



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:48 PM UTC

PDB ID : 3WG7 / pdb_00003wg7
Title : A 1.9 angstrom radiation damage free X-ray structure of large (420KDa) protein by femtosecond crystallography
Authors : Hirata, K.; Shinzawa-Itoh, K.; Yano, N.; Takemura, S.; Kato, K.; Hatanaka, M.; Muramoto, K.; Kawahara, T.; Tsukihara, T.; Yamashita, E.; Tono, K.; Ueno, G.; Hikima, T.; Murakami, H.; Inubushi, Y.; Yabashi, M.; Ishikawa, T.; Yamamoto, M.; Ogura, T.; Sugimoto, H.; Shen, J.R.; Yoshikawa, S.; Ago, H.
Deposited on : 2013-07-29
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

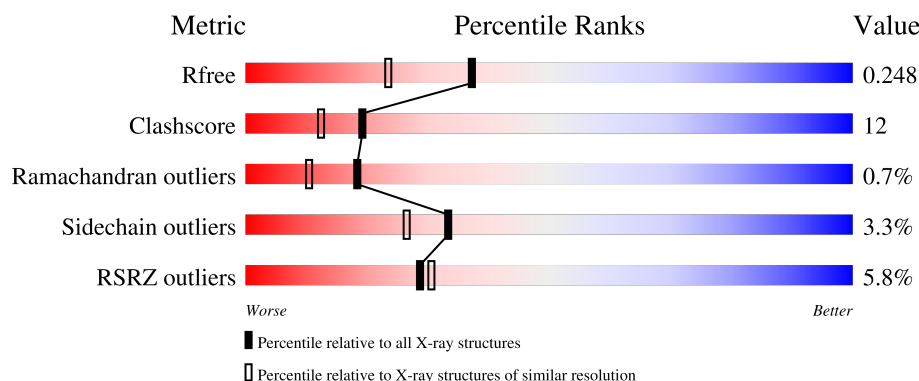
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	N	514	
2	B	227	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FME	O	1	-	-	X	-
23	PSC	N	610	-	-	X	-
25	CDL	C	304	-	-	X	-
25	CDL	G	101	-	-	X	-
25	CDL	T	102	-	-	X	-
27	DMU	M	101	X	-	-	-
27	DMU	Z	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33302 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	6	0
			4074	2725	629	684	36			
1	N	514	Total	C	N	O	S	0	6	0
			4074	2725	629	684	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	1	0
			1832	1189	282	343	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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase 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			

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

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

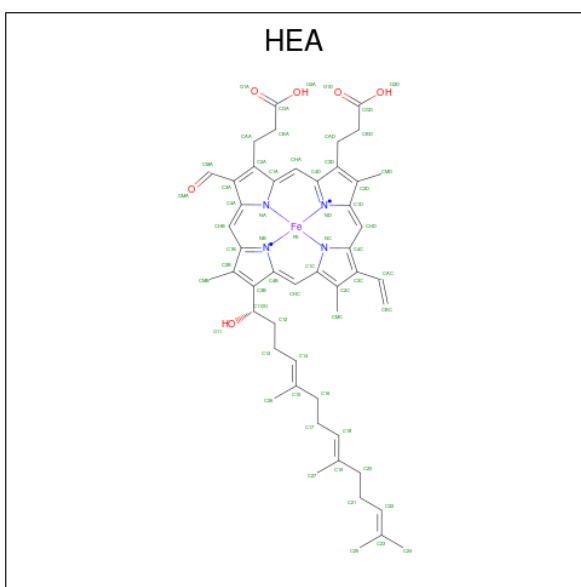
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

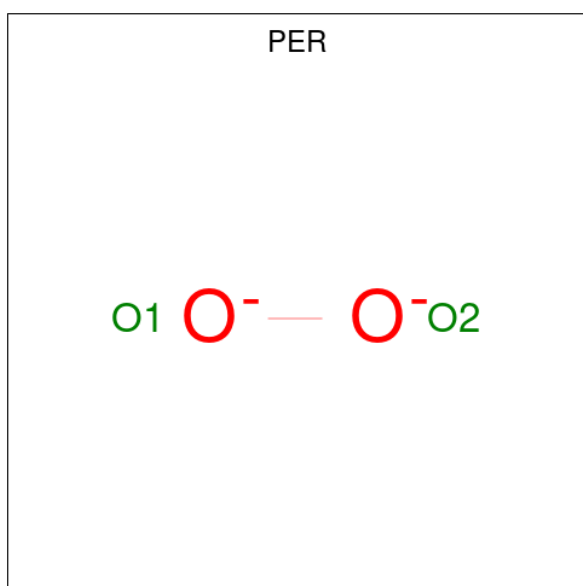
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

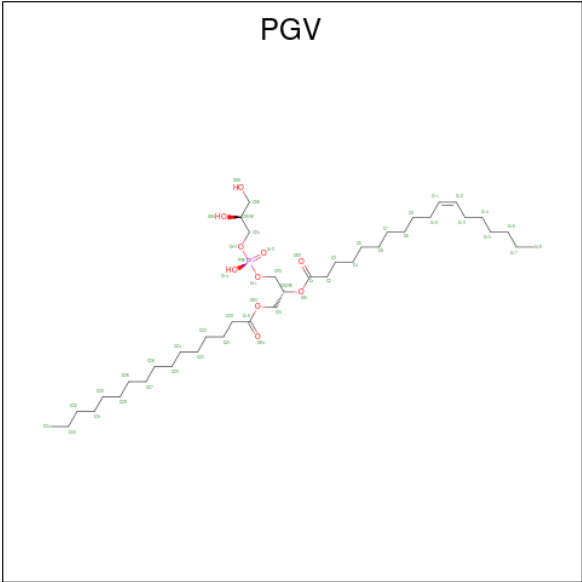
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



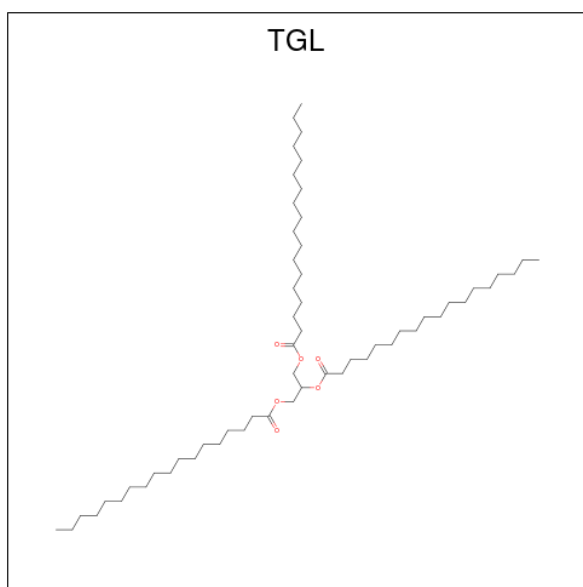
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 4 4	0	1
18	N	1	Total O 4 4	0	1

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



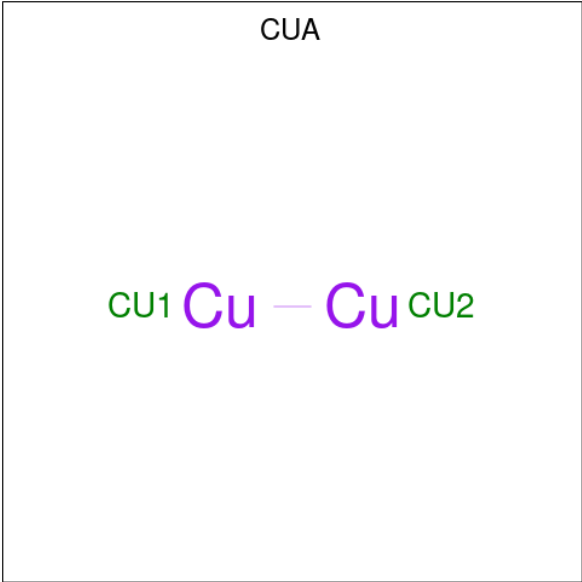
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



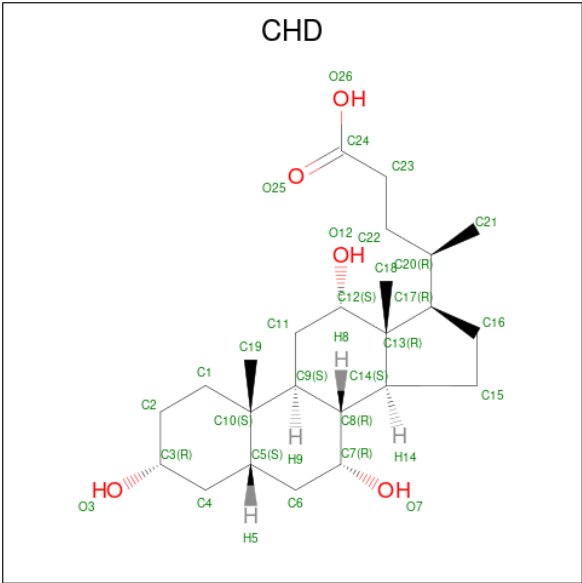
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

- 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).



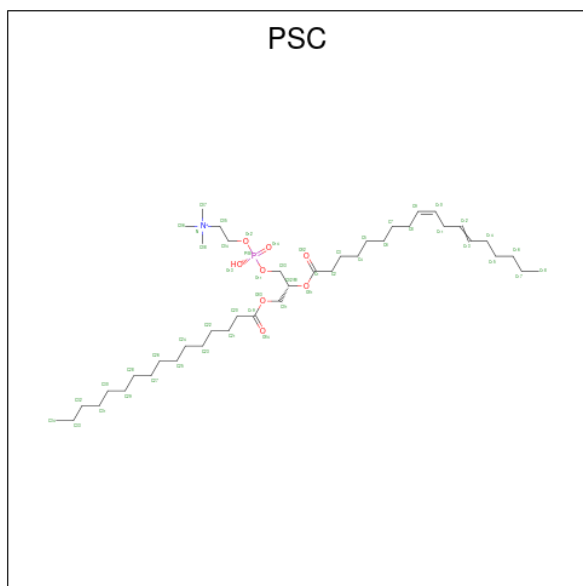
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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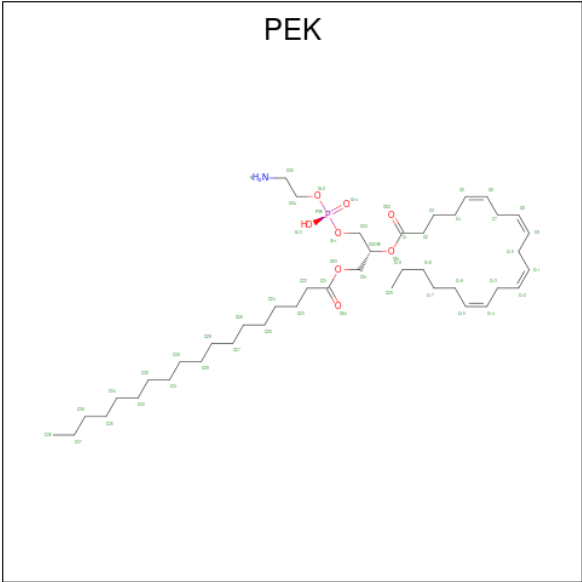
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 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: $C_{42}H_{81}NO_8P$).



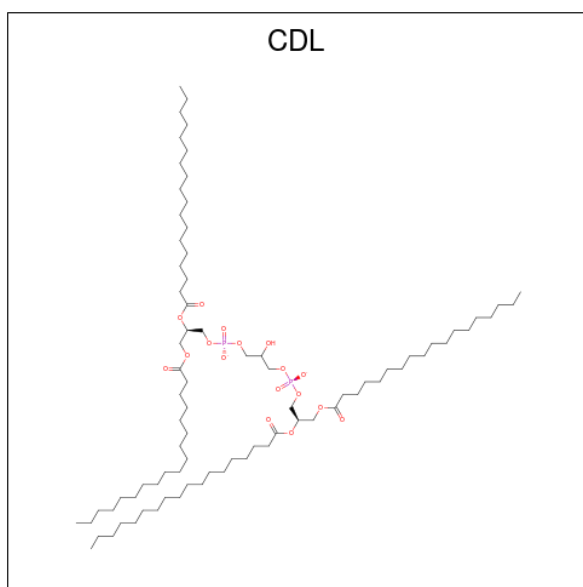
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 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: $C_{43}H_{78}NO_8P$).



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

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

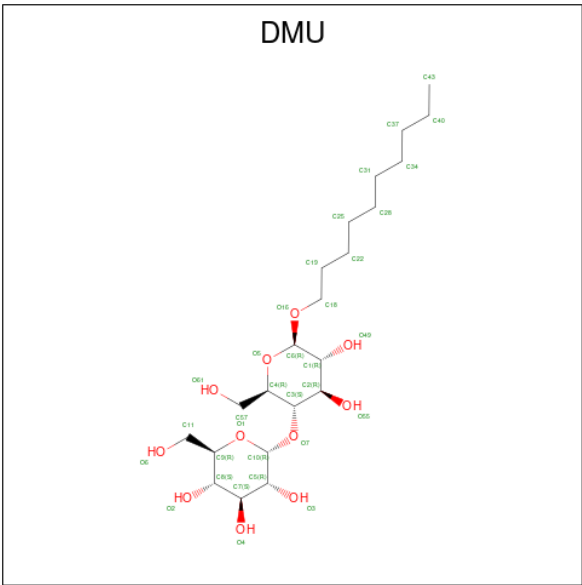


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	265	Total	O	0	0
			265	265		
28	B	194	Total	O	0	0
			194	194		
28	C	141	Total	O	0	0
			141	141		
28	D	160	Total	O	0	0
			160	160		
28	E	125	Total	O	0	0
			125	125		
28	F	112	Total	O	0	0
			112	112		
28	G	70	Total	O	0	0
			70	70		
28	H	70	Total	O	0	0
			70	70		
28	I	52	Total	O	0	0
			52	52		
28	J	31	Total	O	0	0
			31	31		

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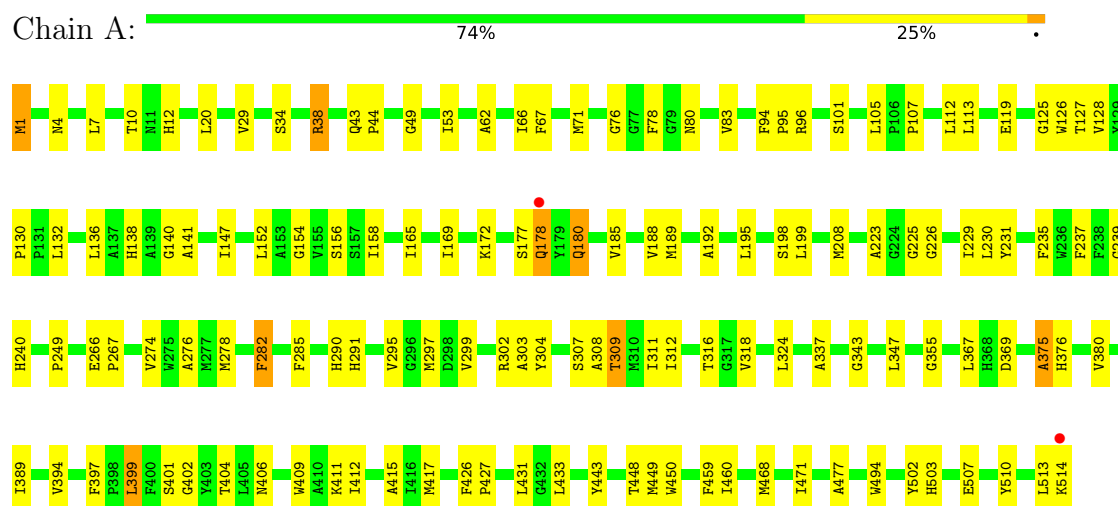
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	40	Total 40	O 40	0	0
28	L	31	Total 31	O 31	0	0
28	M	31	Total 31	O 31	0	0
28	N	259	Total 259	O 259	0	0
28	O	157	Total 157	O 157	0	0
28	P	143	Total 143	O 143	0	0
28	Q	90	Total 90	O 90	0	0
28	R	103	Total 103	O 103	0	0
28	S	122	Total 122	O 122	0	0
28	T	56	Total 56	O 56	0	0
28	U	51	Total 51	O 51	0	0
28	V	42	Total 42	O 42	0	0
28	W	38	Total 38	O 38	0	0
28	X	34	Total 34	O 34	0	0
28	Y	37	Total 37	O 37	0	0
28	Z	24	Total 24	O 24	0	0

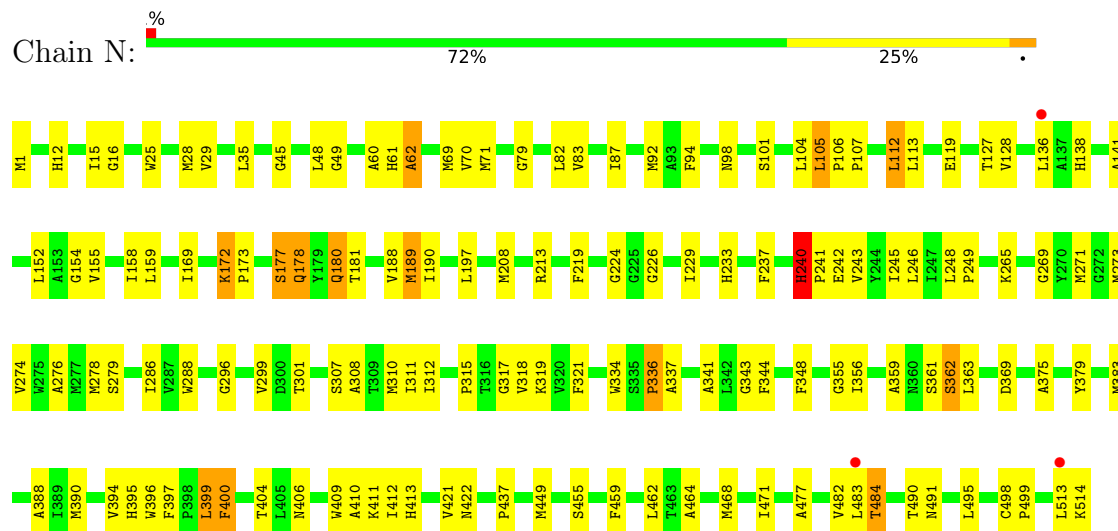
3 Residue-property plots

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

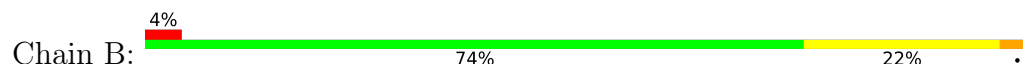
• Molecule 1: Cytochrome c oxidase subunit 1

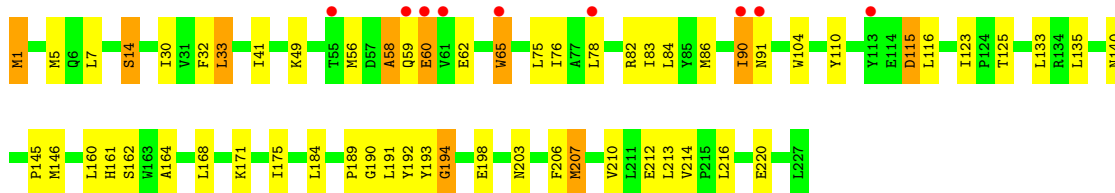


• Molecule 1: Cytochrome c oxidase subunit 1

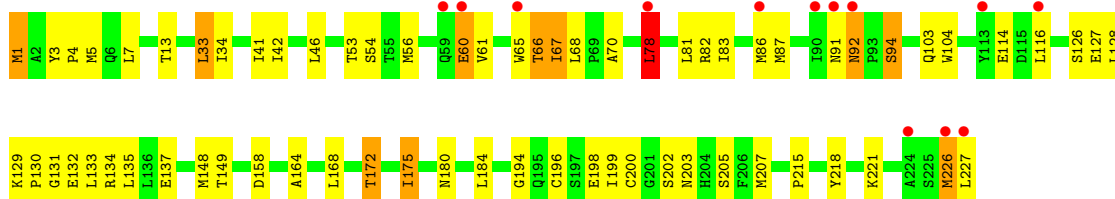


• Molecule 2: Cytochrome c oxidase subunit 2

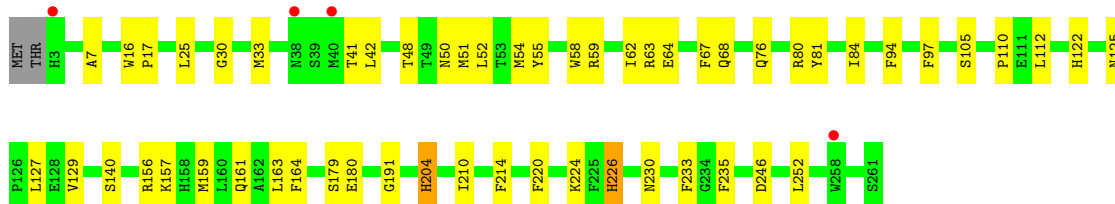
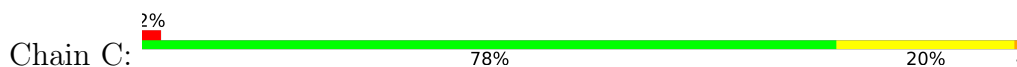




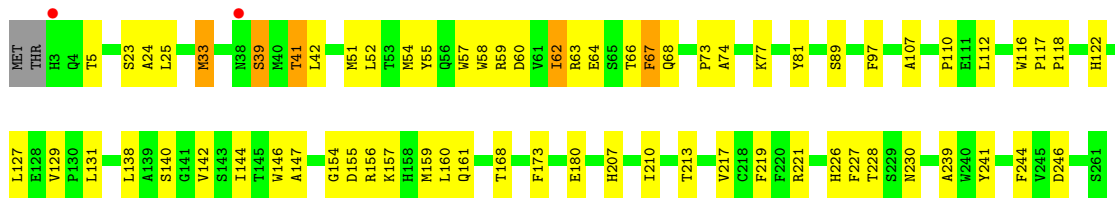
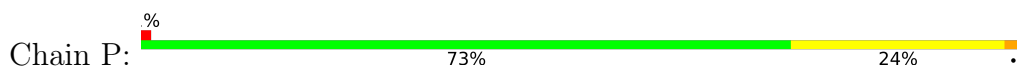
• Molecule 2: Cytochrome c oxidase subunit 2



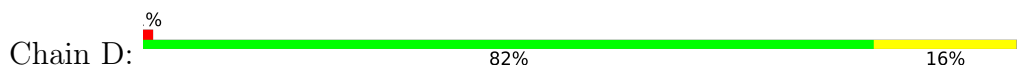
• Molecule 3: Cytochrome c oxidase subunit 3



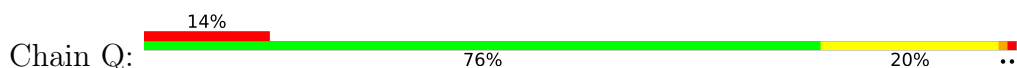
• Molecule 3: Cytochrome c oxidase subunit 3

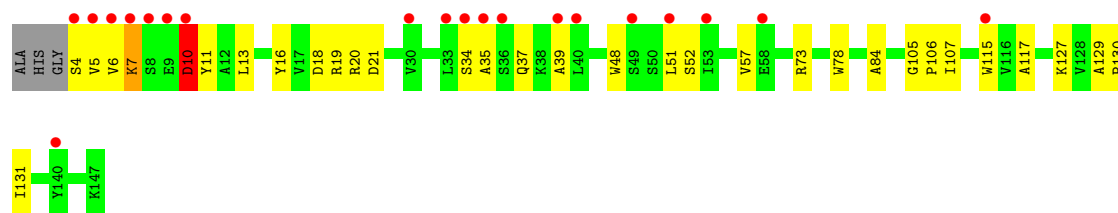


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

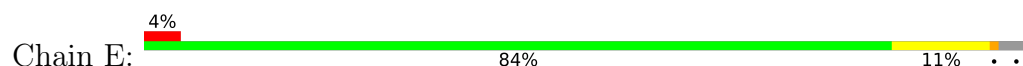


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

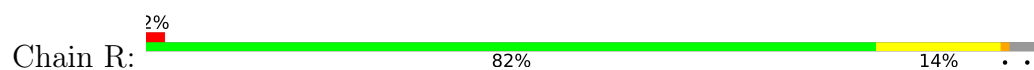




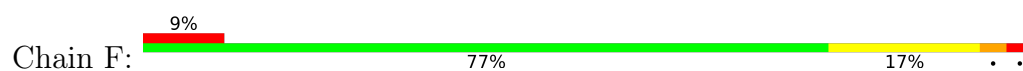
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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



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



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

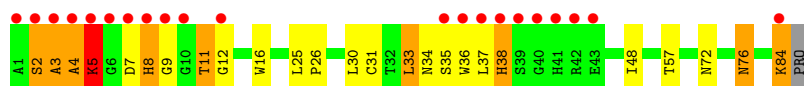


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

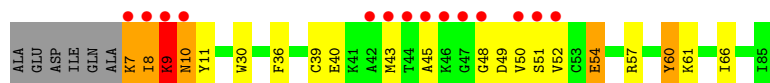


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

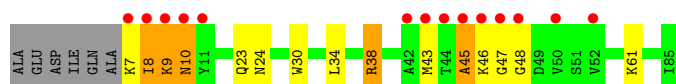
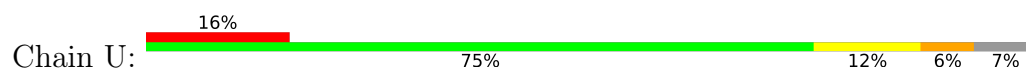




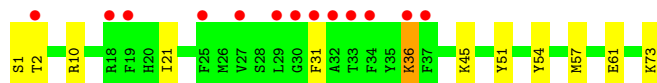
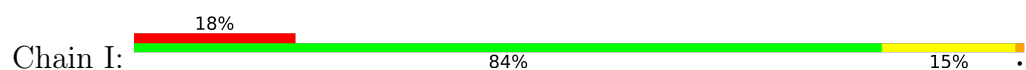
- Molecule 8: Cytochrome c oxidase subunit 6B1



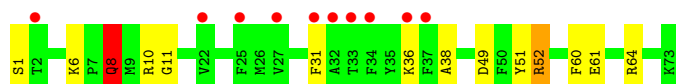
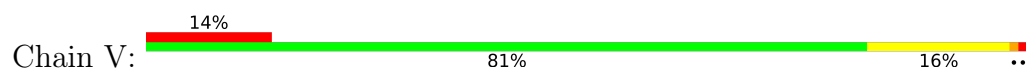
- Molecule 8: Cytochrome c oxidase subunit 6B1



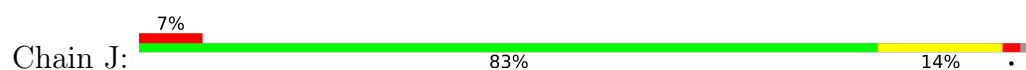
- Molecule 9: Cytochrome c oxidase subunit 6C



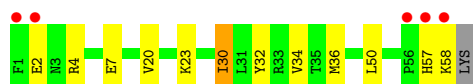
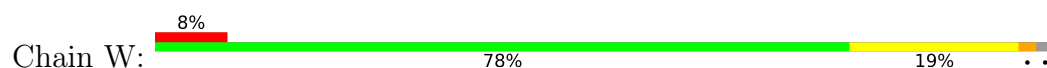
- Molecule 9: Cytochrome c oxidase subunit 6C



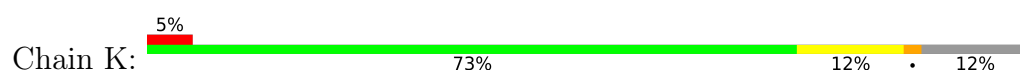
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



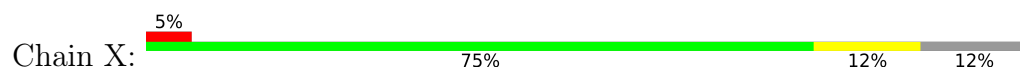
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



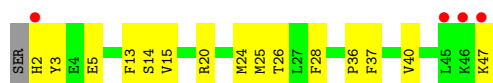
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



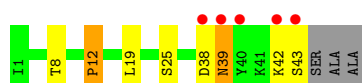
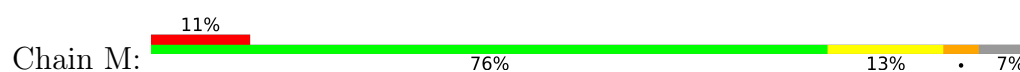
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



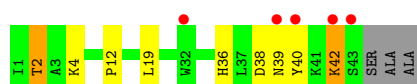
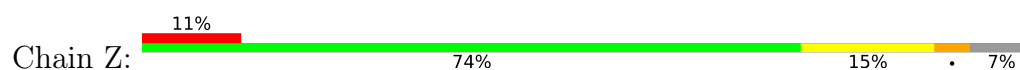
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 40.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-1.90) 96.0 (40.00-1.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.195 , 0.230 0.218 , 0.248	Depositor DCC
R_{free} test set	25229 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: PGV, TGL, HEA, PEK, CUA, PSC, CU, TPO, DMU, CDL, PER, NA, CHD, MG, SAC, ZN, FME

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	1.84	57/4203 (1.4%)	1.44	35/5742 (0.6%)
1	N	1.76	62/4203 (1.5%)	1.43	38/5742 (0.7%)
2	B	1.56	10/1868 (0.5%)	1.37	6/2545 (0.2%)
2	O	1.45	16/1860 (0.9%)	1.28	9/2534 (0.4%)
3	C	1.63	15/2221 (0.7%)	1.28	10/3035 (0.3%)
3	P	1.62	21/2221 (0.9%)	1.28	7/3035 (0.2%)
4	D	1.50	6/1229 (0.5%)	1.32	10/1658 (0.6%)
4	Q	1.21	2/1229 (0.2%)	1.21	8/1658 (0.5%)
5	E	1.53	2/871 (0.2%)	1.23	2/1182 (0.2%)
5	R	1.25	1/871 (0.1%)	1.19	0/1182
6	F	1.47	2/765 (0.3%)	1.33	2/1038 (0.2%)
6	S	1.57	3/765 (0.4%)	1.34	3/1038 (0.3%)
7	G	1.46	4/690 (0.6%)	1.32	6/937 (0.6%)
7	T	1.44	3/690 (0.4%)	1.32	5/937 (0.5%)
8	H	1.40	0/682	1.27	3/921 (0.3%)
8	U	1.26	1/682 (0.1%)	1.21	1/921 (0.1%)
9	I	1.20	0/605	1.26	1/802 (0.1%)
9	V	1.12	1/605 (0.2%)	1.31	2/802 (0.2%)
10	J	1.31	0/471	1.26	1/636 (0.2%)
10	W	1.30	1/471 (0.2%)	1.29	1/636 (0.2%)
11	K	1.43	0/398	1.30	2/546 (0.4%)
11	X	1.27	3/398 (0.8%)	1.23	1/546 (0.2%)
12	L	1.56	5/393 (1.3%)	1.43	3/526 (0.6%)
12	Y	1.45	3/393 (0.8%)	1.27	4/526 (0.8%)
13	M	1.50	1/345 (0.3%)	1.26	0/470
13	Z	1.36	0/345	1.16	0/470
All	All	1.57	219/29474 (0.7%)	1.33	160/40065 (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	N	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
10	W	0	1
All	All	0	6

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	9.91	1.59	1.54
1	N	337	ALA	N-CA	9.89	1.58	1.46
1	A	404	THR	C-O	9.76	1.35	1.23
1	A	154	GLY	N-CA	9.64	1.57	1.45
1	N	288	TRP	N-CA	9.30	1.58	1.46
1	N	359	ALA	N-CA	9.23	1.57	1.46
1	N	69	MET	CA-C	8.99	1.60	1.52
2	B	198	GLU	C-O	8.83	1.33	1.23
1	N	79	GLY	N-CA	8.77	1.56	1.45
3	C	129	VAL	CA-CB	8.60	1.59	1.53
3	P	226	HIS	N-CA	8.43	1.56	1.46
1	A	443	TYR	C-O	8.36	1.33	1.24
1	A	355	GLY	N-CA	8.28	1.56	1.45
1	N	106	PRO	CA-C	8.21	1.59	1.52
1	A	147	ILE	N-CA	8.04	1.56	1.46
1	A	83	VAL	N-CA	7.78	1.55	1.46
7	T	57	THR	C-O	-7.66	1.14	1.24
3	P	129	VAL	CA-CB	7.57	1.59	1.53
6	S	59	GLY	C-O	7.57	1.33	1.23
3	P	147	ALA	N-CA	7.51	1.55	1.46
1	A	295	VAL	CA-CB	7.32	1.63	1.54
1	N	404	THR	C-O	7.31	1.32	1.23
2	O	198	GLU	C-O	7.26	1.31	1.23
1	N	491	ASN	CA-CB	7.25	1.61	1.53
1	N	246	LEU	N-CA	7.15	1.55	1.46
1	A	132	LEU	N-CA	7.11	1.55	1.46
2	O	199	ILE	C-O	7.03	1.32	1.24
1	N	128	VAL	N-CA	6.97	1.55	1.46
2	O	66	THR	CA-C	6.97	1.59	1.52
1	A	158	ILE	N-CA	6.96	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	219	PHE	N-CA	6.92	1.55	1.46
1	N	158	ILE	N-CA	6.91	1.54	1.46
2	O	78	LEU	CA-C	6.91	1.60	1.52
1	A	12	HIS	CA-C	6.87	1.62	1.52
2	B	190	GLY	C-O	-6.83	1.17	1.24
1	N	92	MET	CA-C	6.83	1.61	1.52
4	D	56	LYS	C-O	-6.78	1.16	1.24
1	N	243	VAL	N-CA	6.75	1.55	1.46
1	N	12	HIS	CA-C	6.73	1.61	1.52
3	C	42	LEU	N-CA	-6.69	1.38	1.46
2	O	172	THR	N-CA	6.66	1.54	1.46
1	A	239	GLY	N-CA	6.57	1.54	1.45
2	O	175	ILE	N-CA	6.55	1.52	1.46
1	N	459	PHE	N-CA	6.54	1.54	1.46
1	A	324	LEU	N-CA	6.54	1.54	1.46
2	B	162	SER	CA-C	-6.50	1.44	1.52
3	C	204	HIS	N-CA	6.48	1.54	1.46
1	A	401	SER	N-CA	6.47	1.54	1.46
12	Y	35	ALA	CA-CB	6.42	1.59	1.54
2	O	175	ILE	CA-C	6.38	1.57	1.52
2	O	200	CYS	N-CA	6.35	1.52	1.46
3	P	142	VAL	C-O	6.33	1.31	1.24
2	B	194	GLY	C-O	6.32	1.30	1.23
3	C	58	TRP	N-CA	6.30	1.54	1.46
1	A	156	SER	N-CA	6.29	1.53	1.46
1	A	49	GLY	C-O	6.28	1.31	1.23
2	O	135	LEU	N-CA	6.28	1.54	1.46
3	P	66	THR	N-CA	6.27	1.53	1.46
1	A	397	PHE	CA-CB	6.25	1.59	1.54
1	N	245	ILE	N-CA	6.24	1.53	1.46
4	D	97	ILE	N-CA	6.23	1.53	1.46
1	A	502	TYR	C-O	6.22	1.31	1.24
4	D	94	LEU	N-CA	6.22	1.54	1.46
3	P	129	VAL	CA-C	6.22	1.57	1.52
1	N	61	HIS	CA-CB	6.19	1.62	1.53
1	N	355	GLY	N-CA	6.13	1.53	1.45
13	M	8	THR	C-N	6.13	1.41	1.33
1	N	16	GLY	CA-C	6.11	1.58	1.52
11	X	41	ASN	C-O	6.10	1.26	1.23
1	A	105	LEU	CA-C	6.09	1.60	1.52
3	P	73	PRO	CA-CB	6.08	1.62	1.53
3	C	30	GLY	N-CA	6.07	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	188	VAL	N-CA	6.07	1.53	1.46
1	A	477	ALA	C-O	-6.05	1.17	1.24
2	B	207	MET	CA-CB	6.03	1.60	1.53
3	P	23	SER	CA-C	6.02	1.60	1.52
1	A	460	ILE	C-O	6.02	1.31	1.24
3	P	146	TRP	C-O	6.02	1.31	1.24
7	G	46	ALA	CA-C	6.00	1.60	1.52
6	S	92	VAL	C-O	-6.00	1.16	1.24
1	N	242	GLU	CA-C	5.96	1.60	1.52
1	N	224	GLY	C-O	-5.96	1.20	1.24
3	C	140	SER	CA-C	5.94	1.60	1.52
3	P	89	SER	CA-C	5.92	1.60	1.52
2	B	135	LEU	N-CA	5.90	1.53	1.46
3	C	7	ALA	N-CA	5.90	1.53	1.46
1	N	274	VAL	N-CA	5.89	1.53	1.46
6	S	66	ASN	N-CA	5.89	1.53	1.46
1	A	198	SER	CA-CB	5.86	1.62	1.53
1	N	315	PRO	CA-C	5.86	1.61	1.52
1	A	231	TYR	CA-CB	5.86	1.62	1.53
12	Y	31	SER	CA-C	5.85	1.60	1.52
1	A	199	LEU	N-CA	5.84	1.52	1.46
1	A	282	PHE	CA-C	5.84	1.60	1.52
1	N	276	ALA	CA-CB	5.83	1.62	1.53
1	A	128	VAL	CA-C	5.82	1.60	1.52
2	O	198	GLU	CA-C	5.79	1.59	1.52
1	A	503	HIS	N-CA	5.78	1.53	1.46
1	N	271	MET	N-CA	5.77	1.53	1.46
2	B	192	TYR	CA-CB	5.76	1.64	1.53
4	Q	106	PRO	C-O	5.76	1.30	1.23
1	N	341	ALA	C-O	-5.76	1.17	1.24
5	E	95	GLU	CA-C	5.74	1.60	1.52
1	N	94	PHE	CA-C	5.72	1.58	1.52
1	N	348	PHE	N-CA	5.70	1.53	1.46
1	A	66	ILE	N-CA	5.68	1.53	1.46
1	N	319	LYS	C-O	-5.67	1.17	1.24
4	D	29	HIS	CA-C	5.67	1.60	1.52
1	A	126	TRP	CA-C	5.67	1.62	1.52
1	N	224	GLY	CA-C	5.65	1.57	1.51
1	A	38	ARG	CZ-NH1	5.64	1.40	1.32
6	F	72	PHE	C-O	5.64	1.31	1.23
7	G	58	LYS	C-O	5.64	1.30	1.24
11	X	41	ASN	N-CA	5.64	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	HIS	CA-CB	5.64	1.62	1.53
12	L	15	VAL	CA-CB	5.64	1.60	1.54
1	A	226	GLY	N-CA	5.63	1.51	1.45
1	A	188	VAL	CA-C	5.62	1.60	1.52
3	P	62	ILE	CA-CB	5.62	1.60	1.54
1	N	395	HIS	CA-C	5.60	1.59	1.52
1	A	152	LEU	CA-C	5.57	1.59	1.52
1	N	399	LEU	C-O	5.57	1.30	1.24
1	A	477	ALA	N-CA	5.56	1.53	1.46
7	T	48	ILE	CA-C	5.54	1.58	1.52
1	N	45	GLY	C-O	5.54	1.30	1.23
10	W	20	VAL	CA-CB	5.53	1.61	1.54
2	O	34	ILE	CA-CB	5.52	1.61	1.54
2	O	205	SER	C-O	5.51	1.31	1.24
1	A	230	LEU	CA-CB	5.51	1.62	1.53
1	N	301	THR	CA-C	5.50	1.59	1.52
1	N	237	PHE	CA-CB	5.50	1.61	1.53
1	N	477	ALA	N-CA	5.50	1.52	1.46
4	D	5	VAL	N-CA	5.50	1.52	1.46
1	N	344	PHE	N-CA	5.49	1.52	1.46
3	C	179	SER	CA-C	5.48	1.59	1.52
1	A	240	HIS	CA-CB	5.45	1.60	1.53
12	L	36	PRO	CA-C	5.43	1.60	1.52
12	L	5	GLU	N-CA	-5.41	1.39	1.45
1	A	185	VAL	N-CA	5.40	1.52	1.46
1	N	178	GLN	CA-C	5.40	1.60	1.52
3	C	163	LEU	N-CA	5.39	1.52	1.46
5	E	30	ARG	CZ-NH2	5.38	1.40	1.33
3	C	235	PHE	N-CA	5.38	1.52	1.46
3	P	219	PHE	N-CA	5.37	1.52	1.46
1	A	309	THR	N-CA	5.36	1.52	1.46
1	A	460	ILE	CA-C	5.36	1.59	1.52
6	F	82	CYS	CA-CB	5.35	1.61	1.53
3	C	129	VAL	CA-C	5.35	1.57	1.52
3	P	67	PHE	N-CA	5.35	1.53	1.46
1	A	402	GLY	CA-C	5.34	1.59	1.51
1	N	48	LEU	C-O	-5.34	1.17	1.23
9	V	8	GLN	N-CA	-5.33	1.39	1.46
12	L	37	PHE	N-CA	5.33	1.52	1.46
3	P	138	LEU	N-CA	5.33	1.52	1.46
1	A	347	LEU	CA-C	5.31	1.60	1.52
3	P	58	TRP	N-CA	5.31	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	122	HIS	N-CA	5.31	1.52	1.46
4	D	81	VAL	CA-CB	5.31	1.60	1.54
1	N	413	HIS	C-O	5.31	1.30	1.24
1	A	29	VAL	CA-C	5.30	1.59	1.52
1	N	60	ALA	CA-CB	5.30	1.61	1.53
1	N	172	LYS	CA-CB	5.29	1.60	1.53
1	N	400	PHE	N-CA	5.29	1.53	1.46
2	O	135	LEU	CB-CG	5.29	1.64	1.53
7	G	59	PRO	CA-CB	5.29	1.60	1.53
12	L	28	PHE	N-CA	5.29	1.52	1.46
1	A	127	THR	N-CA	5.28	1.53	1.46
3	C	81	TYR	N-CA	5.28	1.52	1.46
1	A	130	PRO	CA-CB	5.28	1.61	1.54
3	P	244	PHE	CA-CB	5.26	1.61	1.53
1	N	318	VAL	CA-CB	5.25	1.61	1.54
12	Y	28	PHE	N-CA	5.25	1.52	1.46
2	B	14	SER	N-CA	5.24	1.51	1.45
4	Q	117	ALA	CA-C	5.22	1.59	1.52
1	N	226	GLY	N-CA	5.21	1.50	1.45
2	O	158	ASP	C-O	-5.21	1.17	1.24
1	N	177	SER	C-O	5.21	1.30	1.23
1	N	233	HIS	CA-CB	5.20	1.61	1.53
3	P	228	THR	CB-CG2	5.19	1.69	1.52
3	C	214	PHE	CA-C	5.19	1.59	1.52
1	A	389	ILE	CA-C	5.18	1.59	1.52
1	A	309	THR	CA-C	5.17	1.59	1.52
3	C	226	HIS	N-CA	5.17	1.52	1.46
1	N	498	CYS	C-O	-5.16	1.18	1.25
1	A	399	LEU	CA-CB	5.16	1.61	1.53
5	R	53	ARG	N-CA	-5.16	1.39	1.46
8	U	24	ASN	C-O	5.15	1.30	1.24
1	A	235	PHE	N-CA	5.15	1.52	1.46
1	N	62	ALA	C-O	-5.14	1.18	1.24
2	B	160	LEU	CA-C	5.13	1.59	1.52
1	N	127	THR	N-CA	5.13	1.52	1.46
3	P	227	PHE	CG-CD1	5.12	1.49	1.38
1	A	20	LEU	N-CA	5.12	1.52	1.46
2	B	125	THR	CA-C	5.12	1.59	1.52
3	P	217	VAL	CA-CB	5.11	1.60	1.54
1	N	437	PRO	C-O	5.10	1.29	1.23
1	A	375	ALA	CA-C	5.09	1.59	1.52
3	C	105	SER	N-CA	5.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	70	VAL	N-CA	5.08	1.52	1.46
1	N	278	MET	N-CA	5.07	1.52	1.46
1	N	98	ASN	N-CA	5.06	1.52	1.46
1	A	276	ALA	CA-CB	5.06	1.61	1.53
1	N	248	LEU	N-CA	5.06	1.51	1.46
1	N	249	PRO	CA-C	5.05	1.60	1.52
1	N	49	GLY	CA-C	5.05	1.58	1.52
1	N	154	GLY	N-CA	5.05	1.52	1.45
1	A	140	GLY	C-O	5.04	1.29	1.24
1	A	318	VAL	CA-CB	5.04	1.60	1.54
2	O	3	TYR	N-CA	5.04	1.51	1.45
2	O	131	GLY	C-O	-5.04	1.16	1.24
1	A	316	THR	N-CA	5.04	1.52	1.46
11	X	17	VAL	N-CA	5.03	1.52	1.46
1	A	140	GLY	N-CA	5.03	1.51	1.45
1	N	242	GLU	CD-OE1	5.03	1.34	1.25
7	G	53	LEU	N-CA	5.01	1.52	1.45
7	T	36	TRP	CB-CG	5.01	1.65	1.50
3	P	146	TRP	CA-CB	5.01	1.61	1.53
1	A	94	PHE	CA-C	5.00	1.58	1.52
1	A	192	ALA	N-CA	5.00	1.52	1.46

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	8.84	120.85	110.42
1	N	319	LYS	N-CA-C	-8.36	102.11	111.14
1	N	105	LEU	CA-C-N	-8.19	111.95	120.38
1	N	105	LEU	C-N-CA	-8.19	111.95	120.38
1	N	141	ALA	N-CA-C	8.14	122.47	112.54
1	A	240	HIS	N-CA-CB	7.84	121.40	110.11
9	V	8	GLN	CB-CG-CD	-7.76	99.41	112.60
12	Y	20	ARG	N-CA-C	-7.59	103.08	111.36
3	C	125	ASN	CA-C-N	-7.58	111.71	120.12
3	C	125	ASN	C-N-CA	-7.58	111.71	120.12
4	Q	10	ASP	N-CA-C	7.54	121.97	111.56
1	N	240	HIS	CA-C-N	-7.43	110.85	119.32
1	N	240	HIS	C-N-CA	-7.43	110.85	119.32
11	X	36	ILE	N-CA-C	7.34	119.66	111.88
1	A	141	ALA	N-CA-C	7.29	121.44	112.54
2	O	78	LEU	CA-C-N	-7.18	111.58	119.19
2	O	78	LEU	C-N-CA	-7.18	111.58	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	38	ARG	N-CA-C	-7.17	103.54	111.36
5	E	81	ILE	N-CA-C	7.07	117.18	110.53
1	N	375	ALA	N-CA-C	-7.07	103.50	111.14
3	P	74	ALA	N-CA-C	-7.04	103.69	111.36
3	C	157	LYS	N-CA-C	7.00	118.56	111.07
1	A	355	GLY	N-CA-C	-7.00	103.81	112.77
1	N	355	GLY	N-CA-C	-6.93	103.90	112.77
1	N	464	ALA	N-CA-C	6.81	118.70	111.28
3	P	41	THR	N-CA-C	6.78	118.32	111.07
5	E	67	ILE	N-CA-C	-6.73	103.92	110.72
1	N	101	SER	CA-CB-OG	-6.73	97.64	111.10
1	A	105	LEU	CA-C-N	-6.66	113.52	120.38
1	A	105	LEU	C-N-CA	-6.66	113.52	120.38
4	Q	105	GLY	CA-C-N	-6.63	113.81	120.31
4	Q	105	GLY	C-N-CA	-6.63	113.81	120.31
1	A	199	LEU	CA-C-N	-6.56	112.24	119.19
1	A	199	LEU	C-N-CA	-6.56	112.24	119.19
4	D	20	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	A	96	ARG	NE-CZ-NH2	-6.49	113.36	119.20
7	G	8	HIS	N-CA-C	6.48	124.59	110.80
1	A	49	GLY	N-CA-C	-6.44	101.92	110.74
1	A	237	PHE	N-CA-C	-6.38	104.32	111.28
6	F	87	THR	N-CA-CB	6.37	119.34	110.17
7	G	25	LEU	CA-C-N	-6.36	112.28	119.28
7	G	25	LEU	C-N-CA	-6.36	112.28	119.28
1	N	71	MET	CG-SD-CE	-6.34	86.95	100.90
4	Q	11	TYR	N-CA-C	-6.33	105.42	113.01
8	H	9	LYS	N-CA-C	6.33	119.06	109.63
1	N	224	GLY	N-CA-C	-6.32	104.80	115.80
1	A	147	ILE	N-CA-C	-6.32	104.33	110.72
1	A	125	GLY	N-CA-C	-6.32	104.83	112.48
1	A	266	GLU	CA-C-N	6.32	126.23	119.85
1	A	266	GLU	C-N-CA	6.32	126.23	119.85
1	N	299	VAL	N-CA-C	6.20	116.87	110.36
1	A	316	THR	N-CA-C	-6.17	104.64	111.36
1	A	71	MET	CG-SD-CE	-6.08	87.53	100.90
1	A	34	SER	N-CA-C	-6.03	104.82	111.82
1	A	380	VAL	N-CA-C	6.02	120.86	112.50
3	P	140	SER	N-CA-C	-6.02	105.43	112.89
4	D	129	ALA	CA-C-N	6.02	126.54	120.04
4	D	129	ALA	C-N-CA	6.02	126.54	120.04
1	N	410	ALA	N-CA-C	-5.99	104.68	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5	VAL	N-CA-C	5.96	117.03	107.73
3	C	16	TRP	CA-C-N	-5.94	112.45	119.05
3	C	16	TRP	C-N-CA	-5.94	112.45	119.05
1	A	240	HIS	CA-CB-CG	-5.93	107.87	113.80
2	B	65	TRP	CB-CA-C	5.93	121.38	110.11
6	S	45	ASP	CA-C-N	-5.93	114.50	120.31
6	S	45	ASP	C-N-CA	-5.93	114.50	120.31
4	D	100	LYS	N-CA-C	-5.89	104.99	111.82
1	A	119	GLU	CB-CA-C	-5.88	109.81	116.63
2	B	123	ILE	CB-CA-C	-5.88	105.47	110.94
3	P	23	SER	CA-CB-OG	-5.86	99.38	111.10
12	L	15	VAL	N-CA-C	-5.85	105.68	111.88
9	V	38	ALA	N-CA-C	5.85	119.60	112.23
1	A	127	THR	N-CA-C	-5.83	106.00	113.23
4	D	105	GLY	CA-C-N	5.82	125.75	119.76
4	D	105	GLY	C-N-CA	5.82	125.75	119.76
1	N	388	ALA	N-CA-C	-5.80	105.04	111.36
7	G	5	LYS	CB-CA-C	5.74	121.84	110.42
2	O	92	ASN	N-CA-C	5.74	122.50	109.81
12	Y	19	TRP	CA-CB-CG	-5.73	102.72	113.60
1	A	101	SER	CA-CB-OG	-5.73	99.64	111.10
11	K	13	TYR	CA-C-N	5.72	126.46	119.99
11	K	13	TYR	C-N-CA	5.72	126.46	119.99
2	O	65	TRP	N-CA-C	5.72	119.96	113.15
1	N	82	LEU	CA-C-N	-5.71	115.76	120.33
1	N	82	LEU	C-N-CA	-5.71	115.76	120.33
1	A	78	PHE	N-CA-C	5.70	117.50	111.28
1	A	223	ALA	N-CA-C	-5.70	105.21	111.82
1	N	455	SER	N-CA-C	5.70	117.49	111.28
3	P	131	LEU	N-CA-C	-5.68	105.00	111.14
7	T	5	LYS	CB-CA-C	5.66	121.68	110.42
2	B	83	ILE	N-CA-C	5.64	115.84	110.42
1	N	15	ILE	N-CA-C	-5.63	105.03	110.72
10	J	57	HIS	CB-CA-C	5.62	119.96	110.79
1	A	302	ARG	CA-CB-CG	-5.60	102.89	114.10
2	O	67	ILE	N-CA-C	5.56	115.76	110.42
3	C	80	ARG	CG-CD-NE	-5.52	99.86	112.00
1	A	95	PRO	N-CA-C	-5.50	106.54	114.18
8	H	54	GLU	N-CA-C	5.45	117.65	111.11
3	C	48	THR	N-CA-C	5.44	116.89	111.07
1	A	249	PRO	CA-C-N	5.43	125.96	119.94
1	A	249	PRO	C-N-CA	5.43	125.96	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	47	SER	N-CA-C	5.40	118.18	110.24
1	A	10	THR	N-CA-C	-5.40	104.11	111.56
2	B	189	PRO	N-CA-C	-5.39	103.68	111.22
1	N	92	MET	CG-SD-CE	5.39	112.75	100.90
3	C	41	THR	N-CA-C	5.38	116.83	111.07
9	I	21	ILE	N-CA-C	-5.36	105.15	111.00
6	S	49	VAL	N-CA-C	-5.36	101.87	107.60
6	F	94	HIS	N-CA-C	5.33	122.14	110.80
1	N	189	MET	CB-CG-SD	-5.30	96.80	112.70
7	G	58	LYS	CA-C-N	-5.27	114.53	119.85
7	G	58	LYS	C-N-CA	-5.27	114.53	119.85
1	A	67	PHE	N-CA-C	5.27	118.86	112.23
1	N	362	SER	CA-CB-OG	-5.26	100.57	111.10
2	B	58	ALA	N-CA-C	5.25	119.82	113.41
1	A	38	ARG	CG-CD-NE	5.25	123.55	112.00
4	Q	129	ALA	CA-C-N	5.25	124.94	119.64
4	Q	129	ALA	C-N-CA	5.25	124.94	119.64
3	P	161	GLN	N-CA-C	5.23	117.39	111.11
1	N	119	GLU	CB-CA-C	-5.23	110.53	116.54
1	N	343	GLY	N-CA-C	-5.23	106.46	112.73
1	N	482	VAL	CB-CA-C	-5.22	103.32	111.26
2	O	226	MET	N-CA-C	-5.19	104.55	111.87
2	B	161	HIS	N-CA-C	-5.18	101.83	109.18
1	N	29	VAL	CB-CA-C	-5.17	105.15	112.14
4	Q	107	ILE	CA-C-N	-5.17	114.91	120.03
4	Q	107	ILE	C-N-CA	-5.17	114.91	120.03
12	L	25	MET	CA-C-N	5.17	127.16	120.44
12	L	25	MET	C-N-CA	5.17	127.16	120.44
3	C	233	PHE	CA-C-N	-5.14	114.27	119.98
3	C	233	PHE	C-N-CA	-5.14	114.27	119.98
1	A	195	LEU	N-CA-C	-5.12	105.61	111.14
1	N	172	LYS	CA-C-N	-5.12	115.92	119.66
1	N	172	LYS	C-N-CA	-5.12	115.92	119.66
1	N	49	GLY	N-CA-C	-5.11	103.74	110.74
1	N	213	ARG	CA-C-N	-5.11	114.26	122.08
1	N	213	ARG	C-N-CA	-5.11	114.26	122.08
4	D	5	VAL	CA-C-N	-5.11	115.78	122.37
4	D	5	VAL	C-N-CA	-5.11	115.78	122.37
3	P	39	SER	N-CA-C	5.10	117.47	108.75
1	N	477	ALA	N-CA-C	5.10	116.52	111.07
7	T	76	ASN	CA-C-N	-5.08	115.33	120.31
7	T	76	ASN	C-N-CA	-5.08	115.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LEU	N-CA-C	-5.08	105.82	111.36
12	Y	16	GLU	CA-C-N	-5.08	115.83	122.99
12	Y	16	GLU	C-N-CA	-5.08	115.83	122.99
1	A	448	THR	N-CA-C	5.08	116.50	110.97
1	N	271	MET	N-CA-C	-5.08	105.93	111.82
2	O	54	SER	N-CA-C	-5.08	103.98	110.53
8	H	66	ILE	N-CA-C	5.07	115.69	110.36
1	N	112	LEU	CD1-CG-CD2	-5.05	99.68	110.80
1	N	286	ILE	N-CA-C	5.05	117.24	111.88
1	A	267	PRO	N-CA-C	-5.04	103.36	111.38
7	T	25	LEU	CA-C-N	-5.04	113.85	119.19
7	T	25	LEU	C-N-CA	-5.04	113.85	119.19
2	O	202	SER	N-CA-C	5.03	118.19	111.75
10	W	30	ILE	N-CA-C	5.03	115.25	110.42
2	O	221	LYS	N-CA-C	-5.02	105.70	111.07
1	N	336	PRO	CB-CA-C	-5.02	104.34	112.62
1	N	361	SER	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
8	H	9	LYS	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	4074	0	4058	60	0
1	N	4074	0	4058	80	0
2	B	1832	0	1836	38	0
2	O	1824	0	1833	53	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2134	0	2051	41	0
3	P	2134	0	2051	52	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	7	0
5	R	852	0	845	11	2
6	F	748	0	728	16	1
6	S	748	0	728	37	7
7	G	675	0	643	30	0
7	T	675	0	643	34	0
8	H	662	0	623	22	0
8	U	662	0	623	11	0
9	I	601	0	613	8	2
9	V	601	0	613	9	0
10	J	460	0	459	9	0
10	W	460	0	459	8	0
11	K	384	0	366	7	0
11	X	384	0	366	4	0
12	L	380	0	380	14	0
12	Y	380	0	380	17	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	120	0	108	10	0
14	N	120	0	108	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	1	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	1	0
18	N	4	0	0	1	0
19	A	102	0	152	10	0
19	C	102	0	152	6	0
19	N	102	0	152	16	0
19	P	102	0	152	11	0
20	B	63	0	110	3	0
20	D	63	0	110	13	0
20	L	63	0	110	12	0
20	N	63	0	110	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Q	63	0	110	11	0
20	Y	63	0	110	17	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	4	0
22	G	29	0	39	0	0
22	J	29	0	39	5	0
22	P	58	0	78	5	0
22	W	29	0	38	5	0
23	B	52	0	80	13	0
23	N	52	0	80	21	0
24	C	106	0	154	23	0
24	G	53	0	77	6	0
24	P	106	0	154	22	0
24	T	53	0	77	12	0
25	C	100	0	156	23	0
25	G	100	0	156	37	0
25	P	100	0	156	18	0
25	T	100	0	156	29	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	42	1	0
27	Z	33	0	42	0	0
28	A	265	0	0	10	0
28	B	194	0	0	10	2
28	C	141	0	0	8	0
28	D	160	0	0	1	1
28	E	125	0	0	3	0
28	F	112	0	0	2	1
28	G	70	0	0	7	0
28	H	70	0	0	5	0
28	I	52	0	0	1	0
28	J	31	0	0	2	0
28	K	40	0	0	3	1
28	L	31	0	0	1	0
28	M	31	0	0	1	2
28	N	259	0	0	12	0
28	O	157	0	0	11	6
28	P	143	0	0	8	0
28	Q	90	0	0	5	0
28	R	103	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	S	122	0	0	7	1
28	T	56	0	0	2	0
28	U	51	0	0	2	0
28	V	42	0	0	5	0
28	W	38	0	0	2	0
28	X	34	0	0	3	0
28	Y	37	0	0	4	0
28	Z	24	0	0	1	0
All	All	33302	0	31396	727	14

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (727) 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)
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.47	1.41
6:S:43:LYS:H	6:S:43:LYS:CD	1.28	1.39
6:S:43:LYS:HD3	6:S:43:LYS:N	1.33	1.29
6:S:76:LYS:HD3	28:S:271:HOH:O	1.36	1.25
18:A:606[A]:PER:O2	18:A:606[A]:PER:O1	1.55	1.22
18:N:606[A]:PER:O2	18:N:606[A]:PER:O1	1.55	1.19
20:L:101:TGL:OC1	20:L:101:TGL:HC41	1.41	1.18
7:G:5:LYS:HB2	24:G:102:PEK:H362	1.21	1.17
6:S:76:LYS:HE3	6:S:93:PRO:CG	1.80	1.11
1:N:513:LEU:O	1:N:514:LYS:HB2	1.49	1.07
19:P:304:PGV:H172	25:P:305:CDL:H651	1.35	1.07
20:Q:201:TGL:HA91	20:Q:201:TGL:H231	1.29	1.06
23:N:610:PSC:H342	2:O:41:ILE:HD13	1.36	1.04
7:T:5:LYS:HB2	24:T:101:PEK:H351	1.39	1.03
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.04	1.02
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.38	1.01
12:L:20:ARG:HH22	20:L:101:TGL:HC32	1.22	1.01
3:C:67:PHE:HE1	25:C:304:CDL:H1	1.25	1.01
6:S:95:GLN:HB2	28:S:240:HOH:O	1.64	0.97
1:N:321:PHE:CD2	23:N:610:PSC:H341	2.00	0.96
10:W:23:LYS:HE3	28:W:221:HOH:O	1.64	0.95
11:X:47:ARG:HD3	28:X:116:HOH:O	1.67	0.95
7:G:5:LYS:HG3	24:G:102:PEK:H383	1.48	0.94
2:O:1:FME:HE1	2:O:133:LEU:CD1	1.98	0.94
7:G:72:ASN:H	7:G:76:ASN:HD22	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:608:PGV:H02	19:A:608:PGV:O14	1.67	0.93
6:F:85:CYS:SG	6:F:87:THR:HG23	2.08	0.93
23:N:610:PSC:H22	28:V:101:HOH:O	1.68	0.92
3:C:224:LYS:CD	25:C:304:CDL:HB31	1.98	0.92
24:C:307:PEK:H383	25:G:101:CDL:C27	2.01	0.90
17:C:301:NA:NA	28:C:404:HOH:O	1.45	0.89
7:G:5:LYS:HB2	24:G:102:PEK:C36	2.01	0.89
7:T:5:LYS:CB	24:T:101:PEK:H351	2.02	0.89
3:C:67:PHE:CE1	25:C:304:CDL:H1	2.08	0.88
3:P:67:PHE:HE1	25:P:305:CDL:H1	1.36	0.88
6:S:76:LYS:CE	6:S:93:PRO:CG	2.42	0.88
19:N:608:PGV:H343	24:P:303:PEK:H382	1.56	0.87
25:G:101:CDL:H202	25:G:101:CDL:H522	1.58	0.86
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.57	0.86
19:P:301:PGV:H11	22:P:307:CHD:H152	1.58	0.86
6:S:98:HIS:HB3	28:S:268:HOH:O	1.76	0.85
12:L:20:ARG:NH2	20:L:101:TGL:HC32	1.91	0.85
25:T:102:CDL:H511	25:T:102:CDL:H202	1.57	0.85
8:U:7:LYS:O	8:U:8:ILE:HG22	1.77	0.84
1:A:513:LEU:O	1:A:514:LYS:HB2	1.74	0.84
4:D:78:TRP:HB3	20:D:201:TGL:HB22	1.56	0.84
1:N:169[B]:ILE:HD11	1:N:189:MET:HE1	1.60	0.84
25:G:101:CDL:H352	2:O:78:LEU:HD12	1.59	0.83
20:L:101:TGL:OC1	20:L:101:TGL:CC4	2.23	0.83
6:S:85:CYS:SG	6:S:87:THR:HG23	2.19	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.23	0.83
3:C:224:LYS:HD2	25:C:304:CDL:HB31	1.59	0.82
6:S:75:HIS:H	6:S:80:GLN:HE22	1.23	0.82
2:O:1:FME:CE	2:O:133:LEU:HD13	2.10	0.81
3:P:63:ARG:HE	25:P:305:CDL:HA22	1.46	0.81
8:H:40:GLU:OE2	28:H:130:HOH:O	1.98	0.80
14:N:602:HEA:HBC1	14:N:602:HEA:HMC3	1.64	0.80
19:A:608:PGV:H311	13:M:19:LEU:HD23	1.64	0.80
25:C:304:CDL:H522	25:C:304:CDL:OB9	1.81	0.80
12:L:2:HIS:CG	12:L:3:TYR:H	1.99	0.80
7:G:84:LYS:H	7:G:84:LYS:HD2	1.47	0.79
28:A:955:HOH:O	2:B:206:PHE:HE1	1.63	0.79
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.27	0.79
28:C:528:HOH:O	25:G:101:CDL:H673	1.81	0.79
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.63	0.79
3:P:33[A]:MET:HG2	28:P:455:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.16	0.78
1:N:321:PHE:HD2	23:N:610:PSC:H341	1.48	0.78
24:P:303:PEK:H203	24:P:303:PEK:H15	1.65	0.78
3:C:50:ASN:HD22	3:C:51[A]:MET:HE2	1.49	0.77
6:S:43:LYS:CD	6:S:43:LYS:N	2.08	0.77
24:C:307:PEK:H361	25:G:101:CDL:H273	1.66	0.77
25:P:305:CDL:OB6	25:P:305:CDL:HB21	1.82	0.77
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.81	0.77
5:E:90:ARG:HD2	28:E:279:HOH:O	1.83	0.77
7:T:5:LYS:HG3	24:T:101:PEK:H371	1.67	0.77
6:S:52:ILE:O	6:S:94:HIS:CE1	2.37	0.77
28:N:953:HOH:O	24:P:303:PEK:H372	1.83	0.77
24:C:307:PEK:C38	25:G:101:CDL:C27	2.62	0.77
5:R:80:GLU:H	5:R:80:GLU:CD	1.93	0.77
3:P:33[A]:MET:HE2	3:P:42:LEU:H	1.49	0.76
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.16	0.76
23:B:304:PSC:C12	23:B:304:PSC:H342	2.14	0.75
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.67	0.75
28:P:530:HOH:O	6:S:1:ALA:HB2	1.87	0.75
25:T:102:CDL:H311	25:T:102:CDL:CA5	2.17	0.75
25:P:305:CDL:OB9	25:P:305:CDL:H532	1.87	0.74
1:A:311[A]:ILE:HD13	25:T:102:CDL:H221	1.69	0.74
7:G:84:LYS:HD2	7:G:84:LYS:N	2.02	0.74
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.86	0.73
3:C:161:GLN:HE22	24:C:307:PEK:H21	1.52	0.73
8:H:30:TRP:HB2	28:H:158:HOH:O	1.89	0.73
12:L:26:THR:HG23	13:M:25:SER:CB	2.19	0.73
19:N:607:PGV:H302	13:Z:19:LEU:CD2	2.19	0.73
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.70	0.73
4:Q:6:VAL:HG13	4:Q:10:ASP:OD2	1.89	0.72
12:Y:12:PRO:HB2	20:Y:101:TGL:HG11	1.68	0.72
2:O:1:FME:CE	2:O:133:LEU:CD1	2.67	0.72
4:Q:6:VAL:CG1	4:Q:10:ASP:OD2	2.37	0.72
25:G:101:CDL:H111	25:G:101:CDL:HA21	1.71	0.72
28:O:536:HOH:O	4:Q:21:ASP:HB2	1.89	0.72
24:C:307:PEK:C38	25:G:101:CDL:H272	2.20	0.72
1:A:417:MET:HE1	14:A:601:HEA:H263	1.72	0.72
1:N:169[B]:ILE:CD1	1:N:189:MET:HE1	2.18	0.72
25:P:305:CDL:H251	25:P:305:CDL:H391	1.72	0.72
3:C:161:GLN:NE2	24:C:307:PEK:H21	2.05	0.72
25:G:101:CDL:H751	25:G:101:CDL:H561	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:107:ALA:HB2	19:P:301:PGV:H031	1.72	0.72
19:N:607:PGV:H31	19:N:607:PGV:H202	1.72	0.72
3:P:54:MET:HE1	19:P:304:PGV:H131	1.72	0.71
12:Y:20:ARG:HH21	20:Y:101:TGL:HC32	1.55	0.71
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.20	0.71
4:Q:78:TRP:CA	20:Q:201:TGL:HB22	2.21	0.71
24:P:303:PEK:HN2	7:T:76:ASN:HD21	1.34	0.71
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.26	0.71
2:B:56:MET:HG2	23:B:304:PSC:H221	1.73	0.70
1:A:311[B]:ILE:HD11	24:P:308:PEK:H342	1.72	0.70
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.73	0.70
7:T:84:LYS:HZ3	7:T:84:LYS:H	1.39	0.70
12:L:14:SER:H	20:L:101:TGL:HC31	1.55	0.70
20:Q:201:TGL:HG32	20:Q:201:TGL:OB1	1.92	0.70
1:N:28:MET:HE2	14:N:601:HEA:H271	1.74	0.69
7:T:30:LEU:HD21	25:T:102:CDL:H471	1.74	0.69
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	1.91	0.69
4:D:78:TRP:N	20:D:201:TGL:HB21	2.06	0.69
24:C:307:PEK:H382	25:G:101:CDL:H272	1.74	0.69
3:C:63:ARG:HE	25:C:304:CDL:HA22	1.56	0.69
1:N:321:PHE:CD2	23:N:610:PSC:C34	2.75	0.69
7:T:3:ALA:O	7:T:4:ALA:CB	2.40	0.69
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.57	0.69
3:P:63:ARG:HE	25:P:305:CDL:CA2	2.06	0.69
3:C:63:ARG:HE	25:C:304:CDL:CA2	2.06	0.68
1:N:113:LEU:HD12	20:Y:101:TGL:H141	1.75	0.68
4:D:78:TRP:CB	20:D:201:TGL:HB22	2.23	0.68
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.93	0.68
7:G:2:SER:OG	24:G:102:PEK:H301	1.93	0.68
7:G:5:LYS:NZ	28:G:224:HOH:O	2.26	0.68
25:G:101:CDL:H182	25:G:101:CDL:CB5	2.24	0.68
2:B:32:PHE:CE2	20:B:301:TGL:HA52	2.29	0.68
2:O:1:FME:HE2	2:O:133:LEU:HD13	1.76	0.67
3:P:67:PHE:CE1	25:P:305:CDL:H1	2.25	0.67
1:N:321:PHE:CE2	23:N:610:PSC:H341	2.30	0.67
24:P:308:PEK:H382	25:T:102:CDL:H271	1.76	0.67
6:S:64:GLU:O	6:S:65:ASP:HB2	1.94	0.67
23:B:304:PSC:H342	23:B:304:PSC:H12	1.77	0.67
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.77	0.67
4:D:34:SER:H	4:D:37:GLN:HE21	1.43	0.66
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:39:GLU:HB3	28:K:137:HOH:O	1.95	0.66
8:H:9:LYS:O	8:H:10:ASN:HB2	1.94	0.66
1:N:406:ASN:HD21	19:N:607:PGV:H22	1.60	0.66
2:B:115[B]:ASP:OD1	28:B:501:HOH:O	2.13	0.66
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.31	0.66
19:A:608:PGV:H152	19:A:608:PGV:H322	1.77	0.66
7:G:1:ALA:HB2	19:P:301:PGV:H321	1.76	0.66
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.42	0.66
8:H:7:LYS:O	8:H:8:ILE:HB	1.96	0.66
2:O:218:TYR:HB3	28:O:513:HOH:O	1.94	0.66
20:Q:201:TGL:HA91	20:Q:201:TGL:C23	2.15	0.66
1:A:417:MET:CE	14:A:601:HEA:H263	2.25	0.66
7:T:31:CYS:SG	25:T:102:CDL:H551	2.36	0.66
1:N:159:LEU:HD21	28:P:499:HOH:O	1.96	0.65
2:O:1:FME:HE1	2:O:133:LEU:HD11	1.78	0.65
4:Q:78:TRP:CB	20:Q:201:TGL:HB22	2.27	0.65
1:A:406:ASN:HD21	19:A:608:PGV:H22	1.62	0.65
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.77	0.64
25:C:304:CDL:HB21	25:C:304:CDL:OB6	1.98	0.64
4:Q:20:ARG:HG2	28:Q:317:HOH:O	1.96	0.64
6:S:52:ILE:O	6:S:94:HIS:ND1	2.31	0.64
1:N:273:MET:HE2	28:N:921:HOH:O	1.97	0.63
3:C:224:LYS:HD3	25:C:304:CDL:HB31	1.80	0.63
4:Q:78:TRP:HB3	20:Q:201:TGL:HB22	1.79	0.63
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.80	0.63
3:P:33[A]:MET:HE3	3:P:39:SER:OG	1.98	0.63
23:N:610:PSC:H342	2:O:41:ILE:CD1	2.23	0.62
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.29	0.62
23:N:610:PSC:C32	23:N:610:PSC:H12	2.29	0.62
4:D:109:HIS:HD2	28:D:306:HOH:O	1.83	0.62
6:F:95:GLN:C	6:F:97:ALA:H	2.06	0.62
2:O:227:LEU:HD21	28:O:546:HOH:O	2.00	0.61
25:G:101:CDL:H462	2:O:70:ALA:HB1	1.82	0.61
10:J:7:GLU:HG3	28:J:209:HOH:O	2.01	0.61
12:L:26:THR:HG23	13:M:25:SER:HB3	1.81	0.61
5:E:12:ASP:OD1	5:E:44:GLU:HG3	1.98	0.61
1:N:136[B]:LEU:HD21	28:N:892:HOH:O	2.00	0.61
2:B:140:ASN:HB3	28:B:502:HOH:O	2.00	0.61
7:T:3:ALA:O	7:T:4:ALA:HB3	1.99	0.61
12:Y:12:PRO:CB	20:Y:101:TGL:HG11	2.31	0.61
2:B:7:LEU:HD12	20:B:301:TGL:HC52	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.66	0.61
1:N:136[B]:LEU:CD2	28:N:893:HOH:O	2.48	0.61
4:Q:78:TRP:HA	20:Q:201:TGL:HB22	1.83	0.60
12:Y:24:MET:SD	20:Y:101:TGL:H152	2.41	0.60
7:T:2:SER:OG	24:T:101:PEK:H292	2.00	0.60
1:A:311[A]:ILE:HG13	25:T:102:CDL:H432	1.83	0.60
10:J:33:ARG:HG2	22:J:101:CHD:H152	1.82	0.60
3:P:59:ARG:HA	25:P:305:CDL:H512	1.82	0.60
13:M:42:LYS:HB3	28:M:2326:HOH:O	2.01	0.60
3:P:246:ASP:HB2	28:P:473:HOH:O	2.02	0.60
7:T:31:CYS:SG	25:T:102:CDL:C55	2.90	0.60
14:N:602:HEA:HBC1	14:N:602:HEA:CMC	2.32	0.60
6:S:43:LYS:H	6:S:43:LYS:HD3	0.48	0.60
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.83	0.60
3:C:246:ASP:HB2	28:C:459:HOH:O	2.02	0.59
1:N:177:SER:H	1:N:180:GLN:HE21	1.50	0.59
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.37	0.59
9:I:45:LYS:HG3	28:I:144:HOH:O	2.02	0.59
3:C:54:MET:HE1	19:C:303:PGV:H142	1.84	0.59
1:N:484:THR:HG22	13:Z:2:THR:HG23	1.84	0.59
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.84	0.59
3:P:54:MET:HE3	25:P:305:CDL:H612	1.83	0.59
20:D:201:TGL:H242	20:D:201:TGL:H202	1.84	0.59
5:R:80:GLU:HG3	28:R:279:HOH:O	2.02	0.59
2:O:83:ILE:O	2:O:87:MET:HG3	2.02	0.59
3:P:60:ASP:O	3:P:64:GLU:HG3	2.03	0.59
5:R:79:LYS:HD2	5:R:79:LYS:N	2.16	0.59
7:T:31:CYS:SG	25:T:102:CDL:H532	2.42	0.59
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.67	0.59
23:B:304:PSC:H22	23:B:304:PSC:H231	1.83	0.59
3:C:161:GLN:HE22	24:C:307:PEK:C2	2.15	0.59
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.38	0.59
7:G:3:ALA:O	7:G:4:ALA:CB	2.51	0.58
12:Y:12:PRO:CG	20:Y:101:TGL:HG11	2.32	0.58
3:C:210:ILE:HG12	19:C:303:PGV:H132	1.84	0.58
1:N:449:MET:SD	2:O:5:MET:HG2	2.43	0.58
12:Y:20:ARG:NH2	20:Y:101:TGL:HC32	2.18	0.58
4:Q:73:ARG:HH11	4:Q:73:ARG:HG2	1.67	0.58
6:F:75:HIS:H	6:F:80:GLN:HE22	1.51	0.58
20:L:101:TGL:HC61	20:L:101:TGL:HC22	1.86	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:610:PSC:H21	23:N:610:PSC:H222	1.84	0.58
4:Q:127:LYS:HD2	28:V:109:HOH:O	2.04	0.58
1:A:136[B]:LEU:HD11	28:A:927:HOH:O	2.04	0.58
2:O:127:GLU:HG2	28:O:543:HOH:O	2.04	0.58
6:S:94:HIS:CD2	6:S:95:GLN:H	2.21	0.58
10:J:37:THR:OG1	22:J:101:CHD:H5	2.04	0.57
6:F:92:VAL:HG23	6:F:92:VAL:O	2.02	0.57
25:G:101:CDL:H242	25:G:101:CDL:H542	1.86	0.57
25:G:101:CDL:H171	1:N:307:SER:HB3	1.85	0.57
19:N:607:PGV:H322	13:Z:19:LEU:HD23	1.86	0.57
3:C:161:GLN:NE2	24:C:307:PEK:C2	2.67	0.57
1:N:422:ASN:OD1	20:N:609:TGL:H262	2.03	0.57
3:C:33[A]:MET:HE1	10:J:45:TYR:OH	2.04	0.57
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.87	0.57
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.85	0.57
7:G:72:ASN:H	7:G:76:ASN:ND2	1.96	0.57
28:N:945:HOH:O	2:O:56:MET:SD	2.58	0.57
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.18	0.57
24:P:308:PEK:H311	7:T:26:PRO:HB3	1.86	0.57
1:A:177:SER:H	1:A:180:GLN:HE21	1.53	0.57
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.87	0.57
7:T:5:LYS:CG	24:T:101:PEK:H371	2.34	0.57
1:N:400:PHE:O	20:Y:101:TGL:H281	2.04	0.57
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.05	0.57
22:C:305:CHD:C23	22:C:305:CHD:H162	2.35	0.57
12:L:13:PHE:HB3	20:L:101:TGL:HG12	1.85	0.57
6:F:95:GLN:HB3	28:F:280:HOH:O	2.03	0.56
7:G:45:PRO:HD2	28:G:203:HOH:O	2.06	0.56
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	2.04	0.56
1:A:274:VAL:HG12	1:A:278:MET:HE2	1.87	0.56
25:G:101:CDL:H561	25:G:101:CDL:H771	1.87	0.56
12:L:26:THR:HG22	28:L:226:HOH:O	2.05	0.56
25:G:101:CDL:H771	25:G:101:CDL:C56	2.35	0.56
6:S:78:GLU:HB2	28:S:317:HOH:O	2.05	0.56
2:B:32:PHE:HE2	20:B:301:TGL:HA52	1.67	0.56
23:B:304:PSC:H241	23:B:304:PSC:H42	1.86	0.56
7:G:8:HIS:O	7:G:9:GLY:C	2.47	0.56
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.71	0.56
24:C:307:PEK:H361	25:G:101:CDL:C27	2.34	0.56
24:C:307:PEK:H041	7:G:17:ARG:HH22	1.71	0.56
25:G:101:CDL:C35	2:O:78:LEU:HD12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:THR:HG23	13:M:25:SER:HB2	1.88	0.56
1:N:113:LEU:HD12	20:Y:101:TGL:C14	2.36	0.56
24:P:308:PEK:H383	25:T:102:CDL:H273	1.88	0.56
20:L:101:TGL:HC61	20:L:101:TGL:CC1	2.36	0.56
4:Q:6:VAL:HG12	4:Q:7:LYS:N	2.20	0.56
1:A:297:MET:HG2	28:C:531:HOH:O	2.05	0.56
24:G:102:PEK:H241	28:G:266:HOH:O	2.06	0.56
3:P:210:ILE:HD13	19:P:304:PGV:H301	1.87	0.55
7:T:72:ASN:N	7:T:76:ASN:HD22	1.99	0.55
20:Y:101:TGL:OG3	20:Y:101:TGL:OA1	2.24	0.55
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.36	0.55
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.88	0.55
3:P:77:LYS:NZ	28:P:482:HOH:O	2.36	0.55
1:N:483:LEU:HD21	13:Z:4:LYS:HE3	1.87	0.55
20:N:609:TGL:HC31	28:V:102:HOH:O	2.07	0.55
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.88	0.55
6:S:43:LYS:HE3	28:S:282:HOH:O	2.06	0.55
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.88	0.55
1:N:28:MET:HE2	14:N:601:HEA:C27	2.37	0.55
8:U:48:GLY:HA2	28:U:133:HOH:O	2.06	0.55
1:A:1:FME:HE1	28:A:963:HOH:O	2.06	0.54
12:Y:12:PRO:HG2	20:Y:101:TGL:HG11	1.89	0.54
2:B:33:LEU:HD13	9:I:31:PHE:HD1	1.70	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.07	0.54
3:P:168:THR:HG22	24:P:308:PEK:H14	1.88	0.54
3:C:94:PHE:HD2	28:C:509:HOH:O	1.90	0.54
11:X:52:GLU:HG2	28:X:120:HOH:O	2.06	0.54
1:N:308:ALA:O	1:N:311[B]:ILE:HG22	2.08	0.54
14:N:601:HEA:HBC1	14:N:601:HEA:CMC	2.37	0.54
8:H:50:VAL:HG23	28:H:156:HOH:O	2.07	0.54
1:N:321:PHE:HD2	23:N:610:PSC:C34	2.15	0.54
4:Q:10:ASP:HB3	4:Q:13:LEU:HD12	1.88	0.54
1:A:513:LEU:O	1:A:514:LYS:CB	2.46	0.54
3:C:54:MET:HE1	19:C:303:PGV:C14	2.38	0.54
1:N:513:LEU:O	1:N:514:LYS:CB	2.31	0.54
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.37	0.54
2:O:91:ASN:HD22	2:O:149:THR:HG21	1.73	0.54
28:P:529:HOH:O	25:T:102:CDL:H673	2.06	0.54
7:T:5:LYS:HD2	24:T:101:PEK:H371	1.89	0.54
25:G:101:CDL:H171	1:N:307:SER:CB	2.38	0.53
8:H:43:MET:HE1	8:U:43:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.90	0.53
2:O:53:THR:HG21	28:Q:344:HOH:O	2.07	0.53
12:Y:12:PRO:HB2	20:Y:101:TGL:CG1	2.37	0.53
28:B:452:HOH:O	20:D:201:TGL:HC61	2.08	0.53
1:N:113:LEU:HD12	20:Y:101:TGL:C13	2.38	0.53
3:P:77:LYS:NZ	3:P:81:TYR:OH	2.40	0.53
4:Q:19:ARG:CD	4:Q:21:ASP:OD1	2.57	0.53
25:T:102:CDL:H571	25:T:102:CDL:H781	1.91	0.53
25:T:102:CDL:H172	28:T:222:HOH:O	2.07	0.53
1:A:309:THR:O	1:A:312[B]:ILE:HG22	2.08	0.53
7:G:84:LYS:HG2	28:G:253:HOH:O	2.08	0.53
1:N:411:LYS:NZ	28:N:890:HOH:O	2.41	0.53
1:A:311[B]:ILE:CD1	24:P:308:PEK:H342	2.39	0.53
8:H:43:MET:CE	8:H:49:ASP:H	2.22	0.53
8:U:45:ALA:O	8:U:47:GLY:N	2.42	0.53
2:B:49:LYS:HD3	20:D:201:TGL:HC72	1.91	0.53
3:C:191:GLY:HA3	28:G:204:HOH:O	2.09	0.53
25:G:101:CDL:H542	25:G:101:CDL:C24	2.38	0.53
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.44	0.53
1:A:165:ILE:HG22	1:A:169[B]:ILE:HD12	1.91	0.53
23:N:610:PSC:H12	23:N:610:PSC:H321	1.90	0.53
4:Q:6:VAL:HG12	4:Q:10:ASP:OD2	2.07	0.53
7:T:5:LYS:HG3	24:T:101:PEK:C37	2.37	0.53
1:N:152:LEU:HD22	3:P:24:ALA:HB1	1.91	0.53
28:O:479:HOH:O	20:Q:201:TGL:HC72	2.09	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.23	0.53
3:C:156:ARG:HE	22:C:305:CHD:C24	2.22	0.53
1:A:112:LEU:HG	28:A:749:HOH:O	2.10	0.52
10:J:55:PHE:HB2	28:J:230:HOH:O	2.09	0.52
8:H:8:ILE:HG23	8:H:8:ILE:O	2.09	0.52
1:N:321:PHE:CZ	23:N:610:PSC:H162	2.45	0.52
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.92	0.52
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.92	0.52
28:B:582:HOH:O	24:P:308:PEK:H301	2.08	0.52
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.91	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.92	0.52
10:W:2:GLU:HA	28:W:218:HOH:O	2.09	0.52
20:L:101:TGL:HC61	20:L:101:TGL:CC2	2.39	0.52
23:N:610:PSC:H12	23:N:610:PSC:H322	1.92	0.52
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.91	0.52
3:C:84:ILE:HD11	24:T:101:PEK:H031	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:304:PSC:H342	23:B:304:PSC:C13	2.39	0.52
3:C:59:ARG:HG3	25:C:304:CDL:H512	1.90	0.52
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.10	0.52
3:P:168:THR:CG2	24:P:308:PEK:H14	2.40	0.52
19:P:301:PGV:H21	28:P:512:HOH:O	2.09	0.52
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.44	0.51
25:T:102:CDL:HA21	25:T:102:CDL:H122	1.93	0.51
9:V:8:GLN:HG3	28:V:116:HOH:O	2.08	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
20:N:609:TGL:H191	28:N:933:HOH:O	2.09	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
1:A:297:MET:HB2	28:A:924:HOH:O	2.11	0.51
6:S:76:LYS:CD	28:S:271:HOH:O	2.19	0.51
19:P:301:PGV:H42	22:P:307:CHD:H151	1.93	0.51
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.91	0.51
19:A:608:PGV:P	19:A:608:PGV:H061	2.50	0.51
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.93	0.51
5:E:16:VAL:HG21	5:E:46:LYS:HG3	1.92	0.51
1:N:112:LEU:HD23	1:N:113:LEU:HD23	1.93	0.51
23:B:304:PSC:H042	28:E:217:HOH:O	2.10	0.50
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.46	0.50
23:N:610:PSC:H21	23:N:610:PSC:C22	2.40	0.50
1:A:308:ALA:HA	25:T:102:CDL:H212	1.94	0.50
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.93	0.50
24:C:307:PEK:C04	7:G:17:ARG:HH22	2.25	0.50
1:N:136[B]:LEU:HD22	28:N:893:HOH:O	2.09	0.50
1:N:406:ASN:HD21	19:N:607:PGV:C2	2.25	0.50
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.94	0.50
1:A:299:VAL:HG23	2:B:84:LEU:HG	1.94	0.50
28:O:458:HOH:O	8:U:61:LYS:HE3	2.10	0.50
3:P:51[A]:MET:SD	25:P:305:CDL:H621	2.51	0.50
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
3:C:55:TYR:CE1	25:C:304:CDL:H521	2.47	0.50
6:F:87:THR:HG21	28:F:222:HOH:O	2.12	0.50
7:T:2:SER:OG	24:T:101:PEK:C29	2.59	0.50
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.47	0.50
19:C:303:PGV:H12	25:C:304:CDL:H651	1.93	0.50
23:N:610:PSC:H072	9:V:10:ARG:HH21	1.77	0.50
1:A:343:GLY:HA2	20:D:201:TGL:H211	1.92	0.50
7:G:9:GLY:HA3	28:N:812:HOH:O	2.12	0.50
23:B:304:PSC:H212	23:B:304:PSC:O01	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HG3	8:H:11:TYR:H	1.77	0.50
3:P:210:ILE:HG21	19:P:304:PGV:H282	1.93	0.50
19:A:608:PGV:H251	13:M:12:PRO:HG3	1.93	0.49
3:P:107:ALA:HB2	19:P:301:PGV:C03	2.41	0.49
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.65	0.49
3:C:127:LEU:HD13	25:G:101:CDL:OB3	2.11	0.49
25:C:304:CDL:HB22	25:C:304:CDL:CB5	2.42	0.49
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.48	0.49
24:P:303:PEK:H15	24:P:303:PEK:C20	2.36	0.49
3:C:164:PHE:CD1	22:C:305:CHD:H192	2.48	0.49
5:E:86:ILE:O	5:E:90:ARG:HG2	2.12	0.49
1:N:155:VAL:HG21	19:N:608:PGV:H142	1.95	0.49
1:N:169[B]:ILE:HD11	1:N:189:MET:CE	2.36	0.49
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.94	0.49
1:A:415:ALA:HB1	20:D:201:TGL:H132	1.94	0.49
19:N:608:PGV:H61	3:P:54:MET:HG2	1.94	0.49
19:N:608:PGV:H21	3:P:57:TRP:CZ2	2.47	0.49
4:Q:7:LYS:HA	28:Q:373:HOH:O	2.13	0.49
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.49
4:D:34:SER:H	4:D:37:GLN:NE2	2.10	0.49
25:P:305:CDL:H431	10:W:34:VAL:HG11	1.93	0.49
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.49
25:G:101:CDL:HA21	25:G:101:CDL:C11	2.39	0.49
2:O:13:THR:HB	2:O:168:LEU:HD23	1.95	0.49
13:Z:40:TYR:O	13:Z:42:LYS:N	2.45	0.49
3:C:224:LYS:HD3	25:C:304:CDL:CB3	2.42	0.49
24:C:307:PEK:H292	28:O:486:HOH:O	2.13	0.49
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.94	0.49
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.49
1:N:317:GLY:O	1:N:321:PHE:CD1	2.66	0.49
7:T:2:SER:O	7:T:3:ALA:HB3	2.11	0.49
19:N:608:PGV:C34	24:P:303:PEK:H382	2.35	0.48
28:R:294:HOH:O	9:V:11:GLY:HA2	2.12	0.48
1:A:459:PHE:HE2	28:A:949:HOH:O	1.96	0.48
2:B:30:ILE:HD13	28:B:571:HOH:O	2.13	0.48
7:G:2:SER:HB2	1:N:197:LEU:HD21	1.95	0.48
25:G:101:CDL:H522	25:G:101:CDL:C20	2.37	0.48
3:P:62:ILE:HD12	25:P:305:CDL:H511	1.94	0.48
1:A:1:FME:CE	1:A:4:ASN:HD22	2.27	0.48
1:A:303:ALA:HB1	25:T:102:CDL:H132	1.95	0.48
7:G:2:SER:HB2	1:N:197:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:102:CDL:H571	25:T:102:CDL:C78	2.43	0.48
12:Y:25:MET:HE3	20:Y:101:TGL:HA81	1.96	0.48
2:O:1:FME:CE	2:O:133:LEU:HD22	2.43	0.48
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.95	0.48
4:D:78:TRP:CA	20:D:201:TGL:CB2	2.92	0.48
9:I:57:MET:O	9:I:61:GLU:HG2	2.13	0.48
11:K:44:PRO:CA	11:K:47:ARG:HH21	2.27	0.48
24:P:303:PEK:H11	24:P:303:PEK:H161	1.96	0.48
2:B:41:ILE:HD13	23:B:304:PSC:H341	1.96	0.48
2:B:86:MET:HE3	2:B:86:MET:HB2	1.76	0.48
6:S:54:ASN:HD22	6:S:54:ASN:C	2.22	0.48
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.12	0.47
2:B:56:MET:CG	23:B:304:PSC:H221	2.43	0.47
3:C:204:HIS:HB2	3:C:252:LEU:HD11	1.97	0.47
7:G:37:LEU:HD21	25:G:101:CDL:H361	1.96	0.47
23:N:610:PSC:C13	23:N:610:PSC:H343	2.44	0.47
12:Y:46:LYS:HG2	28:Y:229:HOH:O	2.15	0.47
12:L:20:ARG:HH22	20:L:101:TGL:HC52	1.79	0.47
10:W:36:MET:HB3	22:W:101:CHD:H181	1.97	0.47
12:Y:41:ARG:HG3	13:Z:40:TYR:CE1	2.50	0.47
8:H:43:MET:CE	8:U:43:MET:HE1	2.44	0.47
1:N:87:ILE:O	1:N:173:PRO:HD3	2.14	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.45	0.47
3:C:226:HIS:CE1	25:C:304:CDL:HB32	2.50	0.47
8:U:7:LYS:HB2	28:U:139:HOH:O	2.14	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.96	0.47
8:H:9:LYS:O	8:H:10:ASN:CB	2.62	0.47
2:O:94:SER:OG	2:O:148:MET:HE2	2.15	0.47
24:P:308:PEK:C38	25:T:102:CDL:C27	2.93	0.47
22:J:101:CHD:H192	22:J:101:CHD:H3	1.96	0.47
23:N:610:PSC:H42	23:N:610:PSC:H241	1.97	0.47
24:P:308:PEK:H362	24:P:308:PEK:H332	1.78	0.47
1:A:311[A]:ILE:HD13	25:T:102:CDL:C22	2.41	0.47
1:N:104:LEU:C	1:N:107:PRO:HD2	2.40	0.47
19:N:607:PGV:H302	13:Z:19:LEU:HD22	1.96	0.47
6:S:76:LYS:CE	28:S:271:HOH:O	2.57	0.47
7:T:2:SER:O	24:T:101:PEK:H322	2.15	0.47
3:C:52:LEU:HD23	25:C:304:CDL:H362	1.97	0.47
2:O:42:ILE:HG21	20:Q:201:TGL:H232	1.96	0.47
3:P:127:LEU:HD22	25:T:102:CDL:HB62	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:102:CDL:H712	25:T:102:CDL:H521	1.97	0.47
2:B:56:MET:HG2	23:B:304:PSC:H201	1.95	0.46
25:G:101:CDL:H732	25:G:101:CDL:H541	1.97	0.46
12:L:24:MET:SD	20:L:101:TGL:HC82	2.55	0.46
28:C:536:HOH:O	24:T:101:PEK:H262	2.14	0.46
7:G:23:LEU:HD12	25:G:101:CDL:H271	1.97	0.46
9:I:36:LYS:HB2	9:I:36:LYS:HE3	1.64	0.46
2:O:4:PRO:HB2	11:X:43:SER:HA	1.96	0.46
7:T:7:ASP:O	7:T:9:GLY:N	2.49	0.46
24:C:302:PEK:H102	24:C:302:PEK:H72	1.73	0.46
4:D:78:TRP:N	20:D:201:TGL:CB2	2.77	0.46
19:N:607:PGV:H21	19:N:607:PGV:H52	1.64	0.46
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.46	0.46
24:C:302:PEK:H161	24:C:302:PEK:C12	2.45	0.46
4:D:78:TRP:CA	20:D:201:TGL:HB22	2.45	0.46
25:G:101:CDL:H152	1:N:307:SER:OG	2.15	0.46
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.96	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.50	0.46
1:A:468:MET:HG3	28:A:937:HOH:O	2.15	0.46
24:C:307:PEK:H383	25:G:101:CDL:H271	1.89	0.46
1:N:240:HIS:O	1:N:241:PRO:C	2.56	0.46
19:N:608:PGV:H343	24:P:303:PEK:C38	2.36	0.46
2:O:67:ILE:CD1	28:O:486:HOH:O	2.62	0.46
7:T:33:LEU:O	7:T:34:ASN:C	2.59	0.46
25:T:102:CDL:H342	25:T:102:CDL:OA7	2.16	0.46
19:A:607:PGV:H343	24:C:302:PEK:H382	1.97	0.46
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
1:N:310:MET:HE3	1:N:356:ILE:CG2	2.45	0.46
10:W:32:TYR:OH	22:W:101:CHD:H213	2.15	0.46
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.16	0.46
5:R:76:GLY:O	5:R:79:LYS:HE3	2.16	0.46
1:A:507:GLU:CD	28:A:945:HOH:O	2.59	0.45
6:F:95:GLN:O	6:F:97:ALA:N	2.40	0.45
7:T:2:SER:O	7:T:3:ALA:CB	2.64	0.45
2:B:30:ILE:CD1	28:B:571:HOH:O	2.63	0.45
3:C:62:ILE:HD12	25:C:304:CDL:H511	1.99	0.45
11:K:44:PRO:HA	11:K:47:ARG:HH21	1.80	0.45
13:M:39:ASN:OD1	13:M:39:ASN:N	2.49	0.45
2:O:129:LYS:O	2:O:132:GLU:HG3	2.17	0.45
22:W:101:CHD:O12	22:W:101:CHD:H222	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.45
2:O:114:GLU:HG3	28:O:505:HOH:O	2.15	0.45
2:O:128:LEU:HD22	2:O:132:GLU:HB2	1.97	0.45
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.52	0.45
25:P:305:CDL:H561	25:P:305:CDL:H531	1.50	0.45
19:A:608:PGV:H311	13:M:19:LEU:CD2	2.41	0.45
1:N:25:TRP:CH2	20:Y:101:TGL:H292	2.52	0.45
4:D:98:TRP:CE2	27:M:101:DMU:H11	2.52	0.45
20:Q:201:TGL:HG31	20:Q:201:TGL:HC21	1.77	0.45
5:R:77:PRO:O	5:R:79:LYS:HD2	2.16	0.45
7:T:11:TPO:CG2	7:T:11:TPO:O	2.65	0.45
1:A:307:SER:HB2	25:T:102:CDL:H192	1.99	0.45
1:A:311[B]:ILE:HG12	1:A:311[B]:ILE:O	2.15	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
8:H:43:MET:HE3	8:H:48:GLY:HA3	1.98	0.45
13:M:39:ASN:O	13:M:43:SER:HB2	2.16	0.45
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.97	0.45
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.97	0.45
20:Y:101:TGL:H172	28:Y:235:HOH:O	2.17	0.45
23:B:304:PSC:H073	5:E:11:PHE:CG	2.52	0.45
7:G:43:GLU:HA	28:G:269:HOH:O	2.16	0.45
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.52	0.45
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.04	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.97	0.45
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.17	0.45
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.52	0.45
5:E:90:ARG:HG3	28:E:239:HOH:O	2.16	0.45
11:K:8:ASP:HB2	28:K:111:HOH:O	2.16	0.45
11:K:24:PHE:CE1	11:K:28:VAL:HG21	2.52	0.45
1:N:468:MET:HG3	28:N:923:HOH:O	2.17	0.45
7:G:2:SER:CB	1:N:197:LEU:HD11	2.47	0.44
28:B:452:HOH:O	20:D:201:TGL:CC6	2.64	0.44
1:N:321:PHE:HD2	23:N:610:PSC:C33	2.30	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.44
4:Q:73:ARG:HG2	4:Q:73:ARG:NH1	2.32	0.44
22:W:101:CHD:H232	22:W:101:CHD:H211	1.60	0.44
1:A:304:TYR:CD2	1:A:304:TYR:C	2.94	0.44
1:A:411:LYS:NZ	28:A:908:HOH:O	2.50	0.44
3:C:220:PHE:HB2	25:C:304:CDL:H712	1.99	0.44
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.48	0.44
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:GLU:O	6:F:65:ASP:CB	2.62	0.44
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.81	0.44
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.65	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.83	0.44
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.53	0.44
24:P:308:PEK:C38	25:T:102:CDL:H271	2.46	0.44
22:W:101:CHD:H111	22:W:101:CHD:H12A	1.85	0.44
13:Z:40:TYR:C	13:Z:42:LYS:H	2.26	0.44
2:B:76:ILE:HG13	28:B:571:HOH:O	2.18	0.44
19:N:607:PGV:H251	13:Z:12:PRO:HB3	2.00	0.44
3:P:52:LEU:HD23	25:P:305:CDL:H362	2.00	0.44
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.49	0.44
14:A:601:HEA:HHC	14:A:601:HEA:H122	2.00	0.44
2:B:207:MET:HE3	2:B:207:MET:HB2	1.79	0.44
28:N:951:HOH:O	6:S:37:LYS:HE2	2.18	0.44
22:C:306:CHD:H212	22:C:306:CHD:H12	1.99	0.44
24:C:307:PEK:H372	1:N:279:SER:OG	2.18	0.44
1:N:321:PHE:HB3	23:N:610:PSC:H331	2.00	0.44
1:N:379:TYR:CZ	1:N:383:MET:HE1	2.53	0.44
14:A:601:HEA:H212	14:A:601:HEA:H271	1.44	0.43
3:C:55:TYR:CD1	25:C:304:CDL:H181	2.53	0.43
3:C:122:HIS:HD2	28:C:467:HOH:O	2.00	0.43
6:S:52:ILE:C	6:S:94:HIS:HD1	2.25	0.43
8:U:34:LEU:O	8:U:38:ARG:HG3	2.19	0.43
12:Y:42:HIS:O	12:Y:46:LYS:HG3	2.18	0.43
25:G:101:CDL:H352	2:O:78:LEU:CD1	2.38	0.43
1:N:105:LEU:HD23	1:N:105:LEU:HA	1.86	0.43
19:N:607:PGV:H211	28:Z:222:HOH:O	2.18	0.43
23:N:610:PSC:H21	23:N:610:PSC:C21	2.48	0.43
24:P:308:PEK:H382	25:T:102:CDL:C27	2.47	0.43
7:T:12:GLY:CA	28:T:207:HOH:O	2.65	0.43
20:Y:101:TGL:H202	20:Y:101:TGL:H231	1.67	0.43
10:J:29:ASN:HD22	10:J:29:ASN:H	1.66	0.43
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.43
8:H:7:LYS:HA	28:H:145:HOH:O	2.18	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.99	0.43
5:R:44:GLU:OE1	9:V:6:LYS:NZ	2.40	0.43
9:V:51:TYR:O	9:V:52:ARG:C	2.61	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.00	0.43
8:H:43:MET:HE3	8:H:49:ASP:N	2.33	0.43
12:L:2:HIS:CG	12:L:3:TYR:N	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:144:ILE:CD1	3:P:239:ALA:HA	2.48	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.01	0.43
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.54	0.43
1:N:399:LEU:O	1:N:499:PRO:HA	2.18	0.43
6:F:54:ASN:H	6:F:54:ASN:HD22	1.65	0.43
10:J:37:THR:OG1	22:J:101:CHD:H191	2.18	0.43
13:Z:36:HIS:HD2	13:Z:39:ASN:HD22	1.67	0.43
1:A:449:MET:SD	2:B:5:MET:HG2	2.59	0.43
22:B:303:CHD:H12	22:B:303:CHD:H212	2.00	0.43
24:C:302:PEK:H171	24:C:302:PEK:H203	1.81	0.43
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.44	0.43
12:L:20:ARG:HH22	20:L:101:TGL:CC3	2.11	0.43
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.67	0.43
5:R:80:GLU:CD	5:R:80:GLU:N	2.69	0.43
19:A:607:PGV:H183	24:C:302:PEK:H322	2.01	0.43
24:P:308:PEK:H6	24:P:308:PEK:H221	2.01	0.43
14:A:602:HEA:HAD2	14:A:602:HEA:HH4	1.76	0.43
3:P:62:ILE:CD1	3:P:221:ARG:HD2	2.49	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
4:Q:52:SER:HB2	28:Q:340:HOH:O	2.18	0.43
4:D:78:TRP:CA	20:D:201:TGL:HB21	2.49	0.42
7:G:3:ALA:HA	28:G:261:HOH:O	2.19	0.42
25:C:304:CDL:H182	25:C:304:CDL:H352	2.00	0.42
24:C:307:PEK:H383	25:G:101:CDL:H273	1.93	0.42
19:P:301:PGV:H202	19:P:301:PGV:H231	1.74	0.42
25:T:102:CDL:CB5	25:T:102:CDL:H181	2.50	0.42
12:Y:39:ILE:O	12:Y:42:HIS:HB3	2.19	0.42
25:C:304:CDL:OB6	25:C:304:CDL:CB2	2.67	0.42
25:C:304:CDL:CB5	25:C:304:CDL:CB2	2.98	0.42
25:G:101:CDL:H202	25:G:101:CDL:C52	2.39	0.42
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.55	0.42
3:P:213:THR:HG23	25:P:305:CDL:H771	2.01	0.42
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.02	0.42
19:C:308:PGV:H51	19:C:308:PGV:H21	1.88	0.42
1:N:396:TRP:O	1:N:397:PHE:C	2.62	0.42
25:P:305:CDL:H222	25:P:305:CDL:H192	1.80	0.42
20:Q:201:TGL:HA32	20:Q:201:TGL:HB51	2.00	0.42
12:Y:46:LYS:CD	28:Y:229:HOH:O	2.67	0.42
25:G:101:CDL:H591	25:G:101:CDL:C77	2.49	0.42
2:O:60:GLU:CD	2:O:60:GLU:H	2.26	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HA	7:T:4:ALA:CB	2.49	0.42
2:B:216:LEU:O	2:B:220:GLU:HG3	2.20	0.42
23:N:610:PSC:H062	23:N:610:PSC:H042	1.85	0.42
28:A:955:HOH:O	2:B:206:PHE:CE1	2.51	0.42
1:N:269:GLY:HA2	28:O:500:HOH:O	2.19	0.42
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.01	0.42
3:P:155:ASP:OD2	6:S:2:SER:HA	2.20	0.42
28:B:580:HOH:O	4:D:126:MET:SD	2.62	0.42
11:K:52:GLU:HG3	28:K:131:HOH:O	2.18	0.42
3:P:5:THR:HG22	6:S:96:LEU:HD11	1.99	0.42
3:P:173:PHE:CD2	3:P:173:PHE:C	2.98	0.42
6:S:43:LYS:N	6:S:43:LYS:HD2	2.24	0.42
10:W:58:LYS:HD3	10:W:58:LYS:HA	1.70	0.42
13:Z:40:TYR:C	13:Z:42:LYS:N	2.77	0.42
25:G:101:CDL:H132	2:O:81:LEU:HD13	2.01	0.42
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.02	0.42
2:O:1:FME:HE1	2:O:133:LEU:HD21	1.99	0.42
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.54	0.42
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.50	0.42
3:P:157:LYS:HD3	28:P:520:HOH:O	2.20	0.42
2:B:191:LEU:HD23	2:B:212:GLU:HA	2.01	0.41
25:G:101:CDL:H771	25:G:101:CDL:H591	2.02	0.41
19:A:608:PGV:C31	13:M:19:LEU:HD23	2.42	0.41
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.55	0.41
8:H:52:VAL:HG12	28:H:166:HOH:O	2.19	0.41
19:N:607:PGV:H131	19:N:607:PGV:H301	2.02	0.41
20:N:609:TGL:H152	2:O:7:LEU:HD11	2.01	0.41
22:P:307:CHD:H212	22:P:307:CHD:H12	2.01	0.41
7:T:38:HIS:HE1	25:T:102:CDL:H121	1.83	0.41
7:G:5:LYS:CG	24:G:102:PEK:H383	2.35	0.41
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.03	0.41
1:A:468:MET:HE1	14:A:601:HEA:H271	2.02	0.41
3:C:63:ARG:HE	25:C:304:CDL:HA21	1.83	0.41
3:C:76:GLN:NE2	28:C:435:HOH:O	2.46	0.41
3:C:210:ILE:HG21	19:C:303:PGV:H281	2.01	0.41
24:C:307:PEK:C36	25:G:101:CDL:H273	2.45	0.41
5:E:12:ASP:HB3	5:E:46:LYS:HE2	2.03	0.41
4:Q:57:VAL:HG21	28:R:258:HOH:O	2.20	0.41
9:V:49:ASP:HB3	28:V:132:HOH:O	2.20	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.55	0.41
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:303:PEK:H161	24:P:303:PEK:C11	2.49	0.41
7:T:30:LEU:CD2	25:T:102:CDL:H471	2.44	0.41
1:A:375:ALA:O	1:A:376:HIS:C	2.64	0.41
2:B:60:GLU:H	2:B:60:GLU:HG3	1.56	0.41
2:B:90:ILE:H	2:B:90:ILE:HG13	1.73	0.41
6:F:55:LYS:HA	6:F:74:LEU:O	2.20	0.41
4:Q:39:ALA:HB1	28:Q:354:HOH:O	2.21	0.41
7:T:11:TPO:HG22	7:T:11:TPO:O	2.20	0.41
12:Y:20:ARG:HD3	28:Y:211:HOH:O	2.20	0.41
25:G:101:CDL:H602	25:G:101:CDL:H631	1.87	0.41
4:Q:16:TYR:OH	4:Q:18:ASP:OD2	2.37	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.66	0.41
1:A:417:MET:HE1	14:A:601:HEA:C26	2.47	0.41
2:B:145:PRO:HA	2:B:214:VAL:O	2.20	0.41
8:H:43:MET:HE2	8:H:49:ASP:H	1.86	0.41
1:N:136[B]:LEU:HD11	28:N:935:HOH:O	2.20	0.41
1:N:468:MET:HE2	1:N:468:MET:HB3	1.81	0.41
3:P:144:ILE:HD13	3:P:239:ALA:HA	2.03	0.41
1:A:412:ILE:HG12	4:D:84:ALA:HB3	2.03	0.41
6:F:92:VAL:O	6:F:92:VAL:CG2	2.66	0.41
25:G:101:CDL:H541	25:G:101:CDL:H712	2.03	0.41
14:N:601:HEA:HHC	14:N:601:HEA:H122	2.03	0.41
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.03	0.40
2:B:1:FME:HE3	28:B:418:HOH:O	2.21	0.40
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.03	0.40
2:O:67:ILE:HD13	28:O:486:HOH:O	2.20	0.40
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.86	0.40
3:P:156:ARG:HE	22:P:306:CHD:C23	2.33	0.40
7:T:5:LYS:CD	24:T:101:PEK:H371	2.49	0.40
25:T:102:CDL:H712	25:T:102:CDL:C52	2.51	0.40
2:B:168:LEU:HD23	2:B:168:LEU:HA	1.94	0.40
1:A:510:TYR:CD1	1:A:510:TYR:C	3.00	0.40
9:I:73:LYS:HA	9:I:73:LYS:HD2	1.60	0.40
1:N:189:MET:HG3	1:N:190:ILE:N	2.29	0.40
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.40
3:P:160:LEU:HD13	22:P:306:CHD:H181	2.03	0.40
23:B:304:PSC:C07	9:I:10:ARG:HH21	2.34	0.40
10:J:52:TRP:O	10:J:57:HIS:HE1	2.02	0.40
8:H:39:CYS:O	8:H:43:MET:HG2	2.21	0.40
10:J:32:TYR:OH	22:J:101:CHD:H213	2.22	0.40
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.50	0.40
3:P:55:TYR:CE1	25:P:305:CDL:H171	2.57	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.46	0.40
7:T:72:ASN:H	7:T:76:ASN:ND2	2.03	0.40
11:X:54:ARG:NH2	28:X:130:HOH:O	2.53	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:F:294:HOH:O	28:K:114:HOH:O[2_585]	1.63	0.57
9:I:2:THR:CG2	5:R:80:GLU:OE1[3_647]	1.83	0.37
28:B:586:HOH:O	28:M:2318:HOH:O[2_584]	1.90	0.30
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	1.93	0.27
6:S:95:GLN:N	28:O:535:HOH:O[2_685]	1.95	0.25
6:F:94:HIS:CE1	28:D:393:HOH:O[2_585]	1.98	0.22
6:S:94:HIS:CD2	28:O:535:HOH:O[2_685]	2.00	0.20
9:I:2:THR:CB	5:R:80:GLU:OE1[3_647]	2.06	0.14
6:S:94:HIS:CA	28:O:547:HOH:O[2_685]	2.07	0.13
28:B:592:HOH:O	28:M:2318:HOH:O[2_584]	2.09	0.11
28:O:533:HOH:O	28:S:307:HOH:O[2_684]	2.10	0.10
6:S:95:GLN:CA	28:O:535:HOH:O[2_685]	2.10	0.10
2:O:126:SER:O	6:S:94:HIS:CG[2_684]	2.12	0.08
6:S:95:GLN:N	28:O:547:HOH:O[2_685]	2.18	0.02

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	518/514 (101%)	500 (96%)	18 (4%)	0	100	100
1	N	518/514 (101%)	501 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	226/227 (100%)	213 (94%)	13 (6%)	0	100	100
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	30	22
3	C	260/261 (100%)	254 (98%)	6 (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
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	18	10
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%)	91 (95%)	2 (2%)	3 (3%)	3	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	68 (84%)	8 (10%)	5 (6%)	1	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	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%)	41 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3523/3614 (98%)	3376 (96%)	123 (4%)	24 (1%)	18	10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE

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Mol	Chain	Res	Type
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
8	U	46	LYS
6	F	95	GLN
7	G	37	LEU
7	T	38	HIS
7	G	7	ASP
2	O	92	ASN
7	T	4	ALA
8	U	45	ALA
4	Q	35	ALA
6	S	96	LEU
7	G	5	LYS
8	H	10	ASN
8	H	45	ALA

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	432/426 (101%)	425 (98%)	7 (2%)	55	54
1	N	432/426 (101%)	423 (98%)	9 (2%)	47	44
2	B	211/210 (100%)	198 (94%)	13 (6%)	16	9
2	O	210/210 (100%)	203 (97%)	7 (3%)	33	26
3	C	227/226 (100%)	223 (98%)	4 (2%)	51	50
3	P	227/226 (100%)	222 (98%)	5 (2%)	45	42
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	75
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	21
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	18
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	6
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	9
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	9
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	7
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	32
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	50
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	12
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	46
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	35
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	35
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	5
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	5
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	5
All	All	3059/3082 (99%)	2956 (97%)	103 (3%)	33	25

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	38	ARG
1	A	138	HIS
1	A	178	GLN
1	A	180	GLN
1	A	189	MET
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	90	ILE

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	110	TYR
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	159	MET
3	C	180	GLU
3	C	230	ASN
4	D	31	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	54	ASN
6	F	78	GLU
6	F	80	GLN
6	F	87	THR
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	33	LEU
7	G	37	LEU
7	G	79	PRO
8	H	7	LYS
8	H	9	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
11	K	47	ARG
12	L	47	LYS
13	M	12	PRO
13	M	38	ASP
13	M	39	ASN
1	N	138	HIS
1	N	180	GLN
1	N	312[A]	ILE
1	N	312[B]	ILE
1	N	362	SER
1	N	363	LEU
1	N	369	ASP

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Mol	Chain	Res	Type
1	N	484	THR
1	N	495	LEU
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	78	LEU
2	O	94	SER
3	P	33[A]	MET
3	P	33[B]	MET
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	4	SER
4	Q	5	VAL
4	Q	7	LYS
4	Q	10	ASP
4	Q	51	LEU
5	R	5	HIS
5	R	46	LYS
5	R	79	LYS
5	R	109	VAL
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	5	LYS
7	T	8	HIS
7	T	33	LEU
7	T	35	SER
7	T	37	LEU
7	T	84	LYS
8	U	9	LYS
8	U	10	ASN
9	V	8	GLN
9	V	36	LYS
9	V	52	ARG
10	W	50	LEU
12	Y	2	HIS

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Mol	Chain	Res	Type
12	Y	20	ARG
12	Y	26	THR
13	Z	2	THR
13	Z	38	ASP
13	Z	42	LYS

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	55	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	503	HIS
2	B	59	GLN
2	B	92	ASN
3	C	50	ASN
3	C	56	GLN
3	C	68	GLN
3	C	76	GLN
3	C	149	HIS
3	C	161	GLN
3	C	230	ASN
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
8	H	31	GLN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN

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Mol	Chain	Res	Type
1	N	422	ASN
2	O	10	GLN
2	O	91	ASN
3	P	50	ASN
3	P	56	GLN
3	P	68	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	95	GLN
6	S	98	HIS
7	T	76	ASN
8	U	12	GLN
8	U	37	HIS
10	W	29	ASN
10	W	57	HIS
13	Z	36	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	B	1	2	8,9,10	1.39	1 (12%)	8,9,11	7.58	4 (50%)
7	TPO	G	11	7	8,10,11	1.67	2 (25%)	10,14,16	1.56	2 (20%)
7	TPO	T	11	7	8,10,11	1.77	1 (12%)	10,14,16	1.33	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	0.50	0	8,9,11	1.39	1 (12%)
9	SAC	V	1	9	7,8,9	2.22	2 (28%)	7,9,11	1.40	1 (14%)
1	FME	N	1	1	8,9,10	0.88	0	8,9,11	1.48	2 (25%)
2	FME	O	1	2	8,9,10	0.97	0	8,9,11	1.92	3 (37%)
9	SAC	I	1	9	7,8,9	2.29	2 (28%)	7,9,11	1.31	1 (14%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.14	1.34	1.23
9	V	1	SAC	OAC-C1A	4.87	1.34	1.23
7	T	11	TPO	P-O1P	3.48	1.61	1.50
9	V	1	SAC	CA-N	3.04	1.51	1.46
7	G	11	TPO	P-O1P	2.82	1.59	1.50
9	I	1	SAC	CA-N	2.65	1.50	1.46
2	B	1	FME	O1-CN	-2.59	1.12	1.22
7	G	11	TPO	P-OG1	2.51	1.63	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.41	91.43	122.82
2	B	1	FME	O1-CN-N	4.73	137.52	125.32
7	T	11	TPO	CG2-CB-CA	3.19	119.47	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	O1-CN-N	-3.02	117.51	125.32
2	B	1	FME	O-C-CA	-2.95	117.18	124.77
7	G	11	TPO	CG2-CB-CA	2.94	119.00	113.26
1	N	1	FME	C-CA-N	2.89	115.08	109.50
2	O	1	FME	CG-CB-CA	-2.68	104.68	112.87
2	B	1	FME	CB-CA-N	-2.53	105.91	110.52
1	A	1	FME	C-CA-N	2.50	114.32	109.50
9	I	1	SAC	C-CA-N	2.48	114.28	109.50
2	O	1	FME	CB-CA-N	-2.38	106.18	110.52
9	V	1	SAC	C2A-C1A-N	2.34	120.00	116.12
1	N	1	FME	O-C-CA	-2.09	119.39	124.77
7	G	11	TPO	O2P-P-OG1	2.04	113.79	105.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	O-C-CA-CB
9	V	1	SAC	C-CA-CB-OG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
2	B	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
2	O	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	CA-CB-CG-SD
7	G	11	TPO	CB-OG1-P-O1P
7	G	11	TPO	CG2-CB-OG1-P

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	2	0
7	G	11	TPO	1	0
7	T	11	TPO	3	0
1	A	1	FME	3	0
2	O	1	FME	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 10 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
24	PEK	P	303	-	52,52,52	1.09	3 (5%)	55,57,57	1.39	6 (10%)
23	PSC	N	610	-	51,51,51	1.25	3 (5%)	57,59,59	1.27	4 (7%)
19	PGV	P	301	-	50,50,50	1.07	2 (4%)	53,56,56	1.21	5 (9%)
24	PEK	C	302	-	52,52,52	1.00	2 (3%)	55,57,57	1.10	6 (10%)
27	DMU	Z	101	-	34,34,34	0.74	1 (2%)	45,45,45	1.83	12 (26%)
14	HEA	N	602	18,1	67,67,67	2.12	22 (32%)	81,103,103	1.76	28 (34%)
14	HEA	A	602	18,1	67,67,67	2.44	26 (38%)	81,103,103	2.23	25 (30%)
20	TGL	Q	201	-	62,62,62	1.60	7 (11%)	65,65,65	1.33	11 (16%)
18	PER	A	606[B]	15	1,1,1	0.88	0	-		
21	CUA	B	302	2	0,1,1	-	-	-		
19	PGV	N	607	-	50,50,50	1.03	2 (4%)	53,56,56	1.32	8 (15%)
14	HEA	N	601	1	67,67,67	2.11	19 (28%)	81,103,103	1.81	22 (27%)
24	PEK	T	101	-	52,52,52	1.05	2 (3%)	55,57,57	1.24	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	W	101	-	32,32,32	0.83	0	51,51,51	3.06	17 (33%)
18	PER	A	606[A]	15,14	1,1,1	0.90	0	-		
19	PGV	A	608	-	50,50,50	1.23	2 (4%)	53,56,56	1.44	6 (11%)
19	PGV	C	308	-	50,50,50	1.19	2 (4%)	53,56,56	1.22	4 (7%)
19	PGV	C	303	-	50,50,50	0.96	2 (4%)	53,56,56	1.40	7 (13%)
20	TGL	B	301	-	62,62,62	1.36	6 (9%)	65,65,65	1.68	11 (16%)
22	CHD	B	303	-	32,32,32	1.45	4 (12%)	51,51,51	1.92	13 (25%)
27	DMU	M	101	-	34,34,34	0.67	0	45,45,45	2.38	14 (31%)
24	PEK	C	307	-	52,52,52	1.10	2 (3%)	55,57,57	1.20	4 (7%)
20	TGL	L	101	-	62,62,62	1.47	6 (9%)	65,65,65	1.48	10 (15%)
22	CHD	C	306	-	32,32,32	1.20	3 (9%)	51,51,51	1.77	12 (23%)
25	CDL	P	305	-	99,99,99	1.49	15 (15%)	105,111,111	1.40	13 (12%)
19	PGV	P	304	-	50,50,50	0.98	2 (4%)	53,56,56	1.05	2 (3%)
20	TGL	N	609	-	62,62,62	1.39	6 (9%)	65,65,65	1.62	9 (13%)
22	CHD	J	101	-	32,32,32	0.71	0	51,51,51	2.59	25 (49%)
25	CDL	G	101	-	99,99,99	1.45	12 (12%)	105,111,111	1.30	9 (8%)
21	CUA	O	301	2	0,1,1	-	-	-		
20	TGL	Y	101	-	62,62,62	1.44	6 (9%)	65,65,65	1.56	11 (16%)
18	PER	N	606[B]	15	1,1,1	0.90	0	-		
24	PEK	G	102	-	52,52,52	1.13	2 (3%)	55,57,57	1.25	6 (10%)
22	CHD	P	307	-	32,32,32	1.33	4 (12%)	51,51,51	1.40	8 (15%)
25	CDL	C	304	-	99,99,99	1.53	16 (16%)	105,111,111	1.51	13 (12%)
19	PGV	A	607	-	50,50,50	1.16	5 (10%)	53,56,56	1.31	5 (9%)
22	CHD	C	305	-	32,32,32	0.81	0	51,51,51	1.99	18 (35%)
22	CHD	G	103	-	32,32,32	1.56	7 (21%)	51,51,51	2.47	18 (35%)
20	TGL	D	201	-	62,62,62	1.60	7 (11%)	65,65,65	1.64	13 (20%)
19	PGV	N	608	-	50,50,50	1.06	2 (4%)	53,56,56	1.51	6 (11%)
24	PEK	P	308	-	52,52,52	1.15	2 (3%)	55,57,57	1.10	4 (7%)
25	CDL	T	102	-	99,99,99	1.45	12 (12%)	105,111,111	1.35	12 (11%)
18	PER	N	606[A]	15,14	1,1,1	0.91	0	-		
23	PSC	B	304	-	51,51,51	1.21	3 (5%)	57,59,59	1.17	4 (7%)
14	HEA	A	601	1	67,67,67	2.54	25 (37%)	81,103,103	2.32	30 (37%)
22	CHD	P	306	-	32,32,32	0.90	1 (3%)	51,51,51	2.45	19 (37%)

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
24	PEK	P	303	-	-	25/56/56/56	-
23	PSC	N	610	-	-	25/55/55/55	-
27	DMU	Z	101	-	2/2/10/10	7/19/59/59	0/2/2/2
19	PGV	P	301	-	-	30/55/55/55	-
24	PEK	C	302	-	-	17/56/56/56	-
14	HEA	N	602	18,1	-	5/36/76/76	-
14	HEA	A	602	18,1	-	7/36/76/76	-
20	TGL	Q	201	-	-	41/65/65/65	-
19	PGV	N	607	-	-	28/55/55/55	-
14	HEA	N	601	1	-	7/36/76/76	-
24	PEK	T	101	-	-	25/56/56/56	-
22	CHD	W	101	-	-	7/9/74/74	0/4/4/4
19	PGV	A	608	-	-	32/55/55/55	-
19	PGV	C	308	-	-	32/55/55/55	-
19	PGV	C	303	-	-	19/55/55/55	-
20	TGL	B	301	-	-	32/65/65/65	-
22	CHD	B	303	-	-	2/9/74/74	0/4/4/4
27	DMU	M	101	-	2/2/10/10	7/19/59/59	0/2/2/2
24	PEK	C	307	-	-	36/56/56/56	-
20	TGL	L	101	-	-	33/65/65/65	-
22	CHD	C	306	-	-	1/9/74/74	0/4/4/4
25	CDL	P	305	-	-	58/110/110/110	-
19	PGV	P	304	-	-	12/55/55/55	-
20	TGL	N	609	-	-	37/65/65/65	-
22	CHD	J	101	-	-	7/9/74/74	0/4/4/4
25	CDL	G	101	-	-	77/110/110/110	-
20	TGL	Y	101	-	-	39/65/65/65	-
24	PEK	G	102	-	-	29/56/56/56	-
22	CHD	P	307	-	-	2/9/74/74	0/4/4/4
25	CDL	C	304	-	-	62/110/110/110	-
19	PGV	A	607	-	-	9/55/55/55	-
22	CHD	C	305	-	-	6/9/74/74	0/4/4/4
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	TGL	D	201	-	-	38/65/65/65	-
19	PGV	N	608	-	-	12/55/55/55	-
24	PEK	P	308	-	-	36/56/56/56	-
25	CDL	T	102	-	-	65/110/110/110	-
23	PSC	B	304	-	-	34/55/55/55	-
14	HEA	A	601	1	-	8/36/76/76	-
22	CHD	P	306	-	-	8/9/74/74	0/4/4/4

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-NA	9.36	2.26	1.95
14	A	602	HEA	FE-NA	6.84	2.17	1.95
14	N	601	HEA	FE-NC	6.57	2.16	1.95
14	A	601	HEA	CHA-C1A	6.29	1.50	1.38
14	A	601	HEA	FE-NC	6.22	2.15	1.95
14	N	601	HEA	FE-NA	6.02	2.15	1.95
20	L	101	TGL	OG2-CB1	5.99	1.51	1.34
14	A	602	HEA	FE-NC	5.82	2.14	1.95
20	Y	101	TGL	OG2-CB1	5.45	1.49	1.34
19	A	608	PGV	O03-C19	5.44	1.49	1.33
20	D	201	TGL	OB1-CB1	5.44	1.38	1.22
20	Q	201	TGL	OG2-CB1	5.42	1.49	1.34
20	D	201	TGL	OG2-CB1	5.39	1.49	1.34
20	B	301	TGL	OG1-CA1	5.32	1.48	1.33
24	P	308	PEK	O01-C1	5.19	1.48	1.34
20	Q	201	TGL	OG1-CA1	5.17	1.48	1.33
20	Y	101	TGL	OG3-CC1	5.16	1.48	1.33
14	A	602	HEA	CMD-C2D	5.10	1.61	1.50
20	Q	201	TGL	OB1-CB1	5.08	1.37	1.22
23	N	610	PSC	O01-C1	5.06	1.48	1.34
25	G	101	CDL	OB8-CB7	5.06	1.48	1.33
20	D	201	TGL	OG1-CA1	5.06	1.48	1.33
25	C	304	CDL	OA8-CA7	5.05	1.48	1.33
20	N	609	TGL	OG3-CC1	5.04	1.48	1.33
24	C	307	PEK	O03-C21	5.01	1.48	1.33
14	N	602	HEA	FE-NC	5.01	2.11	1.95
14	A	602	HEA	C1C-NC	-5.00	1.30	1.39
24	C	307	PEK	O01-C1	4.98	1.48	1.34
24	G	102	PEK	O03-C21	4.97	1.47	1.33
25	P	305	CDL	OA8-CA7	4.94	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	609	TGL	OG1-CA1	4.89	1.47	1.33
24	G	102	PEK	O01-C1	4.85	1.48	1.34
19	C	308	PGV	O01-C1	4.85	1.48	1.34
20	B	301	TGL	OG3-CC1	4.83	1.47	1.33
19	N	607	PGV	O03-C19	4.83	1.47	1.33
24	T	101	PEK	O03-C21	4.83	1.47	1.33
25	G	101	CDL	OA6-CA5	4.83	1.47	1.34
25	T	102	CDL	OA8-CA7	4.81	1.47	1.33
23	B	304	PSC	O01-C1	4.81	1.47	1.34
25	T	102	CDL	OA6-CA5	4.80	1.47	1.34
25	C	304	CDL	OA6-CA5	4.74	1.47	1.34
19	P	301	PGV	O03-C19	4.70	1.47	1.33
24	P	308	PEK	O03-C21	4.69	1.47	1.33
19	A	608	PGV	O01-C1	4.69	1.47	1.34
20	L	101	TGL	OG1-CA1	4.64	1.46	1.33
14	A	601	HEA	C1A-NA	-4.63	1.30	1.39
20	L	101	TGL	OG3-CC1	4.61	1.46	1.33
19	C	308	PGV	O03-C19	4.58	1.46	1.33
23	N	610	PSC	O03-C19	4.53	1.46	1.33
24	C	302	PEK	O03-C21	4.50	1.46	1.33
25	P	305	CDL	OB8-CB7	4.49	1.46	1.33
19	N	608	PGV	O03-C19	4.48	1.46	1.33
25	P	305	CDL	OA6-CA5	4.47	1.46	1.34
25	G	101	CDL	OB6-CB5	4.47	1.46	1.34
14	N	602	HEA	CHD-C1D	4.42	1.47	1.38
25	T	102	CDL	OB6-CB5	4.41	1.46	1.34
24	T	101	PEK	O01-C1	4.39	1.46	1.34
25	C	304	CDL	OB8-CB7	4.38	1.46	1.33
20	Q	201	TGL	OG3-CC1	4.38	1.46	1.33
14	N	602	HEA	C1A-NA	-4.37	1.31	1.39
14	A	602	HEA	C12-C11	4.36	1.60	1.53
24	P	303	PEK	O03-C21	4.32	1.45	1.33
14	A	602	HEA	CHB-C4A	4.32	1.46	1.38
25	T	102	CDL	C42-C41	-4.30	1.30	1.51
20	N	609	TGL	OG2-CB1	4.30	1.46	1.34
14	N	601	HEA	C1D-ND	-4.26	1.32	1.40
14	N	602	HEA	CMD-C2D	4.25	1.59	1.50
14	N	601	HEA	FE-ND	4.25	2.08	1.94
25	G	101	CDL	OA8-CA7	4.23	1.45	1.33
23	N	610	PSC	C13-C12	4.22	1.55	1.31
23	B	304	PSC	O03-C19	4.21	1.45	1.33
19	P	301	PGV	O01-C1	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	304	PSC	C13-C12	4.14	1.55	1.31
19	A	607	PGV	O03-C19	4.13	1.45	1.33
14	A	602	HEA	CHA-C1A	4.11	1.46	1.38
14	N	602	HEA	FE-NA	4.10	2.08	1.95
25	T	102	CDL	OB8-CB7	4.09	1.45	1.33
19	P	304	PGV	O03-C19	4.09	1.45	1.33
14	A	601	HEA	CHC-C1C	4.08	1.48	1.39
19	N	607	PGV	O01-C1	4.08	1.45	1.34
14	A	601	HEA	C1C-NC	-4.05	1.32	1.39
20	D	201	TGL	OG3-CC1	4.04	1.45	1.33
24	C	302	PEK	O01-C1	3.99	1.45	1.34
25	C	304	CDL	C59-C58	-3.96	1.32	1.51
20	Y	101	TGL	C20-CA9	-3.96	1.32	1.51
14	A	601	HEA	C4C-NC	-3.95	1.32	1.39
14	A	601	HEA	FE-NB	3.95	2.07	1.94
25	C	304	CDL	C79-C78	-3.93	1.32	1.51
14	N	601	HEA	CHA-C1A	3.90	1.46	1.38
20	Y	101	TGL	OG1-CA1	3.89	1.44	1.33
14	A	602	HEA	CMB-C2B	3.88	1.58	1.50
22	G	103	CHD	C10-C5	-3.86	1.49	1.55
14	A	601	HEA	CHB-C4A	3.84	1.45	1.38
20	N	609	TGL	C10-CB9	-3.81	1.32	1.51
25	P	305	CDL	C59-C58	-3.81	1.32	1.51
14	A	601	HEA	CMB-C2B	3.80	1.58	1.50
20	L	101	TGL	C20-CA9	-3.76	1.33	1.51
20	D	201	TGL	C10-CB9	-3.76	1.33	1.51
25	P	305	CDL	OB6-CB5	3.76	1.44	1.34
25	P	305	CDL	C62-C61	-3.73	1.33	1.51
14	N	602	HEA	C1B-C2B	-3.73	1.37	1.44
25	T	102	CDL	C39-C38	-3.70	1.33	1.51
14	N	602	HEA	C4B-C3B	-3.70	1.38	1.44
19	C	303	PGV	O03-C19	3.69	1.44	1.33
20	Q	201	TGL	C10-CB9	-3.68	1.33	1.51
25	P	305	CDL	C79-C78	-3.68	1.33	1.51
25	G	101	CDL	C82-C81	-3.68	1.33	1.51
20	N	609	TGL	C20-CA9	-3.67	1.33	1.51
22	B	303	CHD	C4-C3	3.65	1.58	1.52
14	N	602	HEA	CHA-C1A	3.64	1.45	1.38
14	N	601	HEA	C1B-C2B	-3.62	1.37	1.44
14	N	602	HEA	C3A-C4A	-3.62	1.39	1.46
25	G	101	CDL	C59-C58	-3.61	1.33	1.51
25	T	102	CDL	C59-C58	-3.60	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-ND	3.60	2.06	1.94
25	T	102	CDL	C22-C21	-3.60	1.33	1.51
25	C	304	CDL	C82-C81	-3.59	1.33	1.51
25	G	101	CDL	C79-C78	-3.59	1.33	1.51
25	P	305	CDL	C39-C38	-3.59	1.33	1.51
24	P	303	PEK	C2-C1	3.59	1.61	1.50
25	T	102	CDL	C82-C81	-3.59	1.33	1.51
14	N	601	HEA	C4A-NA	-3.58	1.32	1.39
25	C	304	CDL	C19-C18	-3.57	1.34	1.51
20	L	101	TGL	C10-CB9	-3.55	1.34	1.51
25	C	304	CDL	C22-C21	-3.55	1.34	1.51
25	C	304	CDL	C39-C38	-3.55	1.34	1.51
25	C	304	CDL	C62-C61	-3.53	1.34	1.51
25	C	304	CDL	C42-C41	-3.51	1.34	1.51
25	T	102	CDL	C19-C18	-3.51	1.34	1.51
25	G	101	CDL	C62-C61	-3.51	1.34	1.51
20	Y	101	TGL	C10-CB9	-3.49	1.34	1.51
20	B	301	TGL	C20-CA9	-3.49	1.34	1.51
25	P	305	CDL	C82-C81	-3.48	1.34	1.51
14	A	601	HEA	CMA-C3A	3.48	1.53	1.45
25	T	102	CDL	C79-C78	-3.46	1.34	1.51
20	B	301	TGL	C10-CB9	-3.46	1.34	1.51
25	P	305	CDL	C19-C18	-3.45	1.34	1.51
25	G	101	CDL	C42-C41	-3.45	1.34	1.51
14	A	602	HEA	C4D-ND	-3.43	1.32	1.38
14	A	601	HEA	C4B-NB	-3.43	1.34	1.40
25	P	305	CDL	C42-C41	-3.42	1.34	1.51
25	C	304	CDL	OB6-CB5	3.39	1.43	1.34
14	N	601	HEA	CHC-C4B	3.32	1.45	1.38
25	P	305	CDL	C22-C21	-3.31	1.35	1.51
20	Q	201	TGL	C15-CC9	-3.31	1.35	1.51
14	A	602	HEA	FE-NB	3.30	2.05	1.94
25	G	101	CDL	C39-C38	-3.30	1.35	1.51
20	Y	101	TGL	C15-CC9	-3.29	1.35	1.51
20	D	201	TGL	C15-CC9	-3.28	1.35	1.51
20	B	301	TGL	OG2-CB1	3.24	1.43	1.34
14	N	601	HEA	C1A-C2A	-3.24	1.39	1.45
14	A	602	HEA	FE-ND	3.23	2.04	1.94
14	N	602	HEA	C4D-ND	-3.22	1.32	1.38
20	N	609	TGL	C15-CC9	-3.21	1.35	1.51
20	Q	201	TGL	C20-CA9	-3.21	1.35	1.51
25	T	102	CDL	C62-C61	-3.20	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	CHD-C1D	3.19	1.44	1.38
14	A	601	HEA	C1A-C2A	-3.18	1.39	1.45
20	D	201	TGL	C20-CA9	-3.17	1.36	1.51
14	N	602	HEA	C1A-C2A	-3.17	1.39	1.45
24	P	303	PEK	O01-C1	3.16	1.43	1.34
25	G	101	CDL	C19-C18	-3.16	1.36	1.51
19	C	303	PGV	O01-C1	3.15	1.43	1.34
14	N	602	HEA	CHB-C4A	3.15	1.44	1.38
22	P	307	CHD	C8-C7	3.11	1.59	1.53
19	P	304	PGV	O01-C1	3.10	1.43	1.34
20	L	101	TGL	C15-CC9	-3.09	1.36	1.51
20	B	301	TGL	C15-CC9	-3.04	1.36	1.51
14	A	602	HEA	C11-C3B	3.02	1.55	1.51
14	A	602	HEA	C1A-C2A	-3.02	1.39	1.45
14	A	601	HEA	C1D-ND	-3.02	1.35	1.40
14	A	602	HEA	C18-C19	3.02	1.40	1.33
14	A	602	HEA	C1A-NA	-3.01	1.33	1.39
22	G	103	CHD	C6-C5	3.00	1.58	1.53
22	C	306	CHD	C18-C13	2.99	1.59	1.54
25	G	101	CDL	C22-C21	-2.99	1.36	1.51
14	N	601	HEA	C3A-C4A	-2.97	1.40	1.46
22	G	103	CHD	C18-C13	2.97	1.59	1.54
14	N	602	HEA	C1D-C2D	-2.93	1.38	1.44
14	N	602	HEA	C1C-NC	-2.92	1.34	1.39
22	B	303	CHD	C4-C5	2.92	1.58	1.53
14	N	601	HEA	C1A-NA	-2.90	1.34	1.39
14	A	602	HEA	CHC-C1C	2.89	1.45	1.39
14	A	602	HEA	CHD-C4C	2.87	1.45	1.39
22	P	307	CHD	C11-C12	2.84	1.57	1.53
14	N	601	HEA	CHC-C1C	2.83	1.45	1.39
14	A	602	HEA	C3A-C2A	2.80	1.43	1.37
14	N	601	HEA	C1C-NC	-2.80	1.34	1.39
14	A	602	HEA	CAD-C3D	2.73	1.58	1.51
14	A	602	HEA	C4A-NA	-2.67	1.34	1.39
14	A	601	HEA	C3A-C4A	-2.64	1.41	1.46
14	A	601	HEA	CBD-CGD	2.64	1.56	1.50
14	N	601	HEA	CHA-C4D	2.62	1.45	1.39
14	A	602	HEA	CMC-C2C	2.61	1.56	1.50
14	N	602	HEA	CHC-C4B	2.59	1.43	1.38
19	A	607	PGV	O01-C1	2.58	1.41	1.34
14	N	601	HEA	CMB-C2B	2.55	1.56	1.50
25	C	304	CDL	OB6-CB4	-2.55	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	CHB-C1B	2.53	1.45	1.39
14	A	601	HEA	C1C-C2C	-2.51	1.37	1.43
22	G	103	CHD	C13-C12	2.50	1.58	1.54
14	A	601	HEA	CHB-C1B	2.46	1.44	1.39
22	C	306	CHD	C21-C20	2.45	1.59	1.53
14	A	601	HEA	O1D-CGD	2.44	1.30	1.22
14	A	602	HEA	C4B-NB	-2.44	1.36	1.40
14	N	602	HEA	C4C-NC	-2.43	1.35	1.39
22	G	103	CHD	C11-C9	2.41	1.57	1.53
14	N	601	HEA	O11-C11	2.37	1.48	1.42
14	N	601	HEA	C4D-ND	-2.37	1.34	1.38
14	A	602	HEA	CHC-C4B	2.33	1.43	1.38
27	Z	101	DMU	O16-C6	2.33	1.44	1.40
22	C	306	CHD	C11-C9	2.33	1.57	1.53
14	A	601	HEA	O11-C11	2.32	1.48	1.42
14	A	602	HEA	C20-C19	2.30	1.56	1.51
25	P	305	CDL	PB2-OB3	2.30	1.58	1.50
14	N	602	HEA	OMA-CMA	2.28	1.27	1.22
14	N	602	HEA	CBD-CGD	2.28	1.55	1.50
14	N	602	HEA	FE-ND	2.26	2.01	1.94
19	A	607	PGV	P-O14	-2.24	1.45	1.55
14	N	602	HEA	C16-C15	2.23	1.55	1.51
25	C	304	CDL	CA2-C1	2.22	1.58	1.51
25	P	305	CDL	O1-C1	2.21	1.49	1.43
14	A	601	HEA	C4A-NA	-2.20	1.35	1.39
22	P	306	CHD	C8-C9	2.19	1.58	1.53
25	P	305	CDL	CB2-C1	2.17	1.58	1.51
14	N	602	HEA	C20-C19	2.15	1.55	1.51
22	B	303	CHD	C11-C9	2.15	1.57	1.53
14	A	601	HEA	C1D-C2D	-2.15	1.40	1.44
22	B	303	CHD	C13-C12	2.11	1.57	1.54
14	A	602	HEA	C1D-C2D	-2.08	1.40	1.44
19	N	608	PGV	O06-C06	2.08	1.51	1.42
25	C	304	CDL	PB2-OB3	2.07	1.58	1.50
14	N	601	HEA	C4D-C3D	-2.06	1.41	1.45
25	C	304	CDL	CB2-C1	2.05	1.58	1.51
22	G	103	CHD	C20-C17	2.05	1.57	1.54
22	P	307	CHD	C6-C5	2.04	1.57	1.53
14	A	601	HEA	C3B-C2B	2.03	1.39	1.34
22	P	307	CHD	C21-C20	2.02	1.58	1.53
14	N	602	HEA	CMA-C3A	2.01	1.49	1.45
22	G	103	CHD	O26-C24	-2.01	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	607	PGV	C01-C02	2.00	1.57	1.50
14	A	601	HEA	C4D-ND	-2.00	1.34	1.38
19	A	607	PGV	C8-C7	2.00	1.61	1.51

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C17-C13-C12	9.82	126.50	117.67
22	G	103	CHD	C1-C2-C3	-9.55	97.84	110.48
22	W	101	CHD	C13-C17-C20	8.62	129.93	119.48
22	W	101	CHD	C18-C13-C12	-7.92	101.13	109.06
22	W	101	CHD	C17-C13-C14	-7.30	92.79	100.11
14	A	601	HEA	OMA-CMA-C3A	-6.91	110.01	125.62
20	N	609	TGL	CG2-OG2-CB1	6.85	134.19	117.80
14	A	602	HEA	CHB-C1B-NB	-6.78	117.13	124.42
27	M	101	DMU	O7-C10-C5	-6.69	91.64	108.09
20	Y	101	TGL	OG2-CB1-CB2	6.42	125.37	111.48
25	T	102	CDL	OA6-CA5-C11	6.25	125.01	111.48
14	A	601	HEA	CHB-C4A-NA	-6.16	117.75	124.45
22	G	103	CHD	C4-C5-C10	-6.14	106.12	112.66
22	C	305	CHD	C23-C22-C20	-6.09	103.09	114.46
24	T	101	PEK	O01-C1-C2	6.05	124.56	111.48
22	J	101	CHD	C10-C9-C8	6.03	118.56	111.84
25	C	304	CDL	OA6-CA5-C11	6.02	124.51	111.48
25	G	101	CDL	OB6-CB5-C51	5.96	124.38	111.48
27	M	101	DMU	O1-C9-C8	5.93	120.38	109.70
20	D	201	TGL	OG2-CB1-CB2	-5.90	98.72	111.48
22	P	306	CHD	C18-C13-C12	-5.87	103.18	109.06
22	B	303	CHD	C4-C3-C2	5.69	117.56	110.62
20	D	201	TGL	OG2-CB1-OB1	5.68	136.97	123.70
14	A	601	HEA	C4A-C3A-C2A	-5.51	102.03	106.81
14	A	601	HEA	C4A-CHB-C1B	5.49	137.69	126.02
14	N	602	HEA	OMA-CMA-C3A	-5.41	113.40	125.62
19	N	608	PGV	O03-C19-O04	-5.40	110.13	123.63
22	J	101	CHD	C9-C8-C7	5.40	118.65	111.86
22	J	101	CHD	C6-C5-C4	-5.24	105.24	111.23
24	P	303	PEK	C2-C3-C4	5.21	124.73	113.35
27	Z	101	DMU	C10-O1-C9	5.21	123.89	113.72
14	A	601	HEA	CHA-C4D-ND	5.19	130.00	124.42
14	A	601	HEA	C17-C18-C19	5.16	139.42	127.62
25	G	101	CDL	OA6-CA5-C11	5.15	122.62	111.48
24	G	102	PEK	O01-C1-C2	5.14	122.61	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	301	TGL	CG2-OG2-CB1	5.12	130.04	117.80
27	M	101	DMU	O1-C10-C5	5.06	120.76	110.37
23	N	610	PSC	O01-C1-C2	5.05	122.40	111.48
22	P	306	CHD	C6-C7-C8	5.04	117.01	111.50
14	A	602	HEA	OMA-CMA-C3A	-4.96	114.42	125.62
22	C	306	CHD	C18-C13-C12	4.95	114.01	109.06
19	P	301	PGV	O03-C19-C20	4.93	126.88	111.83
25	P	305	CDL	CB4-OB6-CB5	-4.91	106.03	117.80
14	A	602	HEA	CMB-C2B-C1B	4.91	132.70	125.03
14	A	602	HEA	CHA-C4D-ND	4.82	129.62	124.42
14	A	601	HEA	CHB-C1B-NB	-4.82	119.24	124.42
19	C	308	PGV	O01-C1-C2	4.81	121.89	111.48
27	Z	101	DMU	O1-C9-C8	4.81	118.36	109.70
19	C	303	PGV	O03-C19-O04	-4.74	111.76	123.63
23	B	304	PSC	O01-C1-C2	4.70	121.64	111.48
22	P	306	CHD	C15-C14-C13	4.60	108.00	103.54
22	G	103	CHD	C15-C14-C13	4.59	108.00	103.54
24	P	303	PEK	O01-C1-O02	-4.57	113.02	123.70
14	A	602	HEA	C4A-C3A-C2A	-4.57	102.85	106.81
22	J	101	CHD	C4-C5-C10	4.54	117.49	112.66
22	P	306	CHD	C19-C10-C9	-4.51	105.11	111.18
22	J	101	CHD	C14-C8-C7	4.49	117.80	111.85
25	T	102	CDL	OB6-CB5-C51	4.46	121.14	111.48
14	A	601	HEA	C2B-C1B-NB	4.44	115.04	109.90
14	N	601	HEA	C3A-C2A-C1A	-4.44	102.84	107.05
22	P	306	CHD	C4-C5-C10	4.42	117.37	112.66
24	C	307	PEK	O01-C1-C2	4.40	121.01	111.48
22	W	101	CHD	C14-C8-C7	4.39	117.68	111.85
27	M	101	DMU	C8-C7-C5	4.35	118.47	110.83
25	P	305	CDL	OA6-CA5-C11	4.34	120.88	111.48
22	W	101	CHD	C11-C12-C13	4.31	115.65	111.26
20	B	301	TGL	CG3-OG3-CC1	4.30	132.85	117.12
22	G	103	CHD	C18-C13-C14	4.28	117.91	111.20
14	N	601	HEA	O2D-CGD-CBD	4.28	127.53	114.00
22	J	101	CHD	C14-C8-C9	-4.28	103.78	109.75
19	A	608	PGV	O03-C19-C20	4.28	124.88	111.83
25	P	305	CDL	OB8-CB7-C71	4.27	124.87	111.83
24	C	307	PEK	O03-C21-C22	4.26	124.83	111.83
22	J	101	CHD	C13-C17-C20	4.25	124.63	119.48
20	N	609	TGL	OG2-CB1-CB2	4.24	120.66	111.48
22	B	303	CHD	C19-C10-C5	-4.21	103.40	110.44
20	B	301	TGL	OG1-CA1-CA2	4.19	124.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C13-C12-C11	-4.18	107.72	114.39
20	L	101	TGL	OG3-CC1-CC2	4.17	124.55	111.83
22	P	306	CHD	O7-C7-C6	-4.16	99.52	109.86
19	A	608	PGV	C4-C3-C2	-4.15	97.87	113.13
14	N	602	HEA	CHA-C4D-ND	4.11	128.84	124.42
22	J	101	CHD	C14-C13-C12	4.10	111.16	107.42
25	C	304	CDL	CB4-OB6-CB5	-4.08	108.03	117.80
19	N	608	PGV	O03-C19-C20	4.07	124.24	111.83
20	B	301	TGL	OG2-CB1-CB2	4.06	120.25	111.48
22	J	101	CHD	C11-C12-C13	4.04	115.38	111.26
22	W	101	CHD	C18-C13-C17	3.95	117.40	111.20
22	W	101	CHD	C15-C14-C8	3.94	123.76	118.36
22	P	306	CHD	C19-C10-C1	-3.93	102.06	108.31
19	C	308	PGV	O03-C19-C20	3.92	123.80	111.83
22	B	303	CHD	C15-C14-C13	3.92	107.35	103.54
24	P	303	PEK	O03-C21-C22	3.92	123.78	111.83
19	P	301	PGV	O01-C1-C2	3.90	119.92	111.48
22	G	103	CHD	C19-C10-C1	-3.89	102.12	108.31
14	A	602	HEA	CMD-C2D-C1D	3.86	131.06	125.03
22	J	101	CHD	C19-C10-C9	-3.85	106.00	111.18
20	N	609	TGL	CG3-OG3-CC1	3.82	131.09	117.12
27	M	101	DMU	O7-C10-O1	-3.82	100.64	110.69
27	Z	101	DMU	O49-C1-C2	-3.82	101.38	110.38
14	A	602	HEA	C2B-C1B-NB	3.80	114.29	109.90
19	C	303	PGV	O01-C1-C2	3.79	119.68	111.48
22	P	306	CHD	C16-C17-C13	3.78	107.21	103.54
14	A	602	HEA	C4A-CHB-C1B	3.77	134.04	126.02
14	A	602	HEA	CAD-C3D-C4D	-3.76	118.14	124.70
22	W	101	CHD	C6-C5-C10	3.74	116.64	112.66
22	C	305	CHD	C6-C7-C8	3.74	115.58	111.50
20	B	301	TGL	OG2-CG2-CG1	3.72	121.68	108.34
19	A	607	PGV	O03-C19-C20	3.72	123.17	111.83
22	G	103	CHD	C13-C14-C8	-3.71	110.02	114.72
14	A	601	HEA	CMB-C2B-C1B	3.71	130.82	125.03
14	A	602	HEA	CMB-C2B-C3B	-3.70	123.12	130.28
22	B	303	CHD	C18-C13-C12	-3.70	105.36	109.06
27	Z	101	DMU	C18-O16-C6	-3.67	107.42	113.68
22	P	306	CHD	O3-C3-C4	-3.65	102.57	109.84
14	A	602	HEA	C1D-C2D-C3D	-3.65	103.15	106.98
20	Q	201	TGL	OG2-CB1-CB2	-3.63	103.63	111.48
24	P	308	PEK	O01-C1-C2	3.63	119.33	111.48
25	P	305	CDL	OB6-CB5-C51	3.62	119.31	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	CHC-C4B-NB	3.62	128.84	124.37
14	N	601	HEA	C2B-C1B-NB	3.59	114.05	109.90
24	P	308	PEK	O03-C21-C22	3.58	122.75	111.83
22	C	306	CHD	C1-C2-C3	-3.58	105.74	110.48
22	C	305	CHD	C18-C13-C12	-3.56	105.49	109.06
19	N	607	PGV	O01-C1-C2	3.55	119.17	111.48
14	N	601	HEA	CHA-C1A-NA	-3.55	120.58	124.45
22	C	306	CHD	C16-C17-C13	-3.54	100.11	103.54
22	P	306	CHD	C11-C12-C13	3.53	114.86	111.26
27	M	101	DMU	O3-C5-C7	3.53	118.70	110.38
24	G	102	PEK	O03-C21-C22	3.52	122.57	111.83
22	P	307	CHD	C19-C10-C1	-3.51	102.72	108.31
22	C	305	CHD	C1-C10-C5	3.51	112.79	107.75
19	A	608	PGV	C02-O01-C1	3.50	126.17	117.80
22	C	305	CHD	C17-C13-C12	-3.50	114.52	117.67
20	Y	101	TGL	OG3-CC1-CC2	3.50	122.50	111.83
14	A	602	HEA	CHB-C4A-NA	-3.49	120.65	124.45
23	N	610	PSC	O03-C19-C20	3.49	122.47	111.83
20	B	301	TGL	OG3-CC1-CC2	3.48	122.45	111.83
19	N	608	PGV	O01-C1-O02	-3.47	115.60	123.70
27	Z	101	DMU	O2-C8-C9	3.45	117.83	109.32
14	N	601	HEA	O2D-CGD-O1D	-3.44	114.48	123.33
25	P	305	CDL	OB8-CB7-OB9	-3.44	115.03	123.63
22	W	101	CHD	C1-C10-C5	3.43	112.67	107.75
14	A	601	HEA	CAA-CBA-CGA	-3.43	104.56	113.67
20	L	101	TGL	OG1-CA1-CA2	3.43	122.29	111.83
27	M	101	DMU	C10-C5-C7	3.43	117.22	110.01
14	N	602	HEA	O11-C11-C3B	-3.42	104.98	111.26
24	T	101	PEK	O01-C1-O02	-3.41	115.74	123.70
20	B	301	TGL	CB3-CB2-CB1	-3.40	101.23	113.69
22	B	303	CHD	C6-C5-C10	3.40	116.27	112.66
20	N	609	TGL	OG1-CA1-CA2	3.39	122.19	111.83
22	B	303	CHD	C13-C17-C20	-3.39	115.37	119.48
14	N	601	HEA	CMD-C2D-C1D	3.39	130.33	125.03
19	N	607	PGV	C4-C3-C2	-3.38	100.70	113.13
19	A	607	PGV	O03-C19-O04	-3.38	115.18	123.63
20	Q	201	TGL	OG1-CA1-CA2	3.37	122.12	111.83
14	A	601	HEA	CHA-C4D-C3D	-3.37	119.86	124.77
14	A	601	HEA	C1B-C2B-C3B	-3.36	102.91	106.80
22	G	103	CHD	C17-C13-C12	-3.35	114.65	117.67
14	N	602	HEA	C1A-CHA-C4D	-3.34	118.93	126.02
22	W	101	CHD	C22-C20-C17	3.34	117.25	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	609	TGL	OG2-CG2-CG1	3.32	120.26	108.34
22	B	303	CHD	C1-C10-C5	3.32	112.51	107.75
22	J	101	CHD	C1-C2-C3	3.31	114.87	110.48
27	M	101	DMU	C7-C8-C9	3.30	116.21	110.23
22	J	101	CHD	C19-C10-C1	-3.29	103.08	108.31
20	Y	101	TGL	OG1-CA1-OA1	-3.29	115.40	123.63
14	A	602	HEA	CHA-C4D-C3D	-3.27	120.01	124.77
24	P	308	PEK	O03-C21-O04	-3.26	115.47	123.63
22	P	307	CHD	C4-C5-C10	-3.26	109.19	112.66
22	P	306	CHD	C15-C14-C8	3.25	122.81	118.36
20	D	201	TGL	CB3-CB2-CB1	3.23	125.53	113.69
19	N	607	PGV	C3-C2-C1	-3.23	101.87	113.69
22	W	101	CHD	C6-C5-C4	-3.21	107.56	111.23
19	C	303	PGV	O03-C19-C20	3.21	121.61	111.83
14	N	601	HEA	OMA-CMA-C3A	-3.20	118.41	125.62
25	G	101	CDL	OA8-CA7-C31	3.18	121.53	111.83
27	M	101	DMU	C10-O1-C9	3.18	119.92	113.72
20	Y	101	TGL	OG1-CA1-CA2	3.17	121.51	111.83
24	T	101	PEK	O03-C21-C22	3.17	121.51	111.83
20	Q	201	TGL	OG1-CG1-CG2	3.17	117.53	108.40
25	C	304	CDL	C52-C51-CB5	-3.13	102.22	113.69
22	P	306	CHD	C6-C5-C10	3.13	115.99	112.66
25	T	102	CDL	OA8-CA7-C31	3.13	121.36	111.83
20	B	301	TGL	CG1-OG1-CA1	3.12	128.53	117.12
25	C	304	CDL	OB6-CB5-C51	3.12	118.23	111.48
25	P	305	CDL	OA8-CA7-C31	3.10	121.29	111.83
14	N	601	HEA	C3C-C4C-NC	3.10	112.41	109.80
22	C	306	CHD	C6-C5-C4	-3.09	107.69	111.23
22	G	103	CHD	C18-C13-C12	-3.08	105.97	109.06
25	C	304	CDL	OB8-CB7-C71	3.06	121.17	111.83
22	J	101	CHD	C15-C14-C8	3.05	122.55	118.36
14	A	601	HEA	C26-C15-C16	-3.05	109.93	115.23
14	N	602	HEA	C4C-C3C-C2C	-3.05	103.51	107.30
19	N	608	PGV	C01-O03-C19	-3.03	106.05	117.12
22	C	306	CHD	C5-C6-C7	3.02	117.99	114.40
25	C	304	CDL	OA8-CA7-C31	3.01	121.03	111.83
22	P	306	CHD	C11-C9-C8	3.01	115.34	110.89
14	A	602	HEA	CHD-C4C-NC	3.00	129.30	123.86
20	L	101	TGL	OG2-CB1-CB2	3.00	117.97	111.48
24	G	102	PEK	O03-C01-C02	2.99	117.02	108.40
22	P	306	CHD	C22-C23-C24	-2.96	104.61	112.49
14	A	602	HEA	CAD-C3D-C2D	2.95	133.40	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	306	CHD	C21-C20-C22	-2.94	105.79	110.34
19	A	608	PGV	C01-O03-C19	2.94	127.85	117.12
25	G	101	CDL	OA6-CA5-OA7	-2.93	116.85	123.70
14	N	601	HEA	C17-C18-C19	2.93	134.32	127.62
14	N	602	HEA	C12-C11-C3B	2.93	116.69	112.12
14	A	601	HEA	CHA-C1A-NA	-2.92	121.27	124.45
20	N	609	TGL	OG2-CG2-CG3	2.92	118.80	108.34
14	A	602	HEA	C2D-C1D-ND	2.90	113.18	109.84
14	A	602	HEA	C16-C15-C14	-2.90	114.66	121.17
22	C	305	CHD	C21-C20-C17	2.88	117.20	112.88
20	Q	201	TGL	OG3-CC1-CC2	2.87	120.59	111.83
22	C	306	CHD	C11-C12-C13	2.86	114.18	111.26
20	D	201	TGL	OG3-CG3-CG2	-2.86	100.14	108.40
25	C	304	CDL	OA6-CA5-OA7	-2.86	117.01	123.70
24	C	302	PEK	O03-C21-O04	-2.86	116.47	123.63
20	D	201	TGL	OG1-CG1-CG2	2.85	116.62	108.40
19	C	308	PGV	C01-O03-C19	2.84	127.52	117.12
14	A	601	HEA	C20-C19-C18	2.84	127.55	121.17
20	D	201	TGL	C21-C20-CA9	2.84	128.71	114.37
19	A	607	PGV	C23-C22-C21	-2.81	100.15	114.37
22	G	103	CHD	C16-C15-C14	-2.79	99.67	105.14
14	N	602	HEA	O2A-CGA-CBA	2.78	122.78	114.00
19	A	608	PGV	O03-C19-O04	-2.77	116.69	123.63
25	T	102	CDL	OA6-CA5-OA7	-2.77	117.23	123.70
23	B	304	PSC	O03-C19-C20	2.77	120.27	111.83
25	G	101	CDL	C19-C18-C17	2.76	128.34	114.37
14	N	602	HEA	C13-C12-C11	-2.76	109.98	114.39
22	W	101	CHD	C11-C9-C10	2.76	116.50	113.70
19	P	304	PGV	O01-C1-C2	2.76	117.45	111.48
22	P	306	CHD	C14-C8-C9	-2.76	105.90	109.75
20	Q	201	TGL	OG2-CB1-OB1	2.75	130.14	123.70
25	G	101	CDL	CB6-OB8-CB7	2.75	127.17	117.12
14	N	601	HEA	C12-C11-C3B	2.74	116.40	112.12
22	P	306	CHD	C1-C10-C9	2.74	115.59	111.34
27	M	101	DMU	O16-C6-C1	2.73	112.41	108.27
22	J	101	CHD	C16-C17-C13	2.73	106.19	103.54
25	P	305	CDL	C52-C51-CB5	-2.72	103.72	113.69
27	M	101	DMU	C28-C25-C22	-2.72	100.61	114.37
20	Y	101	TGL	OG1-CG1-CG2	2.71	116.20	108.40
27	M	101	DMU	O7-C3-C4	-2.70	102.39	109.48
22	G	103	CHD	C5-C4-C3	-2.70	108.64	112.71
14	N	602	HEA	CHB-C1B-C2B	-2.68	120.80	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	201	TGL	CG2-OG2-CB1	2.68	124.20	117.80
22	J	101	CHD	C11-C9-C8	-2.68	106.94	110.89
25	G	101	CDL	OA8-CA7-OA9	-2.67	116.95	123.63
25	T	102	CDL	OB8-CB7-OB9	-2.66	116.97	123.63
22	C	305	CHD	C19-C10-C1	-2.66	104.08	108.31
24	C	307	PEK	O03-C01-C02	2.65	116.04	108.40
14	N	602	HEA	C4A-C3A-C2A	-2.65	104.52	106.81
22	G	103	CHD	C14-C8-C9	2.65	113.45	109.75
22	W	101	CHD	O12-C12-C11	2.65	114.51	109.12
22	P	307	CHD	C22-C23-C24	-2.65	105.43	112.49
22	P	307	CHD	C11-C9-C10	-2.65	111.02	113.70
19	C	303	PGV	O01-C1-O02	-2.64	117.53	123.70
25	G	101	CDL	OB6-CB5-OB7	-2.64	117.54	123.70
27	Z	101	DMU	C7-C8-C9	2.63	115.00	110.23
20	Y	101	TGL	OG2-CB1-OB1	-2.63	117.56	123.70
20	Y	101	TGL	OG3-CG3-CG2	2.63	115.97	108.40
22	C	305	CHD	C22-C23-C24	-2.63	105.49	112.49
25	T	102	CDL	OB8-CB7-C71	2.62	119.82	111.83
20	D	201	TGL	OG3-CC1-OC1	-2.62	117.08	123.63
19	N	607	PGV	C02-O01-C1	2.61	124.05	117.80
23	N	610	PSC	O01-C1-O02	-2.61	117.61	123.70
25	C	304	CDL	OA8-CA6-CA4	2.61	115.91	108.40
24	C	302	PEK	O01-C1-C2	2.60	117.10	111.48
20	N	609	TGL	OG3-CC1-CC2	2.60	119.75	111.83
14	N	601	HEA	O11-C11-C3B	-2.59	106.51	111.26
22	C	305	CHD	C14-C13-C12	2.59	109.78	107.42
14	N	601	HEA	C3D-C4D-ND	2.58	112.85	110.35
20	Y	101	TGL	OG3-CC1-OC1	-2.58	117.18	123.63
19	A	608	PGV	O01-C02-C03	2.57	117.56	108.34
27	M	101	DMU	O6-C11-C9	-2.57	102.60	111.33
14	N	601	HEA	C1A-CHA-C4D	2.56	131.45	126.02
19	P	301	PGV	O01-C1-O02	-2.55	117.74	123.70
14	N	601	HEA	O2A-CGA-CBA	2.55	122.05	114.00
20	B	301	TGL	C15-CC9-CC8	2.54	127.22	114.37
14	N	602	HEA	CHA-C1A-NA	2.53	127.21	124.45
22	C	306	CHD	C5-C4-C3	-2.52	108.91	112.71
14	N	601	HEA	O1A-CGA-CBA	-2.52	115.11	123.09
14	A	602	HEA	C21-C20-C19	2.52	121.53	113.19
14	A	602	HEA	CHC-C4B-NB	2.52	127.48	124.37
25	P	305	CDL	OB2-PB2-OB3	2.51	118.90	108.94
14	N	601	HEA	C4A-C3A-C2A	2.51	108.99	106.81
25	C	304	CDL	CA4-OA6-CA5	2.50	123.78	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	303	PGV	C02-O01-C1	2.50	123.78	117.80
19	C	303	PGV	O01-C02-C03	-2.49	99.40	108.34
19	N	607	PGV	O03-C19-C20	2.49	119.42	111.83
22	B	303	CHD	C4-C5-C10	2.49	115.31	112.66
14	N	601	HEA	C13-C12-C11	-2.47	110.45	114.39
22	G	103	CHD	C1-C10-C9	2.47	115.17	111.34
22	C	306	CHD	O25-C24-C23	-2.47	115.27	123.09
14	N	602	HEA	C3C-C4C-NC	2.46	111.87	109.80
22	J	101	CHD	C6-C7-C8	2.46	114.19	111.50
19	P	301	PGV	O04-C19-C20	-2.45	114.18	123.78
14	N	601	HEA	CHB-C1B-C2B	-2.45	121.16	125.03
24	P	303	PEK	O02-C1-C2	2.44	133.34	123.78
20	L	101	TGL	OG3-CC1-OC1	-2.44	117.52	123.63
22	C	305	CHD	C14-C8-C9	-2.44	106.34	109.75
14	A	602	HEA	C17-C18-C19	2.43	133.19	127.62
22	G	103	CHD	C15-C16-C17	2.43	109.90	105.14
27	Z	101	DMU	O4-C7-C8	-2.42	104.66	110.38
24	C	302	PEK	O01-C02-C01	-2.42	99.65	108.34
14	N	602	HEA	CHC-C4B-NB	2.42	127.36	124.37
14	A	602	HEA	C1B-C2B-C3B	-2.42	103.99	106.80
22	W	101	CHD	C19-C10-C1	-2.42	104.46	108.31
20	D	201	TGL	C16-C15-CC9	2.41	126.56	114.37
22	P	306	CHD	C2-C1-C10	2.41	116.81	112.74
22	J	101	CHD	O7-C7-C8	2.41	115.04	109.52
19	C	303	PGV	O14-P-O13	2.40	123.62	112.44
22	G	103	CHD	C14-C13-C12	2.40	109.61	107.42
23	N	610	PSC	C21-C20-C19	-2.39	104.94	113.69
20	Y	101	TGL	CA4-CA3-CA2	-2.39	104.36	113.13
22	J	101	CHD	C22-C20-C17	2.37	115.25	110.33
14	N	602	HEA	CAD-CBD-CGD	-2.37	107.38	113.67
22	J	101	CHD	C23-C22-C20	-2.37	110.04	114.46
22	C	305	CHD	C18-C13-C17	2.37	114.91	111.20
22	G	103	CHD	C19-C10-C5	-2.37	106.48	110.44
25	P	305	CDL	C57-C56-C55	-2.36	102.41	114.37
14	N	602	HEA	C1C-CHC-C4B	-2.36	120.69	126.25
24	C	302	PEK	C2-C3-C4	-2.35	108.22	113.35
22	W	101	CHD	C16-C17-C20	2.34	115.73	112.18
14	N	602	HEA	CHA-C4D-C3D	-2.34	121.36	124.77
14	A	601	HEA	C4C-CHD-C1D	2.34	131.75	126.25
22	C	305	CHD	C16-C17-C13	2.33	105.80	103.54
14	N	601	HEA	C4C-C3C-C2C	-2.33	104.41	107.30
25	P	305	CDL	OA6-CA5-OA7	-2.32	118.27	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	307	CHD	O25-C24-C23	-2.32	115.72	123.09
22	P	307	CHD	C1-C10-C5	2.32	111.07	107.75
14	N	602	HEA	CHC-C1C-C2C	-2.32	120.70	127.43
22	C	305	CHD	C5-C6-C7	2.32	117.16	114.40
20	D	201	TGL	CG3-OG3-CC1	2.32	125.58	117.12
25	G	101	CDL	OB8-CB6-CB4	2.31	115.05	108.40
20	L	101	TGL	CC4-CC3-CC2	-2.31	104.65	113.13
20	Q	201	TGL	OG2-CG2-CG1	2.31	116.62	108.34
24	C	302	PEK	C23-C22-C21	2.30	122.13	113.69
22	B	303	CHD	C10-C9-C8	-2.30	109.27	111.84
20	Q	201	TGL	C15-CC9-CC8	2.30	125.99	114.37
22	C	306	CHD	C17-C13-C14	-2.30	97.81	100.11
22	C	306	CHD	C22-C20-C17	-2.29	105.59	110.33
22	C	305	CHD	O12-C12-C11	2.29	113.77	109.12
20	Q	201	TGL	C16-C15-CC9	2.29	125.92	114.37
27	Z	101	DMU	O1-C10-C5	2.28	115.06	110.37
22	B	303	CHD	C19-C10-C1	-2.28	104.68	108.31
27	Z	101	DMU	O4-C7-C5	-2.28	105.01	110.38
20	N	609	TGL	CG1-OG1-CA1	2.27	125.43	117.12
19	N	607	PGV	O01-C02-C01	2.27	116.49	108.34
20	Y	101	TGL	CG2-OG2-CB1	2.27	123.23	117.80
22	J	101	CHD	C19-C10-C5	2.27	114.22	110.44
23	B	304	PSC	O01-C1-O02	-2.27	118.41	123.70
20	Q	201	TGL	C21-C20-CA9	2.26	125.81	114.37
22	J	101	CHD	C15-C14-C13	2.26	105.74	103.54
22	B	303	CHD	O26-C24-C23	2.26	121.15	114.00
22	B	303	CHD	C16-C17-C20	-2.26	108.75	112.18
20	Y	101	TGL	CG3-OG3-CC1	2.26	125.38	117.12
19	N	607	PGV	C9-C8-C7	-2.26	102.95	114.37
14	A	601	HEA	CMD-C2D-C1D	2.25	128.55	125.03
14	N	601	HEA	C4D-C3D-C2D	-2.25	103.62	106.89
14	A	601	HEA	CHC-C4B-NB	-2.24	121.60	124.37
20	D	201	TGL	OG1-CA1-CA2	2.24	118.66	111.83
25	C	304	CDL	C56-C55-C54	-2.23	103.07	114.37
14	N	602	HEA	CHD-C1D-ND	2.23	127.12	124.37
14	A	601	HEA	C16-C15-C14	2.22	126.16	121.17
22	C	305	CHD	C6-C5-C10	2.22	115.03	112.66
22	P	306	CHD	C1-C10-C5	2.22	110.94	107.75
22	J	101	CHD	C18-C13-C12	-2.22	106.83	109.06
25	C	304	CDL	C39-C38-C37	2.22	125.59	114.37
14	A	602	HEA	CHB-C1B-C2B	2.22	128.53	125.03
20	L	101	TGL	CG2-OG2-CB1	2.21	123.09	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	305	CHD	C16-C17-C20	2.21	115.52	112.18
25	T	102	CDL	C83-C82-C81	2.21	125.53	114.37
25	T	102	CDL	C12-C11-CA5	-2.21	105.61	113.69
19	A	607	PGV	O01-C1-C2	2.20	116.23	111.48
20	Q	201	TGL	CG2-OG2-CB1	2.19	123.04	117.80
25	T	102	CDL	CA4-OA6-CA5	2.19	123.04	117.80
20	D	201	TGL	CG1-OG1-CA1	2.19	125.11	117.12
23	B	304	PSC	O03-C19-O04	-2.18	118.18	123.63
14	A	601	HEA	CAA-C2A-C1A	-2.17	120.44	124.85
25	T	102	CDL	C59-C58-C57	2.17	125.33	114.37
25	T	102	CDL	C63-C62-C61	2.17	125.32	114.37
24	G	102	PEK	O01-C02-C01	2.17	116.11	108.34
20	B	301	TGL	OA1-CA1-CA2	-2.17	115.31	123.78
22	W	101	CHD	C19-C10-C5	-2.16	106.82	110.44
22	B	303	CHD	C11-C12-C13	-2.16	109.06	111.26
22	C	306	CHD	C14-C8-C9	2.16	112.77	109.75
14	A	601	HEA	C1C-CHC-C4B	2.16	131.33	126.25
14	A	601	HEA	C21-C20-C19	-2.16	106.03	113.19
22	G	103	CHD	C6-C5-C10	-2.16	110.36	112.66
22	G	103	CHD	C9-C10-C5	2.16	111.51	108.51
24	C	302	PEK	C03-C02-C01	2.15	116.80	111.78
14	N	602	HEA	CHA-C1A-C2A	-2.15	121.47	124.86
24	C	307	PEK	O03-C21-O04	-2.14	118.27	123.63
22	J	101	CHD	C2-C1-C10	2.14	116.35	112.74
19	N	608	PGV	O01-C1-C2	2.14	116.10	111.48
22	J	101	CHD	C5-C6-C7	-2.14	111.86	114.40
24	P	303	PEK	O03-C21-O04	-2.13	118.30	123.63
14	N	601	HEA	CBC-CAC-C3C	-2.13	116.88	127.53
24	T	101	PEK	C01-O03-C21	2.13	124.90	117.12
14	N	602	HEA	C2B-C1B-NB	2.13	112.36	109.90
22	P	307	CHD	C23-C22-C20	-2.13	110.49	114.46
14	N	602	HEA	C12-C13-C14	-2.12	106.58	112.16
19	N	607	PGV	C26-C25-C24	-2.12	103.63	114.37
24	P	308	PEK	O03-C01-C02	2.12	114.51	108.40
27	Z	101	DMU	C8-C7-C5	2.12	114.55	110.83
14	N	602	HEA	O2D-CGD-CBD	2.12	120.69	114.00
27	Z	101	DMU	O5-C4-C57	2.11	111.68	106.44
14	A	601	HEA	CHB-C4A-C3A	2.11	128.77	125.21
14	A	601	HEA	C25-C23-C22	-2.11	116.31	122.66
22	G	103	CHD	C15-C14-C8	2.11	121.25	118.36
19	P	301	PGV	O03-C01-C02	2.11	114.47	108.40
20	Q	201	TGL	OG3-CC1-OC1	-2.11	118.36	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	306	CHD	C16-C15-C14	-2.10	101.03	105.14
14	A	601	HEA	C1D-ND-C4D	2.10	107.69	105.21
20	N	609	TGL	C15-CC9-CC8	2.10	124.97	114.37
14	N	602	HEA	CHB-C4A-NA	-2.10	122.17	124.45
14	A	601	HEA	O2A-CGA-CBA	2.09	120.62	114.00
25	P	305	CDL	OA4-PA1-OA3	2.09	122.17	112.44
14	A	601	HEA	C12-C11-C3B	2.09	115.38	112.12
20	D	201	TGL	C11-C10-CB9	2.08	124.90	114.37
20	B	301	TGL	C16-C15-CC9	2.08	124.89	114.37
14	A	602	HEA	C21-C22-C23	-2.08	120.70	127.64
14	A	601	HEA	CMB-C2B-C3B	-2.08	126.25	130.28
22	J	101	CHD	C17-C13-C14	-2.08	98.03	100.11
14	N	602	HEA	C21-C20-C19	2.08	120.06	113.19
24	G	102	PEK	O03-C21-O04	-2.07	118.44	123.63
22	C	305	CHD	C11-C9-C8	2.07	113.96	110.89
14	A	602	HEA	C27-C19-C20	2.07	118.82	115.23
22	C	305	CHD	C4-C5-C10	2.07	114.86	112.66
25	P	305	CDL	OB6-CB5-OB7	-2.07	118.87	123.70
19	P	304	PGV	C04-C05-C06	-2.07	104.81	111.77
19	A	607	PGV	C02-O01-C1	2.06	122.73	117.80
25	T	102	CDL	C62-C61-C60	2.06	124.80	114.37
14	A	601	HEA	C4C-NC-C1C	2.06	109.18	105.82
14	N	602	HEA	CHD-C1D-C2D	-2.06	121.09	126.95
27	Z	101	DMU	C10-O7-C3	-2.06	113.10	117.98
22	P	307	CHD	C1-C2-C3	-2.06	107.76	110.48
20	L	101	TGL	C29-C14-C13	-2.06	103.98	114.37
20	L	101	TGL	C16-C15-CC9	2.05	124.72	114.37
25	P	305	CDL	OA8-CA7-OA9	-2.05	118.51	123.63
20	L	101	TGL	OG2-CG2-CG1	2.04	115.67	108.34
25	C	304	CDL	OB6-CB5-OB7	-2.04	118.95	123.70
14	A	601	HEA	CHA-C1A-C2A	2.03	128.07	124.86
27	M	101	DMU	O5-C6-O16	-2.03	105.25	110.04
24	G	102	PEK	C01-O03-C21	2.03	124.54	117.12
19	C	308	PGV	O04-C19-C20	-2.03	115.84	123.78
25	C	304	CDL	CA6-OA8-CA7	2.03	124.53	117.12
20	L	101	TGL	CA9-CA8-CA7	-2.03	104.12	114.37
24	P	303	PEK	O12-P-O14	2.03	116.97	108.94
14	N	602	HEA	O1A-CGA-CBA	-2.03	116.67	123.09
14	N	602	HEA	CHB-C1B-NB	2.02	126.59	124.42
14	N	602	HEA	C13-C14-C15	-2.01	123.02	127.62
19	N	608	PGV	O14-P-O11	2.00	116.63	107.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	M	101	DMU	C9
27	M	101	DMU	C5
27	Z	101	DMU	C9
27	Z	101	DMU	C5

All (959) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C04-O12-P-O11
19	A	608	PGV	C04-O12-P-O13
19	A	608	PGV	C04-O12-P-O14
19	A	608	PGV	C02-C03-O11-P
19	A	608	PGV	C05-C04-O12-P
19	A	608	PGV	C2-C1-O01-C02
19	A	608	PGV	O04-C19-O03-C01
19	A	608	PGV	C20-C19-O03-C01
19	C	308	PGV	C03-O11-P-O12
19	C	308	PGV	C03-O11-P-O13
19	N	607	PGV	O12-C04-C05-C06
19	N	607	PGV	O02-C1-O01-C02
19	N	607	PGV	C2-C1-O01-C02
19	P	301	PGV	C03-O11-P-O12
19	P	301	PGV	C03-O11-P-O13
19	P	301	PGV	C03-O11-P-O14
19	P	301	PGV	C04-O12-P-O11
19	P	301	PGV	C04-O12-P-O14
19	P	301	PGV	O01-C02-C03-O11
19	P	301	PGV	C02-C03-O11-P
20	D	201	TGL	OG1-CG1-CG2-OG2
20	L	101	TGL	CB2-CB1-OG2-CG2
20	Q	201	TGL	CC2-CC1-OG3-CG3
20	Q	201	TGL	OC1-CC1-OG3-CG3
20	Y	101	TGL	CB2-CB1-OG2-CG2
22	J	101	CHD	C13-C17-C20-C21
22	J	101	CHD	C13-C17-C20-C22
22	J	101	CHD	C16-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
22	W	101	CHD	C16-C17-C20-C22
23	B	304	PSC	C03-O11-P-O12
23	B	304	PSC	C03-O11-P-O13
23	B	304	PSC	C04-O12-P-O11
23	B	304	PSC	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
23	B	304	PSC	C04-O12-P-O14
23	N	610	PSC	C03-O11-P-O12
23	N	610	PSC	C03-O11-P-O13
23	N	610	PSC	C2-C1-O01-C02
23	N	610	PSC	O04-C19-O03-C01
23	N	610	PSC	C20-C19-O03-C01
24	C	302	PEK	C5-C6-C7-C8
24	C	307	PEK	C04-O12-P-O11
24	C	307	PEK	O03-C01-C02-O01
24	C	307	PEK	O12-C04-C05-N
24	G	102	PEK	O12-C04-C05-N
24	G	102	PEK	C2-C1-O01-C02
24	G	102	PEK	C9-C10-C11-C12
24	P	308	PEK	C03-O11-P-O12
24	P	308	PEK	C03-O11-P-O13
24	P	308	PEK	C03-O11-P-O14
24	P	308	PEK	C04-O12-P-O11
24	P	308	PEK	O12-C04-C05-N
24	T	101	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O13
24	T	101	PEK	O12-C04-C05-N
24	T	101	PEK	C11-C12-C13-C14
25	C	304	CDL	CA2-OA2-PA1-OA4
25	C	304	CDL	CA2-OA2-PA1-OA5
25	C	304	CDL	CA3-OA5-PA1-OA2
25	C	304	CDL	CA3-OA5-PA1-OA3
25	C	304	CDL	CA4-CA3-OA5-PA1
25	C	304	CDL	OA7-CA5-OA6-CA4
25	C	304	CDL	C11-CA5-OA6-CA4
25	C	304	CDL	CB2-OB2-PB2-OB4
25	G	101	CDL	O1-C1-CA2-OA2
25	G	101	CDL	CB2-C1-CA2-OA2
25	G	101	CDL	CA2-OA2-PA1-OA3
25	G	101	CDL	CA3-OA5-PA1-OA2
25	G	101	CDL	CA3-OA5-PA1-OA4
25	G	101	CDL	OA7-CA5-OA6-CA4
25	G	101	CDL	C11-CA5-OA6-CA4
25	G	101	CDL	C31-CA7-OA8-CA6
25	G	101	CDL	C1-CB2-OB2-PB2
25	G	101	CDL	CB2-OB2-PB2-OB4
25	G	101	CDL	CB2-OB2-PB2-OB5
25	G	101	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	C51-CB5-OB6-CB4
25	P	305	CDL	CA2-OA2-PA1-OA4
25	P	305	CDL	CA2-OA2-PA1-OA5
25	P	305	CDL	CA3-OA5-PA1-OA2
25	P	305	CDL	CA3-OA5-PA1-OA3
25	P	305	CDL	C11-CA5-OA6-CA4
25	P	305	CDL	CB2-OB2-PB2-OB3
25	P	305	CDL	CB2-OB2-PB2-OB4
25	P	305	CDL	CB3-OB5-PB2-OB2
25	P	305	CDL	CB3-OB5-PB2-OB3
25	P	305	CDL	CB3-OB5-PB2-OB4
25	P	305	CDL	OB7-CB5-OB6-CB4
25	P	305	CDL	C51-CB5-OB6-CB4
25	T	102	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CA3-OA5-PA1-OA3
25	T	102	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	OA7-CA5-OA6-CA4
25	T	102	CDL	OA9-CA7-OA8-CA6
25	T	102	CDL	C31-CA7-OA8-CA6
25	T	102	CDL	C1-CB2-OB2-PB2
25	T	102	CDL	CB2-OB2-PB2-OB4
25	T	102	CDL	CB2-OB2-PB2-OB5
25	T	102	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	OA9-CA7-OA8-CA6
19	N	607	PGV	O04-C19-O03-C01
20	D	201	TGL	OC1-CC1-OG3-CG3
20	L	101	TGL	OB1-CB1-OG2-CG2
20	Y	101	TGL	OB1-CB1-OG2-CG2
24	G	102	PEK	O02-C1-O01-C02
25	G	101	CDL	OB7-CB5-OB6-CB4
25	P	305	CDL	OA7-CA5-OA6-CA4
19	N	607	PGV	C20-C19-O03-C01
20	D	201	TGL	CC2-CC1-OG3-CG3
20	L	101	TGL	CA2-CA1-OG1-CG1
23	B	304	PSC	C20-C19-O03-C01
25	T	102	CDL	C11-CA5-OA6-CA4
14	A	601	HEA	C27-C19-C20-C21
14	A	601	HEA	C18-C19-C20-C21
25	C	304	CDL	C31-CA7-OA8-CA6
19	C	303	PGV	C10-C11-C12-C13
19	P	301	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	N	610	PSC	C11-C12-C13-C14
24	C	307	PEK	C4-C5-C6-C7
24	P	308	PEK	C10-C11-C12-C13
20	L	101	TGL	OA1-CA1-OG1-CG1
20	N	609	TGL	OC1-CC1-OG3-CG3
25	C	304	CDL	OA9-CA7-OA8-CA6
19	A	608	PGV	O02-C1-O01-C02
23	N	610	PSC	O02-C1-O01-C02
22	J	101	CHD	C16-C17-C20-C22
19	N	607	PGV	O12-C04-C05-O05
23	B	304	PSC	O04-C19-O03-C01
27	M	101	DMU	O6-C11-C9-C8
27	Z	101	DMU	O6-C11-C9-O1
22	C	305	CHD	C17-C20-C22-C23
20	N	609	TGL	CC2-CC1-OG3-CG3
14	N	601	HEA	C19-C20-C21-C22
25	P	305	CDL	C19-C20-C21-C22
25	G	101	CDL	C58-C59-C60-C61
24	C	302	PEK	C10-C11-C12-C13
24	C	307	PEK	C10-C11-C12-C13
24	C	307	PEK	C13-C14-C15-C16
24	P	303	PEK	C13-C14-C15-C16
24	P	308	PEK	C13-C14-C15-C16
24	T	101	PEK	C7-C8-C9-C10
25	P	305	CDL	C53-C54-C55-C56
19	C	308	PGV	O12-C04-C05-C06
25	C	304	CDL	CB2-C1-CA2-OA2
25	G	101	CDL	CA2-C1-CB2-OB2
25	P	305	CDL	CB2-C1-CA2-OA2
25	P	305	CDL	CA2-C1-CB2-OB2
25	G	101	CDL	C71-CB7-OB8-CB6
25	T	102	CDL	C71-CB7-OB8-CB6
19	A	607	PGV	C26-C27-C28-C29
24	P	308	PEK	C33-C34-C35-C36
25	C	304	CDL	C80-C81-C82-C83
20	D	201	TGL	C20-C21-C22-C23
20	Y	101	TGL	C20-C21-C22-C23
19	C	308	PGV	C20-C21-C22-C23
27	Z	101	DMU	O6-C11-C9-C8
23	N	610	PSC	C20-C21-C22-C23
19	C	308	PGV	O12-C04-C05-O05
25	C	304	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
23	B	304	PSC	C22-C23-C24-C25
25	P	305	CDL	CB5-C51-C52-C53
22	P	306	CHD	C17-C20-C22-C23
25	G	101	CDL	CA5-C11-C12-C13
24	P	303	PEK	C4-C5-C6-C7
19	C	308	PGV	O05-C05-C06-O06
24	G	102	PEK	C33-C34-C35-C36
20	B	301	TGL	OB1-CB1-OG2-CG2
20	Q	201	TGL	C16-C15-CC9-CC8
25	G	101	CDL	C60-C61-C62-C63
19	N	607	PGV	C19-C20-C21-C22
20	D	201	TGL	CB1-CB2-CB3-CB4
20	Y	101	TGL	CA1-CA2-CA3-CA4
20	Y	101	TGL	CB1-CB2-CB3-CB4
24	C	307	PEK	C1-C2-C3-C4
24	G	102	PEK	C21-C22-C23-C24
24	T	101	PEK	C1-C2-C3-C4
25	T	102	CDL	CB5-C51-C52-C53
25	T	102	CDL	CB7-C71-C72-C73
25	T	102	CDL	OB9-CB7-OB8-CB6
20	B	301	TGL	CC2-CC1-OG3-CG3
22	C	305	CHD	C20-C22-C23-C24
25	T	102	CDL	C79-C80-C81-C82
22	C	305	CHD	C21-C20-C22-C23
19	C	308	PGV	C1-C2-C3-C4
20	B	301	TGL	CB1-CB2-CB3-CB4
24	P	303	PEK	C1-C2-C3-C4
25	T	102	CDL	CA7-C31-C32-C33
19	N	607	PGV	C02-C01-O03-C19
23	N	610	PSC	C22-C23-C24-C25
25	G	101	CDL	O1-C1-CB2-OB2
25	P	305	CDL	O1-C1-CA2-OA2
25	P	305	CDL	O1-C1-CB2-OB2
25	T	102	CDL	O1-C1-CB2-OB2
20	B	301	TGL	OC1-CC1-OG3-CG3
22	P	306	CHD	C21-C20-C22-C23
23	B	304	PSC	C11-C12-C13-C14
24	C	307	PEK	C7-C8-C9-C10
24	G	102	PEK	C10-C11-C12-C13
25	G	101	CDL	OB9-CB7-OB8-CB6
22	W	101	CHD	C13-C17-C20-C21
25	C	304	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
25	T	102	CDL	CA2-C1-CB2-OB2
19	C	303	PGV	C24-C25-C26-C27
20	Q	201	TGL	CB1-CB2-CB3-CB4
27	Z	101	DMU	O16-C18-C19-C22
24	C	307	PEK	C22-C21-O03-C01
20	B	301	TGL	CB2-CB1-OG2-CG2
23	B	304	PSC	C2-C1-O01-C02
25	C	304	CDL	C51-CB5-OB6-CB4
23	B	304	PSC	O02-C1-O01-C02
24	G	102	PEK	C7-C8-C9-C10
24	P	308	PEK	C7-C8-C9-C10
24	C	307	PEK	C24-C25-C26-C27
25	C	304	CDL	O1-C1-CB2-OB2
19	C	308	PGV	C04-C05-C06-O06
24	P	308	PEK	C1-C2-C3-C4
19	A	608	PGV	C03-C02-O01-C1
20	D	201	TGL	CG3-CG2-OG2-CB1
20	Q	201	TGL	CG3-CG2-OG2-CB1
23	N	610	PSC	C01-C02-O01-C1
24	C	307	PEK	C2-C3-C4-C5
20	N	609	TGL	OB1-CB1-OG2-CG2
19	P	301	PGV	C2-C1-O01-C02
19	P	301	PGV	C20-C19-O03-C01
20	L	101	TGL	CB1-CB2-CB3-CB4
24	C	307	PEK	O04-C21-O03-C01
19	N	607	PGV	C4-C5-C6-C7
20	B	301	TGL	C10-C11-C12-C13
20	L	101	TGL	CB4-CB5-CB6-CB7
20	N	609	TGL	CC2-CC3-CC4-CC5
20	Q	201	TGL	CA6-CA7-CA8-CA9
20	Q	201	TGL	CB5-CB6-CB7-CB8
23	B	304	PSC	C29-C30-C31-C32
24	P	303	PEK	C16-C17-C18-C19
19	C	303	PGV	C13-C14-C15-C16
19	P	301	PGV	C24-C25-C26-C27
20	D	201	TGL	CC7-CC8-CC9-C15
20	L	101	TGL	C11-C10-CB9-CB8
20	L	101	TGL	C21-C22-C23-C24
20	Y	101	TGL	CA7-CA8-CA9-C20
20	Y	101	TGL	CB6-CB7-CB8-CB9
25	C	304	CDL	C23-C24-C25-C26
25	C	304	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C23-C24-C25-C26
25	G	101	CDL	C36-C37-C38-C39
25	G	101	CDL	C37-C38-C39-C40
25	P	305	CDL	C74-C75-C76-C77
19	A	608	PGV	C10-C11-C12-C13
24	T	101	PEK	C13-C14-C15-C16
20	B	301	TGL	C16-C15-CC9-CC8
20	Y	101	TGL	C18-C19-C33-C34
25	G	101	CDL	C16-C17-C18-C19
25	G	101	CDL	C63-C64-C65-C66
25	P	305	CDL	C22-C23-C24-C25
25	P	305	CDL	C72-C73-C74-C75
25	T	102	CDL	C76-C77-C78-C79
20	L	101	TGL	CB3-CB4-CB5-CB6
20	L	101	TGL	CC5-CC6-CC7-CC8
20	N	609	TGL	CB6-CB7-CB8-CB9
20	N	609	TGL	C12-C13-C14-C29
20	N	609	TGL	C15-C16-C17-C18
25	C	304	CDL	C72-C73-C74-C75
25	C	304	CDL	C79-C80-C81-C82
25	G	101	CDL	C20-C21-C22-C23
27	M	101	DMU	C19-C22-C25-C28
20	D	201	TGL	CB9-C10-C11-C12
20	N	609	TGL	CC5-CC6-CC7-CC8
24	C	302	PEK	C32-C33-C34-C35
24	G	102	PEK	C34-C35-C36-C37
25	T	102	CDL	C75-C76-C77-C78
19	C	303	PGV	C27-C28-C29-C30
25	P	305	CDL	C16-C17-C18-C19
25	T	102	CDL	C72-C73-C74-C75
24	P	303	PEK	C31-C32-C33-C34
25	G	101	CDL	C76-C77-C78-C79
24	C	307	PEK	C2-C1-O01-C02
24	T	101	PEK	C27-C28-C29-C30
19	N	608	PGV	C23-C24-C25-C26
19	P	301	PGV	C26-C27-C28-C29
20	B	301	TGL	C11-C12-C13-C14
20	N	609	TGL	CB5-CB6-CB7-CB8
20	Q	201	TGL	CC5-CC6-CC7-CC8
24	P	303	PEK	C28-C29-C30-C31
25	C	304	CDL	C36-C37-C38-C39
25	C	304	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
20	N	609	TGL	CC4-CC5-CC6-CC7
20	N	609	TGL	C16-C15-CC9-CC8
27	Z	101	DMU	C22-C25-C28-C31
20	D	201	TGL	C11-C12-C13-C14
19	A	608	PGV	C14-C15-C16-C17
19	C	308	PGV	C30-C31-C32-C33
19	N	607	PGV	C14-C15-C16-C17
25	C	304	CDL	C60-C61-C62-C63
25	C	304	CDL	C82-C83-C84-C85
24	G	102	PEK	C22-C21-O03-C01
19	A	608	PGV	C7-C8-C9-C10
19	N	608	PGV	C13-C14-C15-C16
19	P	301	PGV	C30-C31-C32-C33
20	B	301	TGL	CA6-CA7-CA8-CA9
20	B	301	TGL	C22-C23-C24-C25
20	N	609	TGL	CA4-CA5-CA6-CA7
23	B	304	PSC	C28-C29-C30-C31
24	G	102	PEK	C23-C24-C25-C26
25	G	101	CDL	C77-C78-C79-C80
25	G	101	CDL	C80-C81-C82-C83
19	A	608	PGV	C20-C21-C22-C23
19	N	607	PGV	C25-C26-C27-C28
19	P	304	PGV	C30-C31-C32-C33
20	D	201	TGL	CA3-CA4-CA5-CA6
23	B	304	PSC	C30-C31-C32-C33
25	T	102	CDL	C11-C12-C13-C14
27	M	101	DMU	C22-C25-C28-C31
19	N	608	PGV	C27-C28-C29-C30
19	P	301	PGV	C4-C5-C6-C7
20	B	301	TGL	C16-C17-C18-C19
20	N	609	TGL	C10-C11-C12-C13
20	Q	201	TGL	C21-C20-CA9-CA8
24	T	101	PEK	C32-C33-C34-C35
25	C	304	CDL	C53-C54-C55-C56
25	C	304	CDL	C63-C64-C65-C66
25	G	101	CDL	C82-C83-C84-C85
25	P	305	CDL	C37-C38-C39-C40
19	N	607	PGV	C28-C29-C30-C31
20	N	609	TGL	CA5-CA6-CA7-CA8
23	N	610	PSC	C3-C4-C5-C6
19	P	301	PGV	C20-C21-C22-C23
20	D	201	TGL	C14-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
20	N	609	TGL	CB4-CB5-CB6-CB7
20	Q	201	TGL	CC6-CC7-CC8-CC9
24	P	308	PEK	C28-C29-C30-C31
25	G	101	CDL	C73-C74-C75-C76
25	T	102	CDL	C31-C32-C33-C34
19	P	304	PGV	C1-C2-C3-C4
23	B	304	PSC	C19-C20-C21-C22
20	Q	201	TGL	C21-C22-C23-C24
19	A	608	PGV	C11-C10-C9-C8
19	C	303	PGV	C12-C13-C14-C15
19	N	608	PGV	C11-C10-C9-C8
24	P	303	PEK	C2-C3-C4-C5
24	G	102	PEK	C4-C5-C6-C7
19	N	607	PGV	C20-C21-C22-C23
20	B	301	TGL	C12-C13-C14-C29
23	B	304	PSC	C27-C28-C29-C30
25	T	102	CDL	C73-C74-C75-C76
19	C	308	PGV	C2-C3-C4-C5
25	G	101	CDL	C79-C80-C81-C82
19	C	308	PGV	C14-C15-C16-C17
20	Q	201	TGL	CB9-C10-C11-C12
24	G	102	PEK	C26-C27-C28-C29
19	P	301	PGV	C22-C23-C24-C25
23	N	610	PSC	C2-C3-C4-C5
24	C	302	PEK	C23-C24-C25-C26
24	C	307	PEK	C28-C29-C30-C31
19	P	301	PGV	O02-C1-O01-C02
24	C	307	PEK	O02-C1-O01-C02
25	C	304	CDL	OB7-CB5-OB6-CB4
25	C	304	CDL	C20-C21-C22-C23
25	T	102	CDL	C20-C21-C22-C23
25	T	102	CDL	C62-C63-C64-C65
20	B	301	TGL	CB4-CB5-CB6-CB7
20	D	201	TGL	CA7-CA8-CA9-C20
20	Q	201	TGL	C23-C24-C25-C26
25	T	102	CDL	C54-C55-C56-C57
25	T	102	CDL	C55-C56-C57-C58
19	C	308	PGV	C26-C27-C28-C29
20	B	301	TGL	CA5-CA6-CA7-CA8
20	D	201	TGL	C13-C14-C29-C30
20	D	201	TGL	C18-C19-C33-C34
23	B	304	PSC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	P	308	PEK	C32-C33-C34-C35
25	G	101	CDL	C83-C84-C85-C86
20	L	101	TGL	C10-C11-C12-C13
24	C	302	PEK	C28-C29-C30-C31
25	P	305	CDL	C59-C60-C61-C62
19	A	608	PGV	C24-C25-C26-C27
20	B	301	TGL	C17-C18-C19-C33
20	Y	101	TGL	C19-C33-C34-C35
19	C	303	PGV	C26-C27-C28-C29
20	L	101	TGL	CA3-CA4-CA5-CA6
24	C	302	PEK	C16-C17-C18-C19
24	P	308	PEK	C26-C27-C28-C29
25	T	102	CDL	C13-C14-C15-C16
20	L	101	TGL	CB2-CB3-CB4-CB5
20	N	609	TGL	C21-C20-CA9-CA8
20	Y	101	TGL	CB3-CB4-CB5-CB6
24	C	307	PEK	C22-C23-C24-C25
25	C	304	CDL	C57-C58-C59-C60
25	G	101	CDL	C33-C34-C35-C36
20	L	101	TGL	C16-C15-CC9-CC8
20	Y	101	TGL	C10-C11-C12-C13
20	Y	101	TGL	C22-C23-C24-C25
23	N	610	PSC	C29-C30-C31-C32
25	G	101	CDL	C31-C32-C33-C34
20	N	609	TGL	CB2-CB1-OG2-CG2
25	C	304	CDL	C51-C52-C53-C54
25	C	304	CDL	C38-C39-C40-C41
24	G	102	PEK	O04-C21-O03-C01
20	L	101	TGL	C21-C20-CA9-CA8
20	N	609	TGL	CB7-CB8-CB9-C10
25	C	304	CDL	C74-C75-C76-C77
20	N	609	TGL	C14-C29-C30-C31
20	Y	101	TGL	CA9-C20-C21-C22
19	C	308	PGV	C5-C6-C7-C8
25	T	102	CDL	C57-C58-C59-C60
24	P	303	PEK	C26-C27-C28-C29
25	T	102	CDL	C59-C60-C61-C62
19	N	607	PGV	C7-C8-C9-C10
19	P	301	PGV	O04-C19-O03-C01
25	P	305	CDL	C14-C15-C16-C17
25	G	101	CDL	C81-C82-C83-C84
20	Y	101	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
24	P	303	PEK	C2-C1-O01-C02
20	Q	201	TGL	C19-C33-C34-C35
20	B	301	TGL	CC4-CC5-CC6-CC7
20	Q	201	TGL	C12-C13-C14-C29
24	C	307	PEK	C16-C17-C18-C19
25	T	102	CDL	C42-C43-C44-C45
20	Q	201	TGL	OG1-CG1-CG2-OG2
24	G	102	PEK	O03-C01-C02-O01
24	G	102	PEK	C15-C16-C17-C18
24	P	308	PEK	O03-C01-C02-O01
25	C	304	CDL	OA6-CA4-CA6-OA8
25	G	101	CDL	OA6-CA4-CA6-OA8
19	P	301	PGV	C5-C6-C7-C8
20	Q	201	TGL	C16-C17-C18-C19
20	Y	101	TGL	CA4-CA5-CA6-CA7
25	P	305	CDL	C36-C37-C38-C39
25	P	305	CDL	C40-C41-C42-C43
24	T	101	PEK	C22-C21-O03-C01
19	P	304	PGV	C24-C25-C26-C27
25	P	305	CDL	C35-C36-C37-C38
19	N	607	PGV	C13-C14-C15-C16
24	P	308	PEK	C29-C30-C31-C32
25	T	102	CDL	C41-C42-C43-C44
19	P	301	PGV	C29-C30-C31-C32
20	B	301	TGL	C20-C21-C22-C23
20	N	609	TGL	C23-C24-C25-C26
25	C	304	CDL	C58-C59-C60-C61
25	G	101	CDL	C14-C15-C16-C17
20	Q	201	TGL	CC2-CC3-CC4-CC5
25	C	304	CDL	C41-C42-C43-C44
25	P	305	CDL	C79-C80-C81-C82
19	C	308	PGV	C24-C25-C26-C27
23	B	304	PSC	C26-C27-C28-C29
25	P	305	CDL	C41-C42-C43-C44
20	L	101	TGL	C18-C19-C33-C34
24	C	307	PEK	C33-C34-C35-C36
20	D	201	TGL	CC5-CC6-CC7-CC8
25	G	101	CDL	C38-C39-C40-C41
19	P	301	PGV	C1-C2-C3-C4
19	N	607	PGV	C29-C30-C31-C32
20	N	609	TGL	CA3-CA4-CA5-CA6
25	P	305	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C4-C5-C6-C7
20	D	201	TGL	CC6-CC7-CC8-CC9
20	L	101	TGL	C24-C25-C26-C27
19	P	301	PGV	C13-C14-C15-C16
20	D	201	TGL	C19-C33-C34-C35
24	C	307	PEK	C32-C33-C34-C35
25	C	304	CDL	C17-C18-C19-C20
19	P	301	PGV	C11-C10-C9-C8
19	P	304	PGV	C11-C10-C9-C8
24	C	302	PEK	C15-C16-C17-C18
20	B	301	TGL	CA4-CA5-CA6-CA7
20	Y	101	TGL	C13-C14-C29-C30
24	T	101	PEK	C26-C27-C28-C29
25	C	304	CDL	C42-C43-C44-C45
19	A	608	PGV	C01-C02-C03-O11
19	N	607	PGV	C01-C02-C03-O11
19	P	301	PGV	C01-C02-C03-O11
24	P	308	PEK	C01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-CA6
20	Q	201	TGL	CB4-CB5-CB6-CB7
20	Y	101	TGL	C11-C12-C13-C14
25	P	305	CDL	C73-C74-C75-C76
25	P	305	CDL	C81-C82-C83-C84
24	P	308	PEK	C16-C17-C18-C19
19	A	608	PGV	C19-C20-C21-C22
24	C	302	PEK	C24-C25-C26-C27
25	G	101	CDL	C43-C44-C45-C46
20	D	201	TGL	C16-C15-CC9-CC8
19	A	607	PGV	C29-C30-C31-C32
20	Y	101	TGL	CB7-CB8-CB9-C10
25	G	101	CDL	C52-C53-C54-C55
19	C	303	PGV	C19-C20-C21-C22
20	Q	201	TGL	OG1-CG1-CG2-CG3
20	Q	201	TGL	CG1-CG2-CG3-OG3
23	N	610	PSC	O03-C01-C02-C03
24	C	307	PEK	O03-C01-C02-C03
24	G	102	PEK	O03-C01-C02-C03
24	P	308	PEK	O03-C01-C02-C03
25	T	102	CDL	CA3-CA4-CA6-OA8
25	G	101	CDL	C53-C54-C55-C56
27	M	101	DMU	O6-C11-C9-O1
23	B	304	PSC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	307	PEK	C25-C26-C27-C28
23	B	304	PSC	C24-C25-C26-C27
25	G	101	CDL	C59-C60-C61-C62
25	C	304	CDL	C40-C41-C42-C43
19	N	607	PGV	C26-C27-C28-C29
19	C	303	PGV	C20-C21-C22-C23
20	Q	201	TGL	CC7-CC8-CC9-C15
25	G	101	CDL	C62-C63-C64-C65
22	P	306	CHD	C16-C17-C20-C21
20	L	101	TGL	CA6-CA7-CA8-CA9
25	P	305	CDL	C21-C22-C23-C24
24	P	308	PEK	C31-C32-C33-C34
24	T	101	PEK	C25-C26-C27-C28
25	P	305	CDL	C76-C77-C78-C79
20	Q	201	TGL	CA9-C20-C21-C22
24	T	101	PEK	C31-C32-C33-C34
19	P	304	PGV	C19-C20-C21-C22
19	N	607	PGV	C10-C11-C12-C13
14	A	602	HEA	C4D-C3D-CAD-CBD
19	C	308	PGV	O01-C02-C03-O11
24	T	101	PEK	O04-C21-O03-C01
19	A	608	PGV	C29-C30-C31-C32
19	C	303	PGV	C7-C8-C9-C10
20	N	609	TGL	C16-C17-C18-C19
24	P	308	PEK	C35-C36-C37-C38
25	C	304	CDL	C84-C85-C86-C87
19	P	301	PGV	C28-C29-C30-C31
20	D	201	TGL	CA2-CA3-CA4-CA5
20	D	201	TGL	C23-C24-C25-C26
20	L	101	TGL	CC9-C15-C16-C17
20	Y	101	TGL	C14-C29-C30-C31
24	T	101	PEK	C33-C34-C35-C36
19	C	303	PGV	C28-C29-C30-C31
19	N	607	PGV	C5-C6-C7-C8
20	D	201	TGL	CC3-CC4-CC5-CC6
20	Q	201	TGL	CB6-CB7-CB8-CB9
20	Y	101	TGL	CB9-C10-C11-C12
25	T	102	CDL	C36-C37-C38-C39
19	N	608	PGV	C31-C32-C33-C34
24	C	302	PEK	C25-C26-C27-C28
20	L	101	TGL	OG2-CG2-CG3-OG3
20	N	609	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
25	C	304	CDL	OB6-CB4-CB6-OB8
20	L	101	TGL	CC3-CC4-CC5-CC6
19	C	303	PGV	C31-C32-C33-C34
24	C	307	PEK	C26-C27-C28-C29
25	T	102	CDL	C81-C82-C83-C84
19	N	608	PGV	C15-C16-C17-C18
24	C	307	PEK	C35-C36-C37-C38
25	T	102	CDL	C84-C85-C86-C87
19	C	308	PGV	O01-C1-C2-C3
20	L	101	TGL	CB7-CB8-CB9-C10
20	Q	201	TGL	CB7-CB8-CB9-C10
25	T	102	CDL	C63-C64-C65-C66
25	P	305	CDL	C77-C78-C79-C80
20	B	301	TGL	C29-C30-C31-C32
20	D	201	TGL	CC1-CC2-CC3-CC4
19	A	607	PGV	C31-C32-C33-C34
20	D	201	TGL	OG2-CB1-CB2-CB3
20	L	101	TGL	CB6-CB7-CB8-CB9
19	C	303	PGV	C23-C24-C25-C26
25	G	101	CDL	C42-C43-C44-C45
27	Z	101	DMU	C25-C28-C31-C34
19	P	304	PGV	C10-C11-C12-C13
24	P	303	PEK	C7-C8-C9-C10
24	P	308	PEK	C4-C5-C6-C7
19	P	304	PGV	C7-C8-C9-C10
20	B	301	TGL	CA3-CA4-CA5-CA6
25	C	304	CDL	C73-C74-C75-C76
20	B	301	TGL	CA9-C20-C21-C22
25	G	101	CDL	C55-C56-C57-C58
20	B	301	TGL	C21-C22-C23-C24
20	Q	201	TGL	C11-C12-C13-C14
20	B	301	TGL	C18-C19-C33-C34
20	Q	201	TGL	CC3-CC4-CC5-CC6
20	Q	201	TGL	CC9-C15-C16-C17
19	N	607	PGV	C02-C03-O11-P
19	N	607	PGV	C15-C16-C17-C18
19	P	301	PGV	C14-C15-C16-C17
20	B	301	TGL	C21-C20-CA9-CA8
25	G	101	CDL	C71-C72-C73-C74
25	P	305	CDL	C58-C59-C60-C61
20	N	609	TGL	C29-C30-C31-C32
25	C	304	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C22-C23-C24-C25
19	P	304	PGV	C22-C23-C24-C25
19	C	308	PGV	C01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-CA6
25	P	305	CDL	OA5-CA3-CA4-CA6
20	Y	101	TGL	C29-C30-C31-C32
25	C	304	CDL	C64-C65-C66-C67
25	G	101	CDL	C51-C52-C53-C54
19	C	308	PGV	C27-C28-C29-C30
25	P	305	CDL	C63-C64-C65-C66
24	G	102	PEK	C22-C23-C24-C25
19	C	308	PGV	C20-C19-O03-C01
19	A	607	PGV	C23-C24-C25-C26
20	B	301	TGL	C15-C16-C17-C18
24	P	303	PEK	C30-C31-C32-C33
24	P	303	PEK	C33-C34-C35-C36
25	C	304	CDL	C35-C36-C37-C38
14	A	602	HEA	C2D-C3D-CAD-CBD
27	Z	101	DMU	C34-C37-C40-C43
20	N	609	TGL	C22-C23-C24-C25
19	A	608	PGV	O03-C01-C02-C03
19	N	607	PGV	O03-C01-C02-C03
25	C	304	CDL	CA3-CA4-CA6-OA8
25	C	304	CDL	CB3-CB4-CB6-OB8
19	N	608	PGV	C30-C31-C32-C33
24	C	302	PEK	C27-C28-C29-C30
25	T	102	CDL	C12-C13-C14-C15
25	T	102	CDL	C22-C23-C24-C25
20	Y	101	TGL	C24-C25-C26-C27
20	L	101	TGL	CC1-CC2-CC3-CC4
24	C	307	PEK	O01-C02-C03-O11
24	P	308	PEK	O01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-OA6
25	P	305	CDL	OA5-CA3-CA4-OA6
25	P	305	CDL	OB5-CB3-CB4-OB6
27	M	101	DMU	C34-C37-C40-C43
20	Y	101	TGL	CB2-CB3-CB4-CB5
23	B	304	PSC	C21-C22-C23-C24
19	C	303	PGV	C22-C23-C24-C25
19	P	301	PGV	C2-C3-C4-C5
24	G	102	PEK	C24-C25-C26-C27
19	C	308	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
20	B	301	TGL	OG1-CG1-CG2-OG2
25	G	101	CDL	OB6-CB4-CB6-OB8
23	B	304	PSC	C9-C10-C11-C12
23	B	304	PSC	C10-C11-C12-C13
23	N	610	PSC	C9-C10-C11-C12
24	C	307	PEK	C6-C7-C8-C9
24	C	307	PEK	C9-C10-C11-C12
24	G	102	PEK	C5-C6-C7-C8
24	P	303	PEK	C11-C10-C9-C8
24	P	303	PEK	C11-C12-C13-C14
24	P	308	PEK	C9-C10-C11-C12
24	P	308	PEK	C12-C13-C14-C15
24	T	101	PEK	C12-C13-C14-C15
20	L	101	TGL	C20-C21-C22-C23
24	P	303	PEK	C27-C28-C29-C30
25	G	101	CDL	C41-C42-C43-C44
24	P	308	PEK	C30-C31-C32-C33
25	G	101	CDL	C21-C22-C23-C24
25	P	305	CDL	C52-C53-C54-C55
23	N	610	PSC	C15-C16-C17-C18
20	Y	101	TGL	CB4-CB5-CB6-CB7
19	A	608	PGV	C2-C3-C4-C5
20	D	201	TGL	CB4-CB5-CB6-CB7
25	T	102	CDL	C77-C78-C79-C80
19	A	608	PGV	O05-C05-C06-O06
19	N	607	PGV	C30-C31-C32-C33
20	B	301	TGL	CC9-C15-C16-C17
20	Q	201	TGL	C25-C26-C27-C28
24	T	101	PEK	C29-C30-C31-C32
25	T	102	CDL	C78-C79-C80-C81
20	Y	101	TGL	CA2-CA1-OG1-CG1
24	T	101	PEK	C01-C02-C03-O11
19	C	308	PGV	C4-C5-C6-C7
20	D	201	TGL	C17-C18-C19-C33
20	B	301	TGL	CA1-CA2-CA3-CA4
20	D	201	TGL	CB5-CB6-CB7-CB8
20	Y	101	TGL	C25-C26-C27-C28
23	B	304	PSC	C15-C16-C17-C18
25	C	304	CDL	C62-C63-C64-C65
25	T	102	CDL	C21-C22-C23-C24
25	G	101	CDL	C17-C18-C19-C20
19	C	308	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	CA5-C11-C12-C13
22	P	306	CHD	C20-C22-C23-C24
19	A	608	PGV	C31-C32-C33-C34
20	N	609	TGL	C18-C19-C33-C34
19	N	607	PGV	C03-C02-O01-C1
23	B	304	PSC	C01-C02-O01-C1
20	Y	101	TGL	OA1-CA1-OG1-CG1
19	N	607	PGV	O01-C02-C03-O11
24	T	101	PEK	O01-C02-C03-O11
19	C	308	PGV	C25-C26-C27-C28
25	T	102	CDL	C56-C57-C58-C59
20	D	201	TGL	OG1-CG1-CG2-CG3
20	N	609	TGL	C21-C22-C23-C24
25	C	304	CDL	C71-C72-C73-C74
25	P	305	CDL	C80-C81-C82-C83
20	D	201	TGL	CA9-C20-C21-C22
20	Q	201	TGL	OG2-CG2-CG3-OG3
20	Y	101	TGL	OG2-CG2-CG3-OG3
23	B	304	PSC	O03-C01-C02-O01
23	N	610	PSC	O03-C01-C02-O01
23	N	610	PSC	C31-C32-C33-C34
19	N	608	PGV	C24-C25-C26-C27
20	L	101	TGL	C22-C23-C24-C25
25	G	101	CDL	C12-C13-C14-C15
25	P	305	CDL	C34-C35-C36-C37
19	A	607	PGV	C27-C28-C29-C30
20	D	201	TGL	C11-C10-CB9-CB8
20	L	101	TGL	CA2-CA3-CA4-CA5
25	C	304	CDL	C13-C14-C15-C16
20	B	301	TGL	C23-C24-C25-C26
20	L	101	TGL	OG1-CA1-CA2-CA3
25	T	102	CDL	C52-C53-C54-C55
14	A	601	HEA	C26-C15-C16-C17
24	C	307	PEK	C31-C32-C33-C34
20	N	609	TGL	C13-C14-C29-C30
19	N	607	PGV	C31-C32-C33-C34
24	C	302	PEK	C30-C31-C32-C33
25	P	305	CDL	C11-C12-C13-C14
20	D	201	TGL	CA4-CA5-CA6-CA7
25	G	101	CDL	C15-C16-C17-C18
25	T	102	CDL	C33-C34-C35-C36
25	G	101	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C20-C21-C22-C23
19	P	304	PGV	C11-C12-C13-C14
19	C	303	PGV	C02-C03-O11-P
19	P	304	PGV	C02-C03-O11-P
25	G	101	CDL	CB4-CB3-OB5-PB2
19	C	308	PGV	C31-C32-C33-C34
20	L	101	TGL	C17-C18-C19-C33
20	N	609	TGL	C24-C25-C26-C27
23	B	304	PSC	C23-C24-C25-C26
19	A	608	PGV	O01-C02-C03-O11
25	G	101	CDL	OA5-CA3-CA4-OA6
20	Y	101	TGL	CA6-CA7-CA8-CA9
24	P	303	PEK	C32-C33-C34-C35
14	A	601	HEA	C4A-C3A-CMA-OMA
14	N	601	HEA	C4A-C3A-CMA-OMA
25	T	102	CDL	C37-C38-C39-C40
25	T	102	CDL	OA6-CA4-CA6-OA8
19	P	301	PGV	C23-C24-C25-C26
25	C	304	CDL	C16-C17-C18-C19
20	L	101	TGL	CG1-CG2-CG3-OG3
23	B	304	PSC	O03-C01-C02-C03
25	G	101	CDL	CA3-CA4-CA6-OA8
19	P	301	PGV	C31-C32-C33-C34
23	B	304	PSC	C4-C5-C6-C7
19	A	608	PGV	C1-C2-C3-C4
24	P	303	PEK	C15-C16-C17-C18
20	Q	201	TGL	CA5-CA6-CA7-CA8
20	Y	101	TGL	CC5-CC6-CC7-CC8
20	L	101	TGL	C23-C24-C25-C26
19	A	608	PGV	C11-C12-C13-C14
20	D	201	TGL	CA6-CA7-CA8-CA9
19	C	308	PGV	C03-O11-P-O14
24	C	307	PEK	C04-O12-P-O14
24	G	102	PEK	C03-O11-P-O12
24	G	102	PEK	C04-O12-P-O14
24	P	308	PEK	C04-O12-P-O13
25	C	304	CDL	CB2-OB2-PB2-OB3
25	C	304	CDL	CB2-OB2-PB2-OB5
25	G	101	CDL	CA3-OA5-PA1-OA3
25	G	101	CDL	CB3-OB5-PB2-OB4
25	P	305	CDL	CB2-OB2-PB2-OB5
25	T	102	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
25	T	102	CDL	CB3-OB5-PB2-OB4
19	A	608	PGV	C9-C10-C11-C12
22	P	306	CHD	C16-C17-C20-C22
25	T	102	CDL	CB4-CB3-OB5-PB2
27	M	101	DMU	C18-C19-C22-C25
25	G	101	CDL	C34-C35-C36-C37
19	C	308	PGV	C15-C16-C17-C18
19	C	303	PGV	C1-C2-C3-C4
25	T	102	CDL	C53-C54-C55-C56
24	P	303	PEK	C23-C24-C25-C26
27	M	101	DMU	C25-C28-C31-C34
25	C	304	CDL	C12-C13-C14-C15
23	N	610	PSC	C04-C05-N-C06
23	N	610	PSC	C04-C05-N-C07
24	G	102	PEK	C25-C26-C27-C28
24	P	303	PEK	C29-C30-C31-C32
19	A	608	PGV	C27-C28-C29-C30
24	P	308	PEK	C17-C18-C19-C20
20	D	201	TGL	CC9-C15-C16-C17
20	B	301	TGL	C13-C14-C29-C30
20	Y	101	TGL	C12-C13-C14-C29
24	C	302	PEK	C34-C35-C36-C37
23	N	610	PSC	C30-C31-C32-C33
24	C	302	PEK	C13-C14-C15-C16
19	C	303	PGV	C14-C15-C16-C17
14	N	601	HEA	C15-C16-C17-C18
20	Y	101	TGL	CG1-CG2-CG3-OG3
25	T	102	CDL	C60-C61-C62-C63
25	C	304	CDL	C76-C77-C78-C79
19	A	608	PGV	O12-C04-C05-O05
24	P	308	PEK	C15-C16-C17-C18
25	C	304	CDL	C12-C11-CA5-OA6
20	Q	201	TGL	CB2-CB3-CB4-CB5
25	C	304	CDL	C34-C35-C36-C37
20	D	201	TGL	OB1-CB1-CB2-CB3
19	A	608	PGV	O12-C04-C05-C06
22	C	305	CHD	C16-C17-C20-C22
25	C	304	CDL	C1-CA2-OA2-PA1
24	T	101	PEK	C28-C29-C30-C31
20	Q	201	TGL	C10-C11-C12-C13
14	A	601	HEA	C14-C15-C16-C17
19	C	303	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	T	101	PEK	C3-C4-C5-C6
19	N	608	PGV	C25-C26-C27-C28
25	T	102	CDL	C44-C45-C46-C47
20	Q	201	TGL	OG2-CB1-CB2-CB3
25	T	102	CDL	C80-C81-C82-C83
14	A	602	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAD-CBD-CGD-O1D
23	N	610	PSC	C04-C05-N-C08
19	C	308	PGV	O02-C1-C2-C3
19	C	308	PGV	C23-C24-C25-C26
25	P	305	CDL	C60-C61-C62-C63
22	J	101	CHD	C22-C23-C24-O25
25	T	102	CDL	C58-C59-C60-C61
24	C	302	PEK	C7-C8-C9-C10
24	P	308	PEK	C23-C24-C25-C26
25	C	304	CDL	C14-C15-C16-C17
20	B	301	TGL	CG1-CG2-OG2-CB1
20	N	609	TGL	CG1-CG2-OG2-CB1
24	G	102	PEK	C01-C02-O01-C1
25	C	304	CDL	CA3-CA4-OA6-CA5
22	J	101	CHD	C17-C20-C22-C23
25	G	101	CDL	C61-C62-C63-C64
22	B	303	CHD	C22-C23-C24-O25
22	G	103	CHD	C22-C23-C24-O25
25	P	305	CDL	C43-C44-C45-C46
24	P	303	PEK	O02-C1-O01-C02
14	A	602	HEA	CAD-CBD-CGD-O1D
22	C	306	CHD	C22-C23-C24-O25
20	L	101	TGL	CA9-C20-C21-C22
25	G	101	CDL	CA4-CA3-OA5-PA1
25	P	305	CDL	CA4-CA3-OA5-PA1
22	C	305	CHD	C22-C23-C24-O26
22	P	306	CHD	C22-C23-C24-O25
20	D	201	TGL	C12-C13-C14-C29
20	N	609	TGL	C11-C10-CB9-CB8
24	P	303	PEK	C35-C36-C37-C38
20	N	609	TGL	C17-C18-C19-C33
25	P	305	CDL	C51-C52-C53-C54
19	A	607	PGV	C11-C12-C13-C14
25	T	102	CDL	C43-C44-C45-C46
23	N	610	PSC	C10-C11-C12-C13
24	C	302	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	307	PEK	C11-C10-C9-C8
24	C	307	PEK	C12-C13-C14-C15
24	G	102	PEK	C12-C13-C14-C15
24	P	303	PEK	C5-C6-C7-C8
24	P	308	PEK	C5-C6-C7-C8
24	P	308	PEK	C6-C7-C8-C9
24	P	308	PEK	C11-C10-C9-C8
24	T	101	PEK	C5-C6-C7-C8
24	T	101	PEK	C11-C10-C9-C8
14	N	602	HEA	CAD-CBD-CGD-O2D
23	B	304	PSC	C04-C05-N-C08
14	A	602	HEA	C26-C15-C16-C17
14	N	602	HEA	C26-C15-C16-C17
24	C	302	PEK	C17-C18-C19-C20
20	Q	201	TGL	C20-C21-C22-C23
22	G	103	CHD	C22-C23-C24-O26
20	Y	101	TGL	C17-C18-C19-C33
22	P	306	CHD	C13-C17-C20-C21
22	J	101	CHD	C22-C23-C24-O26
24	P	308	PEK	C24-C25-C26-C27
14	A	601	HEA	CAD-CBD-CGD-O1D
19	C	308	PGV	C05-C04-O12-P
25	P	305	CDL	C55-C56-C57-C58
14	N	602	HEA	CAA-CBA-CGA-O2A
14	A	602	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAA-CBA-CGA-O1A
20	Y	101	TGL	C15-C16-C17-C18
19	C	308	PGV	C29-C30-C31-C32
24	P	308	PEK	C3-C4-C5-C6
19	N	608	PGV	O03-C19-C20-C21
20	D	201	TGL	C21-C22-C23-C24
20	D	201	TGL	C29-C30-C31-C32
24	P	303	PEK	O03-C21-C22-C23
22	B	303	CHD	C22-C23-C24-O26
22	C	305	CHD	C22-C23-C24-O25
24	C	307	PEK	C01-C02-C03-O11
25	P	305	CDL	OB5-CB3-CB4-CB6
20	Y	101	TGL	C23-C24-C25-C26
24	C	302	PEK	C21-C22-C23-C24
24	T	101	PEK	O01-C1-C2-C3
19	C	303	PGV	C9-C10-C11-C12
25	T	102	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C16-C17-C18-C19
22	W	101	CHD	C22-C23-C24-O25
25	T	102	CDL	O1-C1-CA2-OA2
19	P	301	PGV	C11-C12-C13-C14
23	B	304	PSC	C12-C13-C14-C15
23	N	610	PSC	C12-C13-C14-C15
19	N	607	PGV	C22-C23-C24-C25
22	W	101	CHD	C22-C23-C24-O26
25	P	305	CDL	C18-C19-C20-C21
25	G	101	CDL	C22-C23-C24-C25
20	Q	201	TGL	CA1-CA2-CA3-CA4
25	C	304	CDL	CA6-CA4-OA6-CA5
19	A	607	PGV	C11-C10-C9-C8
23	N	610	PSC	C6-C7-C8-C9
20	N	609	TGL	C19-C33-C34-C35
22	P	306	CHD	C22-C23-C24-O26
24	T	101	PEK	C21-C22-C23-C24
20	Y	101	TGL	C16-C15-CC9-CC8
25	G	101	CDL	C84-C85-C86-C87
25	T	102	CDL	C83-C84-C85-C86
20	B	301	TGL	C19-C33-C34-C35
20	N	609	TGL	CC7-CC8-CC9-C15
19	C	308	PGV	O03-C01-C02-C03
20	Y	101	TGL	OG1-CG1-CG2-CG3
25	G	101	CDL	CB3-CB4-CB6-OB8
20	N	609	TGL	C25-C26-C27-C28
24	C	307	PEK	C17-C18-C19-C20
25	P	305	CDL	C84-C85-C86-C87
25	G	101	CDL	C52-C51-CB5-OB6
20	N	609	TGL	CA6-CA7-CA8-CA9
25	G	101	CDL	C13-C14-C15-C16
24	P	308	PEK	O01-C1-C2-C3
22	P	307	CHD	C22-C23-C24-O25
25	T	102	CDL	C32-C31-CA7-OA8
22	W	101	CHD	C21-C20-C22-C23
19	N	608	PGV	C11-C12-C13-C14
24	G	102	PEK	C3-C4-C5-C6
24	G	102	PEK	C31-C32-C33-C34
24	P	303	PEK	O01-C1-C2-C3
14	A	601	HEA	CAD-CBD-CGD-O2D
25	G	101	CDL	C12-C11-CA5-OA6
25	G	101	CDL	C32-C31-CA7-OA8

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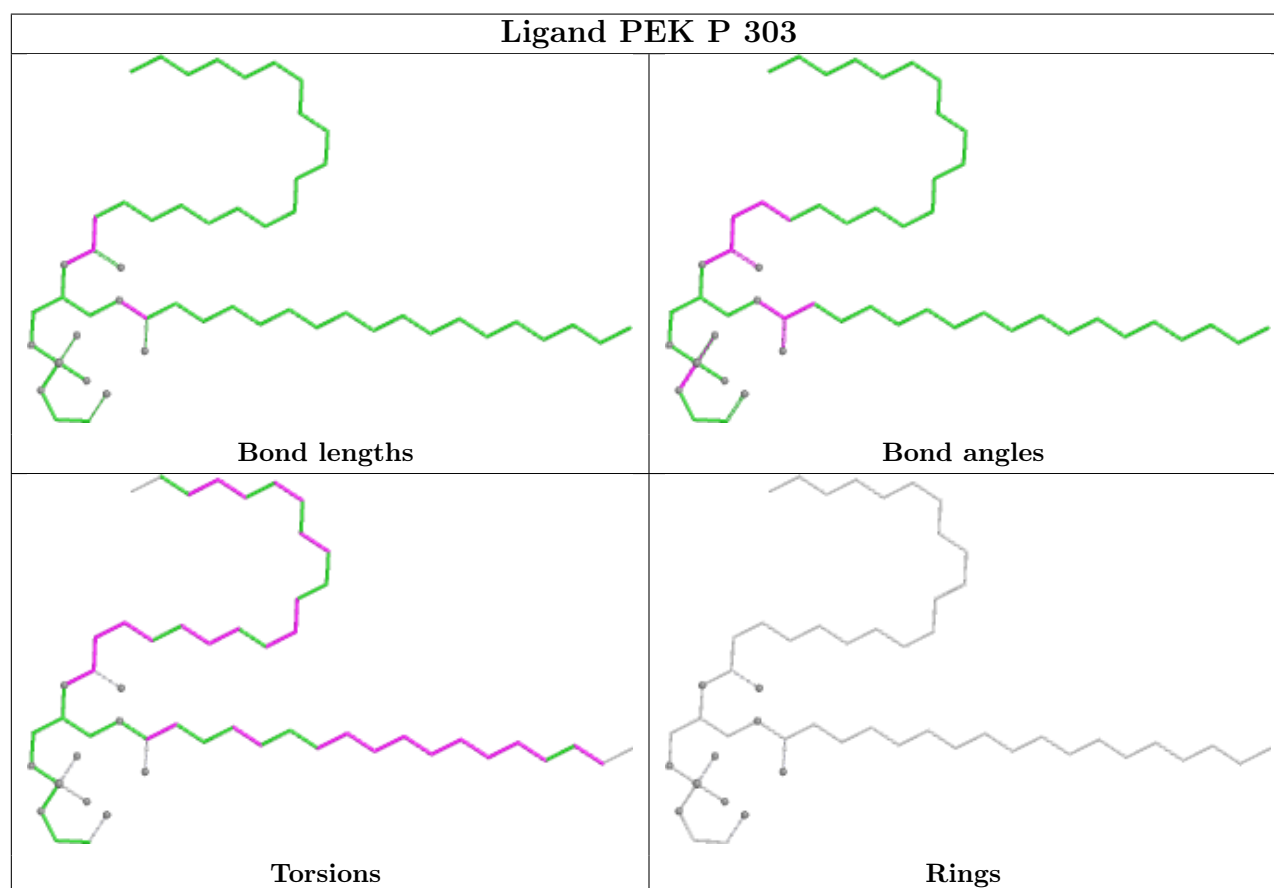
Mol	Chain	Res	Type	Atoms
19	C	308	PGV	C12-C13-C14-C15
20	Y	101	TGL	C33-C34-C35-C36
19	N	608	PGV	C4-C5-C6-C7
20	Q	201	TGL	CA3-CA4-CA5-CA6
24	G	102	PEK	C35-C36-C37-C38
24	C	307	PEK	C21-C22-C23-C24
23	B	304	PSC	O03-C19-C20-C21
14	A	602	HEA	CAA-CBA-CGA-O1A
20	Q	201	TGL	OG3-CC1-CC2-CC3
20	Y	101	TGL	OG1-CG1-CG2-OG2
14	N	601	HEA	CAD-CBD-CGD-O1D
14	N	601	HEA	CAD-CBD-CGD-O2D
25	T	102	CDL	CA4-CA6-OA8-CA7
20	Q	201	TGL	C17-C18-C19-C33
20	L	101	TGL	OA1-CA1-CA2-CA3
23	B	304	PSC	C04-C05-N-C07
20	N	609	TGL	CA7-CA8-CA9-C20
27	Z	101	DMU	C19-C22-C25-C28
20	D	201	TGL	CB2-CB3-CB4-CB5
24	G	102	PEK	C28-C29-C30-C31
19	P	304	PGV	C05-C04-O12-P
14	N	601	HEA	CAA-CBA-CGA-O1A
22	P	307	CHD	C22-C23-C24-O26
24	P	308	PEK	O02-C1-C2-C3
25	T	102	CDL	C64-C65-C66-C67
23	B	304	PSC	O04-C19-C20-C21
20	Q	201	TGL	C13-C14-C29-C30
24	C	307	PEK	O01-C1-C2-C3
20	Q	201	TGL	OC1-CC1-CC2-CC3
25	T	102	CDL	C32-C31-CA7-OA9
24	P	303	PEK	O02-C1-C2-C3
25	G	101	CDL	C12-C11-CA5-OA7
25	G	101	CDL	C32-C31-CA7-OA9
24	C	307	PEK	C14-C15-C16-C17
19	C	303	PGV	C05-C04-O12-P
19	A	607	PGV	C19-C20-C21-C22
24	C	307	PEK	O02-C1-C2-C3
19	P	304	PGV	C23-C24-C25-C26
25	G	101	CDL	C78-C79-C80-C81
19	A	607	PGV	O03-C19-C20-C21
14	A	601	HEA	CAA-CBA-CGA-O1A
14	N	601	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

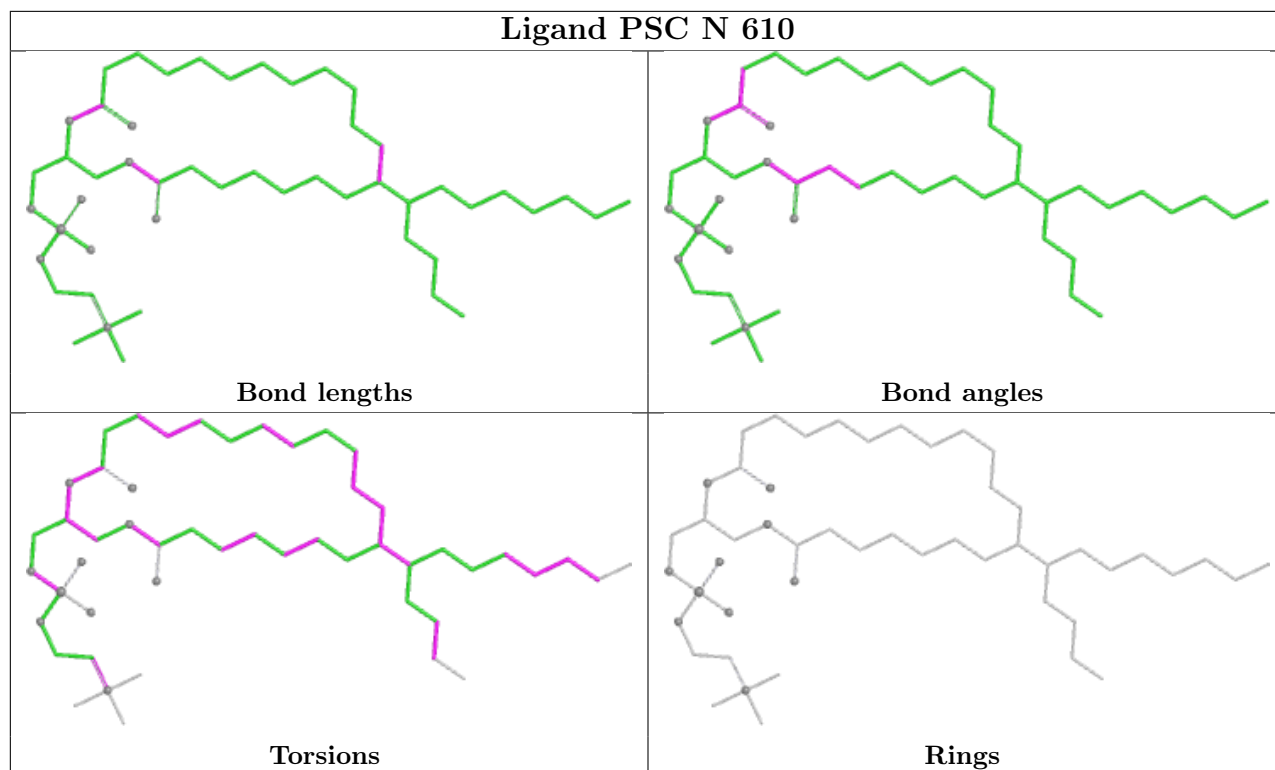
40 monomers are involved in 325 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	303	PEK	9	0
23	N	610	PSC	21	0
19	P	301	PGV	7	0
24	C	302	PEK	6	0
14	N	602	HEA	2	0
14	A	602	HEA	2	0
20	Q	201	TGL	11	0
19	N	607	PGV	10	0
14	N	601	HEA	6	0
24	T	101	PEK	12	0
22	W	101	CHD	5	0
18	A	606[A]	PER	1	0
19	A	608	PGV	8	0
19	C	308	PGV	1	0
19	C	303	PGV	5	0
20	B	301	TGL	3	0
22	B	303	CHD	1	0
27	M	101	DMU	1	0
24	C	307	PEK	17	0
20	L	101	TGL	12	0
22	C	306	CHD	1	0
25	P	305	CDL	18	0
19	P	304	PGV	4	0
20	N	609	TGL	4	0
22	J	101	CHD	5	0
25	G	101	CDL	37	0
20	Y	101	TGL	17	0
24	G	102	PEK	6	0
22	P	307	CHD	3	0
25	C	304	CDL	23	0
19	A	607	PGV	2	0
22	C	305	CHD	3	0
20	D	201	TGL	13	0
19	N	608	PGV	6	0
24	P	308	PEK	13	0
25	T	102	CDL	29	0
18	N	606[A]	PER	1	0
23	B	304	PSC	13	0
14	A	601	HEA	8	0
22	P	306	CHD	2	0

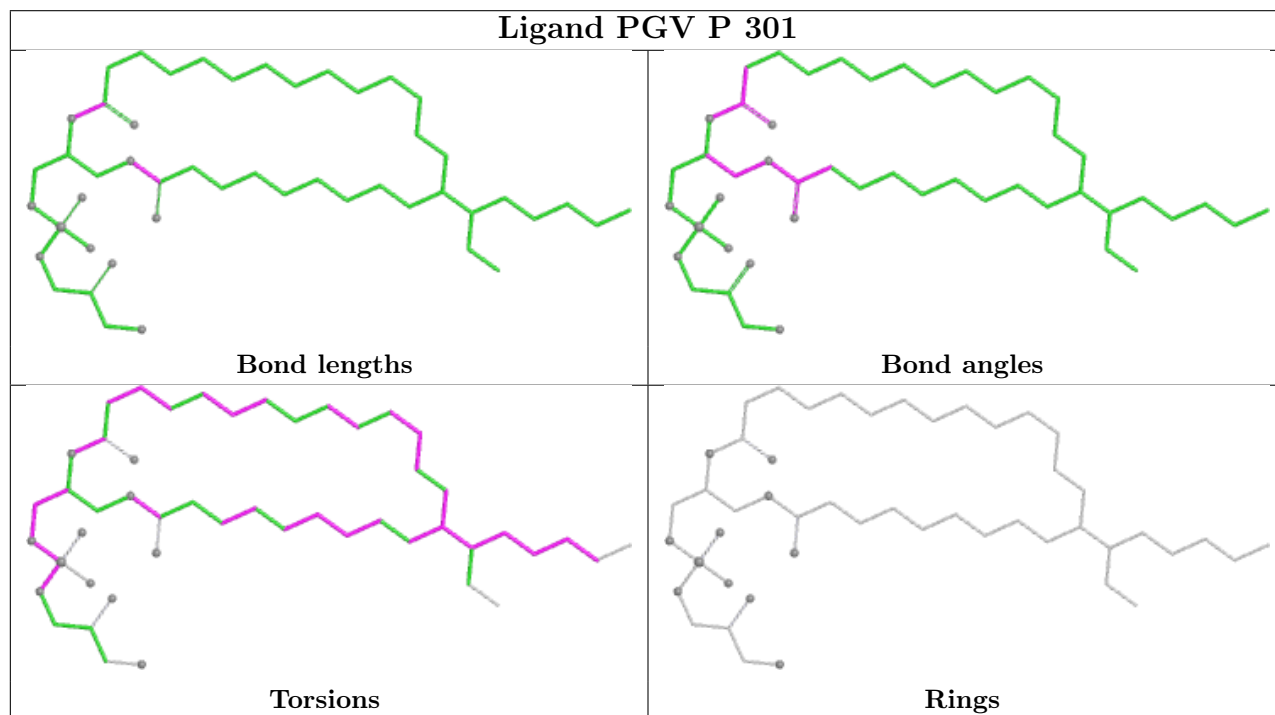
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

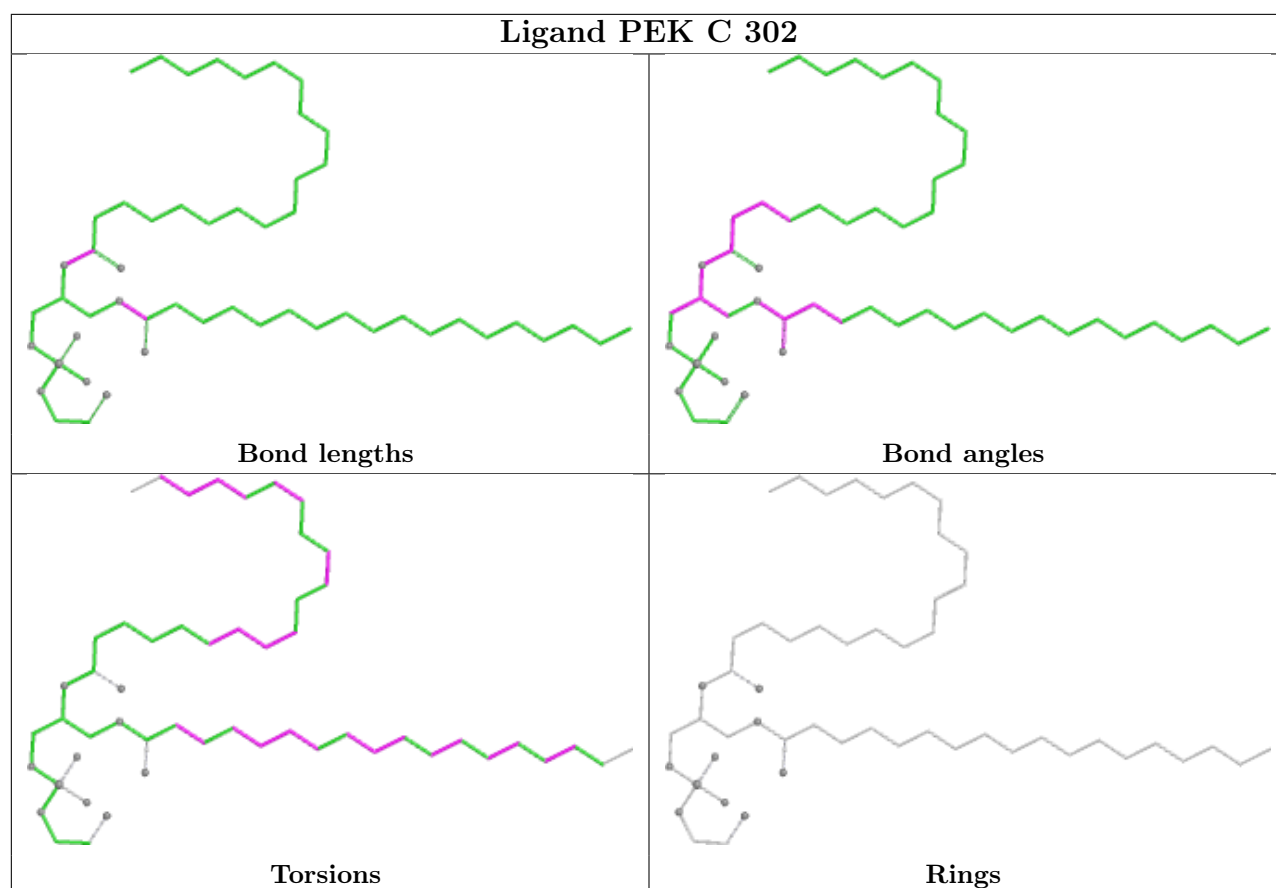


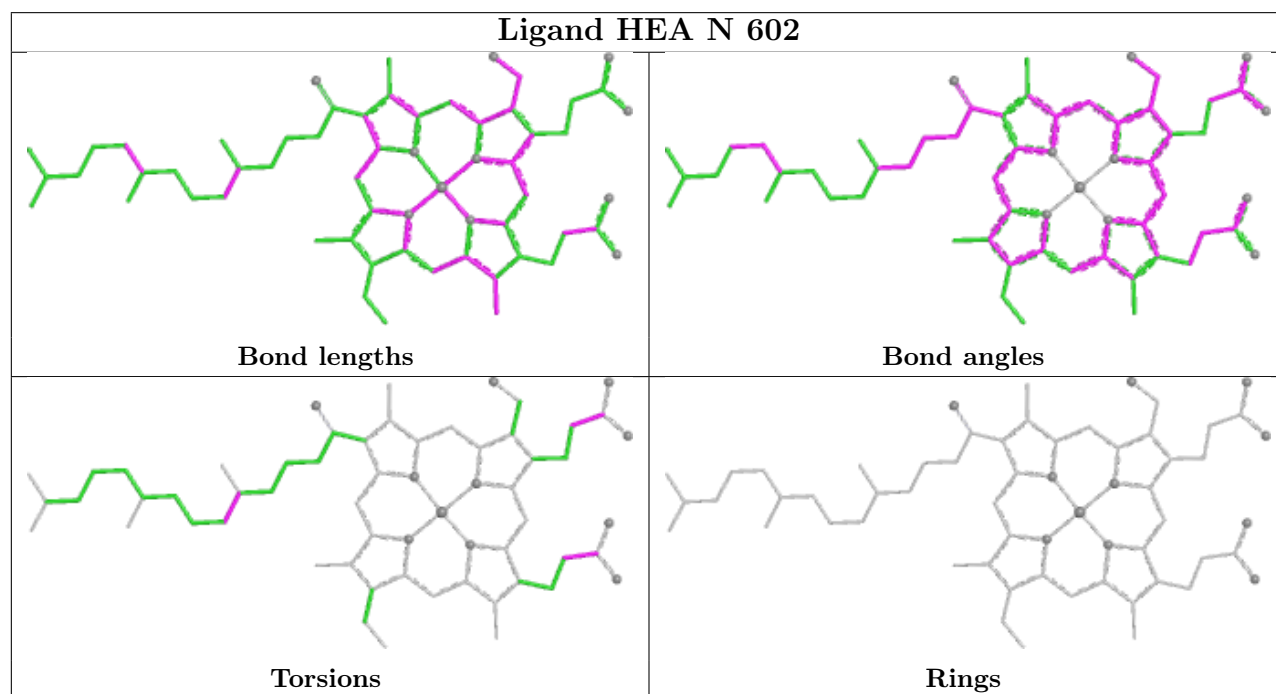
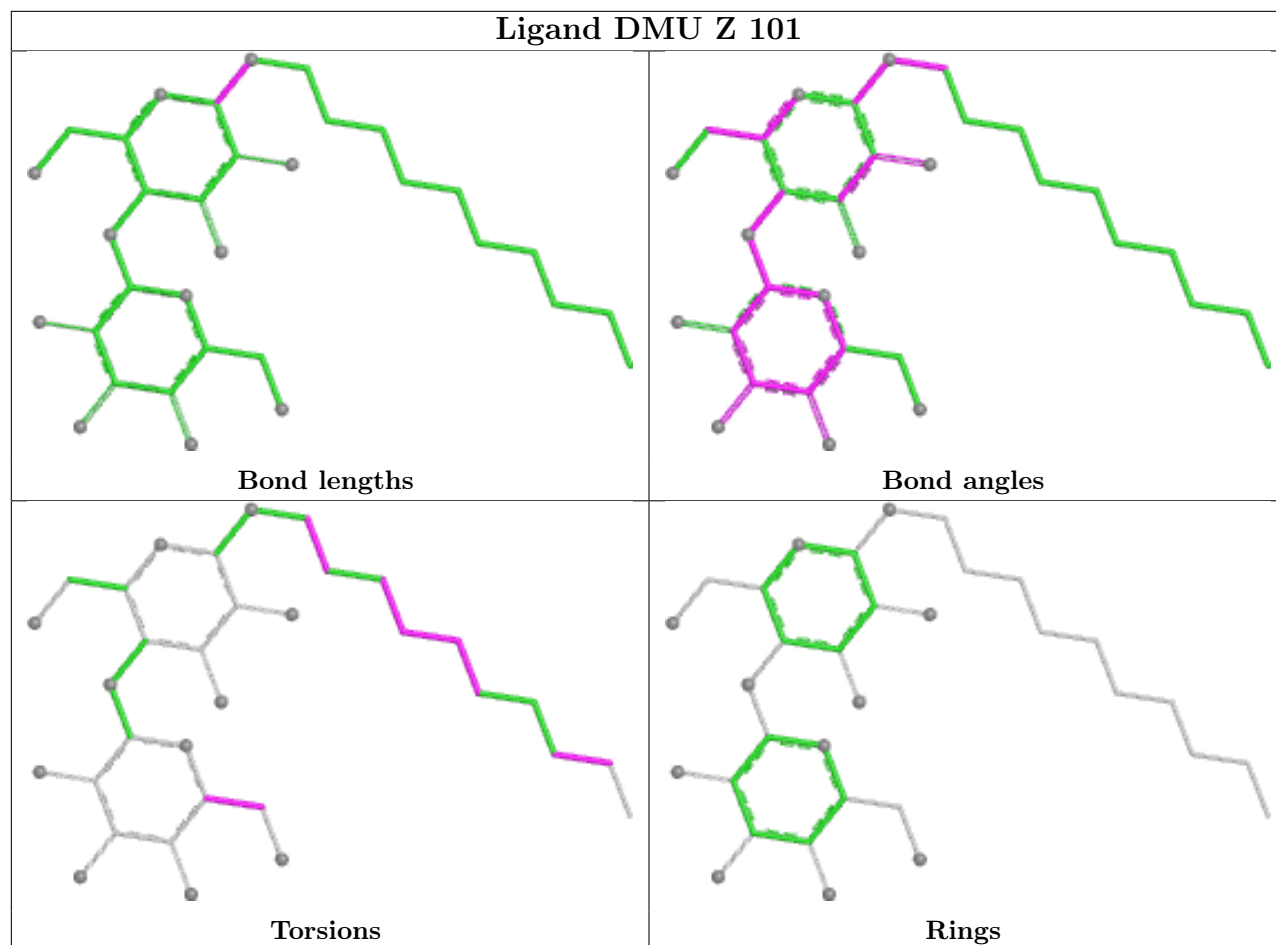
Ligand PSC N 610

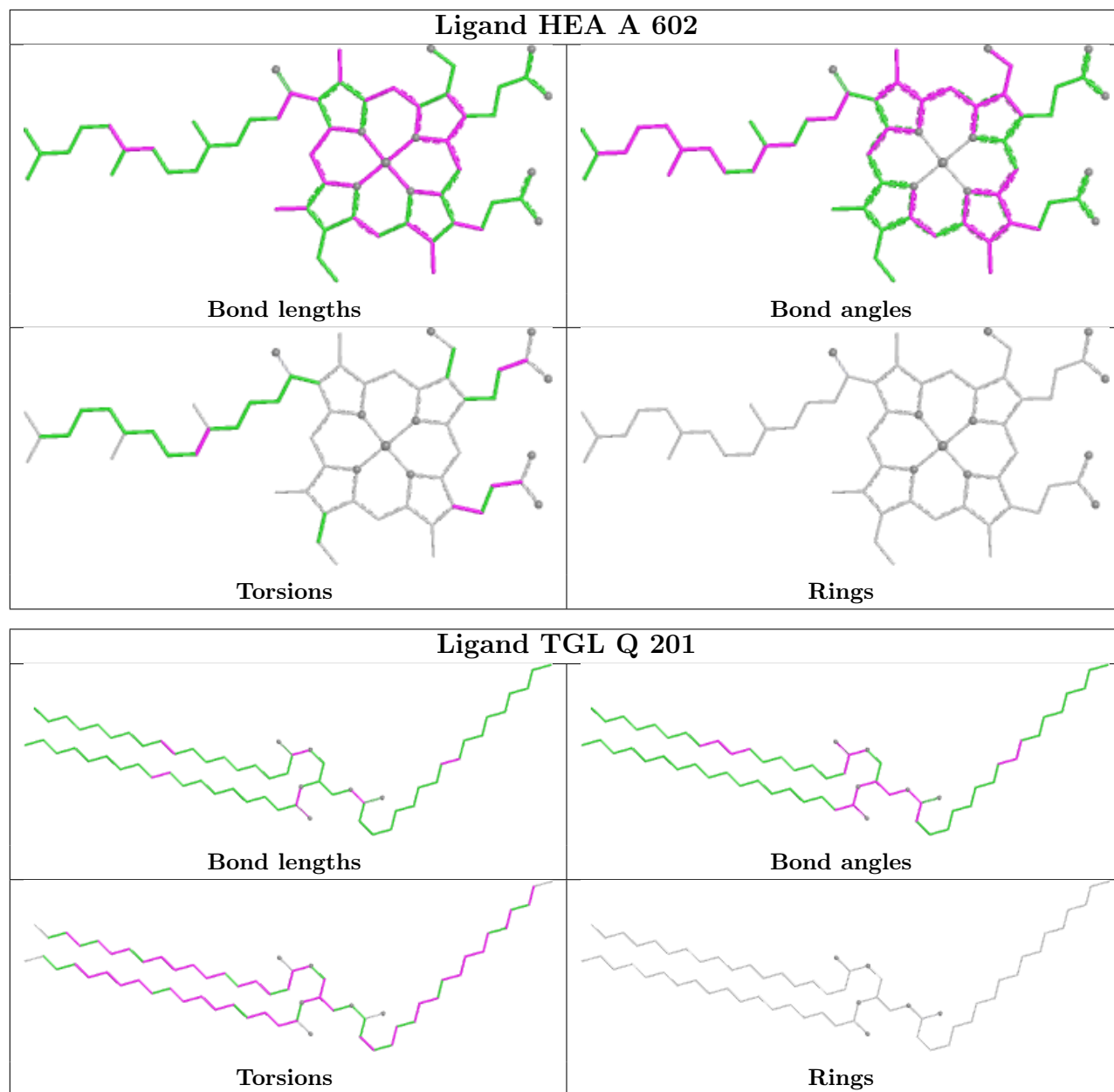


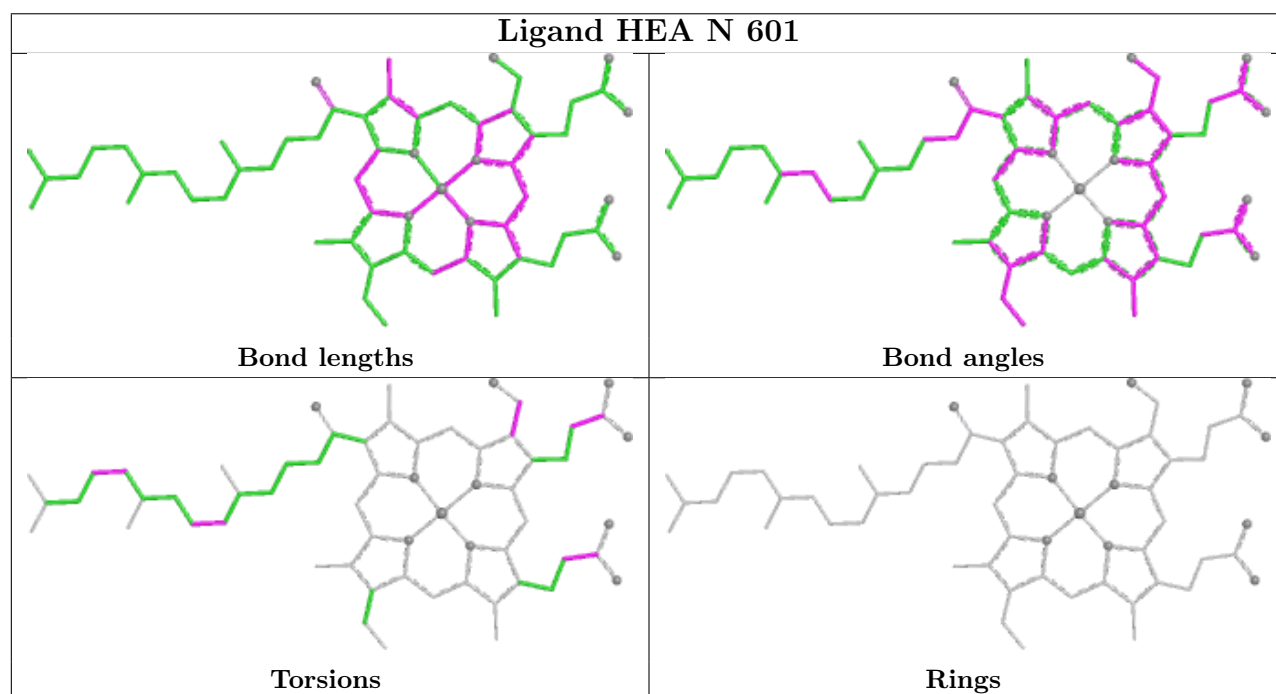
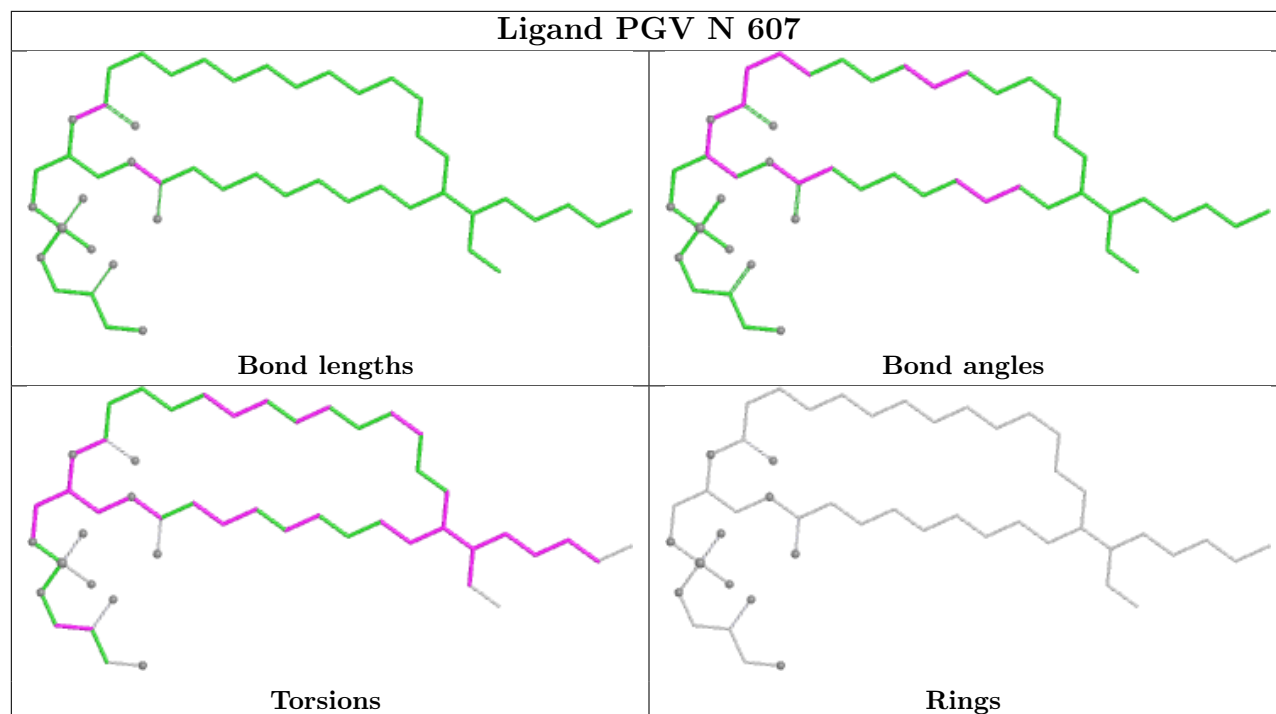
Ligand PGV P 301



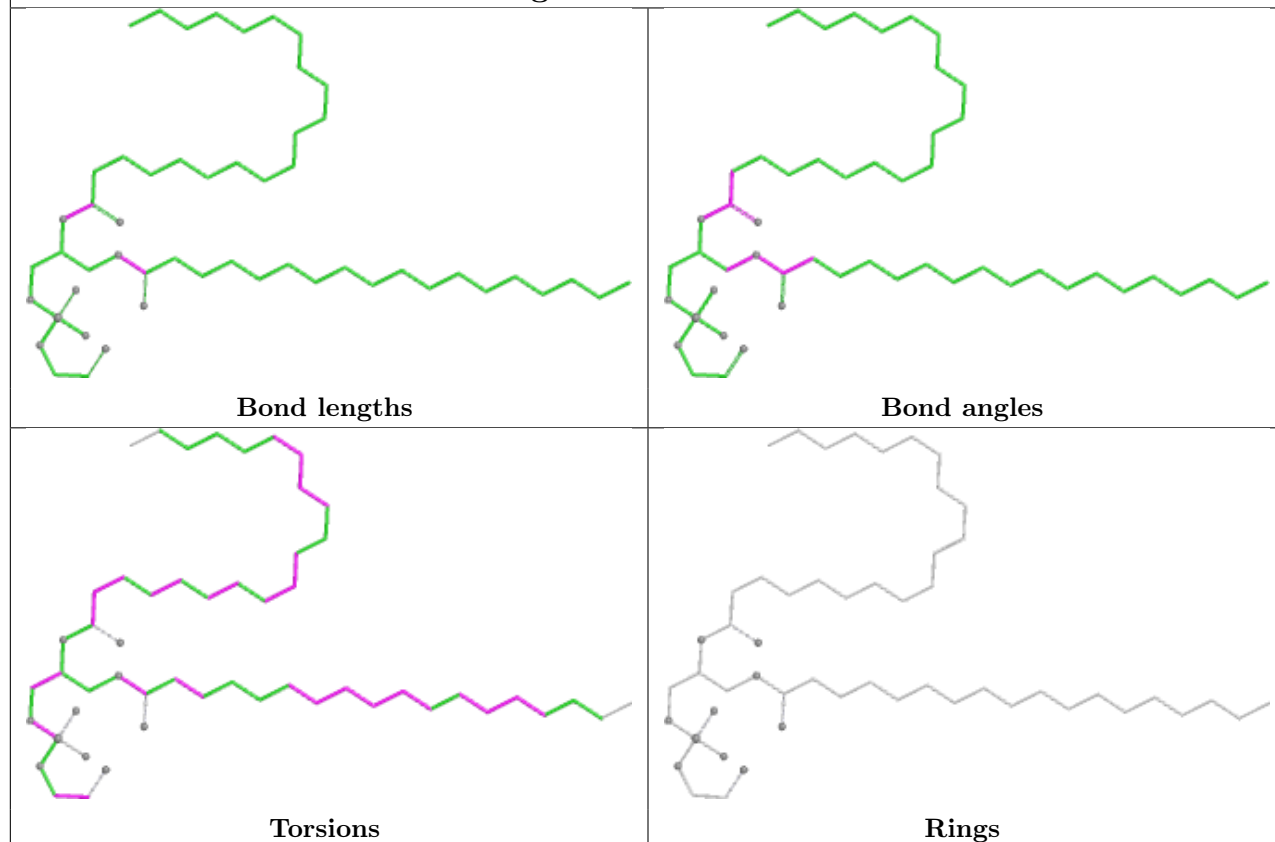




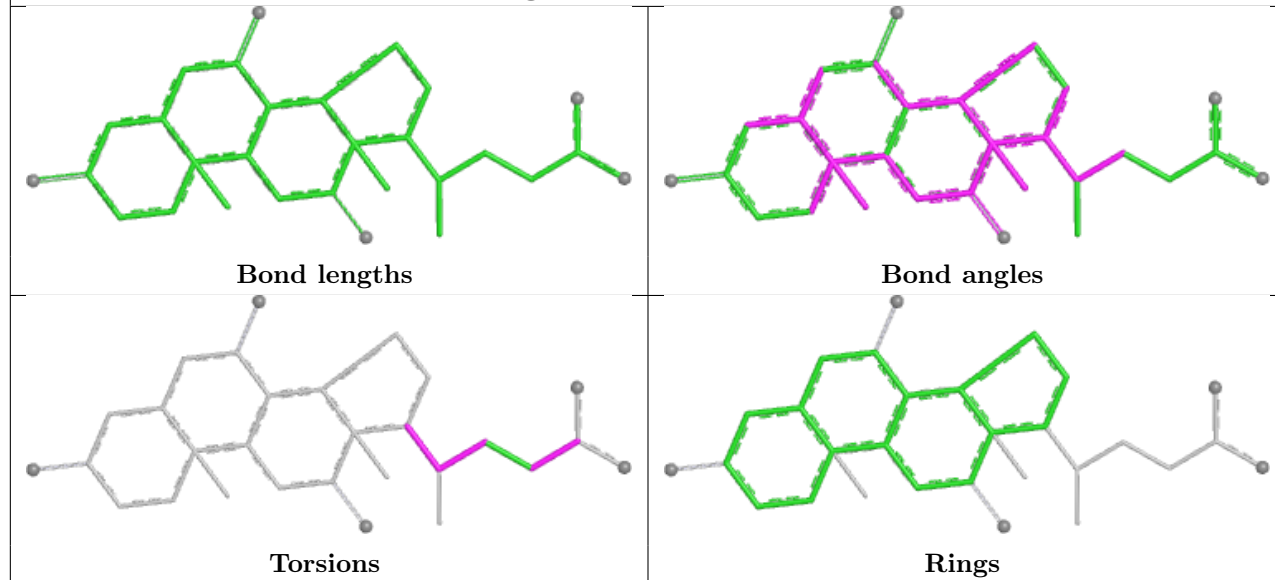


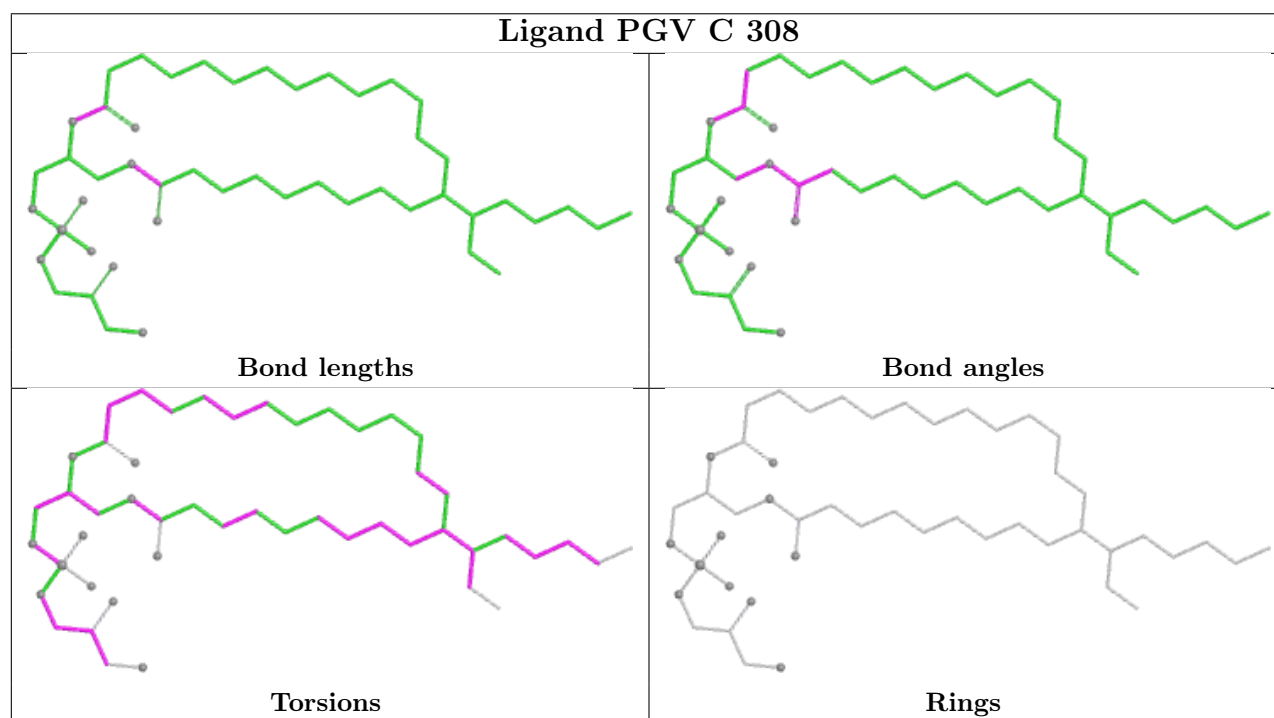
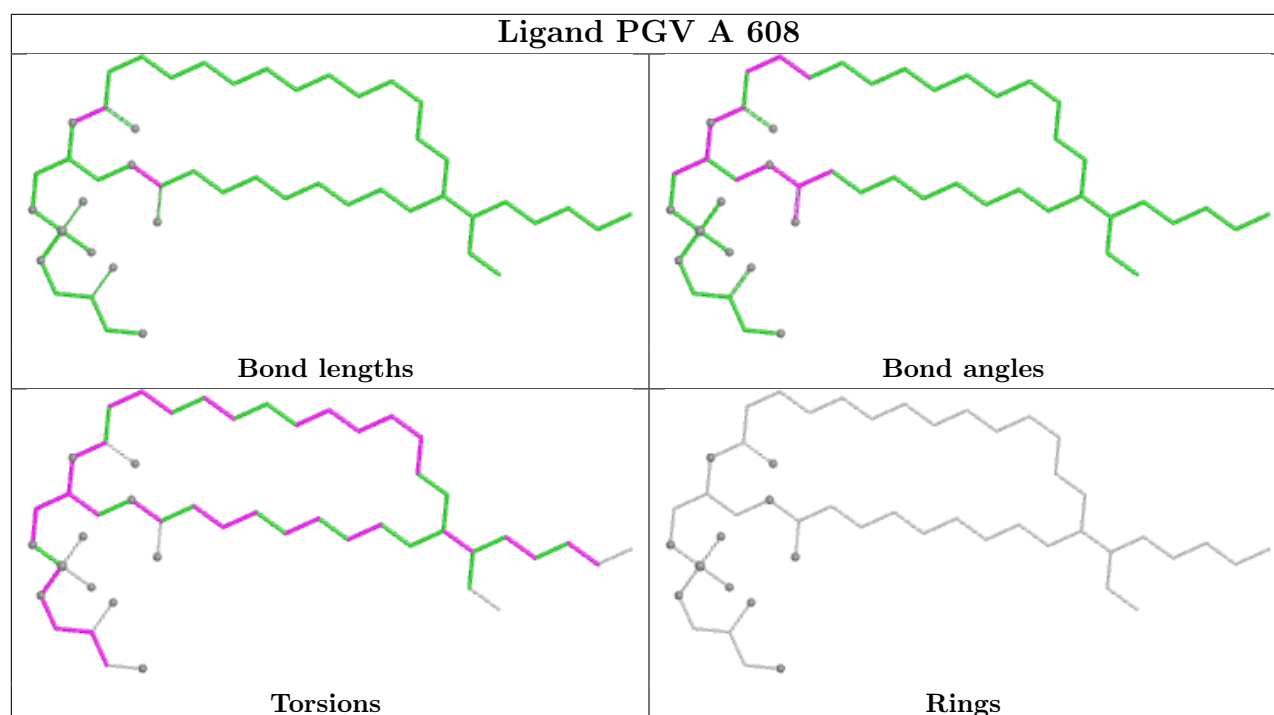


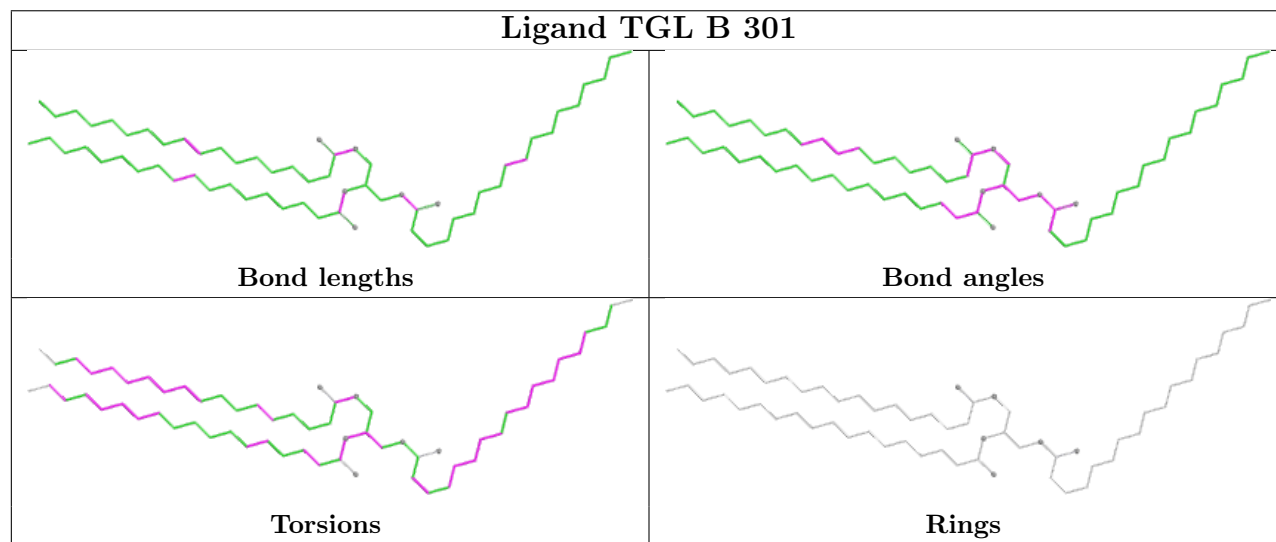
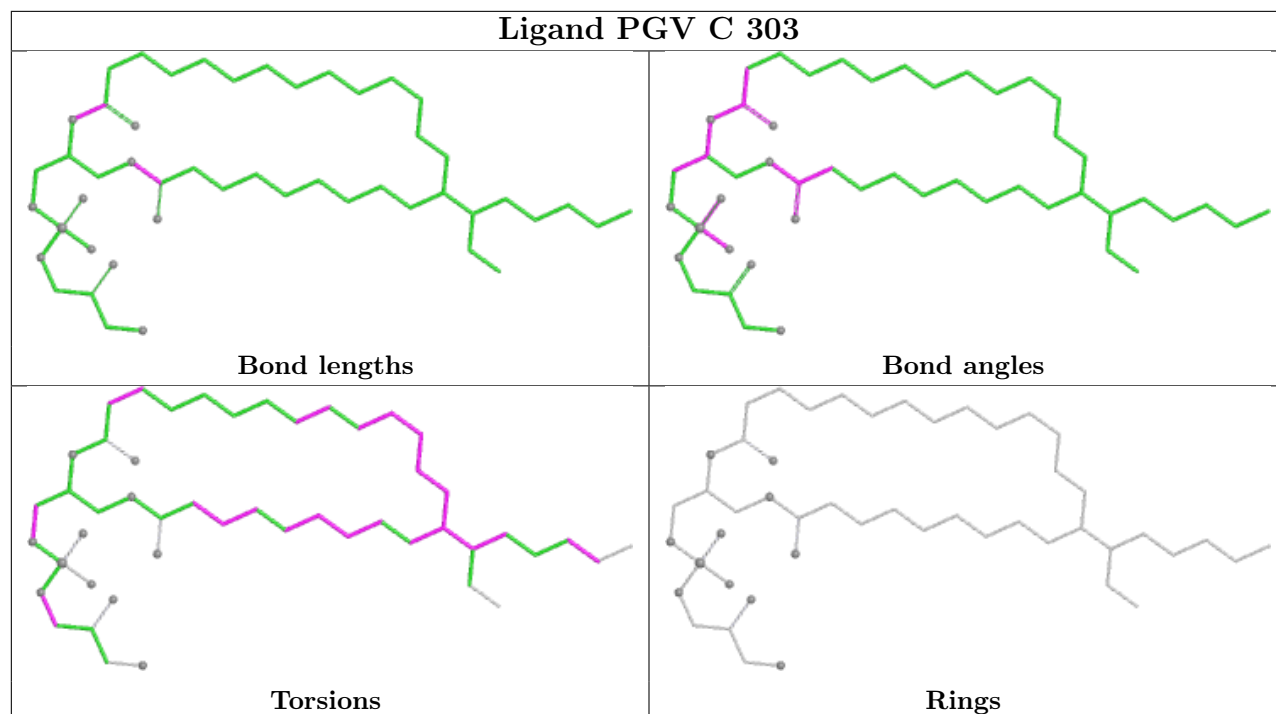
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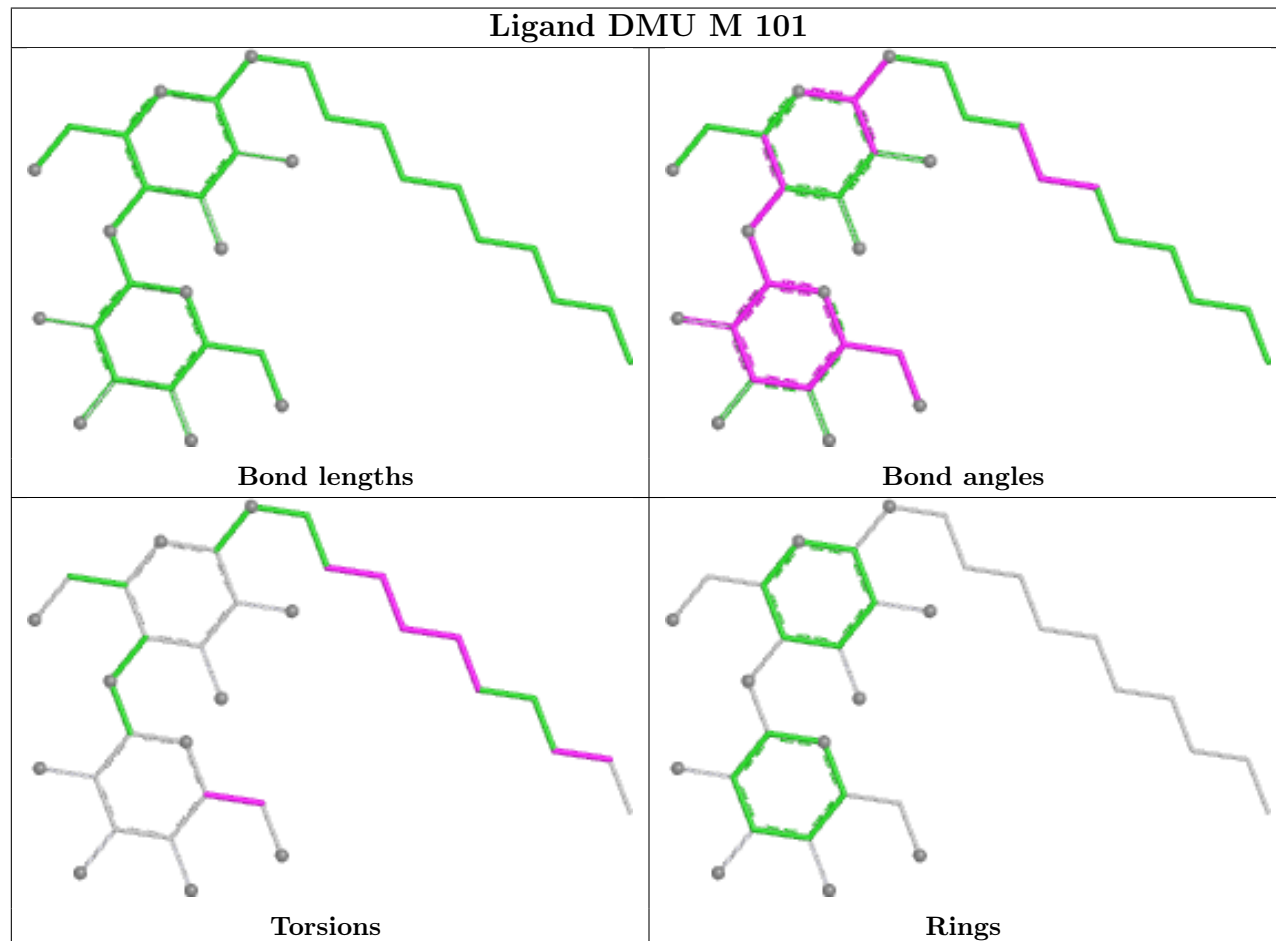
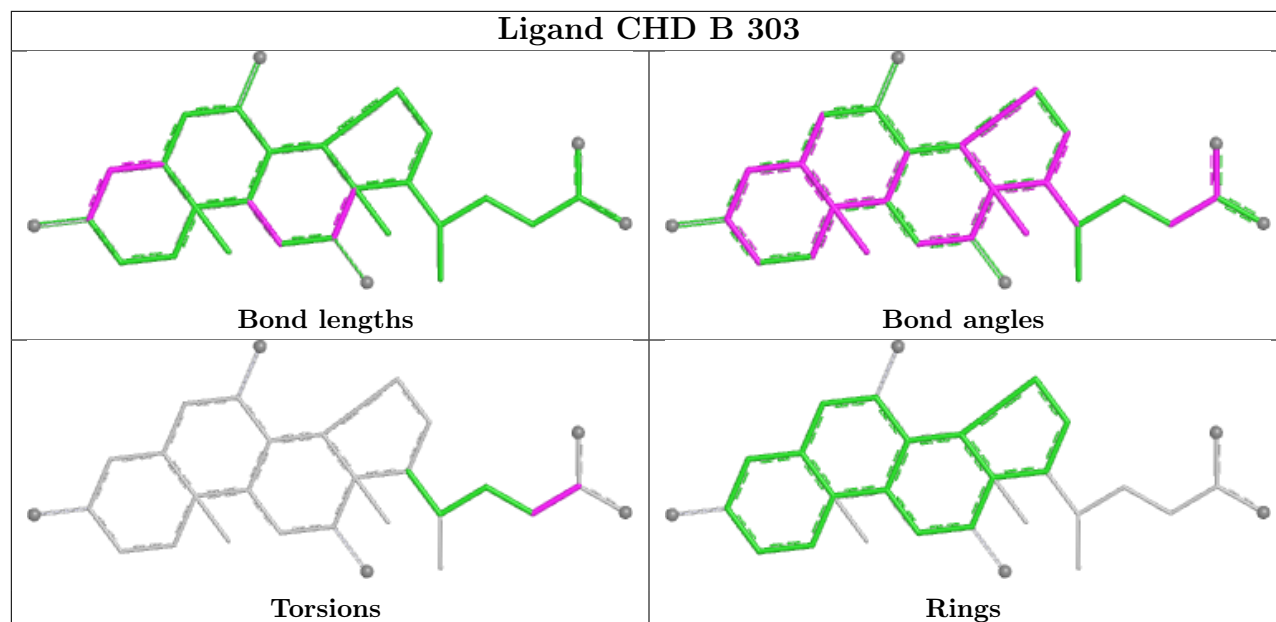


Ligand CHD W 101

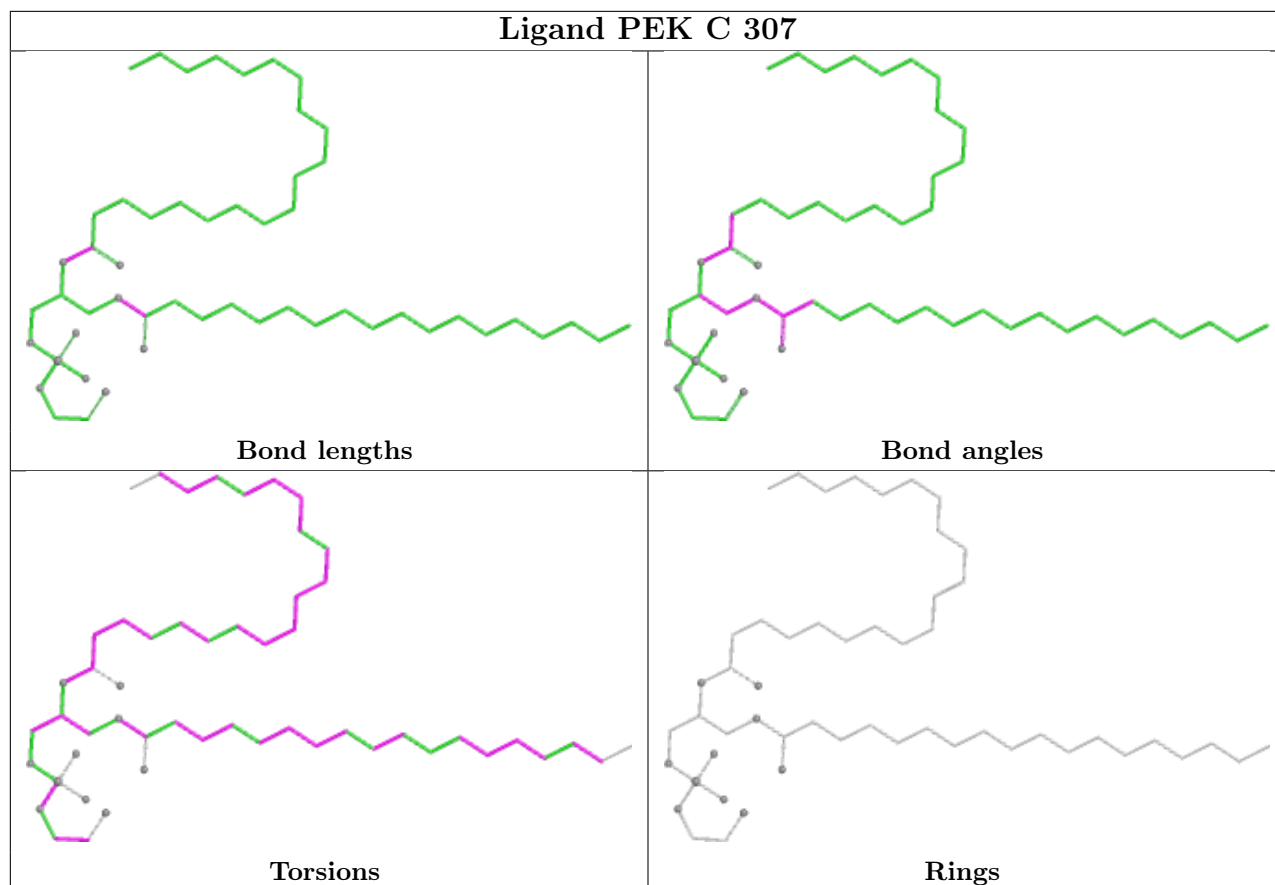




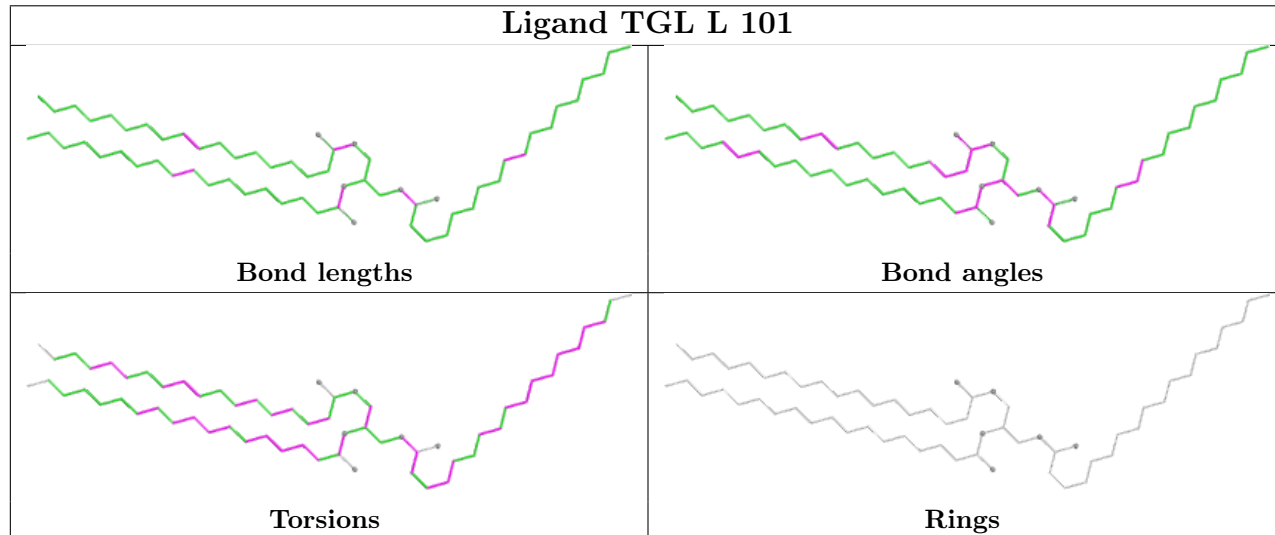


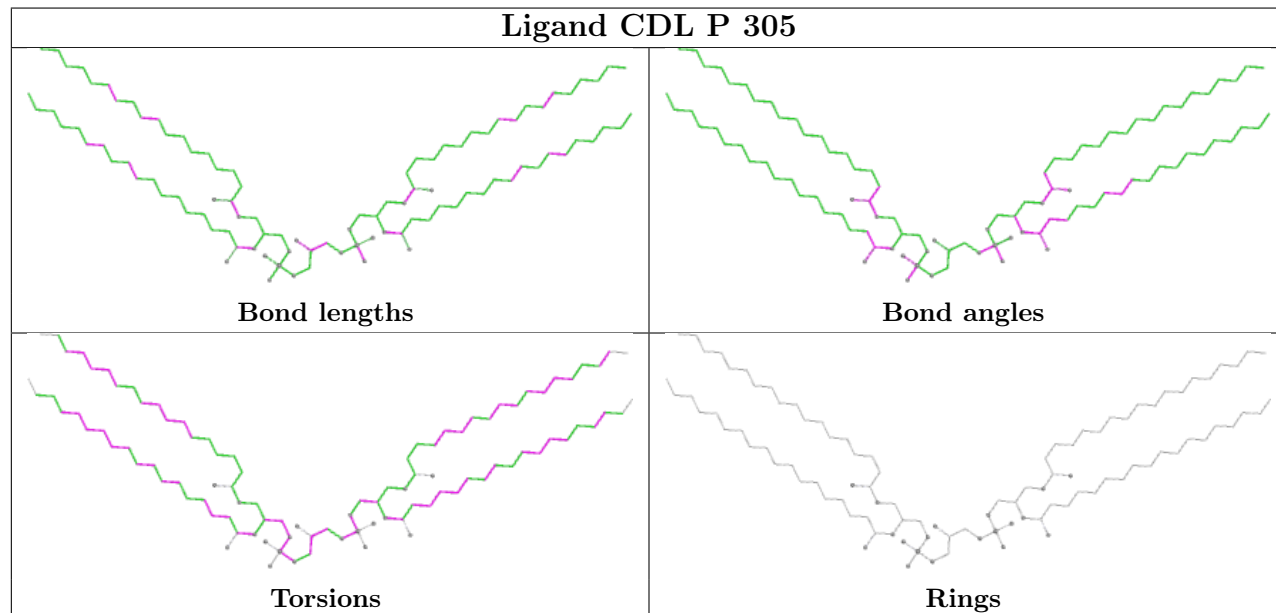
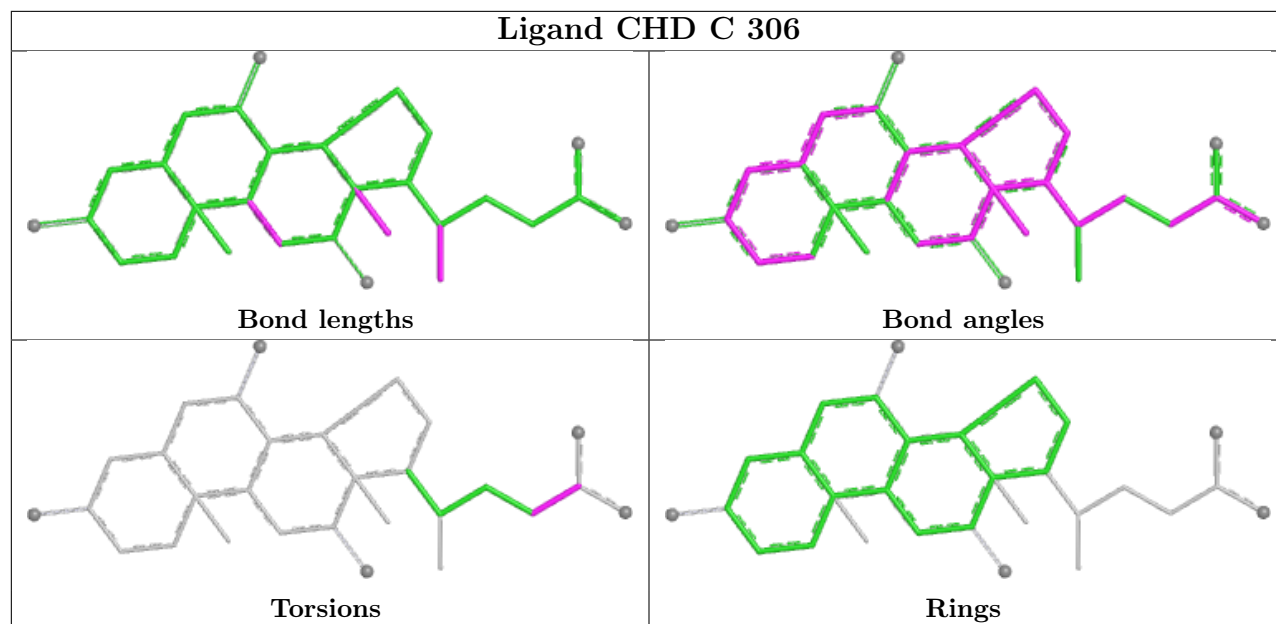


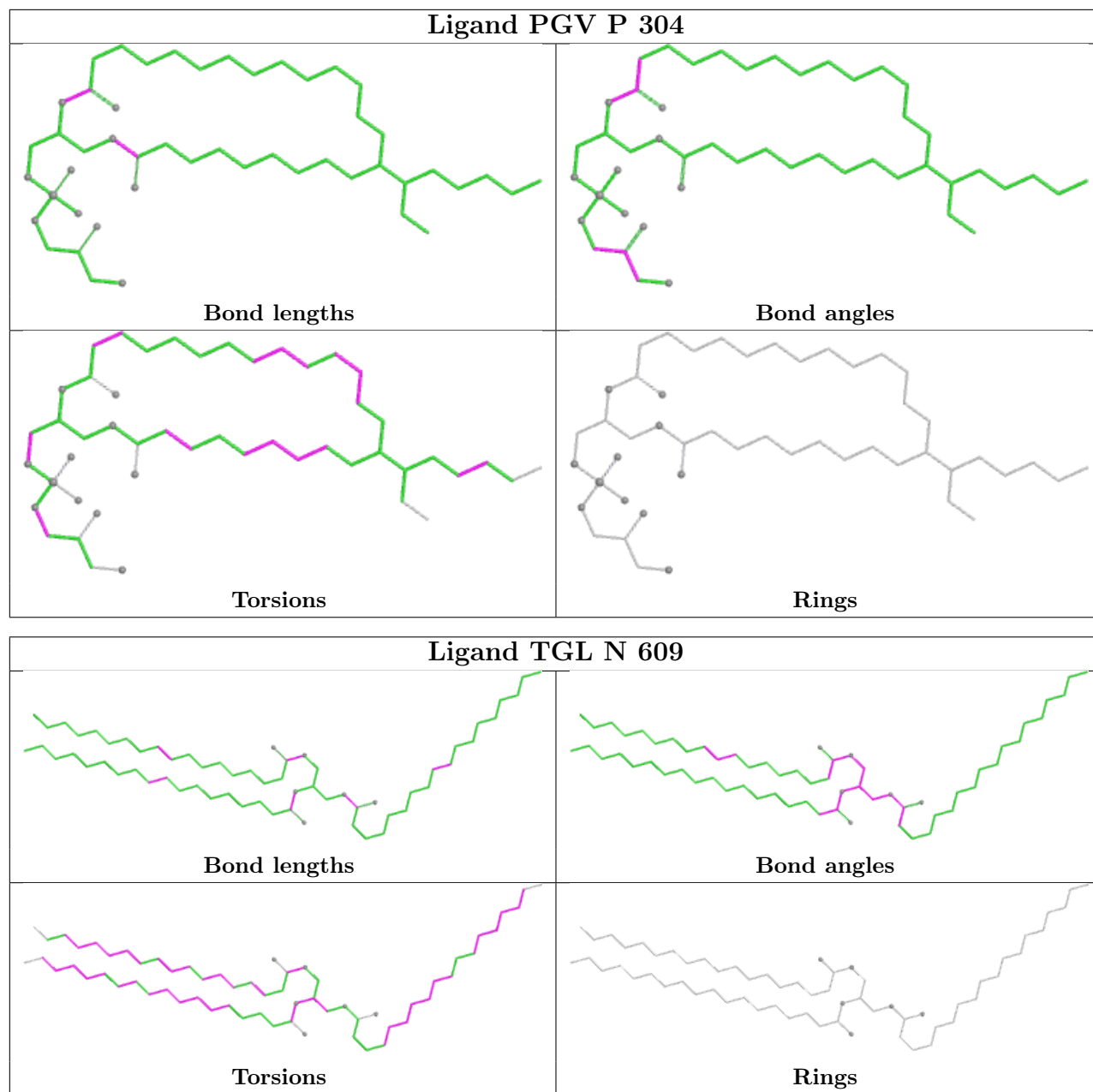
Ligand PEK C 307

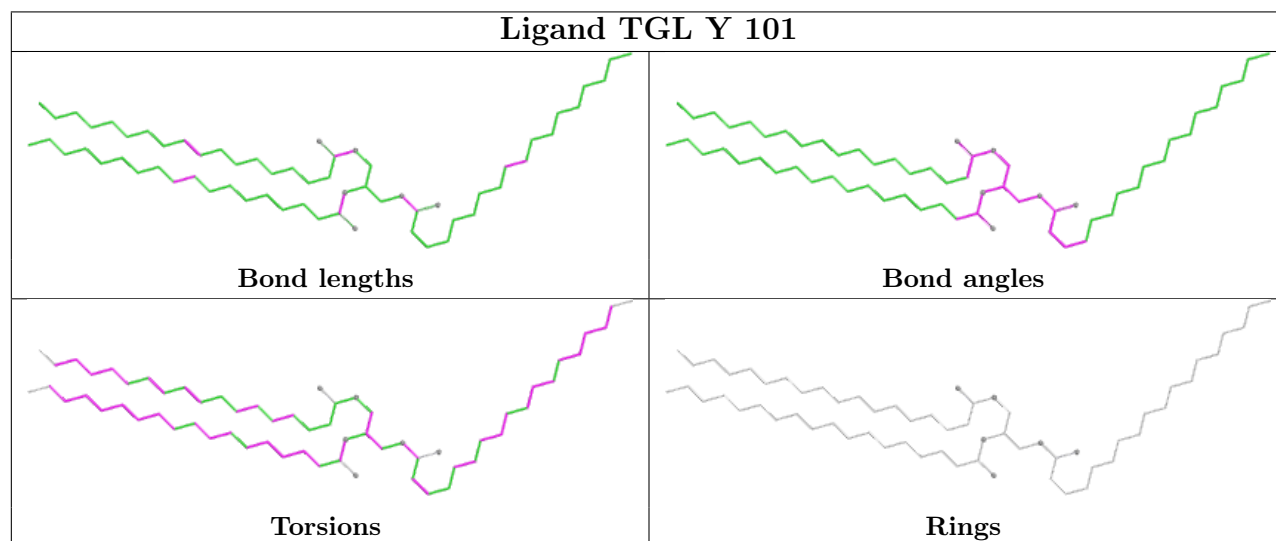
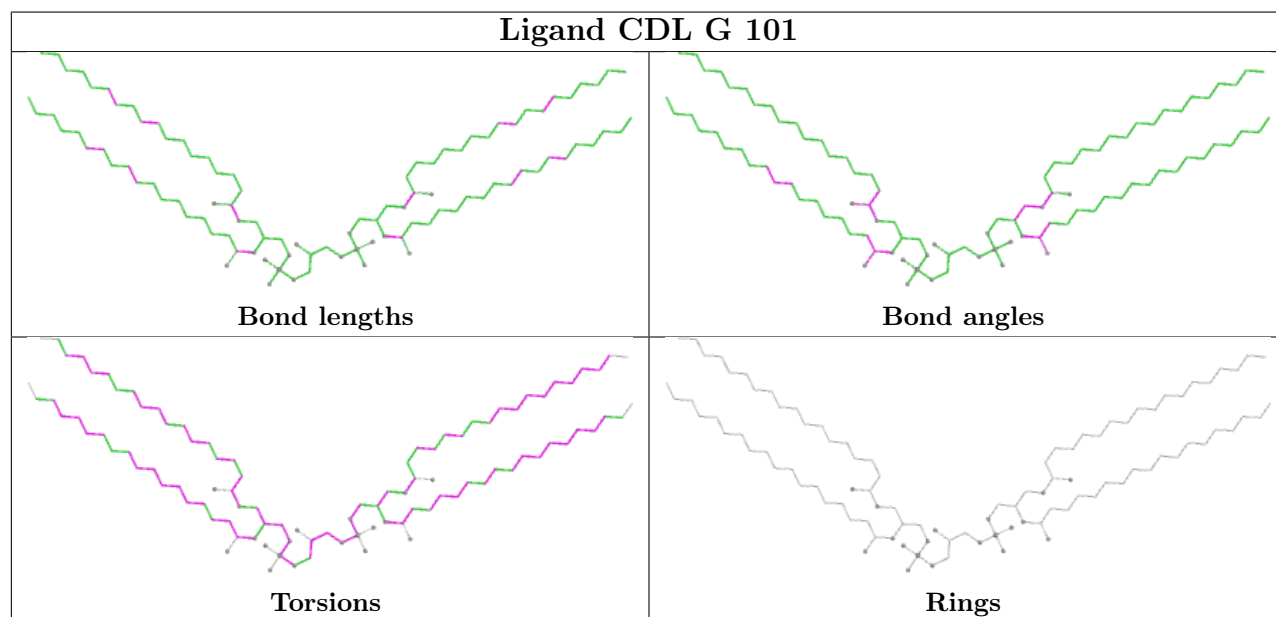
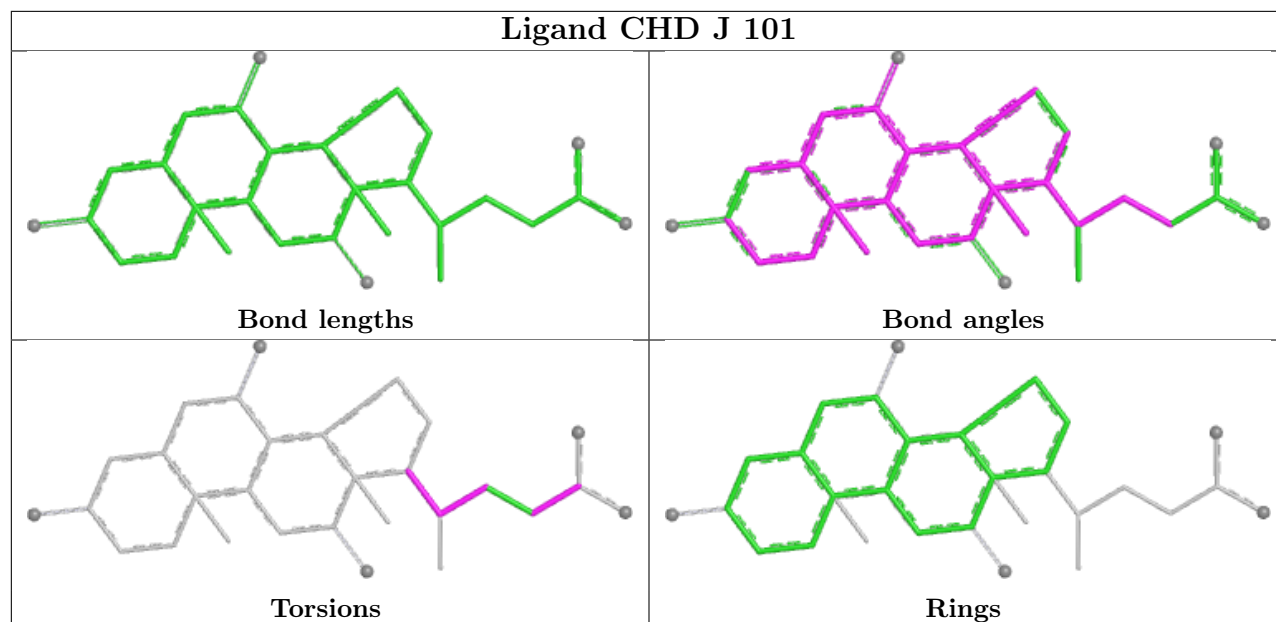


Ligand TGL L 101

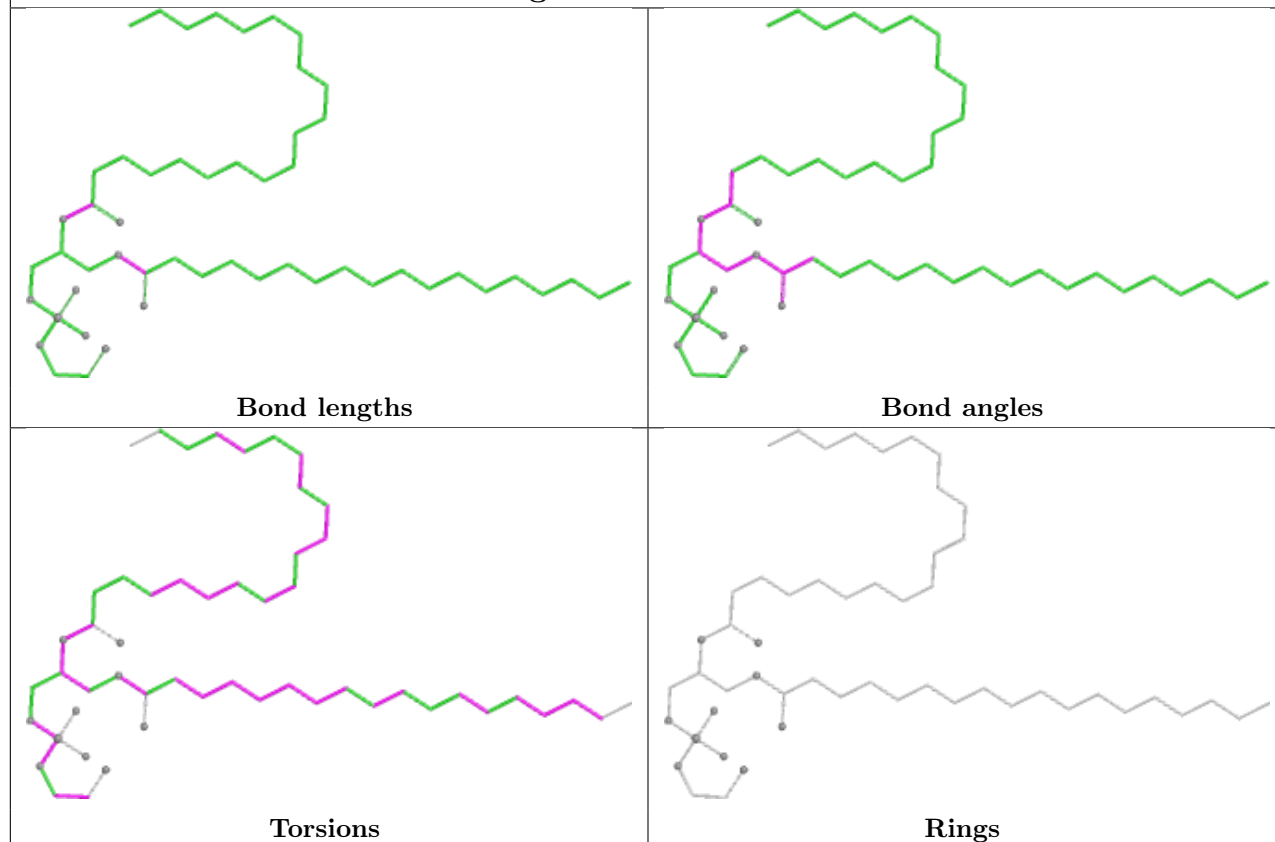




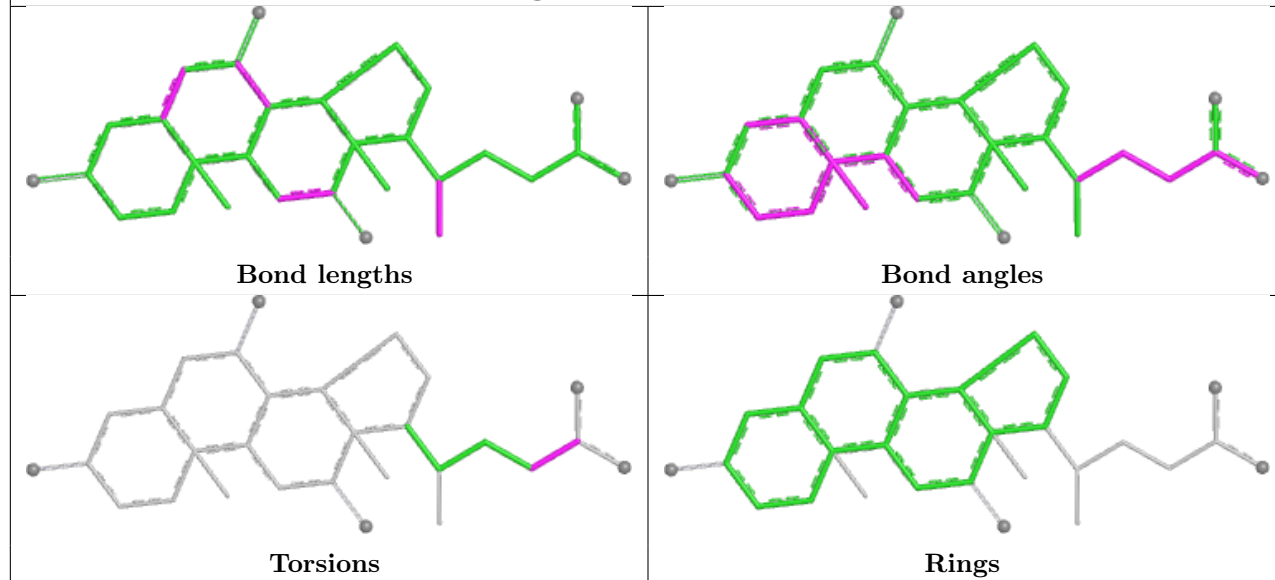


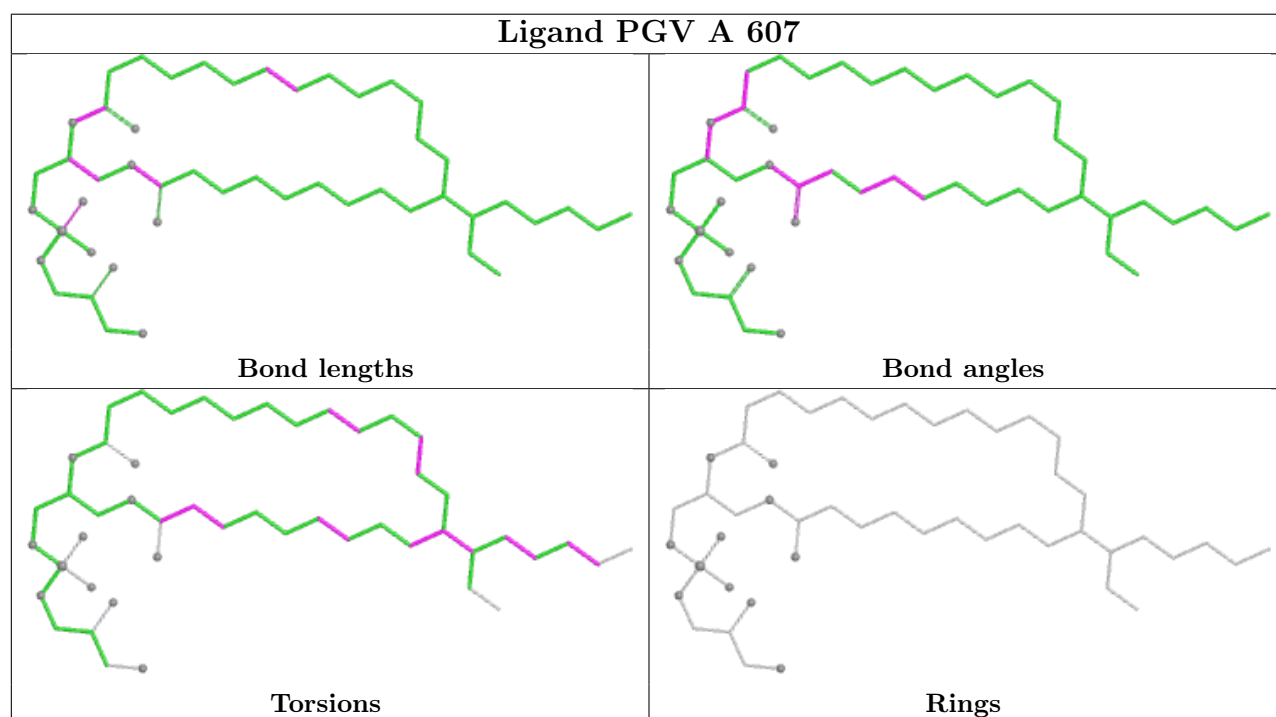
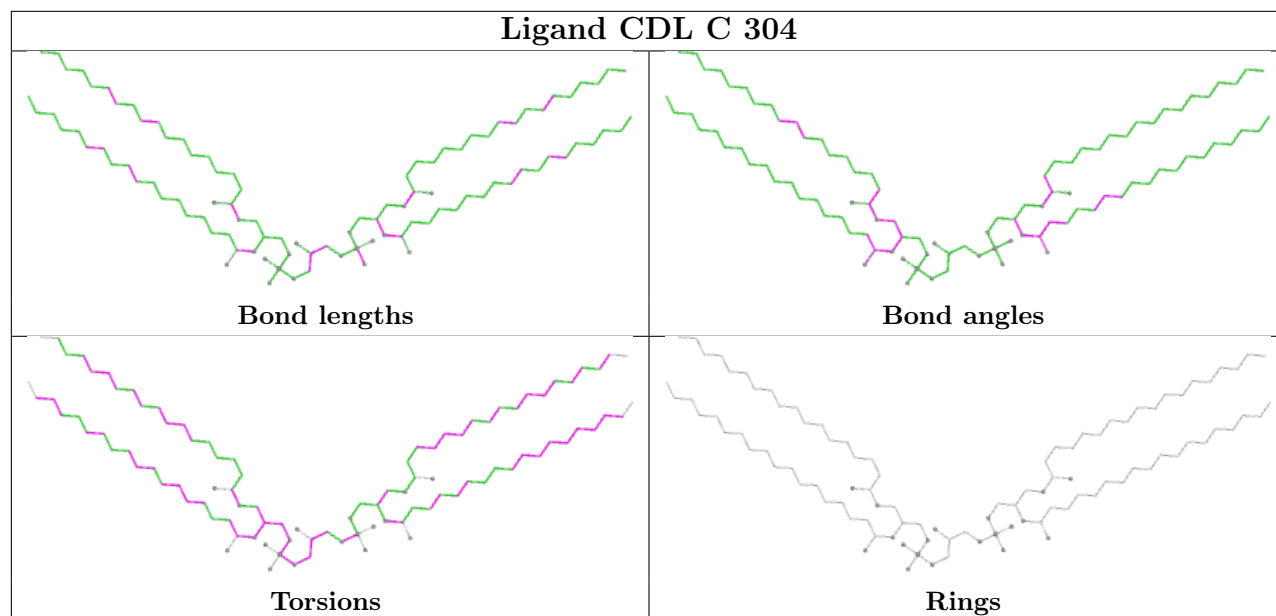


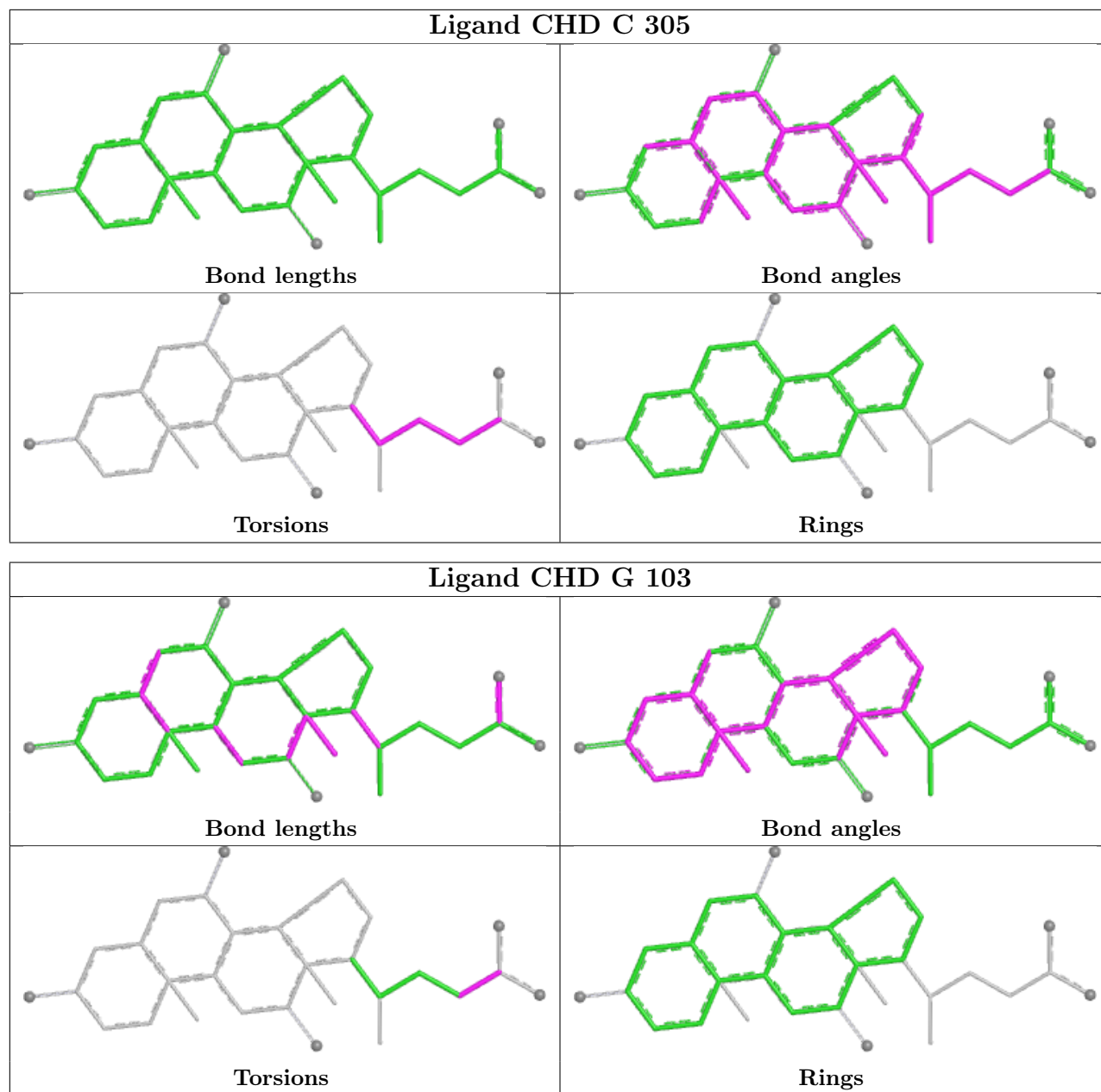
Ligand PEK G 102

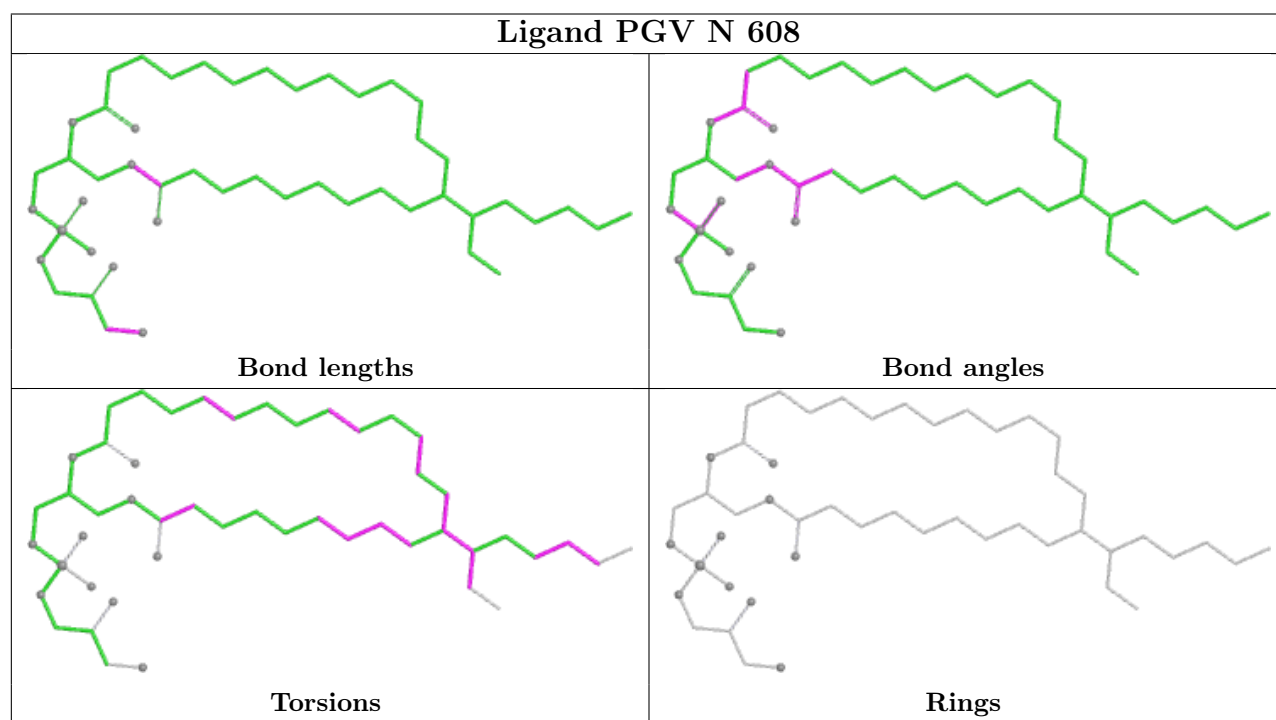
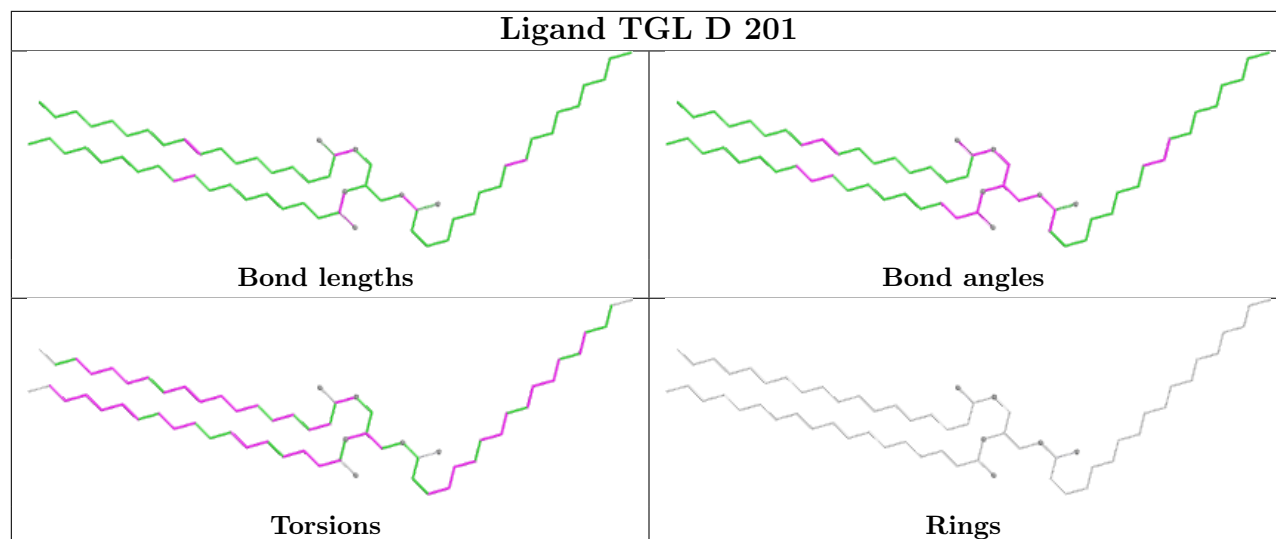


Ligand CHD P 307

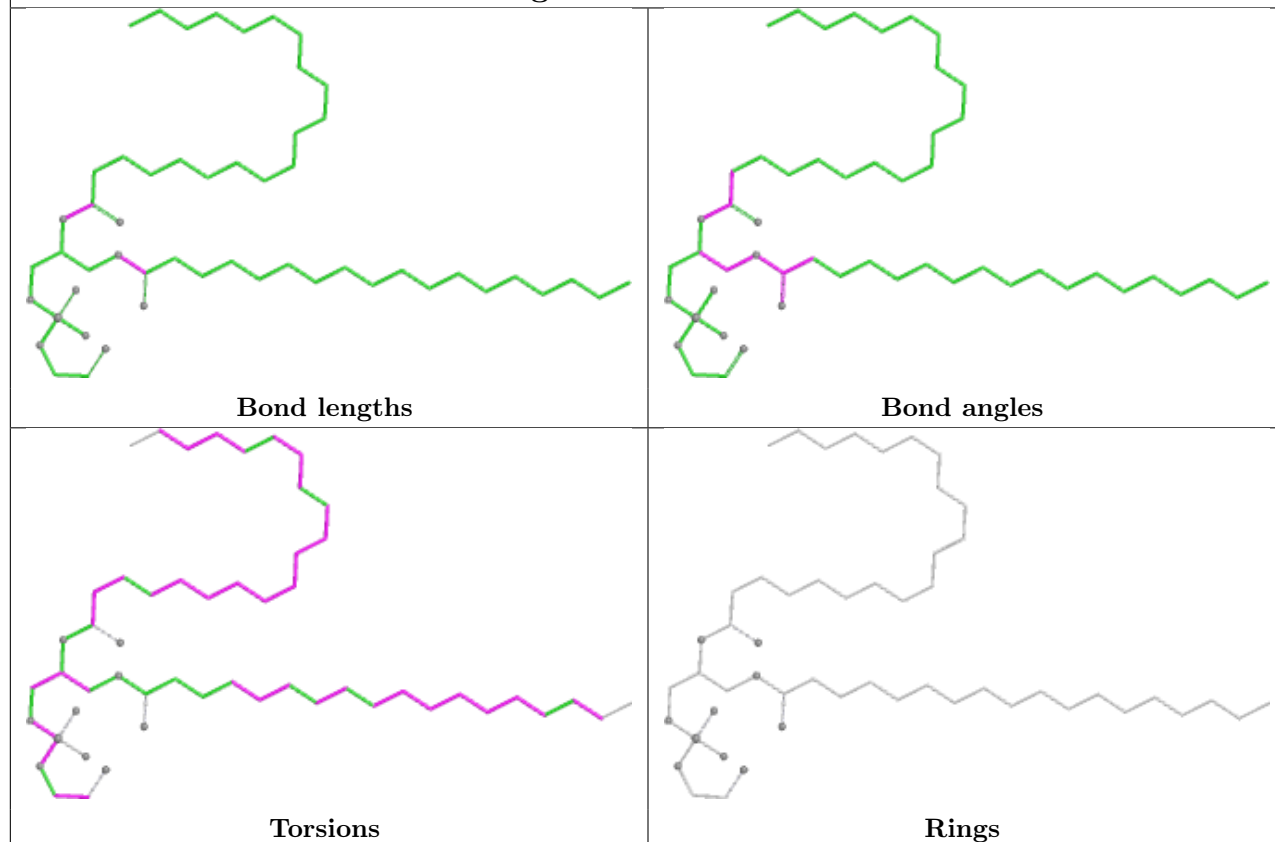




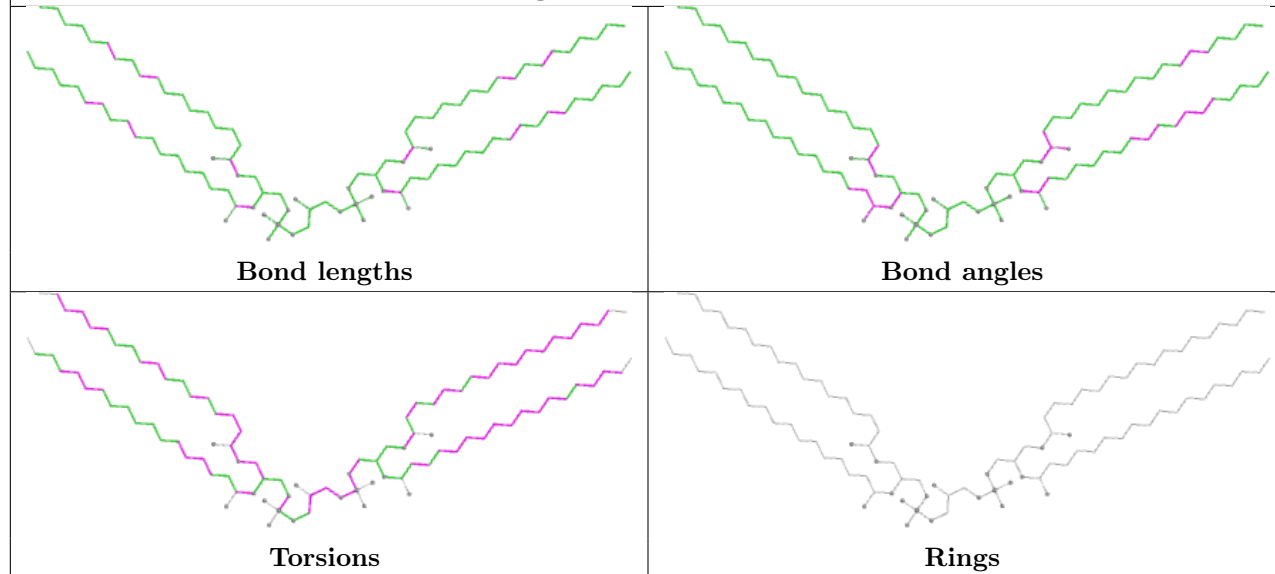




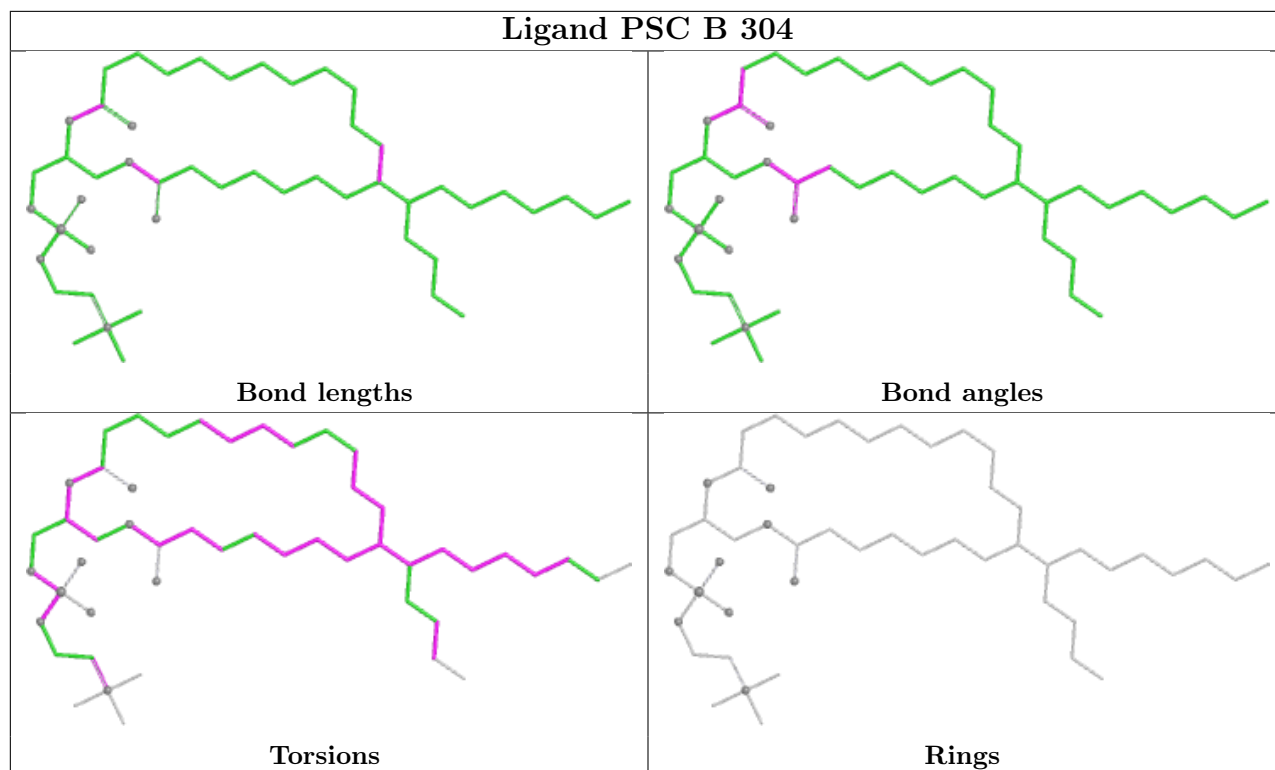
Ligand PEK P 308



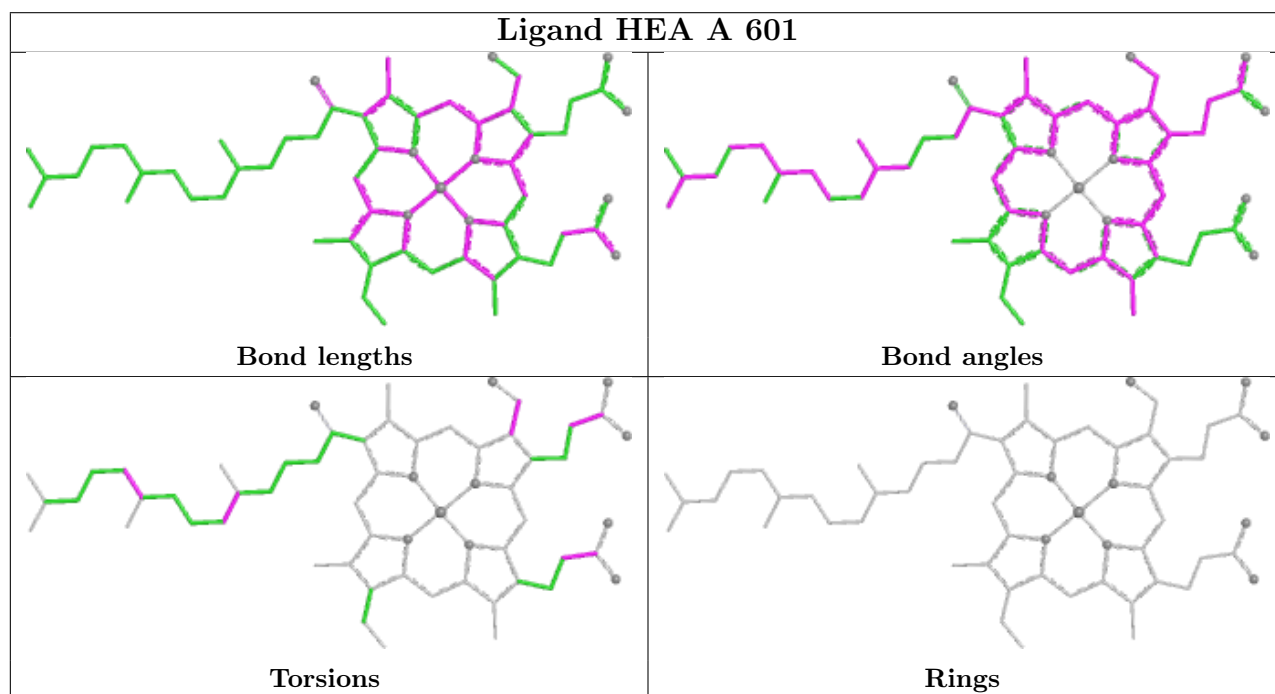
Ligand CDL T 102

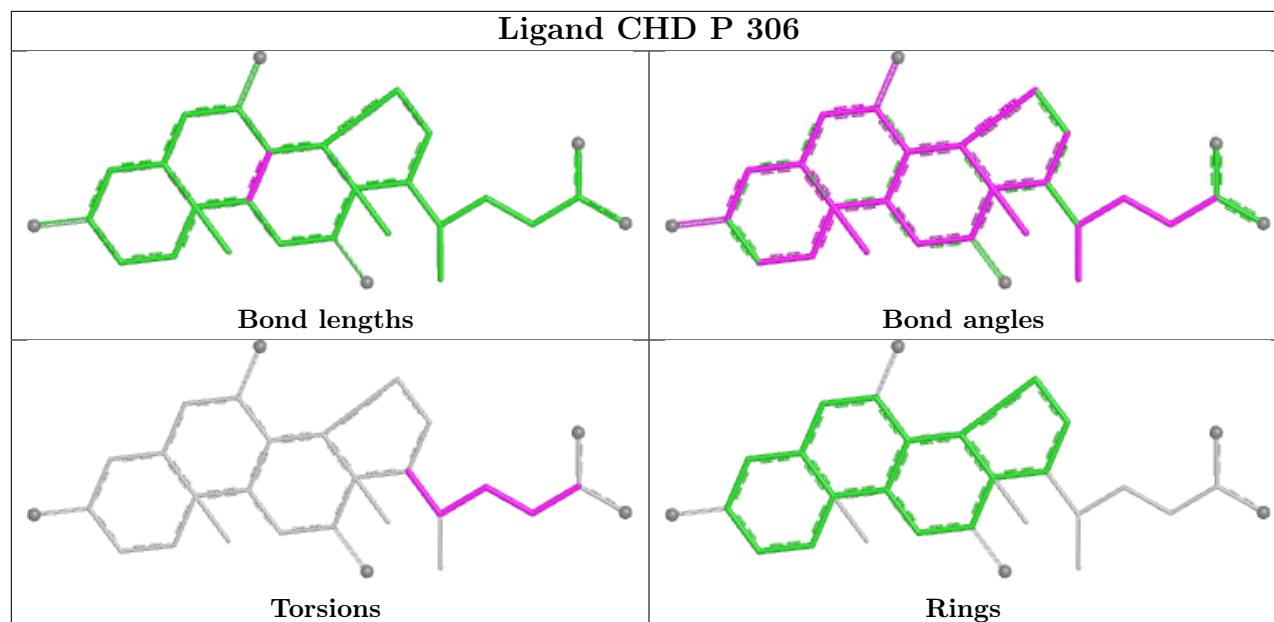


Ligand PSC B 304



Ligand HEA A 601





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%)	-0.21	2 (0%) 88 90	6, 15, 22, 51	6 (1%)
1	N	513/514 (99%)	-0.21	3 (0%) 85 87	6, 14, 20, 51	6 (1%)
2	B	226/227 (99%)	0.16	9 (3%) 42 45	9, 18, 39, 65	1 (0%)
2	O	226/227 (99%)	0.31	13 (5%) 29 30	11, 17, 41, 62	0
3	C	259/261 (99%)	-0.10	4 (1%) 72 75	11, 17, 26, 59	3 (1%)
3	P	259/261 (99%)	-0.08	2 (0%) 82 85	9, 16, 26, 46	3 (1%)
4	D	144/147 (97%)	0.14	2 (1%) 73 76	12, 18, 35, 57	0
4	Q	144/147 (97%)	0.96	20 (13%) 6 6	13, 23, 48, 106	0
5	E	105/109 (96%)	0.08	4 (3%) 44 47	11, 17, 41, 88	0
5	R	105/109 (96%)	0.41	2 (1%) 66 70	13, 18, 36, 89	0
6	F	98/98 (100%)	0.79	9 (9%) 14 15	15, 23, 68, 118	0
6	S	98/98 (100%)	0.67	9 (9%) 14 15	13, 20, 61, 97	0
7	G	83/85 (97%)	0.98	21 (25%) 1 1	11, 20, 73, 90	0
7	T	83/85 (97%)	1.15	21 (25%) 1 1	10, 20, 77, 101	0
8	H	79/85 (92%)	0.83	14 (17%) 4 3	16, 24, 62, 76	0
8	U	79/85 (92%)	0.78	14 (17%) 4 3	14, 21, 63, 76	0
9	I	72/73 (98%)	0.90	13 (18%) 3 3	15, 26, 53, 63	0
9	V	72/73 (98%)	1.02	10 (13%) 6 6	13, 26, 47, 58	0
10	J	58/59 (98%)	0.67	4 (6%) 23 24	17, 25, 45, 86	0
10	W	58/59 (98%)	0.72	5 (8%) 16 17	13, 22, 51, 91	0
11	K	49/56 (87%)	0.54	3 (6%) 27 29	16, 22, 36, 42	0
11	X	49/56 (87%)	0.93	3 (6%) 27 29	16, 21, 37, 43	0
12	L	46/47 (97%)	0.28	4 (8%) 16 17	15, 19, 37, 64	0
12	Y	46/47 (97%)	0.44	4 (8%) 16 17	12, 19, 38, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.31	5 (11%) 9 10	14, 18, 44, 77	0
13	Z	43/46 (93%)	0.64	5 (11%) 9 10	12, 18, 48, 66	0
All	All	3550/3614 (98%)	0.24	205 (5%) 29 30	6, 17, 43, 118	19 (0%)

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.6
6	F	97	ALA	10.6
6	S	97	ALA	10.6
6	F	96	LEU	8.8
6	S	1	ALA	8.7
7	T	36	TRP	8.1
4	Q	6	VAL	7.8
4	Q	5	VAL	7.3
6	S	96	LEU	7.1
7	T	10	GLY	7.0
4	D	4	SER	6.2
6	S	98	HIS	6.2
8	H	44	THR	6.2
8	H	47	GLY	6.0
7	T	8	HIS	5.9
7	G	10	GLY	5.8
6	F	94	HIS	5.8
8	H	8	ILE	5.7
10	W	1	PHE	5.5
9	V	37	PHE	5.5
6	F	98	HIS	5.4
8	U	8	ILE	5.4
6	F	95	GLN	5.4
6	S	95	GLN	5.4
7	T	9	GLY	5.4
4	D	5	VAL	5.3
7	G	7	ASP	5.3
4	Q	8	SER	5.3
7	T	2	SER	5.3
7	T	37	LEU	5.3
7	G	9	GLY	5.2
6	S	94	HIS	5.1
5	E	109	VAL	5.1
6	S	2	SER	5.0

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Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	4.9
7	G	36	TRP	4.8
9	I	37	PHE	4.8
2	B	60	GLU	4.8
5	R	109	VAL	4.6
8	H	10	ASN	4.5
10	W	58	LYS	4.5
8	H	45	ALA	4.4
2	O	227	LEU	4.4
2	O	113	TYR	4.4
7	G	2	SER	4.4
7	G	1	ALA	4.4
7	T	38	HIS	4.3
7	T	7	ASP	4.3
13	M	42	LYS	4.3
4	Q	7	LYS	4.3
6	S	93	PRO	4.3
7	T	84	LYS	4.2
7	G	84	LYS	4.2
8	U	44	THR	4.1
7	T	1	ALA	4.1
12	Y	20	ARG	4.0
7	G	37	LEU	4.0
10	J	58	LYS	4.0
5	R	5	HIS	3.9
3	C	38	ASN	3.9
6	F	2	SER	3.9
7	T	4	ALA	3.9
8	U	47	GLY	3.9
13	Z	43	SER	3.9
5	E	5	HIS	3.8
8	U	45	ALA	3.8
2	O	90	ILE	3.8
6	F	3	GLY	3.8
6	S	3	GLY	3.8
12	L	2	HIS	3.7
9	V	22	VAL	3.7
10	W	57	HIS	3.7
4	Q	35	ALA	3.6
7	G	5	LYS	3.6
12	L	47	LYS	3.6
2	B	65	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	59	GLN	3.5
7	G	41	HIS	3.5
7	G	8	HIS	3.4
7	G	3	ALA	3.4
8	H	7	LYS	3.4
13	M	43	SER	3.4
7	T	39	SER	3.4
9	I	32	ALA	3.4
9	I	33	THR	3.4
7	T	42	ARG	3.3
7	T	5	LYS	3.3
2	O	59	GLN	3.3
3	P	38	ASN	3.3
7	T	3	ALA	3.2
8	U	42	ALA	3.2
9	I	34	PHE	3.2
2	O	116	LEU	3.2
9	V	34	PHE	3.2
5	E	7	THR	3.1
8	U	7	LYS	3.1
7	G	33	LEU	3.1
13	Z	39	ASN	3.1
9	I	25	PHE	3.1
8	H	9	LYS	3.1
7	G	38	HIS	3.1
7	G	6	GLY	3.1
8	H	52	VAL	3.1
2	O	226	MET	3.0
2	B	90	ILE	3.0
2	O	91	ASN	3.0
4	Q	10	ASP	3.0
9	V	2	THR	3.0
4	Q	39	ALA	3.0
3	P	3	HIS	2.9
13	M	38	ASP	2.9
8	U	43	MET	2.9
10	J	1	PHE	2.9
7	G	4	ALA	2.9
4	Q	140	TYR	2.9
12	Y	2	HIS	2.9
2	O	86	MET	2.9
7	T	6	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
8	U	9	LYS	2.8
2	O	224	ALA	2.8
8	U	52	VAL	2.8
8	U	10	ASN	2.8
2	B	61	VAL	2.8
9	V	25	PHE	2.7
9	I	27	VAL	2.7
9	I	36	LYS	2.7
2	B	91	ASN	2.7
10	J	52	TRP	2.7
7	G	42	ARG	2.7
4	Q	9	GLU	2.7
8	H	50	VAL	2.7
8	H	43	MET	2.6
9	I	19	PHE	2.6
7	T	41	HIS	2.6
2	B	78	LEU	2.6
7	G	40	GLY	2.6
7	T	43	GLU	2.6
10	J	57	HIS	2.6
12	L	45	LEU	2.6
7	T	40	GLY	2.6
11	X	6	ALA	2.6
7	G	39	SER	2.6
9	V	33	THR	2.6
3	C	3	HIS	2.5
4	Q	33	LEU	2.5
2	O	65	TRP	2.5
13	Z	40	TYR	2.5
13	Z	42	LYS	2.5
1	N	513	LEU	2.5
8	H	51	SER	2.5
10	W	2	GLU	2.5
11	X	13	TYR	2.4
1	N	136[A]	LEU	2.4
2	O	60	GLU	2.4
2	O	92	ASN	2.4
5	E	6	GLU	2.4
13	M	39	ASN	2.4
9	I	29	LEU	2.4
9	V	36	LYS	2.4
4	Q	30	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	12	GLY	2.4
8	U	50	VAL	2.4
13	Z	32	TRP	2.4
13	M	40	TYR	2.3
9	I	31	PHE	2.3
3	C	40	MET	2.3
4	Q	40	LEU	2.3
12	Y	47	LYS	2.3
9	V	27	VAL	2.3
1	N	483	LEU	2.3
7	T	12	GLY	2.3
2	B	55	THR	2.3
7	G	43	GLU	2.2
9	I	30	GLY	2.2
10	W	56	PRO	2.2
2	O	78	LEU	2.2
8	H	48	GLY	2.2
8	U	11	TYR	2.2
9	I	2	THR	2.2
9	V	32	ALA	2.2
2	B	113	TYR	2.2
4	Q	34	SER	2.2
4	Q	49	SER	2.2
11	X	7	PRO	2.2
8	U	46	LYS	2.2
1	A	178	GLN	2.1
3	C	258	TRP	2.1
4	Q	36	SER	2.1
12	L	46	LYS	2.1
4	Q	53	ILE	2.1
9	I	18	ARG	2.1
8	H	42	ALA	2.1
11	K	47	ARG	2.1
1	A	514	LYS	2.1
8	U	48	GLY	2.1
12	Y	24	MET	2.1
8	H	46	LYS	2.0
9	V	31	PHE	2.0
11	K	7	PRO	2.0
4	Q	51	LEU	2.0
4	Q	115	TRP	2.0
11	K	6	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
4	Q	58	GLU	2.0
7	T	35	SER	2.0
6	F	54	ASN	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
9	SAC	V	1	9/10	0.42	0.23	63,69,72,74	0
9	SAC	I	1	9/10	0.62	0.25	43,49,64,67	0
7	TPO	T	11	11/12	0.65	0.26	52,69,96,97	0
7	TPO	G	11	11/12	0.68	0.26	65,74,106,115	0
1	FME	A	1	10/11	0.89	0.12	25,33,52,71	0
1	FME	N	1	10/11	0.90	0.12	18,28,48,58	0
2	FME	B	1	10/11	0.94	0.09	15,16,24,33	0
2	FME	O	1	10/11	0.96	0.08	15,16,24,24	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
22	CHD	J	101	29/29	0.62	0.27	56,93,101,102	0
22	CHD	W	101	29/29	0.62	0.26	52,82,95,101	0
20	TGL	Q	201	63/63	0.71	0.20	30,47,66,71	0
19	PGV	P	301	51/51	0.73	0.22	45,70,102,114	0
24	PEK	C	307	53/53	0.74	0.22	34,59,94,103	0
19	PGV	C	308	51/51	0.75	0.21	34,64,99,101	0
24	PEK	G	102	53/53	0.75	0.23	37,71,111,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CDL	T	102	100/100	0.75	0.22	31,67,118,128	0
24	PEK	T	101	53/53	0.76	0.26	36,76,114,118	0
25	CDL	G	101	100/100	0.77	0.20	34,66,99,138	0
20	TGL	Y	101	63/63	0.78	0.20	33,49,76,81	0
19	PGV	N	607	51/51	0.78	0.20	27,49,103,114	0
23	PSC	B	304	52/52	0.79	0.22	36,84,130,137	0
22	CHD	P	306	29/29	0.79	0.15	34,44,49,56	0
24	PEK	P	308	53/53	0.80	0.20	25,55,100,118	0
20	TGL	L	101	63/63	0.80	0.19	28,44,70,80	0
19	PGV	A	608	51/51	0.80	0.19	24,51,72,84	0
25	CDL	P	305	100/100	0.80	0.20	28,60,102,116	0
20	TGL	D	201	63/63	0.80	0.18	23,45,66,74	0
23	PSC	N	610	52/52	0.81	0.21	24,61,117,126	0
22	CHD	C	305	29/29	0.81	0.14	41,47,53,59	0
25	CDL	C	304	100/100	0.82	0.19	26,59,88,108	0
20	TGL	N	609	63/63	0.83	0.17	31,54,73,76	0
20	TGL	B	301	63/63	0.84	0.17	28,51,75,84	0
17	NA	P	302	1/1	0.88	0.09	29,29,29,29	0
27	DMU	M	101	33/33	0.88	0.11	25,29,39,40	0
27	DMU	Z	101	33/33	0.88	0.10	18,31,34,39	0
16	MG	N	604	1/1	0.91	0.07	17,17,17,17	0
17	NA	C	301	1/1	0.93	0.22	37,37,37,37	0
22	CHD	B	303	29/29	0.93	0.07	8,10,13,19	0
24	PEK	P	303	53/53	0.94	0.11	13,29,70,77	0
22	CHD	P	307	29/29	0.94	0.07	12,19,23,26	0
24	PEK	C	302	53/53	0.94	0.12	13,33,60,65	0
22	CHD	C	306	29/29	0.95	0.07	17,21,25,29	0
22	CHD	G	103	29/29	0.95	0.06	8,10,12,16	0
17	NA	N	605	1/1	0.95	0.06	12,12,12,12	0
19	PGV	C	303	51/51	0.95	0.10	13,22,55,63	0
19	PGV	N	608	51/51	0.95	0.10	12,30,49,58	0
19	PGV	A	607	51/51	0.96	0.10	13,26,49,57	0
19	PGV	P	304	51/51	0.96	0.09	12,27,51,54	0
14	HEA	A	601	60/60	0.97	0.08	10,12,37,46	0
14	HEA	A	602	60/60	0.97	0.06	9,12,18,19	0
21	CUA	O	301	2/2	0.97	0.04	14,14,14,15	0
14	HEA	N	601	60/60	0.97	0.07	10,13,32,39	0
16	MG	A	604	1/1	0.97	0.06	14,14,14,14	0
14	HEA	N	602	60/60	0.98	0.06	9,12,18,21	0
18	PER	A	606[A]	2/2	0.98	0.18	10,10,10,12	0
18	PER	A	606[B]	2/2	0.98	0.18	11,11,11,11	2
18	PER	N	606[A]	2/2	0.98	0.08	10,10,10,12	0

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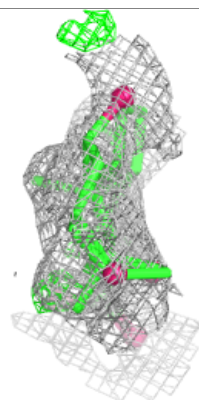
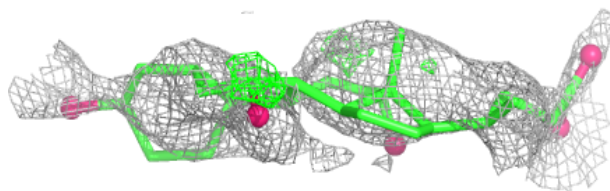
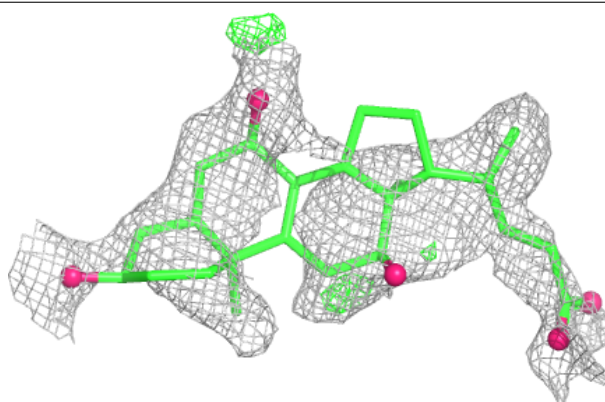
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	PER	N	606[B]	2/2	0.98	0.08	11,11,11,11	2
17	NA	A	605	1/1	0.98	0.04	14,14,14,14	0
26	ZN	F	101	1/1	0.99	0.02	19,19,19,19	0
26	ZN	S	101	1/1	0.99	0.02	18,18,18,18	0
21	CUA	B	302	2/2	0.99	0.03	14,14,14,15	0
15	CU	N	603	1/1	0.99	0.04	14,14,14,14	0
15	CU	A	603	1/1	1.00	0.07	15,15,15,15	0

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

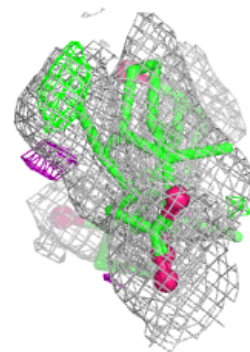
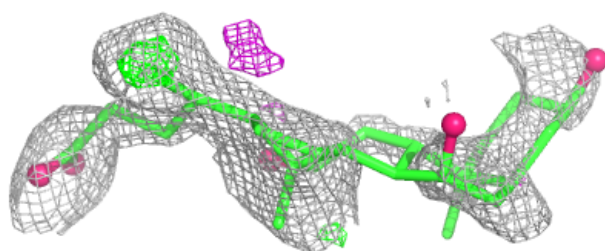
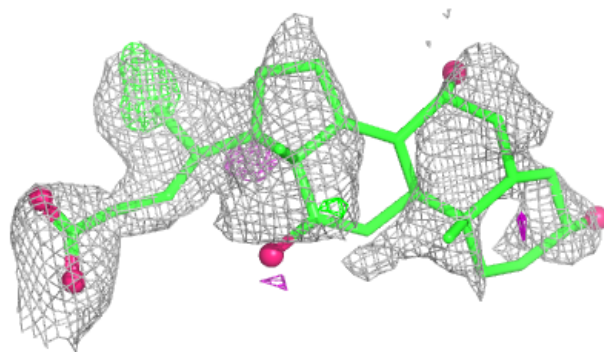
Electron density around CHD J 101:

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

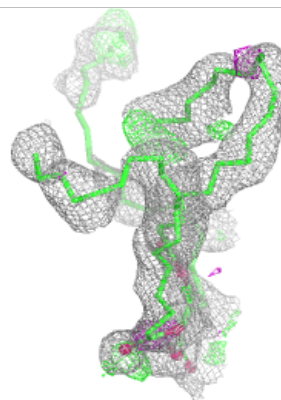
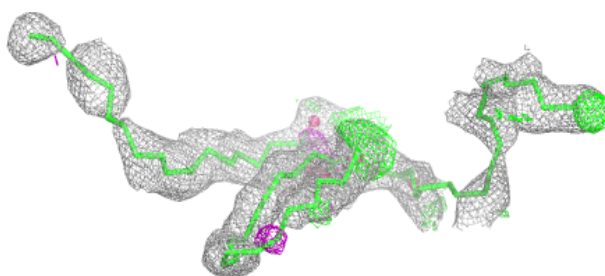
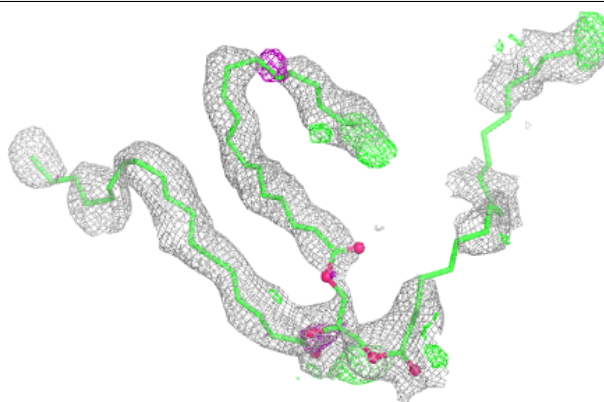


Electron density around CHD W 101:

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

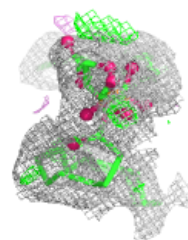
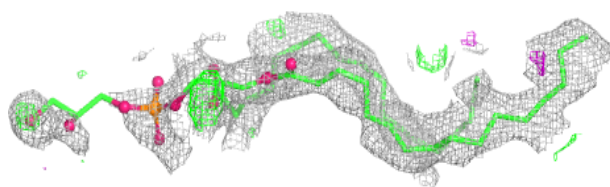
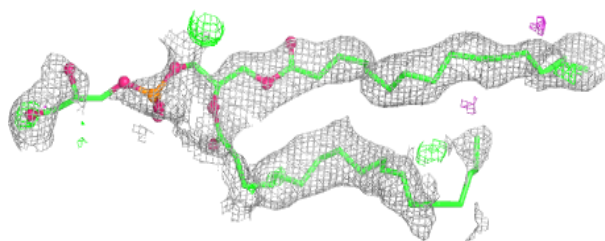
**Electron density around TGL Q 201:**

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



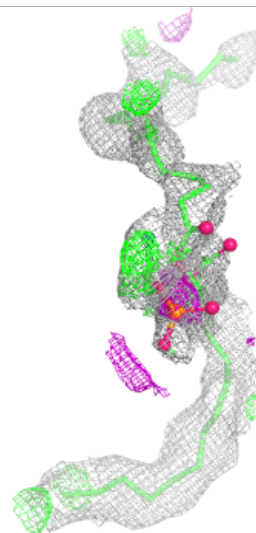
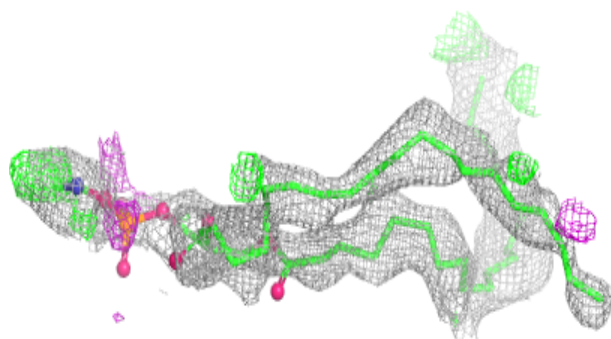
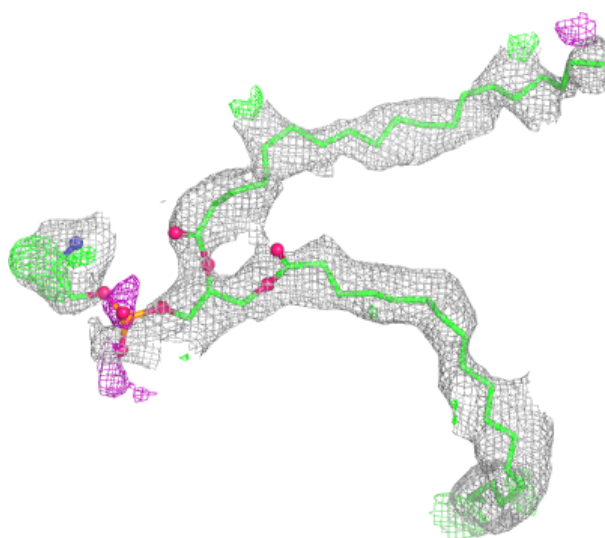
Electron density around PGV P 301:

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



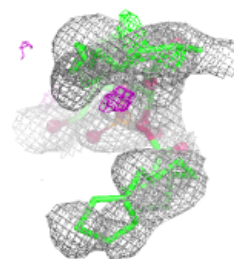
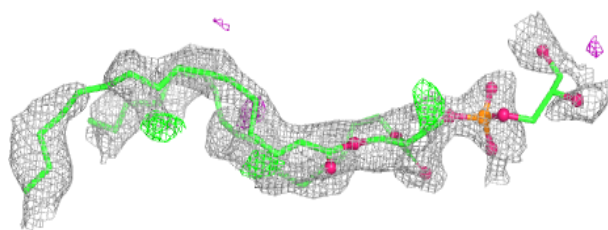
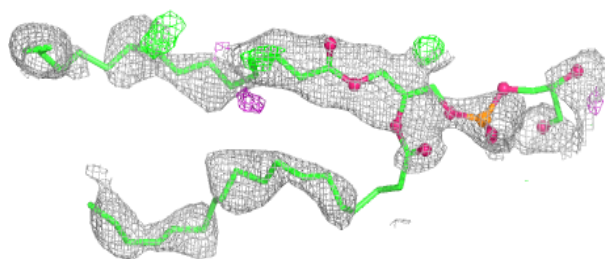
Electron density around PEK C 307:

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



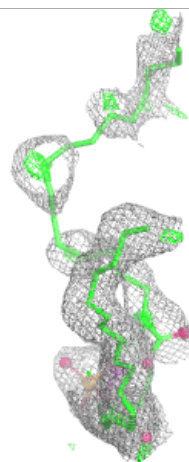
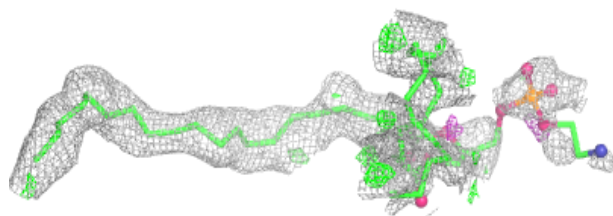
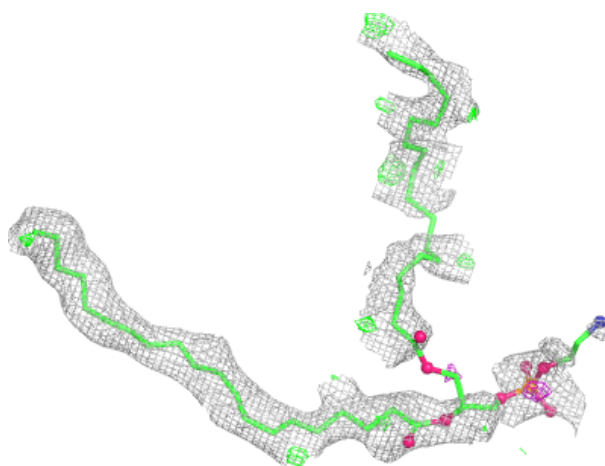
Electron density around PGV C 308:

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



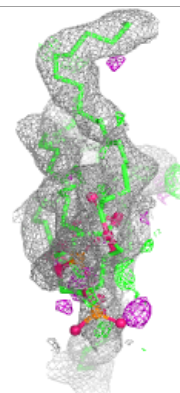
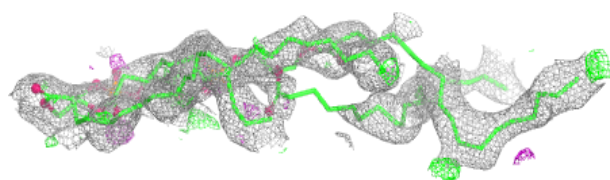
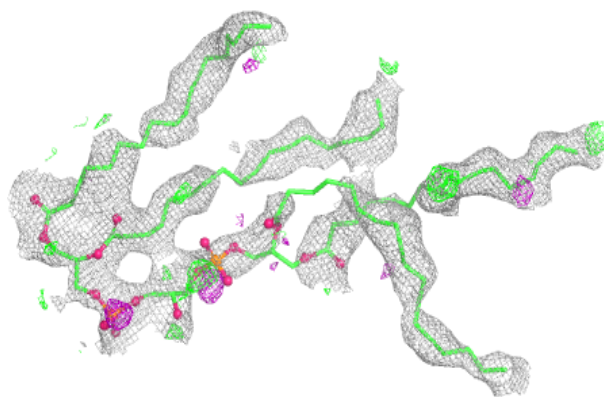
Electron density around PEK G 102:

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

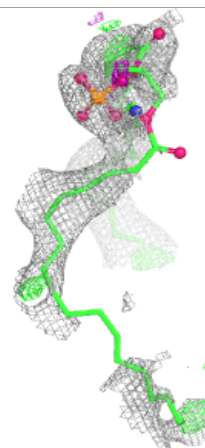
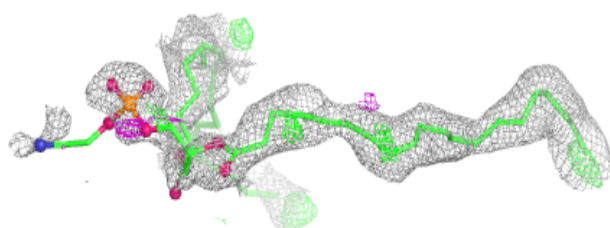
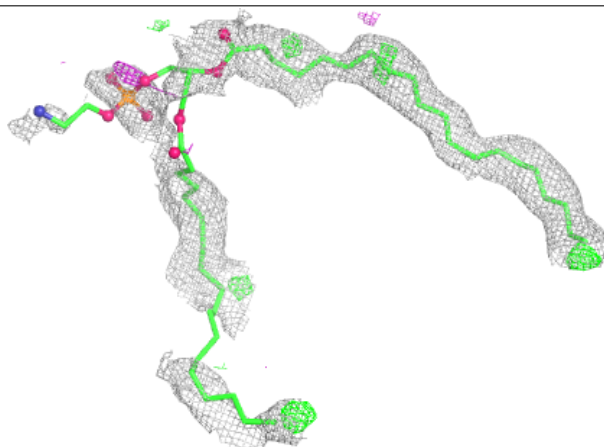


Electron density around CDL T 102:

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

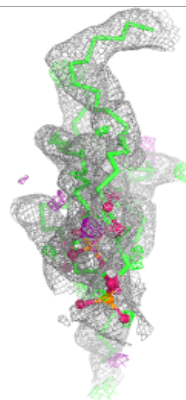
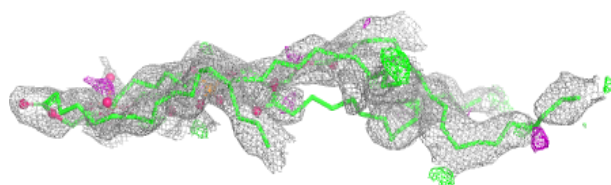
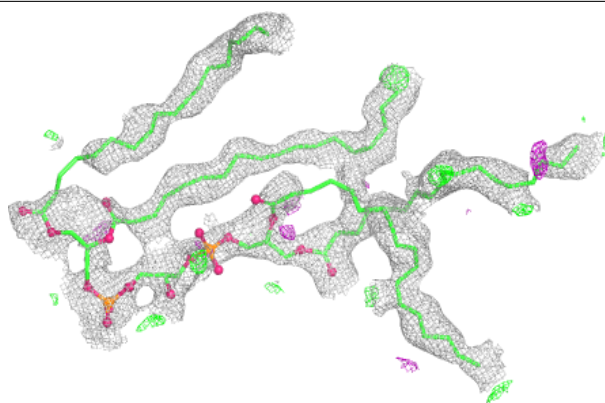
**Electron density around PEK T 101:**

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

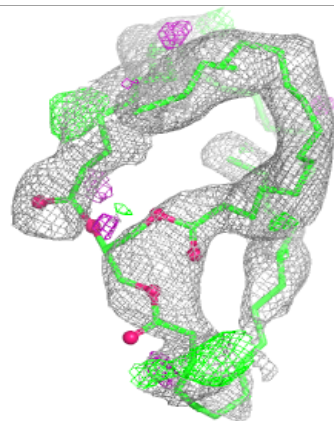
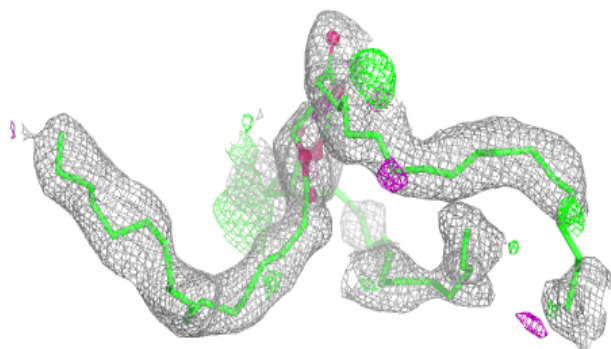
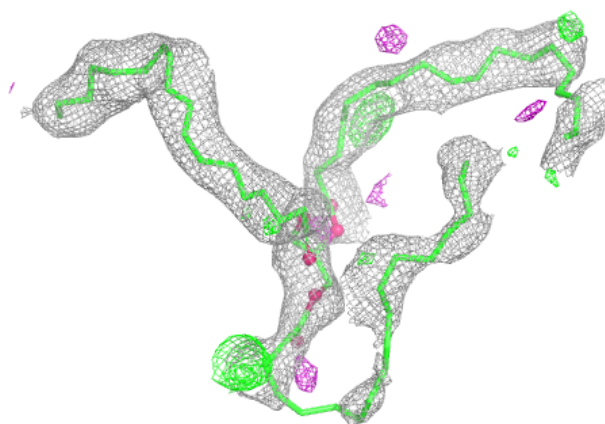


Electron density around CDL G 101:

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

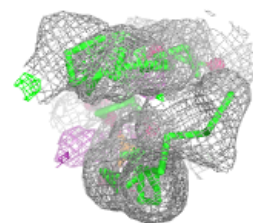
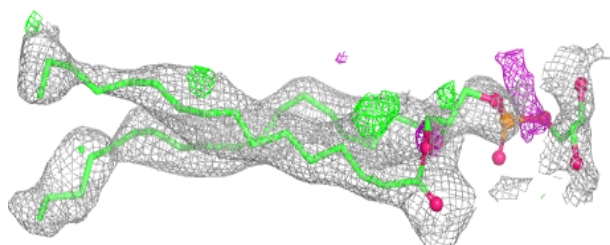
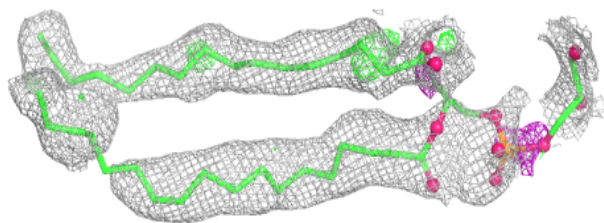
**Electron density around TGL Y 101:**

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

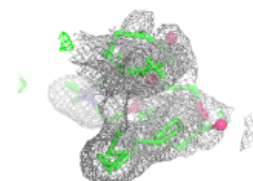
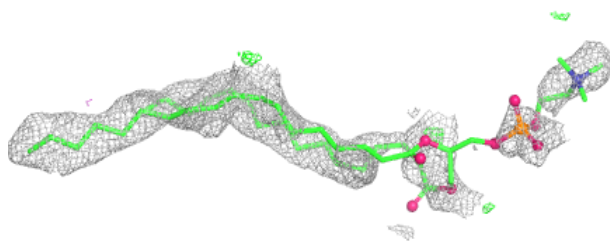
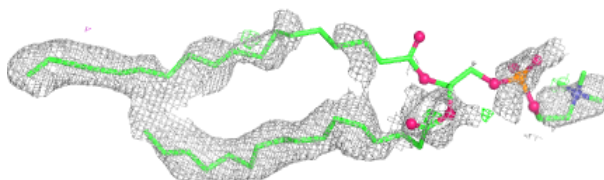


Electron density around PGV N 607:

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

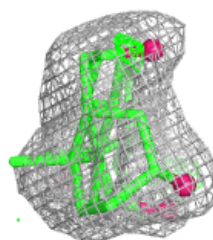
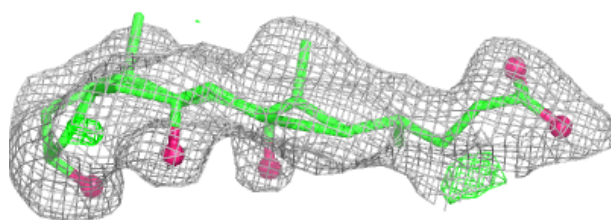
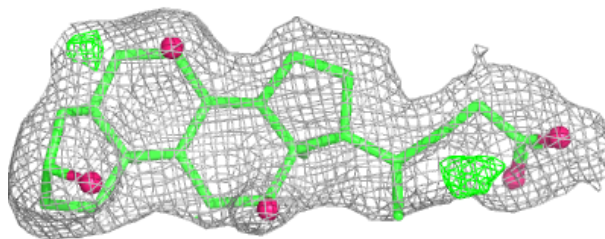
**Electron density around PSC B 304:**

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



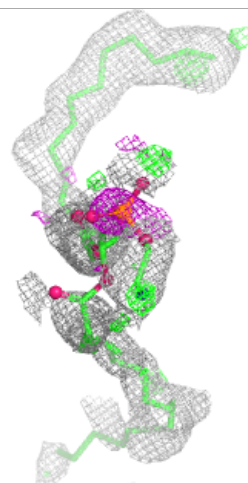
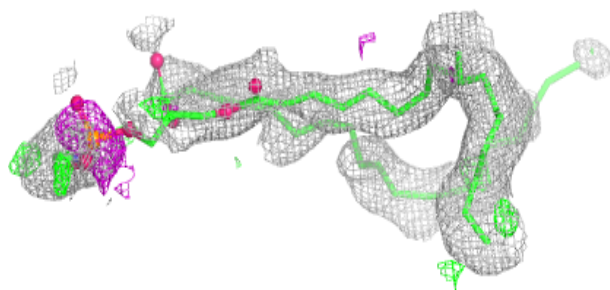
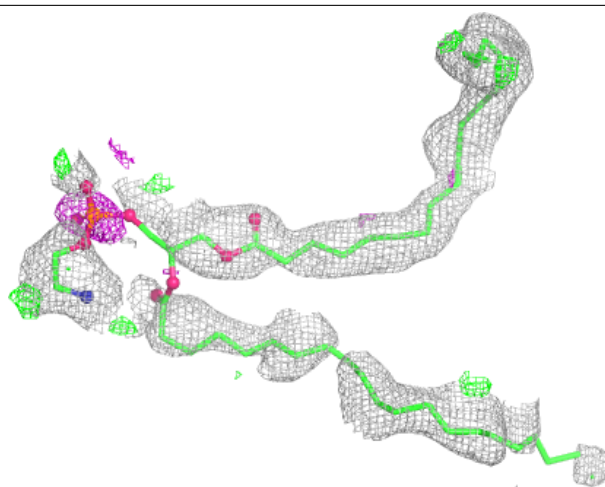
Electron density around CHD P 306:

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



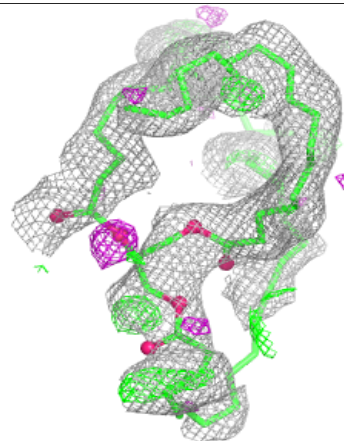
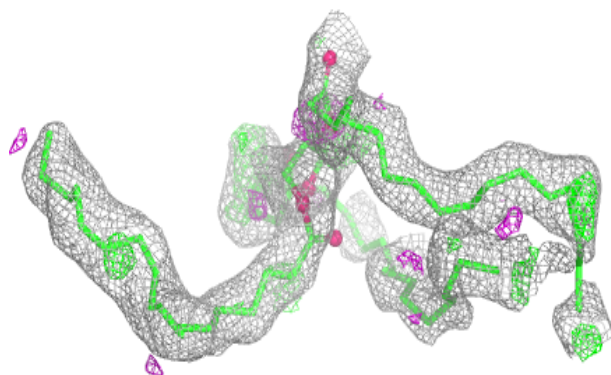
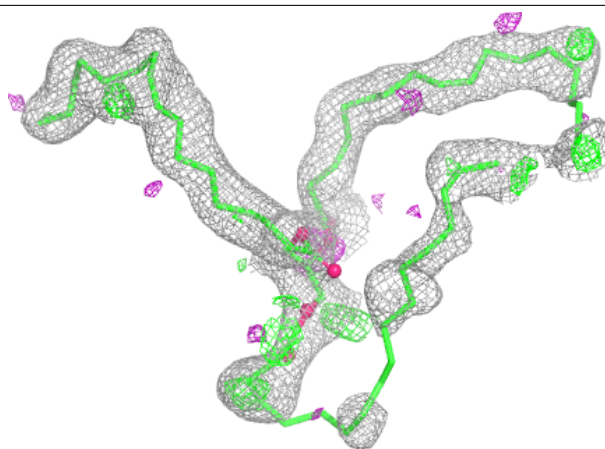
Electron density around PEK P 308:

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

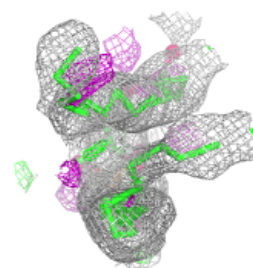
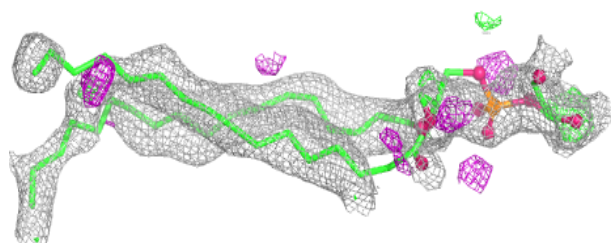
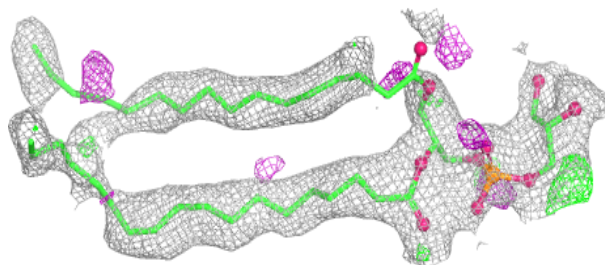


Electron density around TGL L 101:

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

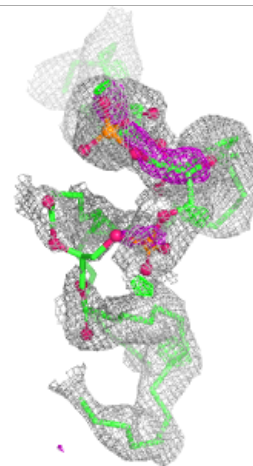
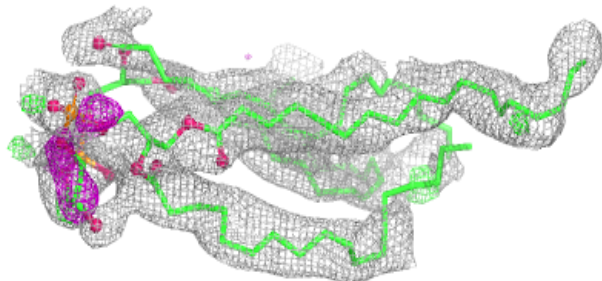
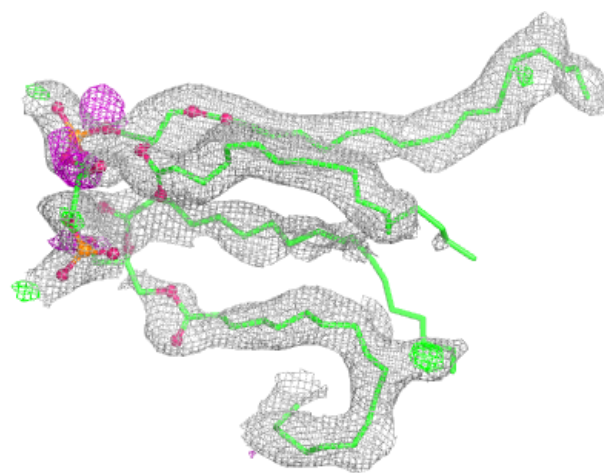
**Electron density around PGV A 608:**

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



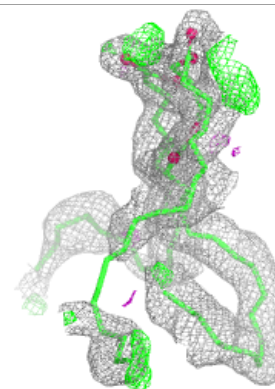
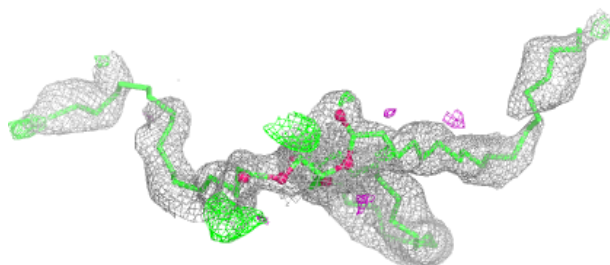
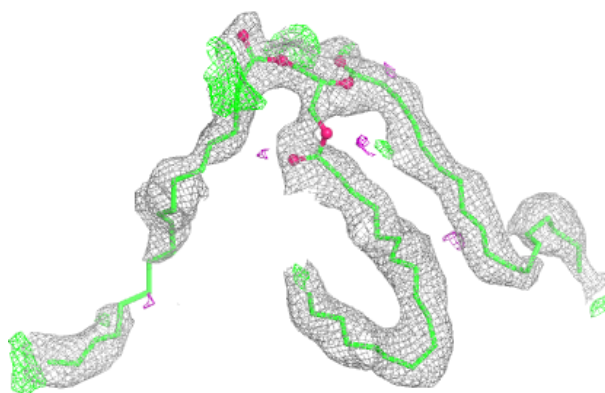
Electron density around CDL P 305:

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

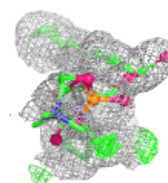
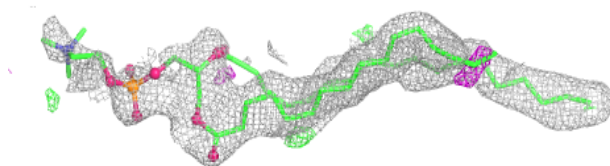
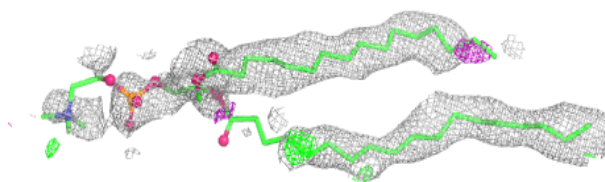


Electron density around TGL D 201:

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

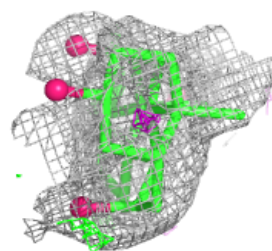
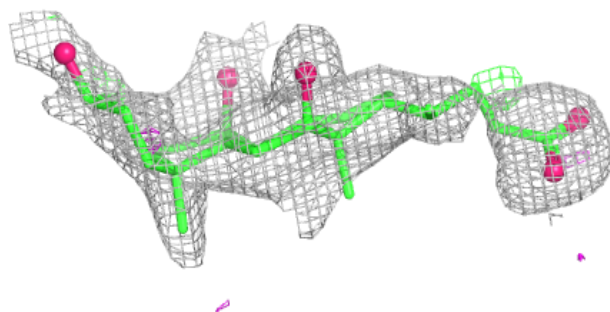
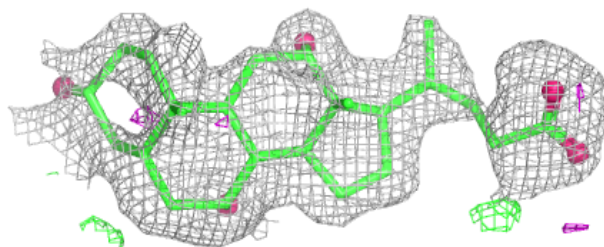
**Electron density around PSC N 610:**

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



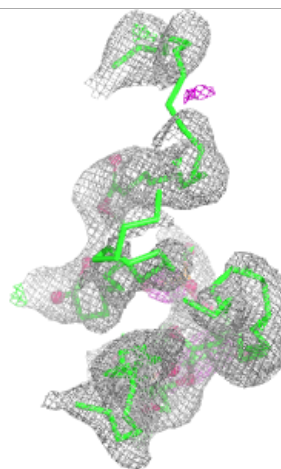
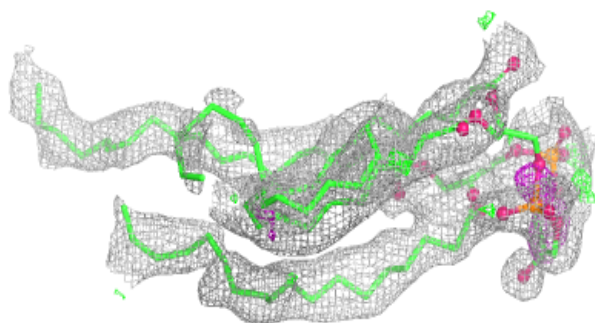
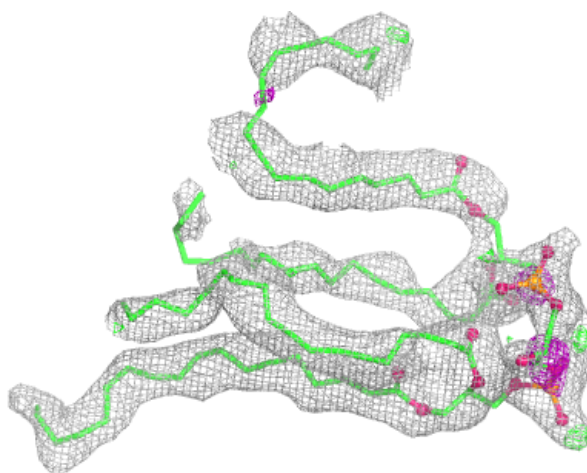
Electron density around CHD C 305:

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



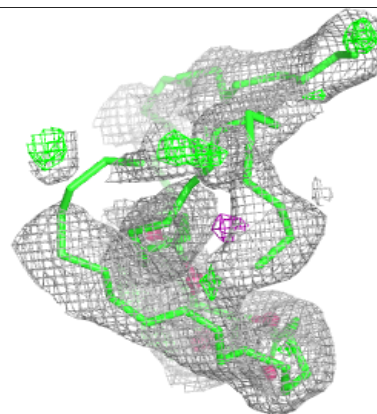
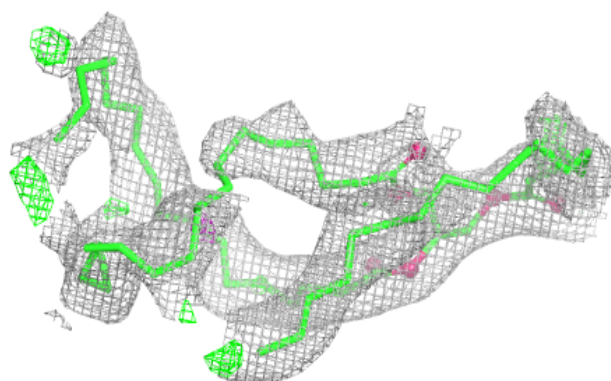
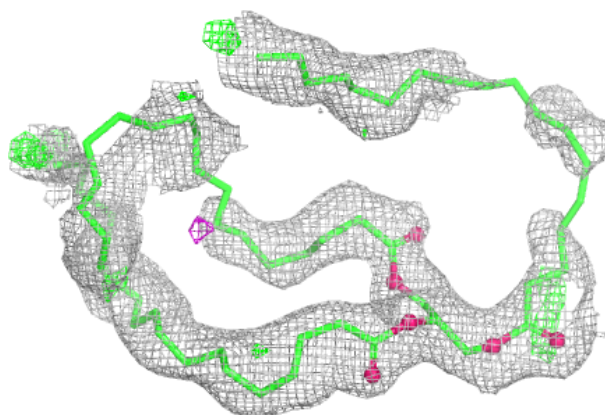
Electron density around CDL C 304:

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

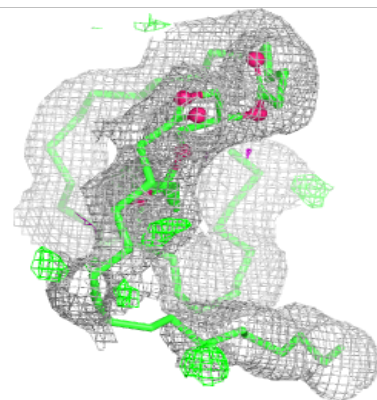
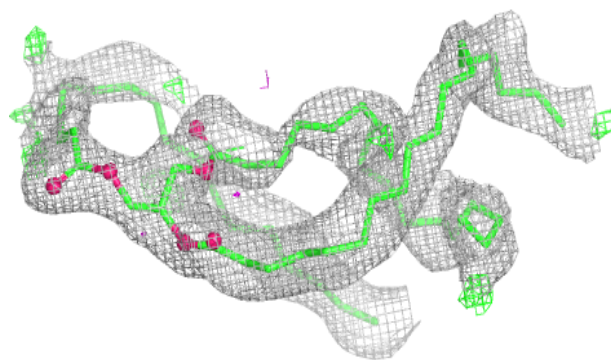
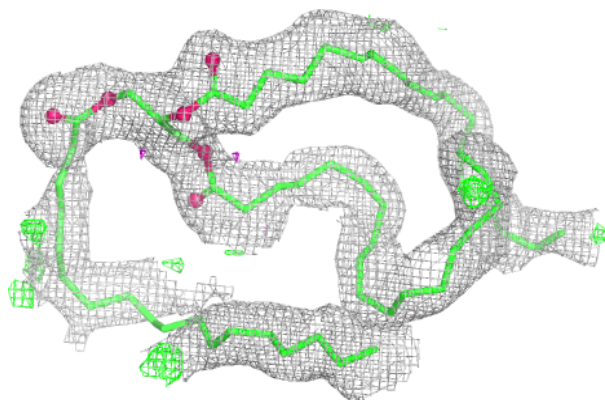


Electron density around TGL N 609:

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

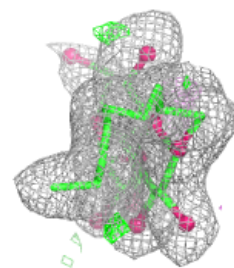
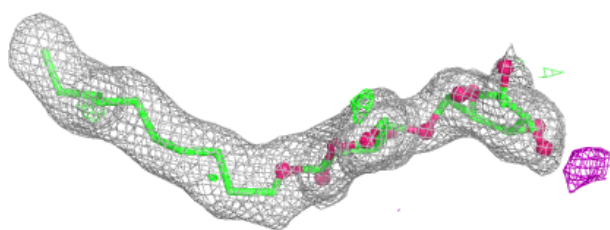
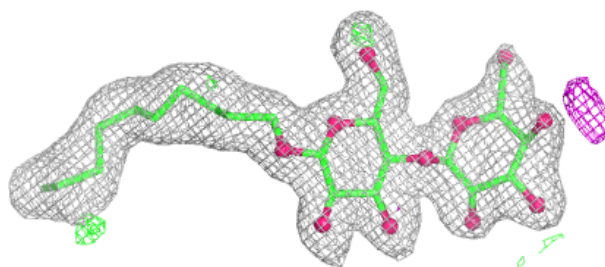
**Electron density around TGL B 301:**

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

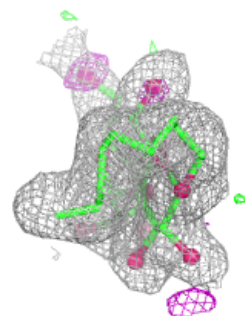
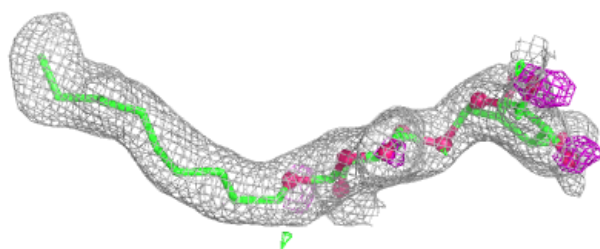
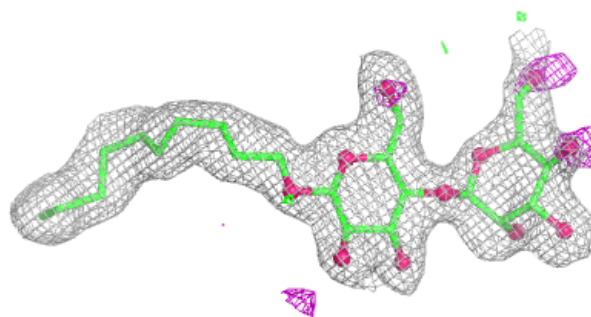


Electron density around DMU M 101:

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

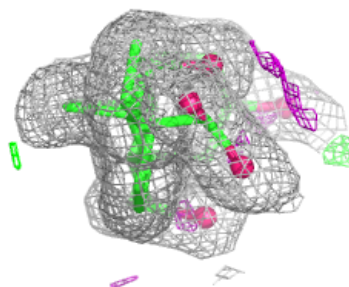
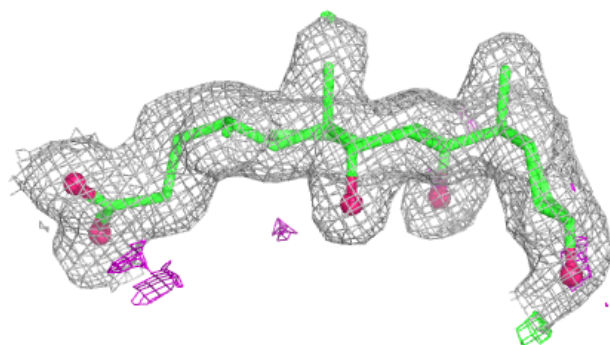
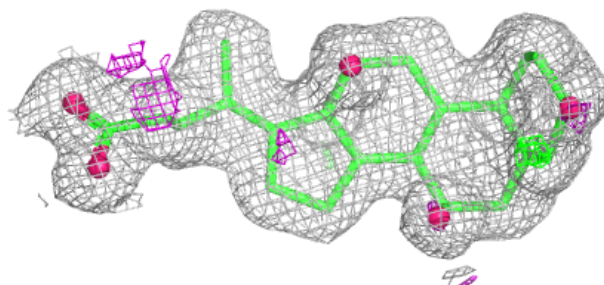
**Electron density around DMU Z 101:**

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

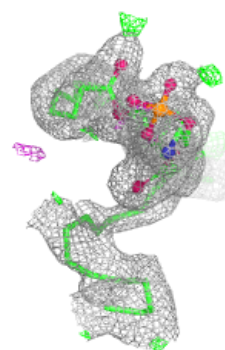
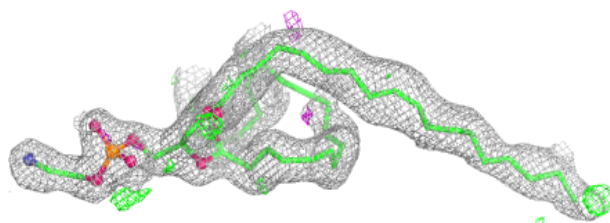
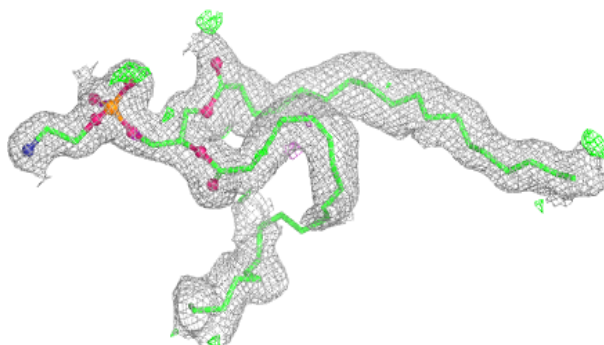


Electron density around CHD B 303:

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

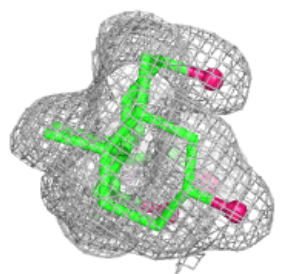
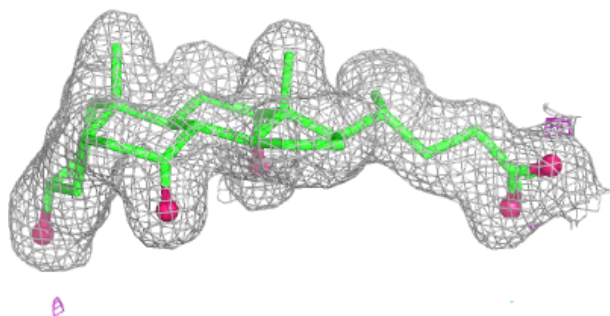
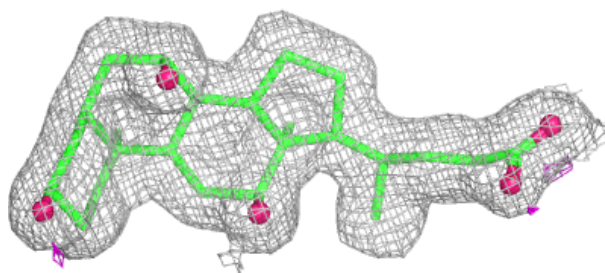
**Electron density around PEK P 303:**

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

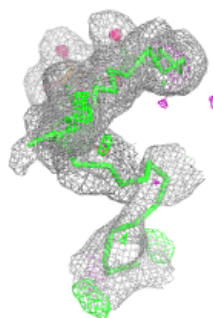
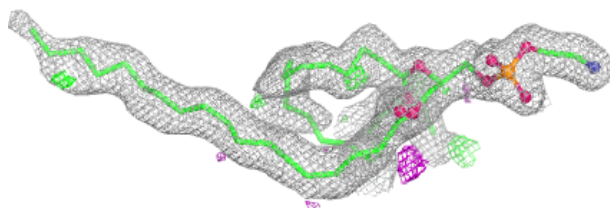
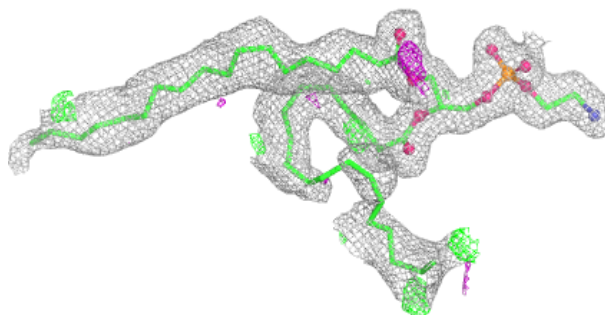


Electron density around CHD P 307:

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

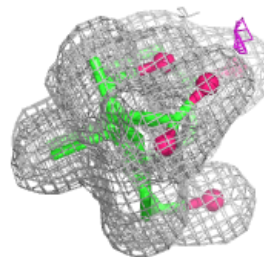
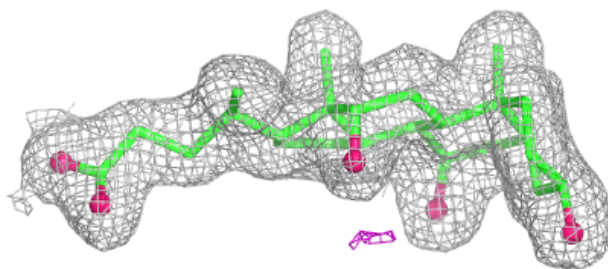
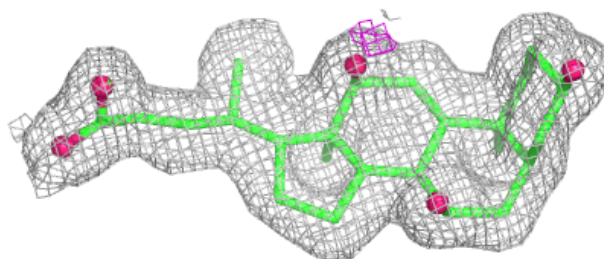
**Electron density around PEK C 302:**

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

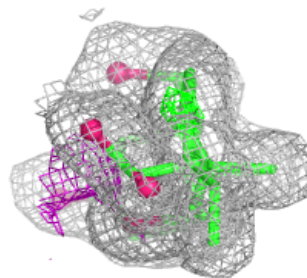
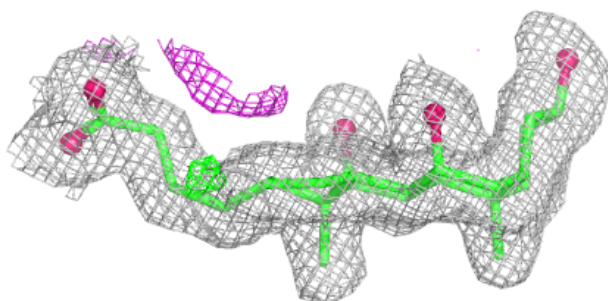
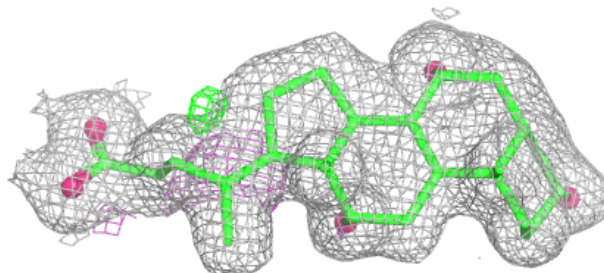


Electron density around CHD C 306:

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

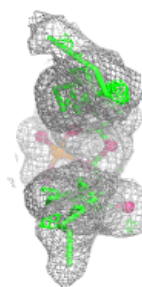
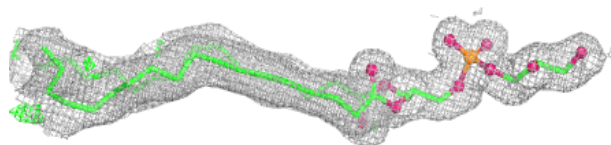
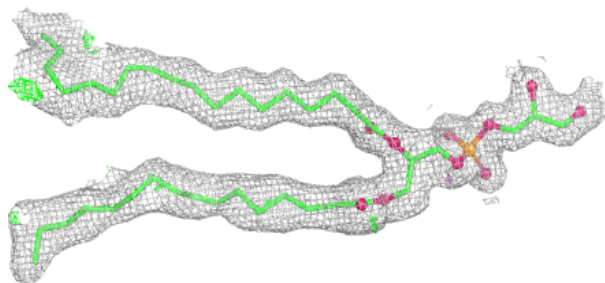
**Electron density around CHD G 103:**

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

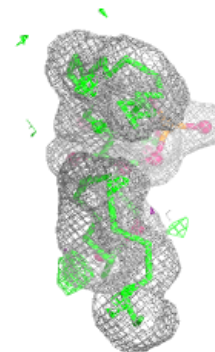
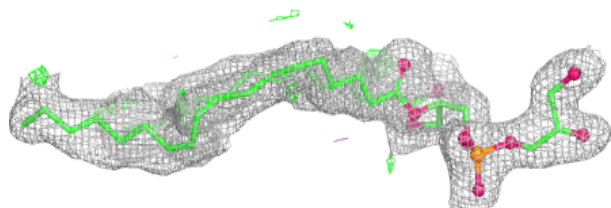
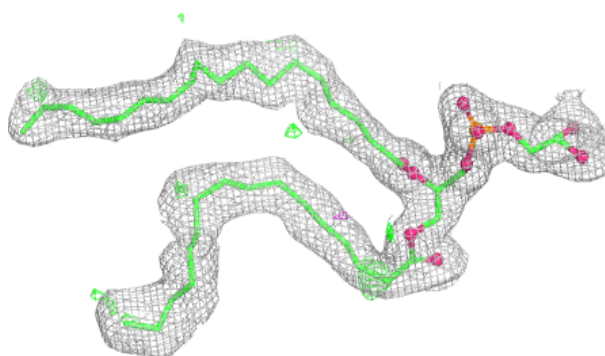


Electron density around PGV C 303:

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

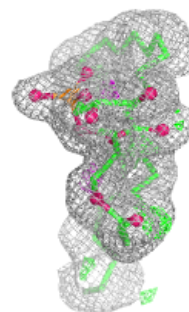
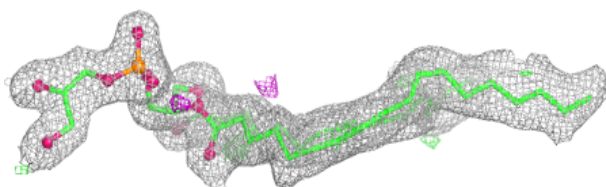
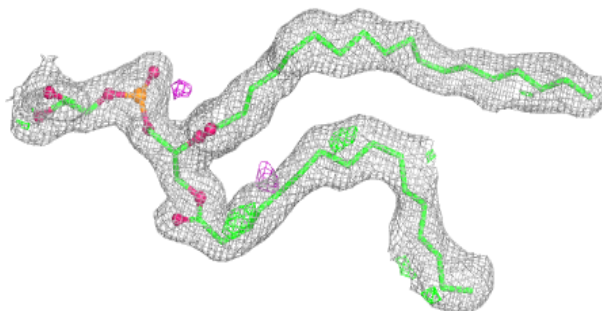
**Electron density around PGV N 608:**

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

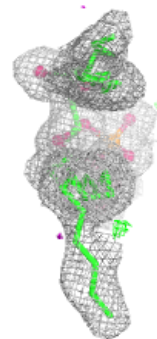
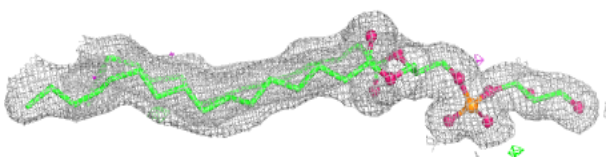
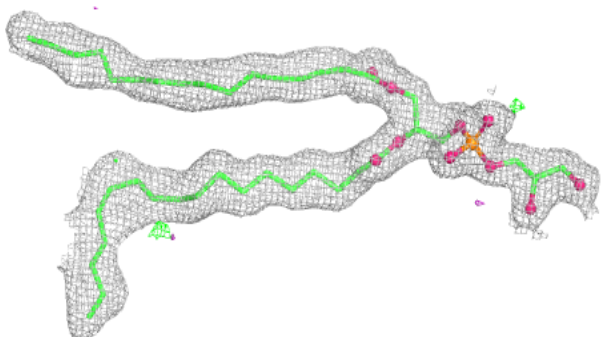


Electron density around PGV A 607:

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

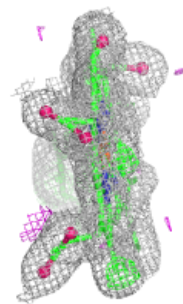
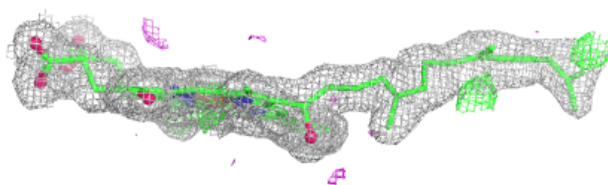
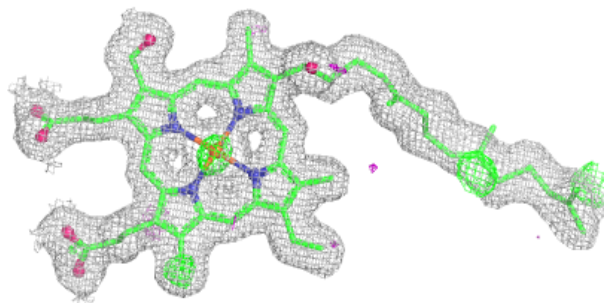
**Electron density around PGV P 304:**

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

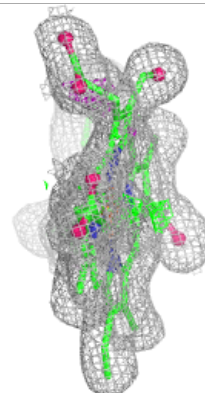
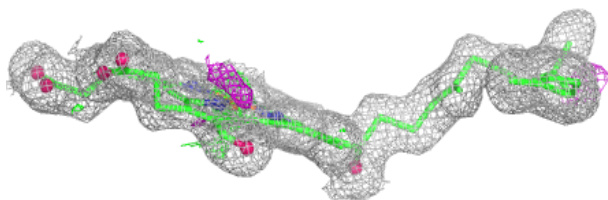
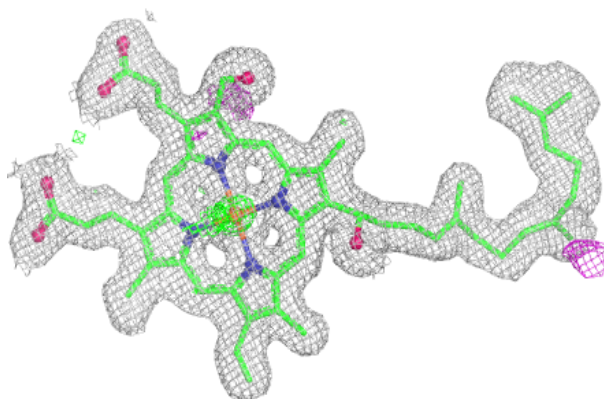


Electron density around HEA A 601:

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

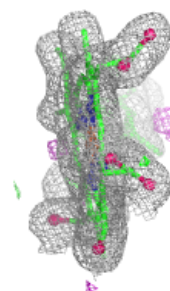
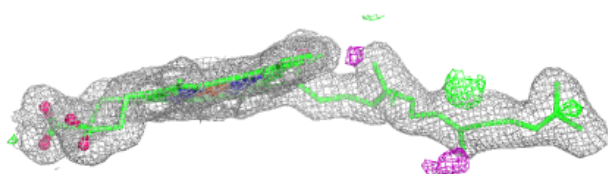
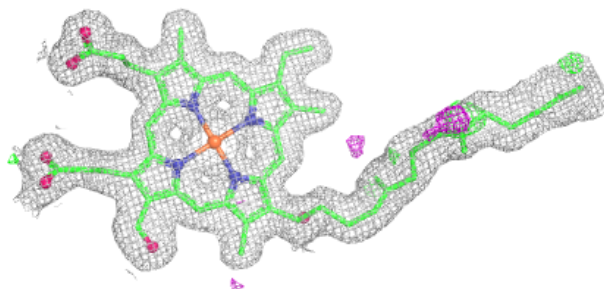
**Electron density around HEA A 602:**

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

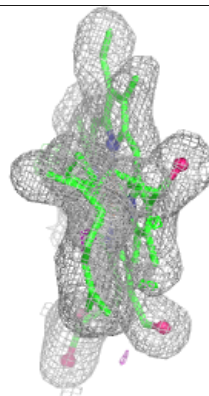
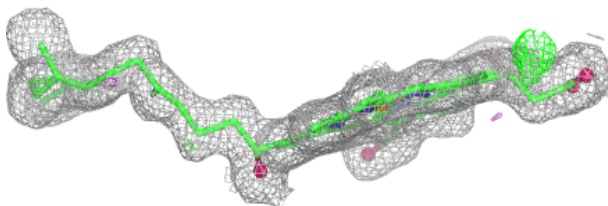
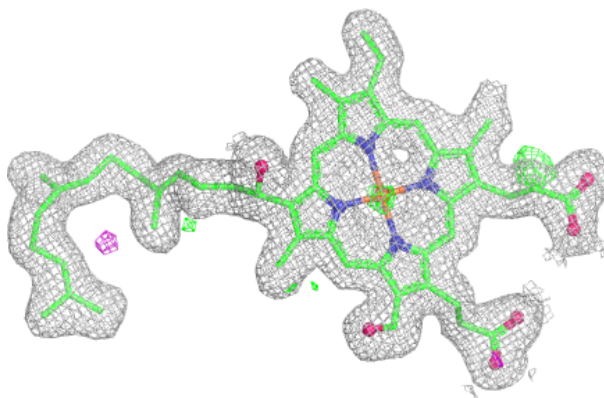


Electron density around HEA N 601:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.