



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:29 AM JST

PDB ID : 5ZCP / pdb_00005zcp
Title : azide-bound cytochrome c oxidase structure determined using the crystals exposed to 20 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-02-19
Resolution : 1.65 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:

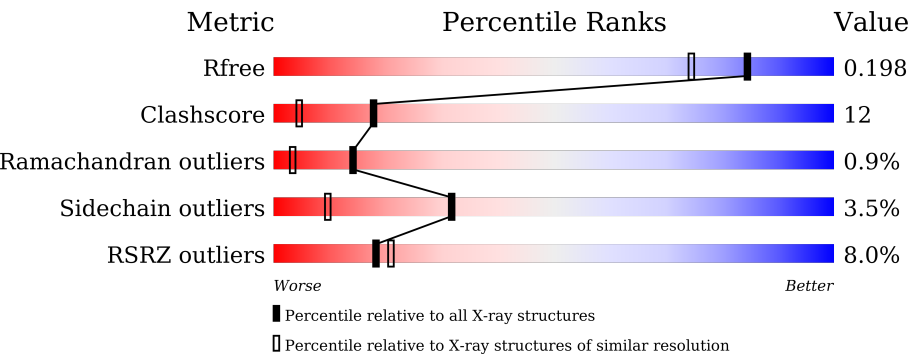
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	74% 22% .
1	N	514	67% 29% .
2	B	227	12% 64% 28% 7% .
2	O	227	11% 70% 26% .
3	C	261	3% 74% 24% ..
3	P	261	3% 73% 25% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
21	EDO	A	616	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	D	202	-	-	X	-
27	CDL	N	601	-	-	X	-
27	CDL	P	305	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33609 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	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

- 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	9	0
			1899	1234	292	353	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

- 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	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- 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	4	0
			1233	803	204	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	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	1	0
			863	550	148	163	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	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0

- 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	1	0
			469	302	79	85	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	1	0
			391	255	66	68	2			

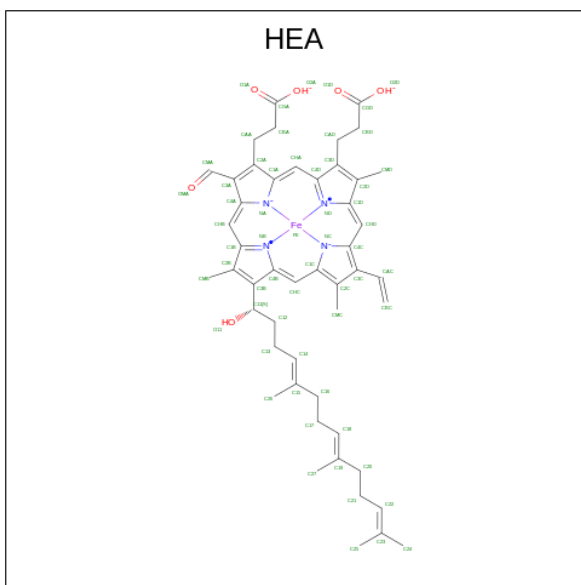
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	1	0
			388	259	65	61	3			

- 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 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

- 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		

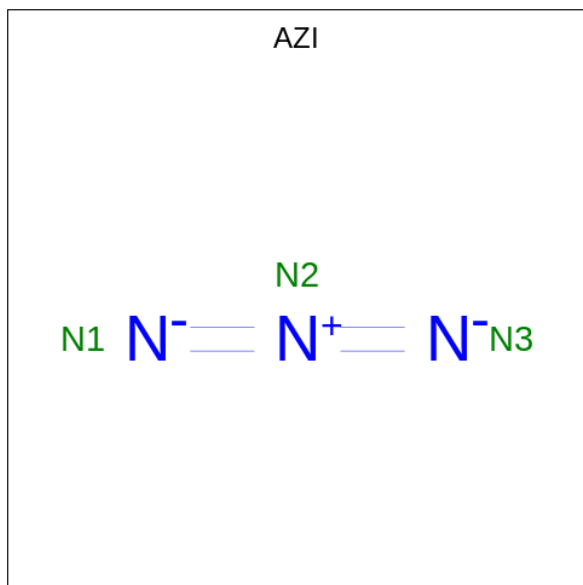
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

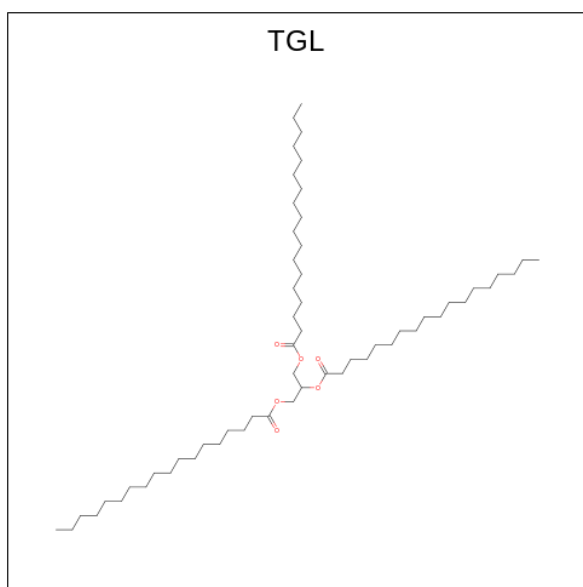
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (CCD ID: AZI) (formula: N₃).



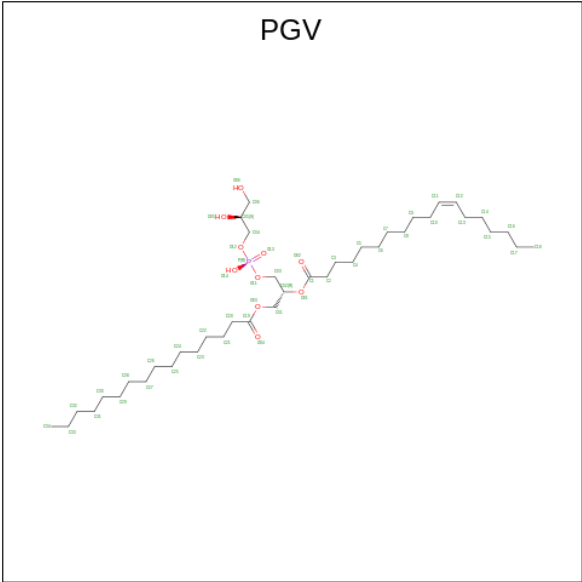
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

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



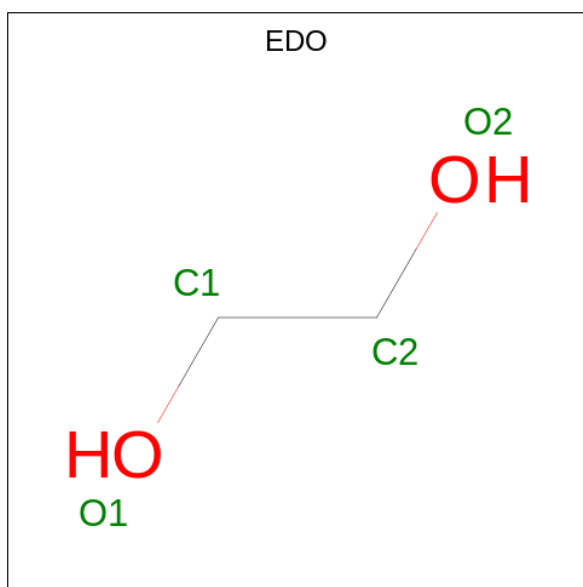
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		

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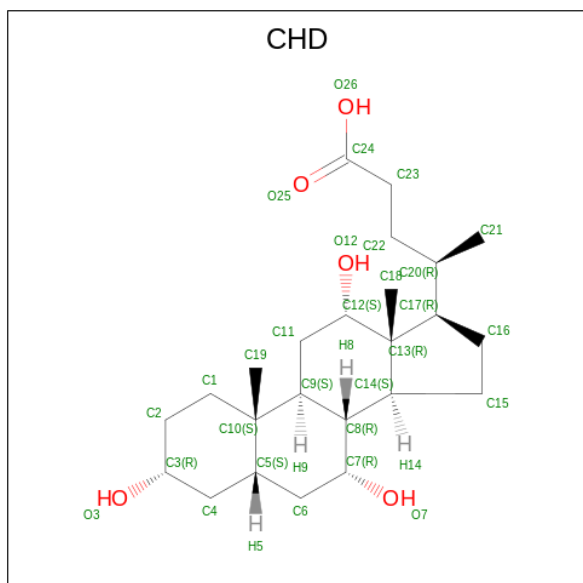
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	M	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



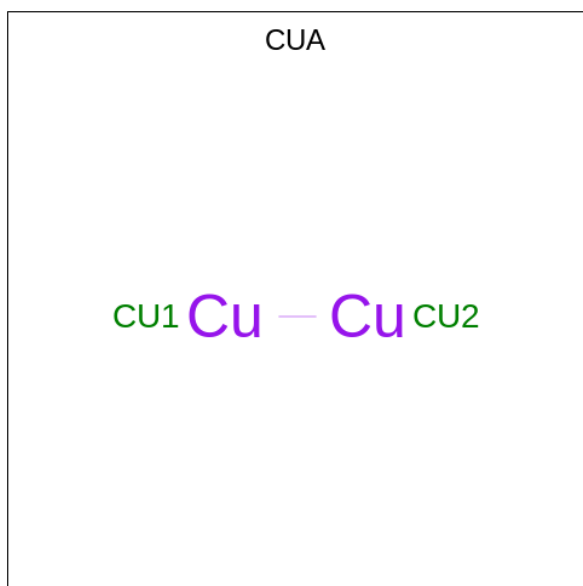
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		

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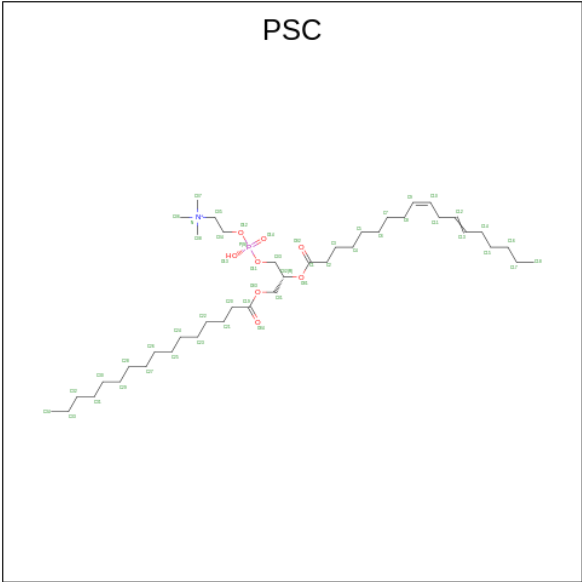
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	G	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



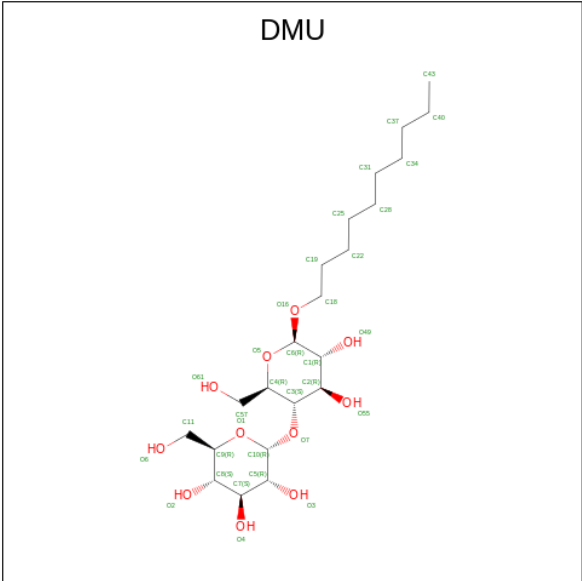
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0
23	O	1	Total Cu 2 2	0	0

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		

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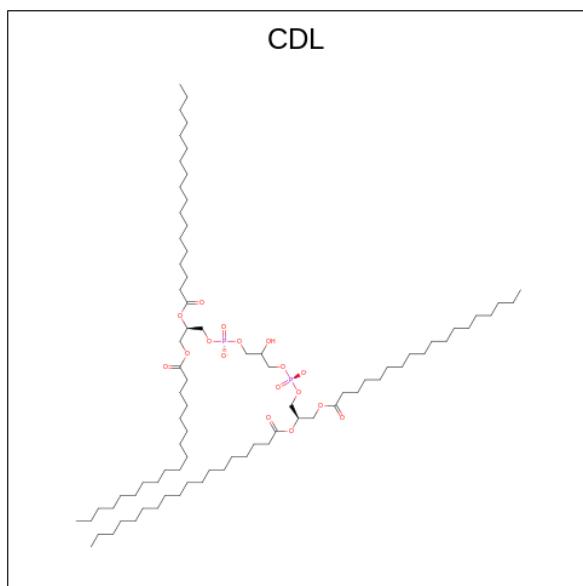
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O 33 22 11	0	0
25	C	1	Total C O 33 22 11	0	0
25	M	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	P	1	Total C O 33 22 11	0	0
25	Z	1	Total C O 33 22 11	0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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

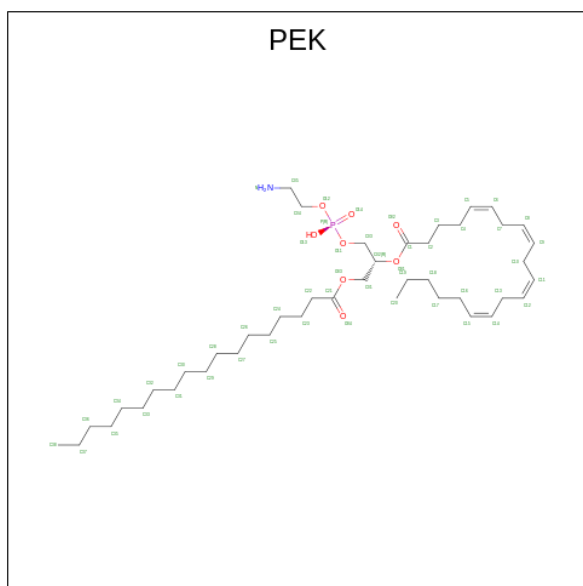
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total X 1 1	0	0
26	P	1	Total X 1 1	0	0

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 28 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	235	Total 235	O 235	0	0
30	B	161	Total 162	O 162	0	1
30	C	110	Total 110	O 110	0	0
30	D	118	Total 118	O 118	0	0
30	E	93	Total 93	O 93	0	0
30	F	94	Total 94	O 94	0	0
30	G	42	Total 42	O 42	0	0
30	H	42	Total 42	O 42	0	0
30	I	27	Total 27	O 27	0	0
30	J	23	Total 23	O 23	0	0
30	K	26	Total 26	O 26	0	0
30	L	38	Total 38	O 38	0	0
30	M	25	Total 25	O 25	0	0
30	N	203	Total 203	O 203	0	0
30	O	99	Total 100	O 100	0	1
30	P	95	Total 95	O 95	0	0
30	Q	29	Total 29	O 29	0	0
30	R	40	Total 40	O 40	0	0

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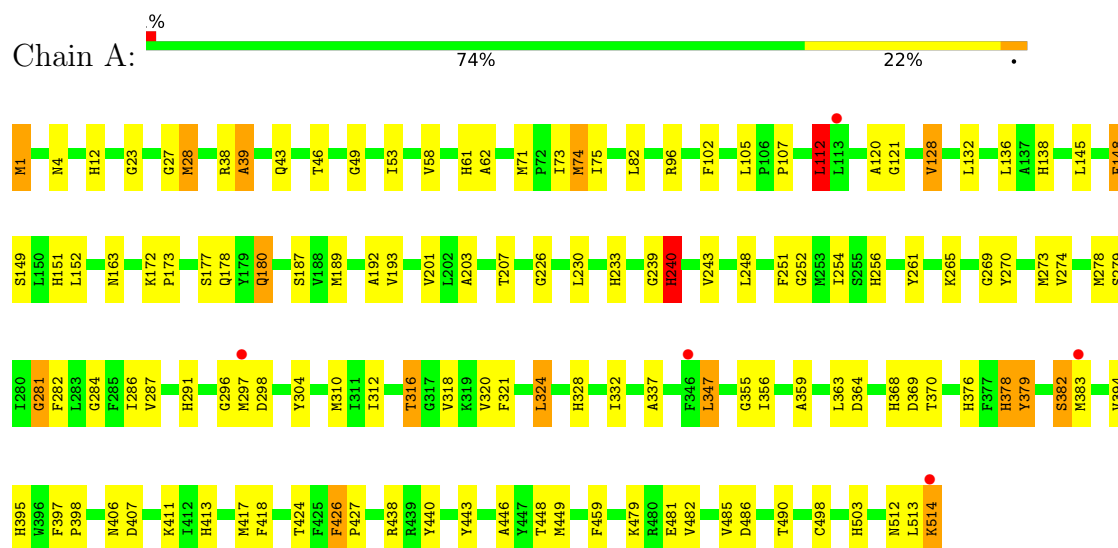
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	45	Total 45	O 45	0	0
30	T	35	Total 35	O 35	0	0
30	U	29	Total 29	O 29	0	0
30	V	16	Total 16	O 16	0	0
30	W	7	Total 7	O 7	0	0
30	X	11	Total 11	O 11	0	0
30	Y	12	Total 12	O 12	0	0
30	Z	12	Total 12	O 12	0	0

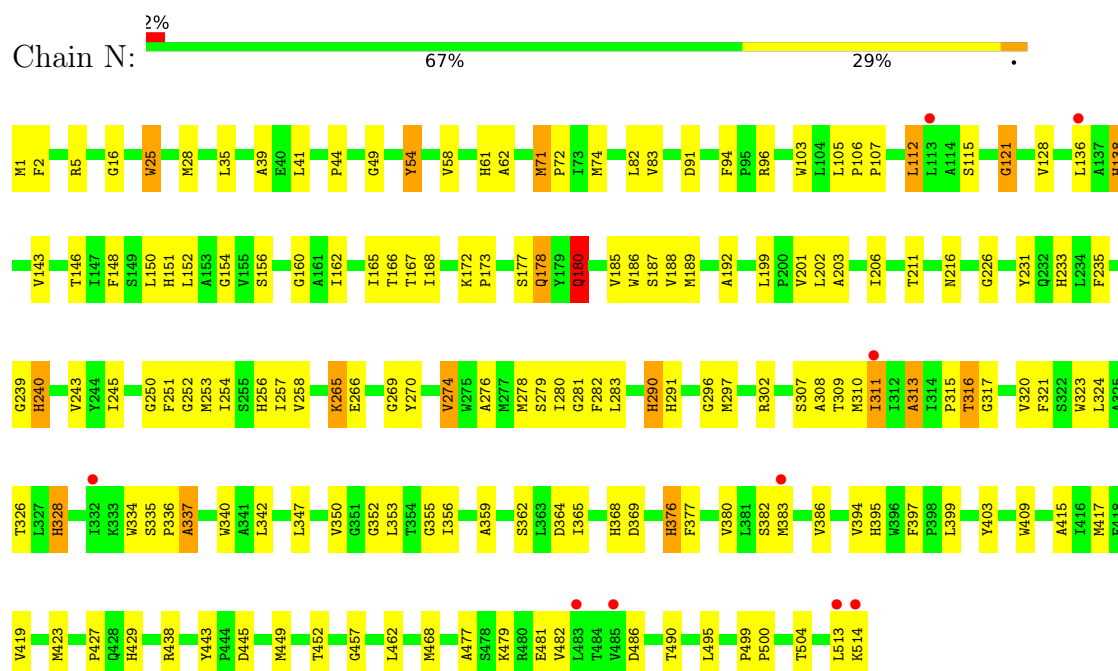
3 Residue-property plots

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.

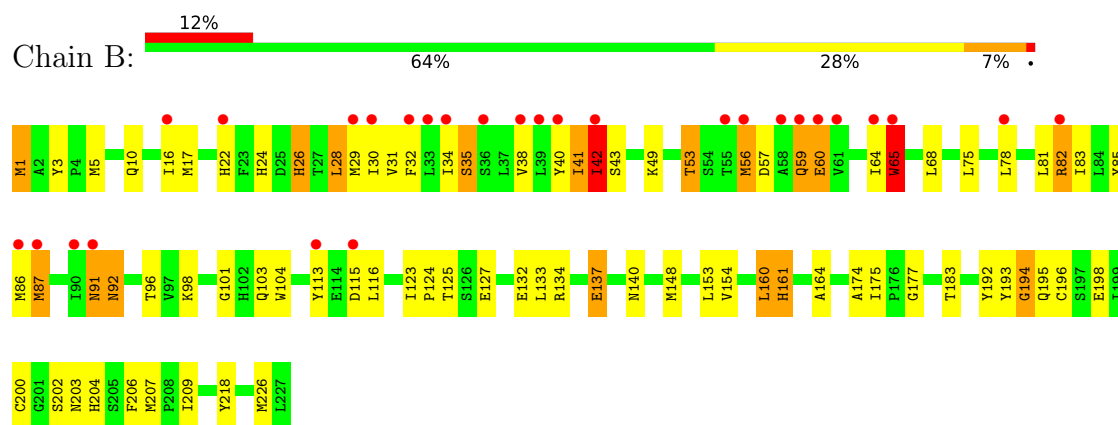
• Molecule 1: Cytochrome c oxidase subunit 1



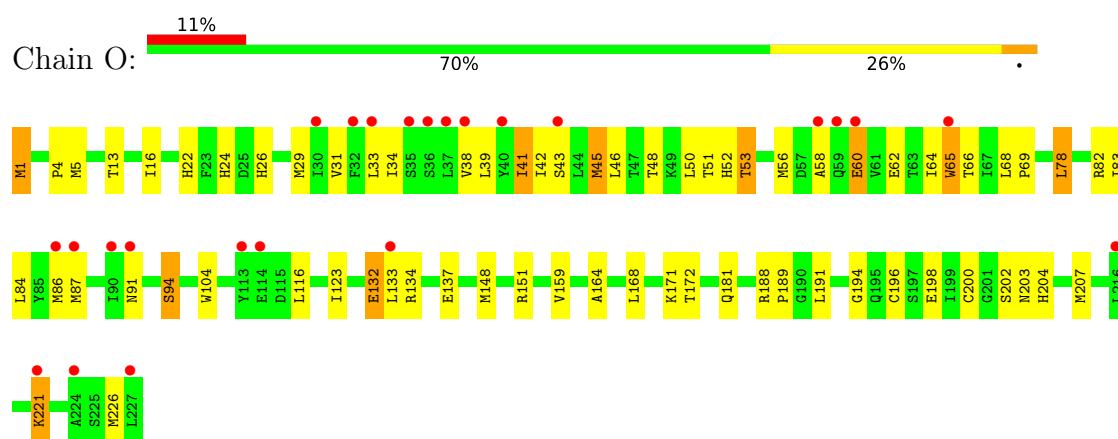
• Molecule 1: Cytochrome c oxidase subunit 1



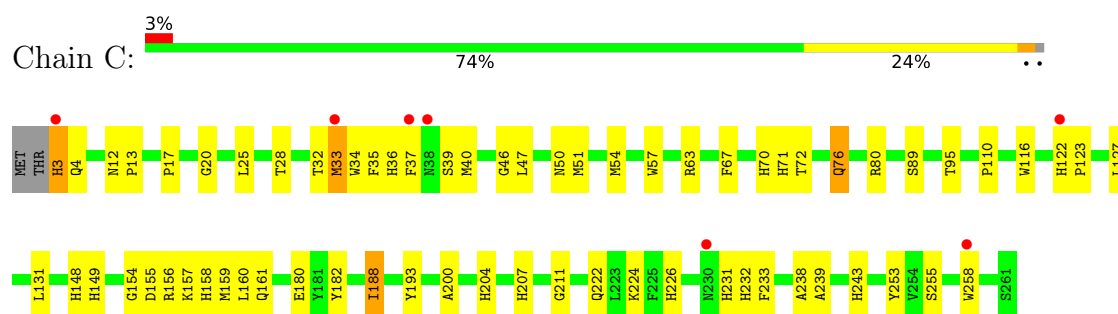
- Molecule 2: Cytochrome c oxidase subunit 2



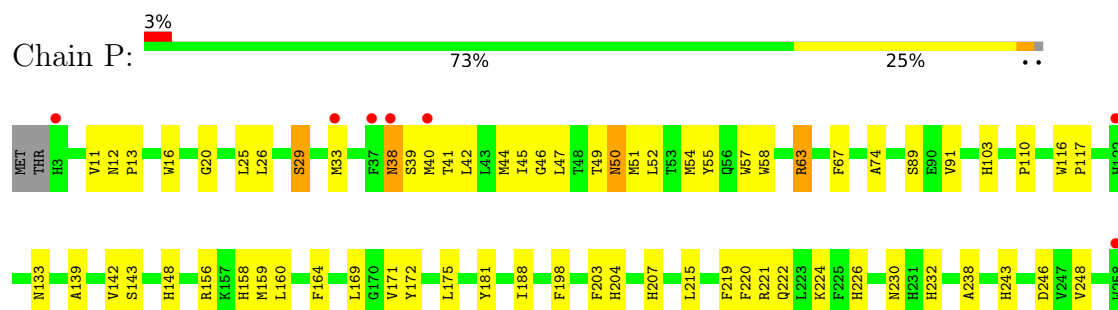
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

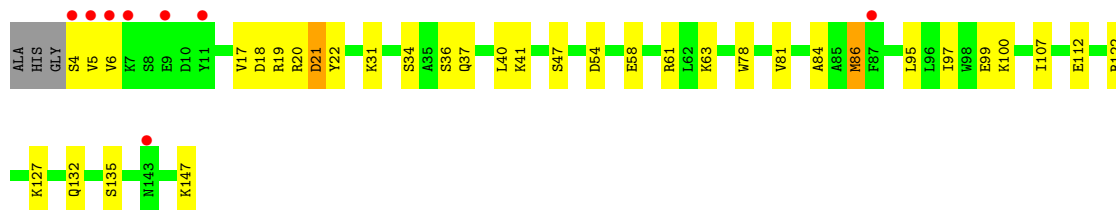
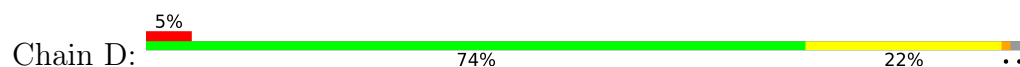


- Molecule 3: Cytochrome c oxidase subunit 3

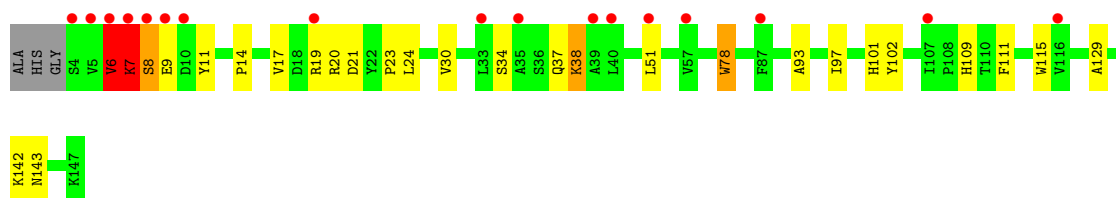
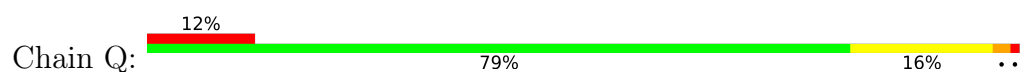




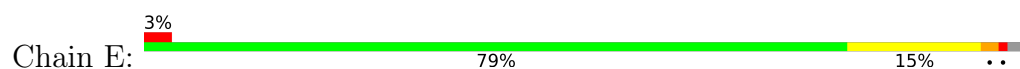
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



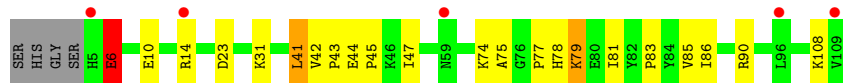
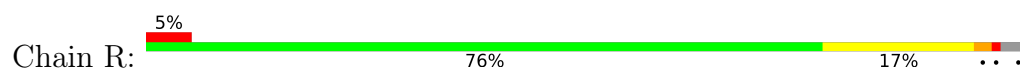
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



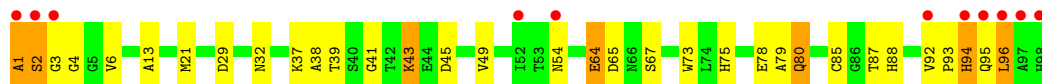
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



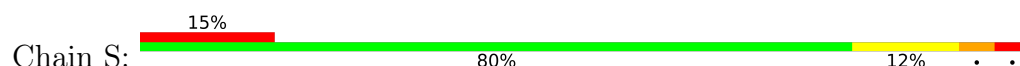
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

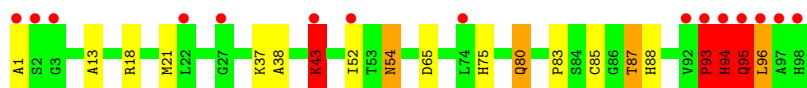


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

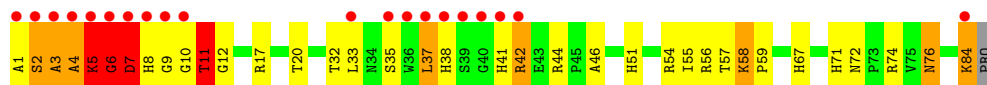


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

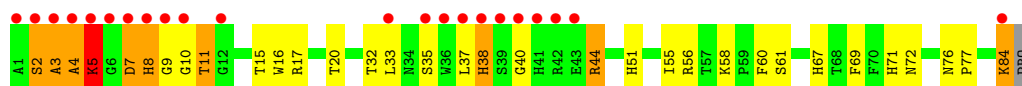




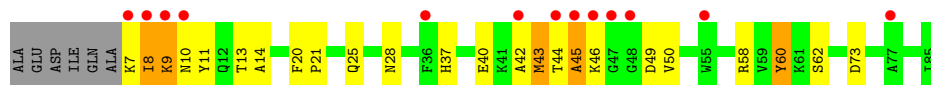
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



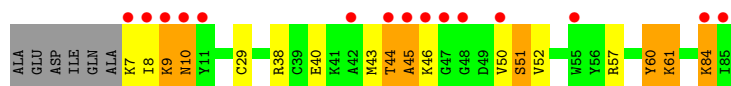
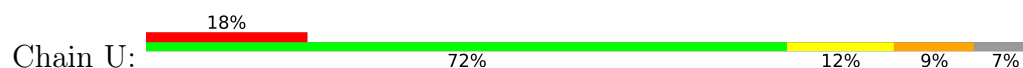
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



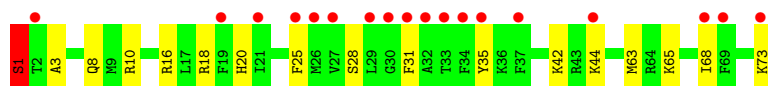
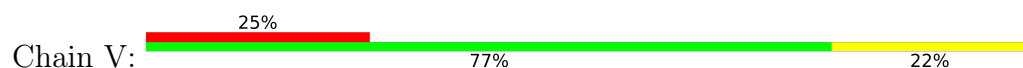
- Molecule 8: Cytochrome c oxidase subunit 6B1



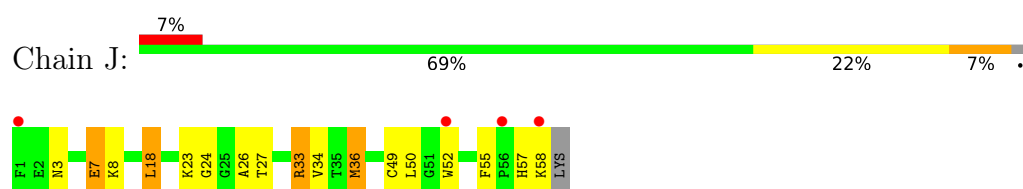
- Molecule 9: Cytochrome c oxidase subunit 6C



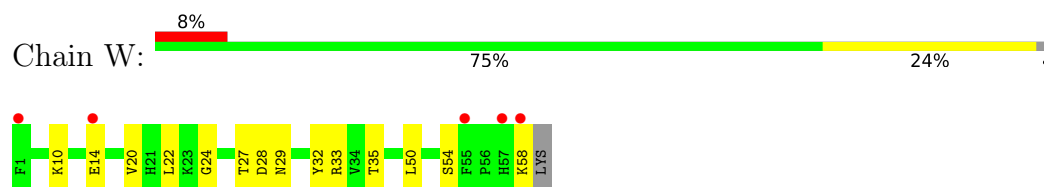
- Molecule 9: Cytochrome c oxidase subunit 6C



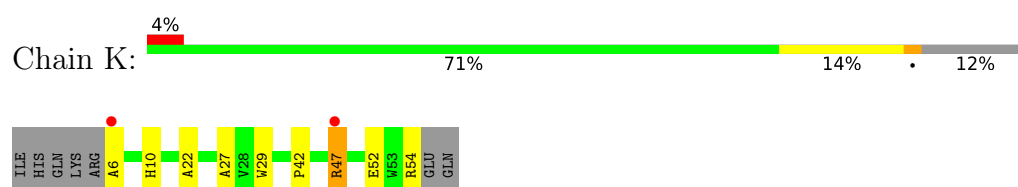
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



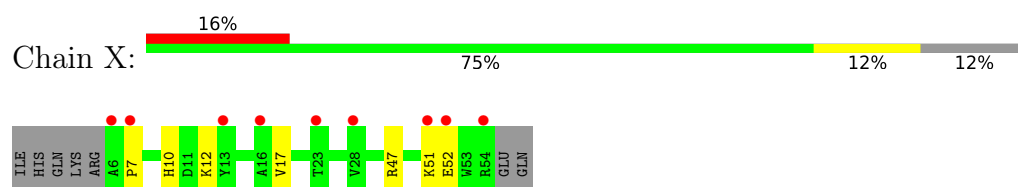
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



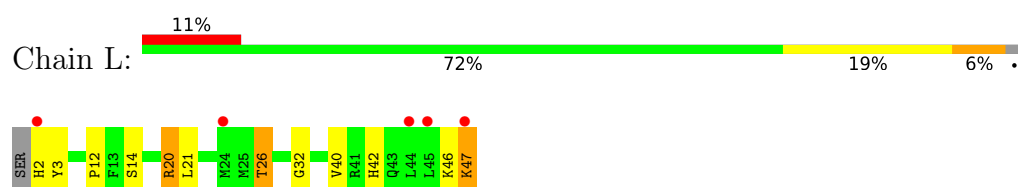
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



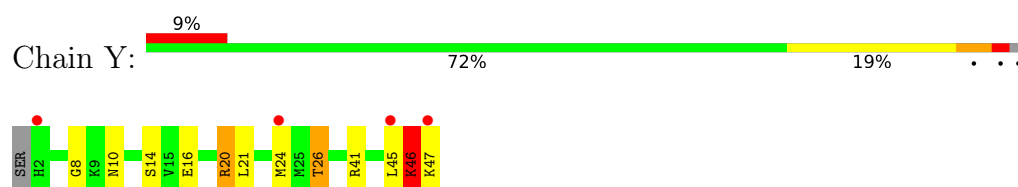
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



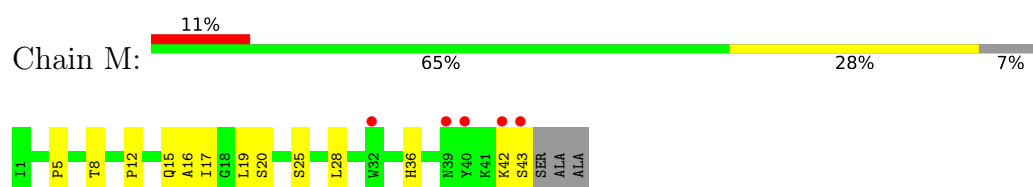
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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

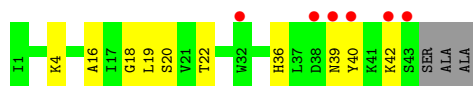


- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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

Chain Z:  13% 72% 22% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.32Å 206.17Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 40.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.65) 99.5 (40.00-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.175 , 0.197 0.177 , 0.198	Depositor DCC
R_{free} test set	39973 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: HEA, PEK, AZI, PSC, EDO, TGL, CU, CUA, FME, UNX, ZN, MG, SAC, DMU, NA, CDL, TPO, CHD, PGV

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	1.96	71/4322 (1.6%)	1.63	38/5897 (0.6%)
1	N	1.97	101/4308 (2.3%)	1.62	52/5878 (0.9%)
2	B	1.89	38/1937 (2.0%)	1.52	22/2637 (0.8%)
2	O	1.64	22/1908 (1.2%)	1.34	8/2597 (0.3%)
3	C	1.85	42/2272 (1.8%)	1.43	6/3102 (0.2%)
3	P	1.93	46/2272 (2.0%)	1.49	11/3102 (0.4%)
4	D	1.78	21/1268 (1.7%)	1.46	6/1709 (0.4%)
4	Q	1.41	8/1259 (0.6%)	1.25	5/1698 (0.3%)
5	E	1.85	13/871 (1.5%)	1.55	8/1182 (0.7%)
5	R	1.67	12/882 (1.4%)	1.39	2/1196 (0.2%)
6	F	1.80	13/795 (1.6%)	1.51	9/1079 (0.8%)
6	S	1.67	5/780 (0.6%)	1.45	2/1058 (0.2%)
7	G	1.95	14/702 (2.0%)	1.48	8/953 (0.8%)
7	T	1.95	19/702 (2.7%)	1.51	11/953 (1.2%)
8	H	1.59	7/682 (1.0%)	1.31	2/921 (0.2%)
8	U	1.29	1/682 (0.1%)	1.24	1/921 (0.1%)
9	I	1.57	5/605 (0.8%)	1.43	1/802 (0.1%)
9	V	1.33	1/605 (0.2%)	1.34	0/802
10	J	1.80	7/471 (1.5%)	1.44	3/636 (0.5%)
10	W	1.68	6/480 (1.2%)	1.38	2/648 (0.3%)
11	K	1.64	4/398 (1.0%)	1.29	1/546 (0.2%)
11	X	1.44	2/405 (0.5%)	1.20	0/556
12	L	1.77	4/393 (1.0%)	1.44	2/526 (0.4%)
12	Y	1.63	2/401 (0.5%)	1.29	2/536 (0.4%)
13	M	1.86	7/345 (2.0%)	1.37	0/470
13	Z	1.60	3/345 (0.9%)	1.28	2/470 (0.4%)
All	All	1.81	474/30090 (1.6%)	1.48	204/40875 (0.5%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	2
6	F	0	1
6	S	0	2
7	G	0	1
9	V	0	1
All	All	0	11

All (474) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	49	GLY	C-O	15.40	1.34	1.23
1	A	310	MET	SD-CE	-10.49	1.53	1.79
5	R	78	HIS	CE1-NE2	10.49	1.43	1.32
1	N	173	PRO	CA-CB	10.26	1.64	1.54
1	A	376	HIS	ND1-CE1	10.18	1.42	1.32
1	N	310	MET	SD-CE	-10.15	1.54	1.79
3	C	149	HIS	ND1-CE1	9.75	1.42	1.32
1	N	192	ALA	N-CA	9.61	1.58	1.46
7	G	51	HIS	ND1-CE1	9.59	1.42	1.32
1	A	482	VAL	CA-CB	9.47	1.64	1.54
2	B	53	THR	N-CA	9.35	1.58	1.45
1	A	61	HIS	ND1-CE1	9.25	1.41	1.32
1	A	270	TYR	N-CA	9.21	1.57	1.46
1	N	395	HIS	CE1-NE2	9.18	1.41	1.32
1	A	368	HIS	ND1-CE1	9.17	1.41	1.32
7	T	67	HIS	ND1-CE1	9.15	1.41	1.32
3	P	158	HIS	ND1-CE1	8.81	1.41	1.32
2	B	161	HIS	ND1-CE1	8.76	1.41	1.32
2	O	204	HIS	ND1-CE1	8.74	1.41	1.32
2	B	127	GLU	CA-C	-8.69	1.41	1.52
3	P	232	HIS	CG-CD2	8.52	1.45	1.35
3	P	226	HIS	CG-CD2	8.41	1.45	1.35
7	T	5	LYS	CA-C	8.40	1.64	1.52
3	C	158	HIS	ND1-CE1	8.30	1.40	1.32
11	K	10	HIS	CE1-NE2	8.29	1.40	1.32
1	N	258	VAL	C-O	8.26	1.33	1.24
7	G	5	LYS	CA-C	8.22	1.63	1.52
1	N	315	PRO	CA-CB	8.18	1.65	1.53
9	I	4	LEU	CA-CB	8.17	1.66	1.53
2	B	31	VAL	N-CA	-8.07	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	232	HIS	ND1-CE1	8.06	1.40	1.32
4	D	40	LEU	N-CA	8.06	1.56	1.46
3	P	20	GLY	N-CA	8.04	1.55	1.45
6	F	2	SER	CA-C	8.02	1.62	1.52
2	O	53	THR	N-CA	8.01	1.56	1.46
1	N	324	LEU	N-CA	7.99	1.55	1.46
1	N	83	VAL	CA-CB	7.96	1.58	1.54
1	N	274	VAL	N-CA	7.85	1.55	1.46
2	O	123	ILE	N-CA	7.83	1.56	1.46
3	C	204	HIS	CE1-NE2	7.82	1.40	1.32
5	E	78	HIS	N-CA	7.78	1.56	1.46
3	C	70	HIS	ND1-CE1	7.76	1.40	1.32
1	A	74	MET	CB-CG	7.75	1.75	1.52
2	B	24	HIS	CG-CD2	7.71	1.44	1.35
7	G	7	ASP	N-CA	7.67	1.54	1.46
1	N	376	HIS	CE1-NE2	7.63	1.40	1.32
1	A	203	ALA	C-O	7.61	1.32	1.24
2	O	34	ILE	CA-CB	7.61	1.64	1.54
5	E	98	ILE	N-CA	7.60	1.55	1.46
6	F	3	GLY	N-CA	7.60	1.53	1.44
5	R	83	PRO	N-CA	7.55	1.57	1.47
1	A	281	GLY	N-CA	7.54	1.55	1.45
1	N	317	GLY	N-CA	7.52	1.55	1.45
1	A	378	HIS	ND1-CE1	7.49	1.40	1.32
1	A	256	HIS	ND1-CE1	7.48	1.40	1.32
5	R	47	ILE	N-CA	7.46	1.55	1.46
1	A	498	CYS	C-O	7.45	1.31	1.25
5	E	51	ALA	N-CA	7.42	1.55	1.46
13	M	28	LEU	N-CA	7.42	1.52	1.46
1	N	254	ILE	N-CA	7.41	1.55	1.46
1	N	168	ILE	N-CA	7.40	1.55	1.46
3	C	226	HIS	CG-CD2	7.39	1.44	1.35
1	N	323	TRP	CA-C	7.38	1.62	1.52
3	P	103	HIS	CE1-NE2	7.37	1.40	1.32
1	A	96	ARG	CZ-NH1	7.37	1.43	1.32
3	P	12	ASN	CA-CB	7.37	1.64	1.53
3	P	26	LEU	N-CA	7.35	1.55	1.46
2	B	113	TYR	N-CA	7.34	1.55	1.46
1	A	413	HIS	ND1-CE1	7.30	1.39	1.32
1	N	240	HIS	N-CA	7.30	1.52	1.46
1	A	376	HIS	CG-CD2	7.28	1.43	1.35
7	G	55	ILE	CA-CB	7.28	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	231	HIS	ND1-CE1	7.23	1.39	1.32
7	T	55	ILE	CA-CB	7.21	1.62	1.54
3	C	76	GLN	CD-OE1	7.20	1.37	1.23
3	P	171	VAL	N-CA	7.20	1.55	1.46
4	D	18	ASP	N-CA	7.19	1.55	1.46
12	Y	26	THR	CA-CB	7.17	1.64	1.53
6	F	4	GLY	N-CA	7.10	1.55	1.45
1	N	368	HIS	ND1-CE1	7.09	1.39	1.32
1	N	150	LEU	N-CA	7.09	1.55	1.46
13	M	36	HIS	ND1-CE1	7.08	1.39	1.32
7	T	33	LEU	N-CA	7.08	1.54	1.46
1	A	121	GLY	N-CA	7.08	1.52	1.45
10	W	28	ASP	N-CA	7.05	1.54	1.46
1	N	146	THR	N-CA	7.03	1.54	1.46
1	A	12	HIS	ND1-CE1	6.96	1.39	1.32
1	N	290	HIS	CE1-NE2	6.92	1.39	1.32
5	E	89	LEU	CA-CB	6.91	1.65	1.53
3	C	46	GLY	N-CA	6.91	1.54	1.45
1	N	482	VAL	CA-CB	6.88	1.62	1.54
1	A	406	ASN	CA-CB	6.87	1.62	1.53
3	P	50	ASN	N-CA	6.87	1.54	1.46
1	A	395	HIS	CG-ND1	6.86	1.45	1.38
1	A	378	HIS	CE1-NE2	6.86	1.39	1.32
5	E	87	GLN	N-CA	6.86	1.54	1.46
1	N	61	HIS	ND1-CE1	6.82	1.39	1.32
4	D	97	ILE	N-CA	6.82	1.54	1.46
2	B	192	TYR	N-CA	6.82	1.54	1.46
1	N	166	THR	CA-CB	6.81	1.64	1.53
10	J	18	LEU	CA-C	6.80	1.61	1.53
1	A	149	SER	CA-C	6.78	1.61	1.52
3	P	204	HIS	CE1-NE2	6.78	1.39	1.32
3	P	232	HIS	ND1-CE1	6.75	1.39	1.32
13	M	36	HIS	CG-CD2	6.74	1.43	1.35
3	C	243	HIS	ND1-CE1	6.74	1.39	1.32
6	F	2	SER	N-CA	6.73	1.54	1.46
7	G	71	HIS	CG-CD2	6.72	1.43	1.35
1	A	378	HIS	CG-CD2	-6.71	1.28	1.35
3	C	182	TYR	N-CA	6.71	1.54	1.46
3	P	215	LEU	CA-C	6.70	1.61	1.52
10	W	35	THR	N-CA	6.64	1.54	1.46
7	T	8	HIS	N-CA	6.63	1.54	1.46
7	G	56	ARG	CA-CB	6.63	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	51	HIS	ND1-CE1	6.63	1.39	1.32
2	O	134	ARG	CA-C	6.61	1.61	1.52
13	Z	22	THR	N-CA	6.61	1.54	1.46
1	N	376	HIS	CG-CD2	6.60	1.43	1.35
7	G	46	ALA	CA-C	6.59	1.60	1.52
5	E	85	VAL	CA-CB	6.57	1.62	1.54
13	M	17	ILE	CA-C	6.56	1.60	1.52
1	N	257	ILE	N-CA	6.55	1.54	1.46
1	N	203	ALA	C-O	6.54	1.31	1.24
7	G	67	HIS	ND1-CE1	6.52	1.39	1.32
1	N	74	MET	CB-CG	6.52	1.72	1.52
1	A	192	ALA	N-CA	6.51	1.54	1.46
1	N	500	PRO	CA-C	6.50	1.58	1.52
5	R	41	LEU	N-CA	6.50	1.54	1.46
2	B	175	ILE	CA-CB	6.49	1.59	1.54
4	D	20	ARG	N-CA	6.48	1.54	1.46
1	N	252	GLY	CA-C	6.47	1.59	1.52
2	O	198	GLU	C-O	6.46	1.31	1.23
2	B	204	HIS	CE1-NE2	6.43	1.39	1.32
1	N	160	GLY	N-CA	6.42	1.53	1.45
1	A	39	ALA	N-CA	6.41	1.54	1.46
2	O	24	HIS	CE1-NE2	6.40	1.39	1.32
1	A	481	GLU	N-CA	6.40	1.54	1.46
13	M	20	SER	CA-CB	6.39	1.63	1.53
2	O	202	SER	N-CA	6.38	1.54	1.46
10	J	34	VAL	CA-C	6.35	1.60	1.52
3	P	55	TYR	CA-CB	6.34	1.63	1.53
1	N	96	ARG	CZ-NH1	6.34	1.41	1.32
6	F	39	THR	N-CA	6.32	1.53	1.45
3	C	13	PRO	C-O	6.31	1.31	1.23
4	D	86	MET	N-CA	6.30	1.53	1.46
1	A	74	MET	CG-SD	-6.30	1.65	1.80
1	A	61	HIS	CE1-NE2	6.28	1.38	1.32
1	N	152	LEU	CA-C	6.28	1.60	1.52
1	N	443	TYR	CA-CB	6.27	1.62	1.54
6	S	88	HIS	ND1-CE1	6.26	1.38	1.32
3	P	207	HIS	ND1-CE1	6.26	1.38	1.32
3	P	55	TYR	N-CA	-6.26	1.38	1.46
7	T	77	PRO	C-O	6.23	1.30	1.23
3	C	36	HIS	CA-CB	-6.22	1.45	1.54
1	N	328	HIS	ND1-CE1	6.22	1.38	1.32
5	R	43	PRO	CA-C	6.22	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	57	TRP	N-CA	6.21	1.53	1.46
4	D	122	ARG	CA-C	6.20	1.60	1.52
9	I	17	LEU	N-CA	6.19	1.53	1.46
1	N	419	VAL	CA-CB	6.19	1.62	1.54
10	J	33	ARG	CA-CB	6.18	1.62	1.53
1	N	121	GLY	N-CA	6.18	1.53	1.45
2	O	26	HIS	CG-CD2	6.18	1.42	1.35
8	H	73	ASP	N-CA	6.18	1.53	1.46
1	A	443	TYR	C-O	6.15	1.30	1.24
3	C	200	ALA	N-CA	6.15	1.53	1.46
12	L	26	THR	CA-CB	6.14	1.62	1.53
1	A	438	ARG	CA-CB	6.14	1.63	1.53
2	O	51	THR	N-CA	6.14	1.53	1.45
5	E	38	GLY	N-CA	6.13	1.54	1.45
8	H	25	GLN	CA-C	-6.13	1.44	1.52
2	B	204	HIS	ND1-CE1	6.12	1.38	1.32
3	P	238	ALA	CA-CB	6.11	1.62	1.53
1	N	429	HIS	ND1-CE1	6.10	1.38	1.32
10	W	33	ARG	CA-CB	6.10	1.62	1.53
1	N	167	THR	CA-C	6.09	1.60	1.52
2	O	45	MET	CA-CB	6.07	1.64	1.53
7	T	20	THR	CA-C	6.07	1.60	1.52
1	N	138	HIS	CG-CD2	6.05	1.42	1.35
5	E	84	TYR	N-CA	6.05	1.53	1.46
1	N	270	TYR	N-CA	6.05	1.53	1.46
1	N	279	SER	CA-CB	6.04	1.62	1.53
1	N	337	ALA	N-CA	6.04	1.53	1.46
2	O	52	HIS	ND1-CE1	6.04	1.38	1.32
3	P	221	ARG	CA-CB	6.03	1.63	1.53
5	E	24	ILE	N-CA	6.03	1.53	1.46
3	C	71	HIS	CG-CD2	6.02	1.42	1.35
3	C	57	TRP	N-CA	6.02	1.53	1.46
2	B	40	TYR	CA-CB	-6.02	1.43	1.53
3	C	188	ILE	N-CA	6.01	1.54	1.46
7	G	56	ARG	CZ-NH1	6.01	1.41	1.32
3	P	226	HIS	CE1-NE2	6.00	1.38	1.32
3	P	175	LEU	N-CA	6.00	1.53	1.46
10	W	27	THR	CA-C	6.00	1.60	1.52
1	N	203	ALA	N-CA	6.00	1.53	1.46
1	A	347	LEU	CA-C	5.99	1.60	1.52
7	G	7	ASP	CA-C	5.98	1.59	1.52
1	A	207	THR	N-CA	5.98	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	139	ALA	CA-CB	5.98	1.62	1.53
3	P	143	SER	CA-CB	5.97	1.63	1.53
2	B	124	PRO	C-O	5.96	1.30	1.23
7	T	71	HIS	ND1-CE1	5.96	1.38	1.32
1	N	266	GLU	C-O	5.95	1.31	1.24
13	Z	18	GLY	N-CA	5.95	1.53	1.45
3	C	160	LEU	CA-CB	5.94	1.62	1.53
1	N	397	PHE	N-CA	5.94	1.52	1.46
1	N	409	TRP	CD2-CE2	5.94	1.51	1.41
1	N	328	HIS	CD2-NE2	5.91	1.44	1.37
1	N	240	HIS	ND1-CE1	5.90	1.38	1.32
3	C	207	HIS	ND1-CE1	5.90	1.38	1.32
4	D	135	SER	N-CA	5.89	1.53	1.46
5	R	81	ILE	CA-CB	5.88	1.62	1.54
1	A	12	HIS	CG-CD2	5.88	1.42	1.35
1	N	103	TRP	NE1-CE2	-5.88	1.30	1.37
1	A	152	LEU	CA-C	5.87	1.60	1.52
1	N	403	TYR	N-CA	5.87	1.53	1.45
2	O	159	VAL	N-CA	5.86	1.53	1.46
1	N	445	ASP	CA-CB	5.86	1.62	1.53
3	C	110	PRO	N-CA	5.85	1.55	1.47
5	R	85	VAL	CA-CB	5.85	1.61	1.54
2	B	160	LEU	C-N	5.84	1.40	1.33
1	N	54	TYR	CA-C	5.84	1.60	1.52
10	J	27	THR	CA-C	5.83	1.60	1.52
1	N	58	VAL	N-CA	5.83	1.53	1.46
3	P	243	HIS	ND1-CE1	5.82	1.38	1.32
5	R	78	HIS	CG-CD2	5.82	1.42	1.35
1	N	269	GLY	CA-C	5.81	1.60	1.51
8	H	13	THR	C-O	5.81	1.30	1.23
1	N	481	GLU	N-CA	5.81	1.53	1.46
8	H	21	PRO	N-CA	-5.80	1.40	1.47
1	N	251	PHE	N-CA	5.79	1.53	1.46
7	G	71	HIS	ND1-CE1	5.79	1.38	1.32
1	N	429	HIS	CG-CD2	5.78	1.42	1.35
1	N	231	TYR	CA-CB	5.78	1.62	1.53
3	P	49	THR	CA-C	5.78	1.60	1.52
4	D	95	LEU	N-CA	-5.78	1.39	1.46
8	H	20	PHE	N-CA	5.78	1.53	1.46
10	J	50	LEU	N-CA	5.78	1.53	1.46
7	T	16	TRP	CA-C	5.78	1.60	1.52
1	N	477	ALA	N-CA	5.76	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	61	SER	N-CA	5.76	1.52	1.46
2	B	24	HIS	CE1-NE2	5.76	1.38	1.32
3	C	89	SER	CB-OG	5.74	1.53	1.42
1	N	328	HIS	N-CA	5.72	1.53	1.46
1	N	290	HIS	CG-CD2	5.72	1.42	1.35
1	A	304	TYR	CA-C	5.72	1.60	1.52
7	T	7	ASP	N-CA	5.71	1.53	1.46
1	N	91	ASP	CA-CB	5.70	1.61	1.53
4	D	21	ASP	CA-CB	5.70	1.63	1.53
3	C	70	HIS	CG-CD2	5.69	1.42	1.35
3	C	238	ALA	CA-CB	5.69	1.62	1.53
1	N	105	LEU	CA-CB	5.69	1.62	1.53
1	A	324	LEU	N-CA	5.68	1.53	1.46
1	A	233	HIS	CE1-NE2	5.66	1.38	1.32
1	N	151	HIS	CD2-NE2	5.66	1.44	1.37
1	N	233	HIS	CA-C	-5.66	1.45	1.52
10	W	22	LEU	N-CA	5.65	1.53	1.45
1	N	256	HIS	ND1-CE1	5.65	1.38	1.32
1	A	320	VAL	N-CA	5.65	1.53	1.46
5	E	82	TYR	CA-C	5.64	1.59	1.52
13	M	15	GLN	N-CA	5.64	1.53	1.46
1	N	5	ARG	CZ-NH1	5.63	1.40	1.32
4	Q	30	VAL	N-CA	5.63	1.53	1.46
1	N	355	GLY	N-CA	5.63	1.53	1.45
1	N	216	ASN	CA-CB	5.63	1.62	1.53
3	P	204	HIS	CG-CD2	5.63	1.42	1.35
11	K	29	TRP	CD2-CE2	5.63	1.50	1.41
3	C	57	TRP	CD2-CE2	5.62	1.50	1.41
4	D	61	ARG	C-O	5.61	1.31	1.24
5	E	73	ASP	CA-CB	5.61	1.62	1.53
1	N	276	ALA	CA-CB	5.61	1.62	1.53
2	B	154	VAL	C-O	5.60	1.29	1.24
6	S	94	HIS	CE1-NE2	5.60	1.38	1.32
4	D	47	SER	C-O	5.60	1.30	1.23
3	C	32	THR	CA-C	5.59	1.59	1.52
1	A	446	ALA	CA-C	5.58	1.60	1.52
13	M	5	PRO	CA-CB	5.58	1.61	1.53
7	T	51	HIS	CG-CD2	5.58	1.42	1.35
4	Q	129	ALA	CA-C	5.57	1.59	1.53
11	X	10	HIS	CE1-NE2	5.57	1.38	1.32
1	N	25	TRP	CD2-CE2	5.57	1.50	1.41
7	T	60	PHE	C-O	5.57	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	45	ASP	CA-C	5.55	1.59	1.52
1	A	43	GLN	N-CA	5.55	1.50	1.45
3	C	57	TRP	CD1-NE1	5.54	1.49	1.37
2	B	123	ILE	N-CA	5.53	1.53	1.46
2	B	125	THR	CA-C	5.53	1.60	1.52
3	P	158	HIS	CG-CD2	5.52	1.42	1.35
5	R	78	HIS	N-CA	5.52	1.53	1.46
1	N	438	ARG	CA-CB	5.51	1.62	1.53
3	C	122	HIS	CG-CD2	5.50	1.42	1.35
2	B	82	ARG	N-CA	5.50	1.52	1.46
1	A	332	ILE	N-CA	5.50	1.53	1.46
1	N	340	TRP	CA-CB	5.49	1.61	1.53
3	C	70	HIS	N-CA	5.48	1.53	1.46
5	R	44	GLU	N-CA	5.48	1.53	1.45
6	S	88	HIS	CG-CD2	5.48	1.41	1.35
1	N	245	ILE	CA-CB	5.48	1.61	1.54
1	N	269	GLY	N-CA	5.48	1.53	1.45
3	P	220	PHE	N-CA	5.48	1.53	1.46
5	R	23	ASP	N-CA	5.48	1.52	1.46
11	K	52	GLU	C-O	5.47	1.30	1.23
6	F	88	HIS	ND1-CE1	5.46	1.38	1.32
3	P	29	SER	N-CA	5.46	1.53	1.46
6	F	88	HIS	CA-C	-5.46	1.45	1.52
2	O	4	PRO	CA-CB	5.46	1.60	1.53
2	O	43	SER	CA-C	5.46	1.59	1.52
1	N	201	VAL	CA-CB	5.44	1.61	1.54
12	L	32	GLY	N-CA	5.43	1.52	1.45
6	S	18	ARG	CA-C	5.43	1.59	1.52
1	A	284	GLY	C-O	-5.43	1.18	1.24
2	B	218	TYR	C-O	5.43	1.30	1.24
9	I	8	GLN	CA-C	5.42	1.59	1.52
2	O	189	PRO	CA-CB	5.42	1.61	1.53
6	S	94	HIS	CG-CD2	5.42	1.41	1.35
3	C	239	ALA	N-CA	5.42	1.53	1.46
1	A	448	THR	CA-CB	5.41	1.61	1.53
1	N	320	VAL	N-CA	5.41	1.52	1.46
2	B	193	TYR	CA-C	5.41	1.59	1.52
2	B	3	TYR	N-CA	5.41	1.50	1.45
9	I	28	SER	CA-C	5.41	1.59	1.52
1	N	138	HIS	ND1-CE1	5.40	1.38	1.32
1	A	128	VAL	CA-C	5.40	1.59	1.52
1	N	106	PRO	CA-C	5.40	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	342	LEU	CA-CB	5.39	1.61	1.53
7	T	56	ARG	CA-CB	5.39	1.60	1.52
1	N	281	GLY	N-CA	5.39	1.52	1.45
3	C	149	HIS	CE1-NE2	5.39	1.38	1.32
3	P	248	VAL	N-CA	5.39	1.52	1.46
1	N	427	PRO	CA-CB	5.38	1.61	1.53
3	P	203	PHE	C-O	-5.38	1.17	1.24
2	O	132	GLU	N-CA	5.38	1.52	1.45
7	T	56	ARG	CZ-NH1	5.38	1.40	1.32
2	B	26	HIS	CG-CD2	5.38	1.41	1.35
2	B	26	HIS	N-CA	5.37	1.52	1.46
3	P	13	PRO	C-O	5.37	1.29	1.23
4	D	63	LYS	C-O	5.37	1.30	1.24
6	F	29	ASP	N-CA	5.37	1.52	1.46
4	D	132	GLN	C-O	-5.37	1.17	1.24
3	C	35	PHE	CG-CD2	5.37	1.50	1.38
3	C	116	TRP	CA-C	-5.36	1.48	1.52
2	B	38	VAL	C-O	5.36	1.30	1.24
1	A	273	MET	N-CA	5.36	1.52	1.46
10	J	26	ALA	CA-CB	5.36	1.62	1.53
1	A	413	HIS	CG-ND1	-5.35	1.32	1.38
1	N	326	THR	CA-C	5.35	1.59	1.52
1	N	376	HIS	ND1-CE1	5.35	1.37	1.32
2	B	123	ILE	C-N	5.34	1.40	1.33
7	G	54	ARG	CA-CB	5.34	1.61	1.53
3	C	123	PRO	N-CA	5.33	1.53	1.47
1	A	226	GLY	N-CA	5.33	1.50	1.45
1	N	347	LEU	CA-C	5.33	1.59	1.52
3	P	89	SER	CA-C	5.32	1.59	1.52
2	B	137	GLU	C-O	5.32	1.30	1.23
7	T	15	THR	CA-CB	5.31	1.61	1.53
1	A	251	PHE	N-CA	5.31	1.52	1.46
1	A	132	LEU	N-CA	5.30	1.52	1.46
3	C	35	PHE	CA-CB	5.30	1.62	1.53
4	D	6	VAL	CA-C	-5.30	1.46	1.52
1	N	94	PHE	N-CA	5.30	1.52	1.46
1	A	193	VAL	N-CA	5.30	1.52	1.46
8	U	38	ARG	N-CA	5.30	1.52	1.46
4	Q	23	PRO	CA-CB	5.29	1.61	1.53
2	B	30	ILE	CA-C	-5.29	1.45	1.52
1	N	452	THR	CA-CB	5.28	1.61	1.53
1	N	395	HIS	CG-ND1	5.28	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	GLU	CA-CB	-5.27	1.45	1.53
2	B	202	SER	N-CA	5.27	1.52	1.46
2	O	41	ILE	CA-C	-5.27	1.46	1.52
3	C	71	HIS	CA-CB	5.27	1.59	1.52
6	F	67	SER	N-CA	5.27	1.53	1.46
1	N	39	ALA	CA-CB	-5.27	1.45	1.53
1	A	368	HIS	CE1-NE2	5.25	1.37	1.32
1	N	16	GLY	N-CA	5.25	1.52	1.45
1	N	211	THR	N-CA	5.25	1.53	1.46
8	H	58	ARG	CZ-NH1	5.25	1.40	1.32
4	Q	8	SER	N-CA	5.25	1.52	1.46
1	N	479	LYS	CA-C	-5.25	1.47	1.53
2	B	10	GLN	N-CA	5.25	1.52	1.46
11	K	27	ALA	N-CA	5.24	1.52	1.46
1	A	248	LEU	C-O	-5.24	1.19	1.24
1	A	376	HIS	CE1-NE2	5.24	1.37	1.32
2	O	204	HIS	CG-CD2	5.24	1.41	1.35
11	X	17	VAL	N-CA	5.24	1.52	1.46
2	O	26	HIS	CE1-NE2	5.23	1.37	1.32
3	P	45	ILE	CA-C	5.23	1.59	1.52
1	A	395	HIS	CE1-NE2	5.22	1.37	1.32
12	L	42	HIS	CG-CD2	5.22	1.41	1.35
1	A	286	ILE	N-CA	5.22	1.51	1.46
4	D	36	SER	N-CA	5.22	1.52	1.46
10	J	7	GLU	N-CA	5.22	1.52	1.46
3	P	198	PHE	CA-CB	5.22	1.61	1.53
3	P	160	LEU	CA-CB	5.21	1.61	1.53
4	D	112	GLU	N-CA	5.21	1.52	1.46
4	Q	14	PRO	N-CA	5.21	1.53	1.47
9	V	65	LYS	N-CA	5.21	1.52	1.46
1	N	162	ILE	CA-CB	5.21	1.60	1.54
1	N	352	GLY	N-CA	5.21	1.52	1.45
2	B	3	TYR	CA-CB	5.21	1.60	1.54
3	P	16	TRP	CG-CD2	5.20	1.53	1.43
7	G	20	THR	N-CA	5.19	1.52	1.46
3	C	232	HIS	CG-CD2	5.19	1.41	1.35
1	A	252	GLY	CA-C	5.19	1.57	1.52
5	E	77	PRO	CA-C	5.18	1.59	1.52
13	Z	20	SER	CA-CB	5.18	1.61	1.53
3	P	46	GLY	N-CA	5.18	1.52	1.45
7	T	7	ASP	CA-C	5.18	1.59	1.52
7	G	57	THR	CA-CB	5.18	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	115	TRP	N-CA	5.17	1.52	1.46
1	A	163	ASN	CG-ND2	5.17	1.44	1.33
3	P	148	HIS	ND1-CE1	5.16	1.37	1.32
3	P	63	ARG	CZ-NH2	5.16	1.40	1.33
4	D	41	LYS	N-CA	5.15	1.52	1.46
3	P	11	VAL	N-CA	5.15	1.52	1.46
1	A	424	THR	C-O	5.15	1.30	1.24
1	N	482	VAL	N-CA	-5.15	1.39	1.46
2	B	194	GLY	N-CA	5.14	1.50	1.45
3	P	181	TYR	CA-C	5.14	1.59	1.52
9	I	12	LEU	CA-C	5.14	1.59	1.52
6	F	79	ALA	N-CA	5.14	1.52	1.46
1	A	151	HIS	CD2-NE2	5.12	1.43	1.37
1	A	203	ALA	N-CA	5.12	1.52	1.46
2	B	206	PHE	N-CA	5.12	1.53	1.46
3	P	103	HIS	CG-CD2	5.12	1.41	1.35
6	F	49	VAL	CA-C	-5.11	1.48	1.53
1	N	313	ALA	CA-CB	5.11	1.61	1.53
1	A	27	GLY	CA-C	5.11	1.57	1.52
2	B	56	MET	N-CA	5.11	1.52	1.46
1	N	283	LEU	CA-CB	5.11	1.61	1.53
3	C	148	HIS	ND1-CE1	5.11	1.37	1.32
4	Q	78	TRP	CD2-CE2	5.10	1.50	1.41
1	A	279	SER	CA-CB	5.10	1.61	1.53
1	A	254	ILE	N-CA	5.10	1.52	1.46
3	C	226	HIS	CE1-NE2	5.10	1.37	1.32
4	Q	24	LEU	CA-C	5.10	1.58	1.52
12	Y	8	GLY	N-CA	5.09	1.52	1.45
1	A	128	VAL	N-CA	5.09	1.52	1.46
1	A	148	PHE	CA-CB	5.09	1.61	1.53
2	B	103	GLN	CA-C	5.09	1.59	1.52
3	C	20	GLY	N-CA	5.08	1.52	1.45
1	A	269	GLY	CA-C	5.08	1.59	1.51
1	A	46	THR	C-O	5.08	1.30	1.24
4	D	81	VAL	N-CA	5.08	1.52	1.46
1	N	226	GLY	N-CA	5.08	1.51	1.45
1	A	28	MET	CA-C	5.07	1.59	1.52
1	A	298[A]	ASP	CA-C	5.07	1.59	1.52
1	A	298[B]	ASP	CA-C	5.07	1.59	1.52
5	E	86	ILE	CB-CG1	5.07	1.63	1.53
3	P	169	LEU	CA-CB	5.07	1.61	1.53
3	C	3	HIS	CG-CD2	5.06	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	28	ASN	N-CA	5.06	1.52	1.46
4	D	58	GLU	CD-OE1	5.06	1.34	1.25
4	D	107	ILE	C-O	5.06	1.30	1.24
5	R	75	ALA	CA-CB	5.06	1.62	1.53
7	T	67	HIS	CG-CD2	5.06	1.41	1.35
2	B	134	ARG	CA-C	5.05	1.59	1.52
6	F	73	TRP	C-O	5.05	1.30	1.24
2	O	200	CYS	N-CA	5.05	1.51	1.46
1	N	188	VAL	N-CA	5.05	1.52	1.46
3	P	222	GLN	CA-C	5.04	1.59	1.52
2	B	161	HIS	CG-ND1	5.04	1.43	1.38
3	P	188	ILE	N-CA	5.04	1.53	1.46
1	A	58	VAL	N-CA	5.03	1.52	1.46
4	D	54	ASP	N-CA	5.03	1.52	1.46
2	B	34	ILE	CA-CB	5.03	1.60	1.54
3	C	72	THR	CA-C	5.03	1.59	1.53
1	A	287	VAL	CA-CB	5.02	1.60	1.54
3	C	193	TYR	CA-CB	5.02	1.61	1.53
3	P	207	HIS	CA-CB	5.02	1.61	1.53
10	W	20	VAL	CA-CB	5.01	1.61	1.54
1	N	185	VAL	N-CA	5.01	1.52	1.46
2	O	172	THR	N-CA	5.00	1.52	1.46
12	L	21	LEU	N-CA	5.00	1.52	1.46
1	N	41	LEU	CA-C	5.00	1.59	1.52

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-12.09	74.31	100.90
5	E	90	ARG	NE-CZ-NH1	11.79	133.29	121.50
1	A	71	MET	CG-SD-CE	-11.38	75.86	100.90
1	A	112	LEU	CD1-CG-CD2	-10.41	87.89	110.80
7	G	7	ASP	N-CA-C	10.17	123.45	108.60
4	Q	20	ARG	NE-CZ-NH2	-9.52	110.63	119.20
5	E	90	ARG	NE-CZ-NH2	-9.51	110.64	119.20
7	T	7	ASP	N-CA-C	9.38	130.79	110.80
1	A	189	MET	CG-SD-CE	-8.80	81.53	100.90
7	T	58	LYS	CA-C-N	-8.39	111.37	119.85
7	T	58	LYS	C-N-CA	-8.39	111.37	119.85
1	N	240	HIS	CA-CB-CG	-8.39	105.41	113.80
1	A	240	HIS	CA-CB-CG	-8.28	105.52	113.80
1	N	187	SER	O-C-N	7.77	130.36	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	CB-CG-CD	7.70	129.02	111.30
5	R	86	ILE	N-CA-C	-7.47	103.18	110.72
6	S	94	HIS	N-CA-C	7.47	126.71	110.80
5	E	90	ARG	CD-NE-CZ	7.45	134.83	124.40
4	D	58	GLU	CB-CG-CD	7.44	125.25	112.60
1	A	74	MET	CB-CG-SD	-7.42	90.43	112.70
1	A	49	GLY	N-CA-C	-7.39	99.10	111.08
4	Q	20	ARG	CG-CD-NE	-7.37	95.79	112.00
5	E	11	PHE	N-CA-C	-7.36	103.19	111.07
2	B	65	TRP	CB-CA-C	7.34	123.44	110.37
1	A	105	LEU	CA-C-N	-7.28	112.88	120.38
1	A	105	LEU	C-N-CA	-7.28	112.88	120.38
12	L	20	ARG	CG-CD-NE	-7.24	96.08	112.00
1	N	316	THR	O-C-N	7.09	129.63	122.12
5	R	42	VAL	N-CA-C	-7.02	99.76	108.05
6	F	2	SER	N-CA-C	6.97	119.46	108.79
1	N	202	LEU	O-C-N	6.97	129.25	122.07
1	N	323	TRP	O-C-N	6.93	129.47	122.12
9	I	21	ILE	N-CA-C	-6.82	103.83	110.72
1	N	83	VAL	CA-C-O	6.82	123.26	118.69
4	Q	20	ARG	NE-CZ-NH1	6.82	128.32	121.50
2	B	59	GLN	N-CA-CB	6.76	119.81	110.01
1	N	82	LEU	CA-C-N	-6.74	114.94	120.33
1	N	82	LEU	C-N-CA	-6.74	114.94	120.33
1	N	395	HIS	N-CA-C	6.73	118.27	111.07
3	C	222	GLN	O-C-N	6.70	129.79	122.15
1	N	112	LEU	CD1-CG-CD2	-6.62	96.23	110.80
1	A	187	SER	O-C-N	6.62	129.69	122.15
1	N	189	MET	CG-SD-CE	-6.60	86.38	100.90
7	T	32	THR	N-CA-C	-6.55	104.22	111.36
7	G	6	GLY	N-CA-C	6.53	128.65	113.18
1	A	485	VAL	N-CA-CB	-6.48	102.02	111.48
1	N	152	LEU	O-C-N	6.39	128.90	122.12
7	G	58	LYS	CA-C-N	-6.39	113.20	119.78
7	G	58	LYS	C-N-CA	-6.39	113.20	119.78
3	C	255	SER	N-CA-C	6.39	118.12	111.03
1	A	149	SER	N-CA-C	-6.36	104.35	111.28
1	N	445	ASP	N-CA-C	6.32	118.98	111.71
6	F	49	VAL	CA-C-N	-6.25	113.54	119.85
6	F	49	VAL	C-N-CA	-6.25	113.54	119.85
3	P	222	GLN	O-C-N	6.22	129.24	122.15
12	Y	46	LYS	N-CA-C	6.18	123.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	20	ARG	N-CA-C	-6.18	104.63	111.36
2	B	41[A]	ILE	CA-C-O	6.16	127.69	121.17
2	B	41[B]	ILE	CA-C-O	6.16	127.69	121.17
1	N	54	TYR	N-CA-C	-6.10	104.55	111.07
1	N	154	GLY	O-C-N	-6.09	116.28	122.19
1	A	239	GLY	CA-C-N	-6.07	112.25	119.78
1	A	239	GLY	C-N-CA	-6.07	112.25	119.78
7	T	33	LEU	N-CA-C	6.05	117.56	110.97
2	B	43	SER	N-CA-C	-6.03	104.63	112.23
4	D	84	ALA	N-CA-C	-6.03	104.79	111.36
1	N	280	ILE	O-C-N	6.01	128.02	121.83
4	D	58	GLU	CA-CB-CG	-5.98	102.13	114.10
6	F	64	GLU	CA-C-N	-5.97	114.52	125.02
6	F	64	GLU	C-N-CA	-5.97	114.52	125.02
4	Q	24	LEU	O-C-N	5.96	127.18	120.68
7	T	2	SER	N-CA-C	-5.95	106.66	114.04
2	O	188	ARG	CA-C-N	-5.93	114.51	120.21
2	O	188	ARG	C-N-CA	-5.93	114.51	120.21
7	T	40	GLY	N-CA-C	-5.93	99.11	113.18
1	N	240	HIS	N-CA-CB	5.92	117.41	110.42
1	A	75	ILE	CA-C-N	-5.91	112.72	120.22
1	A	75	ILE	C-N-CA	-5.91	112.72	120.22
2	O	65	TRP	CB-CA-C	5.89	121.26	110.36
1	N	148	PHE	N-CA-C	5.88	117.68	111.28
10	J	24	GLY	N-CA-C	-5.86	107.39	114.66
10	W	24	GLY	N-CA-C	-5.81	107.46	114.66
1	A	145	LEU	O-C-N	5.81	128.27	122.12
1	N	189	MET	CB-CG-SD	-5.78	95.35	112.70
6	F	1	ALA	CA-C-N	5.78	132.19	121.62
6	F	1	ALA	C-N-CA	5.78	132.19	121.62
6	S	43	LYS	CG-CD-CE	5.77	124.56	111.30
4	D	5	VAL	N-CA-C	5.75	115.89	107.37
10	J	36	MET	CG-SD-CE	-5.75	88.25	100.90
1	N	185	VAL	O-C-N	-5.70	115.97	121.90
1	N	323	TRP	N-CA-C	-5.66	105.12	111.28
2	B	38	VAL	N-CA-C	5.65	116.38	110.62
1	N	280	ILE	N-CA-C	-5.65	105.02	110.72
1	A	82	LEU	CA-C-N	-5.63	115.83	120.33
1	A	82	LEU	C-N-CA	-5.63	115.83	120.33
3	P	142	VAL	CA-C-N	-5.61	111.78	120.31
3	P	142	VAL	C-N-CA	-5.61	111.78	120.31
4	D	22	TYR	N-CA-C	-5.60	99.23	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	235	PHE	N-CA-C	-5.59	105.09	111.07
5	E	86	ILE	N-CA-C	-5.57	105.07	110.42
1	N	250	GLY	N-CA-C	-5.56	105.76	112.49
2	O	41	ILE	CA-CB-CG1	-5.55	100.96	110.40
3	P	91	VAL	N-CA-C	-5.54	105.12	110.72
1	N	167	THR	N-CA-C	-5.53	105.33	111.36
1	N	202	LEU	CA-C-O	-5.51	115.04	120.82
2	B	64	ILE	CA-C-N	-5.49	113.12	122.56
2	B	64	ILE	C-N-CA	-5.49	113.12	122.56
4	D	61	ARG	N-CA-C	-5.49	106.54	113.18
1	A	152	LEU	O-C-N	5.49	127.93	122.12
1	A	438	ARG	CA-CB-CG	-5.48	103.14	114.10
3	P	164	PHE	N-CA-C	5.48	117.25	111.28
4	Q	38	LYS	N-CA-C	5.48	117.25	111.28
2	O	202	SER	CB-CA-C	-5.47	101.39	110.68
1	N	74	MET	CB-CG-SD	-5.46	96.30	112.70
1	A	310	MET	CG-SD-CE	-5.46	88.89	100.90
1	N	173	PRO	N-CA-C	-5.45	104.75	110.58
1	A	102	PHE	CA-CB-CG	-5.45	108.35	113.80
1	N	180	GLN	CA-CB-CG	-5.43	103.25	114.10
1	A	4	ASN	CB-CA-C	-5.42	101.64	110.85
1	A	173	PRO	N-CA-C	-5.38	105.31	110.47
1	A	426	PHE	CA-CB-CG	-5.38	108.42	113.80
12	L	12	PRO	N-CA-C	-5.36	107.19	114.80
1	N	253	MET	N-CA-C	-5.36	105.52	111.36
8	U	9	LYS	N-CA-C	5.35	118.78	110.17
2	B	59	GLN	CB-CG-CD	5.33	121.67	112.60
1	A	310	MET	CA-CB-CG	-5.33	103.45	114.10
1	N	397	PHE	CA-C-N	-5.32	114.19	119.56
1	N	397	PHE	C-N-CA	-5.32	114.19	119.56
1	N	187	SER	CA-C-O	-5.32	114.92	120.55
1	N	239	GLY	CA-C-N	-5.31	113.19	119.78
1	N	239	GLY	C-N-CA	-5.31	113.19	119.78
3	P	219	PHE	N-CA-C	-5.31	105.41	111.14
1	N	235	PHE	O-C-N	5.30	127.53	122.07
1	A	378	HIS	ND1-CG-CD2	5.30	111.40	106.10
2	B	177	GLY	N-CA-C	-5.30	108.32	115.21
3	C	131	LEU	N-CA-C	-5.28	105.60	111.36
1	A	187	SER	CA-C-O	-5.28	114.82	120.42
1	A	316	THR	O-C-N	5.28	128.17	122.15
7	G	44	ARG	N-CA-C	5.28	116.35	109.64
2	O	50	LEU	O-C-N	5.27	129.08	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	LEU	CA-C-N	5.27	129.03	120.60
2	B	28	LEU	C-N-CA	5.27	129.03	120.60
2	B	59	GLN	N-CA-C	5.27	116.70	111.07
7	T	8	HIS	N-CA-C	5.26	122.01	110.80
1	A	376	HIS	CA-C-N	-5.26	112.41	121.66
1	A	376	HIS	C-N-CA	-5.26	112.41	121.66
1	N	160	GLY	N-CA-C	-5.25	106.33	113.37
7	G	32	THR	N-CA-C	-5.23	105.66	111.36
3	P	74	ALA	N-CA-C	-5.22	105.67	111.36
1	A	120	ALA	CA-C-N	-5.22	115.37	121.85
1	A	120	ALA	C-N-CA	-5.22	115.37	121.85
1	N	156	SER	O-C-N	5.22	127.52	122.09
2	B	42	ILE	CG1-CB-CG2	-5.22	95.05	110.70
1	N	206	ILE	N-CA-C	-5.21	105.26	112.50
2	B	41[A]	ILE	CA-C-N	-5.21	113.19	120.53
2	B	41[A]	ILE	C-N-CA	-5.21	113.19	120.53
2	B	41[B]	ILE	CA-C-N	-5.21	113.19	120.53
2	B	41[B]	ILE	C-N-CA	-5.21	113.19	120.53
3	P	38	ASN	N-CA-C	5.21	118.62	111.54
13	Z	4	LYS	CA-C-N	-5.20	114.42	119.78
13	Z	4	LYS	C-N-CA	-5.20	114.42	119.78
3	C	239	ALA	N-CA-C	-5.19	105.70	111.36
10	J	23	LYS	CG-CD-CE	-5.18	99.40	111.30
2	B	209	ILE	CA-C-N	-5.17	115.65	122.98
2	B	209	ILE	C-N-CA	-5.17	115.65	122.98
7	T	69	PHE	N-CA-C	5.16	117.12	111.50
3	P	181	TYR	N-CA-C	-5.16	105.66	111.28
2	O	202	SER	N-CA-C	5.15	117.56	111.33
11	K	47	ARG	NE-CZ-NH1	5.14	126.64	121.50
6	F	94	HIS	N-CA-C	5.14	121.75	110.80
1	A	201	VAL	N-CA-C	-5.14	105.40	111.00
3	C	211	GLY	O-C-N	5.13	127.11	122.19
1	N	165	ILE	N-CA-C	5.13	115.75	110.36
1	A	251	PHE	CB-CA-C	-5.13	102.28	110.79
2	O	38	VAL	N-CA-C	5.12	115.84	110.62
3	C	12	ASN	CB-CA-C	-5.12	101.03	109.27
8	H	14	ALA	CA-C-N	-5.12	114.96	120.03
8	H	14	ALA	C-N-CA	-5.12	114.96	120.03
1	N	143	VAL	O-C-N	-5.12	116.56	121.83
1	N	324	LEU	N-CA-C	-5.11	105.60	111.07
6	F	45	ASP	O-C-N	5.11	125.92	121.17
1	A	355	GLY	N-CA-C	-5.10	106.58	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	W	33	ARG	CA-CB-CG	-5.09	103.91	114.10
5	E	63	SER	CA-C-N	-5.08	113.07	120.29
5	E	63	SER	C-N-CA	-5.08	113.07	120.29
1	N	350	VAL	CA-C-N	-5.08	113.76	120.22
1	N	350	VAL	C-N-CA	-5.08	113.76	120.22
1	N	310	MET	CG-SD-CE	-5.08	89.73	100.90
1	N	280	ILE	CA-C-N	-5.08	114.42	120.00
1	N	280	ILE	C-N-CA	-5.08	114.42	120.00
3	P	215	LEU	O-C-N	5.08	128.51	122.27
7	G	5	LYS	CB-CA-C	5.07	120.50	110.42
1	N	167	THR	O-C-N	5.05	127.91	122.15
1	N	199	LEU	CA-C-N	-5.05	113.83	119.19
1	N	199	LEU	C-N-CA	-5.05	113.83	119.19
1	N	323	TRP	CA-C-O	-5.04	115.20	120.55
1	A	370	THR	CB-CA-C	-5.04	100.77	110.24
7	T	16	TRP	O-C-N	5.03	129.07	122.33
3	P	133	ASN	CA-CB-CG	-5.02	107.58	112.60
7	T	44	ARG	N-CA-C	5.02	116.01	109.64
1	A	318	VAL	O-C-N	-5.02	116.92	121.94
2	B	92	ASN	CA-C-N	-5.02	114.82	120.14
2	B	92	ASN	C-N-CA	-5.02	114.82	120.14
7	G	76	ASN	O-C-N	5.00	126.13	120.83

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	379	TYR	Mainchain
1	A	38	ARG	Sidechain
6	F	93	PRO	Peptide
7	G	11	TPO	Peptide
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide
9	V	1	SAC	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	4193	0	4162	98	0
1	N	4179	0	4154	95	0
2	B	1899	0	1898	69	0
2	O	1870	0	1868	51	0
3	C	2185	0	2097	48	0
3	P	2185	0	2097	38	0
4	D	1233	0	1223	37	0
4	Q	1224	0	1211	21	0
5	E	852	0	845	4	0
5	R	863	0	857	6	0
6	F	778	0	754	26	0
6	S	763	0	742	24	0
7	G	686	0	652	32	0
7	T	686	0	651	21	0
8	H	662	0	623	19	0
8	U	662	0	623	12	0
9	I	601	0	613	20	0
9	V	601	0	613	15	0
10	J	460	0	459	9	0
10	W	469	0	464	4	0
11	K	384	0	366	3	0
11	X	391	0	374	3	0
12	L	380	0	380	16	0
12	Y	388	0	388	14	0
13	M	335	0	352	8	0
13	Z	335	0	352	8	0
14	A	180	0	162	18	0
14	N	180	0	162	22	0
15	A	1	0	0	1	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	N	1	0	0	0	0
18	A	9	0	0	7	0
18	N	9	0	0	2	0
19	A	126	0	220	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	13	0
19	N	63	0	110	7	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	13	0
20	C	102	0	152	5	0
20	N	102	0	152	10	0
20	P	102	0	152	3	0
21	A	36	0	52	8	0
21	B	16	0	24	2	0
21	C	4	0	6	0	0
21	D	8	0	12	9	0
21	E	12	0	18	0	0
21	F	12	0	18	0	0
21	G	8	0	12	3	0
21	L	4	0	6	0	0
21	M	4	0	6	0	0
21	N	36	0	54	1	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	12	0	18	0	0
21	T	4	0	6	0	0
21	W	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	1	0
22	P	58	0	78	6	0
22	W	29	0	38	1	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	15	0
24	N	52	0	80	16	0
25	C	99	0	126	15	0
25	M	33	0	42	0	0
25	P	99	0	126	15	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	1	0
27	C	100	0	156	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	N	100	0	156	29	0
27	P	100	0	156	24	0
27	T	100	0	156	16	0
28	C	106	0	154	16	0
28	G	106	0	154	8	0
28	P	53	0	77	6	0
28	T	53	0	77	3	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	235	0	0	32	0
30	B	162	0	0	25	2
30	C	110	0	0	3	0
30	D	118	0	0	12	1
30	E	93	0	0	1	0
30	F	94	0	0	5	0
30	G	42	0	0	5	0
30	H	42	0	0	1	0
30	I	27	0	0	6	1
30	J	23	0	0	2	0
30	K	26	0	0	1	0
30	L	38	0	0	4	1
30	M	25	0	0	7	1
30	N	203	0	0	13	0
30	O	100	0	0	1	0
30	P	95	0	0	3	0
30	Q	29	0	0	5	0
30	R	40	0	0	1	0
30	S	45	0	0	3	0
30	T	35	0	0	3	0
30	U	29	0	0	0	0
30	V	16	0	0	3	0
30	W	7	0	0	0	0
30	X	11	0	0	0	0
30	Y	12	0	0	0	0
30	Z	12	0	0	0	0
All	All	33609	0	32570	796	3

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:CG	1:A:74:MET:CB	1.75	1.61
6:S:43:LYS:H	6:S:43:LYS:CD	1.08	1.49
20:N:609:PGV:H011	20:N:609:PGV:C2	1.38	1.33
24:B:303:PSC:O02	9:I:14:ALA:HB2	1.16	1.31
30:A:709:HOH:O	19:D:201:TGL:HG11	1.23	1.29
19:A:611:TGL:HC32	12:L:20:ARG:NH2	1.50	1.27
1:A:39:ALA:HA	21:D:202:EDO:O1	1.33	1.26
1:A:297[B]:MET:CB	30:A:794:HOH:O	1.75	1.26
21:B:304:EDO:H12	30:C:412:HOH:O	1.13	1.25
1:A:512:ASN:HB3	30:A:701:HOH:O	1.35	1.22
20:N:609:PGV:C01	20:N:609:PGV:H21	1.70	1.21
19:D:201:TGL:HG31	30:D:366:HOH:O	1.34	1.20
6:S:43:LYS:CD	6:S:43:LYS:N	1.90	1.17
27:P:305:CDL:H381	27:P:305:CDL:H272	1.21	1.15
3:C:51[B]:MET:HE2	27:C:305:CDL:H392	1.29	1.15
26:P:303:UNX:UNK	30:P:441:HOH:O	1.28	1.14
1:N:297[B]:MET:HB2	30:N:765:HOH:O	1.44	1.14
2:B:98:LYS:HG3	30:B:522:HOH:O	1.47	1.13
19:N:611:TGL:H281	19:N:611:TGL:HB92	1.31	1.13
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.50	1.11
4:D:19[A]:ARG:HD2	4:D:21:ASP:OD1	1.51	1.11
19:N:611:TGL:HC42	30:N:903:HOH:O	1.51	1.11
2:B:32[A]:PHE:O	2:B:35[A]:SER:OG	1.67	1.10
6:S:43:LYS:H	6:S:43:LYS:HD3	0.98	1.10
1:A:297[B]:MET:HB3	30:A:794:HOH:O	1.41	1.10
1:N:302[B]:ARG:HH12	1:N:365:ILE:HD11	1.00	1.10
2:B:160:LEU:HB2	30:B:424:HOH:O	1.53	1.08
1:N:297[B]:MET:CB	30:N:765:HOH:O	1.97	1.08
1:A:512:ASN:CB	30:A:701:HOH:O	1.88	1.08
3:P:67:PHE:HE2	27:P:305:CDL:H1	1.10	1.08
1:A:74:MET:CB	1:A:74:MET:SD	2.41	1.07
19:A:611:TGL:HC32	12:L:20:ARG:HH22	0.97	1.07
27:N:601:CDL:H371	2:O:78:LEU:HD12	1.34	1.07
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.03	1.06
8:H:9:LYS:HG3	8:H:10:ASN:H	1.11	1.06
1:N:302[B]:ARG:NH1	1:N:365:ILE:HD11	1.71	1.05
20:N:609:PGV:H011	20:N:609:PGV:H22	1.39	1.04
1:A:39:ALA:HA	21:D:202:EDO:HO1	0.92	1.04
3:C:67:PHE:HE2	27:C:305:CDL:H1	1.15	1.04
6:S:95:GLN:HA	6:S:95:GLN:HE21	1.21	1.04
6:S:43:LYS:H	6:S:43:LYS:HD2	0.88	1.03
5:E:90:ARG:HD2	30:E:374:HOH:O	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:O	1:A:514:LYS:HB2	1.50	1.03
24:N:612:PSC:H1	24:N:612:PSC:H343	1.37	1.02
24:B:303:PSC:O02	9:I:14:ALA:CB	2.07	1.01
6:S:43:LYS:N	6:S:43:LYS:HD2	1.50	1.01
7:G:10:GLY:O	7:G:11:TPO:HB	1.56	1.00
4:D:4:SER:HB3	30:D:302:HOH:O	1.60	1.00
1:A:297[B]:MET:HB2	30:A:794:HOH:O	1.42	1.00
1:N:513:LEU:O	1:N:514:LYS:HB2	1.61	1.00
25:P:307:DMU:H29	25:P:307:DMU:H35	1.43	0.99
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.61	0.99
20:N:609:PGV:C2	20:N:609:PGV:C01	2.25	0.99
3:P:67:PHE:CE2	27:P:305:CDL:H1	1.98	0.98
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.61	0.98
1:A:39:ALA:CA	21:D:202:EDO:O1	2.11	0.98
3:P:224:LYS:CD	27:P:305:CDL:HB31	1.94	0.97
19:N:611:TGL:HB92	19:N:611:TGL:C28	1.94	0.97
1:A:512:ASN:ND2	30:A:701:HOH:O	1.96	0.97
30:B:423:HOH:O	8:H:62:SER:HA	1.63	0.96
9:I:73:LYS:HE2	30:I:104:HOH:O	1.65	0.96
19:A:611:TGL:HC31	12:L:14:SER:H	1.28	0.96
10:J:55:PHE:HB2	30:J:208:HOH:O	1.65	0.95
6:S:43:LYS:N	6:S:43:LYS:HD3	1.61	0.95
1:A:479:LYS:HB2	30:M:201:HOH:O	1.66	0.95
4:Q:19[A]:ARG:CG	4:Q:21:ASP:OD1	2.14	0.94
1:A:282:PHE:HA	7:T:4:ALA:CB	1.97	0.94
1:A:328:HIS:NE2	24:B:303:PSC:H31	1.83	0.94
28:G:103:PEK:H312	28:G:103:PEK:H272	1.50	0.93
1:A:136[B]:LEU:HD11	30:A:933:HOH:O	1.67	0.93
2:B:49:LYS:HE2	30:D:395:HOH:O	1.68	0.93
30:A:925:HOH:O	19:D:201:TGL:HC31	1.68	0.93
3:C:67:PHE:CE2	27:C:305:CDL:H1	2.03	0.93
19:Y:101:TGL:HG11	19:Y:101:TGL:HA31	1.48	0.93
27:N:601:CDL:H661	27:N:601:CDL:H611	1.50	0.92
11:K:6:ALA:N	30:K:101:HOH:O	2.01	0.92
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.10	0.91
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.52	0.91
24:B:303:PSC:H62	24:B:303:PSC:H261	1.50	0.91
27:N:601:CDL:H321	27:N:601:CDL:OA7	1.70	0.90
19:N:611:TGL:H281	19:N:611:TGL:CB9	2.01	0.90
2:B:200:CYS:HB3	30:B:402:HOH:O	1.70	0.90
19:A:611:TGL:CC3	12:L:20:ARG:HH22	1.82	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:HIS:CD2	30:A:903:HOH:O	2.24	0.89
1:A:398:PRO:HG3	30:A:738:HOH:O	1.70	0.89
20:A:610:PGV:H221	30:M:222:HOH:O	1.72	0.89
20:N:609:PGV:H011	20:N:609:PGV:H21	0.89	0.89
2:B:161:HIS:HA	30:B:402:HOH:O	1.74	0.88
1:A:503:HIS:HD2	30:A:903:HOH:O	1.56	0.88
22:C:306:CHD:H162	22:C:306:CHD:H231	1.56	0.87
1:A:230:LEU:HB3	30:A:704:HOH:O	1.74	0.87
21:A:616:EDO:H11	30:M:220:HOH:O	1.75	0.87
3:C:33[A]:MET:HB2	25:C:302:DMU:C22	2.05	0.87
1:N:417[A]:MET:CE	30:N:788:HOH:O	2.21	0.86
7:G:84:LYS:H	7:G:84:LYS:HD2	1.37	0.85
1:N:302[B]:ARG:HH12	1:N:365:ILE:CD1	1.86	0.85
7:G:84:LYS:HD2	7:G:84:LYS:N	1.90	0.85
1:N:136[B]:LEU:HG	30:T:222:HOH:O	1.76	0.85
27:N:601:CDL:H611	27:N:601:CDL:C66	2.05	0.85
3:P:224:LYS:HD2	27:P:305:CDL:HB31	1.58	0.85
3:C:33[A]:MET:HB2	25:C:302:DMU:H13	1.58	0.85
12:Y:45:LEU:HD22	13:Z:42:LYS:HE3	1.57	0.84
3:C:63:ARG:HE	27:C:305:CDL:HA21	1.43	0.84
3:C:51[B]:MET:CE	27:C:305:CDL:H392	2.08	0.84
4:D:4:SER:HA	30:D:387:HOH:O	1.78	0.84
1:N:136[B]:LEU:HD11	30:N:902:HOH:O	1.78	0.84
28:T:101:PEK:H242	28:T:101:PEK:H12	1.60	0.83
6:S:75:HIS:H	6:S:80:GLN:HE22	1.25	0.83
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.19	0.83
24:N:612:PSC:H02	24:N:612:PSC:H212	1.61	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.27	0.83
1:A:112:LEU:HG	30:A:906:HOH:O	1.78	0.83
19:A:608:TGL:HA42	19:A:608:TGL:HA91	1.60	0.82
15:A:603:CU:CU	18:A:607[B]:AZI:N1	1.44	0.81
4:Q:19[A]:ARG:CD	4:Q:21:ASP:OD1	2.28	0.81
27:T:102:CDL:H361	27:T:102:CDL:H121	1.63	0.80
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	1.80	0.80
4:D:19[A]:ARG:CD	4:D:21:ASP:OD1	2.28	0.80
7:G:7:ASP:HB2	1:N:178[A]:GLN:HG2	1.61	0.80
8:H:9:LYS:HG3	8:H:10:ASN:N	1.88	0.80
19:N:611:TGL:CC4	30:N:903:HOH:O	2.16	0.80
7:G:72:ASN:H	7:G:76:ASN:HD22	1.30	0.79
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.17	0.79
7:T:76:ASN:HD21	28:T:101:PEK:HN2	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.82	0.79
8:H:43:MET:O	8:H:45:ALA:N	2.14	0.79
4:D:4:SER:CB	30:D:302:HOH:O	2.23	0.78
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.78
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	1.90	0.78
27:T:102:CDL:H161	27:T:102:CDL:OB3	1.84	0.78
3:C:63:ARG:HE	27:C:305:CDL:CA2	1.96	0.78
28:P:308:PEK:H042	6:S:1:ALA:H1	1.48	0.78
2:B:174:ALA:HB1	30:B:528:HOH:O	1.84	0.78
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.66	0.78
7:T:38:HIS:CE1	27:T:102:CDL:H141	2.19	0.77
6:F:92:VAL:HG21	30:F:290:HOH:O	1.83	0.77
27:P:305:CDL:H272	27:P:305:CDL:C38	2.11	0.77
20:A:609:PGV:H183	28:G:101:PEK:H322	1.65	0.77
1:A:514:LYS:NZ	30:A:702:HOH:O	2.11	0.76
24:N:612:PSC:C07	9:V:10:ARG:HH21	1.98	0.76
3:P:33[B]:MET:SD	25:P:307:DMU:H8	2.25	0.76
27:N:601:CDL:H591	27:N:601:CDL:H761	1.68	0.76
3:C:161[A]:GLN:HE22	28:C:307:PEK:H41	1.51	0.76
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.68	0.76
22:P:306:CHD:H162	22:P:306:CHD:H231	1.67	0.75
27:P:305:CDL:H391	27:P:305:CDL:H351	1.66	0.75
6:S:95:GLN:HA	6:S:95:GLN:NE2	2.00	0.75
27:N:601:CDL:H611	27:N:601:CDL:C65	2.16	0.75
24:N:612:PSC:H343	24:N:612:PSC:C13	2.16	0.75
27:T:102:CDL:OB3	27:T:102:CDL:H142	1.86	0.75
20:A:609:PGV:H343	28:G:101:PEK:H382	1.69	0.75
7:G:76:ASN:HD21	28:G:101:PEK:HN2	1.33	0.75
3:P:63:ARG:HE	27:P:305:CDL:HA21	1.51	0.74
3:C:33[A]:MET:HB2	25:C:302:DMU:C25	2.15	0.74
30:B:553:HOH:O	19:D:201:TGL:C28	2.34	0.74
3:C:224:LYS:HD2	27:C:305:CDL:HB31	1.68	0.74
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.67	0.74
6:F:75:HIS:H	6:F:80:GLN:HE22	1.33	0.74
2:B:53:THR:HG21	30:D:311:HOH:O	1.87	0.74
20:C:304:PGV:H181	27:C:305:CDL:H652	1.68	0.74
12:Y:20:ARG:HH12	19:Y:101:TGL:HC32	1.51	0.73
3:P:33[A]:MET:HE3	3:P:39:SER:OG	1.89	0.73
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.88	0.73
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.25	0.72
4:Q:6:VAL:O	4:Q:7:LYS:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:43:LYS:HE3	30:S:225:HOH:O	1.89	0.72
1:A:39:ALA:CA	21:D:202:EDO:HO1	1.87	0.72
8:H:9:LYS:HZ1	8:H:9:LYS:HA	1.55	0.72
9:V:18:ARG:HG3	30:V:110:HOH:O	1.89	0.72
9:I:73:LYS:O	30:I:102:HOH:O	2.07	0.72
14:N:603[B]:HEA:HMD1	14:N:603[B]:HEA:HBD2	1.71	0.72
3:P:63:ARG:HE	27:P:305:CDL:CA2	2.03	0.71
28:C:307:PEK:H382	27:N:601:CDL:H271	1.71	0.71
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.71	0.71
28:P:308:PEK:H042	6:S:1:ALA:N	2.06	0.71
7:G:38:HIS:CE1	27:N:601:CDL:H141	2.25	0.71
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.21	0.70
1:N:307:SER:CB	27:N:601:CDL:H191	2.22	0.70
4:D:100[B]:LYS:HE3	30:D:358:HOH:O	1.91	0.70
6:F:1:ALA:HB3	6:S:65:ASP:OD2	1.92	0.70
9:V:18:ARG:HD3	30:V:114:HOH:O	1.90	0.70
2:B:174:ALA:CB	30:B:528:HOH:O	2.37	0.69
2:B:57:ASP:H	24:B:303:PSC:H221	1.56	0.69
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.08	0.69
19:N:611:TGL:C28	19:N:611:TGL:CB9	2.66	0.69
30:B:553:HOH:O	19:D:201:TGL:H281	1.91	0.69
7:G:38:HIS:HE1	27:N:601:CDL:H141	1.58	0.69
4:D:99:GLU:OE2	21:D:202:EDO:H22	1.93	0.68
19:Y:101:TGL:HC41	19:Y:101:TGL:OC1	1.92	0.68
27:N:601:CDL:C37	2:O:78:LEU:HD12	2.19	0.68
3:C:3:HIS:N	30:C:402:HOH:O	2.26	0.68
4:D:19[A]:ARG:HH21	4:D:21:ASP:CG	2.01	0.68
2:B:148:MET:HE2	30:B:547:HOH:O	1.94	0.68
3:C:224:LYS:CD	27:C:305:CDL:HB31	2.24	0.68
9:I:35:TYR:CD1	9:I:35:TYR:C	2.72	0.68
3:P:33[A]:MET:HE1	3:P:41:THR:HB	1.75	0.67
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.75	0.67
4:D:100[B]:LYS:CE	30:D:358:HOH:O	2.42	0.67
7:G:6:GLY:H	1:N:278[B]:MET:HE1	1.58	0.67
3:P:224:LYS:HD3	27:P:305:CDL:HB31	1.75	0.67
3:C:37:PHE:CG	25:C:302:DMU:H8	2.30	0.67
4:D:100[B]:LYS:HE3	30:D:301:HOH:O	1.94	0.67
1:N:136[B]:LEU:HD11	30:T:233:HOH:O	1.95	0.67
13:M:8:THR:OG1	30:M:201:HOH:O	2.13	0.67
1:A:324:LEU:HD22	2:B:42:ILE:HG13	1.76	0.67
3:P:33[A]:MET:HB2	25:P:307:DMU:H9	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.09	0.66
3:C:47:LEU:O	3:C:51[A]:MET:HG2	1.95	0.66
19:Q:201:TGL:H352	9:V:16:ARG:HE	1.60	0.66
9:I:15:ARG:NH2	30:I:101:HOH:O	1.99	0.66
27:P:305:CDL:H411	27:P:305:CDL:H452	1.75	0.66
1:A:459:PHE:CE1	21:D:202:EDO:H11	2.30	0.66
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	1.94	0.66
24:B:303:PSC:C1	9:I:14:ALA:HB2	2.17	0.66
1:N:136[B]:LEU:CD1	30:N:902:HOH:O	2.40	0.66
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	1.93	0.65
2:B:60:GLU:H	2:B:60:GLU:CD	2.04	0.65
24:N:612:PSC:H111	24:N:612:PSC:C32	2.26	0.65
30:A:877:HOH:O	4:D:17[A]:VAL:CG1	2.45	0.65
2:B:101:GLY:HA3	30:B:528:HOH:O	1.97	0.65
4:D:100[A]:LYS:NZ	30:D:301:HOH:O	1.88	0.65
3:C:180[B]:GLU:HG2	30:C:428:HOH:O	1.95	0.65
27:P:305:CDL:OB9	27:P:305:CDL:H532	1.96	0.65
1:N:382[B]:SER:CB	1:N:383[B]:MET:HE2	2.26	0.65
1:N:362[B]:SER:OG	30:N:702:HOH:O	2.15	0.65
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE3	2.31	0.65
1:A:312:ILE:HD12	30:A:707:HOH:O	1.96	0.65
9:I:73:LYS:CE	30:I:104:HOH:O	2.31	0.65
1:N:297[B]:MET:HB3	30:N:765:HOH:O	1.78	0.65
19:Y:101:TGL:HG11	19:Y:101:TGL:CA3	2.23	0.65
1:A:177:SER:H	1:A:180:GLN:HE21	1.45	0.64
27:C:305:CDL:HB21	27:C:305:CDL:OB6	1.97	0.64
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.64
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.09	0.64
1:A:417[B]:MET:CE	30:A:873:HOH:O	2.45	0.64
8:H:46:LYS:NZ	8:U:51:SER:O	2.29	0.64
2:O:39:LEU:HD11	19:Q:201:TGL:H221	1.79	0.64
3:P:33[A]:MET:HB2	25:P:307:DMU:C19	2.27	0.64
20:A:610:PGV:H311	13:M:19:LEU:HD23	1.79	0.64
14:N:602:HEA:H122	14:N:602:HEA:H262	1.80	0.64
24:N:612:PSC:H1	24:N:612:PSC:C34	2.22	0.64
7:G:8:HIS:CD2	7:G:9:GLY:H	2.15	0.64
1:A:356:ILE:HD13	14:A:602[B]:HEA:HMB1	1.79	0.64
7:T:7:ASP:O	7:T:9:GLY:N	2.25	0.64
1:A:513:LEU:O	1:A:514:LYS:CB	2.32	0.64
19:Q:201:TGL:HG31	30:Q:302:HOH:O	1.97	0.64
27:C:305:CDL:HB21	27:C:305:CDL:CB3	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:305:CDL:H211	27:C:305:CDL:H772	1.80	0.64
27:N:601:CDL:H161	27:N:601:CDL:OB3	1.97	0.63
1:A:281:GLY:C	7:T:4:ALA:HB1	2.22	0.63
22:C:306:CHD:H162	22:C:306:CHD:C23	2.28	0.63
12:L:47:LYS:HB3	30:L:222:HOH:O	1.98	0.63
27:N:601:CDL:H322	2:O:82:ARG:HA	1.80	0.63
7:G:8:HIS:O	1:N:178[A]:GLN:NE2	2.32	0.63
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.46	0.63
2:B:198:GLU:O	30:B:402:HOH:O	2.16	0.63
3:C:80[B]:ARG:HG2	3:C:233:PHE:CE1	2.33	0.63
20:A:610:PGV:H062	20:A:610:PGV:O14	1.99	0.63
19:Y:101:TGL:HA31	19:Y:101:TGL:CG1	2.27	0.62
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.62
2:O:83:ILE:O	2:O:87[A]:MET:HG3	1.99	0.62
28:C:307:PEK:O14	28:C:307:PEK:N	2.32	0.62
7:G:4:ALA:CB	1:N:282:PHE:HA	2.28	0.62
1:N:28:MET:CE	14:N:602:HEA:H271	2.30	0.62
27:C:305:CDL:HB21	27:C:305:CDL:HB32	1.80	0.62
1:N:302[B]:ARG:HE	2:O:84:LEU:HD11	1.62	0.62
19:A:608:TGL:HA72	19:A:608:TGL:H101	1.82	0.62
3:C:33[A]:MET:CB	25:C:302:DMU:H11	2.29	0.62
27:P:305:CDL:H392	27:P:305:CDL:H252	1.81	0.62
1:A:112:LEU:C	1:A:112:LEU:HD23	2.24	0.62
3:C:33[B]:MET:HA	25:C:302:DMU:H11	1.82	0.62
1:N:417[A]:MET:HE1	30:N:788:HOH:O	1.91	0.62
19:Q:201:TGL:H362	9:V:20:HIS:CE1	2.35	0.62
10:W:10:LYS:O	10:W:14[B]:GLU:HG3	2.00	0.62
7:G:12:GLY:N	30:G:202:HOH:O	2.30	0.61
1:A:407:ASP:OD2	21:A:619:EDO:H11	2.00	0.61
2:B:16[B]:ILE:HG23	30:B:523:HOH:O	1.99	0.61
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.83	0.61
24:B:303:PSC:H211	24:B:303:PSC:H251	1.83	0.61
19:Y:101:TGL:OG1	19:Y:101:TGL:OG3	2.18	0.61
28:P:308:PEK:H041	7:T:17:ARG:HH22	1.66	0.61
4:Q:78:TRP:HB3	19:Q:201:TGL:HB22	1.81	0.61
6:F:87[A]:THR:HG21	30:F:266:HOH:O	1.99	0.61
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	2.00	0.61
1:A:417[A]:MET:HE1	14:A:601:HEA:H263	1.82	0.61
1:N:178[B]:GLN:CG	1:N:186:TRP:CZ2	2.83	0.61
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	2.00	0.61
3:P:67:PHE:HE2	27:P:305:CDL:C1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.81	0.61
28:C:309:PEK:H351	7:T:5:LYS:HG3	1.83	0.61
21:A:618:EDO:O1	30:A:703:HOH:O	2.16	0.61
7:G:8:HIS:HD2	7:G:9:GLY:H	1.49	0.60
12:L:47:LYS:HB3	12:L:47:LYS:NZ	2.15	0.60
19:Y:101:TGL:OC1	19:Y:101:TGL:CC4	2.49	0.60
27:T:102:CDL:H111	27:T:102:CDL:OA5	2.01	0.60
1:A:261:TYR:OH	21:A:616:EDO:H12	2.01	0.60
9:I:31:PHE:C	9:I:31:PHE:CD2	2.79	0.60
2:O:13:THR:HB	2:O:168:LEU:HD23	1.84	0.60
12:Y:24[A]:MET:SD	19:Y:101:TGL:H172	2.42	0.60
6:S:13:ALA:CB	6:S:21[B]:MET:HE1	2.31	0.60
28:C:307:PEK:P	28:C:307:PEK:HN1	2.24	0.60
1:N:307:SER:HB3	27:N:601:CDL:H191	1.84	0.60
2:B:87[B]:MET:HB3	30:B:494:HOH:O	2.02	0.60
7:T:38:HIS:HE1	27:T:102:CDL:H141	1.64	0.60
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC3	1.84	0.60
19:D:201:TGL:H242	19:D:201:TGL:HA91	1.83	0.59
30:L:225:HOH:O	13:M:43:SER:HB2	2.02	0.59
1:A:28:MET:CE	14:A:601:HEA:C27	2.80	0.59
30:A:706:HOH:O	6:F:96:LEU:HD13	2.02	0.59
1:N:311[A]:ILE:HD13	27:N:601:CDL:H221	1.83	0.59
1:A:28:MET:CE	14:A:601:HEA:H271	2.33	0.59
30:A:877:HOH:O	4:D:17[A]:VAL:HG11	2.02	0.59
22:P:306:CHD:H231	22:P:306:CHD:C16	2.32	0.59
20:N:609:PGV:H311	13:Z:19:LEU:HD23	1.85	0.59
7:G:6:GLY:N	1:N:278[B]:MET:HE1	2.18	0.59
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:OD1	2.01	0.59
2:B:96:THR:HG22	30:B:522:HOH:O	2.01	0.58
1:N:28:MET:HE2	14:N:602:HEA:C27	2.33	0.58
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.21	0.58
1:N:178[B]:GLN:HG3	1:N:186:TRP:CE2	2.37	0.58
1:N:243:VAL:HB	14:N:603[B]:HEA:HAC	1.83	0.58
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.58
1:A:514:LYS:CE	30:A:702:HOH:O	2.47	0.58
1:A:397:PHE:HD2	30:A:738:HOH:O	1.85	0.58
20:A:610:PGV:H152	20:A:610:PGV:H322	1.84	0.58
22:C:306:CHD:H231	22:C:306:CHD:C16	2.30	0.58
6:F:87[B]:THR:HG21	30:F:262:HOH:O	2.04	0.58
4:Q:78:TRP:CB	19:Q:201:TGL:HB22	2.33	0.58
2:B:198:GLU:HG3	30:B:424:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.86	0.57
3:C:33[B]:MET:HG2	3:C:39:SER:O	2.03	0.57
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.86	0.57
3:C:33[A]:MET:HB2	25:C:302:DMU:H11	1.80	0.57
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.87	0.57
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.87	0.57
20:C:304:PGV:H12	20:C:304:PGV:H171	1.87	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.03	0.57
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.02	0.57
20:A:609:PGV:H312	20:C:304:PGV:H321	1.86	0.57
30:A:706:HOH:O	6:F:96:LEU:CD1	2.53	0.57
3:C:157:LYS:HZ1	28:C:307:PEK:H051	1.69	0.57
1:N:307:SER:O	1:N:311[B]:ILE:HG23	2.04	0.57
27:P:305:CDL:H651	27:P:305:CDL:H222	1.86	0.57
13:M:8:THR:N	30:M:201:HOH:O	2.38	0.57
19:A:611:TGL:HC31	12:L:14:SER:N	2.10	0.56
22:P:306:CHD:H12	22:P:306:CHD:H212	1.86	0.56
4:D:34:SER:H	4:D:37:GLN:NE2	2.02	0.56
1:N:28:MET:HE2	14:N:602:HEA:H271	1.86	0.56
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.86	0.56
2:B:140:ASN:HB3	30:B:520:HOH:O	2.05	0.56
24:B:303:PSC:H061	5:E:5:HIS:N	2.20	0.56
4:D:78:TRP:CA	19:D:201:TGL:HB21	2.35	0.56
12:L:47:LYS:CB	30:L:222:HOH:O	2.52	0.56
1:N:178[B]:GLN:HG3	1:N:178[B]:GLN:O	2.04	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
1:A:514:LYS:HE3	30:A:702:HOH:O	2.04	0.56
25:P:309:DMU:H12	25:P:309:DMU:H20	1.88	0.56
4:Q:109:HIS:HD2	30:Q:319:HOH:O	1.88	0.56
24:N:612:PSC:H211	2:O:56:MET:HG2	1.87	0.56
21:A:619:EDO:H12	30:A:796:HOH:O	2.05	0.56
3:P:33[B]:MET:SD	25:P:307:DMU:C19	2.93	0.56
21:A:620:EDO:H22	6:F:32:ASN:HD21	1.71	0.56
27:T:102:CDL:H321	27:T:102:CDL:OA7	2.05	0.56
1:N:112:LEU:HD23	1:N:112:LEU:C	2.32	0.55
24:B:303:PSC:H011	24:B:303:PSC:H41	1.88	0.55
1:A:291:HIS:NE2	18:A:607[B]:AZI:N1	2.53	0.55
1:A:291:HIS:CE1	18:A:607[B]:AZI:N2	2.74	0.55
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.41	0.55
22:C:306:CHD:C23	22:C:306:CHD:C16	2.84	0.55
1:N:115[A]:SER:O	1:N:121:GLY:HA2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HG3	6:F:38:ALA:CB	2.37	0.55
19:Q:201:TGL:H362	9:V:20:HIS:HE1	1.70	0.55
21:A:618:EDO:C1	30:A:703:HOH:O	2.54	0.55
3:C:157:LYS:NZ	28:C:307:PEK:H051	2.22	0.55
7:G:84:LYS:H	7:G:84:LYS:CD	2.17	0.55
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.89	0.55
28:P:308:PEK:H382	27:T:102:CDL:H271	1.88	0.55
2:B:81:LEU:HD12	27:T:102:CDL:H382	1.88	0.54
2:B:85:TYR:CE2	27:T:102:CDL:H112	2.41	0.54
4:D:78:TRP:N	19:D:201:TGL:HB21	2.23	0.54
4:Q:19[B]:ARG:NH1	30:Q:301:HOH:O	2.26	0.54
14:A:601:HEA:H262	14:A:601:HEA:H122	1.89	0.54
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.89	0.54
7:G:59:PRO:O	21:G:105:EDO:H12	2.07	0.54
21:N:621:EDO:H11	12:Y:10:ASN:HD22	1.72	0.54
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
4:Q:9:GLU:HG3	4:Q:11:TYR:CE2	2.41	0.54
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.89	0.54
11:X:47:ARG:CZ	11:X:47:ARG:HB3	2.35	0.54
1:N:54:TYR:HB2	30:N:859:HOH:O	2.07	0.54
3:P:33[A]:MET:CB	25:P:307:DMU:H9	2.37	0.54
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.07	0.54
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.90	0.54
1:A:1:FME:HE2	1:A:1:FME:HA	1.89	0.54
1:A:282:PHE:CA	7:T:4:ALA:CB	2.81	0.54
1:N:382[B]:SER:HB2	1:N:383[B]:MET:HE2	1.88	0.54
2:B:57:ASP:N	24:B:303:PSC:H221	2.22	0.54
2:B:82:ARG:HD2	2:B:86:MET:HE3	1.90	0.54
28:C:309:PEK:H292	30:T:201:HOH:O	2.06	0.54
5:R:6:GLU:HA	5:R:10:GLU:OE1	2.08	0.54
2:B:32[B]:PHE:CD1	2:B:32[B]:PHE:C	2.87	0.54
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.38	0.54
1:A:178[B]:GLN:HG2	7:T:7:ASP:OD1	2.07	0.53
1:A:379:TYR:CZ	1:A:383[A]:MET:HE1	2.43	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.48	0.53
27:N:601:CDL:H511	27:N:601:CDL:H222	1.90	0.53
27:T:102:CDL:H571	27:T:102:CDL:H782	1.90	0.53
1:A:449:MET:SD	2:B:5:MET:HG2	2.48	0.53
24:B:303:PSC:H32	9:I:14:ALA:HA	1.90	0.53
4:D:19[A]:ARG:HG3	4:D:21:ASP:OD1	2.08	0.53
11:X:7:PRO:HB2	11:X:12:LYS:HZ3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:P:308:PEK:C04	6:S:1:ALA:N	2.70	0.53
28:C:307:PEK:N	28:C:307:PEK:P	2.82	0.53
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.57	0.53
14:N:602:HEA:HBC1	14:N:602:HEA:HMC3	1.91	0.53
24:N:612:PSC:H342	2:O:41:ILE:HD13	1.91	0.53
3:P:54[A]:MET:HE1	20:P:304:PGV:H131	1.91	0.53
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.08	0.53
14:N:603[A]:HEA:HMC3	14:N:603[A]:HEA:HBC1	1.90	0.53
24:N:612:PSC:H342	2:O:41:ILE:CD1	2.39	0.53
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.73	0.53
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.91	0.53
1:A:178[B]:GLN:OE1	7:T:10:GLY:HA3	2.09	0.53
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.73	0.52
3:P:52:LEU:HG	27:P:305:CDL:H382	1.90	0.52
1:A:459:PHE:CE1	21:D:202:EDO:C1	2.93	0.52
2:B:60:GLU:CD	2:B:60:GLU:N	2.66	0.52
4:D:19[A]:ARG:CG	4:D:21:ASP:OD1	2.57	0.52
8:H:8:ILE:CG2	8:H:8:ILE:O	2.57	0.52
11:X:7:PRO:HB2	11:X:12:LYS:NZ	2.24	0.52
21:A:619:EDO:H22	30:M:220:HOH:O	2.08	0.52
2:B:116:LEU:HD11	2:B:226:MET:HB3	1.92	0.52
9:I:70:GLN:NE2	30:I:103:HOH:O	2.41	0.52
24:N:612:PSC:H111	24:N:612:PSC:H322	1.91	0.52
25:P:307:DMU:H29	25:P:307:DMU:C9	2.28	0.52
4:Q:19[A]:ARG:HD2	4:Q:21:ASP:CG	2.35	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.52
14:A:602[B]:HEA:HBD2	14:A:602[B]:HEA:HMD1	1.90	0.52
24:B:303:PSC:O03	24:B:303:PSC:H232	2.09	0.52
28:G:101:PEK:O04	30:G:201:HOH:O	2.19	0.52
27:N:601:CDL:H661	27:N:601:CDL:C61	2.32	0.52
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.09	0.52
1:A:324:LEU:CD2	2:B:42:ILE:HG13	2.40	0.52
20:A:610:PGV:C22	30:M:222:HOH:O	2.46	0.52
2:B:1:FME:HE1	2:B:133:LEU:HD13	1.92	0.52
3:C:95:THR:HG21	20:C:308:PGV:H312	1.91	0.52
1:N:307:SER:HB2	27:N:601:CDL:H191	1.90	0.51
3:C:33[A]:MET:CB	25:C:302:DMU:C22	2.80	0.51
2:O:221:LYS:HD2	2:O:221:LYS:O	2.10	0.51
28:G:101:PEK:H12	28:G:101:PEK:H161	1.90	0.51
3:P:38:ASN:O	25:P:310:DMU:H32	2.09	0.51
19:D:201:TGL:H363	9:I:20:HIS:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:514:LYS:HE2	30:S:212:HOH:O	2.11	0.51
27:N:601:CDL:H371	2:O:78:LEU:CD1	2.24	0.51
9:V:1:SAC:OAC	9:V:3:ALA:HB3	2.10	0.51
2:B:26:HIS:O	2:B:29[B]:MET:HB3	2.10	0.51
8:H:9:LYS:CG	8:H:10:ASN:N	2.69	0.51
3:P:224:LYS:HD3	27:P:305:CDL:CB3	2.41	0.51
8:H:43:MET:HE1	8:U:43:MET:HE1	1.92	0.51
8:U:44:THR:C	8:U:46:LYS:H	2.18	0.51
13:Z:36:HIS:CD2	13:Z:39:ASN:ND2	2.79	0.51
1:N:28:MET:CE	14:N:602:HEA:C27	2.89	0.51
1:N:513:LEU:O	1:N:514:LYS:CB	2.39	0.51
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.41	0.51
5:E:86:ILE:O	5:E:90:ARG:HG2	2.11	0.51
14:A:601:HEA:H122	14:A:601:HEA:HHC	1.93	0.50
10:J:52:TRP:O	10:J:57:HIS:HE1	1.94	0.50
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.46	0.50
1:A:411:LYS:NZ	30:A:709:HOH:O	2.45	0.50
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.77	0.50
20:N:609:PGV:C01	20:N:609:PGV:H22	2.18	0.50
7:T:3:ALA:O	7:T:4:ALA:CB	2.59	0.50
4:D:100[B]:LYS:HE2	30:D:358:HOH:O	2.10	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.50
1:A:28:MET:HE1	14:A:601:HEA:C27	2.41	0.50
20:A:610:PGV:H312	13:M:16:ALA:HA	1.92	0.50
1:N:302[B]:ARG:HE	2:O:84:LEU:CD1	2.24	0.50
30:P:447:HOH:O	8:U:84:LYS:HE3	2.11	0.50
28:T:101:PEK:H32	28:T:101:PEK:H71	1.91	0.50
1:A:74:MET:SD	1:A:74:MET:HB2	2.45	0.50
11:K:42:PRO:O	11:K:47:ARG:NH2	2.45	0.50
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.75	0.50
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.92	0.50
27:P:305:CDL:OB6	27:P:305:CDL:HB21	2.11	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.50
9:V:31:PHE:C	9:V:31:PHE:CD2	2.89	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.49
2:B:198:GLU:CG	30:B:424:HOH:O	2.58	0.49
4:D:78:TRP:HA	19:D:201:TGL:HB21	1.94	0.49
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.46	0.49
8:U:57:ARG:O	8:U:61:LYS:HB2	2.13	0.49
20:P:302:PGV:H72	20:P:302:PGV:H22	1.94	0.49
27:P:305:CDL:H411	27:P:305:CDL:C45	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:17[A]:VAL:O	4:Q:17[A]:VAL:HG23	2.12	0.49
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.32	0.49
3:C:156:ARG:HE	22:C:306:CHD:C24	2.25	0.49
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.94	0.49
3:C:37:PHE:CD2	25:C:302:DMU:H8	2.47	0.49
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.49
2:O:29[B]:MET:O	2:O:29[B]:MET:HG2	2.10	0.49
3:P:33[A]:MET:HE2	3:P:42:LEU:H	1.77	0.49
12:Y:20:ARG:HH22	19:Y:101:TGL:HC82	1.76	0.49
3:C:76:GLN:O	3:C:80[A]:ARG:HG3	2.12	0.49
8:U:44:THR:C	8:U:46:LYS:N	2.71	0.49
2:O:64:ILE:HG23	2:O:68:LEU:HD13	1.94	0.49
25:P:307:DMU:O6	25:P:310:DMU:H40	2.13	0.49
8:U:60:TYR:CD1	8:U:60:TYR:C	2.90	0.49
30:A:877:HOH:O	4:D:17[A]:VAL:HG12	2.09	0.48
25:C:302:DMU:H12	10:J:49:CYS:HB3	1.94	0.48
20:A:610:PGV:H202	20:A:610:PGV:H231	1.61	0.48
3:C:253:TYR:HE2	27:N:601:CDL:H641	1.77	0.48
6:S:95:GLN:HE21	6:S:95:GLN:CA	2.09	0.48
1:A:347:LEU:HD11	1:A:418:PHE:CE2	2.48	0.48
28:G:101:PEK:H101	28:G:101:PEK:H42	1.95	0.48
8:H:40:GLU:OE1	8:H:50:VAL:HG11	2.13	0.48
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.31	0.48
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.78	0.48
3:C:161[A]:GLN:NE2	28:C:307:PEK:H41	2.23	0.48
8:H:43:MET:HE3	8:H:49:ASP:N	2.29	0.48
1:A:378:HIS:O	1:A:383[B]:MET:HG2	2.13	0.48
12:Y:14:SER:H	19:Y:101:TGL:HC31	1.78	0.48
1:A:240:HIS:ND1	18:A:607[B]:AZI:N1	2.62	0.48
3:C:51[A]:MET:HE1	20:C:304:PGV:H161	1.95	0.48
1:N:321:PHE:CD1	24:N:612:PSC:H332	2.49	0.48
2:B:1:FME:CE	2:B:133:LEU:HD13	2.43	0.48
4:D:17[A]:VAL:HG23	4:D:17[A]:VAL:O	2.13	0.48
28:C:309:PEK:H361	27:T:102:CDL:H871	1.95	0.48
4:D:78:TRP:HB3	19:D:201:TGL:CB2	2.39	0.48
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.47
4:D:99:GLU:OE2	21:D:202:EDO:C2	2.61	0.47
9:I:22:VAL:O	9:I:26:MET:HG2	2.14	0.47
2:B:32[A]:PHE:C	2:B:35[A]:SER:OG	2.55	0.47
2:B:161:HIS:HB3	30:B:403:HOH:O	2.12	0.47
27:N:601:CDL:OA7	27:N:601:CDL:H342	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:73:LYS:NZ	30:I:104:HOH:O	2.42	0.47
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.49	0.47
27:P:305:CDL:H381	27:P:305:CDL:C27	2.15	0.47
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.97	0.47
2:B:56:MET:HG2	24:B:303:PSC:H231	1.94	0.47
4:D:100[B]:LYS:O	4:D:100[B]:LYS:CD	2.63	0.47
6:F:54[A]:ASN:ND2	6:F:54[A]:ASN:H	2.13	0.47
1:A:417[B]:MET:HE1	30:A:873:HOH:O	2.13	0.47
6:F:75:HIS:H	6:F:80:GLN:NE2	2.08	0.47
6:F:92:VAL:HG23	6:F:92:VAL:O	2.14	0.47
7:G:1:ALA:O	7:G:3:ALA:N	2.47	0.47
8:H:37:HIS:HD2	30:H:101:HOH:O	1.96	0.47
24:N:612:PSC:H12	2:O:64:ILE:HG21	1.97	0.47
3:P:63:ARG:HE	27:P:305:CDL:HA22	1.78	0.47
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.15	0.47
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.47
3:C:51[A]:MET:SD	27:C:305:CDL:H612	2.54	0.47
3:C:157:LYS:NZ	28:C:307:PEK:C05	2.77	0.47
27:N:601:CDL:H241	27:N:601:CDL:H531	1.97	0.47
20:N:609:PGV:H291	13:Z:16:ALA:HA	1.97	0.47
24:N:612:PSC:H111	24:N:612:PSC:H321	1.97	0.47
14:N:603[A]:HEA:C4B	18:N:608[A]:AZI:N1	2.64	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.46
25:P:309:DMU:H36	25:P:309:DMU:H34	1.35	0.46
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.16	0.46
2:O:53:THR:HG21	30:Q:308:HOH:O	2.14	0.46
2:B:153:LEU:HD12	30:B:522:HOH:O	2.16	0.46
5:R:14[B]:ARG:HG2	30:R:303:HOH:O	2.15	0.46
6:S:85:CYS:SG	6:S:87[B]:THR:HG22	2.55	0.46
1:N:243:VAL:HG11	18:N:608[B]:AZI:N2	2.30	0.46
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.15	0.46
19:N:611:TGL:HB92	19:N:611:TGL:H283	1.92	0.46
2:O:60:GLU:CD	2:O:60:GLU:H	2.21	0.46
3:C:33[A]:MET:HE3	25:C:302:DMU:H10	1.97	0.46
7:G:3:ALA:O	7:G:4:ALA:CB	2.64	0.46
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.97	0.46
20:N:610:PGV:H262	20:P:304:PGV:H292	1.97	0.46
12:Y:21:LEU:HA	12:Y:24[B]:MET:HE2	1.97	0.46
3:C:258:TRP:CZ3	27:N:601:CDL:H642	2.49	0.46
6:F:64:GLU:O	6:F:65:ASP:HB2	2.15	0.46
7:G:12:GLY:N	30:G:203:HOH:O	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.98	0.46
12:Y:24[B]:MET:SD	19:Y:101:TGL:HC21	2.56	0.46
1:A:28:MET:HE2	14:A:601:HEA:C27	2.46	0.46
24:N:612:PSC:H22	30:N:890:HOH:O	2.15	0.46
2:O:39:LEU:CD1	19:Q:201:TGL:H221	2.45	0.46
12:Y:47:LYS:HG3	12:Y:47:LYS:OXT	2.16	0.46
21:B:304:EDO:H22	30:B:527:HOH:O	2.16	0.46
25:C:310:DMU:H36	25:C:310:DMU:H34	0.99	0.46
22:G:102:CHD:H12	22:G:102:CHD:H212	1.98	0.46
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	1.97	0.46
5:R:41:LEU:HA	30:V:109:HOH:O	2.15	0.46
12:Y:20:ARG:HH22	19:Y:101:TGL:HC62	1.80	0.46
1:N:382[B]:SER:C	1:N:383[B]:MET:HE2	2.41	0.46
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.97	0.46
8:H:42:ALA:C	8:H:43:MET:O	2.59	0.46
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.98	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.45
7:G:42:ARG:NH1	7:G:42:ARG:HB2	2.30	0.45
8:H:60:TYR:CD1	8:H:60:TYR:C	2.94	0.45
1:N:172:LYS:NZ	1:N:178[A]:GLN:NE2	2.63	0.45
1:N:386:VAL:HG21	14:N:602:HEA:H261	1.98	0.45
19:A:608:TGL:HA52	19:A:608:TGL:HA22	1.86	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.45
3:C:63:ARG:HE	27:C:305:CDL:HA22	1.76	0.45
25:C:310:DMU:H32	25:C:310:DMU:H29	1.98	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.81	0.45
1:A:364:ASP:OD1	14:A:602[B]:HEA:O1A	2.34	0.45
19:A:611:TGL:HC32	12:L:20:ARG:HH21	1.64	0.45
19:Y:101:TGL:CA3	19:Y:101:TGL:CG1	2.91	0.45
1:A:148:PHE:HB3	3:C:28:THR:HB	1.98	0.45
19:A:608:TGL:HC22	30:A:919:HOH:O	2.15	0.45
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.47	0.45
12:L:26:THR:HG23	13:M:25:SER:HB3	1.99	0.45
1:N:311[A]:ILE:CD1	27:N:601:CDL:H221	2.45	0.45
24:N:612:PSC:C13	24:N:612:PSC:C34	2.87	0.45
2:O:221:LYS:HD2	2:O:221:LYS:C	2.42	0.45
3:P:156:ARG:HE	22:P:306:CHD:C24	2.29	0.45
22:P:306:CHD:C16	22:P:306:CHD:C23	2.94	0.45
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.46	0.45
20:N:609:PGV:C31	13:Z:19:LEU:HD23	2.46	0.45
2:O:41:ILE:O	2:O:42:ILE:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:HG3	8:U:10:ASN:N	2.31	0.45
2:B:41[B]:ILE:O	2:B:42:ILE:C	2.54	0.45
1:N:382[B]:SER:HB3	14:N:602:HEA:C2C	2.47	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.44
3:C:33[A]:MET:HE3	25:C:302:DMU:O16	2.17	0.44
7:G:11:TPO:C	30:G:202:HOH:O	2.64	0.44
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.99	0.44
9:V:25:PHE:O	9:V:28:SER:HB2	2.18	0.44
1:N:415:ALA:HB1	19:Q:201:TGL:H132	1.99	0.44
19:Y:101:TGL:H181	19:Y:101:TGL:OA1	2.17	0.44
4:D:99:GLU:OE1	21:D:202:EDO:H11	2.17	0.44
1:N:311[B]:ILE:HD11	27:N:601:CDL:H232	1.99	0.44
1:A:281:GLY:O	7:T:4:ALA:HB1	2.17	0.44
2:B:160:LEU:HD22	30:B:463:HOH:O	2.17	0.44
3:P:116:TRP:HA	3:P:117:PRO:C	2.42	0.44
2:B:82:ARG:HH11	2:B:86:MET:CE	2.30	0.44
3:C:33[B]:MET:CG	3:C:39:SER:HB3	2.48	0.44
7:G:42:ARG:HB2	7:G:42:ARG:HH11	1.82	0.44
27:N:601:CDL:H591	27:N:601:CDL:H561	1.76	0.44
2:O:29[B]:MET:HB2	9:V:35:TYR:CE1	2.52	0.44
3:P:33[B]:MET:CB	25:P:307:DMU:H9	2.46	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.44
3:P:29:SER:HB2	25:P:307:DMU:H21	1.98	0.44
1:A:74:MET:CG	1:A:74:MET:CA	2.81	0.44
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.32	0.44
6:F:87[A]:THR:HG21	30:F:209:HOH:O	2.17	0.44
2:O:48:THR:HB	9:V:16:ARG:CZ	2.47	0.44
7:G:58:LYS:HG2	21:G:105:EDO:H21	2.00	0.44
14:N:603[A]:HEA:HBC1	14:N:603[A]:HEA:CMC	2.48	0.44
24:N:612:PSC:O02	24:N:612:PSC:H011	2.18	0.44
8:U:7:LYS:HA	8:U:7:LYS:HE3	1.98	0.44
1:A:136[B]:LEU:CD1	30:A:933:HOH:O	2.43	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.74	0.44
22:P:301:CHD:H12	22:P:301:CHD:H212	2.00	0.44
27:T:102:CDL:H651	27:T:102:CDL:H602	2.00	0.44
2:B:32[A]:PHE:HD1	2:B:32[A]:PHE:HA	1.50	0.43
10:J:7:GLU:HG3	30:J:213:HOH:O	2.18	0.43
1:N:316:THR:HG21	14:N:603[A]:HEA:H14	2.00	0.43
2:O:191:LEU:HG	9:V:68:ILE:HD12	1.99	0.43
27:P:305:CDL:H222	27:P:305:CDL:C65	2.48	0.43
4:Q:19[A]:ARG:CD	4:Q:21:ASP:CG	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:21[B]:MET:HB2	6:S:21[B]:MET:HE3	1.49	0.43
10:W:54:SER:O	12:Y:46:LYS:HE2	2.18	0.43
1:A:243:VAL:HG11	18:A:607[B]:AZI:N3	2.33	0.43
30:B:423:HOH:O	8:H:62:SER:CA	2.41	0.43
10:J:36:MET:HB2	10:J:36:MET:HE2	1.76	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
2:O:116:LEU:HD13	2:O:226:MET:HG2	2.01	0.43
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.48	0.43
10:W:29:ASN:HD22	10:W:29:ASN:H	1.66	0.43
2:B:91:ASN:C	2:B:91:ASN:HD22	2.25	0.43
1:N:468:MET:HE1	14:N:602:HEA:H212	2.00	0.43
27:N:601:CDL:H181	27:N:601:CDL:HB32	2.00	0.43
27:T:102:CDL:H752	27:T:102:CDL:H562	1.99	0.43
2:B:28:LEU:HG	2:B:32[A]:PHE:CE2	2.53	0.43
2:B:91:ASN:OD1	2:B:183[B]:THR:HG21	2.18	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.00	0.43
20:A:609:PGV:H343	28:G:101:PEK:C38	2.44	0.43
2:B:28:LEU:O	2:B:29[A]:MET:C	2.58	0.43
6:F:43:LYS:HB2	6:F:43:LYS:HE2	1.59	0.43
6:F:54[A]:ASN:H	6:F:54[A]:ASN:HD22	1.65	0.43
2:O:5:MET:HE2	2:O:5:MET:HB3	1.84	0.43
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.47	0.43
1:A:426:PHE:N	1:A:427:PRO:CD	2.81	0.43
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
3:P:259:TRP:CD1	25:P:309:DMU:H30	2.53	0.43
6:S:54:ASN:HD22	6:S:54:ASN:C	2.26	0.43
2:B:56:MET:HB3	24:B:303:PSC:H252	2.00	0.43
28:C:307:PEK:H31	28:C:307:PEK:H02	1.99	0.43
7:G:1:ALA:C	7:G:3:ALA:H	2.27	0.43
1:N:112:LEU:HG	30:N:881:HOH:O	2.17	0.43
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.19	0.43
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.01	0.43
13:Z:36:HIS:HD2	13:Z:39:ASN:HD22	1.67	0.43
14:A:602[A]:HEA:HHA	14:A:602[A]:HEA:HAD2	1.69	0.43
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	2.00	0.43
7:G:59:PRO:HB2	21:G:105:EDO:H22	2.01	0.43
2:B:91:ASN:HD22	2:B:92:ASN:N	2.17	0.43
8:H:9:LYS:HE3	8:H:11:TYR:H	1.83	0.43
3:P:54[B]:MET:HB3	3:P:58:TRP:CZ3	2.54	0.43
6:S:52:ILE:O	6:S:94:HIS:CE1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ASN:OD1	1:A:514:LYS:HD2	2.19	0.42
28:C:307:PEK:H382	27:N:601:CDL:C27	2.43	0.42
10:J:33:ARG:HG2	22:J:101:CHD:H151	2.00	0.42
12:L:47:LYS:HB3	12:L:47:LYS:HZ3	1.83	0.42
27:P:305:CDL:H651	27:P:305:CDL:C22	2.49	0.42
2:B:16[A]:ILE:CD1	2:B:87[A]:MET:HG2	2.48	0.42
22:C:301:CHD:H212	22:C:301:CHD:H12	2.00	0.42
9:I:23:GLY:O	9:I:27:VAL:HG23	2.19	0.42
1:N:328:HIS:HB2	2:O:45:MET:SD	2.59	0.42
19:A:608:TGL:H242	19:A:608:TGL:HA92	2.01	0.42
24:B:303:PSC:H062	24:B:303:PSC:H042	1.72	0.42
4:D:17[A]:VAL:O	4:D:17[A]:VAL:CG2	2.67	0.42
1:N:316:THR:HG21	14:N:603[A]:HEA:C14	2.49	0.42
1:A:514:LYS:HG3	6:F:38:ALA:HB3	2.01	0.42
2:O:94:SER:OG	2:O:148:MET:HE2	2.19	0.42
6:S:94:HIS:HA	30:S:223:HOH:O	2.20	0.42
2:B:148:MET:HB3	30:B:547:HOH:O	2.19	0.42
3:C:3:HIS:HD2	3:C:4:GLN:O	2.02	0.42
3:C:157:LYS:HZ1	28:C:307:PEK:C05	2.31	0.42
1:N:353:LEU:HB3	2:O:31:VAL:HG13	2.00	0.42
12:Y:20:ARG:NH1	19:Y:101:TGL:HC32	2.27	0.42
28:C:309:PEK:C35	7:T:5:LYS:HG3	2.49	0.42
8:H:7:LYS:HG2	8:U:45:ALA:O	2.20	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.42
1:N:423[A]:MET:HG2	1:N:457:GLY:CA	2.50	0.42
3:P:172:TYR:CD2	28:P:308:PEK:H15	2.55	0.42
12:Y:24[B]:MET:SD	19:Y:101:TGL:CC2	3.07	0.42
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:N	2.68	0.42
1:A:316:THR:HG21	14:A:602[A]:HEA:C14	2.50	0.42
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:HA	1.82	0.42
1:N:311[B]:ILE:HG22	27:N:601:CDL:H442	2.02	0.42
20:A:610:PGV:H011	20:A:610:PGV:C3	2.50	0.42
27:C:305:CDL:H522	27:C:305:CDL:OB9	2.20	0.42
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.50	0.42
10:J:18:LEU:HD23	10:J:18:LEU:HA	1.92	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.42
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	2.02	0.42
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.33	0.42
3:P:224:LYS:HE3	27:P:305:CDL:OA7	2.19	0.42
7:G:35:SER:C	7:G:37:LEU:H	2.27	0.41
12:L:2:HIS:CG	12:L:3:TYR:H	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:602:HEA:H122	14:N:602:HEA:HHC	2.02	0.41
27:T:102:CDL:H421	27:T:102:CDL:H452	1.73	0.41
1:A:243:VAL:HG21	18:A:607[A]:AZI:N2	2.35	0.41
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.34	0.41
10:J:3:ASN:OD1	10:J:3:ASN:C	2.62	0.41
1:N:25:TRP:CE3	19:Y:101:TGL:HB91	2.55	0.41
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.02	0.41
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.85	0.41
2:B:49:LYS:CE	30:D:395:HOH:O	2.47	0.41
10:J:8:LYS:HA	10:J:8:LYS:HD3	1.87	0.41
5:R:31:LYS:HE2	6:S:83:PRO:O	2.19	0.41
8:U:50:VAL:C	8:U:52:VAL:N	2.78	0.41
19:Y:101:TGL:HC32	19:Y:101:TGL:HC62	1.70	0.41
2:B:42:ILE:HD13	2:B:42:ILE:HG21	1.77	0.41
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	2.01	0.41
8:H:7:LYS:O	8:H:8:ILE:HD12	2.20	0.41
3:P:246:ASP:HB2	30:P:486:HOH:O	2.19	0.41
20:A:610:PGV:H241	13:M:12:PRO:HG3	2.01	0.41
9:I:57:MET:O	9:I:61:GLU:HG2	2.20	0.41
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	2.02	0.41
19:Q:201:TGL:HA32	19:Q:201:TGL:HB51	2.03	0.41
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.56	0.41
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.46	0.41
7:T:44:ARG:HH22	7:T:84:LYS:NZ	2.18	0.41
9:V:35:TYR:CD1	9:V:35:TYR:C	2.98	0.41
1:A:378:HIS:HA	1:A:382[B]:SER:CB	2.51	0.41
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.47	0.41
3:C:155:ASP:OD2	6:F:2:SER:HA	2.21	0.41
4:D:17[B]:VAL:HG22	4:D:19[B]:ARG:HG3	2.02	0.41
8:U:50:VAL:O	8:U:51:SER:C	2.63	0.41
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.03	0.41
3:C:188:ILE:HG21	30:G:201:HOH:O	2.19	0.41
1:A:243:VAL:HG11	18:A:607[A]:AZI:N3	2.36	0.41
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.56	0.41
2:O:53:THR:CG2	30:Q:308:HOH:O	2.69	0.41
3:P:33[A]:MET:HB2	25:P:307:DMU:H8	2.00	0.41
19:Y:101:TGL:OC1	19:Y:101:TGL:HC51	2.21	0.41
12:L:46:LYS:HA	30:L:203:HOH:O	2.20	0.41
12:L:47:LYS:NZ	12:L:47:LYS:CB	2.83	0.41
1:N:2:PHE:HZ	19:Y:101:TGL:HG32	1.86	0.41
1:N:399:LEU:O	1:N:499:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:603[B]:HEA:C24	2:O:69:PRO:HB3	2.51	0.41
1:A:28:MET:HE2	14:A:601:HEA:H273	2.03	0.40
2:B:174:ALA:HB3	30:B:528:HOH:O	2.14	0.40
5:E:81:ILE:HD11	9:I:12:LEU:HD11	2.03	0.40
6:F:87[B]:THR:HG21	30:F:266:HOH:O	2.21	0.40
10:W:32:TYR:OH	22:W:101:CHD:H213	2.21	0.40
1:N:423[A]:MET:HG2	1:N:457:GLY:HA3	2.03	0.40
2:O:66:THR:HG22	30:O:493:HOH:O	2.20	0.40
1:A:240:HIS:CD2	1:A:240:HIS:C	2.99	0.40
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.21	0.40
2:B:16[A]:ILE:HD13	2:B:16[A]:ILE:HA	1.93	0.40
2:B:81:LEU:HD13	27:T:102:CDL:H151	2.03	0.40
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.56	0.40
5:R:77:PRO:O	5:R:79:LYS:HD2	2.22	0.40
3:C:258:TRP:CH2	25:C:310:DMU:H12	2.57	0.40
2:O:60:GLU:CD	2:O:60:GLU:N	2.79	0.40

All (3) 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)
30:B:491:HOH:O	30:D:341:HOH:O[2_584]	1.22	0.98
30:I:126:HOH:O	30:M:216:HOH:O[2_584]	1.92	0.28
30:B:541:HOH:O	30:L:228:HOH:O[2_584]	2.14	0.06

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	534/514 (104%)	516 (97%)	18 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/227 (103%)	227 (97%)	5 (2%)	2 (1%)	14	3
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	142 (97%)	4 (3%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	4 (3%)	3 (2%)	5	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	104/109 (95%)	103 (99%)	0	1 (1%)	12	2
6	F	100/98 (102%)	96 (96%)	1 (1%)	3 (3%)	3	0
6	S	98/98 (100%)	91 (93%)	3 (3%)	4 (4%)	2	0
7	G	82/85 (96%)	68 (83%)	9 (11%)	5 (6%)	1	0
7	T	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	1	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	0
13	M	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	4	0
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3597/3614 (100%)	3457 (96%)	109 (3%)	31 (1%)	14	3

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	2	SER
7	G	3	ALA
7	G	4	ALA
7	G	5	LYS

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Mol	Chain	Res	Type
8	H	43	MET
8	H	44	THR
13	M	42	LYS
4	Q	7	LYS
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	10	ASN
12	Y	46	LYS
5	R	6	GLU
6	S	96	LEU
7	T	4	ALA
8	U	8	ILE
6	F	95	GLN
8	H	45	ALA
6	F	96	LEU
4	Q	8	SER
8	U	45	ALA
8	U	51	SER
2	B	87[A]	MET
2	B	87[B]	MET
7	G	6	GLY
4	Q	6	VAL
6	S	93	PRO

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	447/426 (105%)	438 (98%)	9 (2%)	48	26
1	N	445/426 (104%)	434 (98%)	11 (2%)	42	18
2	B	219/210 (104%)	208 (95%)	11 (5%)	22	5
2	O	215/210 (102%)	207 (96%)	8 (4%)	30	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	233/226 (103%)	228 (98%)	5 (2%)	47	24
3	P	233/226 (103%)	230 (99%)	3 (1%)	61	42
4	D	132/129 (102%)	129 (98%)	3 (2%)	44	21
4	Q	131/129 (102%)	126 (96%)	5 (4%)	29	7
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	11
5	R	93/95 (98%)	88 (95%)	5 (5%)	20	4
6	F	85/81 (105%)	81 (95%)	4 (5%)	23	5
6	S	83/81 (102%)	73 (88%)	10 (12%)	5	1
7	G	68/68 (100%)	62 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	63 (93%)	5 (7%)	13	2
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	6
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	1
9	I	57/57 (100%)	55 (96%)	2 (4%)	32	10
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	26
10	W	50/50 (100%)	48 (96%)	2 (4%)	28	7
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	17
11	X	40/46 (87%)	38 (95%)	2 (5%)	22	5
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	17
12	Y	40/40 (100%)	38 (95%)	2 (5%)	22	5
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	37 (100%)	0	100	100
All	All	3131/3082 (102%)	3020 (96%)	111 (4%)	32	10

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	128	VAL
1	A	138	HIS
1	A	180	GLN
1	A	363	LEU
1	A	369	ASP
1	A	382[A]	SER

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Mol	Chain	Res	Type
1	A	382[B]	SER
1	A	514	LYS
2	B	35[A]	SER
2	B	35[B]	SER
2	B	42	ILE
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
3	C	17	PRO
3	C	33[A]	MET
3	C	33[B]	MET
3	C	127	LEU
3	C	159	MET
4	D	31	LYS
4	D	127	LYS
4	D	147	LYS
5	E	5	HIS
5	E	90	ARG
5	E	109	VAL
6	F	37	LYS
6	F	43	LYS
6	F	78	GLU
6	F	80	GLN
7	G	2	SER
7	G	7	ASP
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	60	TYR
9	I	2	THR
9	I	37	PHE
10	J	58	LYS
11	K	54	ARG
12	L	47	LYS

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Mol	Chain	Res	Type
1	N	128	VAL
1	N	138	HIS
1	N	178[A]	GLN
1	N	178[B]	GLN
1	N	180	GLN
1	N	265	LYS
1	N	311[A]	ILE
1	N	311[B]	ILE
1	N	369	ASP
1	N	495	LEU
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	171	LYS
2	O	221	LYS
3	P	110	PRO
3	P	159	MET
3	P	230	ASN
4	Q	6	VAL
4	Q	7	LYS
4	Q	51	LEU
4	Q	142	LYS
4	Q	143	ASN
5	R	6	GLU
5	R	45	PRO
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	93	PRO
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU

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Mol	Chain	Res	Type
7	T	2	SER
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	84	LYS
8	U	29	CYS
8	U	40	GLU
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	8	GLN
9	V	42	LYS
9	V	73	LYS
10	W	50	LEU
10	W	58	LYS
11	X	51	LYS
11	X	52	GLU
12	Y	16	GLU
12	Y	26	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	180	GLN
1	A	503	HIS
2	B	140	ASN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	101	HIS
4	D	119	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	32	ASN
6	F	80	GLN
7	G	8	HIS
7	G	76	ASN

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Mol	Chain	Res	Type
8	H	10	ASN
8	H	22	ASN
8	H	28	ASN
8	H	32	ASN
9	I	20	HIS
9	I	53	ASN
10	J	57	HIS
11	K	35	GLN
1	N	180	GLN
1	N	422	ASN
1	N	503	HIS
2	O	91	ASN
2	O	181	GLN
3	P	38	ASN
3	P	50	ASN
3	P	68	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	76	ASN
4	Q	101	HIS
4	Q	109	HIS
5	R	78	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	88	HIS
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	8	HIS
7	T	76	ASN
8	U	25	GLN
8	U	28	ASN
8	U	32	ASN
9	V	20	HIS
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN
13	Z	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.96	1 (12%)	7,9,11	1.84	3 (42%)
2	FME	O	1	2	8,9,10	1.26	1 (12%)	7,9,11	2.00	2 (28%)
7	TPO	G	11	7	8,10,11	2.03	3 (37%)	10,14,16	0.88	0
7	TPO	T	11	7	8,10,11	1.74	2 (25%)	10,14,16	1.28	1 (10%)
9	SAC	V	1	9	7,8,9	1.66	1 (14%)	8,9,11	1.35	2 (25%)
1	FME	N	1	1	8,9,10	1.26	1 (12%)	7,9,11	1.30	1 (14%)
9	SAC	I	1	9	7,8,9	1.50	1 (14%)	8,9,11	1.89	2 (25%)
2	FME	B	1	2	8,9,10	2.06	4 (50%)	7,9,11	1.90	2 (28%)

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
1	FME	A	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
7	TPO	T	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	7/7/8/10	-
1	FME	N	1	1	-	3/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.24	1.52	1.46
2	B	1	FME	CB-CA	3.59	1.59	1.53
9	I	1	SAC	CA-N	3.50	1.51	1.46
7	G	11	TPO	P-O1P	3.29	1.61	1.50
7	T	11	TPO	P-O1P	3.09	1.60	1.50
7	G	11	TPO	P-OG1	2.78	1.64	1.59
2	B	1	FME	CB-CG	2.65	1.61	1.51
1	N	1	FME	CA-N	2.40	1.49	1.46
2	B	1	FME	O-C	2.37	1.29	1.19
7	T	11	TPO	P-OG1	2.18	1.63	1.59
7	G	11	TPO	CB-CA	2.16	1.58	1.53
1	A	1	FME	O-C	2.13	1.28	1.19
2	O	1	FME	CB-CG	2.08	1.59	1.51
2	B	1	FME	CG-SD	-2.01	1.70	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OG-CB-CA	-3.53	101.96	110.97
9	I	1	SAC	C-CA-N	3.46	115.97	109.73
2	O	1	FME	CA-N-CN	3.36	127.98	122.82
1	A	1	FME	CE-SD-CG	3.23	111.50	100.40
2	B	1	FME	C-CA-N	-3.20	103.96	109.73
2	B	1	FME	CG-CB-CA	-3.02	104.55	112.95
9	V	1	SAC	CA-N-C1A	2.62	127.99	123.15
2	O	1	FME	CG-CB-CA	-2.59	105.74	112.95
1	A	1	FME	O-C-CA	-2.42	118.44	124.78
1	A	1	FME	C-CA-N	2.26	113.81	109.73
1	N	1	FME	O-C-CA	-2.11	119.26	124.78
7	T	11	TPO	CG2-CB-CA	2.08	117.27	113.16
9	V	1	SAC	O-C-CA	-2.00	119.54	124.78

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	CA-CB-OG1-P
7	T	11	TPO	CB-OG1-P-O2P
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	O-C-CA-CB
9	I	1	SAC	N-CA-CB-OG
1	N	1	FME	CA-CB-CG-SD
2	B	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
7	T	11	TPO	CB-OG1-P-O1P
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-CG2
9	V	1	SAC	C-CA-N-C1A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	TGL	Q	201	-	62,62,62	1.51	4 (6%)	65,65,65	1.47	7 (10%)
24	PSC	N	612	-	51,51,51	1.29	3 (5%)	57,59,59	1.19	4 (7%)
14	HEA	A	602[A]	18,1	66,67,67	1.94	22 (33%)	78,103,103	2.20	27 (34%)
21	EDO	A	613	-	3,3,3	0.58	0	2,2,2	1.32	0
21	EDO	A	612	-	3,3,3	0.40	0	2,2,2	1.48	0
28	PEK	G	101	-	52,52,52	1.08	6 (11%)	55,57,57	1.45	8 (14%)
21	EDO	A	619	-	3,3,3	0.26	0	2,2,2	0.78	0
21	EDO	S	103	-	3,3,3	1.30	0	2,2,2	0.49	0
27	CDL	C	305	-	99,99,99	1.50	17 (17%)	105,111,111	1.53	15 (14%)
21	EDO	N	613	-	3,3,3	1.61	1 (33%)	2,2,2	0.51	0
27	CDL	P	305	-	99,99,99	1.53	18 (18%)	105,111,111	1.63	18 (17%)
28	PEK	T	101	-	52,52,52	1.37	6 (11%)	55,57,57	2.47	8 (14%)
21	EDO	G	105	-	3,3,3	0.59	0	2,2,2	0.30	0
20	PGV	P	302	-	50,50,50	1.16	2 (4%)	53,56,56	1.32	4 (7%)
21	EDO	N	618	-	3,3,3	0.64	0	2,2,2	0.66	0
22	CHD	B	301	-	32,32,32	1.79	10 (31%)	51,51,51	2.26	22 (43%)
28	PEK	G	103	-	52,52,52	1.11	2 (3%)	55,57,57	1.19	4 (7%)
21	EDO	T	103	-	3,3,3	1.00	0	2,2,2	0.82	0
21	EDO	N	621	-	3,3,3	0.79	0	2,2,2	1.29	0
25	DMU	Z	101	-	34,34,34	0.80	1 (2%)	45,45,45	1.21	3 (6%)
22	CHD	P	301	-	32,32,32	1.60	8 (25%)	51,51,51	2.05	16 (31%)
22	CHD	J	101	-	32,32,32	0.91	0	51,51,51	2.27	20 (39%)
21	EDO	A	614	-	3,3,3	1.58	1 (33%)	2,2,2	0.78	0
21	EDO	O	302	-	3,3,3	0.65	0	2,2,2	0.58	0
24	PSC	B	303	-	51,51,51	1.28	4 (7%)	57,59,59	1.38	4 (7%)
21	EDO	A	620	-	3,3,3	0.45	0	2,2,2	0.84	0
21	EDO	F	104	-	3,3,3	0.68	0	2,2,2	0.34	0
23	CUA	O	301	2	0,1,1	-	-	-	-	-
18	AZI	N	608[A]	15,14	0,2,2	-	-	0,1,1	-	-
20	PGV	A	609	-	50,50,50	1.19	5 (10%)	53,56,56	1.30	6 (11%)
21	EDO	A	615	-	3,3,3	0.62	0	2,2,2	1.83	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CDL	N	601	-	99,99,99	1.53	15 (15%)	105,111,111	1.51	16 (15%)
20	PGV	P	304	-	50,50,50	1.07	4 (8%)	53,56,56	1.35	6 (11%)
25	DMU	P	307	-	34,34,34	0.94	1 (2%)	45,45,45	1.46	8 (17%)
19	TGL	A	608	-	62,62,62	1.31	6 (9%)	65,65,65	2.24	10 (15%)
21	EDO	N	619	-	3,3,3	1.21	0	2,2,2	0.19	0
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	N	616	-	3,3,3	1.04	0	2,2,2	0.19	0
19	TGL	D	201	-	62,62,62	2.00	5 (8%)	65,65,65	2.58	11 (16%)
27	CDL	T	102	-	99,99,99	1.45	13 (13%)	105,111,111	1.36	17 (16%)
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
25	DMU	P	309	-	34,34,34	0.81	1 (2%)	45,45,45	2.15	12 (26%)
21	EDO	D	202	-	3,3,3	1.05	0	2,2,2	0.36	0
19	TGL	Y	101	-	62,62,62	1.49	5 (8%)	65,65,65	1.81	10 (15%)
21	EDO	B	305	-	3,3,3	1.59	0	2,2,2	0.24	0
25	DMU	C	310	-	34,34,34	0.91	1 (2%)	45,45,45	2.51	13 (28%)
14	HEA	N	603[B]	18,1	66,67,67	1.65	13 (19%)	78,103,103	2.43	30 (38%)
21	EDO	L	101	-	3,3,3	0.74	0	2,2,2	0.84	0
21	EDO	S	102	-	3,3,3	1.07	0	2,2,2	0.43	0
21	EDO	R	201	-	3,3,3	0.87	0	2,2,2	0.63	0
21	EDO	B	304	-	3,3,3	0.16	0	2,2,2	1.40	0
20	PGV	C	304	-	50,50,50	0.98	3 (6%)	53,56,56	1.12	4 (7%)
28	PEK	C	309	-	52,52,52	1.19	2 (3%)	55,57,57	1.37	5 (9%)
21	EDO	F	103	-	3,3,3	1.11	0	2,2,2	0.11	0
21	EDO	E	202	-	3,3,3	0.93	0	2,2,2	0.66	0
22	CHD	P	306	-	32,32,32	1.49	6 (18%)	51,51,51	3.47	22 (43%)
21	EDO	N	620	-	3,3,3	0.57	0	2,2,2	0.05	0
25	DMU	P	310	-	34,34,34	1.11	2 (5%)	45,45,45	1.79	10 (22%)
25	DMU	C	311	-	34,34,34	1.04	1 (2%)	45,45,45	2.33	13 (28%)
14	HEA	N	602	1	66,67,67	1.88	26 (39%)	78,103,103	2.41	29 (37%)
20	PGV	C	308	-	50,50,50	1.26	2 (4%)	53,56,56	1.44	7 (13%)
21	EDO	W	102	-	3,3,3	0.49	0	2,2,2	0.65	0
21	EDO	A	618	-	3,3,3	0.41	0	2,2,2	1.03	0
25	DMU	M	101	-	34,34,34	0.90	1 (2%)	45,45,45	1.44	6 (13%)
14	HEA	A	602[B]	18,1	66,67,67	1.87	19 (28%)	78,103,103	2.20	22 (28%)
18	AZI	N	607[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	P	311	-	3,3,3	0.87	0	2,2,2	0.50	0
21	EDO	A	616	-	3,3,3	3.00	1 (33%)	2,2,2	5.57	1 (50%)
14	HEA	A	601	1	66,67,67	1.91	22 (33%)	78,103,103	2.84	31 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	E	203	-	3,3,3	0.77	0	2,2,2	0.53	0
21	EDO	C	312	-	3,3,3	0.64	0	2,2,2	0.60	0
19	TGL	N	611	-	62,62,62	1.12	4 (6%)	65,65,65	1.69	10 (15%)
21	EDO	B	307	-	3,3,3	0.67	0	2,2,2	0.04	0
18	AZI	A	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
21	EDO	P	312	-	3,3,3	0.77	0	2,2,2	1.65	1 (50%)
22	CHD	G	102	-	32,32,32	1.98	10 (31%)	51,51,51	1.98	14 (27%)
20	PGV	A	610	-	50,50,50	1.41	5 (10%)	53,56,56	1.88	7 (13%)
20	PGV	N	610	-	50,50,50	1.15	6 (12%)	53,56,56	1.48	9 (16%)
21	EDO	M	102	-	3,3,3	0.24	0	2,2,2	1.04	0
28	PEK	C	307	-	52,52,52	1.50	4 (7%)	55,57,57	1.50	9 (16%)
21	EDO	S	104	-	3,3,3	0.63	0	2,2,2	1.66	1 (50%)
21	EDO	D	203	-	3,3,3	0.56	0	2,2,2	0.35	0
14	HEA	N	603[A]	18,1	66,67,67	2.00	28 (42%)	78,103,103	2.06	32 (41%)
25	DMU	C	302	-	34,34,34	0.75	1 (2%)	45,45,45	1.47	7 (15%)
21	EDO	G	104	-	3,3,3	0.99	0	2,2,2	0.62	0
18	AZI	N	608[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	F	102	-	3,3,3	0.94	0	2,2,2	0.20	0
21	EDO	E	201	-	3,3,3	0.70	0	2,2,2	0.77	0
21	EDO	Y	102	-	3,3,3	0.53	0	2,2,2	0.61	0
21	EDO	N	614	-	3,3,3	0.47	0	2,2,2	1.07	0
22	CHD	C	306	-	32,32,32	1.30	5 (15%)	51,51,51	3.30	19 (37%)
22	CHD	C	301	-	32,32,32	1.77	6 (18%)	51,51,51	2.31	19 (37%)
22	CHD	W	101	-	32,32,32	1.27	4 (12%)	51,51,51	2.62	27 (52%)
21	EDO	A	617	-	3,3,3	1.38	0	2,2,2	0.41	0
21	EDO	B	306	-	3,3,3	0.58	0	2,2,2	0.30	0
21	EDO	N	617	-	3,3,3	0.65	0	2,2,2	0.84	0
28	PEK	P	308	-	52,52,52	1.24	2 (3%)	55,57,57	1.37	5 (9%)
23	CUA	B	302	30,2	0,1,1	-	-	-	-	-
20	PGV	N	609	-	50,50,50	1.20	2 (4%)	53,56,56	1.23	6 (11%)
21	EDO	N	615	-	3,3,3	0.69	0	2,2,2	1.27	0
19	TGL	A	611	-	62,62,62	1.28	3 (4%)	65,65,65	1.83	13 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	Q	201	-	-	30/65/65/65	-
24	PSC	N	612	-	-	28/55/55/55	-
14	HEA	A	602[A]	18,1	-	7/36/76/76	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
28	PEK	G	101	-	-	19/56/56/56	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
27	CDL	C	305	-	-	53/110/110/110	-
21	EDO	N	613	-	-	0/1/1/1	-
27	CDL	P	305	-	-	54/110/110/110	-
28	PEK	T	101	-	-	23/56/56/56	-
21	EDO	G	105	-	-	0/1/1/1	-
20	PGV	P	302	-	-	24/55/55/55	-
21	EDO	N	618	-	-	1/1/1/1	-
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
28	PEK	G	103	-	-	31/56/56/56	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	N	621	-	-	1/1/1/1	-
25	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
22	CHD	P	301	-	-	3/9/74/74	0/4/4/4
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	O	302	-	-	0/1/1/1	-
24	PSC	B	303	-	-	33/55/55/55	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	A	615	-	-	1/1/1/1	-
27	CDL	N	601	-	-	59/110/110/110	-
20	PGV	P	304	-	-	13/55/55/55	-
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
19	TGL	A	608	-	-	34/65/65/65	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
19	TGL	D	201	-	-	36/65/65/65	-
27	CDL	T	102	-	-	51/110/110/110	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	D	202	-	-	1/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
21	EDO	B	305	-	-	1/1/1/1	-
25	DMU	C	310	-	-	7/19/59/59	0/2/2/2
14	HEA	N	603[B]	18,1	-	7/36/76/76	-
21	EDO	L	101	-	-	1/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
20	PGV	C	304	-	-	17/55/55/55	-
28	PEK	C	309	-	-	26/56/56/56	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
22	CHD	P	306	-	-	5/9/74/74	0/4/4/4
21	EDO	N	620	-	-	0/1/1/1	-
25	DMU	P	310	-	-	10/19/59/59	0/2/2/2
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
14	HEA	N	602	1	-	6/36/76/76	-
20	PGV	C	308	-	-	23/55/55/55	-
21	EDO	W	102	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
25	DMU	M	101	-	-	4/19/59/59	0/2/2/2
14	HEA	A	602[B]	18,1	-	6/36/76/76	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	A	616	-	-	1/1/1/1	-
14	HEA	A	601	1	-	7/36/76/76	-
21	EDO	E	203	-	-	0/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
19	TGL	N	611	-	-	39/65/65/65	-
21	EDO	B	307	-	-	0/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
22	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	PGV	A	610	-	-	28/55/55/55	-
20	PGV	N	610	-	-	11/55/55/55	-
21	EDO	M	102	-	-	0/1/1/1	-
28	PEK	C	307	-	-	31/56/56/56	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	D	203	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	603[A]	18,1	-	6/36/76/76	-
25	DMU	C	302	-	-	9/19/59/59	0/2/2/2
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	1/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
22	CHD	C	306	-	-	5/9/74/74	0/4/4/4
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
28	PEK	P	308	-	-	25/56/56/56	-
20	PGV	N	609	-	-	35/55/55/55	-
21	EDO	N	615	-	-	0/1/1/1	-
19	TGL	A	611	-	-	39/65/65/65	-

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	10.00	1.52	1.22
19	D	201	TGL	OG2-CB1	7.60	1.55	1.34
19	Y	101	TGL	OG2-CB1	6.73	1.53	1.34
19	Q	201	TGL	OG2-CB1	6.52	1.52	1.34
28	C	307	PEK	O01-C1	6.35	1.52	1.34
19	D	201	TGL	OG1-CA1	6.26	1.51	1.33
19	A	611	TGL	OG2-CB1	6.21	1.51	1.34
19	Y	101	TGL	OG3-CC1	6.00	1.50	1.33
20	N	609	PGV	O03-C19	5.93	1.50	1.33
20	A	610	PGV	O01-C1	5.92	1.51	1.34
28	C	307	PEK	O03-C21	5.87	1.50	1.33
27	N	601	CDL	OB8-CB7	5.79	1.50	1.33
27	N	601	CDL	OB6-CB5	5.76	1.50	1.34
19	Q	201	TGL	OB1-CB1	5.76	1.39	1.22
28	T	101	PEK	C2-C1	5.63	1.67	1.50
27	P	305	CDL	OA8-CA7	5.63	1.49	1.33
27	P	305	CDL	OB8-CB7	5.62	1.49	1.33
24	N	612	PSC	O01-C1	5.52	1.49	1.34
28	P	308	PEK	O01-C1	5.49	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	102	CDL	OB8-CB7	5.47	1.49	1.33
27	T	102	CDL	OB6-CB5	5.35	1.49	1.34
20	C	308	PGV	O01-C1	5.35	1.49	1.34
20	C	308	PGV	O03-C19	5.18	1.48	1.33
27	C	305	CDL	OA8-CA7	5.17	1.48	1.33
27	T	102	CDL	OA6-CA5	5.12	1.48	1.34
28	C	309	PEK	O01-C1	5.12	1.48	1.34
19	A	608	TGL	OG1-CA1	5.12	1.48	1.33
28	C	309	PEK	O03-C21	5.06	1.48	1.33
21	A	616	EDO	C2-C1	5.02	1.83	1.48
27	N	601	CDL	OA6-CA5	5.00	1.48	1.34
14	N	603[A]	HEA	FE-NC	4.90	2.11	1.95
22	G	102	CHD	C8-C7	4.83	1.61	1.53
24	N	612	PSC	O03-C19	4.80	1.47	1.33
27	T	102	CDL	OA8-CA7	4.79	1.47	1.33
27	N	601	CDL	OA8-CA7	4.78	1.47	1.33
28	G	103	PEK	O01-C1	4.78	1.47	1.34
19	N	611	TGL	OG1-CA1	4.75	1.47	1.33
19	Q	201	TGL	OG1-CA1	4.73	1.47	1.33
22	C	301	CHD	C11-C12	4.72	1.61	1.53
20	P	302	PGV	O01-C1	4.71	1.47	1.34
28	P	308	PEK	O03-C21	4.70	1.47	1.33
24	B	303	PSC	O01-C1	4.69	1.47	1.34
20	P	302	PGV	O03-C19	4.68	1.47	1.33
19	A	611	TGL	OG3-CC1	4.66	1.47	1.33
20	A	610	PGV	O03-C19	4.65	1.46	1.33
19	Q	201	TGL	OG3-CC1	4.64	1.46	1.33
27	C	305	CDL	PB2-OB3	4.60	1.67	1.50
27	P	305	CDL	OA6-CA5	4.58	1.47	1.34
19	A	608	TGL	OG2-CB1	4.53	1.47	1.34
28	G	103	PEK	O03-C21	4.53	1.46	1.33
24	B	303	PSC	O03-C19	4.49	1.46	1.33
19	A	611	TGL	OG1-CA1	4.45	1.46	1.33
14	A	602[A]	HEA	C4D-C3D	-4.43	1.37	1.45
14	A	601	HEA	CHA-C1A	4.42	1.47	1.38
19	Y	101	TGL	OG1-CA1	4.39	1.46	1.33
19	N	611	TGL	OG2-CB1	4.35	1.46	1.34
14	A	601	HEA	CHB-C4A	4.31	1.46	1.38
27	C	305	CDL	OA6-CA5	4.25	1.46	1.34
25	C	311	DMU	O16-C6	4.21	1.47	1.40
14	A	602[A]	HEA	FE-ND	4.21	2.07	1.94
20	N	609	PGV	O01-C1	4.15	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[A]	HEA	CHB-C4A	4.10	1.46	1.38
14	A	602[B]	HEA	FE-ND	4.08	2.07	1.94
14	A	601	HEA	C12-C11	-4.03	1.45	1.52
14	A	602[B]	HEA	C4B-C3B	-4.03	1.37	1.44
14	A	601	HEA	CHD-C1D	4.00	1.46	1.38
14	N	603[A]	HEA	C4C-NC	-4.00	1.32	1.39
27	C	305	CDL	OB8-CB7	3.97	1.45	1.33
24	B	303	PSC	C13-C12	3.96	1.54	1.31
27	C	305	CDL	OB6-CB5	3.94	1.45	1.34
14	A	601	HEA	C3A-C4A	-3.91	1.39	1.46
14	N	603[A]	HEA	O11-C11	3.90	1.51	1.42
14	A	602[A]	HEA	FE-NC	3.88	2.08	1.95
24	N	612	PSC	C13-C12	3.83	1.54	1.31
14	N	603[A]	HEA	FE-ND	3.81	2.06	1.94
14	A	602[A]	HEA	FE-NA	3.78	2.07	1.95
19	A	608	TGL	OG3-CC1	3.75	1.44	1.33
22	G	102	CHD	C4-C5	3.75	1.59	1.53
27	P	305	CDL	PB2-OB3	3.74	1.64	1.50
14	N	602	HEA	C3A-C4A	-3.73	1.39	1.46
14	N	603[A]	HEA	C4D-C3D	-3.72	1.38	1.45
19	N	611	TGL	OG3-CC1	3.68	1.44	1.33
14	A	602[B]	HEA	C3A-C4A	-3.67	1.39	1.46
22	G	102	CHD	C11-C9	3.65	1.59	1.53
14	A	602[A]	HEA	CHD-C1D	3.64	1.45	1.38
19	D	201	TGL	OG3-CC1	3.62	1.43	1.33
14	A	602[B]	HEA	FE-NC	3.60	2.07	1.95
14	A	602[B]	HEA	C4A-NA	-3.58	1.32	1.39
25	P	307	DMU	O16-C6	3.57	1.46	1.40
14	N	603[B]	HEA	CHA-C1A	3.53	1.45	1.38
25	P	310	DMU	O16-C6	3.52	1.46	1.40
14	N	602	HEA	CMA-C3A	3.48	1.52	1.45
14	A	602[B]	HEA	C1A-C2A	-3.47	1.39	1.45
22	B	301	CHD	O7-C7	3.47	1.50	1.43
14	N	603[B]	HEA	C4B-NB	-3.43	1.34	1.40
14	N	602	HEA	CMB-C2B	3.42	1.58	1.50
27	P	305	CDL	OB6-CB5	3.41	1.43	1.34
14	N	603[B]	HEA	CHB-C4A	3.40	1.45	1.38
22	P	301	CHD	C23-C24	3.38	1.58	1.50
14	N	603[B]	HEA	C1B-C2B	-3.38	1.38	1.44
22	G	102	CHD	O7-C7	3.33	1.50	1.43
14	N	603[B]	HEA	C4B-C3B	-3.32	1.39	1.44
14	A	602[B]	HEA	CHD-C1D	3.31	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CHD-C1D	3.30	1.45	1.38
22	P	306	CHD	C11-C9	3.30	1.59	1.53
22	G	102	CHD	C1-C2	3.29	1.60	1.53
28	T	101	PEK	P-O14	3.29	1.62	1.50
14	A	602[A]	HEA	CHC-C1C	3.26	1.46	1.39
14	N	603[B]	HEA	C4A-NA	-3.24	1.33	1.39
19	A	608	TGL	OG2-CG2	3.23	1.54	1.46
28	G	101	PEK	O01-C02	3.19	1.54	1.46
22	G	102	CHD	C19-C10	3.18	1.59	1.54
22	P	301	CHD	C11-C12	3.17	1.58	1.53
27	N	601	CDL	C59-C58	-3.17	1.33	1.51
27	N	601	CDL	C22-C21	-3.16	1.33	1.51
27	C	305	CDL	C79-C78	-3.16	1.33	1.51
14	N	602	HEA	C12-C11	-3.14	1.47	1.52
14	N	603[B]	HEA	FE-NB	3.14	2.04	1.94
20	N	610	PGV	C01-C02	3.13	1.60	1.50
22	B	301	CHD	C8-C7	3.12	1.58	1.53
27	T	102	CDL	C59-C58	-3.11	1.34	1.51
14	N	603[A]	HEA	CHC-C1C	3.09	1.46	1.39
25	C	310	DMU	O16-C6	3.09	1.45	1.40
20	P	304	PGV	O05-C05	3.08	1.52	1.43
27	C	305	CDL	C59-C58	-3.07	1.34	1.51
14	A	602[B]	HEA	CHC-C4B	3.07	1.44	1.38
14	N	602	HEA	C1A-C2A	-3.06	1.39	1.45
27	C	305	CDL	O1-C1	3.04	1.52	1.43
22	P	301	CHD	C11-C9	3.04	1.58	1.53
20	A	609	PGV	C01-C02	3.04	1.60	1.50
27	P	305	CDL	C19-C18	-3.02	1.34	1.51
22	C	301	CHD	C11-C9	3.01	1.58	1.53
20	N	610	PGV	O01-C1	3.01	1.42	1.34
14	A	602[A]	HEA	C4C-NC	-3.00	1.33	1.39
22	B	301	CHD	C19-C10	2.99	1.59	1.54
22	B	301	CHD	C10-C9	-2.99	1.50	1.56
27	C	305	CDL	C82-C81	-2.98	1.34	1.51
27	T	102	CDL	C79-C78	-2.98	1.34	1.51
20	A	610	PGV	O02-C1	2.97	1.31	1.22
25	M	101	DMU	O16-C6	2.97	1.45	1.40
27	C	305	CDL	C62-C61	-2.97	1.34	1.51
22	C	301	CHD	C23-C24	2.96	1.57	1.50
27	N	601	CDL	C82-C81	-2.96	1.35	1.51
14	N	603[A]	HEA	CHD-C1D	2.95	1.44	1.38
22	P	306	CHD	C16-C17	2.94	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	305	CDL	C62-C61	-2.94	1.35	1.51
14	A	602[B]	HEA	CHB-C4A	2.93	1.44	1.38
20	N	610	PGV	O03-C01	2.93	1.51	1.45
14	A	601	HEA	C12-C13	2.92	1.63	1.53
14	N	602	HEA	CHC-C1C	2.92	1.45	1.39
14	N	603[A]	HEA	CHC-C4B	2.91	1.44	1.38
27	P	305	CDL	C42-C41	-2.91	1.35	1.51
27	P	305	CDL	C22-C21	-2.91	1.35	1.51
27	T	102	CDL	C22-C21	-2.89	1.35	1.51
27	N	601	CDL	C79-C78	-2.89	1.35	1.51
27	N	601	CDL	C19-C18	-2.89	1.35	1.51
14	N	602	HEA	CHA-C1A	2.89	1.44	1.38
19	A	608	TGL	OC1-CC1	-2.88	1.14	1.22
28	T	101	PEK	C3-C2	2.87	1.62	1.52
28	G	101	PEK	P-O14	2.86	1.61	1.50
27	N	601	CDL	C62-C61	-2.86	1.35	1.51
28	T	101	PEK	O11-C03	2.85	1.55	1.44
14	N	602	HEA	C1B-C2B	-2.85	1.39	1.44
27	C	305	CDL	C22-C21	-2.83	1.35	1.51
20	P	304	PGV	C01-C02	2.83	1.59	1.50
22	C	301	CHD	C8-C7	2.83	1.58	1.53
27	P	305	CDL	C59-C58	-2.82	1.35	1.51
22	C	306	CHD	O26-C24	-2.82	1.21	1.30
14	N	603[B]	HEA	C1D-ND	-2.82	1.35	1.40
14	A	601	HEA	CBD-CAD	2.81	1.60	1.52
27	N	601	CDL	C42-C41	-2.79	1.35	1.51
20	A	609	PGV	O01-C1	2.78	1.42	1.34
14	N	603[A]	HEA	C1D-C2D	-2.78	1.39	1.44
14	A	602[A]	HEA	C1D-C2D	-2.78	1.39	1.44
27	C	305	CDL	C19-C18	-2.77	1.36	1.51
22	C	301	CHD	C2-C3	2.77	1.58	1.51
25	P	310	DMU	C10-C5	2.77	1.60	1.52
27	T	102	CDL	C62-C61	-2.76	1.36	1.51
25	Z	101	DMU	O16-C6	2.75	1.44	1.40
22	C	301	CHD	C4-C3	2.75	1.57	1.51
27	T	102	CDL	C39-C38	-2.73	1.36	1.51
22	C	306	CHD	C16-C17	2.73	1.60	1.54
27	N	601	CDL	C39-C38	-2.73	1.36	1.51
27	P	305	CDL	C39-C38	-2.72	1.36	1.51
14	A	602[A]	HEA	CBD-CGD	2.70	1.56	1.50
22	P	301	CHD	C6-C7	2.69	1.57	1.52
14	N	602	HEA	CMD-C2D	2.69	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	304	PGV	O01-C02	-2.68	1.39	1.46
14	N	602	HEA	C4B-NB	-2.68	1.35	1.40
14	N	602	HEA	C3A-C2A	2.68	1.42	1.36
14	N	603[A]	HEA	CMA-C3A	2.67	1.50	1.45
22	P	301	CHD	C16-C17	2.67	1.59	1.54
14	A	601	HEA	CHC-C4B	2.67	1.43	1.38
14	N	603[B]	HEA	C3A-C4A	-2.66	1.41	1.46
14	N	603[B]	HEA	C1A-C2A	-2.66	1.40	1.45
27	P	305	CDL	C79-C78	-2.65	1.36	1.51
14	N	602	HEA	CBA-CAA	2.65	1.60	1.52
14	A	601	HEA	CHC-C1C	2.63	1.45	1.39
20	C	304	PGV	O01-C02	-2.63	1.40	1.46
14	A	601	HEA	CHD-C4C	2.63	1.45	1.39
28	G	101	PEK	O01-C1	2.63	1.41	1.34
27	C	305	CDL	C42-C41	-2.63	1.36	1.51
14	A	602[B]	HEA	CHD-C4C	2.62	1.45	1.39
14	N	602	HEA	C1D-C2D	-2.62	1.39	1.44
27	T	102	CDL	C42-C41	-2.61	1.36	1.51
14	N	603[A]	HEA	C1A-NA	-2.60	1.34	1.39
19	Y	101	TGL	CG3-CG2	2.57	1.58	1.50
19	Y	101	TGL	CB2-CB1	2.57	1.58	1.50
20	C	304	PGV	O05-C05	2.56	1.51	1.43
14	N	603[A]	HEA	C1B-NB	-2.56	1.33	1.38
27	T	102	CDL	C19-C18	-2.55	1.37	1.51
14	N	602	HEA	CHB-C4A	2.55	1.43	1.38
28	C	307	PEK	O02-C1	2.53	1.30	1.22
14	A	602[B]	HEA	C18-C19	2.53	1.39	1.33
27	P	305	CDL	C82-C81	-2.52	1.37	1.51
20	P	304	PGV	O03-C19	2.52	1.40	1.33
14	A	602[B]	HEA	C4C-NC	-2.51	1.34	1.39
27	C	305	CDL	C39-C38	-2.51	1.37	1.51
14	N	603[A]	HEA	C4B-NB	-2.51	1.36	1.40
20	A	609	PGV	C3-C2	2.50	1.61	1.52
14	A	601	HEA	CHA-C4D	2.50	1.44	1.39
27	C	305	CDL	CB2-C1	2.49	1.60	1.51
22	B	301	CHD	C18-C13	2.49	1.58	1.54
21	N	613	EDO	O2-C2	2.49	1.54	1.42
22	C	306	CHD	O25-C24	2.48	1.30	1.22
14	A	602[A]	HEA	C4B-C3B	-2.48	1.40	1.44
14	N	603[A]	HEA	CHA-C1A	2.47	1.43	1.38
14	A	601	HEA	C1D-C2D	-2.47	1.39	1.44
22	B	301	CHD	C20-C17	2.47	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	101	PEK	C3-C4	2.47	1.62	1.52
14	A	602[B]	HEA	CMC-C2C	2.43	1.55	1.50
28	T	101	PEK	O03-C21	2.43	1.40	1.33
27	T	102	CDL	C82-C81	-2.42	1.38	1.51
14	N	602	HEA	O11-C11	2.41	1.48	1.42
14	A	602[A]	HEA	CHD-C4C	2.41	1.44	1.39
14	A	602[A]	HEA	C4A-NA	-2.41	1.35	1.39
14	A	602[A]	HEA	CHC-C4B	2.41	1.43	1.38
14	N	602	HEA	C12-C13	2.40	1.61	1.53
27	P	305	CDL	PA1-OA5	2.40	1.69	1.59
14	A	602[A]	HEA	C1A-C2A	-2.40	1.40	1.45
21	A	614	EDO	O2-C2	2.40	1.54	1.42
22	C	306	CHD	C20-C17	2.40	1.58	1.54
19	A	608	TGL	CG3-CG2	2.39	1.58	1.50
27	C	305	CDL	PB2-OB2	2.39	1.69	1.59
14	N	603[B]	HEA	CMA-C3A	2.39	1.50	1.45
14	A	602[A]	HEA	CHA-C1A	2.38	1.43	1.38
14	N	603[A]	HEA	CHB-C1B	2.37	1.44	1.39
14	N	603[A]	HEA	CHD-C4C	2.36	1.44	1.39
14	N	603[A]	HEA	CHB-C4A	2.36	1.43	1.38
14	N	602	HEA	OMA-CMA	2.35	1.27	1.22
14	A	602[B]	HEA	C1A-NA	-2.34	1.35	1.39
22	C	306	CHD	C4-C3	2.33	1.56	1.51
20	A	610	PGV	P-O11	2.33	1.68	1.59
22	W	101	CHD	C8-C14	2.32	1.58	1.53
14	A	602[A]	HEA	CHA-C4D	2.32	1.44	1.39
14	N	603[A]	HEA	C1C-C2C	-2.31	1.37	1.43
22	P	301	CHD	C8-C7	2.30	1.57	1.53
24	B	303	PSC	C3-C2	2.30	1.60	1.52
14	A	602[B]	HEA	CHA-C4D	2.30	1.44	1.39
14	A	601	HEA	C1A-NA	-2.30	1.35	1.39
22	W	101	CHD	C13-C17	2.29	1.59	1.55
20	A	610	PGV	C2-C1	-2.29	1.44	1.50
14	N	603[A]	HEA	C1C-NC	-2.29	1.35	1.39
27	P	305	CDL	CB2-C1	2.29	1.59	1.51
20	N	610	PGV	C3-C2	2.28	1.60	1.52
14	N	603[A]	HEA	C3A-C4A	-2.27	1.42	1.46
27	P	305	CDL	O1-C1	2.27	1.50	1.43
27	N	601	CDL	CB3-CB4	2.27	1.57	1.50
14	N	602	HEA	C22-C23	2.26	1.38	1.32
22	P	306	CHD	C4-C5	2.26	1.57	1.53
14	N	603[A]	HEA	CHA-C4D	2.26	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	301	CHD	C13-C17	-2.25	1.51	1.55
20	N	610	PGV	C06-C05	2.25	1.61	1.51
19	D	201	TGL	OC1-CC1	2.25	1.29	1.22
28	G	101	PEK	O11-C03	2.23	1.53	1.44
22	P	306	CHD	O25-C24	2.22	1.29	1.22
22	W	101	CHD	C20-C17	2.22	1.58	1.54
20	A	609	PGV	O03-C19	2.22	1.39	1.33
28	C	307	PEK	C2-C1	2.21	1.57	1.50
14	N	603[A]	HEA	C3C-C4C	-2.21	1.37	1.42
27	P	305	CDL	PB2-OB2	2.21	1.68	1.59
14	A	602[A]	HEA	CMC-C2C	2.20	1.55	1.50
14	A	601	HEA	CMA-C3A	2.20	1.49	1.45
27	C	305	CDL	PA1-OA5	2.20	1.68	1.59
14	N	603[A]	HEA	C4A-NA	-2.19	1.35	1.39
14	A	602[A]	HEA	C1D-ND	-2.18	1.36	1.40
27	N	601	CDL	CB6-CB4	2.18	1.57	1.50
14	A	602[B]	HEA	FE-NB	2.18	2.01	1.94
14	N	602	HEA	C1A-NA	-2.18	1.35	1.39
22	P	306	CHD	C23-C24	-2.18	1.45	1.50
27	P	305	CDL	OB8-CB6	2.17	1.50	1.45
22	B	301	CHD	C21-C20	2.16	1.58	1.53
14	A	601	HEA	C1A-C2A	-2.15	1.41	1.45
14	N	602	HEA	FE-ND	2.15	2.01	1.94
22	P	301	CHD	C1-C10	-2.14	1.50	1.54
28	G	101	PEK	C05-C04	2.13	1.58	1.50
14	A	601	HEA	CHB-C1B	2.13	1.44	1.39
14	A	601	HEA	FE-NA	2.13	2.02	1.95
14	N	602	HEA	C27-C19	2.13	1.56	1.50
19	N	611	TGL	OC1-CC1	-2.12	1.16	1.22
14	A	602[A]	HEA	C18-C19	2.12	1.38	1.33
14	N	603[A]	HEA	C1A-C2A	-2.12	1.41	1.45
27	T	102	CDL	CB6-CB4	2.11	1.57	1.50
14	N	602	HEA	CMC-C2C	2.11	1.55	1.50
22	W	101	CHD	C8-C7	2.11	1.57	1.53
14	N	603[B]	HEA	FE-ND	2.11	2.01	1.94
20	C	304	PGV	O03-C19	2.10	1.39	1.33
14	N	603[A]	HEA	FE-NA	2.10	2.02	1.95
14	A	601	HEA	C4D-ND	-2.09	1.34	1.38
14	N	602	HEA	C4D-ND	-2.09	1.34	1.38
14	N	603[B]	HEA	FE-NA	2.09	2.02	1.95
14	A	602[A]	HEA	C4D-ND	-2.09	1.34	1.38
22	G	102	CHD	C20-C17	2.08	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[B]	HEA	CHA-C1A	2.08	1.42	1.38
14	A	601	HEA	C16-C17	-2.08	1.46	1.53
14	A	601	HEA	O1A-CGA	2.08	1.29	1.22
22	G	102	CHD	O3-C3	2.06	1.49	1.43
22	B	301	CHD	C16-C15	2.06	1.59	1.54
14	N	603[A]	HEA	C12-C11	2.06	1.56	1.52
14	A	601	HEA	CAC-C3C	2.06	1.53	1.47
14	N	603[A]	HEA	C4B-C3B	-2.05	1.41	1.44
20	N	610	PGV	O03-C19	2.05	1.39	1.33
14	A	601	HEA	C4A-NA	-2.04	1.35	1.39
25	C	302	DMU	O16-C6	2.04	1.43	1.40
22	B	301	CHD	C16-C17	2.04	1.58	1.54
14	N	603[A]	HEA	C1D-ND	-2.04	1.36	1.40
22	G	102	CHD	O25-C24	2.03	1.28	1.22
22	G	102	CHD	C16-C17	2.02	1.58	1.54
25	P	309	DMU	O16-C6	2.02	1.43	1.40
20	A	609	PGV	O03-C01	2.02	1.49	1.45
22	P	306	CHD	O12-C12	2.02	1.47	1.43
14	A	602[B]	HEA	CBD-CAD	2.02	1.58	1.52
14	N	602	HEA	C16-C17	-2.01	1.46	1.53
27	N	601	CDL	C71-CB7	2.01	1.56	1.50
14	N	602	HEA	C1D-ND	-2.01	1.36	1.40
28	G	101	PEK	P-O13	-2.01	1.45	1.55
14	A	602[A]	HEA	CHB-C1B	2.00	1.43	1.39
22	P	301	CHD	C16-C15	2.00	1.59	1.54
14	A	602[B]	HEA	C14-C15	2.00	1.37	1.33

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	306	CHD	C23-C22-C20	-17.95	81.74	114.52
22	P	306	CHD	C23-C22-C20	-17.82	81.97	114.52
28	T	101	PEK	C2-C3-C4	15.35	140.59	113.23
19	D	201	TGL	OG2-CB1-CB2	-12.32	84.94	111.50
25	C	311	DMU	O16-C6-C1	11.07	125.59	108.30
19	D	201	TGL	OG2-CB1-OB1	10.53	149.14	123.70
14	A	601	HEA	C3C-C4C-NC	10.52	116.72	110.25
20	A	610	PGV	C02-O01-C1	9.46	141.09	117.79
14	N	603[B]	HEA	C3C-C4C-NC	8.89	115.72	110.25
19	A	608	TGL	OG2-CB1-CB2	8.87	130.61	111.50
14	N	602	HEA	C3C-C4C-NC	8.49	115.47	110.25
19	A	608	TGL	OG3-CC1-OC1	-8.38	102.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	310	DMU	C10-O1-C9	-8.02	97.95	113.69
22	W	101	CHD	C13-C17-C20	7.93	128.96	119.50
21	A	616	EDO	O1-C1-C2	-7.88	55.25	111.91
19	Y	101	TGL	OG2-CB1-CB2	7.70	128.10	111.50
14	A	601	HEA	C3D-C4D-ND	6.95	117.08	110.36
14	N	602	HEA	C4C-NC-C1C	-6.84	98.65	105.35
24	B	303	PSC	O01-C1-C2	6.79	126.14	111.50
19	D	201	TGL	CB3-CB2-CB1	6.72	138.04	113.62
28	C	309	PEK	O01-C1-C2	6.71	125.96	111.50
25	C	310	DMU	C10-C5-C7	-6.70	96.03	110.00
28	P	308	PEK	O01-C1-C2	6.67	125.88	111.50
14	A	602[A]	HEA	OMA-CMA-C3A	-6.56	110.85	125.69
25	C	310	DMU	O7-C10-C5	6.52	125.00	108.10
19	Q	201	TGL	OG2-CB1-CB2	-6.36	97.79	111.50
27	C	305	CDL	OA2-PA1-OA3	6.28	133.60	109.07
19	N	611	TGL	OG2-CB1-CB2	6.28	125.03	111.50
22	C	306	CHD	C21-C20-C17	6.25	122.49	112.92
14	A	601	HEA	C4C-NC-C1C	-6.20	99.28	105.35
19	A	608	TGL	OG2-CG2-CG3	6.15	130.68	108.40
14	N	603[B]	HEA	C27-C19-C20	6.08	125.50	115.27
14	N	603[B]	HEA	C13-C12-C11	-6.07	105.24	114.35
20	P	302	PGV	O03-C19-C20	5.96	130.61	111.91
14	N	603[B]	HEA	C4C-NC-C1C	-5.94	99.53	105.35
14	A	602[B]	HEA	C13-C12-C11	-5.93	105.45	114.35
14	A	602[B]	HEA	C4B-NB-C1B	-5.91	98.97	105.07
28	G	103	PEK	O01-C1-C2	5.89	124.20	111.50
14	N	602	HEA	OMA-CMA-C3A	-5.89	112.38	125.69
22	P	301	CHD	C6-C7-C8	-5.88	105.20	111.48
19	A	611	TGL	CC4-CC3-CC2	-5.87	92.07	113.19
14	N	603[A]	HEA	C26-C15-C16	5.85	125.11	115.27
25	P	309	DMU	O16-C6-C1	5.72	117.24	108.30
25	P	309	DMU	O7-C10-C5	5.65	122.75	108.10
14	A	601	HEA	C4B-NB-C1B	-5.63	99.26	105.07
14	A	601	HEA	C13-C12-C11	-5.58	105.97	114.35
25	C	310	DMU	O16-C6-C1	5.58	117.01	108.30
22	J	101	CHD	C17-C13-C14	-5.55	94.50	100.09
27	N	601	CDL	OB6-CB5-C51	5.54	123.45	111.50
19	A	611	TGL	OG2-CB1-CB2	5.52	123.40	111.50
22	W	101	CHD	C1-C10-C5	5.50	115.91	107.77
27	P	305	CDL	OA6-CA5-C11	5.50	123.36	111.50
22	C	301	CHD	C6-C7-C8	-5.42	105.69	111.48
20	A	610	PGV	O01-C1-O02	5.41	136.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C13-C17-C20	5.40	125.94	119.50
14	N	603[A]	HEA	CAD-CBD-CGD	-5.34	102.11	113.60
28	C	307	PEK	O01-C1-C2	5.34	123.00	111.50
14	A	602[B]	HEA	C27-C19-C20	5.33	124.23	115.27
19	N	611	TGL	CG3-CG2-CG1	-5.32	99.21	111.79
22	G	102	CHD	C19-C10-C1	-5.30	99.71	108.26
14	A	602[B]	HEA	C3B-C4B-NB	5.27	116.08	109.84
22	P	301	CHD	C22-C20-C17	-5.20	99.54	110.28
25	P	310	DMU	O7-C10-C5	5.19	121.56	108.10
25	P	309	DMU	C10-O1-C9	-5.11	103.65	113.69
24	N	612	PSC	O01-C1-C2	5.11	122.51	111.50
22	B	301	CHD	C11-C9-C10	-5.08	108.49	113.73
19	Q	201	TGL	OG2-CB1-OB1	5.06	135.94	123.70
22	C	301	CHD	C23-C22-C20	-5.04	105.32	114.52
19	N	611	TGL	OG3-CC1-OC1	-5.03	110.89	123.59
22	P	306	CHD	C15-C14-C13	5.03	108.49	103.55
27	C	305	CDL	OA6-CA5-C11	5.01	122.30	111.50
27	N	601	CDL	CB2-C1-CA2	-5.00	98.08	112.79
14	A	601	HEA	C1D-ND-C4D	-4.96	99.95	105.07
22	P	301	CHD	C21-C20-C22	-4.91	102.67	110.36
22	W	101	CHD	C13-C14-C8	4.91	121.00	114.74
14	A	601	HEA	CHA-C4D-C3D	-4.89	117.65	124.84
14	A	602[A]	HEA	C3C-C2C-C1C	-4.86	101.29	107.16
14	A	602[B]	HEA	CAA-CBA-CGA	-4.86	103.15	113.60
14	A	601	HEA	C2B-C1B-NB	4.85	115.69	109.88
19	A	611	TGL	OG3-CC1-CC2	4.84	127.10	111.91
22	P	306	CHD	C13-C17-C20	-4.84	113.72	119.50
19	A	608	TGL	CG3-CG2-CG1	-4.79	100.47	111.79
20	N	610	PGV	O01-C1-O02	-4.78	112.15	123.70
14	N	602	HEA	C2C-C1C-NC	4.77	117.34	110.08
22	B	301	CHD	C13-C17-C20	-4.74	113.83	119.50
19	Y	101	TGL	OG2-CB1-OB1	-4.73	112.26	123.70
19	A	608	TGL	OG3-CC1-CC2	4.73	126.75	111.91
14	A	602[A]	HEA	CMB-C2B-C1B	4.72	132.23	125.04
22	B	301	CHD	C19-C10-C1	-4.69	100.70	108.26
14	A	601	HEA	CAD-CBD-CGD	-4.62	103.66	113.60
14	A	601	HEA	C13-C14-C15	-4.57	116.66	127.66
22	P	301	CHD	C23-C22-C20	-4.57	106.17	114.52
25	P	310	DMU	O3-C5-C10	4.56	121.12	110.05
22	P	306	CHD	C5-C4-C3	-4.54	106.09	112.76
19	N	611	TGL	OG1-CA1-CA2	4.53	126.12	111.91
25	P	309	DMU	O49-C1-C2	-4.52	99.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	306	CHD	O26-C24-C23	-4.51	99.52	114.03
19	Y	101	TGL	CG2-OG2-CB1	4.51	128.90	117.79
27	N	601	CDL	CB4-OB6-CB5	4.49	128.85	117.79
28	G	101	PEK	C24-C23-C22	-4.45	97.20	113.19
14	N	602	HEA	C20-C21-C22	-4.44	97.28	111.88
22	J	101	CHD	C1-C10-C5	4.44	114.34	107.77
20	C	308	PGV	O01-C1-C2	4.44	121.06	111.50
14	N	603[B]	HEA	C3D-C4D-ND	4.43	114.64	110.36
22	C	301	CHD	C5-C6-C7	4.41	119.32	114.46
28	C	307	PEK	O03-C21-C22	4.40	125.71	111.91
22	C	306	CHD	C1-C10-C5	4.38	114.24	107.77
19	A	608	TGL	CG3-OG3-CC1	4.37	133.32	117.12
19	D	201	TGL	OG1-CA1-CA2	4.37	125.63	111.91
22	W	101	CHD	C18-C13-C14	-4.37	104.37	111.21
22	P	306	CHD	C19-C10-C9	-4.36	105.18	111.18
27	P	305	CDL	OB8-CB7-C71	4.35	125.57	111.91
14	N	602	HEA	C13-C14-C15	-4.34	117.21	127.66
14	A	602[B]	HEA	C2B-C1B-NB	4.33	115.07	109.88
22	C	301	CHD	C11-C9-C10	-4.33	109.26	113.73
19	N	611	TGL	OG3-CC1-CC2	4.28	125.35	111.91
22	G	102	CHD	C6-C5-C10	4.28	117.20	112.66
22	G	102	CHD	C6-C5-C4	-4.28	106.27	111.19
27	N	601	CDL	CB6-OB8-CB7	4.27	132.95	117.12
22	P	306	CHD	C16-C17-C20	4.26	118.74	112.15
19	D	201	TGL	CG1-OG1-CA1	4.24	132.82	117.12
22	W	101	CHD	C11-C12-C13	4.22	115.58	111.24
14	A	602[A]	HEA	C26-C15-C16	4.21	122.35	115.27
22	J	101	CHD	C18-C13-C17	4.20	117.79	111.21
27	T	102	CDL	OA6-CA5-C11	4.20	120.56	111.50
19	Q	201	TGL	OG3-CC1-CC2	4.19	125.07	111.91
22	P	306	CHD	C21-C20-C17	4.17	119.30	112.92
22	C	301	CHD	C1-C2-C3	-4.13	105.17	110.47
22	P	306	CHD	C16-C17-C13	4.11	107.58	103.55
14	A	602[A]	HEA	CHA-C4D-ND	4.10	128.88	124.42
25	P	309	DMU	C18-O16-C6	-4.08	107.07	113.84
24	B	303	PSC	O01-C1-O02	-4.07	113.86	123.70
22	P	306	CHD	O26-C24-O25	4.07	133.44	123.30
25	C	311	DMU	C18-O16-C6	4.06	120.58	113.84
20	C	308	PGV	O03-C19-C20	4.05	124.62	111.91
14	N	603[B]	HEA	CHC-C1C-C2C	-4.04	115.84	127.24
14	A	601	HEA	C27-C19-C20	-4.03	108.48	115.27
28	T	101	PEK	O03-C21-C22	4.03	124.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CMC-C2C-C1C	4.03	131.51	125.37
19	D	201	TGL	CG3-OG3-CC1	4.03	132.04	117.12
14	N	602	HEA	C3C-C2C-C1C	-4.01	102.32	107.16
22	C	306	CHD	C6-C7-C8	4.01	115.76	111.48
22	C	301	CHD	C9-C11-C12	-4.00	109.01	114.30
27	N	601	CDL	OA6-CA5-C11	3.99	120.10	111.50
27	T	102	CDL	OB6-CB5-C51	3.96	120.03	111.50
14	N	603[B]	HEA	C20-C19-C18	-3.95	113.12	121.12
14	A	602[B]	HEA	C20-C19-C18	-3.95	113.12	121.12
27	C	305	CDL	OA5-PA1-OA3	-3.95	93.65	109.07
14	N	603[B]	HEA	C2D-C1D-ND	3.93	114.50	109.84
22	W	101	CHD	C6-C7-C8	3.93	115.67	111.48
25	C	302	DMU	C18-O16-C6	-3.92	107.34	113.84
19	A	608	TGL	OG2-CB1-OB1	-3.89	114.29	123.70
22	B	301	CHD	C9-C8-C7	-3.89	107.23	111.88
19	Y	101	TGL	OG3-CG3-CG2	3.88	119.74	108.43
19	Y	101	TGL	OG3-CC1-CC2	3.88	124.08	111.91
20	N	610	PGV	O03-C19-O04	-3.88	113.81	123.59
22	P	306	CHD	C14-C13-C12	3.87	111.00	107.40
25	P	310	DMU	C1-C2-C3	3.86	118.50	109.68
14	A	602[B]	HEA	CMB-C2B-C1B	3.81	130.84	125.04
22	W	101	CHD	C6-C5-C10	3.80	116.70	112.66
20	P	304	PGV	O01-C1-O02	-3.80	114.51	123.70
19	A	611	TGL	OG3-CC1-OC1	-3.77	114.07	123.59
22	B	301	CHD	O12-C12-C13	-3.77	104.66	111.03
14	A	601	HEA	C2D-C1D-ND	3.76	114.30	109.84
22	J	101	CHD	C6-C5-C10	3.76	116.65	112.66
14	A	602[A]	HEA	C20-C19-C18	-3.74	113.54	121.12
14	N	602	HEA	CHC-C4B-NB	3.73	128.98	124.37
28	T	101	PEK	O01-C1-O02	-3.73	114.68	123.70
14	A	601	HEA	C2A-C1A-NA	3.73	113.95	110.32
14	A	601	HEA	C20-C19-C18	3.71	128.62	121.12
14	A	602[A]	HEA	C27-C19-C20	3.70	121.49	115.27
14	N	603[B]	HEA	CMD-C2D-C1D	3.69	130.66	125.04
22	B	301	CHD	C18-C13-C12	-3.69	105.31	109.07
14	A	602[B]	HEA	CAD-CBD-CGD	-3.68	105.68	113.60
28	G	103	PEK	O01-C1-O02	-3.68	114.81	123.70
22	J	101	CHD	C16-C17-C13	3.68	107.16	103.55
22	C	306	CHD	C16-C17-C20	3.66	117.81	112.15
14	N	603[A]	HEA	O2A-CGA-CBA	3.65	125.76	114.03
25	P	310	DMU	O16-C6-C1	3.63	113.97	108.30
22	J	101	CHD	C6-C5-C4	-3.63	107.02	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	301	CHD	C18-C13-C12	3.62	112.76	109.07
14	N	603[B]	HEA	CHA-C4D-ND	-3.61	120.49	124.42
19	Q	201	TGL	OG1-CA1-CA2	3.61	123.25	111.91
14	A	602[A]	HEA	CAD-CBD-CGD	-3.61	105.83	113.60
14	A	602[A]	HEA	C13-C14-C15	-3.61	118.97	127.66
14	A	602[B]	HEA	C3C-C4C-NC	3.59	112.46	110.25
22	W	101	CHD	C17-C13-C12	3.59	120.94	117.67
20	P	304	PGV	C03-C02-C01	-3.58	103.32	111.79
22	G	102	CHD	C2-C1-C10	-3.57	106.66	112.78
22	C	306	CHD	O26-C24-O25	3.57	132.19	123.30
25	M	101	DMU	O49-C1-C6	-3.56	101.39	110.05
22	B	301	CHD	C19-C10-C9	3.56	116.09	111.18
25	C	310	DMU	C7-C8-C9	3.55	116.57	110.24
25	M	101	DMU	C18-O16-C6	-3.54	107.97	113.84
22	J	101	CHD	C1-C10-C9	-3.53	105.80	111.35
27	P	305	CDL	CB6-CB4-CB3	-3.53	103.44	111.79
22	C	301	CHD	C22-C23-C24	-3.53	103.14	112.51
14	N	603[B]	HEA	CAA-CBA-CGA	-3.53	106.01	113.60
22	G	102	CHD	C9-C8-C7	-3.51	107.67	111.88
25	M	101	DMU	C22-C19-C18	-3.50	97.96	113.49
14	A	602[A]	HEA	CAD-C3D-C4D	-3.50	118.54	124.66
14	A	601	HEA	CHB-C1B-NB	-3.50	120.61	124.42
25	C	302	DMU	C25-C22-C19	-3.49	96.69	114.42
22	P	306	CHD	O3-C3-C4	-3.49	102.89	109.85
14	A	602[A]	HEA	CMB-C2B-C3B	-3.49	123.68	130.34
14	A	601	HEA	C3A-C2A-C1A	-3.48	103.75	107.08
20	P	302	PGV	O01-C1-C2	3.48	119.00	111.50
14	A	602[B]	HEA	C12-C13-C14	-3.47	103.08	112.23
20	A	610	PGV	C4-C3-C2	-3.47	100.73	113.19
14	A	601	HEA	C2C-C1C-NC	3.46	115.35	110.08
22	P	306	CHD	C4-C5-C10	3.46	116.33	112.66
22	C	301	CHD	C17-C13-C14	-3.46	96.61	100.09
27	P	305	CDL	OB8-CB7-OB9	-3.45	114.88	123.59
14	A	602[B]	HEA	CMB-C2B-C3B	-3.42	123.83	130.34
14	A	602[A]	HEA	CAD-C3D-C2D	3.41	134.23	127.88
22	W	101	CHD	C10-C9-C8	3.41	115.48	111.82
22	P	301	CHD	C18-C13-C12	3.40	112.52	109.07
28	G	101	PEK	C02-O01-C1	-3.39	109.43	117.79
20	N	609	PGV	C3-C2-C1	-3.39	101.28	113.62
22	C	306	CHD	C5-C4-C3	-3.39	107.79	112.76
20	C	304	PGV	C30-C29-C28	-3.38	97.25	114.42
19	D	201	TGL	OG3-CC1-OC1	-3.37	115.09	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	301	CHD	C22-C20-C17	-3.36	103.34	110.28
14	N	603[B]	HEA	C2C-C1C-NC	3.36	115.19	110.08
25	C	302	DMU	C10-O7-C3	-3.35	109.67	117.96
27	P	305	CDL	OA8-CA7-C31	3.34	122.39	111.91
14	A	601	HEA	C4D-C3D-C2D	-3.34	102.03	106.90
28	T	101	PEK	O02-C1-C2	3.34	136.75	123.73
27	P	305	CDL	C56-C55-C54	3.33	131.34	114.42
19	A	611	TGL	CG2-OG2-CB1	3.33	125.98	117.79
14	A	602[B]	HEA	CHC-C4B-NB	-3.32	120.28	124.37
25	P	309	DMU	C10-C5-C7	-3.32	103.08	110.00
22	G	102	CHD	C1-C2-C3	-3.32	106.21	110.47
22	G	102	CHD	C23-C22-C20	-3.32	108.46	114.52
20	N	610	PGV	O02-C1-C2	3.31	136.66	123.73
22	B	301	CHD	C23-C22-C20	-3.31	108.47	114.52
22	W	101	CHD	C4-C5-C10	3.31	116.17	112.66
19	Q	201	TGL	OG3-CC1-OC1	-3.31	115.24	123.59
20	P	302	PGV	O04-C19-C20	-3.31	110.83	123.73
19	A	611	TGL	OG1-CA1-CA2	3.30	122.28	111.91
27	P	305	CDL	OA6-CA5-OA7	-3.29	115.74	123.70
20	A	610	PGV	O02-C1-C2	-3.29	110.90	123.73
28	G	101	PEK	O01-C1-O02	3.28	131.63	123.70
20	C	308	PGV	O03-C01-C02	3.28	117.98	108.43
25	P	309	DMU	C8-C7-C5	-3.27	105.11	110.82
22	J	101	CHD	C16-C17-C20	3.26	117.20	112.15
20	N	609	PGV	O03-C19-C20	3.25	122.11	111.91
22	B	301	CHD	C17-C13-C12	3.25	120.63	117.67
22	P	306	CHD	C1-C10-C9	3.25	116.46	111.35
20	C	308	PGV	O03-C19-O04	-3.25	115.40	123.59
27	P	305	CDL	C83-C82-C81	3.24	130.88	114.42
28	C	309	PEK	C2-C3-C4	3.24	119.00	113.23
22	C	301	CHD	C15-C14-C8	-3.23	113.81	118.33
22	C	306	CHD	C15-C14-C13	3.23	106.72	103.55
22	B	301	CHD	C2-C1-C10	-3.22	107.26	112.78
19	A	611	TGL	C26-C25-C24	-3.22	98.10	114.42
20	N	609	PGV	O01-C02-C01	3.22	120.04	108.40
25	C	311	DMU	O1-C9-C11	3.21	114.42	106.44
25	P	307	DMU	O16-C18-C19	3.21	120.81	109.56
28	P	308	PEK	O03-C21-O04	-3.20	115.52	123.59
22	J	101	CHD	C4-C5-C10	3.20	116.05	112.66
20	A	609	PGV	O03-C19-O04	-3.20	115.52	123.59
25	C	311	DMU	O16-C18-C19	3.20	120.76	109.56
22	B	301	CHD	C16-C17-C20	-3.18	107.22	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	CDL	CB6-OB8-CB7	3.17	128.86	117.12
22	G	102	CHD	C11-C12-C13	3.16	114.49	111.24
14	N	603[A]	HEA	C1D-C2D-C3D	3.16	110.27	106.96
14	N	603[A]	HEA	CHA-C4D-C3D	-3.15	120.21	124.84
25	C	311	DMU	O5-C4-C57	3.15	114.27	106.44
27	C	305	CDL	OB2-PB2-OB3	3.15	121.36	109.07
14	N	602	HEA	O2A-CGA-CBA	3.14	124.13	114.03
28	C	307	PEK	O03-C21-O04	-3.14	115.68	123.59
20	C	304	PGV	C22-C21-C20	-3.13	101.93	113.19
14	N	602	HEA	C25-C23-C24	-3.13	107.70	114.60
22	P	306	CHD	C6-C7-C8	3.12	114.81	111.48
25	C	311	DMU	C6-C1-C2	3.11	116.48	110.00
25	C	311	DMU	O5-C4-C3	-3.11	103.19	109.75
20	N	610	PGV	O03-C19-C20	3.11	121.67	111.91
22	C	306	CHD	C4-C5-C10	3.10	115.95	112.66
14	N	603[A]	HEA	CAA-CBA-CGA	-3.09	106.95	113.60
27	C	305	CDL	CB6-CB4-CB3	-3.09	104.48	111.79
14	A	602[A]	HEA	CHD-C4C-NC	3.08	129.51	123.85
19	A	608	TGL	OG1-CA1-CA2	3.08	121.58	111.91
20	A	610	PGV	O03-C19-C20	3.08	121.57	111.91
22	C	301	CHD	C5-C4-C3	-3.07	108.25	112.76
22	W	101	CHD	C19-C10-C5	-3.07	105.15	110.36
19	A	611	TGL	CA4-CA3-CA2	-3.07	102.17	113.19
20	C	308	PGV	C03-C02-C01	-3.06	104.54	111.79
19	Q	201	TGL	OG1-CA1-OA1	-3.06	115.86	123.59
19	N	611	TGL	OG1-CA1-OA1	-3.06	115.86	123.59
25	P	307	DMU	O55-C2-C3	3.06	118.05	109.94
14	A	601	HEA	C3B-C4B-NB	3.06	113.46	109.84
14	N	603[A]	HEA	CHC-C4B-NB	3.05	128.14	124.37
14	N	603[B]	HEA	OMA-CMA-C3A	-3.05	118.79	125.69
14	N	602	HEA	O2D-CGD-CBD	3.05	123.83	114.03
19	A	608	TGL	CC3-CC2-CC1	3.05	124.72	113.62
22	J	101	CHD	C21-C20-C17	-3.05	108.25	112.92
22	C	301	CHD	C16-C15-C14	-3.05	99.09	105.13
14	A	602[A]	HEA	CMC-C2C-C1C	3.05	130.01	125.37
28	G	101	PEK	O03-C21-O04	-3.05	115.91	123.59
22	C	306	CHD	C19-C10-C5	-3.05	105.20	110.36
20	A	609	PGV	O01-C1-O02	-3.04	116.34	123.70
14	A	601	HEA	C4A-NA-C1A	-3.04	102.37	105.35
25	P	310	DMU	O1-C9-C11	3.03	113.97	106.44
22	W	101	CHD	C6-C5-C4	-3.03	107.70	111.19
14	N	602	HEA	C2B-C1B-NB	3.02	113.50	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	310	DMU	O7-C10-O1	3.02	119.11	110.67
14	N	603[A]	HEA	CMB-C2B-C1B	3.02	129.64	125.04
22	P	306	CHD	C18-C13-C12	-3.01	106.00	109.07
14	A	602[A]	HEA	CAA-C2A-C1A	3.00	130.55	124.89
27	P	305	CDL	OA2-PA1-OA3	2.99	120.74	109.07
28	T	101	PEK	O11-P-O14	-2.99	97.40	109.07
20	P	302	PGV	C21-C20-C19	-2.99	102.76	113.62
22	W	101	CHD	C14-C8-C7	2.98	115.75	111.81
24	B	303	PSC	O01-C02-C03	2.97	119.17	108.40
14	A	602[B]	HEA	OMA-CMA-C3A	-2.97	118.97	125.69
28	G	101	PEK	O11-P-O14	-2.96	97.49	109.07
27	P	305	CDL	C53-C52-C51	2.96	123.83	113.19
22	P	301	CHD	C17-C13-C12	-2.96	114.97	117.67
14	N	603[A]	HEA	C2A-C1A-NA	2.95	113.19	110.32
19	Y	101	TGL	CG3-OG3-CC1	2.94	128.02	117.12
27	C	305	CDL	OA6-CA5-OA7	-2.94	116.61	123.70
14	N	603[B]	HEA	C1D-ND-C4D	-2.93	102.04	105.07
28	C	307	PEK	C02-O01-C1	2.93	125.01	117.79
22	P	301	CHD	C5-C4-C3	-2.92	108.46	112.76
27	C	305	CDL	C39-C38-C37	2.92	129.26	114.42
25	C	310	DMU	O2-C8-C7	2.92	117.10	110.35
14	N	602	HEA	C2A-C1A-NA	2.92	113.16	110.32
19	Y	101	TGL	CB4-CB3-CB2	2.91	123.67	113.19
14	A	601	HEA	CAA-CBA-CGA	-2.90	107.35	113.60
19	A	611	TGL	C25-C24-C23	-2.90	99.71	114.42
27	T	102	CDL	OB8-CB6-CB4	2.89	116.84	108.43
27	N	601	CDL	OA8-CA7-C31	2.89	120.97	111.91
22	B	301	CHD	O26-C24-O25	-2.89	116.10	123.30
22	W	101	CHD	C9-C11-C12	2.88	118.11	114.30
25	P	307	DMU	C2-C3-C4	-2.88	104.32	110.93
14	N	602	HEA	C27-C19-C18	-2.86	116.33	123.68
27	P	305	CDL	PA1-OA2-CA2	2.86	138.46	121.68
20	P	304	PGV	C27-C26-C25	-2.86	99.90	114.42
25	P	309	DMU	O7-C3-C4	-2.85	101.64	109.45
14	A	601	HEA	C16-C17-C18	-2.85	102.52	111.88
28	P	308	PEK	O01-C1-O02	-2.85	116.82	123.70
22	G	102	CHD	C1-C10-C9	2.85	115.83	111.35
22	J	101	CHD	C22-C20-C17	2.84	116.15	110.28
20	C	308	PGV	O01-C02-C01	2.83	118.66	108.40
14	A	602[A]	HEA	CHB-C1B-C2B	-2.83	120.56	124.98
14	N	603[A]	HEA	CMB-C2B-C3B	-2.83	124.95	130.34
22	J	101	CHD	C10-C9-C8	2.81	114.84	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	309	DMU	O4-C7-C8	2.81	116.83	110.35
27	T	102	CDL	C83-C82-C81	2.80	128.66	114.42
27	C	305	CDL	PA1-OA2-CA2	2.80	138.10	121.68
14	N	603[B]	HEA	C1D-C2D-C3D	-2.80	104.02	106.96
22	G	102	CHD	C4-C5-C10	-2.79	109.69	112.66
28	C	307	PEK	C36-C35-C34	-2.78	100.33	114.42
25	C	310	DMU	O55-C2-C1	2.77	116.75	110.35
20	N	609	PGV	C01-O03-C19	2.76	127.35	117.12
14	A	601	HEA	C21-C20-C19	2.76	122.06	112.98
22	C	306	CHD	C16-C17-C13	2.76	106.26	103.55
20	A	609	PGV	O03-C19-C20	2.76	120.56	111.91
27	T	102	CDL	OB8-CB7-C71	2.75	120.54	111.91
25	P	309	DMU	O5-C6-O16	-2.74	103.48	109.97
14	A	602[A]	HEA	C1D-ND-C4D	2.74	107.90	105.07
14	N	603[A]	HEA	OMA-CMA-C3A	-2.73	119.51	125.69
25	Z	101	DMU	C10-O7-C3	-2.72	111.22	117.96
27	C	305	CDL	O1-C1-CB2	2.72	119.10	109.56
24	B	303	PSC	O03-C19-C20	2.72	120.44	111.91
28	C	309	PEK	O03-C21-C22	2.71	120.41	111.91
14	N	602	HEA	CMB-C2B-C1B	-2.70	120.93	125.04
14	N	603[A]	HEA	CHC-C4B-C3B	-2.69	118.88	125.80
14	A	601	HEA	O2A-CGA-CBA	2.68	122.64	114.03
20	A	610	PGV	C3-C2-C1	2.67	123.35	113.62
22	B	301	CHD	C16-C17-C13	2.67	106.17	103.55
14	N	603[B]	HEA	CMB-C2B-C1B	2.67	129.10	125.04
25	C	302	DMU	C6-C1-C2	-2.66	104.46	110.00
25	C	311	DMU	O49-C1-C2	-2.66	104.20	110.35
25	M	101	DMU	C31-C28-C25	-2.65	100.95	114.42
14	A	602[A]	HEA	C4C-CHD-C1D	-2.65	120.04	126.34
22	P	306	CHD	C11-C12-C13	-2.65	108.52	111.24
14	N	602	HEA	O2D-CGD-O1D	-2.65	116.69	123.30
14	N	603[A]	HEA	C3B-C4B-NB	2.65	112.98	109.84
22	P	306	CHD	O26-C24-C23	-2.65	105.52	114.03
14	N	602	HEA	C20-C19-C18	2.65	126.47	121.12
20	C	304	PGV	O14-P-O13	2.64	125.30	112.24
22	C	306	CHD	C2-C1-C10	-2.63	108.26	112.78
14	N	603[B]	HEA	CAA-C2A-C1A	2.63	129.85	124.89
14	N	603[A]	HEA	C4D-C3D-C2D	-2.63	103.07	106.90
19	D	201	TGL	OC1-CC1-CC2	2.62	133.97	123.73
28	C	307	PEK	O01-C1-O02	-2.62	117.37	123.70
25	C	302	DMU	O55-C2-C3	2.61	116.87	109.94
14	N	602	HEA	CHC-C1C-C2C	-2.61	119.86	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	610	PGV	C4-C3-C2	-2.61	103.81	113.19
25	P	310	DMU	O5-C6-C1	-2.61	104.83	110.35
19	A	611	TGL	C20-CA9-CA8	-2.61	101.19	114.42
14	A	602[A]	HEA	C2B-C1B-NB	2.61	113.00	109.88
25	C	311	DMU	O49-C1-C6	-2.60	103.73	110.05
22	G	102	CHD	C13-C17-C20	-2.60	116.39	119.50
25	P	307	DMU	C8-C7-C5	2.60	115.36	110.82
14	A	602[A]	HEA	C4A-CHB-C1B	-2.59	120.47	126.06
22	W	101	CHD	C2-C1-C10	2.59	117.23	112.78
27	P	305	CDL	OA8-CA6-CA4	2.59	115.98	108.43
22	C	306	CHD	C14-C13-C12	2.59	109.81	107.40
14	A	602[B]	HEA	CHA-C1A-NA	2.59	127.24	124.44
22	B	301	CHD	O3-C3-C4	-2.59	104.70	109.85
14	A	602[A]	HEA	C2A-C1A-NA	2.58	112.84	110.32
20	A	609	PGV	C30-C29-C28	2.58	127.53	114.42
14	N	603[A]	HEA	CHB-C1B-C2B	-2.57	120.96	124.98
27	N	601	CDL	C23-C22-C21	2.57	127.48	114.42
28	G	101	PEK	O03-C01-C02	-2.57	100.95	108.43
14	N	603[A]	HEA	C2B-C1B-NB	2.57	112.96	109.88
27	C	305	CDL	C42-C41-C40	2.56	127.43	114.42
22	P	301	CHD	C10-C9-C8	-2.56	109.07	111.82
14	N	603[B]	HEA	C2B-C1B-NB	2.56	112.95	109.88
22	C	301	CHD	C11-C9-C8	2.55	114.60	110.88
22	C	306	CHD	C5-C6-C7	2.54	117.27	114.46
14	N	603[A]	HEA	O2A-CGA-O1A	-2.54	116.96	123.30
14	N	603[A]	HEA	CHA-C1A-C2A	-2.54	120.83	124.94
25	C	311	DMU	C10-O7-C3	-2.54	111.69	117.96
25	C	311	DMU	C6-O5-C4	-2.53	108.72	113.69
14	A	602[B]	HEA	CHB-C1B-NB	-2.53	121.67	124.42
24	N	612	PSC	C02-O01-C1	2.53	124.02	117.79
14	N	603[A]	HEA	C3C-C2C-C1C	-2.52	104.11	107.16
22	C	306	CHD	C13-C17-C20	-2.52	116.48	119.50
20	N	610	PGV	C03-C02-C01	-2.52	105.82	111.79
22	W	101	CHD	C19-C10-C1	-2.52	104.20	108.26
22	P	301	CHD	C11-C12-C13	-2.52	108.66	111.24
22	P	306	CHD	C11-C9-C10	2.52	116.32	113.73
14	N	603[B]	HEA	C3B-C4B-NB	2.51	112.82	109.84
28	C	307	PEK	C24-C23-C22	2.51	122.20	113.19
14	N	603[A]	HEA	C3A-C2A-C1A	-2.50	104.69	107.08
14	N	602	HEA	C12-C13-C14	2.50	118.83	112.23
25	Z	101	DMU	C34-C31-C28	-2.50	101.75	114.42
24	N	612	PSC	O03-C19-C20	2.49	119.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[A]	HEA	C1C-CHC-C4B	-2.49	120.44	126.34
22	B	301	CHD	C1-C10-C9	2.48	115.26	111.35
27	N	601	CDL	C44-C43-C42	-2.48	101.82	114.42
28	G	103	PEK	O03-C21-C22	2.48	119.69	111.91
25	P	307	DMU	O16-C6-C1	2.46	112.15	108.30
27	C	305	CDL	OB6-CB5-OB7	-2.46	117.75	123.70
14	N	602	HEA	C2D-C1D-ND	2.46	112.75	109.84
22	G	102	CHD	C11-C9-C10	-2.46	111.19	113.73
25	C	311	DMU	C1-C2-C3	2.46	115.30	109.68
22	J	101	CHD	C11-C9-C8	2.45	114.46	110.88
14	A	602[A]	HEA	O2A-CGA-CBA	2.45	121.89	114.03
14	A	601	HEA	OMA-CMA-C3A	-2.44	120.16	125.69
14	A	601	HEA	CHC-C1C-C2C	-2.44	120.34	127.24
25	Z	101	DMU	O3-C5-C7	2.44	116.00	110.35
22	C	301	CHD	C6-C5-C10	-2.43	110.08	112.66
27	T	102	CDL	C63-C62-C61	2.43	126.76	114.42
19	Y	101	TGL	OG3-CC1-OC1	-2.43	117.47	123.59
22	B	301	CHD	O7-C7-C6	2.43	115.96	109.94
19	N	611	TGL	OG1-CG1-CG2	2.42	115.48	108.43
27	T	102	CDL	OA8-CA7-C31	2.42	119.49	111.91
27	P	305	CDL	OB2-PB2-OB3	2.42	118.51	109.07
22	J	101	CHD	C15-C14-C13	2.41	105.92	103.55
27	P	305	CDL	C39-C38-C37	2.41	126.67	114.42
14	A	601	HEA	O2D-CGD-CBD	2.41	121.77	114.03
22	W	101	CHD	C14-C8-C9	2.41	113.02	109.71
27	N	601	CDL	C80-C79-C78	2.40	126.63	114.42
14	A	602[B]	HEA	CHA-C1A-C2A	-2.40	121.04	124.94
22	P	301	CHD	C4-C3-C2	-2.40	107.69	110.55
14	N	603[B]	HEA	CMB-C2B-C3B	-2.40	125.76	130.34
28	C	309	PEK	O01-C1-O02	-2.40	117.90	123.70
19	Y	101	TGL	OG2-CG2-CG3	2.40	117.08	108.40
22	W	101	CHD	C23-C22-C20	2.40	118.89	114.52
14	A	602[A]	HEA	CHA-C4D-C3D	-2.40	121.32	124.84
20	P	304	PGV	O03-C01-C02	-2.39	101.47	108.43
20	P	304	PGV	C22-C21-C20	-2.39	104.59	113.19
28	T	101	PEK	O03-C21-O04	-2.39	117.56	123.59
14	A	601	HEA	CBD-CAD-C3D	-2.39	105.98	112.63
14	N	603[A]	HEA	C27-C19-C20	2.39	119.29	115.27
20	N	610	PGV	C5-C4-C3	-2.38	102.34	114.42
20	N	610	PGV	O01-C02-C03	2.38	117.02	108.40
22	W	101	CHD	C17-C13-C14	-2.38	97.69	100.09
22	W	101	CHD	C9-C10-C5	2.38	111.92	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	609	PGV	C03-C02-C01	-2.38	106.17	111.79
25	C	310	DMU	C8-C7-C5	-2.38	106.67	110.82
25	C	302	DMU	C7-C8-C9	2.37	114.47	110.24
22	P	306	CHD	C15-C14-C8	2.37	121.64	118.33
14	A	602[A]	HEA	CMD-C2D-C1D	2.37	128.64	125.04
22	B	301	CHD	C22-C20-C17	2.37	115.17	110.28
14	N	603[B]	HEA	CHD-C1D-C2D	-2.37	120.16	126.73
14	N	603[B]	HEA	CHC-C1C-NC	2.37	128.20	123.85
14	N	602	HEA	O2A-CGA-O1A	-2.36	117.42	123.30
14	N	603[B]	HEA	C4B-NB-C1B	-2.36	102.64	105.07
20	A	609	PGV	C34-C33-C32	-2.36	95.52	113.42
14	A	602[B]	HEA	CAD-C3D-C2D	2.36	132.27	127.88
14	A	602[A]	HEA	C3A-C2A-C1A	-2.35	104.83	107.08
14	N	603[A]	HEA	C16-C17-C18	2.35	119.60	111.88
27	C	305	CDL	OA8-CA7-C31	2.35	119.27	111.91
28	C	307	PEK	C01-O03-C21	2.34	125.80	117.12
22	W	101	CHD	C15-C14-C13	-2.34	101.26	103.55
25	C	310	DMU	O5-C4-C57	2.34	112.25	106.44
25	P	310	DMU	C10-O1-C9	-2.34	109.10	113.69
27	T	102	CDL	C12-C11-CA5	2.33	122.10	113.62
21	P	312	EDO	O1-C1-C2	-2.33	95.15	111.91
22	P	301	CHD	C14-C8-C7	-2.33	108.72	111.81
27	N	601	CDL	OB7-CB5-C51	-2.33	114.65	123.73
14	N	603[A]	HEA	C2D-C1D-ND	-2.33	107.08	109.84
25	M	101	DMU	O3-C5-C10	-2.32	104.40	110.05
20	N	610	PGV	C3-C2-C1	-2.32	105.20	113.62
28	C	307	PEK	C3-C2-C1	2.31	122.03	113.62
22	C	306	CHD	O12-C12-C13	-2.31	107.13	111.03
28	C	309	PEK	C01-O03-C21	2.31	125.66	117.12
14	N	603[A]	HEA	CMC-C2C-C3C	2.30	132.15	126.59
22	W	101	CHD	C1-C10-C9	-2.29	107.75	111.35
27	C	305	CDL	C43-C42-C41	2.29	126.06	114.42
14	A	602[B]	HEA	CAD-C3D-C4D	-2.29	120.66	124.66
14	N	603[A]	HEA	CHA-C4D-ND	2.29	126.90	124.42
14	A	602[A]	HEA	C1B-C2B-C3B	-2.29	104.07	106.80
22	C	301	CHD	O3-C3-C2	-2.28	104.36	110.16
19	D	201	TGL	CB5-CB4-CB3	2.28	125.98	114.42
14	N	602	HEA	CAA-CBA-CGA	-2.27	108.71	113.60
22	W	101	CHD	C5-C6-C7	2.27	116.97	114.46
22	B	301	CHD	C15-C14-C13	2.27	105.78	103.55
14	N	602	HEA	C16-C17-C18	-2.27	104.42	111.88
25	P	310	DMU	C10-C5-C7	2.27	114.72	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	305	CDL	CB4-OB6-CB5	2.27	123.37	117.79
25	C	310	DMU	O5-C4-C3	-2.27	104.97	109.75
19	D	201	TGL	OG1-CA1-OA1	-2.27	117.87	123.59
27	T	102	CDL	C80-C79-C78	2.27	125.93	114.42
14	N	603[B]	HEA	C12-C13-C14	-2.27	106.25	112.23
19	A	608	TGL	OB1-CB1-CB2	-2.26	114.90	123.73
25	M	101	DMU	O3-C5-C7	2.26	115.58	110.35
14	N	603[A]	HEA	C12-C13-C14	-2.26	106.28	112.23
14	N	603[B]	HEA	C3A-C2A-C1A	-2.26	104.92	107.08
25	P	307	DMU	O1-C9-C11	2.25	112.04	106.44
27	P	305	CDL	OA5-PA1-OA3	-2.25	100.27	109.07
22	G	102	CHD	C16-C17-C20	-2.25	108.67	112.15
22	B	301	CHD	O26-C24-C23	2.24	121.22	114.03
22	P	306	CHD	C21-C20-C22	2.24	113.87	110.36
14	A	602[B]	HEA	CBA-CAA-C2A	-2.24	106.41	112.63
27	N	601	CDL	OA6-CA5-OA7	-2.24	118.30	123.70
25	P	309	DMU	C7-C8-C9	2.24	114.23	110.24
19	Q	201	TGL	OG2-CG2-CG3	2.23	116.48	108.40
19	N	611	TGL	OG2-CB1-OB1	-2.23	118.32	123.70
27	T	102	CDL	C39-C38-C37	2.22	125.71	114.42
19	A	611	TGL	OG1-CA1-OA1	-2.22	117.99	123.59
14	A	601	HEA	CMC-C2C-C1C	2.22	128.75	125.37
14	N	603[A]	HEA	C3D-C4D-ND	2.21	112.50	110.36
27	T	102	CDL	C19-C18-C17	2.21	125.65	114.42
20	A	609	PGV	C25-C24-C23	2.21	125.65	114.42
22	B	301	CHD	C5-C4-C3	-2.21	109.52	112.76
19	N	611	TGL	CB3-CB2-CB1	-2.21	105.60	113.62
22	C	301	CHD	C19-C10-C9	-2.21	108.14	111.18
14	N	603[A]	HEA	C26-C15-C14	-2.20	118.02	123.68
14	N	602	HEA	CAD-CBD-CGD	-2.20	108.87	113.60
27	P	305	CDL	OB6-CB4-CB3	-2.19	100.46	108.40
27	T	102	CDL	CB4-OB6-CB5	2.19	123.18	117.79
19	D	201	TGL	CG3-CG2-CG1	2.19	116.96	111.79
20	N	609	PGV	C26-C25-C24	-2.19	103.33	114.42
21	S	104	EDO	O1-C1-C2	-2.18	96.21	111.91
19	Y	101	TGL	CC3-CC2-CC1	2.18	121.54	113.62
22	P	301	CHD	C1-C2-C3	-2.18	107.67	110.47
20	C	308	PGV	C26-C25-C24	2.17	125.46	114.42
22	C	306	CHD	C21-C20-C22	2.17	113.77	110.36
27	N	601	CDL	OB8-CB6-CB4	2.17	114.75	108.43
22	J	101	CHD	O26-C24-C23	2.17	121.00	114.03
22	B	301	CHD	C11-C12-C13	2.16	113.46	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	CHD-C1D-ND	-2.16	121.71	124.37
14	N	603[A]	HEA	CHC-C1C-C2C	-2.16	121.13	127.24
25	C	310	DMU	C6-C1-C2	-2.16	105.50	110.00
25	P	307	DMU	C31-C28-C25	-2.15	103.50	114.42
14	N	603[A]	HEA	C16-C15-C14	-2.15	116.77	121.12
28	T	101	PEK	O01-C02-C03	-2.14	100.66	108.40
25	P	310	DMU	C6-C1-C2	2.13	114.44	110.00
22	W	101	CHD	C18-C13-C17	2.13	114.55	111.21
27	C	305	CDL	OB4-PB2-OB5	-2.13	97.86	107.75
14	N	602	HEA	CAA-C2A-C1A	2.13	128.91	124.89
20	C	304	PGV	C4-C3-C2	-2.12	105.55	113.19
14	N	603[B]	HEA	C3C-C2C-C1C	-2.12	104.60	107.16
28	G	101	PEK	C3-C2-C1	-2.12	105.92	113.62
14	A	602[A]	HEA	O2A-CGA-O1A	-2.11	118.03	123.30
14	A	602[B]	HEA	C1D-ND-C4D	2.11	107.25	105.07
27	N	601	CDL	CA6-OA8-CA7	2.11	124.94	117.12
25	P	310	DMU	C6-O5-C4	2.11	117.83	113.69
28	G	101	PEK	O02-C1-C2	-2.11	115.52	123.73
22	J	101	CHD	C19-C10-C1	-2.10	104.87	108.26
20	P	304	PGV	C3-C2-C1	-2.10	105.98	113.62
22	C	301	CHD	C2-C1-C10	2.10	116.39	112.78
22	J	101	CHD	C1-C2-C3	-2.10	107.78	110.47
27	T	102	CDL	OA6-CA5-OA7	-2.09	118.65	123.70
22	P	306	CHD	C11-C9-C8	2.09	113.93	110.88
22	P	306	CHD	C18-C13-C14	2.09	114.48	111.21
22	B	301	CHD	C19-C10-C5	-2.09	106.82	110.36
22	P	301	CHD	O26-C24-O25	-2.09	118.10	123.30
28	G	103	PEK	C01-O03-C21	2.08	124.84	117.12
22	J	101	CHD	O7-C7-C8	2.08	114.08	109.43
25	P	307	DMU	C22-C19-C18	-2.08	104.28	113.49
14	N	603[B]	HEA	CBA-CAA-C2A	-2.08	106.86	112.63
27	T	102	CDL	CB2-C1-CA2	-2.07	106.69	112.79
22	W	101	CHD	O12-C12-C13	2.07	114.53	111.03
27	P	305	CDL	OB4-PB2-OB5	-2.07	98.12	107.75
24	N	612	PSC	C26-C25-C24	-2.07	103.91	114.42
21	A	615	EDO	O1-C1-C2	-2.07	97.02	111.91
22	P	301	CHD	C5-C6-C7	2.07	116.74	114.46
28	T	101	PEK	C24-C23-C22	-2.07	105.76	113.19
25	P	309	DMU	O5-C4-C57	2.06	111.56	106.44
22	G	102	CHD	O26-C24-C23	2.06	120.65	114.03
27	T	102	CDL	C62-C61-C60	2.06	124.88	114.42
22	J	101	CHD	C14-C8-C7	2.06	114.53	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602[B]	HEA	CMD-C2D-C3D	2.05	131.69	126.12
27	N	601	CDL	C63-C62-C61	2.05	124.84	114.42
14	N	602	HEA	CHA-C1A-C2A	-2.05	121.61	124.94
28	P	308	PEK	C35-C34-C33	2.05	124.81	114.42
14	N	602	HEA	C3A-C2A-C1A	-2.04	105.12	107.08
19	A	611	TGL	CG3-OG3-CC1	2.04	124.68	117.12
28	P	308	PEK	O03-C21-C22	2.04	118.31	111.91
22	W	101	CHD	C21-C20-C17	2.04	116.04	112.92
25	C	311	DMU	O7-C3-C2	2.03	112.67	107.28
14	A	601	HEA	CHB-C4A-NA	-2.03	122.25	124.44
14	N	602	HEA	C1C-CHC-C4B	-2.03	121.53	126.34
22	W	101	CHD	C5-C4-C3	2.02	115.73	112.76
20	A	610	PGV	O03-C19-O04	-2.02	118.49	123.59
27	T	102	CDL	C59-C58-C57	2.02	124.68	114.42
22	P	301	CHD	C17-C13-C14	2.02	102.13	100.09
25	C	310	DMU	O5-C6-C1	-2.02	106.08	110.35
14	N	603[B]	HEA	C1C-CHC-C4B	-2.02	121.55	126.34
14	N	603[A]	HEA	C3C-C4C-NC	-2.02	109.01	110.25
22	P	301	CHD	C1-C10-C5	2.02	110.75	107.77
27	C	305	CDL	C22-C21-C20	2.01	124.65	114.42
27	N	601	CDL	C43-C42-C41	2.01	124.65	114.42
14	N	603[B]	HEA	C17-C18-C19	2.01	132.50	127.66
19	N	611	TGL	OG2-CG2-CG1	2.01	115.68	108.40
19	A	611	TGL	OG2-CB1-OB1	-2.01	118.84	123.70
14	N	603[B]	HEA	CHA-C1A-NA	2.01	126.61	124.44
25	C	302	DMU	C57-C4-C3	2.01	119.17	113.33
27	N	601	CDL	C20-C19-C18	2.01	124.63	114.42
22	C	301	CHD	C4-C3-C2	-2.01	108.16	110.55
22	C	306	CHD	C18-C13-C17	-2.00	108.08	111.21

There are no chirality outliers.

All (946) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C2A-C3A-CMA-OMA
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[A]	HEA	C2A-C3A-CMA-OMA
19	A	611	TGL	CB2-CB1-OG2-CG2
19	A	611	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CG2-CG1-OG1-CA1
19	Y	101	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	610	PGV	C04-O12-P-O11
20	A	610	PGV	C02-C03-O11-P
20	A	610	PGV	C2-C1-O01-C02
20	C	308	PGV	C03-O11-P-O13
20	C	308	PGV	C03-O11-P-O14
20	C	308	PGV	O03-C01-C02-O01
20	C	308	PGV	C02-C03-O11-P
20	N	609	PGV	C04-O12-P-O13
20	N	609	PGV	C04-O12-P-O14
20	N	609	PGV	C02-C03-O11-P
20	N	609	PGV	O02-C1-O01-C02
20	N	609	PGV	C2-C1-O01-C02
20	P	302	PGV	C02-C03-O11-P
21	N	621	EDO	O1-C1-C2-O2
24	B	303	PSC	C03-O11-P-O12
24	B	303	PSC	C03-O11-P-O14
24	B	303	PSC	O12-C04-C05-N
24	N	612	PSC	C04-O12-P-O14
24	N	612	PSC	O12-C04-C05-N
25	C	302	DMU	C19-C18-O16-C6
25	C	311	DMU	C1-C6-O16-C18
25	C	311	DMU	O5-C6-O16-C18
25	C	311	DMU	C19-C18-O16-C6
25	P	307	DMU	O5-C6-O16-C18
25	P	310	DMU	C1-C6-O16-C18
25	P	310	DMU	O5-C6-O16-C18
27	C	305	CDL	CA2-OA2-PA1-OA4
27	C	305	CDL	CA3-OA5-PA1-OA2
27	C	305	CDL	C11-CA5-OA6-CA4
27	C	305	CDL	CB2-OB2-PB2-OB3
27	C	305	CDL	CB2-OB2-PB2-OB4
27	C	305	CDL	C51-CB5-OB6-CB4
27	N	601	CDL	CB2-C1-CA2-OA2
27	N	601	CDL	CA2-OA2-PA1-OA4
27	N	601	CDL	CA3-OA5-PA1-OA3
27	N	601	CDL	OA6-CA4-CA6-OA8
27	N	601	CDL	C11-CA5-OA6-CA4
27	N	601	CDL	CB3-OB5-PB2-OB2
27	N	601	CDL	CB3-OB5-PB2-OB3
27	N	601	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	OB6-CB4-CB6-OB8
27	P	305	CDL	CA2-OA2-PA1-OA5
27	P	305	CDL	CA3-OA5-PA1-OA3
27	P	305	CDL	C11-CA5-OA6-CA4
27	P	305	CDL	CB2-OB2-PB2-OB3
27	P	305	CDL	CB2-OB2-PB2-OB4
27	P	305	CDL	CB2-OB2-PB2-OB5
27	P	305	CDL	C51-CB5-OB6-CB4
27	T	102	CDL	CA3-OA5-PA1-OA2
27	T	102	CDL	CA3-OA5-PA1-OA3
27	T	102	CDL	OA6-CA4-CA6-OA8
27	T	102	CDL	OA7-CA5-OA6-CA4
27	T	102	CDL	CB3-OB5-PB2-OB3
28	C	307	PEK	C04-O12-P-O11
28	C	307	PEK	O12-C04-C05-N
28	C	307	PEK	O02-C1-O01-C02
28	C	307	PEK	C2-C1-O01-C02
28	C	309	PEK	C03-O11-P-O12
28	C	309	PEK	C03-O11-P-O13
28	C	309	PEK	C03-O11-P-O14
28	C	309	PEK	C04-O12-P-O14
28	C	309	PEK	O12-C04-C05-N
28	G	101	PEK	C7-C8-C9-C10
28	G	101	PEK	C10-C11-C12-C13
28	G	101	PEK	C12-C13-C14-C15
28	G	103	PEK	C04-O12-P-O11
28	G	103	PEK	C04-O12-P-O13
28	G	103	PEK	C04-O12-P-O14
28	G	103	PEK	O02-C1-O01-C02
28	G	103	PEK	C2-C1-O01-C02
28	P	308	PEK	C03-O11-P-O14
28	P	308	PEK	C04-O12-P-O11
28	P	308	PEK	C04-O12-P-O13
28	P	308	PEK	C04-O12-P-O14
28	P	308	PEK	O02-C1-O01-C02
28	P	308	PEK	C2-C1-O01-C02
28	T	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C12-C13-C14-C15
19	D	201	TGL	OC1-CC1-OG3-CG3
20	A	610	PGV	O04-C19-O03-C01
20	N	609	PGV	O04-C19-O03-C01
24	N	612	PSC	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
25	P	309	DMU	C5-C10-O7-C3
25	C	310	DMU	C5-C10-O7-C3
20	A	610	PGV	C20-C19-O03-C01
20	N	609	PGV	C20-C19-O03-C01
24	N	612	PSC	C20-C19-O03-C01
19	D	201	TGL	OA1-CA1-OG1-CG1
19	N	611	TGL	OC1-CC1-OG3-CG3
24	B	303	PSC	O04-C19-O03-C01
20	A	610	PGV	O02-C1-O01-C02
27	C	305	CDL	OA7-CA5-OA6-CA4
27	C	305	CDL	OB7-CB5-OB6-CB4
27	N	601	CDL	OA7-CA5-OA6-CA4
27	P	305	CDL	OA7-CA5-OA6-CA4
27	P	305	CDL	OB7-CB5-OB6-CB4
19	A	608	TGL	OC1-CC1-OG3-CG3
19	N	611	TGL	CC2-CC1-OG3-CG3
24	B	303	PSC	C20-C19-O03-C01
27	T	102	CDL	C11-CA5-OA6-CA4
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
19	A	608	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
19	D	201	TGL	CC2-CC1-OG3-CG3
19	Q	201	TGL	CC2-CC1-OG3-CG3
25	P	309	DMU	O6-C11-C9-O1
28	C	307	PEK	C4-C5-C6-C7
28	C	307	PEK	C7-C8-C9-C10
28	G	103	PEK	C7-C8-C9-C10
28	P	308	PEK	C13-C14-C15-C16
28	T	101	PEK	C4-C5-C6-C7
28	T	101	PEK	C7-C8-C9-C10
19	N	611	TGL	C20-C21-C22-C23
14	N	603[B]	HEA	C4D-C3D-CAD-CBD
19	A	611	TGL	CA9-C20-C21-C22
19	D	201	TGL	C16-C17-C18-C19
25	C	302	DMU	C25-C28-C31-C34
27	T	102	CDL	C79-C80-C81-C82
19	A	611	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	CC3-CC4-CC5-CC6
27	C	305	CDL	C76-C77-C78-C79
27	T	102	CDL	C51-CB5-OB6-CB4
19	Y	101	TGL	CC1-CC2-CC3-CC4

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C24-C25-C26-C27
27	T	102	CDL	C61-C62-C63-C64
19	Q	201	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	C21-C22-C23-C24
20	A	610	PGV	C20-C21-C22-C23
25	M	101	DMU	C28-C31-C34-C37
27	N	601	CDL	C58-C59-C60-C61
27	P	305	CDL	C75-C76-C77-C78
25	P	309	DMU	O6-C11-C9-C8
24	B	303	PSC	C19-C20-C21-C22
19	A	611	TGL	CC1-CC2-CC3-CC4
19	Q	201	TGL	CC1-CC2-CC3-CC4
27	N	601	CDL	C81-C82-C83-C84
25	Z	101	DMU	O6-C11-C9-O1
14	A	601	HEA	C15-C16-C17-C18
24	B	303	PSC	C30-C31-C32-C33
22	J	101	CHD	C13-C17-C20-C22
22	C	306	CHD	C17-C20-C22-C23
22	P	306	CHD	C17-C20-C22-C23
19	A	611	TGL	OA1-CA1-OG1-CG1
25	C	302	DMU	O6-C11-C9-C8
19	A	608	TGL	CA2-CA3-CA4-CA5
24	N	612	PSC	C20-C21-C22-C23
20	A	610	PGV	O12-C04-C05-C06
27	C	305	CDL	CB2-C1-CA2-OA2
27	C	305	CDL	CA2-C1-CB2-OB2
27	P	305	CDL	CB2-C1-CA2-OA2
27	P	305	CDL	CA2-C1-CB2-OB2
27	T	102	CDL	OB7-CB5-OB6-CB4
27	T	102	CDL	C42-C43-C44-C45
19	A	608	TGL	CA2-CA1-OG1-CG1
27	N	601	CDL	C31-CA7-OA8-CA6
25	Z	101	DMU	O6-C11-C9-C8
19	D	201	TGL	CC2-CC3-CC4-CC5
27	N	601	CDL	C61-C62-C63-C64
22	W	101	CHD	C13-C17-C20-C21
24	B	303	PSC	C21-C22-C23-C24
20	A	610	PGV	O12-C04-C05-O05
27	C	305	CDL	O1-C1-CB2-OB2
27	N	601	CDL	O1-C1-CA2-OA2
27	P	305	CDL	O1-C1-CB2-OB2
19	N	611	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
28	T	101	PEK	C1-C2-C3-C4
27	P	305	CDL	C81-C82-C83-C84
27	N	601	CDL	OA9-CA7-OA8-CA6
19	A	608	TGL	OB1-CB1-OG2-CG2
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C17-C20-C22-C23
27	T	102	CDL	C31-CA7-OA8-CA6
27	N	601	CDL	CA5-C11-C12-C13
28	P	308	PEK	C21-C22-C23-C24
25	P	310	DMU	C4-C3-O7-C10
19	A	608	TGL	CA1-CA2-CA3-CA4
19	A	608	TGL	CB1-CB2-CB3-CB4
19	D	201	TGL	CA1-CA2-CA3-CA4
20	N	609	PGV	C19-C20-C21-C22
27	C	305	CDL	CA7-C31-C32-C33
27	C	305	CDL	CB7-C71-C72-C73
21	L	101	EDO	O1-C1-C2-O2
19	Y	101	TGL	CA2-CA3-CA4-CA5
22	C	306	CHD	C20-C22-C23-C24
25	P	310	DMU	O16-C18-C19-C22
22	C	306	CHD	C21-C20-C22-C23
22	P	306	CHD	C21-C20-C22-C23
19	A	608	TGL	OA1-CA1-OG1-CG1
28	G	103	PEK	C21-C22-C23-C24
20	N	609	PGV	O12-C04-C05-O05
27	C	305	CDL	O1-C1-CA2-OA2
27	P	305	CDL	O1-C1-CA2-OA2
22	J	101	CHD	C13-C17-C20-C21
27	T	102	CDL	OA9-CA7-OA8-CA6
25	P	310	DMU	C2-C3-O7-C10
20	N	609	PGV	C10-C11-C12-C13
24	B	303	PSC	C11-C10-C9-C8
19	A	608	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C23-C24-C25-C26
20	A	610	PGV	C03-O11-P-O12
20	C	308	PGV	C03-O11-P-O12
20	C	308	PGV	C04-O12-P-O11
20	N	609	PGV	C04-O12-P-O11
20	P	302	PGV	C03-O11-P-O12
24	N	612	PSC	C03-O11-P-O12
27	C	305	CDL	CA2-OA2-PA1-OA5
27	C	305	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	CA2-OA2-PA1-OA5
27	N	601	CDL	CB2-OB2-PB2-OB5
27	P	305	CDL	CA3-OA5-PA1-OA2
28	C	309	PEK	C04-O12-P-O11
27	C	305	CDL	C71-CB7-OB8-CB6
22	W	101	CHD	C16-C17-C20-C21
20	C	308	PGV	C1-C2-C3-C4
20	N	609	PGV	O12-C04-C05-C06
22	J	101	CHD	C16-C17-C20-C21
20	P	302	PGV	C1-C2-C3-C4
19	N	611	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	CC6-CC7-CC8-CC9
27	P	305	CDL	C80-C81-C82-C83
19	N	611	TGL	C21-C22-C23-C24
19	Y	101	TGL	CC4-CC5-CC6-CC7
19	Y	101	TGL	C14-C29-C30-C31
25	P	309	DMU	C19-C22-C25-C28
27	N	601	CDL	C14-C15-C16-C17
27	N	601	CDL	C56-C57-C58-C59
27	P	305	CDL	C57-C58-C59-C60
27	T	102	CDL	C14-C15-C16-C17
19	A	611	TGL	CA3-CA4-CA5-CA6
19	N	611	TGL	CB7-CB8-CB9-C10
19	Y	101	TGL	C21-C20-CA9-CA8
20	A	609	PGV	C26-C27-C28-C29
24	N	612	PSC	C29-C30-C31-C32
28	C	307	PEK	C25-C26-C27-C28
20	N	609	PGV	C01-C02-O01-C1
24	N	612	PSC	C01-C02-O01-C1
27	T	102	CDL	CA7-C31-C32-C33
19	A	608	TGL	C21-C22-C23-C24
19	A	611	TGL	CB5-CB6-CB7-CB8
19	Q	201	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CB3-CB4-CB5-CB6
20	C	304	PGV	C7-C8-C9-C10
27	C	305	CDL	C56-C57-C58-C59
27	C	305	CDL	C63-C64-C65-C66
20	A	610	PGV	C05-C04-O12-P
20	P	304	PGV	C10-C11-C12-C13
28	T	101	PEK	C10-C11-C12-C13
19	N	611	TGL	C19-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	C14-C15-C16-C17
28	G	101	PEK	C34-C35-C36-C37
28	G	103	PEK	C34-C35-C36-C37
19	A	608	TGL	C20-C21-C22-C23
19	Y	101	TGL	CB5-CB6-CB7-CB8
19	Y	101	TGL	CC6-CC7-CC8-CC9
27	N	601	CDL	C79-C80-C81-C82
27	P	305	CDL	C20-C21-C22-C23
25	C	302	DMU	C1-C6-O16-C18
19	Q	201	TGL	CA6-CA7-CA8-CA9
20	P	302	PGV	C26-C27-C28-C29
28	G	101	PEK	C16-C17-C18-C19
19	A	611	TGL	CC7-CC8-CC9-C15
27	N	601	CDL	C22-C23-C24-C25
27	N	601	CDL	C32-C33-C34-C35
27	P	305	CDL	C40-C41-C42-C43
27	P	305	CDL	C52-C53-C54-C55
19	A	611	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	CC9-C15-C16-C17
19	Y	101	TGL	CB6-CB7-CB8-CB9
20	C	304	PGV	C13-C14-C15-C16
20	N	609	PGV	C29-C30-C31-C32
27	C	305	CDL	C20-C21-C22-C23
27	N	601	CDL	C77-C78-C79-C80
27	P	305	CDL	C61-C62-C63-C64
28	T	101	PEK	C26-C27-C28-C29
25	C	302	DMU	O6-C11-C9-O1
24	B	303	PSC	C5-C6-C7-C8
27	C	305	CDL	C83-C84-C85-C86
27	N	601	CDL	C13-C14-C15-C16
27	P	305	CDL	C82-C83-C84-C85
27	T	102	CDL	C13-C14-C15-C16
28	C	307	PEK	C32-C33-C34-C35
20	A	610	PGV	C04-C05-C06-O06
20	N	609	PGV	C04-C05-C06-O06
20	P	302	PGV	C04-C05-C06-O06
19	N	611	TGL	OB1-CB1-OG2-CG2
19	A	608	TGL	C12-C13-C14-C29
19	Q	201	TGL	C10-C11-C12-C13
19	Y	101	TGL	C12-C13-C14-C29
20	P	302	PGV	C2-C3-C4-C5
20	P	302	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
27	T	102	CDL	C59-C60-C61-C62
19	A	608	TGL	C21-C20-CA9-CA8
19	D	201	TGL	C15-C16-C17-C18
20	P	304	PGV	C24-C25-C26-C27
24	N	612	PSC	C5-C6-C7-C8
25	C	311	DMU	O16-C18-C19-C22
25	P	310	DMU	C22-C25-C28-C31
27	C	305	CDL	C71-C72-C73-C74
27	N	601	CDL	C63-C64-C65-C66
27	P	305	CDL	C17-C18-C19-C20
27	T	102	CDL	C36-C37-C38-C39
28	G	101	PEK	C23-C24-C25-C26
28	G	103	PEK	C31-C32-C33-C34
25	C	311	DMU	C18-C19-C22-C25
19	A	608	TGL	CA5-CA6-CA7-CA8
19	A	611	TGL	C12-C13-C14-C29
19	D	201	TGL	CA7-CA8-CA9-C20
19	D	201	TGL	C19-C33-C34-C35
19	N	611	TGL	CA7-CA8-CA9-C20
19	Q	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	C19-C33-C34-C35
27	N	601	CDL	C18-C19-C20-C21
27	N	601	CDL	C55-C56-C57-C58
28	C	307	PEK	C28-C29-C30-C31
25	C	302	DMU	C18-C19-C22-C25
19	A	611	TGL	C11-C12-C13-C14
19	D	201	TGL	CC7-CC8-CC9-C15
19	N	611	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	CA3-CA4-CA5-CA6
20	N	609	PGV	C25-C26-C27-C28
27	C	305	CDL	C77-C78-C79-C80
27	N	601	CDL	C17-C18-C19-C20
27	N	601	CDL	C60-C61-C62-C63
27	P	305	CDL	C15-C16-C17-C18
27	P	305	CDL	C16-C17-C18-C19
27	T	102	CDL	C41-C42-C43-C44
27	T	102	CDL	C71-C72-C73-C74
20	A	610	PGV	C19-C20-C21-C22
27	C	305	CDL	OB9-CB7-OB8-CB6
27	C	305	CDL	C18-C19-C20-C21
28	T	101	PEK	C30-C31-C32-C33
19	N	611	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	C10-C11-C12-C13
19	A	608	TGL	C16-C15-CC9-CC8
19	Y	101	TGL	C10-C11-C12-C13
20	A	610	PGV	C14-C15-C16-C17
20	P	302	PGV	C24-C25-C26-C27
27	C	305	CDL	C11-C12-C13-C14
27	T	102	CDL	CB3-CB4-CB6-OB8
20	A	610	PGV	C10-C11-C12-C13
28	C	309	PEK	C10-C11-C12-C13
19	A	608	TGL	C16-C17-C18-C19
19	N	611	TGL	CB9-C10-C11-C12
19	N	611	TGL	CC4-CC5-CC6-CC7
19	Y	101	TGL	C22-C23-C24-C25
27	P	305	CDL	C78-C79-C80-C81
27	T	102	CDL	C75-C76-C77-C78
19	N	611	TGL	CB1-CB2-CB3-CB4
19	Y	101	TGL	C18-C19-C33-C34
19	N	611	TGL	CB2-CB1-OG2-CG2
24	B	303	PSC	C2-C1-O01-C02
19	Q	201	TGL	CA5-CA6-CA7-CA8
27	T	102	CDL	C32-C33-C34-C35
20	N	609	PGV	O05-C05-C06-O06
19	A	608	TGL	C15-C16-C17-C18
25	Z	101	DMU	O16-C18-C19-C22
25	C	311	DMU	O5-C4-C57-O61
25	P	310	DMU	C19-C22-C25-C28
25	C	311	DMU	C3-C4-C57-O61
20	P	304	PGV	C7-C8-C9-C10
27	N	601	CDL	C34-C35-C36-C37
27	T	102	CDL	C52-C53-C54-C55
19	Y	101	TGL	C16-C17-C18-C19
25	Z	101	DMU	C28-C31-C34-C37
19	A	611	TGL	CC6-CC7-CC8-CC9
19	A	611	TGL	C21-C22-C23-C24
19	A	611	TGL	C19-C33-C34-C35
19	N	611	TGL	CC5-CC6-CC7-CC8
27	N	601	CDL	C59-C60-C61-C62
19	A	611	TGL	C15-C16-C17-C18
20	N	609	PGV	C3-C4-C5-C6
27	P	305	CDL	C18-C19-C20-C21
27	P	305	CDL	C51-C52-C53-C54
21	A	618	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	A	608	TGL	CC4-CC5-CC6-CC7
28	C	309	PEK	C31-C32-C33-C34
28	G	103	PEK	C24-C25-C26-C27
24	N	612	PSC	C4-C5-C6-C7
27	P	305	CDL	C60-C61-C62-C63
19	A	611	TGL	CB2-CB3-CB4-CB5
20	A	609	PGV	C28-C29-C30-C31
20	P	302	PGV	C30-C31-C32-C33
20	C	308	PGV	C10-C11-C12-C13
28	P	308	PEK	C10-C11-C12-C13
28	T	101	PEK	C13-C14-C15-C16
19	Q	201	TGL	C13-C14-C29-C30
19	Y	101	TGL	C11-C12-C13-C14
25	C	311	DMU	C31-C34-C37-C40
27	T	102	CDL	C76-C77-C78-C79
28	C	307	PEK	C24-C25-C26-C27
28	T	101	PEK	C22-C23-C24-C25
22	W	101	CHD	C16-C17-C20-C22
28	T	101	PEK	C2-C3-C4-C5
24	B	303	PSC	O02-C1-O01-C02
19	A	608	TGL	C14-C29-C30-C31
28	G	103	PEK	C29-C30-C31-C32
20	P	302	PGV	C22-C23-C24-C25
27	N	601	CDL	C35-C36-C37-C38
27	P	305	CDL	C19-C20-C21-C22
27	P	305	CDL	C39-C40-C41-C42
27	P	305	CDL	C31-C32-C33-C34
28	G	103	PEK	C25-C26-C27-C28
19	D	201	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB9-C10-C11-C12
19	Y	101	TGL	CC9-C15-C16-C17
19	Q	201	TGL	C22-C23-C24-C25
20	A	610	PGV	C22-C23-C24-C25
20	N	609	PGV	C27-C28-C29-C30
19	A	611	TGL	CC2-CC3-CC4-CC5
19	N	611	TGL	CA5-CA6-CA7-CA8
28	P	308	PEK	C33-C34-C35-C36
24	N	612	PSC	C2-C1-O01-C02
27	P	305	CDL	C43-C44-C45-C46
19	A	611	TGL	C21-C20-CA9-CA8
19	Y	101	TGL	C24-C25-C26-C27
25	M	101	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	C42-C43-C44-C45
24	N	612	PSC	O02-C1-O01-C02
27	T	102	CDL	CB5-C51-C52-C53
20	P	304	PGV	C22-C23-C24-C25
24	N	612	PSC	C2-C3-C4-C5
27	T	102	CDL	OB6-CB4-CB6-OB8
28	C	309	PEK	O03-C01-C02-O01
19	Q	201	TGL	CB5-CB6-CB7-CB8
28	C	309	PEK	C24-C25-C26-C27
28	C	309	PEK	C25-C26-C27-C28
19	A	608	TGL	CB4-CB5-CB6-CB7
20	P	304	PGV	C11-C10-C9-C8
28	C	307	PEK	C15-C16-C17-C18
25	P	307	DMU	O6-C11-C9-C8
27	N	601	CDL	C72-C73-C74-C75
19	A	611	TGL	CC5-CC6-CC7-CC8
19	N	611	TGL	CB6-CB7-CB8-CB9
19	Q	201	TGL	C17-C18-C19-C33
27	C	305	CDL	C19-C20-C21-C22
28	G	101	PEK	C25-C26-C27-C28
27	N	601	CDL	C16-C17-C18-C19
27	N	601	CDL	CA3-OA5-PA1-OA2
28	P	308	PEK	C03-O11-P-O12
27	C	305	CDL	C36-C37-C38-C39
27	N	601	CDL	C11-C12-C13-C14
20	A	609	PGV	C30-C31-C32-C33
20	C	304	PGV	C27-C28-C29-C30
28	G	103	PEK	C32-C33-C34-C35
24	B	303	PSC	C01-C02-C03-O11
27	T	102	CDL	OB5-CB3-CB4-CB6
28	C	309	PEK	C01-C02-C03-O11
19	A	611	TGL	C22-C23-C24-C25
19	Q	201	TGL	CC7-CC8-CC9-C15
28	P	308	PEK	C30-C31-C32-C33
24	B	303	PSC	C2-C3-C4-C5
28	C	309	PEK	C27-C28-C29-C30
20	C	304	PGV	C12-C13-C14-C15
28	C	307	PEK	C2-C3-C4-C5
19	D	201	TGL	C21-C20-CA9-CA8
19	N	611	TGL	C14-C29-C30-C31
25	C	310	DMU	O16-C18-C19-C22
27	P	305	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
19	A	611	TGL	C14-C29-C30-C31
20	P	302	PGV	C6-C7-C8-C9
25	Z	101	DMU	C25-C28-C31-C34
28	C	307	PEK	C29-C30-C31-C32
27	C	305	CDL	C40-C41-C42-C43
28	C	307	PEK	C35-C36-C37-C38
19	A	608	TGL	CA6-CA7-CA8-CA9
19	A	608	TGL	C11-C12-C13-C14
19	D	201	TGL	OG1-CG1-CG2-CG3
19	N	611	TGL	OG1-CG1-CG2-CG3
20	C	308	PGV	O03-C01-C02-C03
20	N	609	PGV	O03-C01-C02-C03
24	B	303	PSC	O03-C01-C02-C03
24	N	612	PSC	O03-C01-C02-C03
27	C	305	CDL	CB3-CB4-CB6-OB8
27	C	305	CDL	C52-C53-C54-C55
27	P	305	CDL	CB3-CB4-CB6-OB8
27	P	305	CDL	C79-C80-C81-C82
27	T	102	CDL	CA3-CA4-CA6-OA8
28	C	309	PEK	O03-C01-C02-C03
20	C	304	PGV	C15-C16-C17-C18
25	C	310	DMU	C34-C37-C40-C43
27	N	601	CDL	C44-C45-C46-C47
27	T	102	CDL	C81-C82-C83-C84
19	Q	201	TGL	CB2-CB3-CB4-CB5
20	A	610	PGV	C29-C30-C31-C32
24	N	612	PSC	C31-C32-C33-C34
20	A	609	PGV	C31-C32-C33-C34
20	P	302	PGV	C13-C14-C15-C16
19	Y	101	TGL	C15-C16-C17-C18
24	B	303	PSC	C25-C26-C27-C28
25	M	101	DMU	C19-C22-C25-C28
28	C	307	PEK	C33-C34-C35-C36
20	P	304	PGV	C11-C12-C13-C14
28	T	101	PEK	C3-C4-C5-C6
20	P	302	PGV	O05-C05-C06-O06
19	A	608	TGL	C25-C26-C27-C28
19	A	611	TGL	C16-C17-C18-C19
28	C	307	PEK	C26-C27-C28-C29
20	A	610	PGV	C11-C10-C9-C8
20	N	610	PGV	C11-C10-C9-C8
20	N	610	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	P	308	PEK	C2-C3-C4-C5
20	P	304	PGV	C1-C2-C3-C4
20	C	308	PGV	C29-C30-C31-C32
19	Y	101	TGL	C25-C26-C27-C28
20	A	610	PGV	C21-C22-C23-C24
20	P	302	PGV	C29-C30-C31-C32
24	N	612	PSC	C15-C16-C17-C18
27	T	102	CDL	C72-C73-C74-C75
28	C	307	PEK	C17-C18-C19-C20
25	P	310	DMU	O6-C11-C9-C8
19	A	611	TGL	C23-C24-C25-C26
27	C	305	CDL	C12-C13-C14-C15
27	T	102	CDL	C38-C39-C40-C41
19	Y	101	TGL	C29-C30-C31-C32
28	G	103	PEK	O01-C02-C03-O11
28	P	308	PEK	O01-C02-C03-O11
28	G	101	PEK	C13-C14-C15-C16
20	C	308	PGV	C31-C32-C33-C34
21	A	612	EDO	O1-C1-C2-O2
19	Q	201	TGL	C21-C20-CA9-CA8
28	G	101	PEK	C28-C29-C30-C31
22	W	101	CHD	C21-C20-C22-C23
25	P	307	DMU	C1-C6-O16-C18
19	Q	201	TGL	C12-C13-C14-C29
20	C	304	PGV	C24-C25-C26-C27
19	A	611	TGL	OG1-CG1-CG2-OG2
19	N	611	TGL	OG1-CG1-CG2-OG2
20	P	302	PGV	O03-C01-C02-O01
27	C	305	CDL	C59-C60-C61-C62
19	D	201	TGL	C10-C11-C12-C13
27	N	601	CDL	C31-C32-C33-C34
27	C	305	CDL	C41-C42-C43-C44
19	A	611	TGL	CB1-CB2-CB3-CB4
19	N	611	TGL	CA2-CA3-CA4-CA5
28	G	103	PEK	C23-C24-C25-C26
19	N	611	TGL	CA4-CA5-CA6-CA7
27	P	305	CDL	C36-C37-C38-C39
19	D	201	TGL	C11-C10-CB9-CB8
27	T	102	CDL	C34-C35-C36-C37
19	A	608	TGL	C23-C24-C25-C26
19	A	611	TGL	CA2-CA3-CA4-CA5
19	A	611	TGL	CC4-CC5-CC6-CC7

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Mol	Chain	Res	Type	Atoms
20	C	308	PGV	C15-C16-C17-C18
20	C	304	PGV	C10-C11-C12-C13
27	T	102	CDL	C37-C38-C39-C40
20	C	308	PGV	C01-C02-C03-O11
27	C	305	CDL	OA5-CA3-CA4-CA6
28	G	101	PEK	C26-C27-C28-C29
19	N	611	TGL	C33-C34-C35-C36
19	Y	101	TGL	C13-C14-C29-C30
27	C	305	CDL	C37-C38-C39-C40
20	P	304	PGV	C02-C03-O11-P
19	A	608	TGL	OG1-CG1-CG2-CG3
20	P	302	PGV	O03-C01-C02-C03
27	N	601	CDL	CA3-CA4-CA6-OA8
27	N	601	CDL	CB3-CB4-CB6-OB8
27	P	305	CDL	CA3-CA4-CA6-OA8
27	C	305	CDL	C31-C32-C33-C34
28	C	309	PEK	C13-C14-C15-C16
20	C	308	PGV	C6-C7-C8-C9
19	A	608	TGL	C17-C18-C19-C33
19	Y	101	TGL	C11-C10-CB9-CB8
14	A	602[A]	HEA	C2A-C3A-CMA-OMA
14	N	603[B]	HEA	C2A-C3A-CMA-OMA
24	B	303	PSC	C9-C10-C11-C12
24	B	303	PSC	C10-C11-C12-C13
24	N	612	PSC	C10-C11-C12-C13
28	C	307	PEK	C5-C6-C7-C8
28	C	307	PEK	C6-C7-C8-C9
28	C	307	PEK	C11-C10-C9-C8
28	C	309	PEK	C11-C10-C9-C8
28	C	309	PEK	C9-C10-C11-C12
28	C	309	PEK	C12-C13-C14-C15
28	G	101	PEK	C9-C10-C11-C12
28	G	103	PEK	C6-C7-C8-C9
28	G	103	PEK	C11-C12-C13-C14
28	G	103	PEK	C12-C13-C14-C15
28	P	308	PEK	C9-C10-C11-C12
28	P	308	PEK	C12-C13-C14-C15
28	T	101	PEK	C11-C10-C9-C8
27	T	102	CDL	C21-C22-C23-C24
20	N	609	PGV	O01-C02-C03-O11
28	C	307	PEK	O01-C02-C03-O11
28	P	308	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	CB5-C51-C52-C53
27	N	601	CDL	O1-C1-CB2-OB2
19	A	611	TGL	C10-C11-C12-C13
20	A	610	PGV	C15-C16-C17-C18
27	T	102	CDL	C62-C63-C64-C65
19	D	201	TGL	OG1-CG1-CG2-OG2
20	N	609	PGV	O03-C01-C02-O01
27	C	305	CDL	OB6-CB4-CB6-OB8
27	P	305	CDL	OA6-CA4-CA6-OA8
20	N	609	PGV	C20-C21-C22-C23
20	N	610	PGV	C30-C31-C32-C33
28	P	308	PEK	C35-C36-C37-C38
20	C	308	PGV	O12-C04-C05-C06
27	N	601	CDL	CA2-C1-CB2-OB2
19	Q	201	TGL	C15-C16-C17-C18
20	C	304	PGV	C22-C23-C24-C25
19	N	611	TGL	C13-C14-C29-C30
20	C	304	PGV	C02-C03-O11-P
24	N	612	PSC	C02-C03-O11-P
27	C	305	CDL	C1-CA2-OA2-PA1
24	N	612	PSC	C6-C7-C8-C9
25	Z	101	DMU	C31-C34-C37-C40
27	C	305	CDL	C53-C54-C55-C56
25	P	307	DMU	C22-C25-C28-C31
21	A	616	EDO	O1-C1-C2-O2
21	B	304	EDO	O1-C1-C2-O2
21	D	202	EDO	O1-C1-C2-O2
20	N	610	PGV	C13-C14-C15-C16
19	A	611	TGL	C33-C34-C35-C36
20	N	610	PGV	C27-C28-C29-C30
27	C	305	CDL	C24-C25-C26-C27
28	G	101	PEK	C35-C36-C37-C38
19	Y	101	TGL	C20-C21-C22-C23
20	N	609	PGV	C01-C02-C03-O11
20	P	302	PGV	C23-C24-C25-C26
28	C	309	PEK	C7-C8-C9-C10
19	A	611	TGL	CA6-CA7-CA8-CA9
20	C	308	PGV	C14-C15-C16-C17
25	P	310	DMU	C34-C37-C40-C43
27	T	102	CDL	C64-C65-C66-C67
19	N	611	TGL	C11-C12-C13-C14
28	G	103	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	C53-C54-C55-C56
20	N	609	PGV	C30-C31-C32-C33
19	A	611	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	CA3-CA4-CA5-CA6
20	P	304	PGV	C28-C29-C30-C31
19	A	611	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	CG1-CG2-CG3-OG3
20	N	609	PGV	C05-C04-O12-P
27	N	601	CDL	C21-C22-C23-C24
20	C	308	PGV	O01-C02-C03-O11
27	C	305	CDL	OA5-CA3-CA4-OA6
27	T	102	CDL	OB5-CB3-CB4-OB6
19	N	611	TGL	CA9-C20-C21-C22
27	C	305	CDL	C84-C85-C86-C87
27	N	601	CDL	OB7-CB5-OB6-CB4
25	C	302	DMU	O16-C18-C19-C22
19	A	611	TGL	C20-C21-C22-C23
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
24	B	303	PSC	O03-C01-C02-O01
24	N	612	PSC	O03-C01-C02-O01
27	P	305	CDL	OB6-CB4-CB6-OB8
20	A	610	PGV	O05-C05-C06-O06
19	A	611	TGL	C29-C30-C31-C32
28	C	309	PEK	C22-C23-C24-C25
20	N	609	PGV	C11-C10-C9-C8
20	N	609	PGV	C12-C13-C14-C15
19	D	201	TGL	CA3-CA4-CA5-CA6
20	C	304	PGV	C1-C2-C3-C4
19	D	201	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CB2-CB3-CB4-CB5
24	N	612	PSC	C11-C12-C13-C14
22	P	306	CHD	C20-C22-C23-C24
25	P	307	DMU	O16-C18-C19-C22
28	P	308	PEK	C26-C27-C28-C29
19	Y	101	TGL	CA9-C20-C21-C22
20	C	308	PGV	C3-C4-C5-C6
27	P	305	CDL	C22-C23-C24-C25
24	B	303	PSC	C4-C5-C6-C7
20	A	609	PGV	C11-C10-C9-C8
24	B	303	PSC	C6-C7-C8-C9
24	N	612	PSC	C04-O12-P-O11
27	T	102	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	CA5-C11-C12-C13
27	C	305	CDL	CA4-CA3-OA5-PA1
27	T	102	CDL	OB9-CB7-OB8-CB6
20	A	610	PGV	C03-O11-P-O13
20	A	610	PGV	C04-O12-P-O14
20	C	308	PGV	C04-O12-P-O13
20	P	302	PGV	C03-O11-P-O13
24	N	612	PSC	C03-O11-P-O13
27	C	305	CDL	CA3-OA5-PA1-OA3
27	N	601	CDL	CA2-OA2-PA1-OA3
27	N	601	CDL	CB2-OB2-PB2-OB3
27	P	305	CDL	CA2-OA2-PA1-OA4
28	C	307	PEK	C04-O12-P-O13
28	C	309	PEK	C04-O12-P-O13
28	P	308	PEK	C03-O11-P-O13
19	Q	201	TGL	C29-C30-C31-C32
27	T	102	CDL	C55-C56-C57-C58
28	G	103	PEK	C35-C36-C37-C38
25	C	302	DMU	O5-C6-O16-C18
27	T	102	CDL	C71-CB7-OB8-CB6
27	P	305	CDL	OA5-CA3-CA4-CA6
28	G	103	PEK	C01-C02-C03-O11
28	P	308	PEK	C01-C02-C03-O11
27	N	601	CDL	C20-C21-C22-C23
21	A	619	EDO	O1-C1-C2-O2
21	N	618	EDO	O1-C1-C2-O2
27	T	102	CDL	C73-C74-C75-C76
25	M	101	DMU	C22-C25-C28-C31
28	C	307	PEK	C05-C04-O12-P
20	A	610	PGV	C12-C13-C14-C15
25	C	310	DMU	O6-C11-C9-C8
27	C	305	CDL	C55-C56-C57-C58
24	B	303	PSC	O01-C02-C03-O11
27	P	305	CDL	OA5-CA3-CA4-OA6
28	C	309	PEK	O01-C02-C03-O11
27	C	305	CDL	C17-C18-C19-C20
27	N	601	CDL	C51-CB5-OB6-CB4
20	N	609	PGV	C28-C29-C30-C31
14	A	602[B]	HEA	C4A-C3A-CMA-OMA
14	N	603[A]	HEA	C4A-C3A-CMA-OMA
14	N	603[B]	HEA	C4A-C3A-CMA-OMA
28	C	307	PEK	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	P	308	PEK	C4-C5-C6-C7
24	N	612	PSC	C30-C31-C32-C33
20	P	302	PGV	C9-C10-C11-C12
28	G	101	PEK	C24-C25-C26-C27
20	P	302	PGV	C31-C32-C33-C34
19	D	201	TGL	C33-C34-C35-C36
28	G	103	PEK	C33-C34-C35-C36
28	G	101	PEK	C33-C34-C35-C36
20	C	304	PGV	C20-C21-C22-C23
25	C	310	DMU	C19-C22-C25-C28
20	P	304	PGV	C12-C13-C14-C15
19	D	201	TGL	C16-C15-CC9-CC8
20	A	609	PGV	C10-C11-C12-C13
20	N	610	PGV	C10-C11-C12-C13
28	G	101	PEK	C4-C5-C6-C7
28	G	103	PEK	C4-C5-C6-C7
19	D	201	TGL	CB2-CB1-OG2-CG2
28	T	101	PEK	O03-C21-C22-C23
19	Y	101	TGL	CC5-CC6-CC7-CC8
27	N	601	CDL	C75-C76-C77-C78
19	D	201	TGL	CG3-CG2-OG2-CB1
28	T	101	PEK	O02-C1-O01-C02
19	N	611	TGL	CA2-CA1-OG1-CG1
25	Z	101	DMU	C19-C22-C25-C28
24	B	303	PSC	C02-C03-O11-P
24	B	303	PSC	C22-C23-C24-C25
21	Y	102	EDO	O1-C1-C2-O2
24	N	612	PSC	C7-C8-C9-C10
20	N	609	PGV	C03-O11-P-O12
20	P	302	PGV	C04-O12-P-O11
24	B	303	PSC	C04-O12-P-O11
27	T	102	CDL	CA2-OA2-PA1-OA5
27	T	102	CDL	CB2-OB2-PB2-OB5
28	C	307	PEK	C03-O11-P-O12
28	G	103	PEK	C03-O11-P-O12
27	C	305	CDL	CA3-CA4-CA6-OA8
19	N	611	TGL	C21-C20-CA9-CA8
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
20	P	302	PGV	C19-C20-C21-C22
19	D	201	TGL	OG2-CB1-CB2-CB3
20	N	610	PGV	C28-C29-C30-C31
20	P	304	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
20	N	609	PGV	C13-C14-C15-C16
19	N	611	TGL	CB2-CB3-CB4-CB5
14	N	602	HEA	C12-C13-C14-C15
27	T	102	CDL	C80-C81-C82-C83
19	A	608	TGL	CA7-CA8-CA9-C20
19	N	611	TGL	OA1-CA1-OG1-CG1
20	P	304	PGV	C19-C20-C21-C22
19	A	608	TGL	CA4-CA5-CA6-CA7
19	Q	201	TGL	OG1-CA1-CA2-CA3
19	D	201	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C3-C4-C5-C6
25	C	302	DMU	C19-C22-C25-C28
19	A	608	TGL	C22-C23-C24-C25
27	N	601	CDL	C64-C65-C66-C67
27	T	102	CDL	C74-C75-C76-C77
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
14	N	603[B]	HEA	CAA-CBA-CGA-O1A
22	B	301	CHD	C22-C23-C24-O25
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
22	G	102	CHD	C22-C23-C24-O26
25	C	310	DMU	C25-C28-C31-C34
25	P	309	DMU	C34-C37-C40-C43
27	C	305	CDL	C51-C52-C53-C54
20	C	308	PGV	C27-C28-C29-C30
14	N	603[A]	HEA	CAA-CBA-CGA-O1A
22	B	301	CHD	C22-C23-C24-O26
22	P	301	CHD	C16-C17-C20-C22
20	N	610	PGV	C31-C32-C33-C34
25	P	309	DMU	O16-C18-C19-C22
19	N	611	TGL	C15-C16-C17-C18
14	A	601	HEA	CAD-CBD-CGD-O2D
22	G	102	CHD	C22-C23-C24-O25
20	C	304	PGV	C30-C31-C32-C33
19	D	201	TGL	CG1-CG2-OG2-CB1
20	N	610	PGV	C11-C12-C13-C14
28	C	307	PEK	C9-C10-C11-C12
28	C	307	PEK	C11-C12-C13-C14
28	T	101	PEK	C5-C6-C7-C8
20	C	304	PGV	C05-C04-O12-P
19	A	611	TGL	OG1-CA1-CA2-CA3
19	Q	201	TGL	OG2-CB1-CB2-CB3
14	A	602[A]	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	N	603[B]	HEA	CAA-CBA-CGA-O2A
20	P	304	PGV	C21-C22-C23-C24
28	C	307	PEK	C01-C02-C03-O11
20	N	609	PGV	C24-C25-C26-C27
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
14	N	603[A]	HEA	CAA-CBA-CGA-O2A
27	P	305	CDL	C12-C13-C14-C15
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
27	P	305	CDL	C56-C57-C58-C59
14	N	602	HEA	CAD-CBD-CGD-O2D
22	J	101	CHD	C22-C23-C24-O26
19	D	201	TGL	C12-C13-C14-C29
27	P	305	CDL	C41-C42-C43-C44
28	C	309	PEK	C15-C16-C17-C18
28	G	103	PEK	C13-C14-C15-C16
27	C	305	CDL	C62-C63-C64-C65
22	J	101	CHD	C22-C23-C24-O25
24	B	303	PSC	C26-C27-C28-C29
19	N	611	TGL	OG1-CA1-CA2-CA3
27	N	601	CDL	C83-C84-C85-C86
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O1D
20	A	609	PGV	O03-C19-C20-C21
27	T	102	CDL	C20-C21-C22-C23
19	D	201	TGL	C20-C21-C22-C23
24	N	612	PSC	C14-C15-C16-C17
14	A	601	HEA	C26-C15-C16-C17
28	C	307	PEK	O01-C1-C2-C3
19	Y	101	TGL	CC2-CC3-CC4-CC5
28	P	308	PEK	C32-C33-C34-C35
19	Q	201	TGL	C16-C17-C18-C19
22	P	306	CHD	C22-C23-C24-O26
24	N	612	PSC	C22-C23-C24-C25
28	G	101	PEK	C22-C23-C24-C25
20	C	304	PGV	C9-C10-C11-C12
28	G	103	PEK	C3-C4-C5-C6
22	C	306	CHD	C22-C23-C24-O26
24	B	303	PSC	C04-C05-N-C06
14	N	602	HEA	C26-C15-C16-C17
19	N	611	TGL	CC7-CC8-CC9-C15
28	G	101	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
25	C	310	DMU	C31-C34-C37-C40
28	G	103	PEK	O03-C21-C22-C23
19	A	611	TGL	OC1-CC1-OG3-CG3
22	C	306	CHD	C22-C23-C24-O25
27	N	601	CDL	C78-C79-C80-C81
28	G	101	PEK	C27-C28-C29-C30
20	C	304	PGV	C25-C26-C27-C28
20	N	609	PGV	O03-C19-C20-C21
19	A	608	TGL	CC9-C15-C16-C17
28	T	101	PEK	C15-C16-C17-C18
27	C	305	CDL	C22-C23-C24-C25
22	W	101	CHD	C22-C23-C24-O25
25	P	310	DMU	C31-C34-C37-C40
28	G	101	PEK	C17-C18-C19-C20
20	C	304	PGV	C11-C12-C13-C14
24	B	303	PSC	C7-C8-C9-C10
22	C	301	CHD	C22-C23-C24-O26
19	Q	201	TGL	OB1-CB1-OG2-CG2
24	N	612	PSC	C28-C29-C30-C31
14	N	602	HEA	C11-C12-C13-C14
19	D	201	TGL	OG1-CA1-CA2-CA3
20	C	308	PGV	C13-C14-C15-C16
27	N	601	CDL	C41-C42-C43-C44
20	N	610	PGV	O03-C19-C20-C21
28	T	101	PEK	O01-C1-C2-C3
20	A	610	PGV	C24-C25-C26-C27
28	P	308	PEK	C3-C4-C5-C6
14	A	601	HEA	C12-C11-C3B-C2B
20	A	610	PGV	O03-C01-C02-C03
22	P	306	CHD	C22-C23-C24-O25
20	C	304	PGV	C28-C29-C30-C31
27	N	601	CDL	C73-C74-C75-C76
19	A	608	TGL	OG3-CC1-CC2-CC3
14	N	603[A]	HEA	CAD-CBD-CGD-O2D
22	C	301	CHD	C22-C23-C24-O25
20	C	308	PGV	C2-C3-C4-C5
21	A	613	EDO	O1-C1-C2-O2
21	E	202	EDO	O1-C1-C2-O2
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
22	P	301	CHD	C22-C23-C24-O25
24	B	303	PSC	C12-C13-C14-C15
28	C	307	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
19	N	611	TGL	C22-C23-C24-C25
20	P	302	PGV	C5-C6-C7-C8
20	P	302	PGV	C11-C10-C9-C8
27	N	601	CDL	C19-C20-C21-C22
19	Q	201	TGL	CB2-CB1-OG2-CG2
22	P	301	CHD	C22-C23-C24-O26
19	Q	201	TGL	CC2-CC3-CC4-CC5
20	A	610	PGV	O03-C01-C02-O01
19	A	608	TGL	CB5-CB6-CB7-CB8
24	B	303	PSC	C04-C05-N-C08
22	W	101	CHD	C22-C23-C24-O26
27	P	305	CDL	C58-C59-C60-C61
28	T	101	PEK	C2-C1-O01-C02
28	P	308	PEK	C17-C18-C19-C20
19	D	201	TGL	CB4-CB5-CB6-CB7
27	T	102	CDL	C12-C13-C14-C15
20	N	610	PGV	C14-C15-C16-C17
24	B	303	PSC	C20-C21-C22-C23
27	P	305	CDL	C84-C85-C86-C87
19	D	201	TGL	OA1-CA1-CA2-CA3
28	G	103	PEK	O04-C21-C22-C23
28	C	309	PEK	C26-C27-C28-C29
19	A	608	TGL	OC1-CC1-CC2-CC3
19	Y	101	TGL	CG1-CG2-CG3-OG3
20	A	610	PGV	C31-C32-C33-C34
14	N	603[B]	HEA	C26-C15-C16-C17
20	N	609	PGV	O04-C19-C20-C21
20	N	609	PGV	C03-O11-P-O13
24	B	303	PSC	C04-C05-N-C07
27	T	102	CDL	CA2-OA2-PA1-OA3
27	T	102	CDL	CB2-OB2-PB2-OB3
28	C	307	PEK	C03-O11-P-O14
28	G	103	PEK	C27-C28-C29-C30
21	A	615	EDO	O1-C1-C2-O2
21	B	305	EDO	O1-C1-C2-O2
28	T	101	PEK	O04-C21-C22-C23
19	N	611	TGL	C10-C11-C12-C13
28	G	103	PEK	C05-C04-O12-P
28	T	101	PEK	C05-C04-O12-P
28	T	101	PEK	O02-C1-C2-C3
28	T	101	PEK	C33-C34-C35-C36
27	C	305	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
19	N	611	TGL	C16-C17-C18-C19
19	N	611	TGL	OG3-CC1-CC2-CC3
28	C	309	PEK	C33-C34-C35-C36
19	A	611	TGL	C18-C19-C33-C34
14	A	601	HEA	O11-C11-C3B-C2B
14	A	601	HEA	CAA-CBA-CGA-O1A
14	N	602	HEA	CAA-CBA-CGA-O2A
28	C	309	PEK	O03-C21-C22-C23
27	P	305	CDL	C44-C45-C46-C47
28	G	103	PEK	C22-C23-C24-C25
19	D	201	TGL	OC1-CC1-CC2-CC3
19	A	611	TGL	CC2-CC1-OG3-CG3
19	Y	101	TGL	C19-C33-C34-C35
25	P	309	DMU	C25-C28-C31-C34

There are no ring outliers.

56 monomers are involved in 349 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	201	TGL	12	0
24	N	612	PSC	16	0
14	A	602[A]	HEA	3	0
28	G	101	PEK	7	0
21	A	619	EDO	3	0
27	C	305	CDL	16	0
27	P	305	CDL	24	0
28	T	101	PEK	3	0
21	G	105	EDO	3	0
20	P	302	PGV	1	0
28	G	103	PEK	1	0
21	N	621	EDO	1	0
22	P	301	CHD	1	0
22	J	101	CHD	1	0
24	B	303	PSC	15	0
21	A	620	EDO	1	0
18	N	608[A]	AZI	1	0
20	A	609	PGV	4	0
27	N	601	CDL	29	0
20	P	304	PGV	2	0
25	P	307	DMU	11	0
19	A	608	TGL	5	0
19	D	201	TGL	13	0

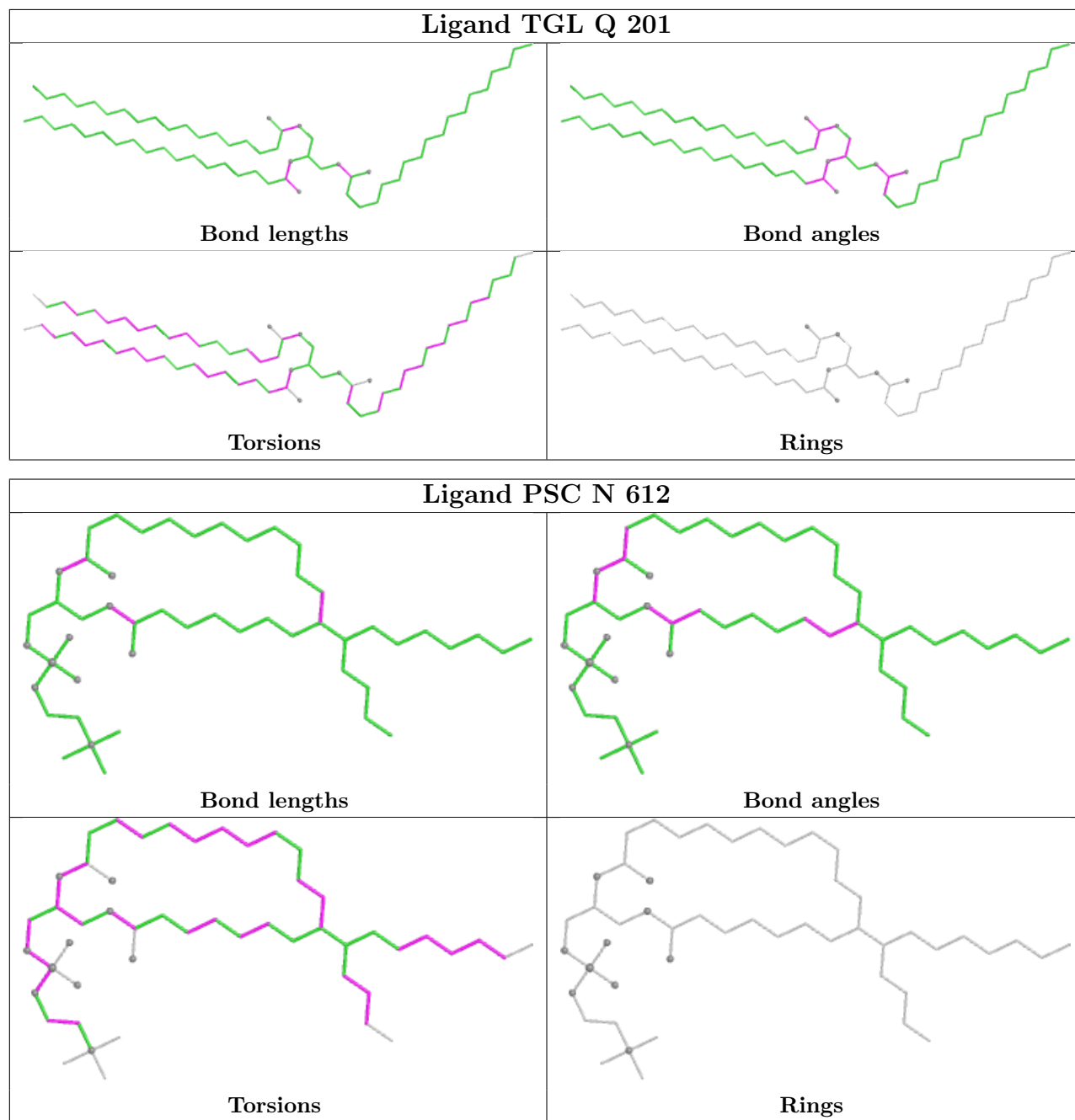
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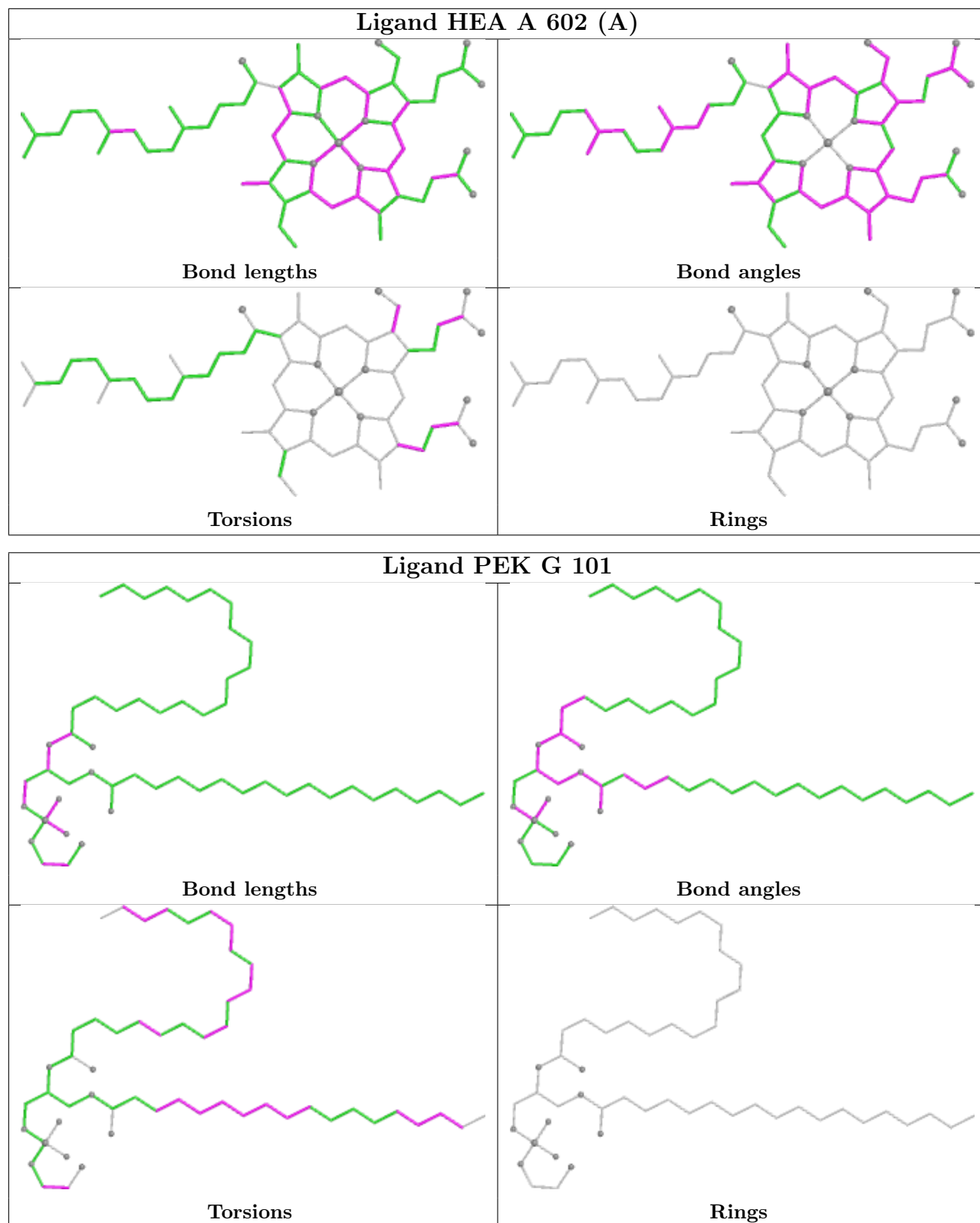
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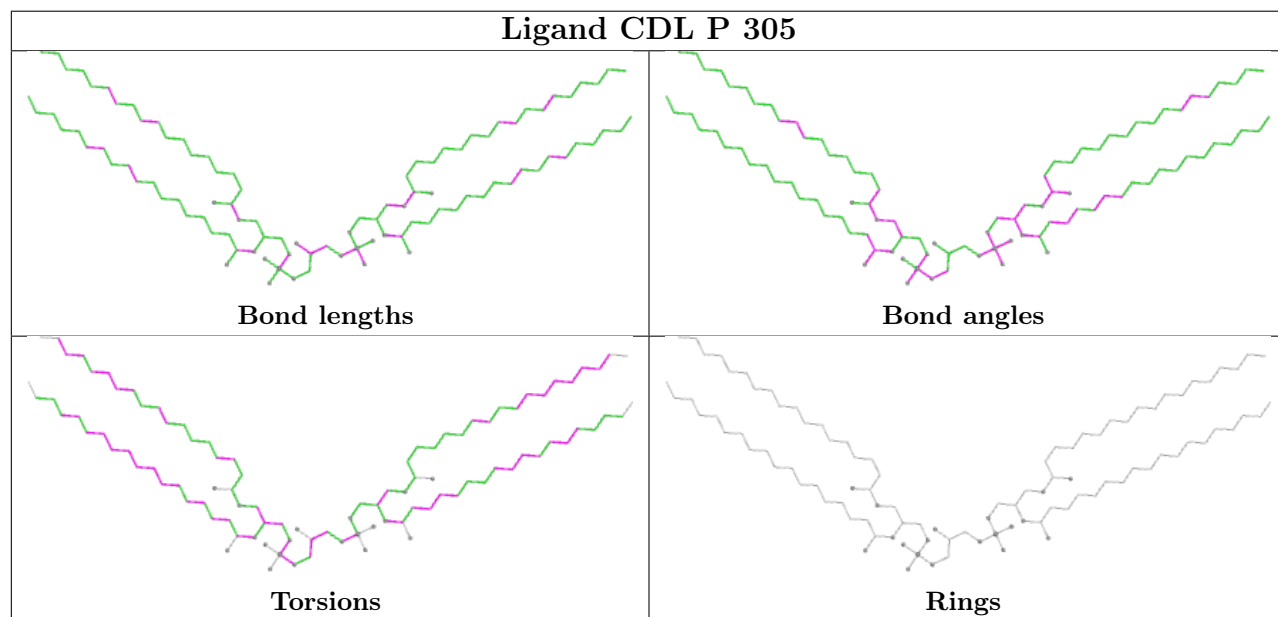
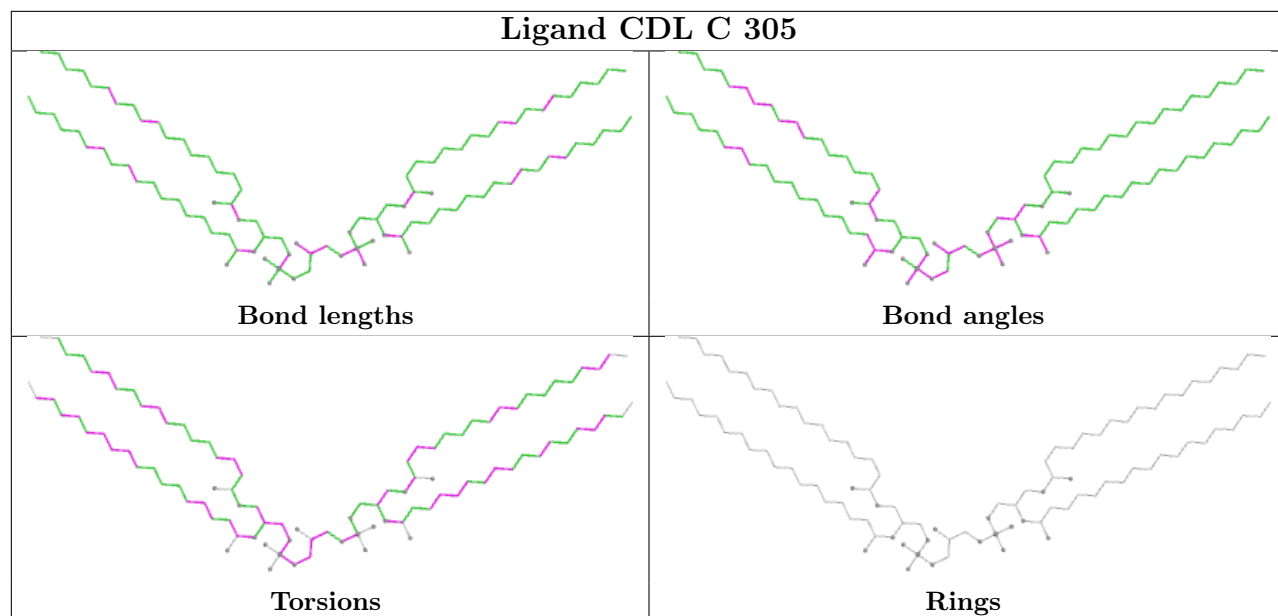
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	T	102	CDL	16	0
18	A	607[B]	AZI	5	0
25	P	309	DMU	3	0
21	D	202	EDO	9	0
19	Y	101	TGL	20	0
25	C	310	DMU	3	0
14	N	603[B]	HEA	6	0
21	B	304	EDO	2	0
20	C	304	PGV	4	0
28	C	309	PEK	4	0
22	P	306	CHD	5	0
25	P	310	DMU	2	0
14	N	602	HEA	11	0
20	C	308	PGV	1	0
21	A	618	EDO	2	0
14	A	602[B]	HEA	5	0
21	A	616	EDO	2	0
14	A	601	HEA	10	0
19	N	611	TGL	7	0
18	A	607[A]	AZI	2	0
22	G	102	CHD	1	0
20	A	610	PGV	9	0
20	N	610	PGV	1	0
28	C	307	PEK	12	0
14	N	603[A]	HEA	5	0
25	C	302	DMU	12	0
18	N	608[B]	AZI	1	0
22	C	306	CHD	5	0
22	C	301	CHD	1	0
22	W	101	CHD	1	0
28	P	308	PEK	6	0
20	N	609	PGV	9	0
19	A	611	TGL	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

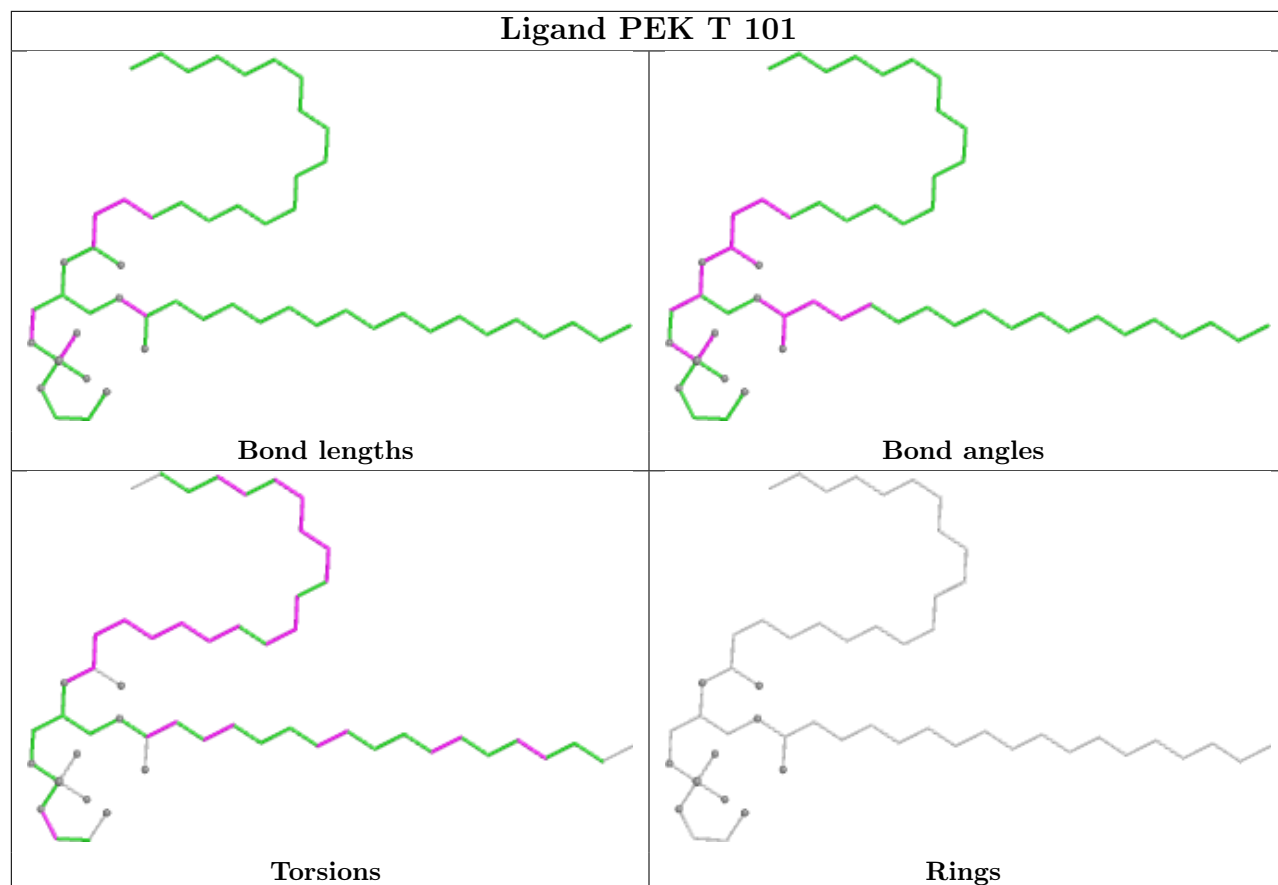
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



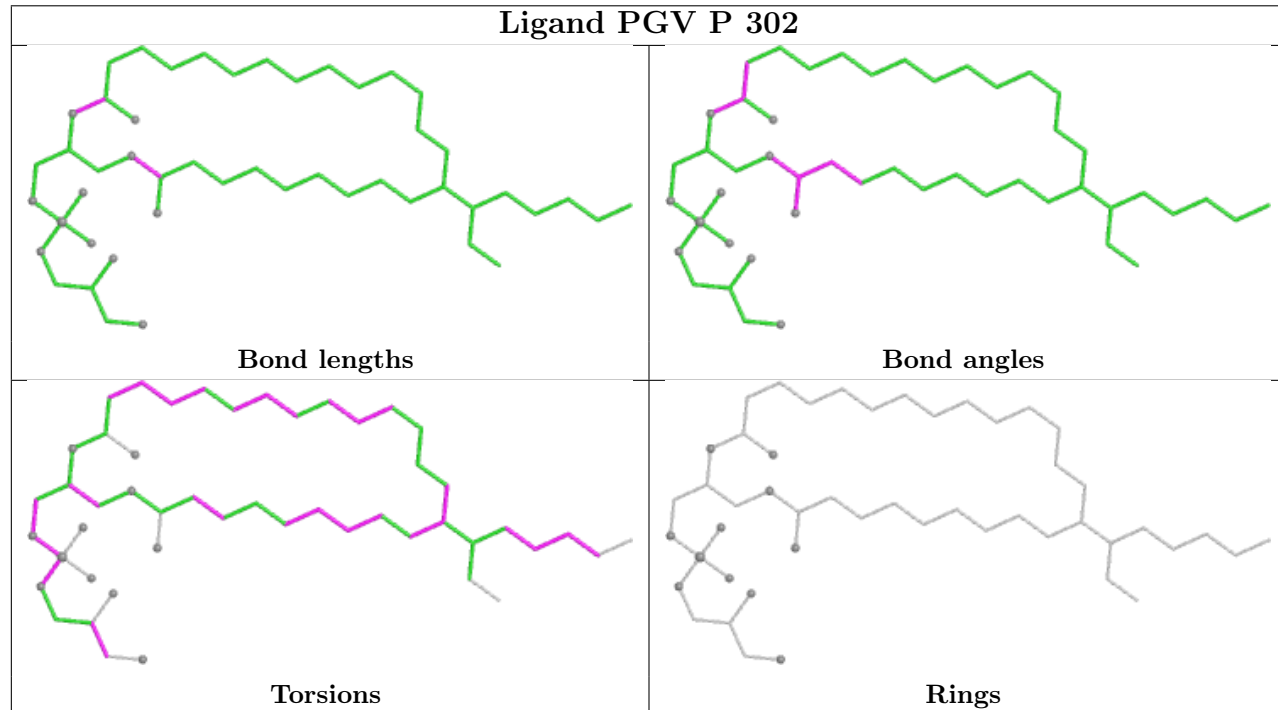


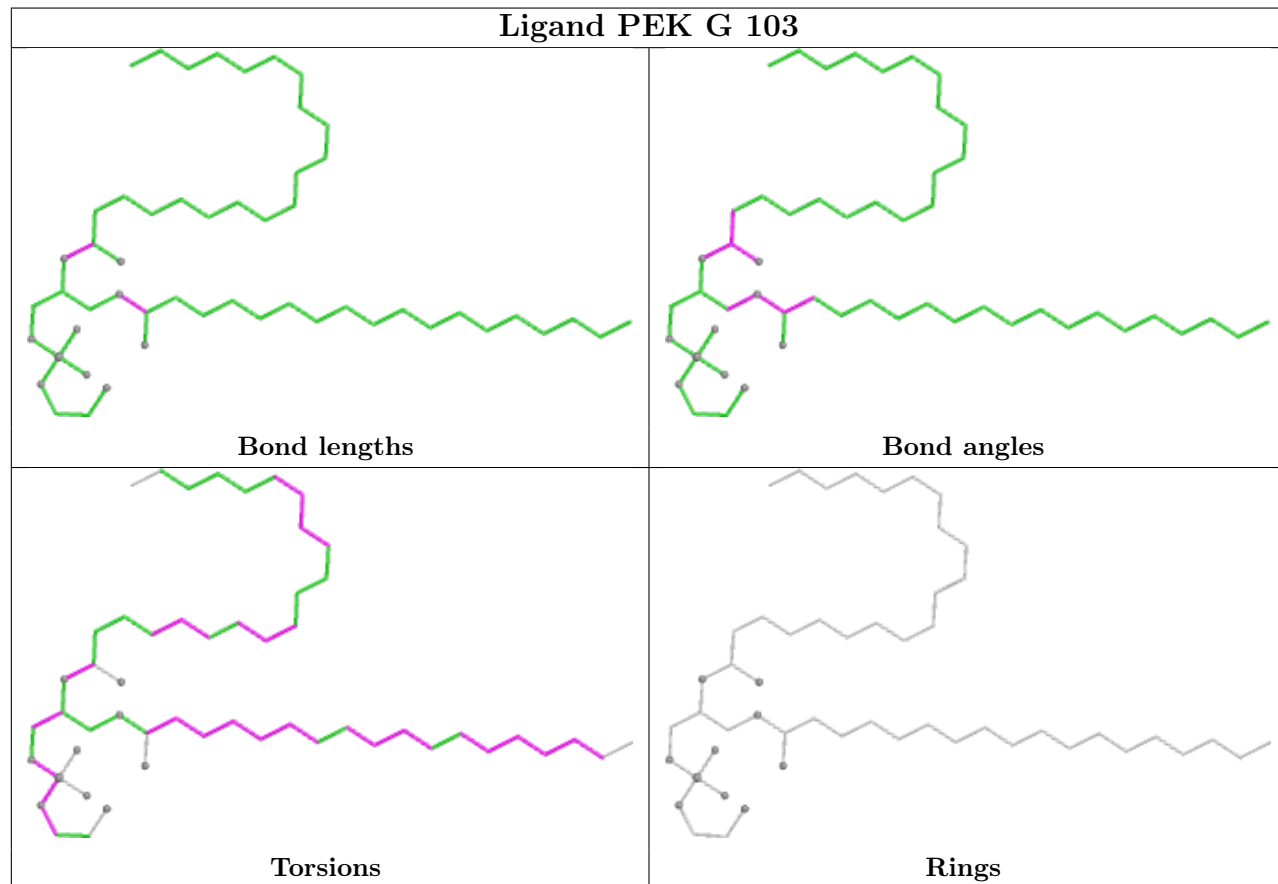
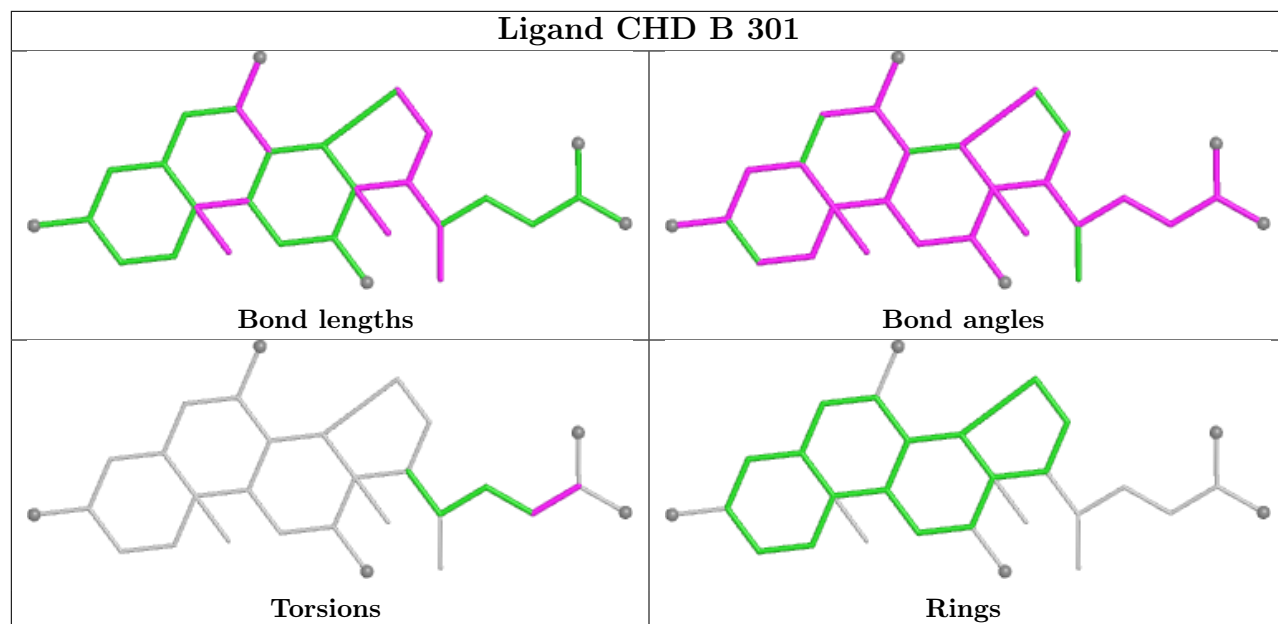


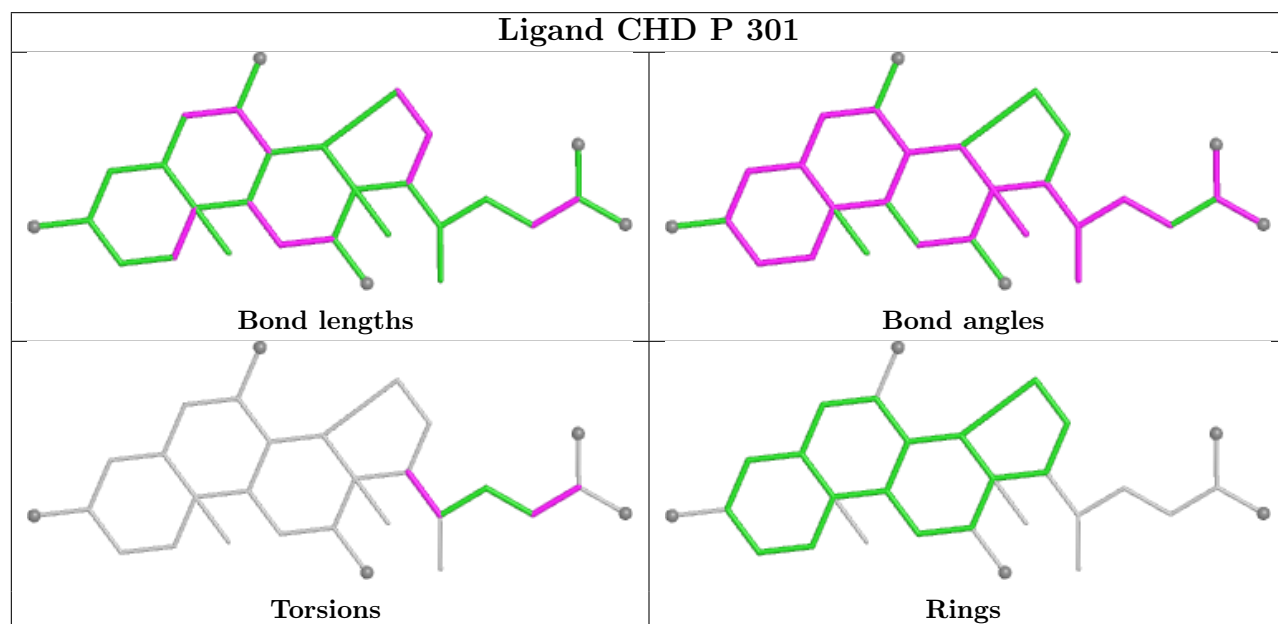
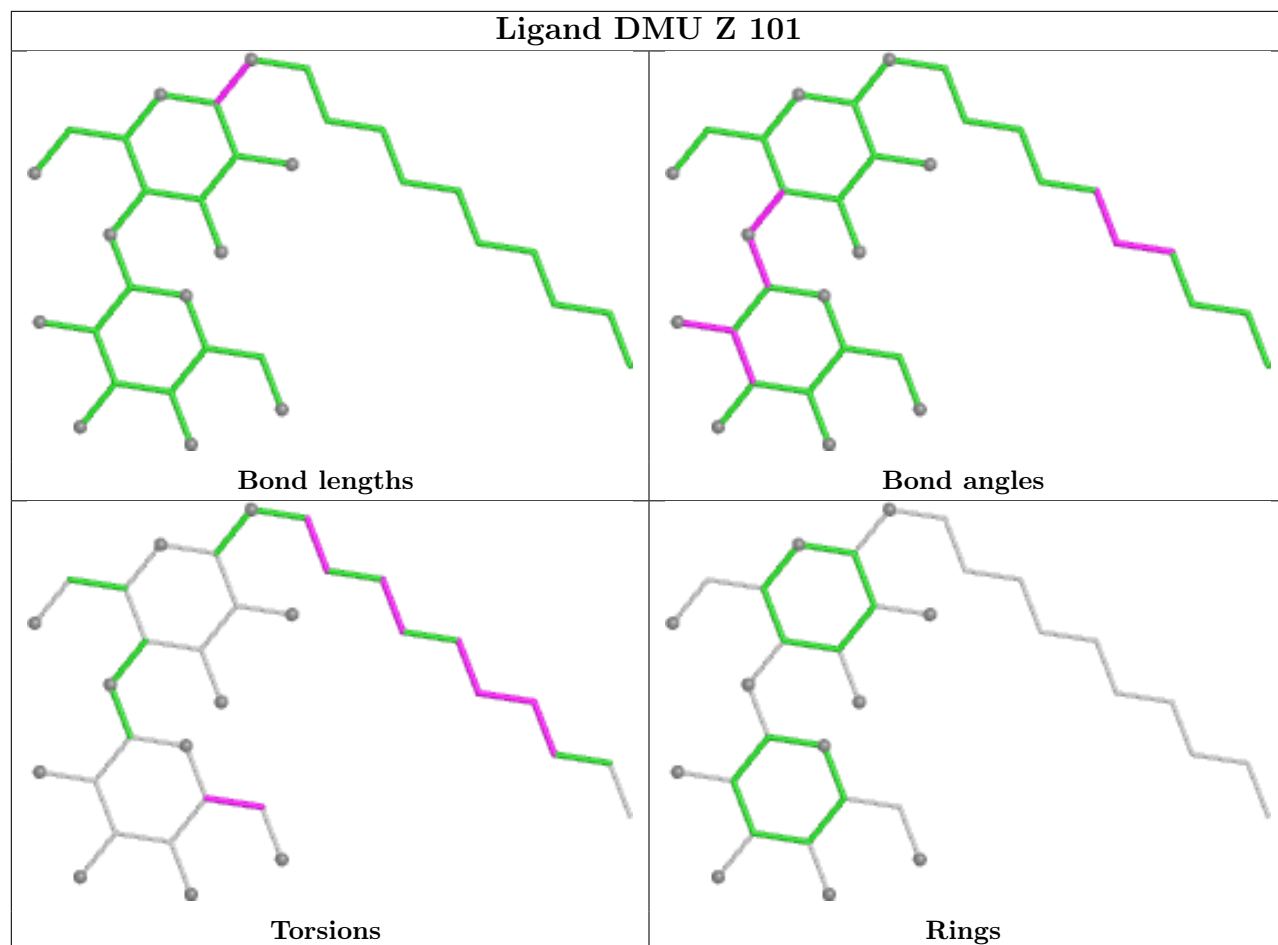
Ligand PEK T 101



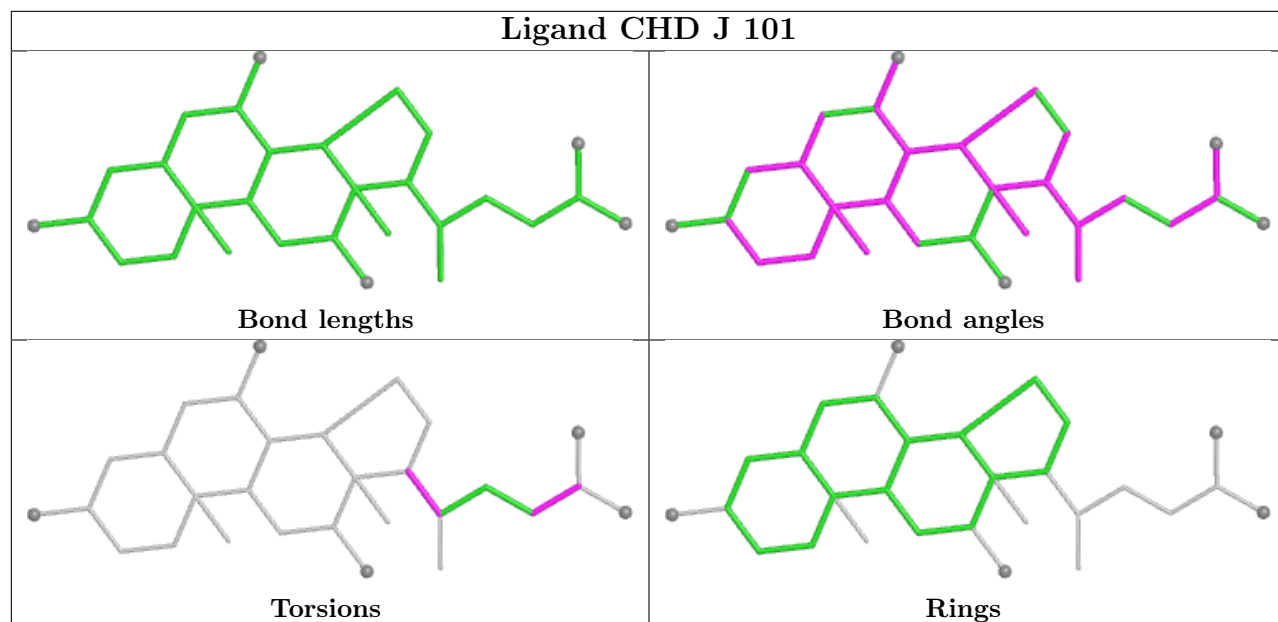
Ligand PGV P 302



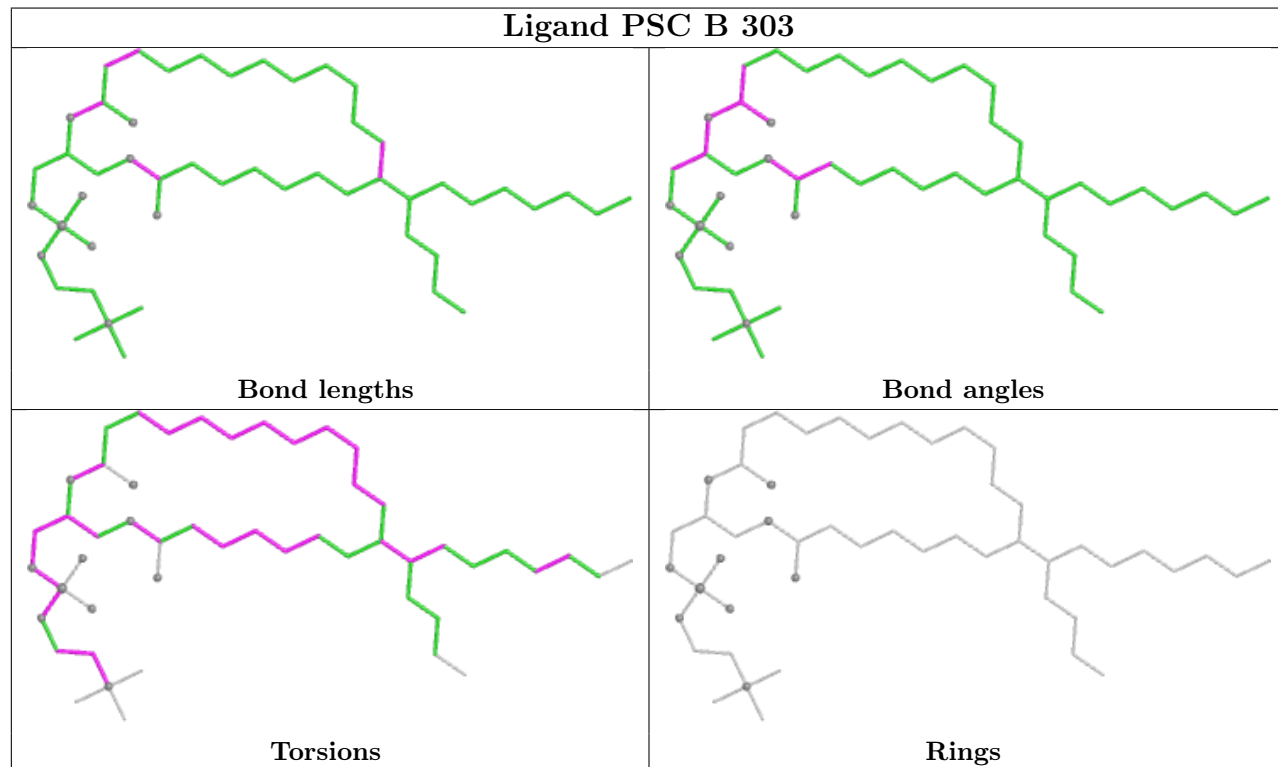


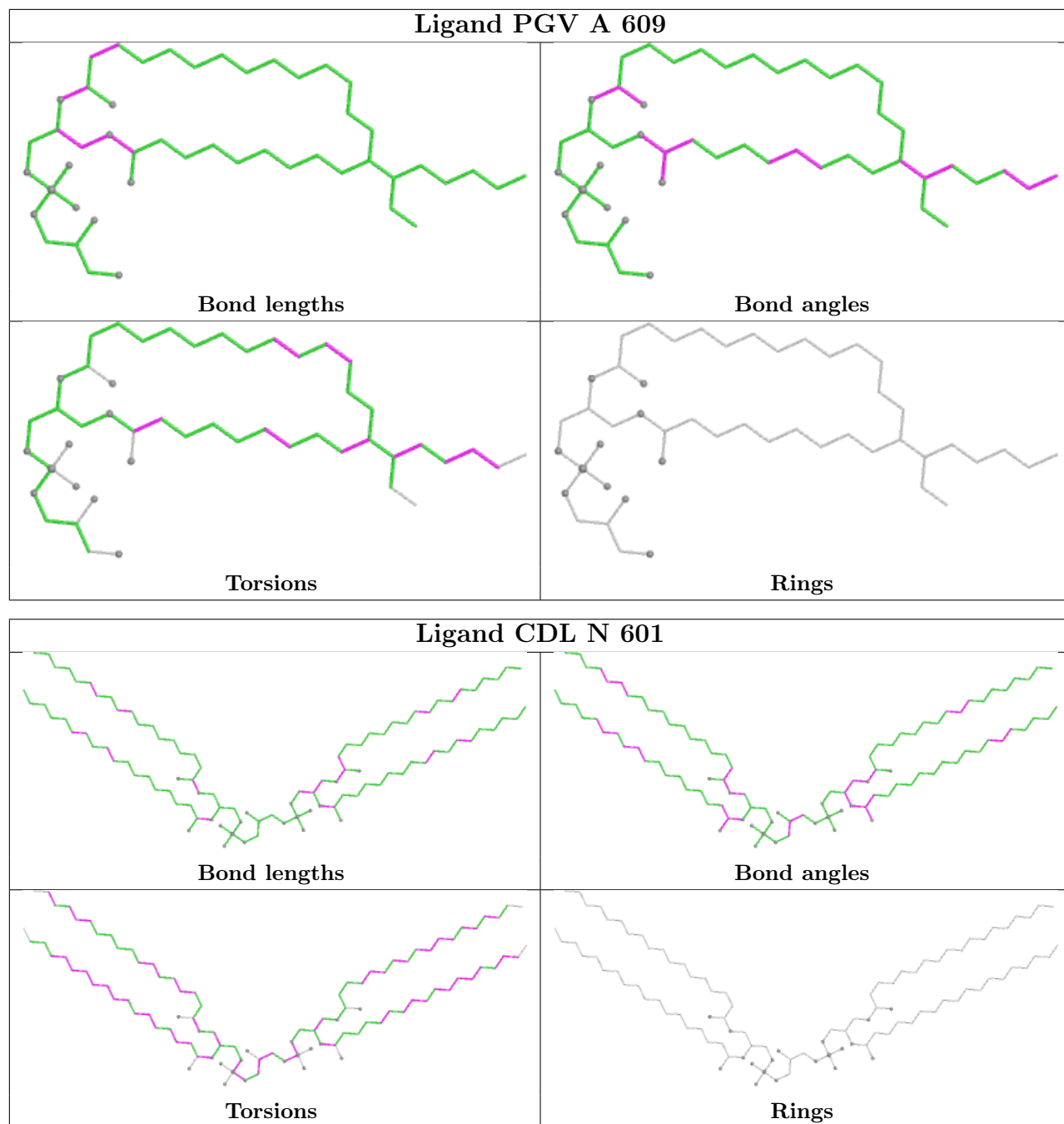


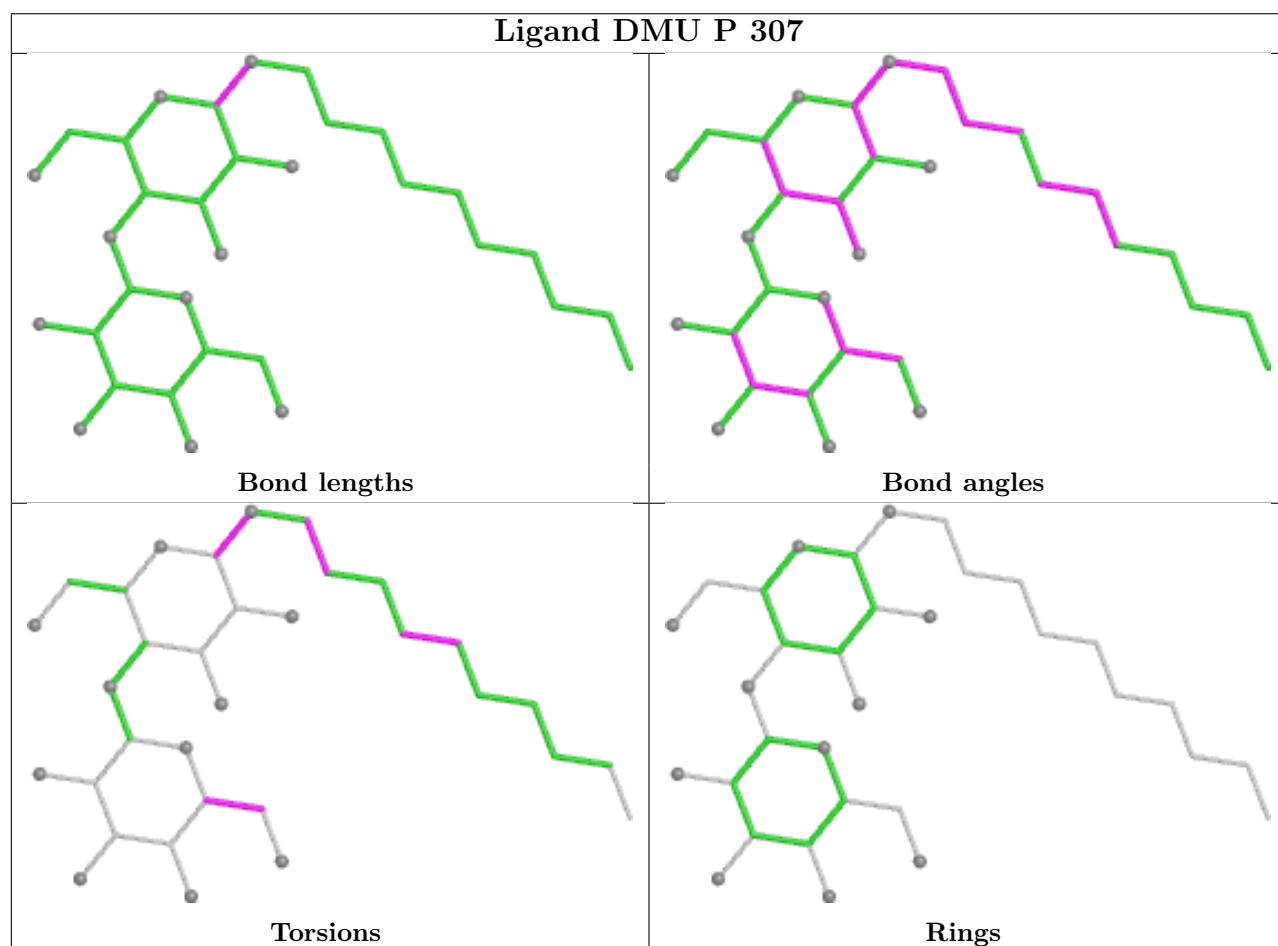
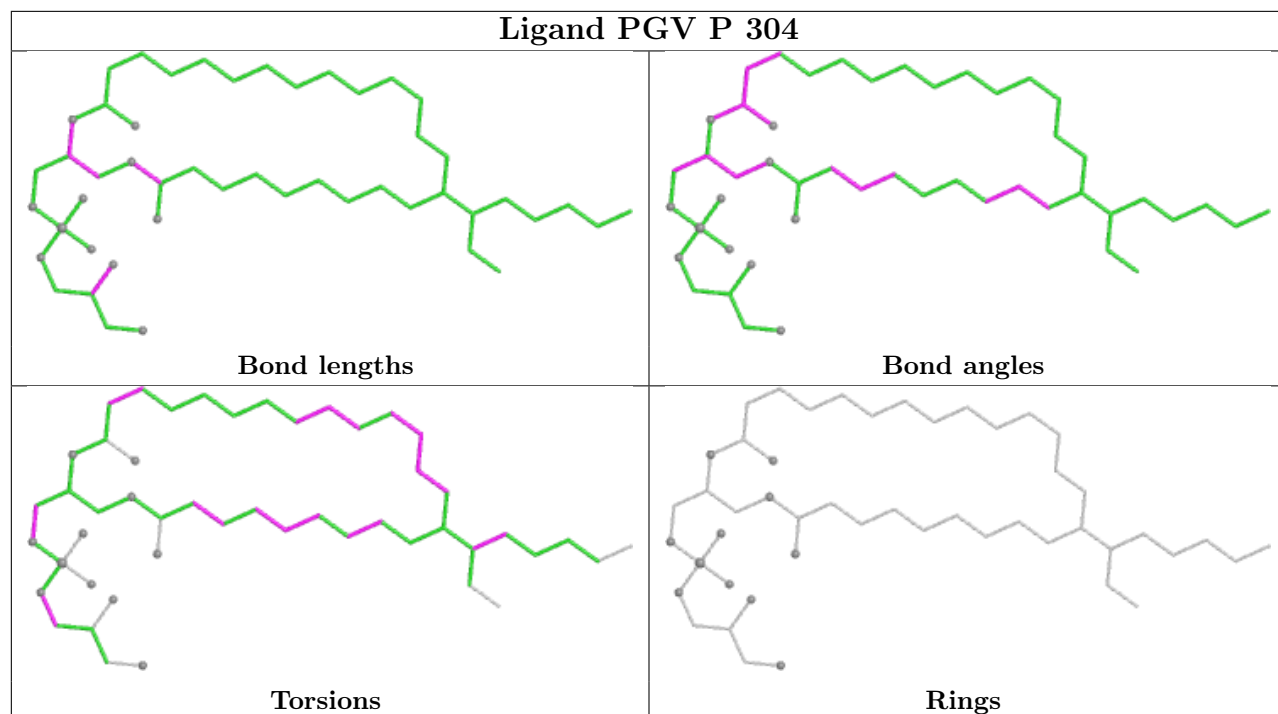
Ligand CHD J 101

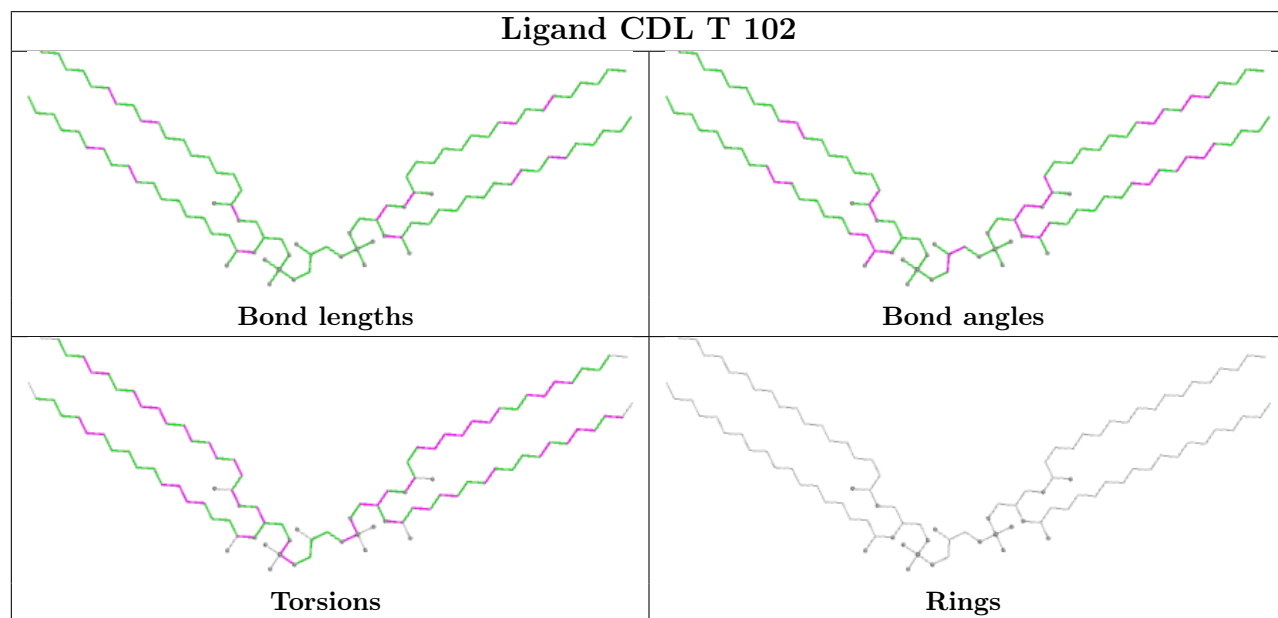
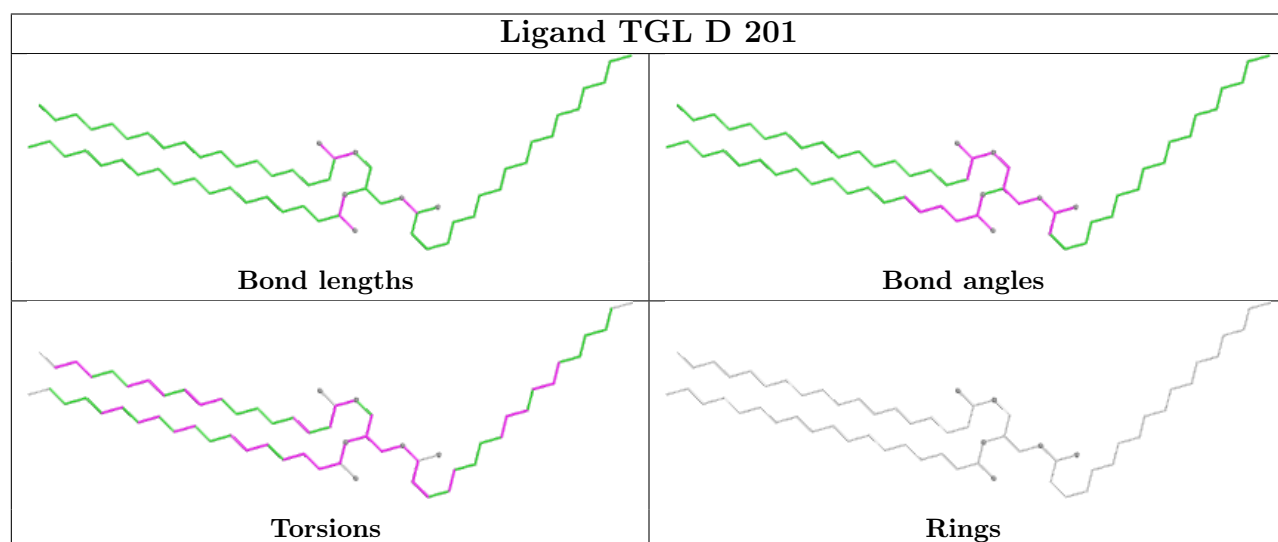
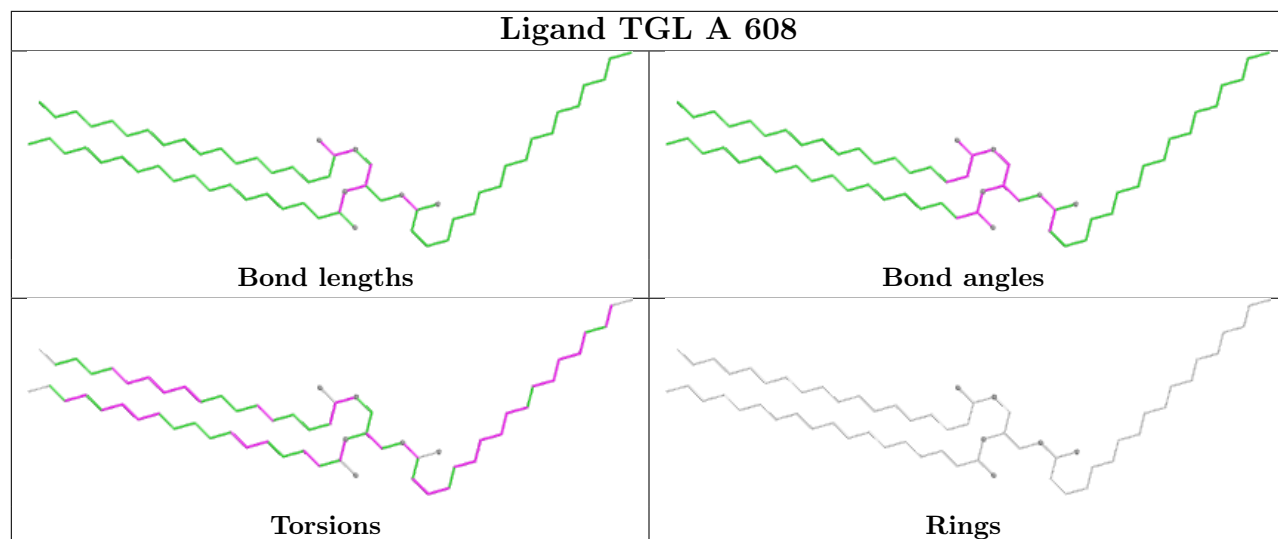


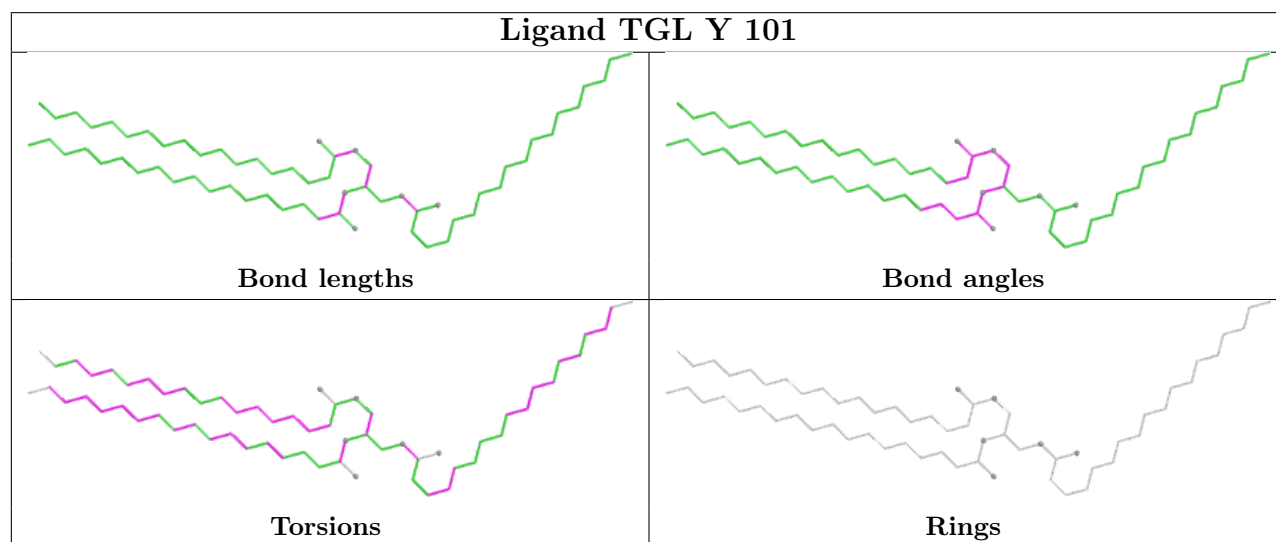
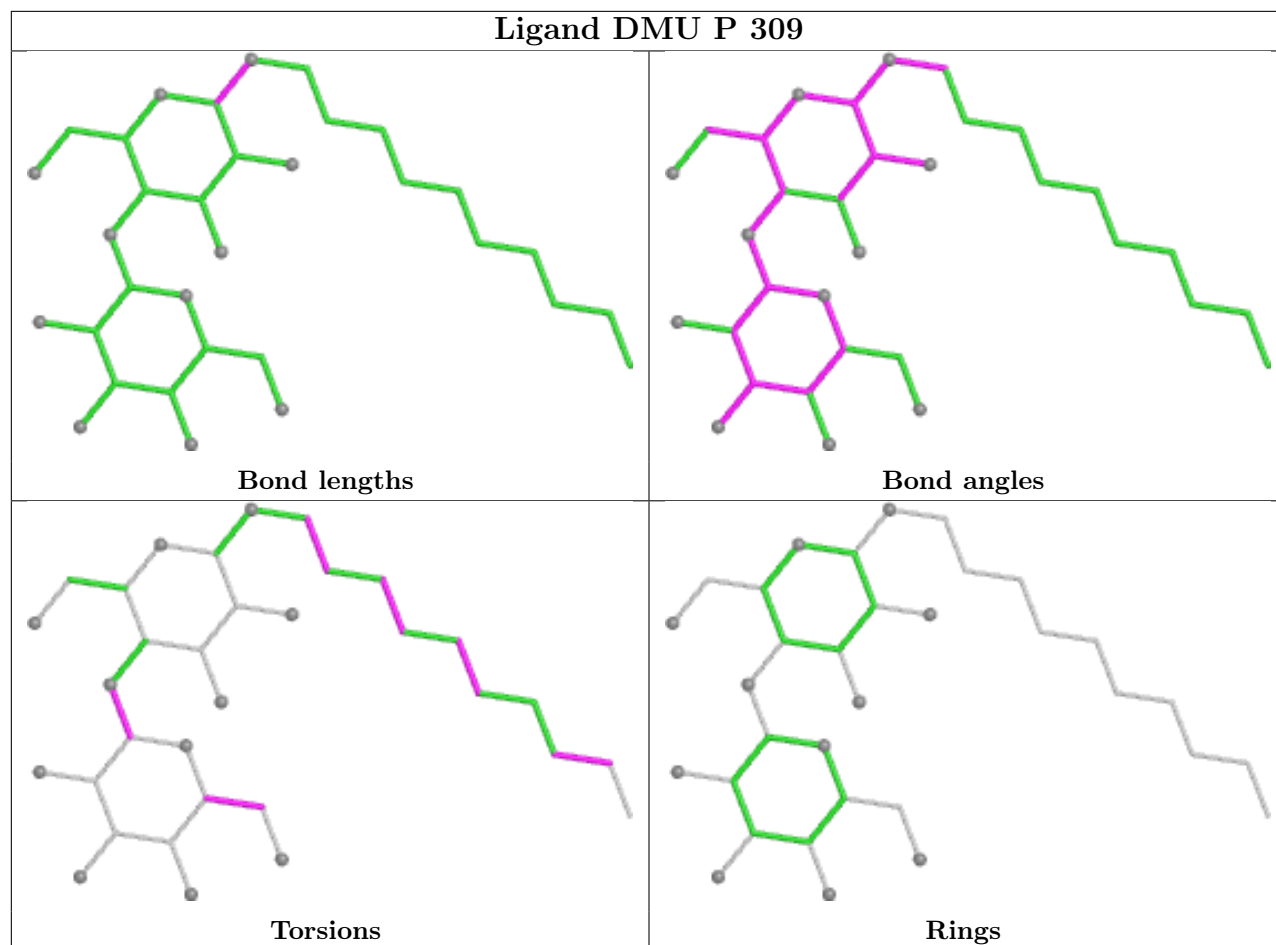
Ligand PSC B 303

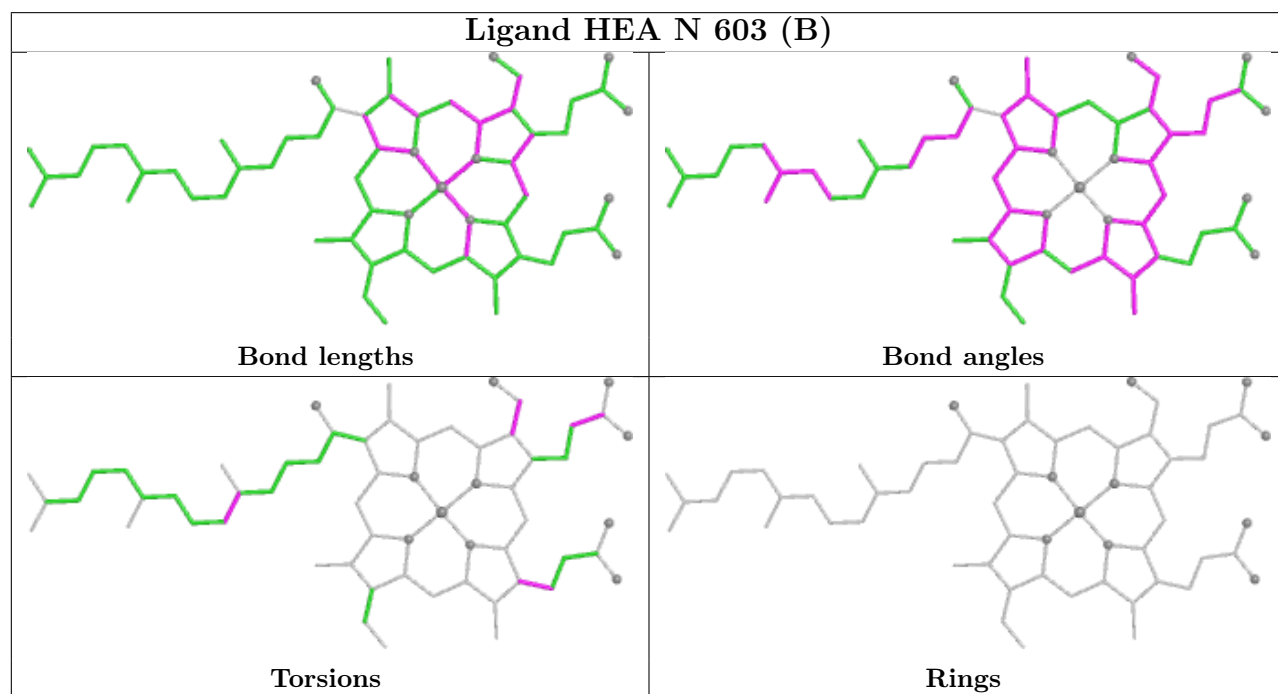
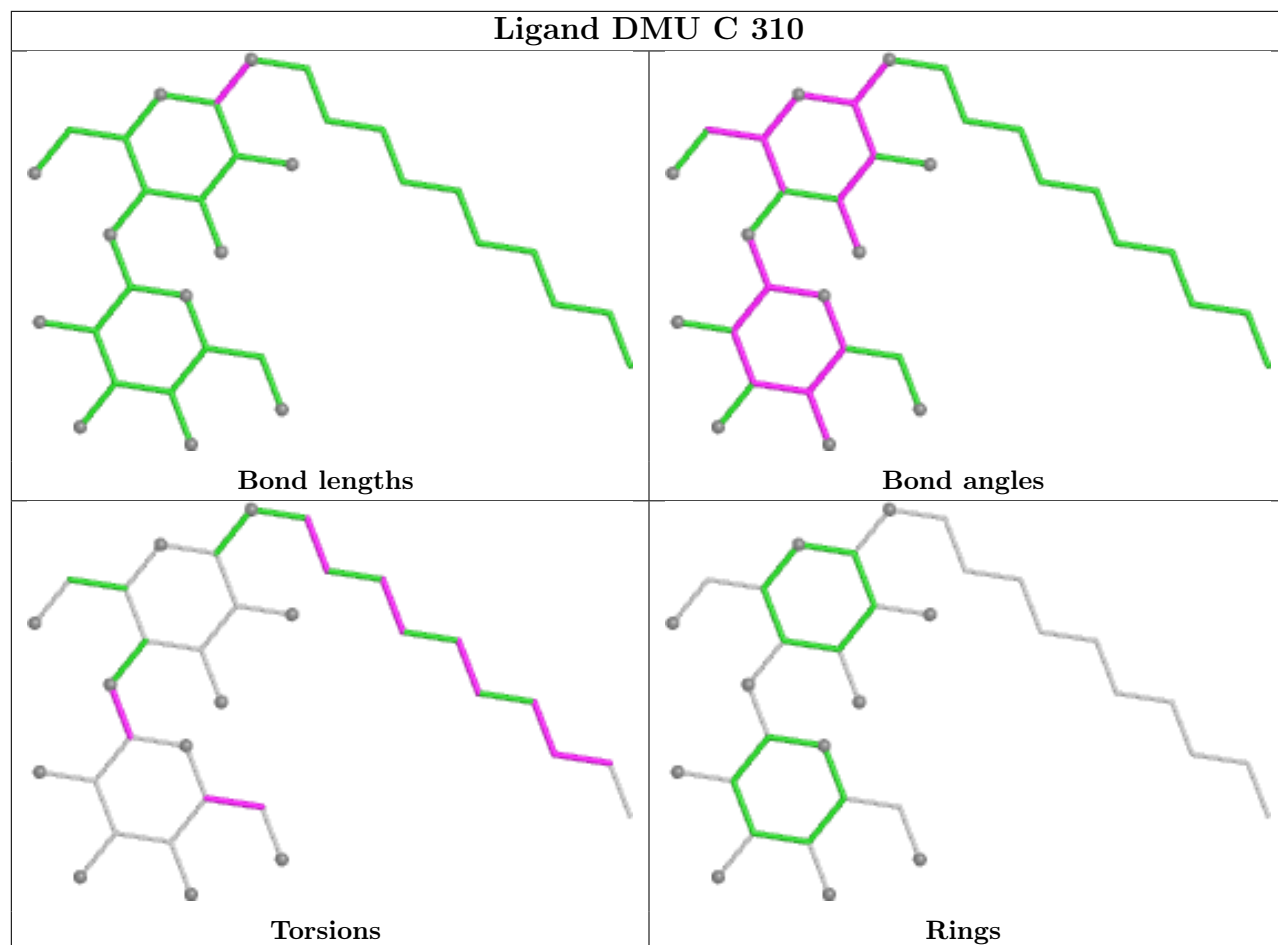


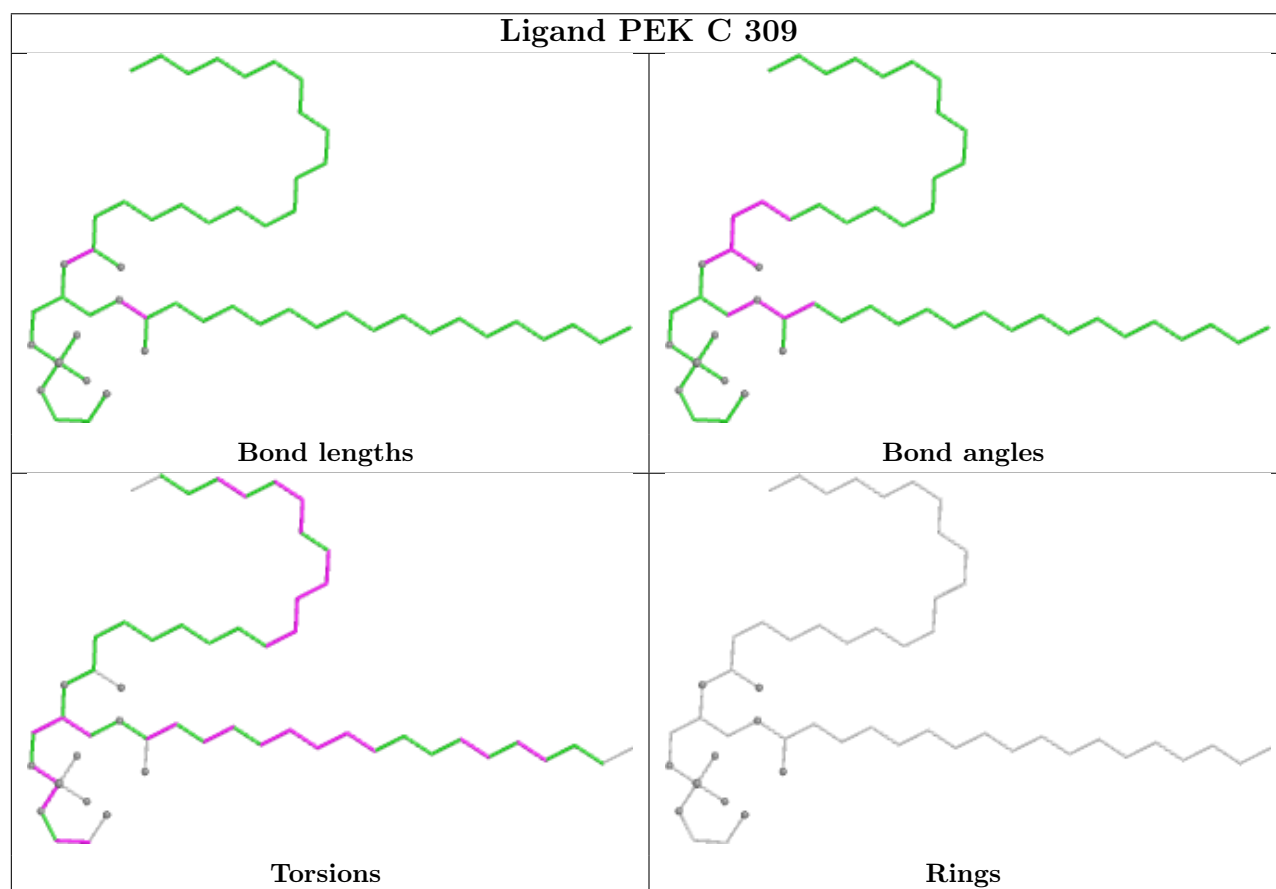
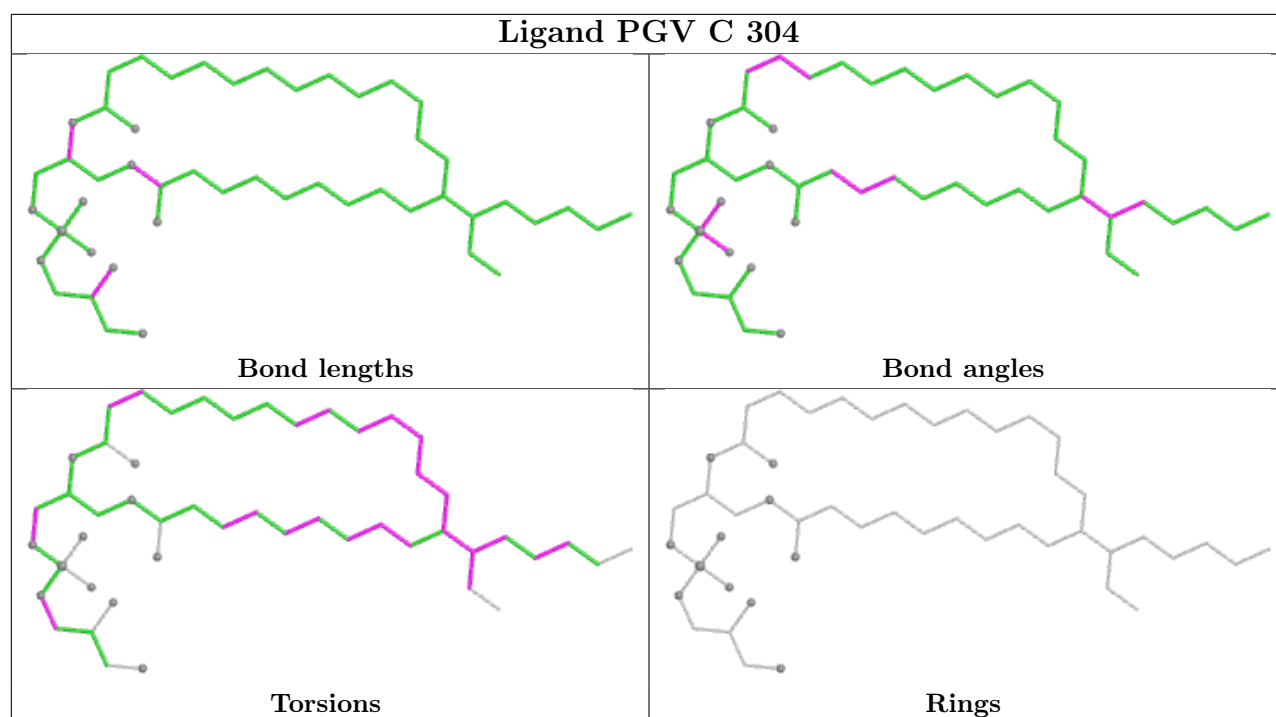


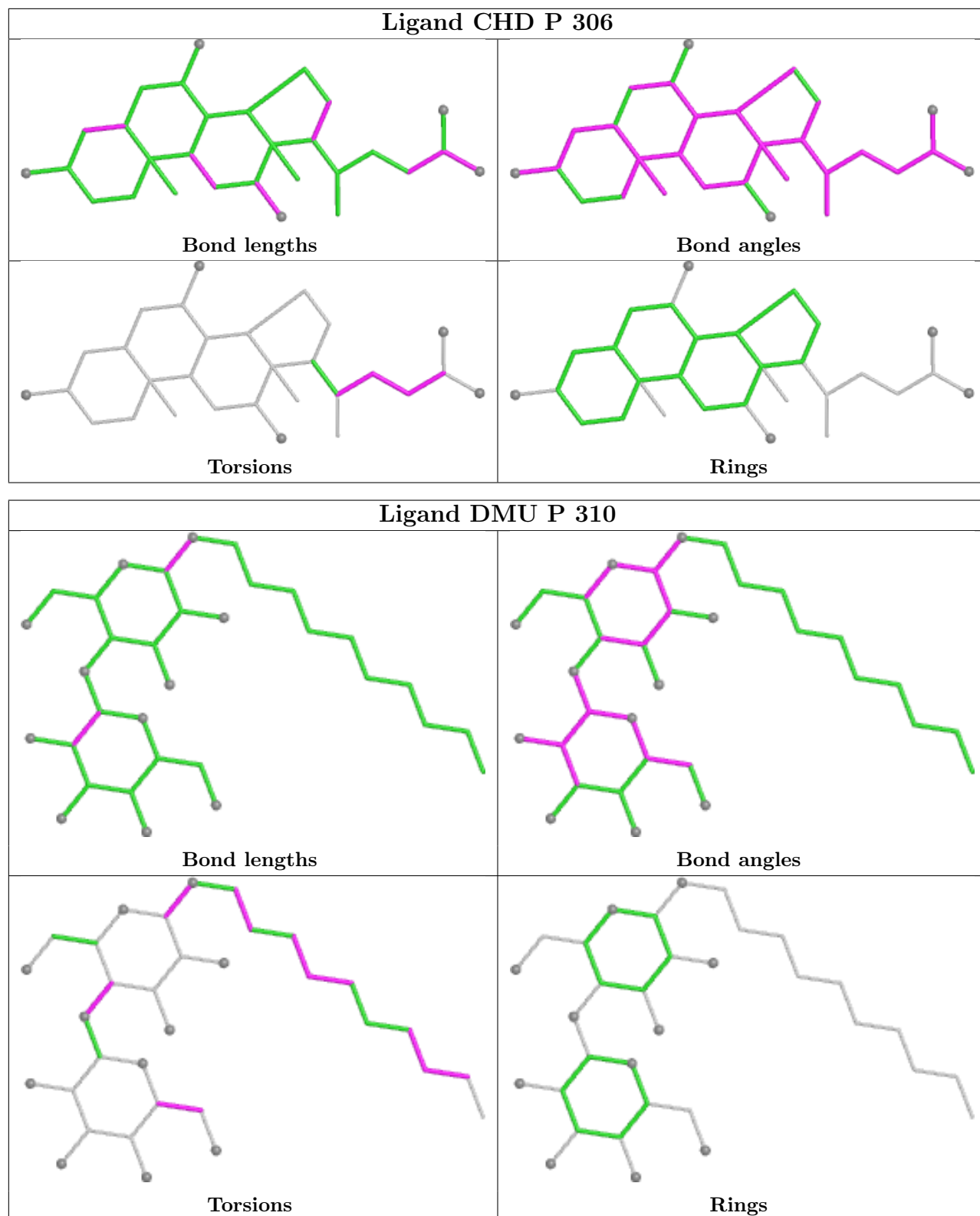


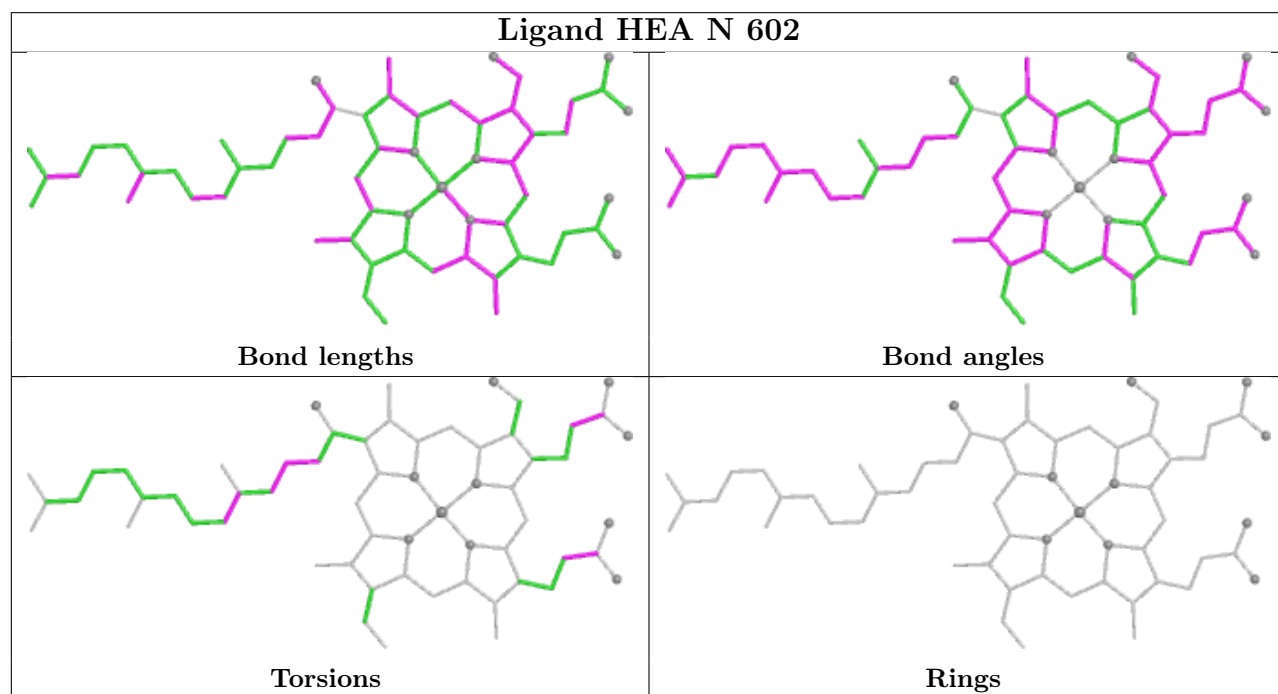
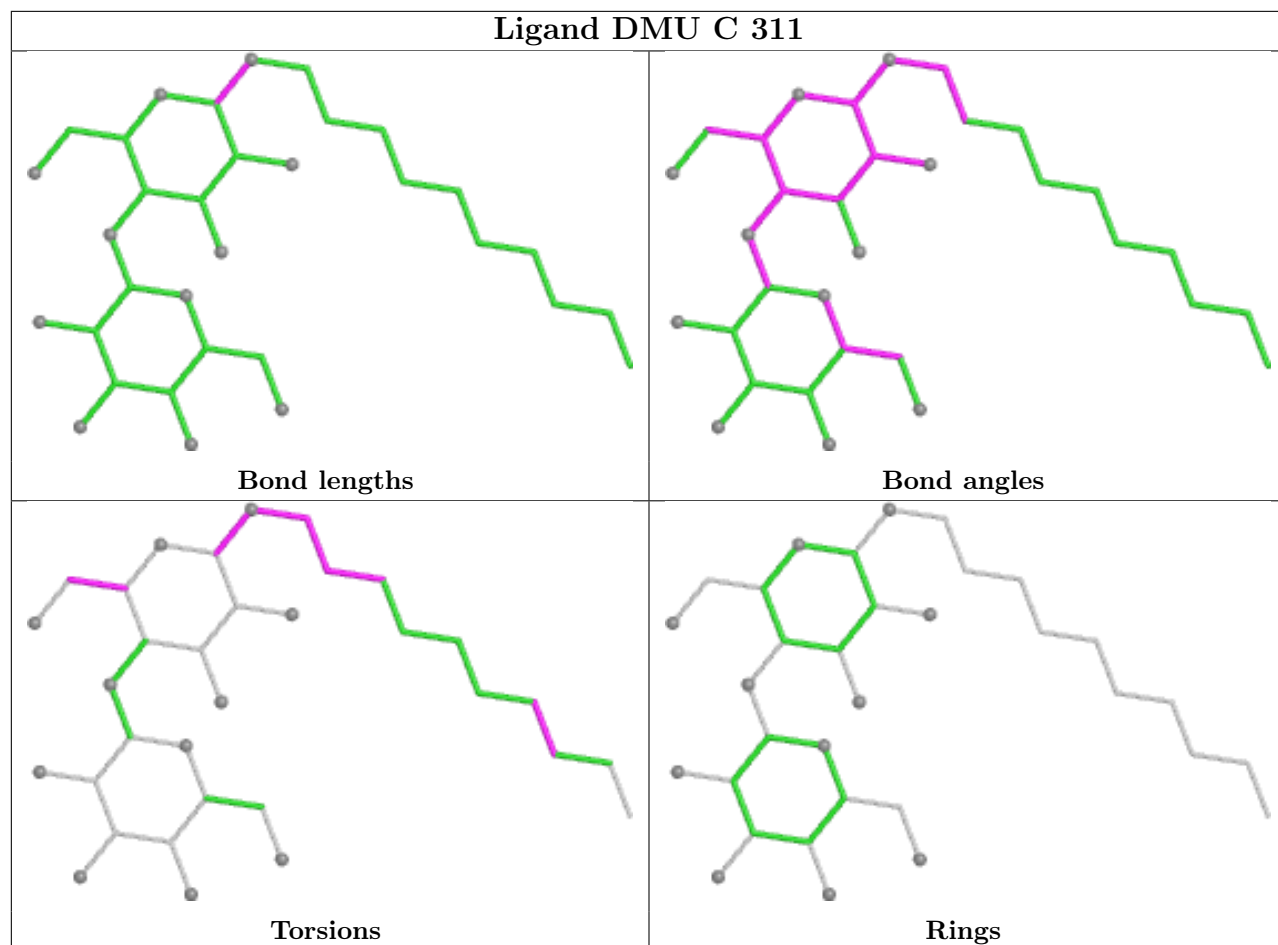


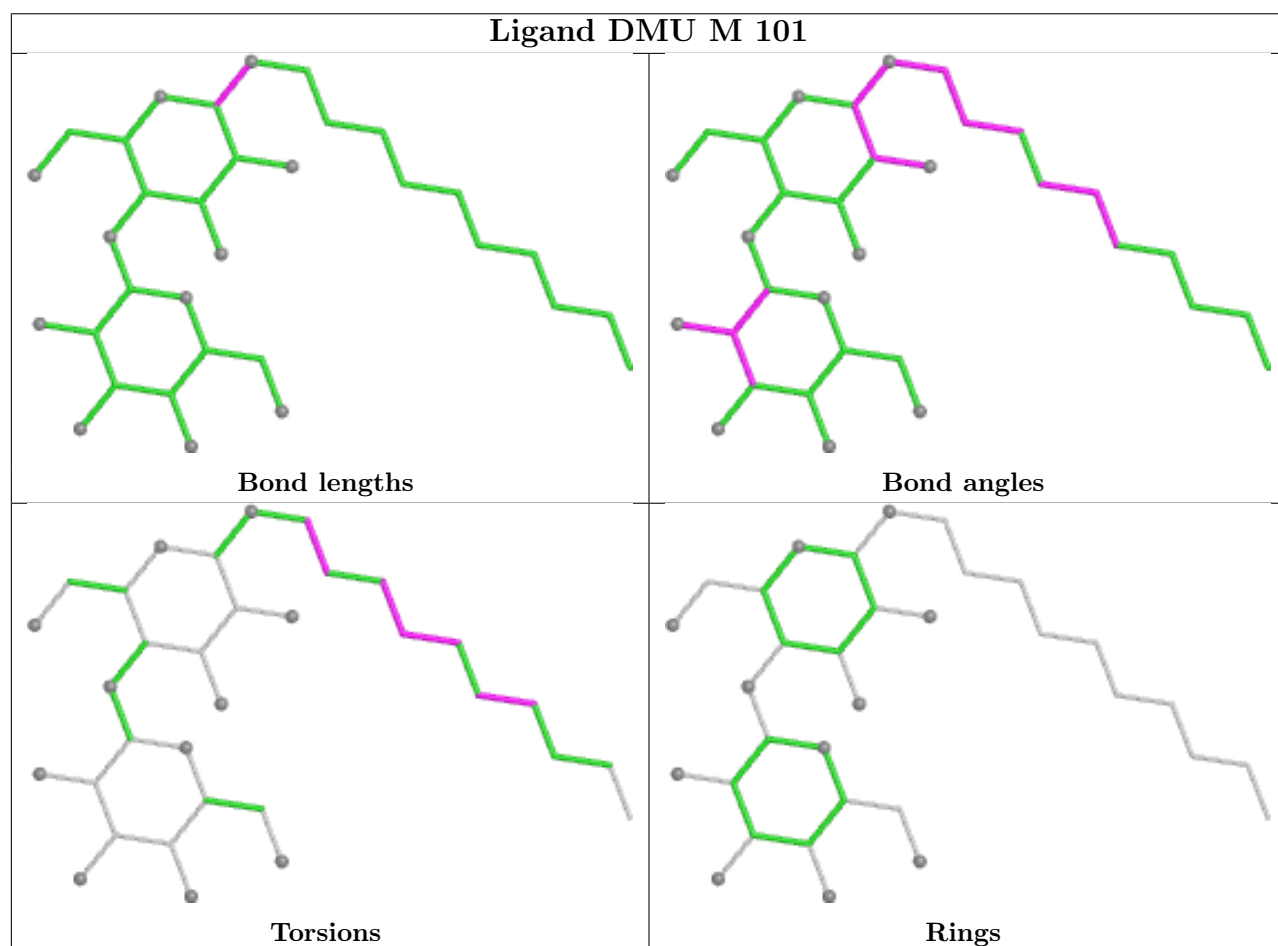
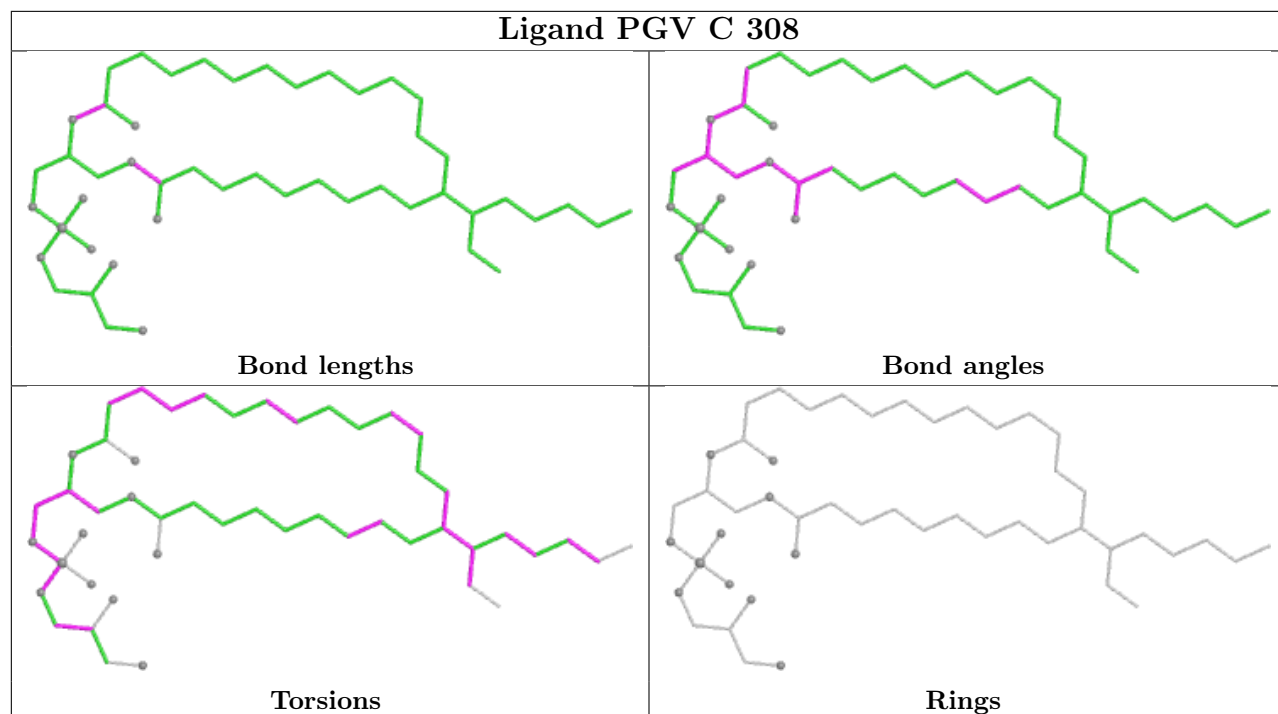


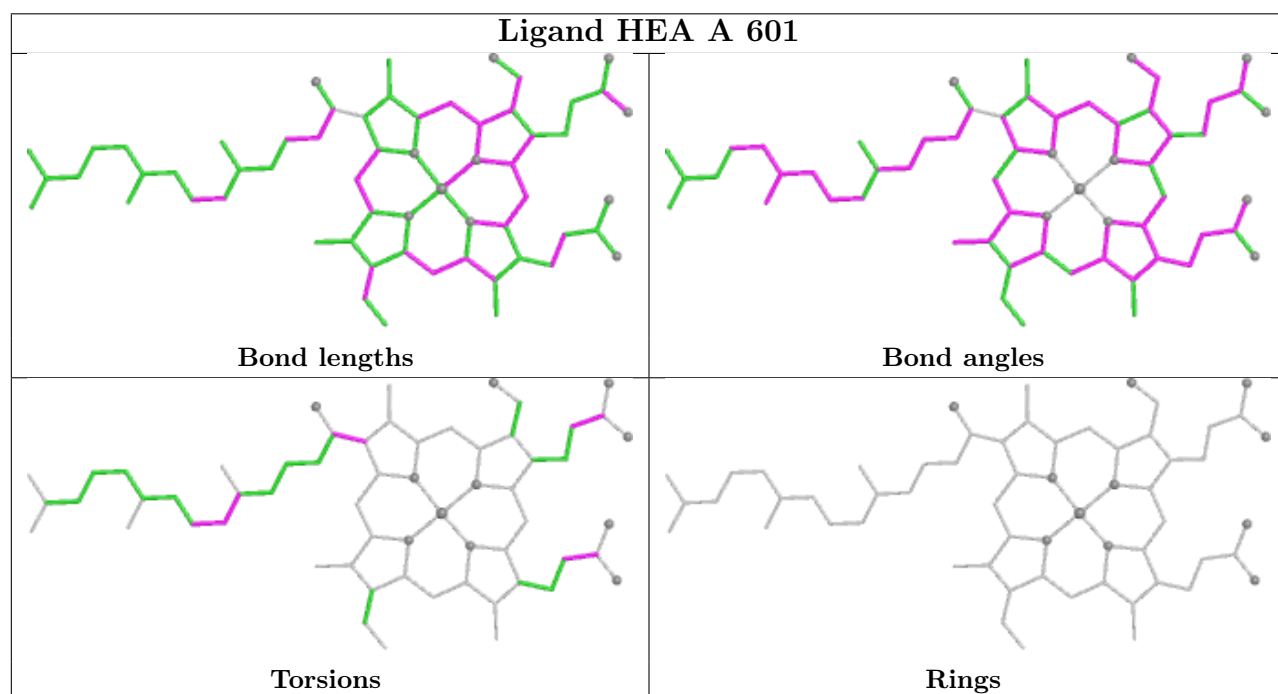
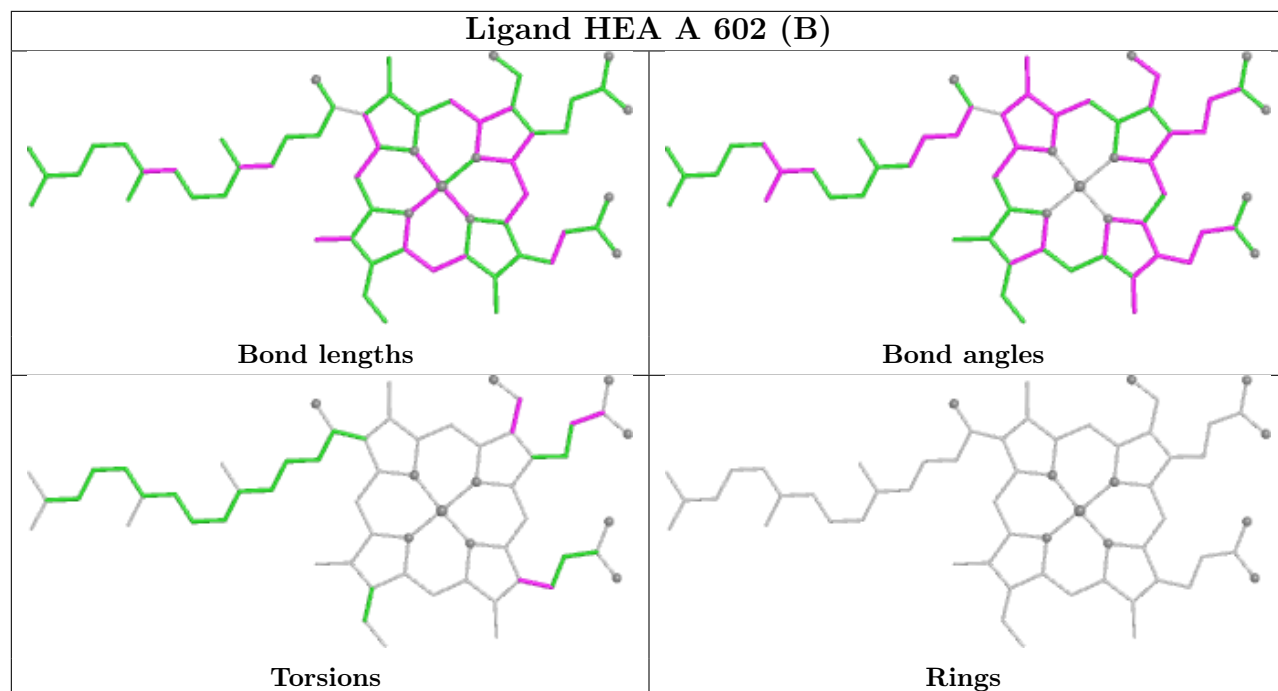


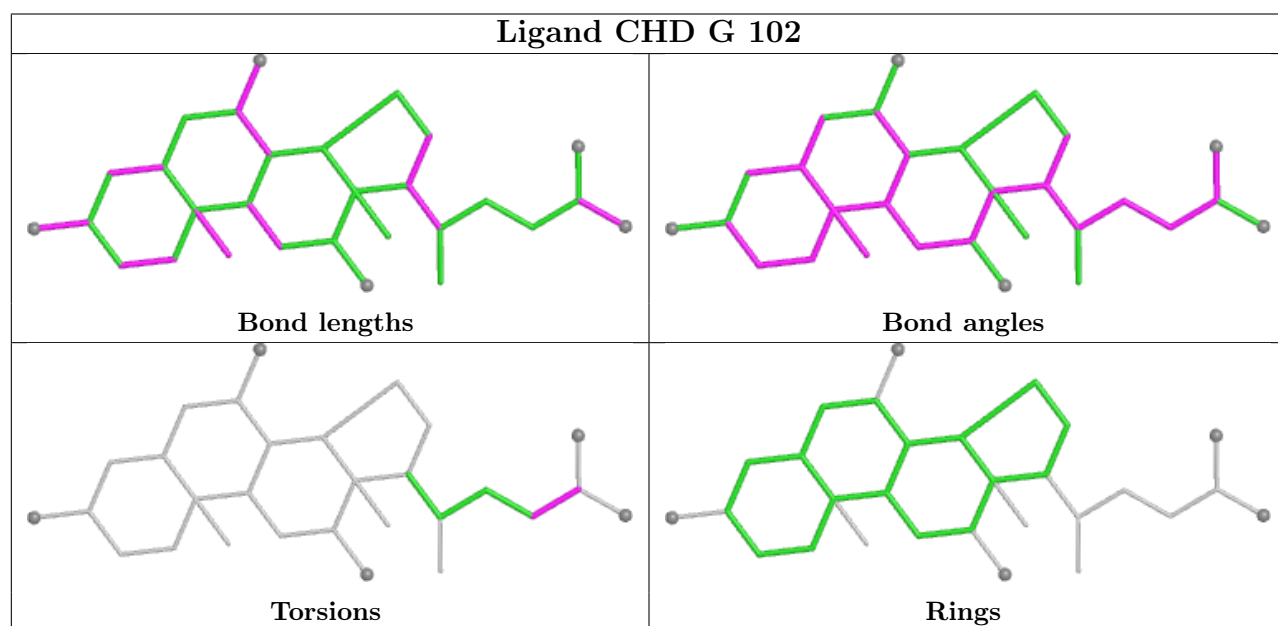
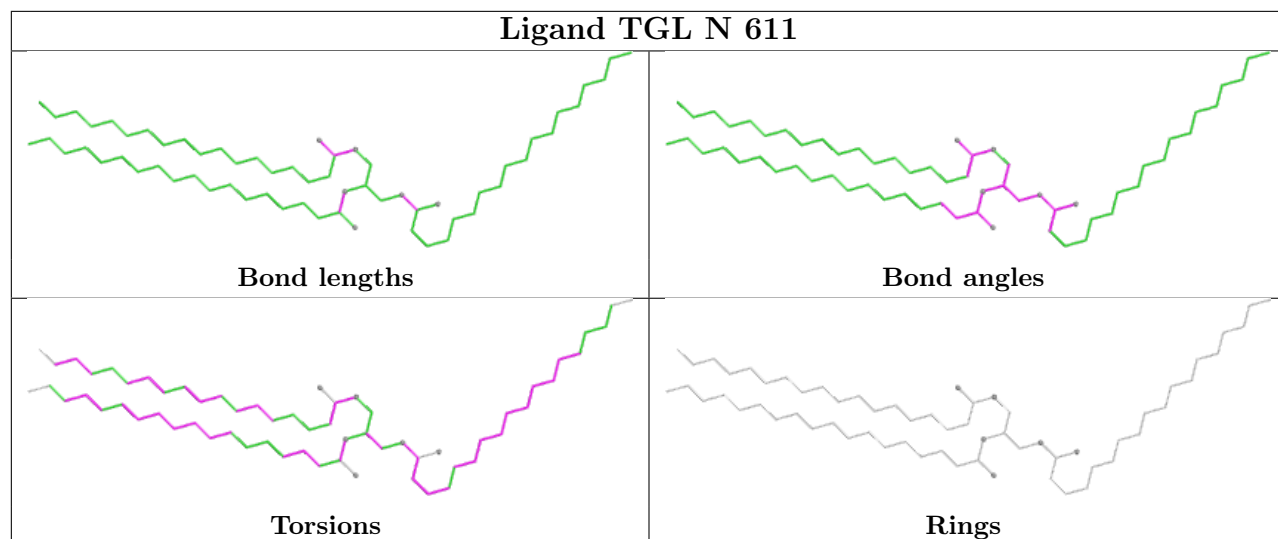


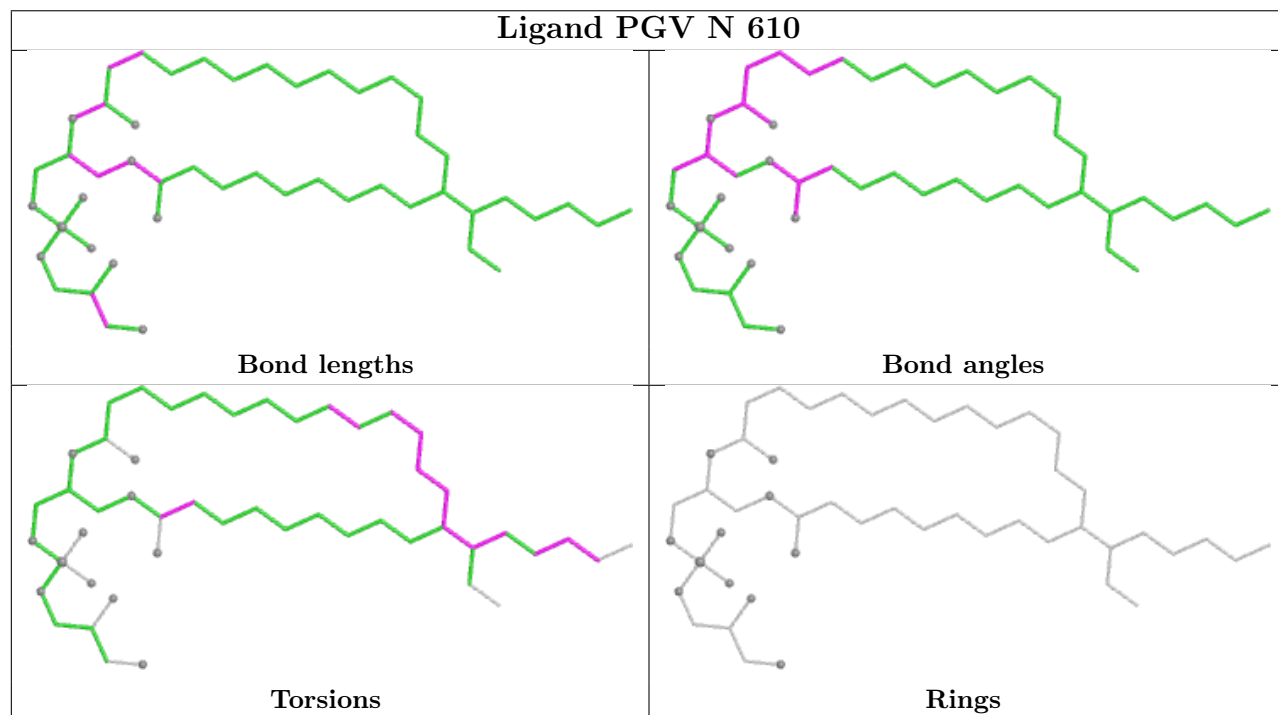
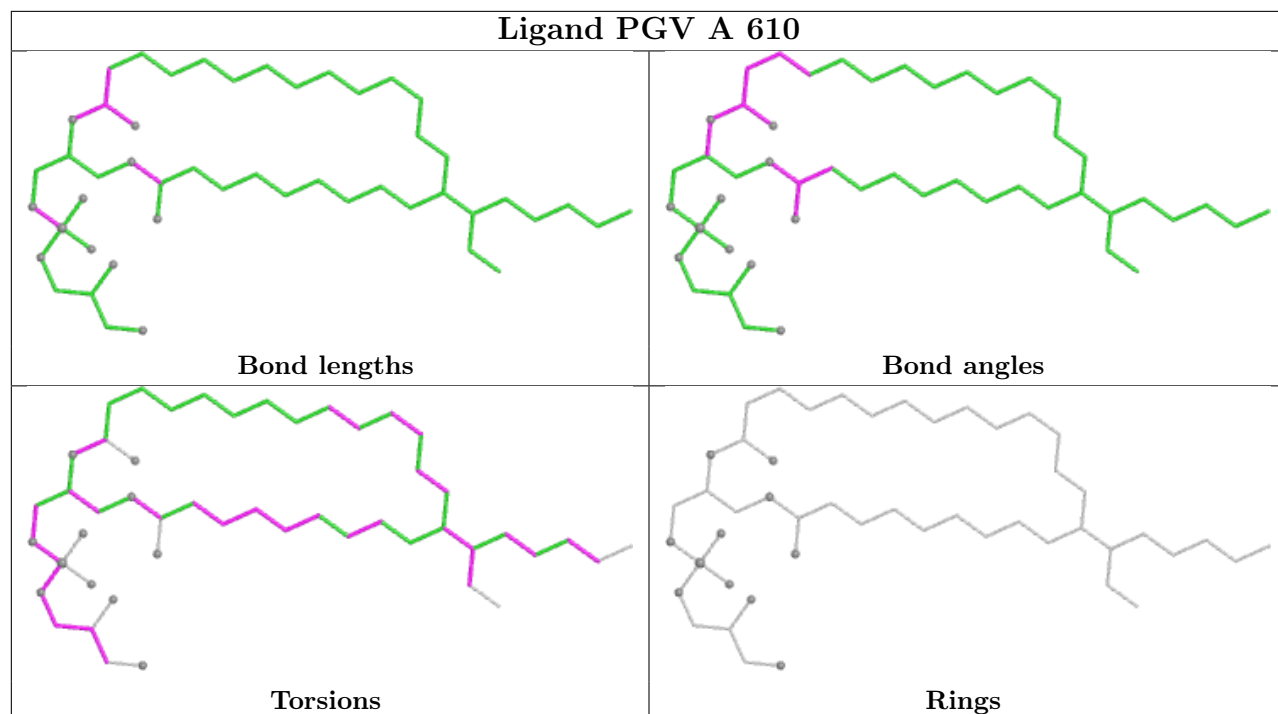


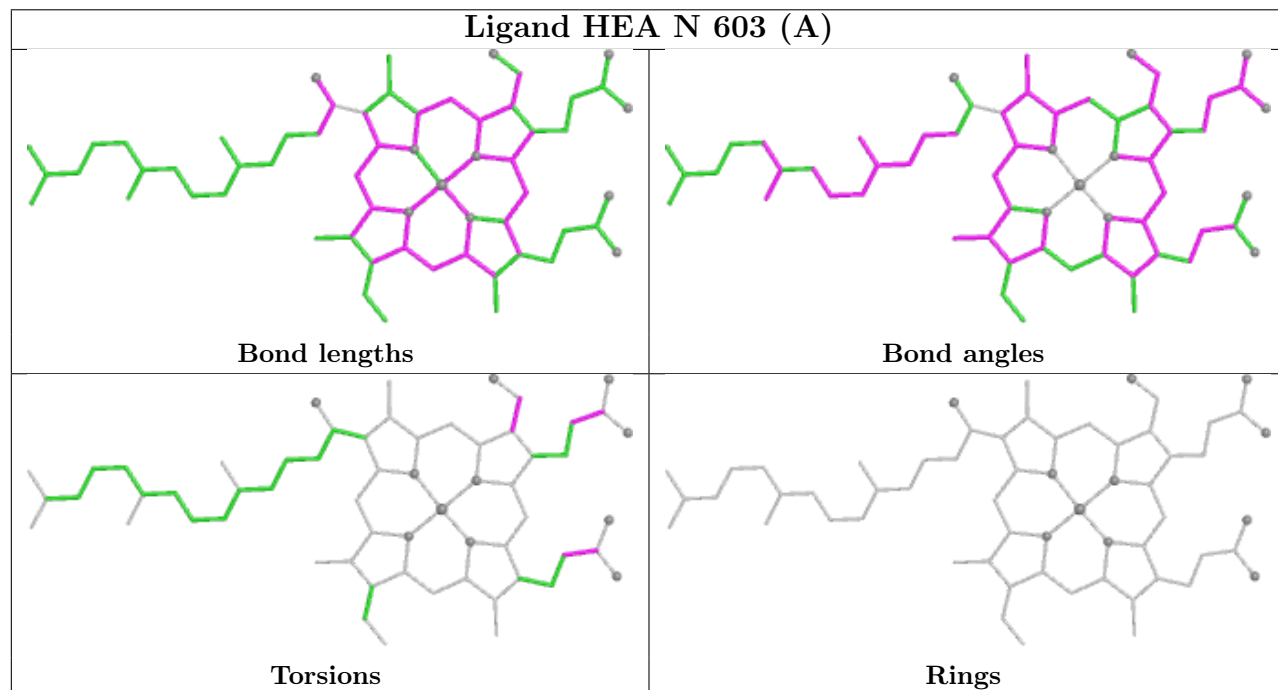
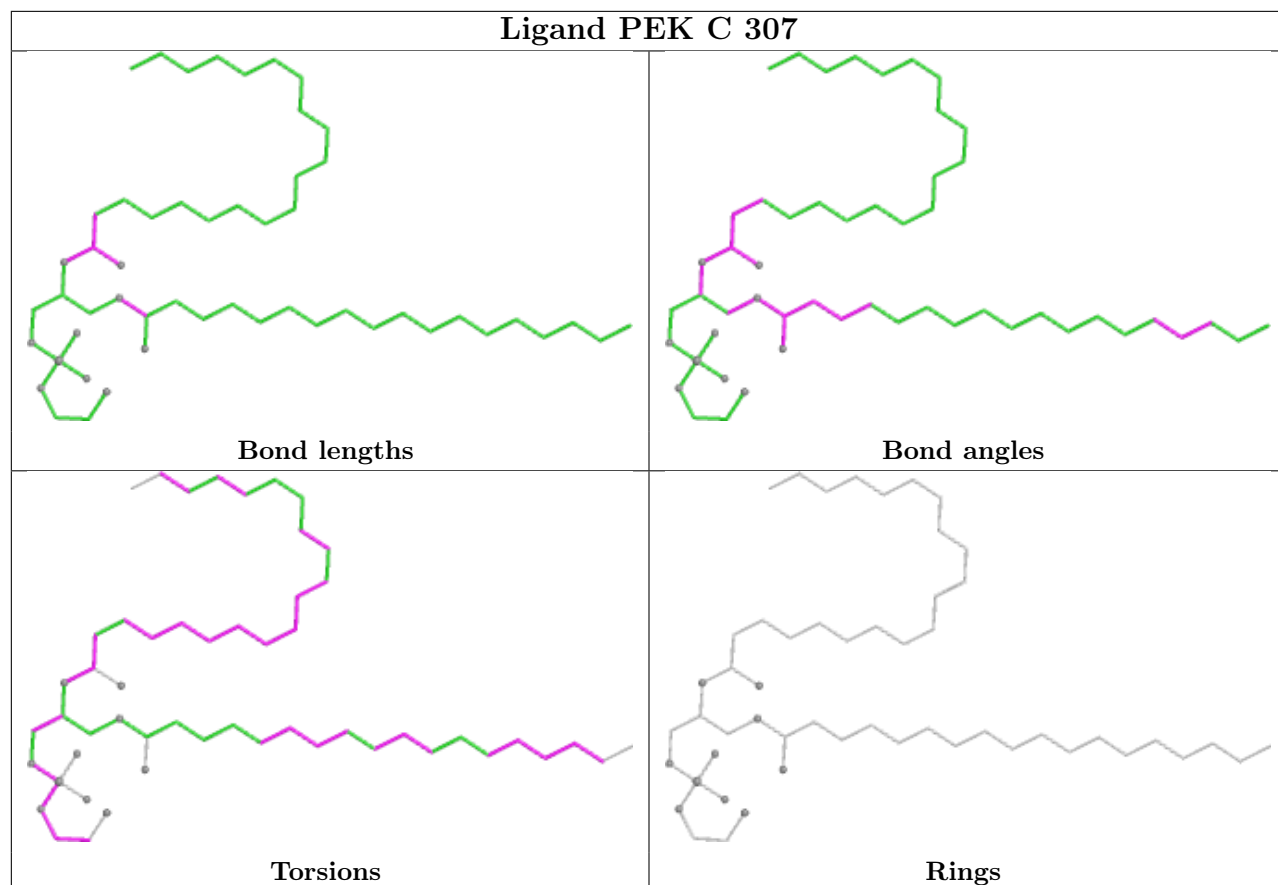


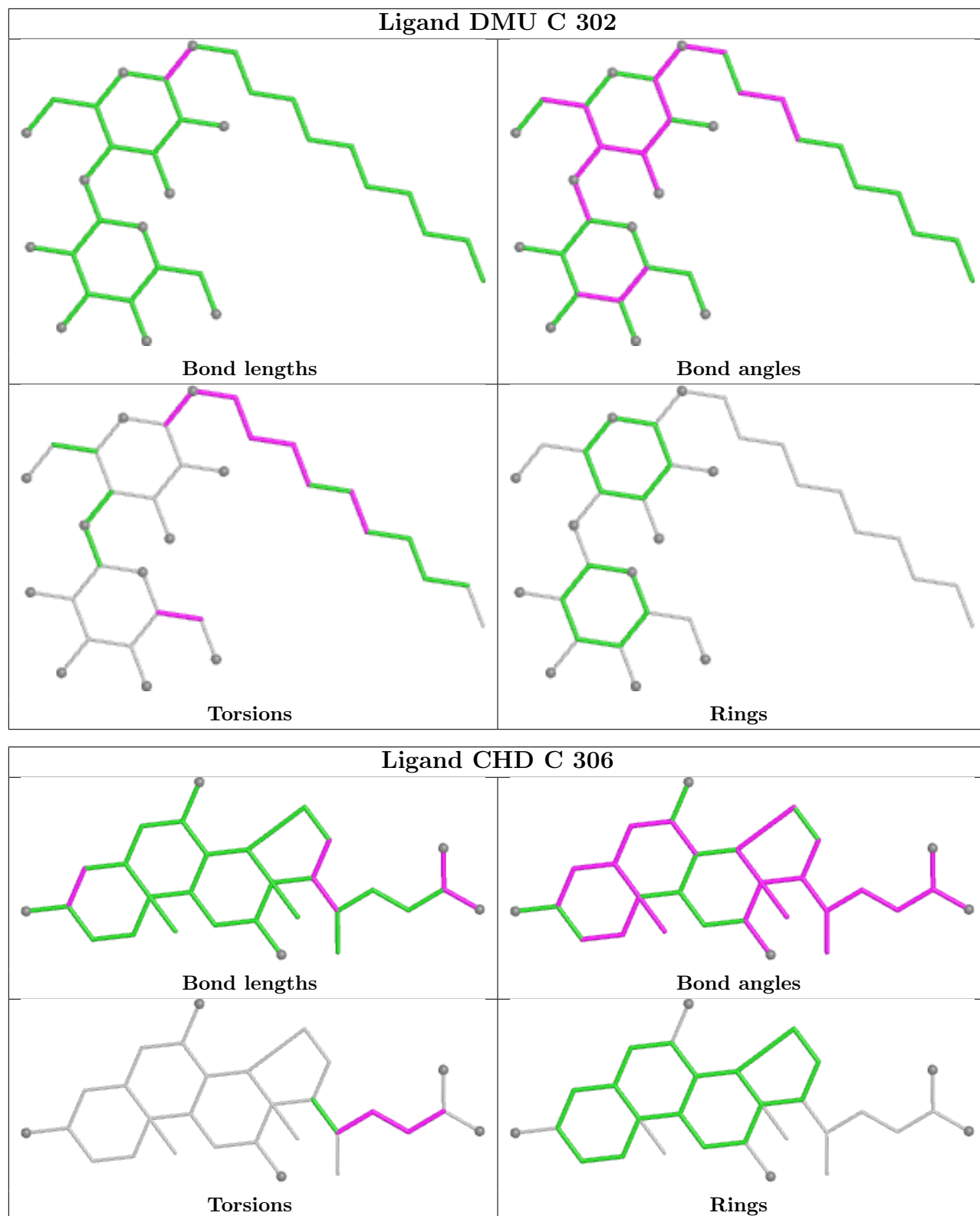


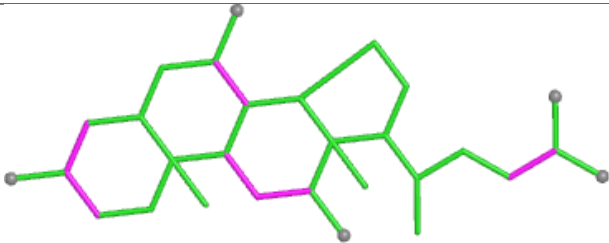
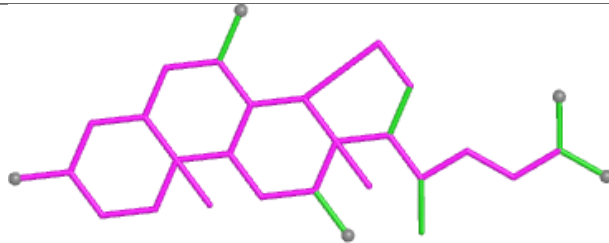
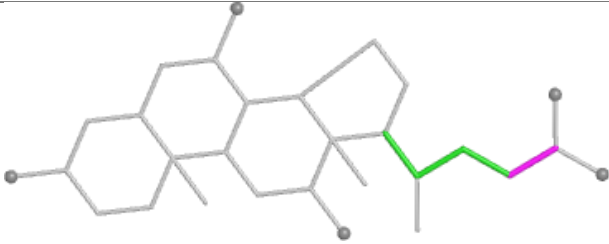
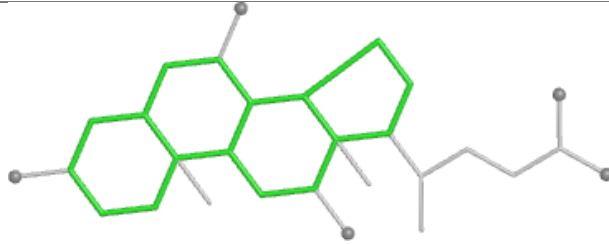


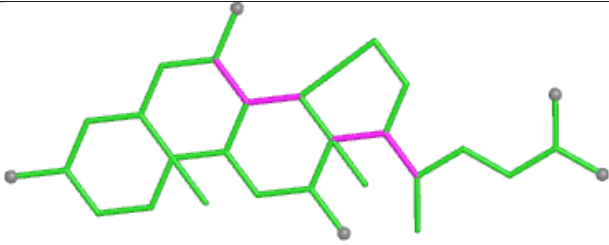
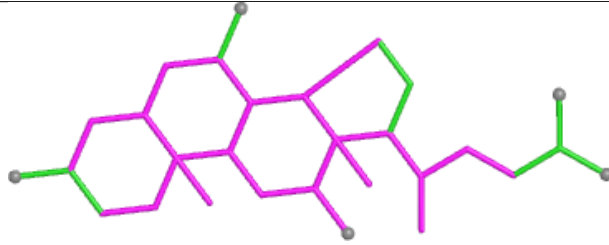
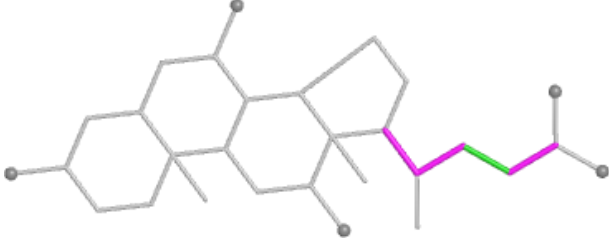
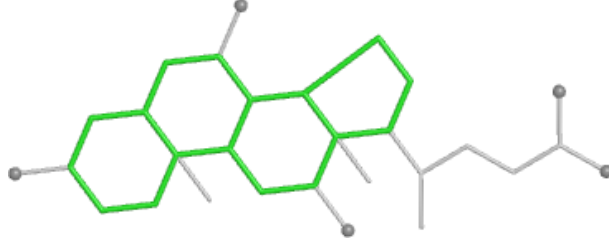




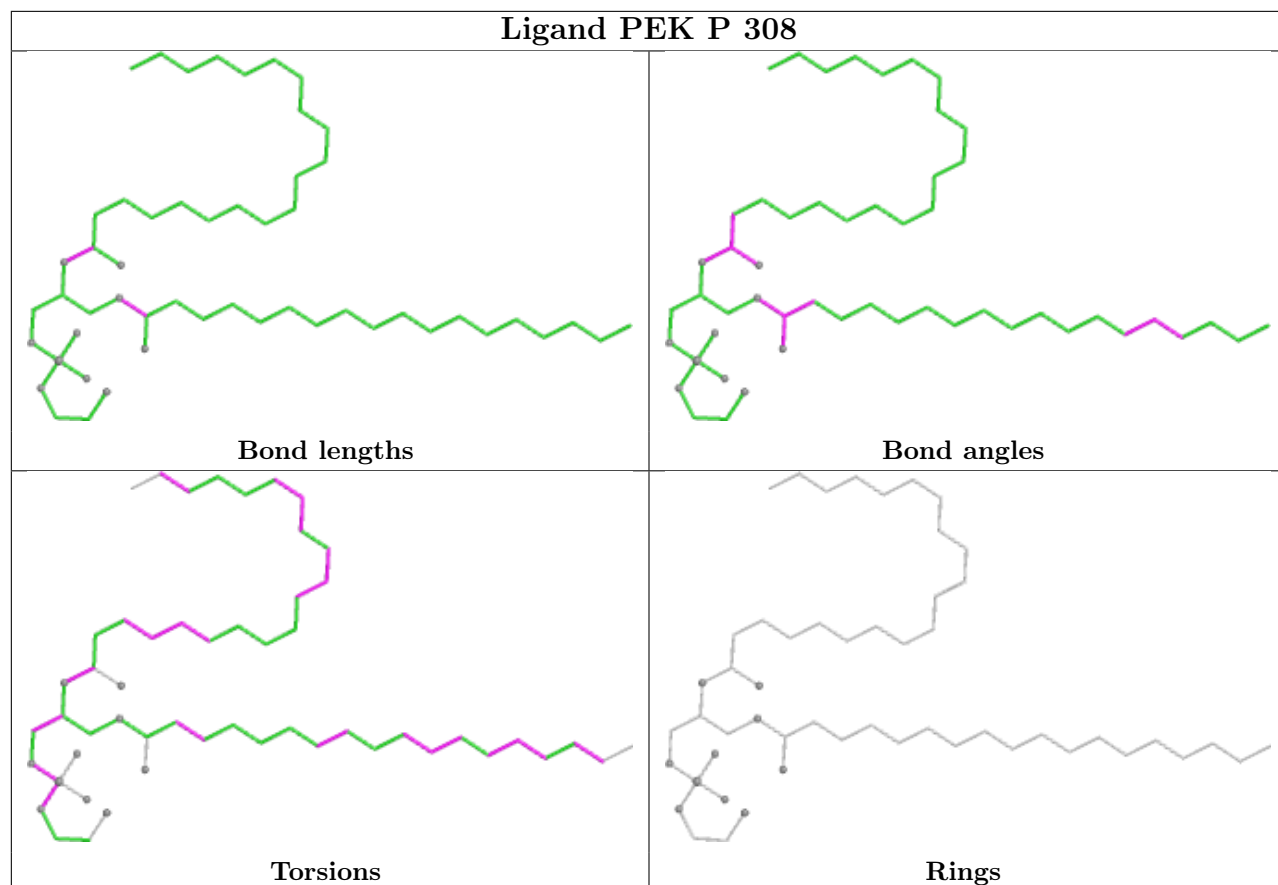




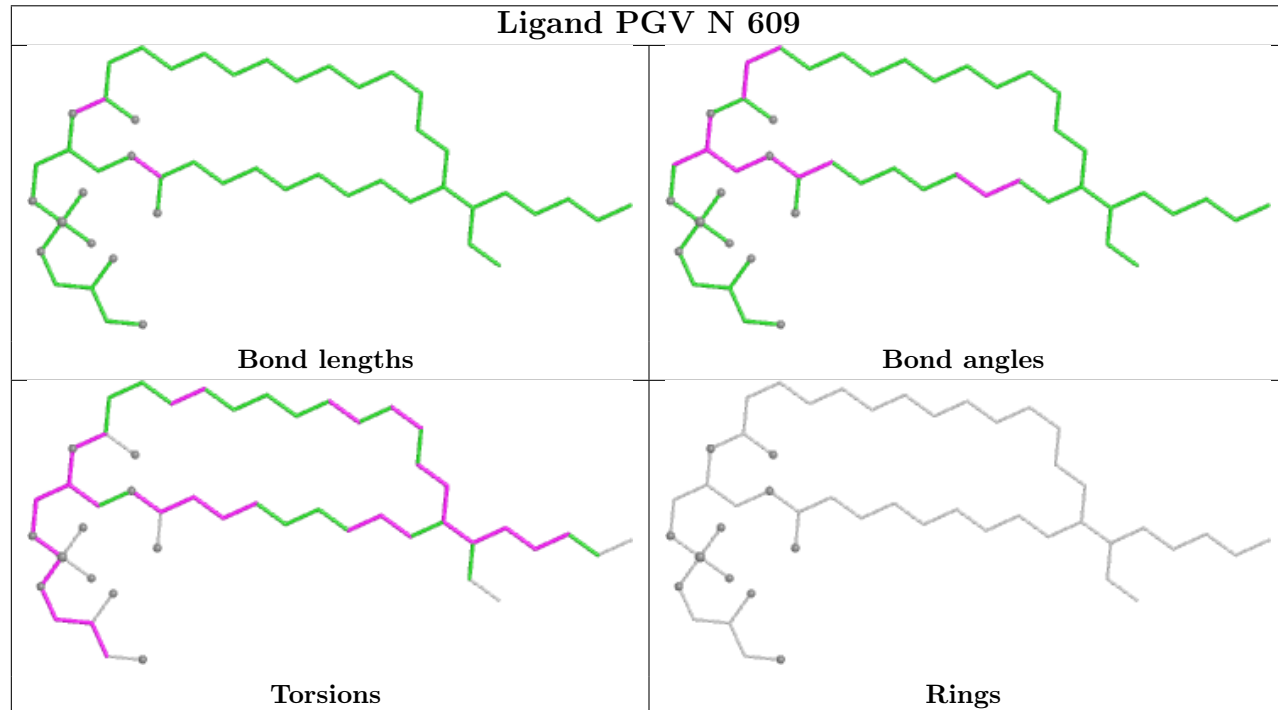
Ligand CHD C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

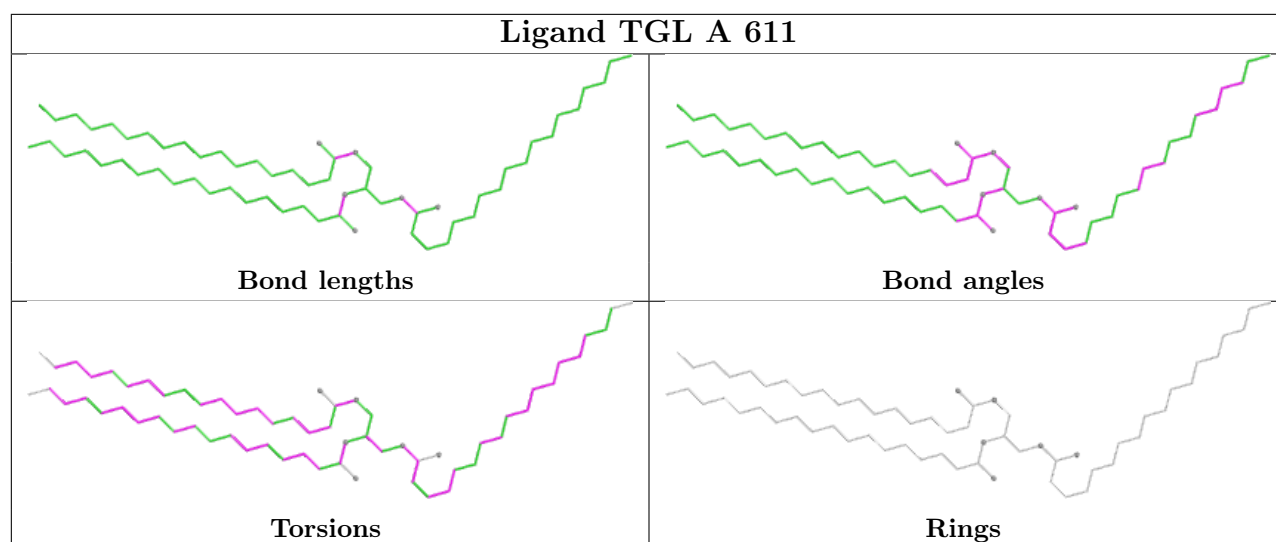
Ligand CHD W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEK P 308



Ligand PGV N 609





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	5 (0%) 79 84	12, 27, 34, 70	22 (4%)
1	N	513/514 (99%)	0.10	9 (1%) 67 73	14, 31, 39, 74	20 (3%)
2	B	226/227 (99%)	0.57	28 (12%) 8 9	19, 34, 54, 68	9 (3%)
2	O	226/227 (99%)	0.78	24 (10%) 11 12	21, 41, 65, 88	5 (2%)
3	C	259/261 (99%)	0.04	7 (2%) 56 61	13, 30, 40, 75	9 (3%)
3	P	259/261 (99%)	0.06	7 (2%) 56 61	12, 31, 41, 80	9 (3%)
4	D	144/147 (97%)	0.45	8 (5%) 30 34	16, 35, 57, 79	4 (2%)
4	Q	144/147 (97%)	1.25	17 (11%) 9 9	19, 48, 74, 136	3 (2%)
5	E	105/109 (96%)	0.33	3 (2%) 53 58	27, 34, 57, 118	0
5	R	105/109 (96%)	0.63	5 (4%) 35 39	24, 40, 58, 121	1 (0%)
6	F	98/98 (100%)	0.86	11 (11%) 10 11	17, 37, 90, 148	4 (4%)
6	S	98/98 (100%)	1.22	15 (15%) 5 5	18, 37, 99, 143	2 (2%)
7	G	83/85 (97%)	1.47	20 (24%) 2 2	17, 39, 108, 141	1 (1%)
7	T	83/85 (97%)	1.46	22 (26%) 1 1	19, 39, 101, 131	1 (1%)
8	H	79/85 (92%)	1.15	13 (16%) 4 4	33, 44, 91, 101	0
8	U	79/85 (92%)	1.18	15 (18%) 3 3	37, 47, 103, 123	0
9	I	72/73 (98%)	1.47	18 (25%) 2 1	33, 44, 83, 90	0
9	V	72/73 (98%)	1.50	18 (25%) 2 1	32, 54, 80, 104	0
10	J	58/59 (98%)	0.78	4 (6%) 23 26	30, 39, 63, 121	0
10	W	58/59 (98%)	0.92	5 (8%) 16 18	22, 42, 69, 127	1 (1%)
11	K	49/56 (87%)	0.74	2 (4%) 41 45	34, 41, 54, 61	0
11	X	49/56 (87%)	1.23	9 (18%) 3 4	23, 50, 70, 81	1 (2%)
12	L	46/47 (97%)	0.44	5 (10%) 10 11	28, 33, 52, 91	0
12	Y	46/47 (97%)	0.92	4 (8%) 16 17	23, 40, 65, 114	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.58	5 (11%) 9 10	30, 33, 68, 118	0
13	Z	43/46 (93%)	1.05	6 (13%) 6 7	39, 44, 78, 108	0
All	All	3550/3614 (98%)	0.51	285 (8%) 18 21	12, 34, 66, 148	93 (2%)

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	14.7
6	F	1	ALA	13.5
6	S	97	ALA	12.4
6	S	1	ALA	10.4
6	S	94	HIS	9.2
4	Q	6	VAL	9.0
7	G	1	ALA	8.3
7	G	9	GLY	8.0
6	S	98	HIS	8.0
6	S	96	LEU	7.6
6	F	96	LEU	7.2
7	T	9	GLY	7.1
7	G	36	TRP	7.1
6	S	93	PRO	7.0
7	G	6	GLY	6.8
9	I	37	PHE	6.8
8	H	8	ILE	6.7
6	F	2	SER	6.7
6	F	97	ALA	6.7
7	G	5	LYS	6.6
7	T	3	ALA	6.6
5	E	109	VAL	6.5
6	S	3	GLY	6.4
9	V	37	PHE	6.4
8	U	8	ILE	6.3
4	D	5	VAL	6.2
6	F	3	GLY	6.2
1	N	113[A]	LEU	6.2
2	O	113	TYR	6.0
7	G	3	ALA	6.0
4	Q	7	LYS	5.9
6	S	95	GLN	5.9
12	L	2	HIS	5.8
7	T	38	HIS	5.7

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Mol	Chain	Res	Type	RSRZ
9	I	27	VAL	5.7
7	T	1	ALA	5.6
6	F	94	HIS	5.6
7	G	10	GLY	5.6
9	V	2	THR	5.6
4	Q	4	SER	5.6
2	O	32[A]	PHE	5.5
5	R	109	VAL	5.4
4	D	4	SER	5.4
7	G	8	HIS	5.4
7	T	10	GLY	5.3
7	T	37	LEU	5.2
3	P	3	HIS	5.2
4	Q	87[A]	PHE	5.2
4	Q	8	SER	5.2
8	U	45	ALA	5.1
7	T	8	HIS	5.1
6	F	98	HIS	5.0
7	T	5	LYS	5.0
7	T	6	GLY	5.0
13	M	43	SER	4.9
12	Y	2	HIS	4.9
6	S	2	SER	4.8
8	H	44	THR	4.8
7	T	2	SER	4.7
1	A	113[A]	LEU	4.7
7	T	36	TRP	4.7
7	G	2	SER	4.7
10	W	58	LYS	4.6
7	G	37	LEU	4.6
9	I	29	LEU	4.6
2	B	16[A]	ILE	4.6
7	T	4	ALA	4.5
9	I	25	PHE	4.5
7	T	33	LEU	4.5
9	I	30	GLY	4.4
7	G	4	ALA	4.4
2	B	65	TRP	4.4
9	I	33	THR	4.4
9	I	35	TYR	4.4
7	T	7	ASP	4.4
9	V	33	THR	4.4

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Mol	Chain	Res	Type	RSRZ
7	T	84	LYS	4.4
2	B	33	LEU	4.3
2	B	59	GLN	4.2
2	O	227	LEU	4.2
7	G	40	GLY	4.2
2	B	60	GLU	4.1
2	B	32[A]	PHE	4.1
13	M	42	LYS	4.1
5	E	5	HIS	4.0
5	R	14[A]	ARG	4.0
5	R	5	HIS	4.0
7	G	41	HIS	4.0
4	D	87[A]	PHE	4.0
8	H	10	ASN	3.9
9	I	34	PHE	3.9
8	U	47	GLY	3.9
12	Y	47	LYS	3.9
7	T	39	SER	3.8
10	J	58	LYS	3.8
11	X	6	ALA	3.8
9	I	31	PHE	3.8
8	U	50	VAL	3.8
8	U	44	THR	3.8
2	B	55	THR	3.7
4	Q	19[A]	ARG	3.7
7	G	84	LYS	3.7
7	G	38	HIS	3.7
10	J	1	PHE	3.6
8	U	55	TRP	3.6
9	I	21	ILE	3.6
2	O	90	ILE	3.5
2	O	33	LEU	3.5
9	I	32	ALA	3.5
9	I	26	MET	3.5
9	V	31	PHE	3.5
7	G	42	ARG	3.5
8	H	7	LYS	3.4
9	V	34	PHE	3.4
3	C	38	ASN	3.4
3	C	3	HIS	3.4
2	B	113	TYR	3.4
8	H	9	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
7	G	7	ASP	3.3
1	N	383[A]	MET	3.3
9	V	73	LYS	3.2
6	F	95	GLN	3.2
13	Z	40	TYR	3.2
8	U	11	TYR	3.2
13	M	40	TYR	3.2
8	U	9	LYS	3.2
2	B	82	ARG	3.2
8	H	36	PHE	3.2
5	E	39	TYR	3.1
11	K	47	ARG	3.1
2	O	86	MET	3.1
7	T	40	GLY	3.1
1	N	483	LEU	3.1
8	U	7	LYS	3.1
8	U	46	LYS	3.1
12	L	45	LEU	3.1
13	Z	32	TRP	3.0
2	B	30	ILE	3.0
4	Q	9	GLU	3.0
8	H	45	ALA	3.0
6	S	43	LYS	3.0
7	T	42	ARG	3.0
4	Q	39	ALA	3.0
4	Q	116	VAL	3.0
2	B	87[A]	MET	3.0
8	H	55	TRP	2.9
1	A	383[A]	MET	2.9
2	B	40	TYR	2.9
4	Q	35	ALA	2.9
1	N	513	LEU	2.9
12	Y	45	LEU	2.9
2	O	30	ILE	2.9
11	X	51	LYS	2.9
8	U	10	ASN	2.9
2	O	58	ALA	2.8
2	O	87[A]	MET	2.8
11	X	52	GLU	2.8
6	S	92	VAL	2.8
9	V	35	TYR	2.8
12	L	47	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
12	Y	24[A]	MET	2.8
2	B	61	VAL	2.8
2	B	56	MET	2.8
4	Q	10	ASP	2.8
7	T	35	SER	2.8
13	Z	43	SER	2.8
13	M	32	TRP	2.7
8	U	42	ALA	2.7
10	J	52	TRP	2.7
4	Q	57	VAL	2.7
4	Q	40	LEU	2.7
9	V	30	GLY	2.7
2	B	86	MET	2.7
9	V	29	LEU	2.6
2	O	65	TRP	2.6
8	U	85	ILE	2.6
2	B	29[A]	MET	2.6
13	M	39	ASN	2.6
7	T	12	GLY	2.6
9	V	25	PHE	2.6
1	N	332	ILE	2.6
3	P	40	MET	2.6
2	O	60	GLU	2.6
8	U	84	LYS	2.5
7	G	35	SER	2.5
2	O	91	ASN	2.5
11	X	54	ARG	2.5
8	H	77	ALA	2.5
11	X	7	PRO	2.5
3	C	258	TRP	2.5
7	G	33	LEU	2.5
12	L	24	MET	2.5
4	D	9	GLU	2.5
2	O	43	SER	2.5
2	B	91	ASN	2.5
5	R	59	ASN	2.5
6	F	92	VAL	2.5
2	O	59	GLN	2.4
6	S	22	LEU	2.4
9	V	68	ILE	2.4
2	O	221	LYS	2.4
3	C	33[A]	MET	2.4

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Mol	Chain	Res	Type	RSRZ
10	W	57	HIS	2.4
6	S	74	LEU	2.4
8	H	47	GLY	2.4
10	W	55	PHE	2.4
2	B	58	ALA	2.4
2	O	36	SER	2.4
7	G	39	SER	2.4
4	D	11	TYR	2.4
1	N	514	LYS	2.4
2	O	37	LEU	2.4
4	Q	51	LEU	2.4
9	V	44	LYS	2.4
2	B	42	ILE	2.4
10	W	1	PHE	2.3
3	C	230	ASN	2.3
9	I	40	ALA	2.3
9	V	32	ALA	2.3
9	V	69	PHE	2.3
6	F	54[A]	ASN	2.3
6	S	52	ILE	2.3
8	H	46	LYS	2.3
3	P	122	HIS	2.3
2	B	78	LEU	2.3
7	T	43	GLU	2.3
2	B	36	SER	2.3
2	B	34	ILE	2.3
6	S	27	GLY	2.3
2	B	38	VAL	2.3
3	P	258	TRP	2.2
7	T	41	HIS	2.2
10	W	14[A]	GLU	2.2
9	I	24	ALA	2.2
9	I	28	SER	2.2
13	Z	38	ASP	2.2
1	N	311[A]	ILE	2.2
9	V	27	VAL	2.2
2	O	216	LEU	2.2
5	R	96	LEU	2.2
1	A	514	LYS	2.2
1	A	346	PHE	2.2
2	O	40	TYR	2.2
9	V	21	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
11	X	23	THR	2.2
2	O	224	ALA	2.1
8	H	42	ALA	2.1
9	I	15	ARG	2.1
3	C	122	HIS	2.1
12	L	44	LEU	2.1
3	P	38	ASN	2.1
4	D	7	LYS	2.1
13	Z	39	ASN	2.1
13	Z	42	LYS	2.1
3	P	33[A]	MET	2.1
2	O	114	GLU	2.1
11	X	13	TYR	2.1
2	O	38	VAL	2.1
2	B	22[A]	HIS	2.1
8	U	48	GLY	2.1
2	B	39	LEU	2.1
2	B	115	ASP	2.1
3	P	37	PHE	2.1
9	V	19	PHE	2.1
2	B	90	ILE	2.1
11	X	16	ALA	2.1
1	N	485	VAL	2.1
1	A	297[A]	MET	2.1
10	J	56	PRO	2.1
9	I	73	LYS	2.1
3	C	37	PHE	2.1
2	B	64	ILE	2.1
4	D	143	ASN	2.0
11	K	6	ALA	2.0
2	O	35	SER	2.0
4	D	6	VAL	2.0
11	X	28[A]	VAL	2.0
1	N	136[A]	LEU	2.0
2	O	133	LEU	2.0
4	Q	33	LEU	2.0
8	H	48	GLY	2.0
9	V	26	MET	2.0
4	Q	107	ILE	2.0
6	F	52	ILE	2.0
9	I	36	LYS	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($\text{\AA}^2$)	Q<0.9
7	TPO	G	11	11/12	0.51	0.26	90,110,131,132	0
9	SAC	V	1	9/10	0.59	0.21	102,119,126,133	0
9	SAC	I	1	9/10	0.73	0.22	60,74,81,81	0
7	TPO	T	11	11/12	0.74	0.22	94,107,122,130	0
1	FME	A	1	10/11	0.91	0.15	38,45,74,86	0
1	FME	N	1	10/11	0.92	0.14	42,51,69,79	0
2	FME	O	1	10/11	0.94	0.11	38,39,48,53	0
2	FME	B	1	10/11	0.96	0.10	29,32,42,66	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($\text{\AA}^2$)	Q<0.9
22	CHD	W	101	29/29	0.65	0.24	61,91,115,121	0
22	CHD	J	101	29/29	0.70	0.20	51,75,90,93	0
28	PEK	C	309	53/53	0.70	0.28	48,90,151,153	0
27	CDL	T	102	100/100	0.74	0.28	49,89,137,155	0
24	PSC	B	303	52/52	0.74	0.27	36,84,154,154	0
28	PEK	G	103	53/53	0.74	0.23	48,86,146,153	0
28	PEK	C	307	53/53	0.75	0.26	38,77,135,141	0
25	DMU	C	310	33/33	0.75	0.17	52,73,102,105	0
20	PGV	C	308	51/51	0.75	0.26	44,74,136,146	0
20	PGV	P	302	51/51	0.76	0.25	51,81,132,151	0
27	CDL	N	601	100/100	0.76	0.28	54,90,129,155	0
27	CDL	P	305	100/100	0.77	0.27	36,82,118,137	0
19	TGL	Y	101	63/63	0.78	0.27	45,74,111,138	0
25	DMU	P	309	33/33	0.78	0.17	45,72,92,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	TGL	Q	201	63/63	0.78	0.27	52,75,93,100	0
24	PSC	N	612	52/52	0.78	0.28	42,83,154,156	0
25	DMU	P	307	33/33	0.79	0.16	38,67,118,121	0
21	EDO	A	613	4/4	0.79	0.21	49,53,56,57	0
28	PEK	P	308	53/53	0.79	0.25	41,72,131,139	0
19	TGL	A	608	63/63	0.80	0.23	40,75,93,101	0
25	DMU	P	310	33/33	0.80	0.16	62,79,108,112	0
25	DMU	C	302	33/33	0.80	0.19	30,73,105,109	0
20	PGV	N	609	51/51	0.81	0.21	43,77,115,131	0
19	TGL	N	611	63/63	0.81	0.24	51,77,97,104	0
19	TGL	A	611	63/63	0.81	0.25	34,60,92,110	0
21	EDO	L	101	4/4	0.81	0.23	55,62,78,81	0
20	PGV	A	610	51/51	0.82	0.23	34,75,106,125	0
27	CDL	C	305	100/100	0.82	0.22	35,75,109,115	0
19	TGL	D	201	63/63	0.82	0.24	32,62,89,92	0
25	DMU	C	311	33/33	0.84	0.15	46,77,99,109	0
22	CHD	P	306	29/29	0.86	0.14	43,49,52,68	0
22	CHD	C	306	29/29	0.86	0.14	43,49,54,66	0
21	EDO	S	104	4/4	0.86	0.14	40,52,60,65	0
21	EDO	W	102	4/4	0.87	0.21	50,55,66,73	0
21	EDO	C	312	4/4	0.87	0.20	41,43,72,85	0
21	EDO	A	617	4/4	0.87	0.17	40,42,43,44	0
26	UNX	C	303	1/1	0.87	0.25	35,35,35,35	0
21	EDO	N	620	4/4	0.87	0.18	47,49,54,58	0
21	EDO	A	618	4/4	0.87	0.19	51,51,53,63	0
21	EDO	Y	102	4/4	0.88	0.17	61,65,66,67	0
21	EDO	N	616	4/4	0.88	0.14	52,54,55,56	0
25	DMU	Z	101	33/33	0.89	0.13	45,54,70,76	0
21	EDO	N	617	4/4	0.89	0.16	52,55,58,61	0
21	EDO	N	621	4/4	0.90	0.17	41,51,53,61	0
21	EDO	A	619	4/4	0.90	0.19	44,60,74,82	0
21	EDO	B	305	4/4	0.91	0.17	35,45,48,51	0
21	EDO	D	202	4/4	0.91	0.15	33,38,47,66	0
21	EDO	G	105	4/4	0.91	0.13	53,56,64,79	0
21	EDO	A	614	4/4	0.92	0.12	30,31,32,37	0
21	EDO	A	620	4/4	0.92	0.15	52,56,57,64	0
21	EDO	M	102	4/4	0.92	0.18	60,63,63,69	0
21	EDO	B	304	4/4	0.92	0.14	46,59,60,85	0
21	EDO	A	615	4/4	0.93	0.14	53,63,65,70	0
21	EDO	B	306	4/4	0.93	0.15	50,51,55,57	0
25	DMU	M	101	33/33	0.93	0.11	38,44,58,67	0
21	EDO	P	312	4/4	0.93	0.13	33,36,43,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	S	103	4/4	0.93	0.12	39,42,45,47	0
21	EDO	D	203	4/4	0.93	0.19	63,67,71,74	0
21	EDO	E	202	4/4	0.93	0.11	38,40,44,47	0
21	EDO	E	203	4/4	0.93	0.11	42,42,50,55	0
21	EDO	N	615	4/4	0.94	0.11	41,53,57,60	0
21	EDO	O	302	4/4	0.94	0.11	38,39,40,42	0
21	EDO	F	104	4/4	0.94	0.11	36,36,38,42	0
21	EDO	F	103	4/4	0.94	0.13	37,41,42,52	0
21	EDO	N	619	4/4	0.94	0.12	40,43,46,49	0
21	EDO	N	614	4/4	0.94	0.11	29,33,36,36	0
28	PEK	T	101	53/53	0.94	0.15	29,49,85,92	0
18	AZI	A	606[B]	3/3	0.95	0.11	22,22,23,24	3
21	EDO	P	311	4/4	0.95	0.10	39,42,43,46	0
21	EDO	A	616	4/4	0.95	0.10	22,27,28,42	0
21	EDO	N	618	4/4	0.95	0.10	37,40,43,45	0
21	EDO	N	613	4/4	0.95	0.10	33,34,37,41	0
28	PEK	G	101	53/53	0.95	0.14	29,46,79,95	0
21	EDO	T	103	4/4	0.95	0.11	36,37,42,44	0
18	AZI	N	607[B]	3/3	0.95	0.12	23,23,27,28	3
21	EDO	B	307	4/4	0.95	0.10	29,30,35,37	0
20	PGV	A	609	51/51	0.96	0.10	25,33,67,71	0
22	CHD	C	301	29/29	0.96	0.07	27,30,34,36	0
20	PGV	N	610	51/51	0.96	0.11	27,35,68,72	0
21	EDO	R	201	4/4	0.96	0.09	44,45,45,45	0
22	CHD	P	301	29/29	0.96	0.07	28,32,36,39	0
18	AZI	N	608[A]	3/3	0.96	0.13	29,29,38,40	3
21	EDO	A	612	4/4	0.96	0.10	37,41,41,53	0
20	PGV	C	304	51/51	0.96	0.12	27,34,86,96	0
18	AZI	N	608[B]	3/3	0.96	0.13	24,24,26,26	3
26	UNX	P	303	1/1	0.96	0.09	32,32,32,32	0
18	AZI	A	607[A]	3/3	0.97	0.09	20,20,24,27	3
18	AZI	A	607[B]	3/3	0.97	0.09	23,23,24,29	3
22	CHD	B	301	29/29	0.97	0.07	25,30,33,41	0
16	MG	N	605	1/1	0.97	0.06	31,31,31,31	0
20	PGV	P	304	51/51	0.97	0.09	26,36,79,89	0
22	CHD	G	102	29/29	0.97	0.06	28,30,36,39	0
21	EDO	G	104	4/4	0.97	0.07	34,37,38,41	0
21	EDO	E	201	4/4	0.97	0.07	40,41,43,44	0
14	HEA	A	601	60/60	0.98	0.07	21,24,48,50	0
17	NA	N	606	1/1	0.98	0.07	35,35,35,35	0
14	HEA	A	602[A]	60/60	0.98	0.07	18,22,26,28	60
14	HEA	A	602[B]	60/60	0.98	0.07	21,25,34,37	60

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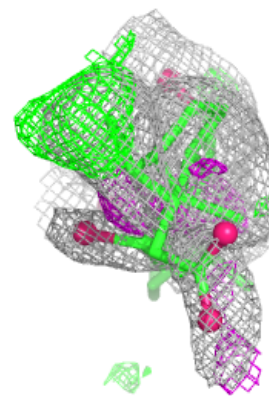
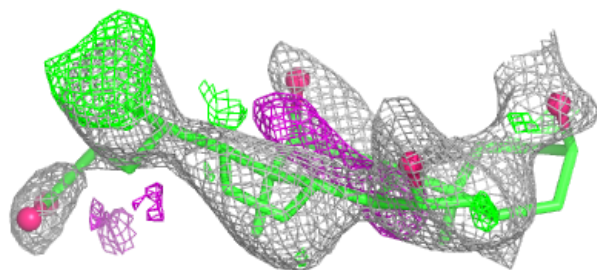
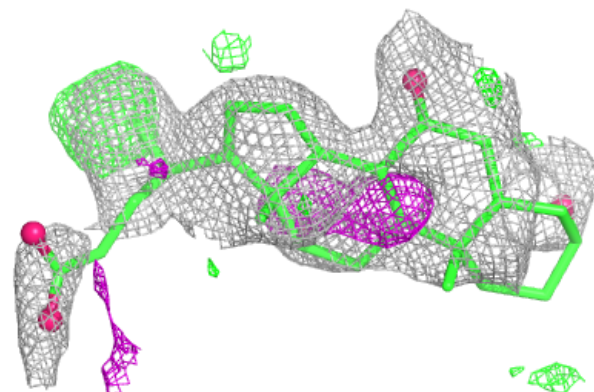
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	S	102	4/4	0.98	0.07	29,29,30,30	0
14	HEA	N	602	60/60	0.98	0.08	26,30,49,52	0
14	HEA	N	603[A]	60/60	0.98	0.07	21,25,28,30	60
14	HEA	N	603[B]	60/60	0.98	0.07	24,29,42,46	60
21	EDO	F	102	4/4	0.99	0.06	27,27,28,30	0
23	CUA	O	301	2/2	0.99	0.02	32,32,32,32	0
16	MG	A	604	1/1	0.99	0.02	26,26,26,26	0
17	NA	A	605	1/1	0.99	0.04	30,30,30,30	0
29	ZN	S	101	1/1	0.99	0.03	33,33,33,33	0
15	CU	N	604	1/1	1.00	0.02	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.01	26,26,26,26	0
29	ZN	F	101	1/1	1.00	0.02	31,31,31,31	0
23	CUA	B	302	2/2	1.00	0.02	27,27,27,28	0

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

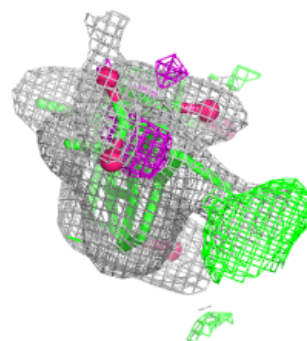
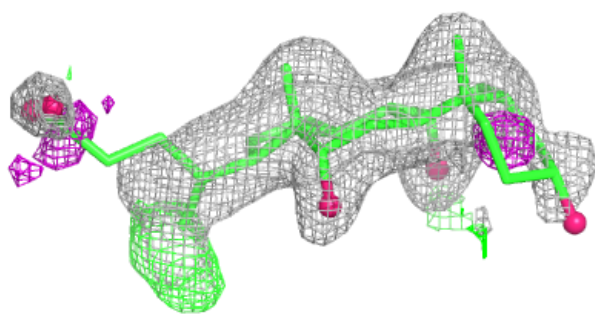
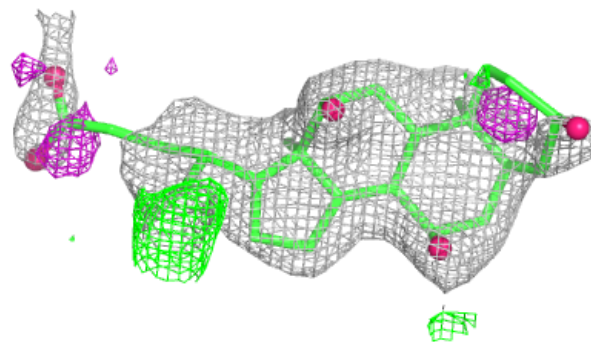
Electron density around CHD W 101:

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



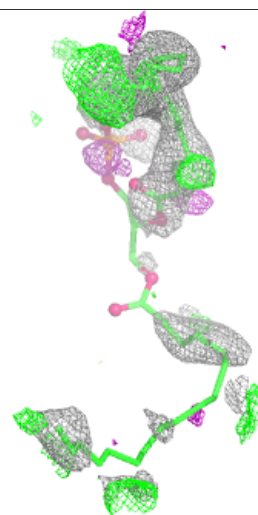
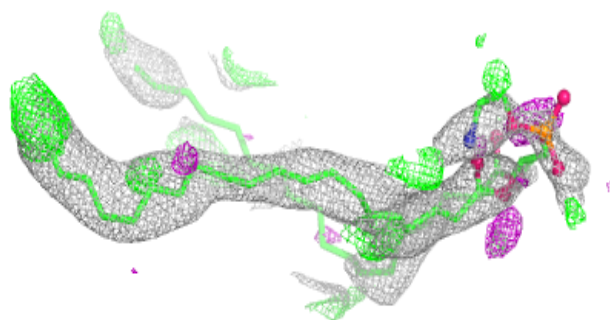
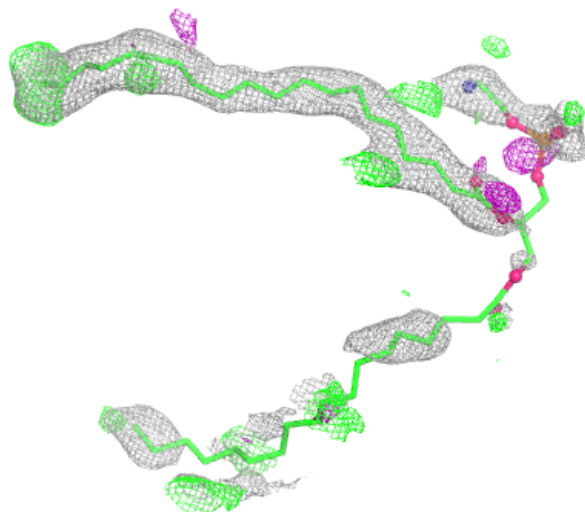
Electron density around CHD J 101:

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



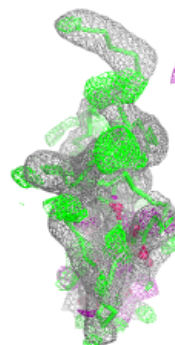
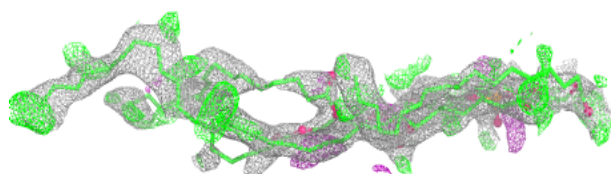
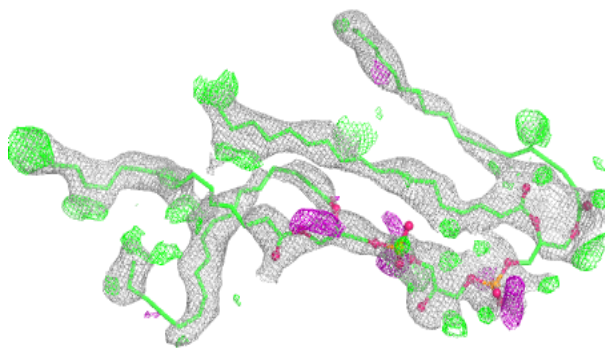
Electron density around PEK C 309:

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

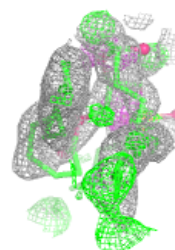
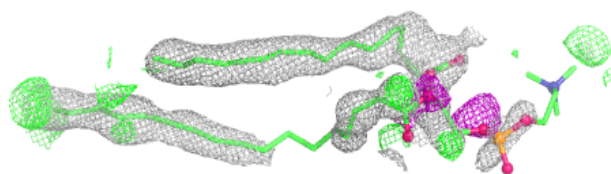
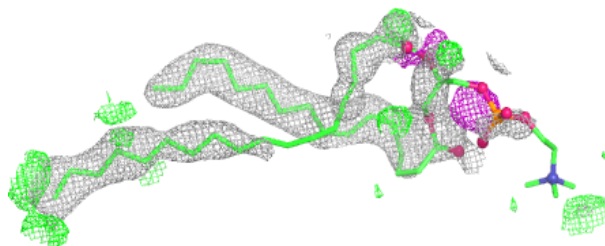


Electron density around CDL T 102:

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

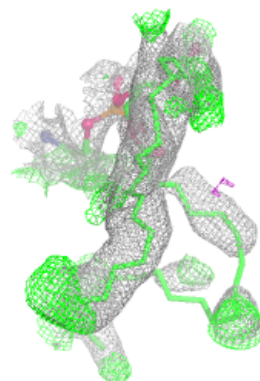
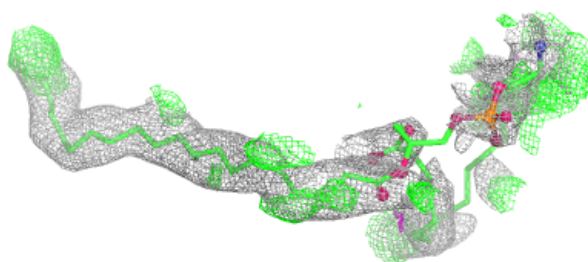
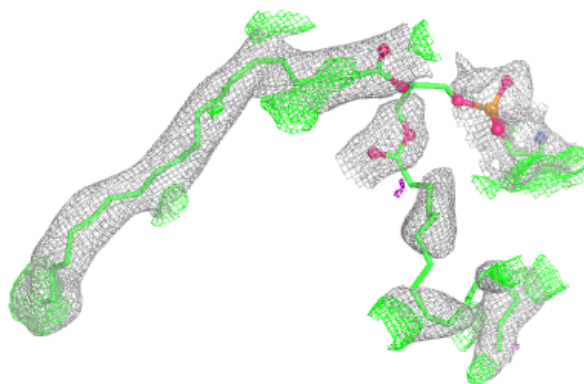
**Electron density around PSC B 303:**

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



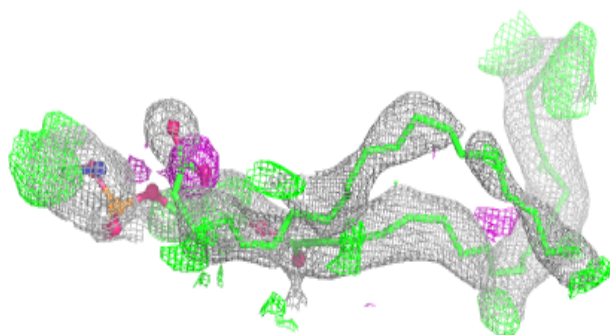
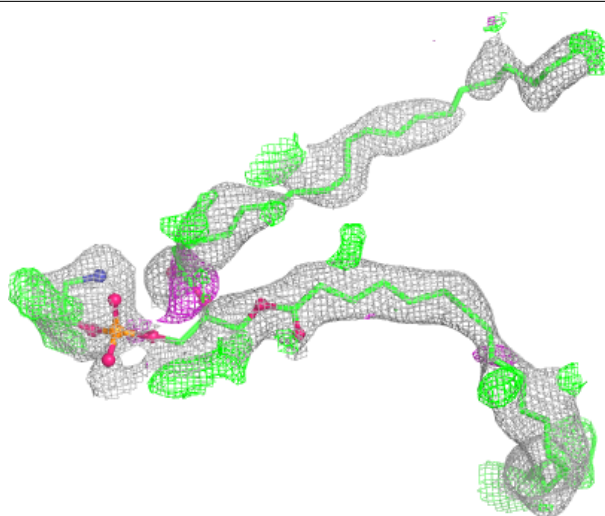
Electron density around PEK G 103:

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



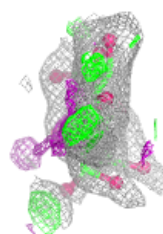
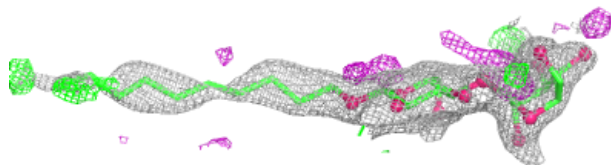
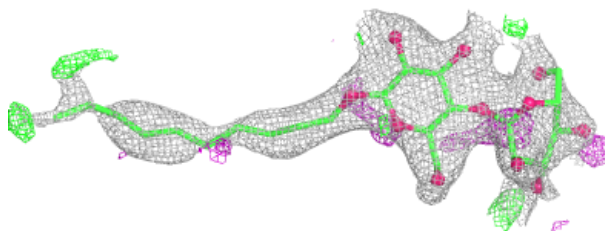
Electron density around PEK C 307:

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

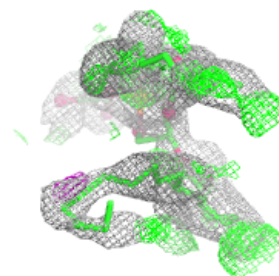
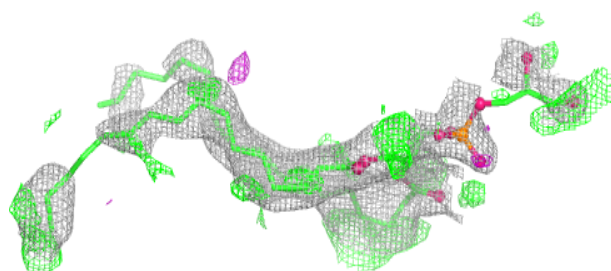
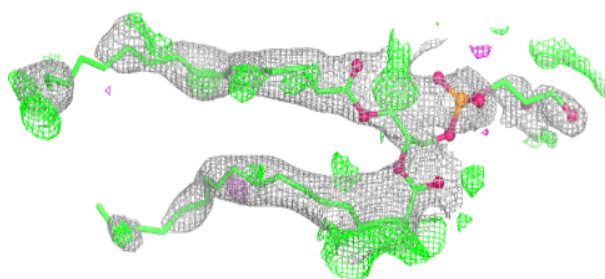


Electron density around DMU C 310:

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

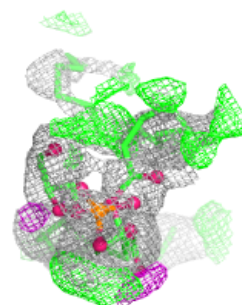
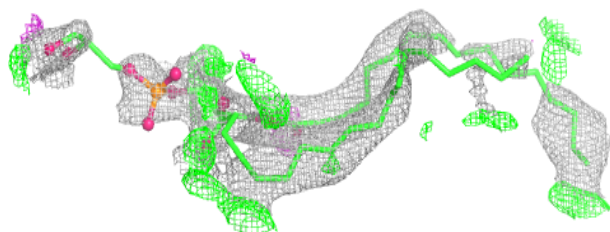
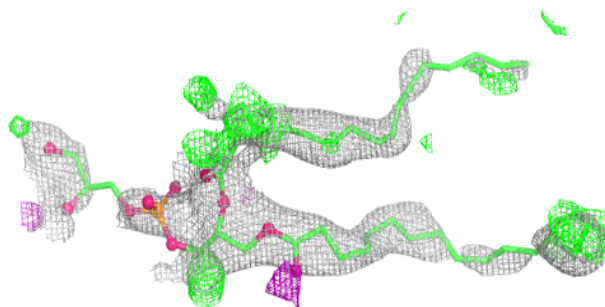
**Electron density around PGV C 308:**

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

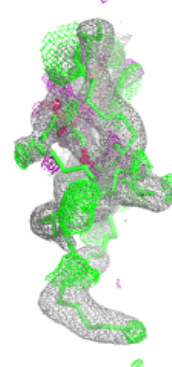
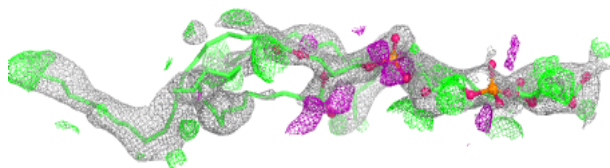
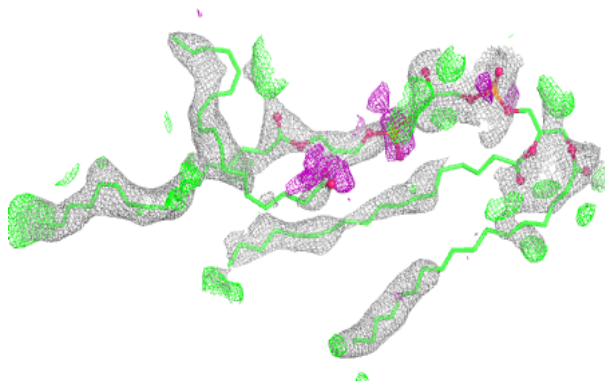


Electron density around PGV P 302:

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

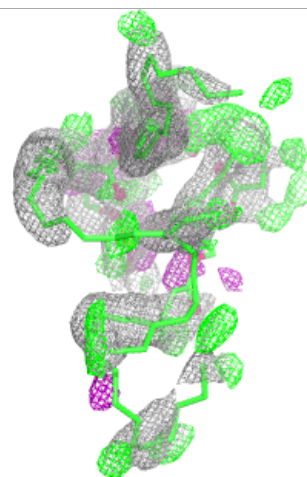
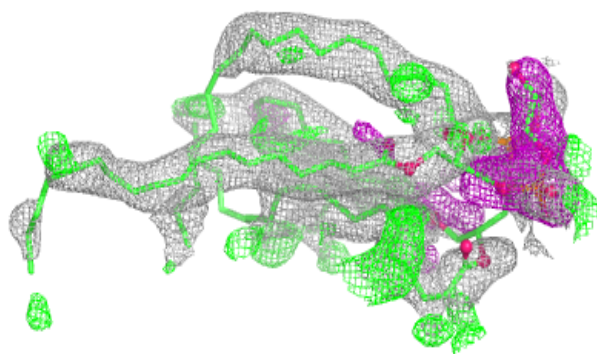
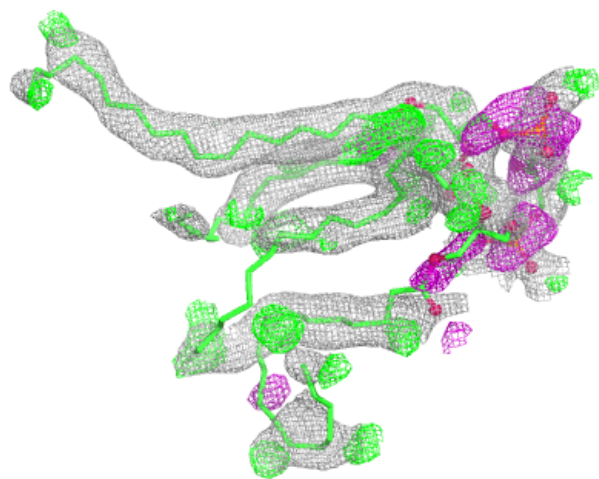
**Electron density around CDL N 601:**

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and green (positive)



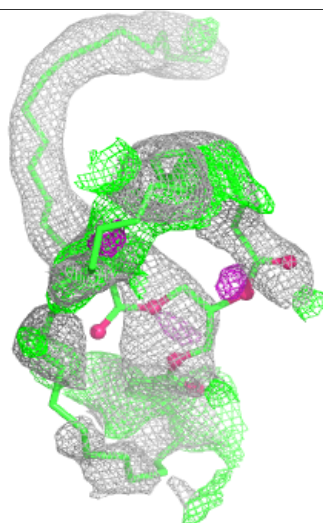
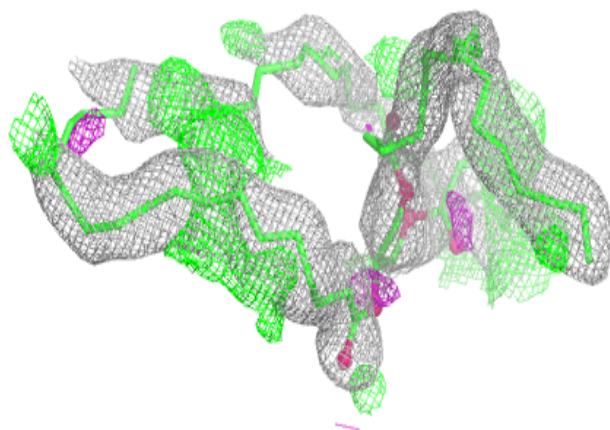
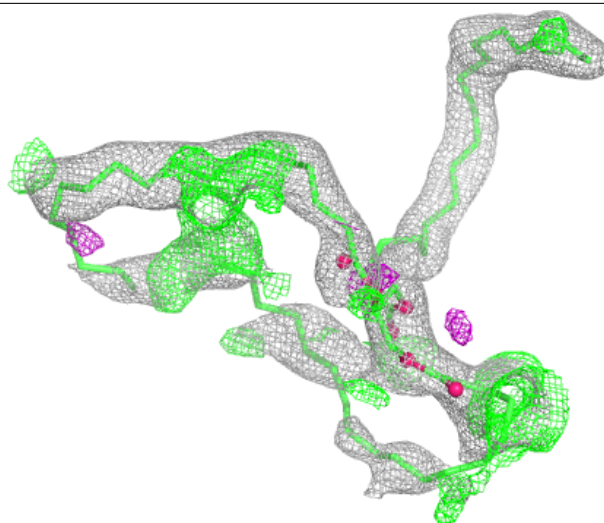
Electron density around CDL P 305:

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



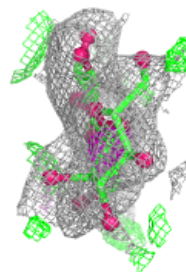
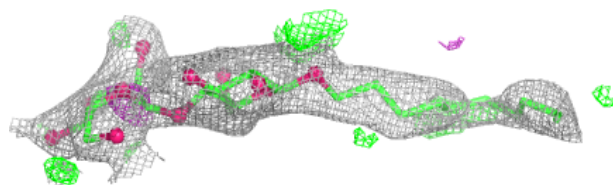
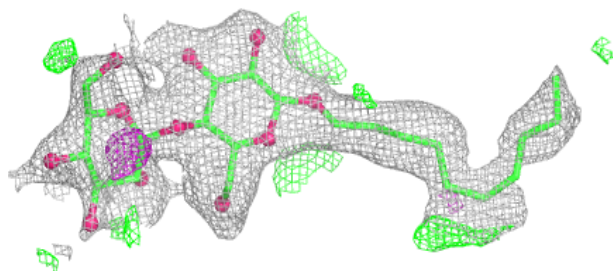
Electron density around TGL Y 101:

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

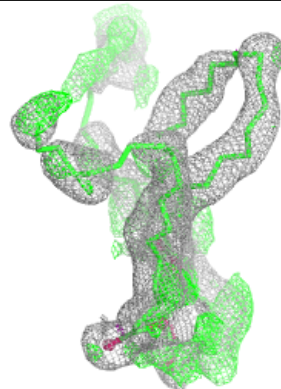
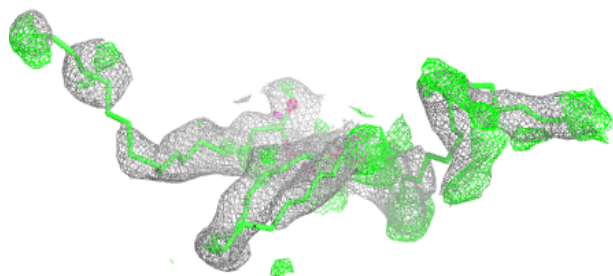
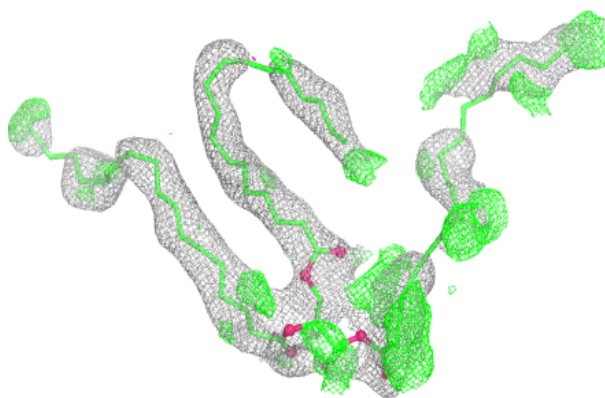


Electron density around DMU P 309:

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

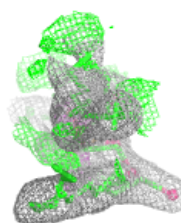
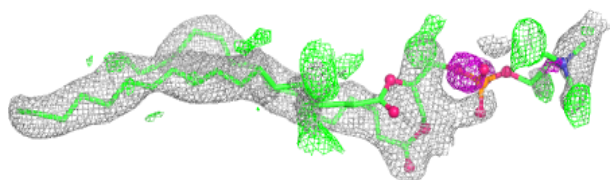
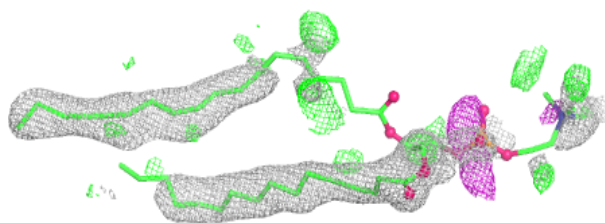
**Electron density around TGL Q 201:**

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

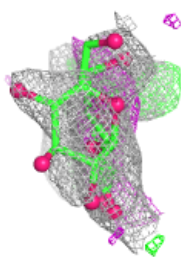
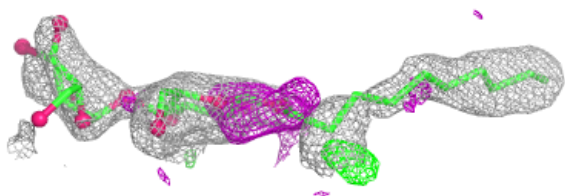
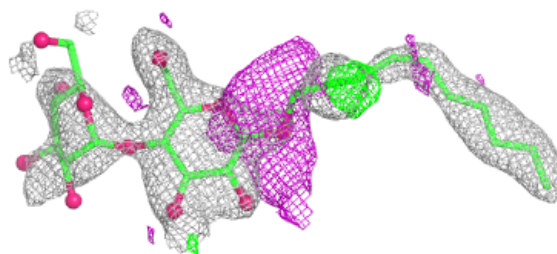


Electron density around PSC N 612:

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

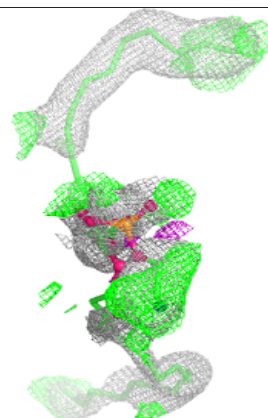
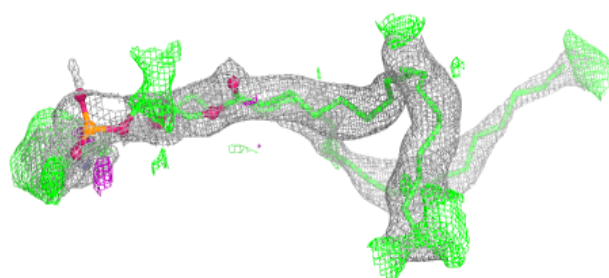
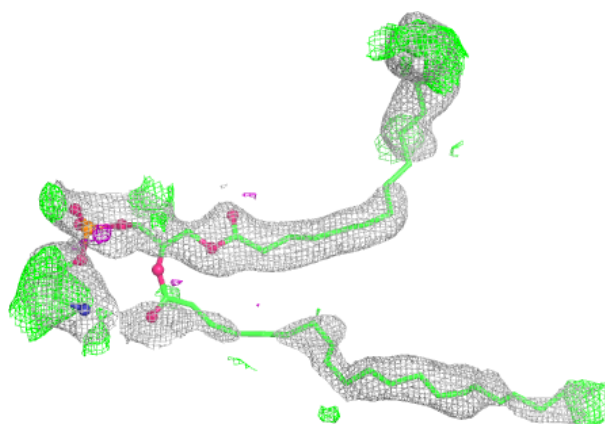
**Electron density around DMU P 307:**

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

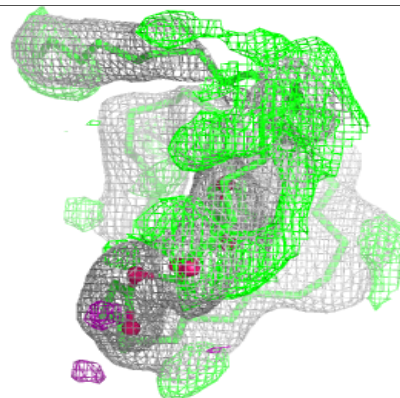
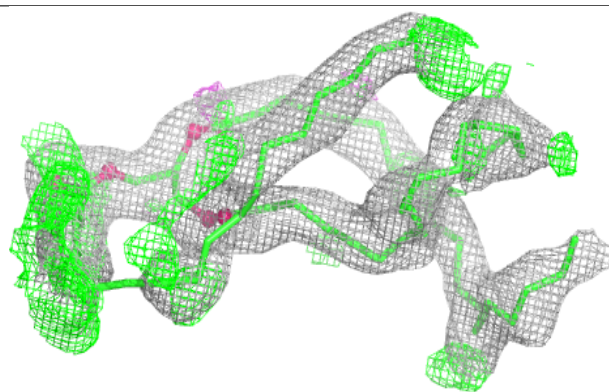
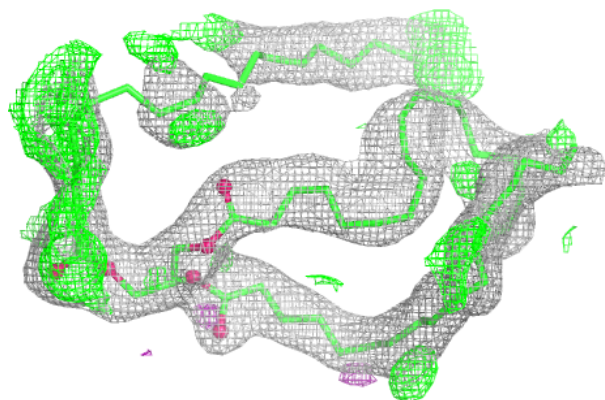


Electron density around PEK P 308:

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

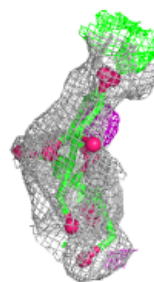
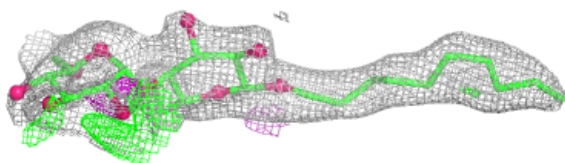
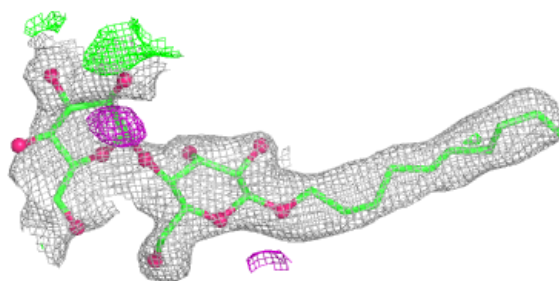
**Electron density around TGL A 608:**

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

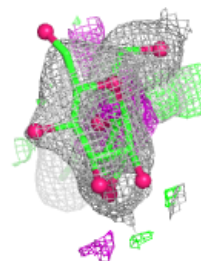
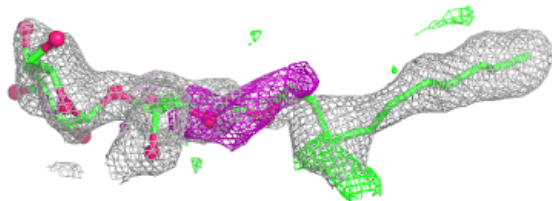
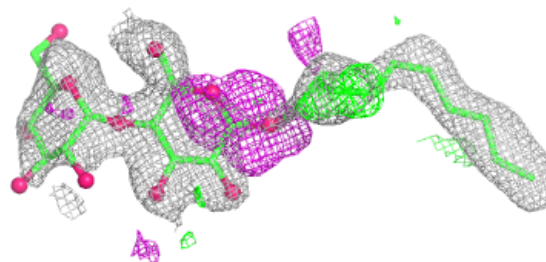


Electron density around DMU P 310:

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

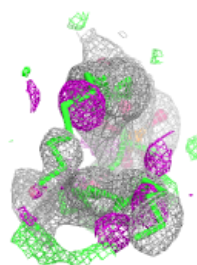
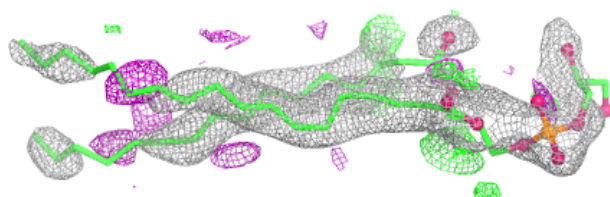
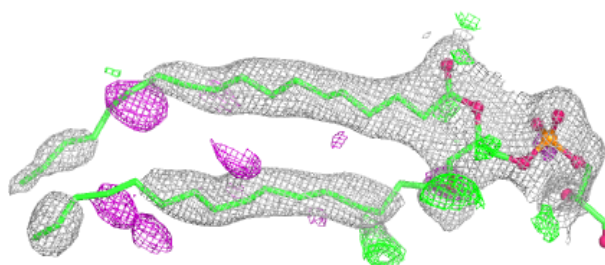
**Electron density around DMU C 302:**

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

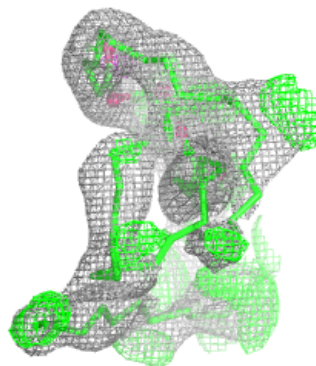
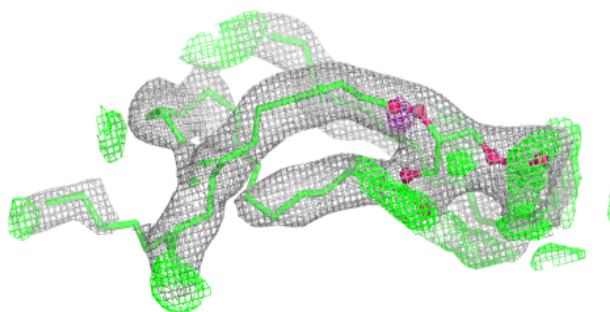
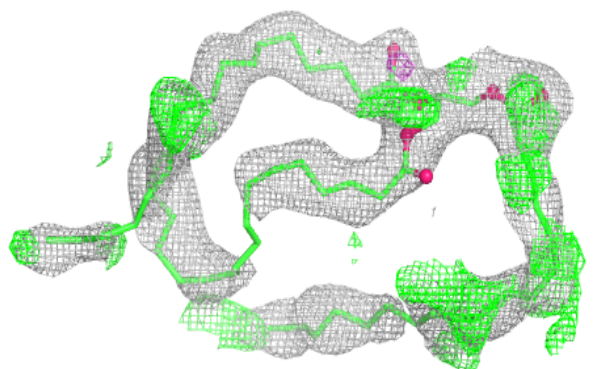


Electron density around PGL N 609:

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

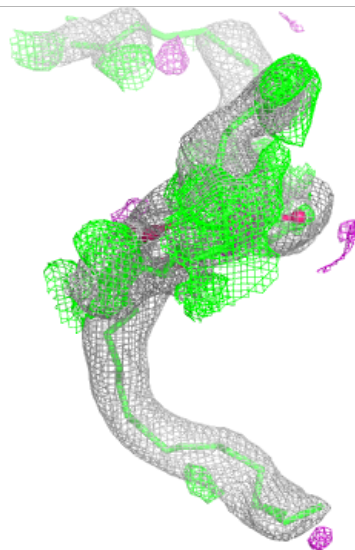
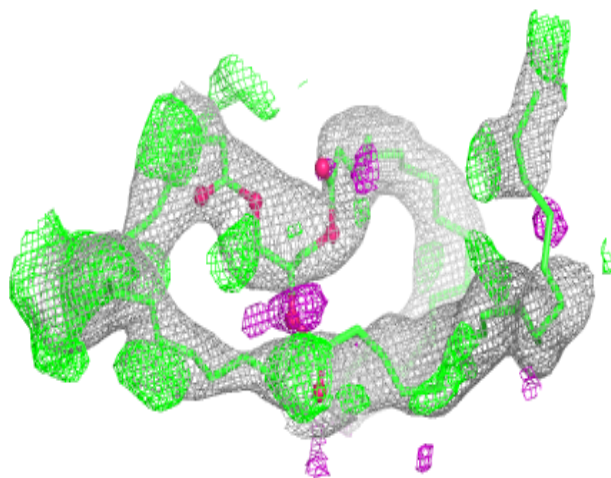
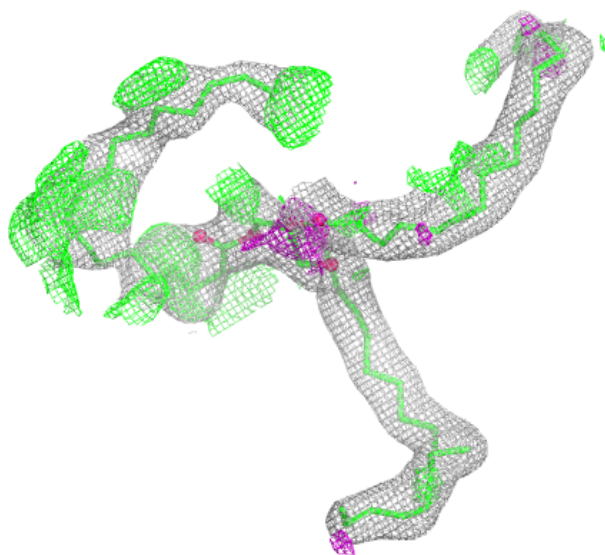
**Electron density around TGL N 611:**

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



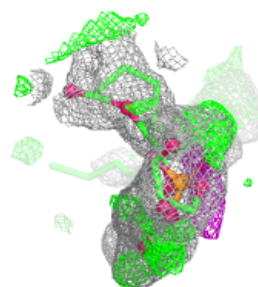
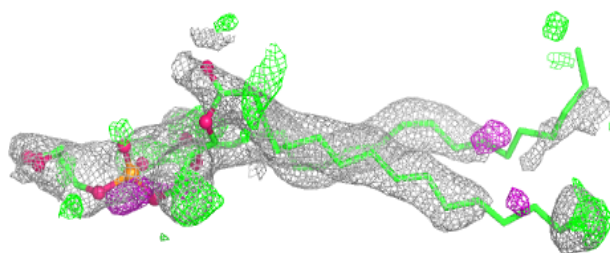
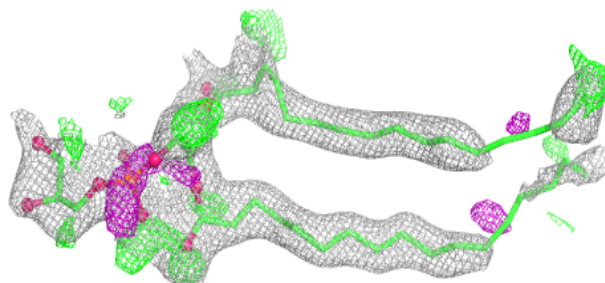
Electron density around TGL A 611:

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



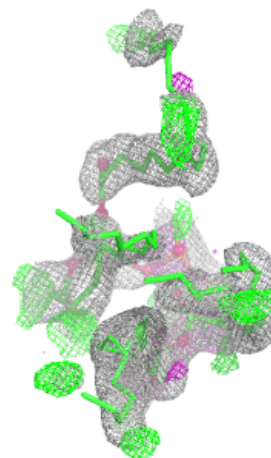
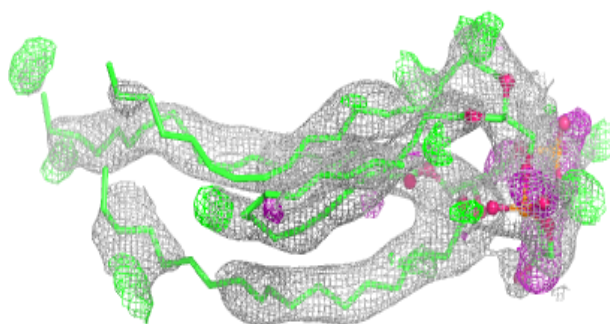
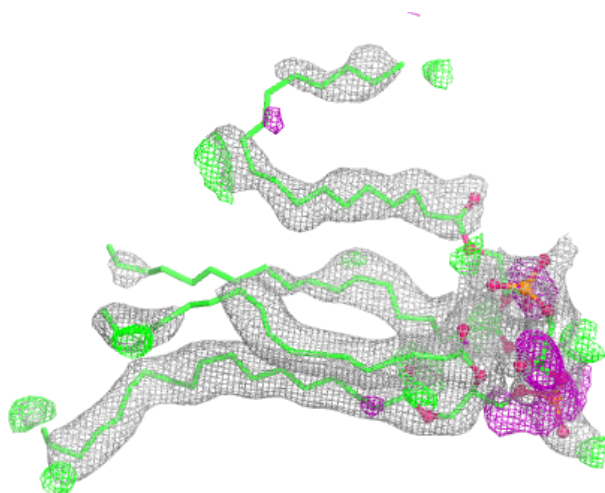
Electron density around PGV A 610:

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



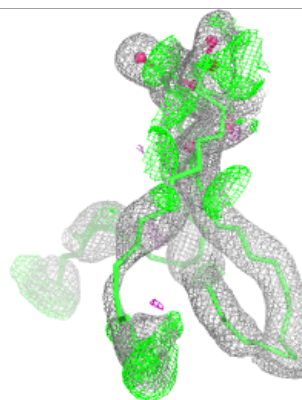
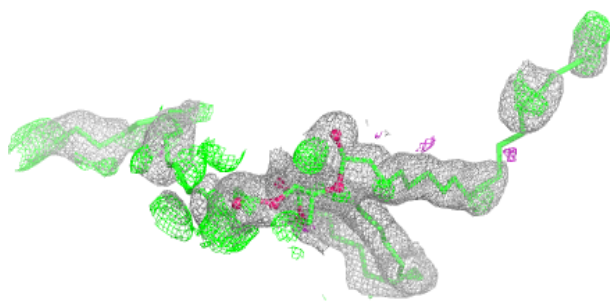
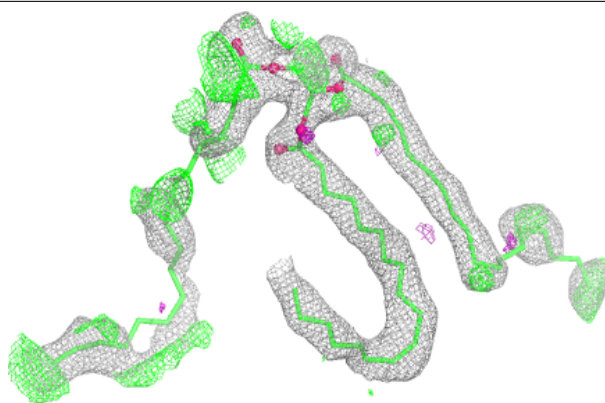
Electron density around CDL C 305:

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

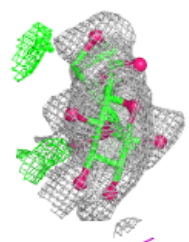
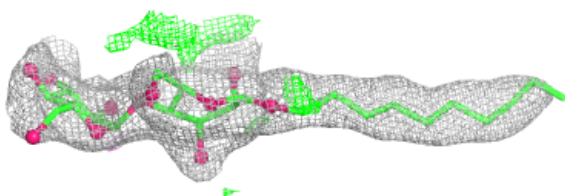
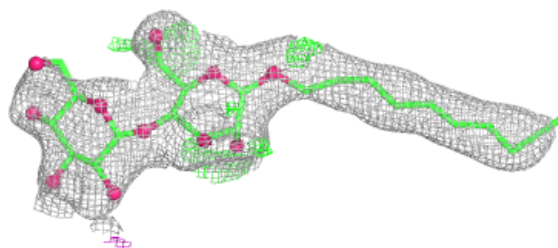


Electron density around TGL D 201:

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

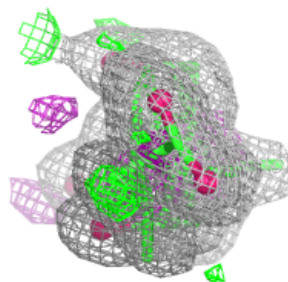
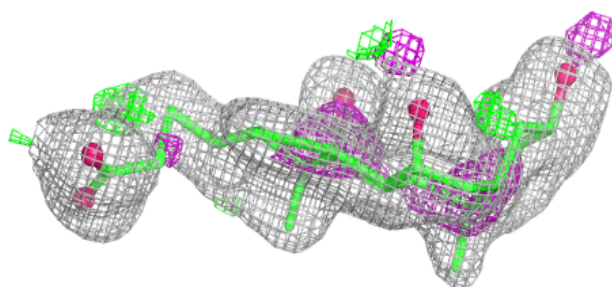
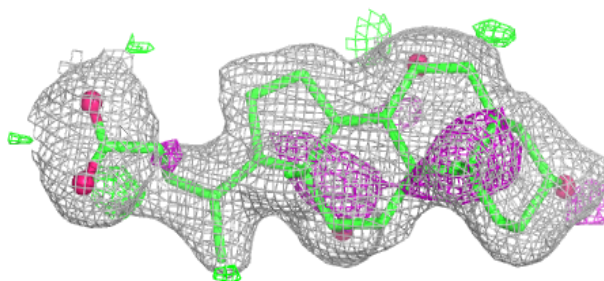
**Electron density around DMU C 311:**

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

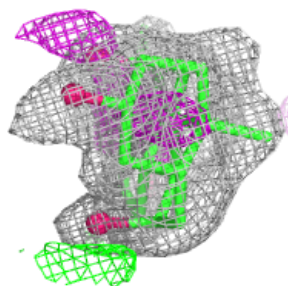
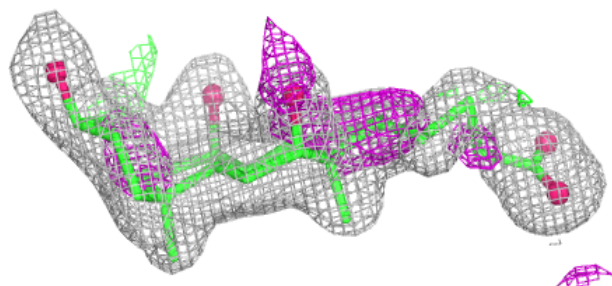
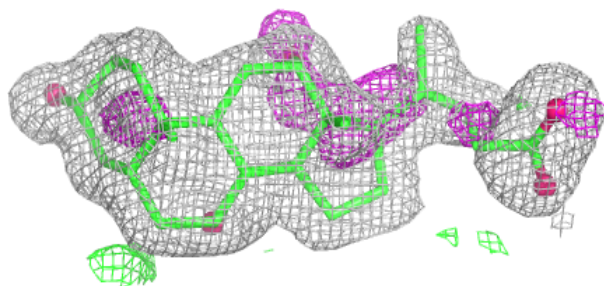


Electron density around CHD P 306:

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

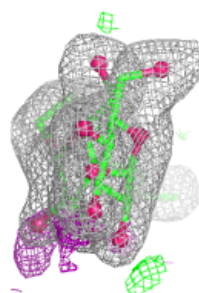
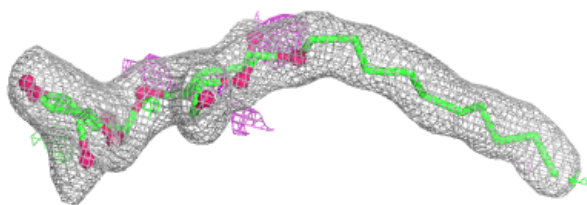
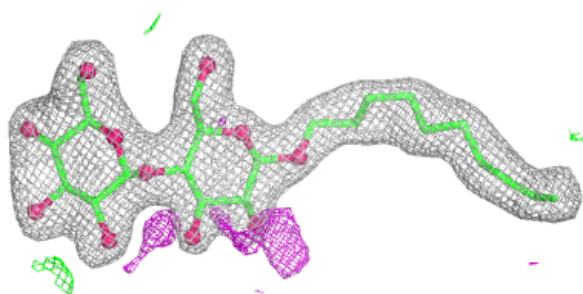
**Electron density around CHD C 306:**

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

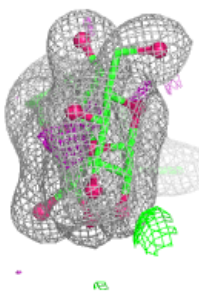
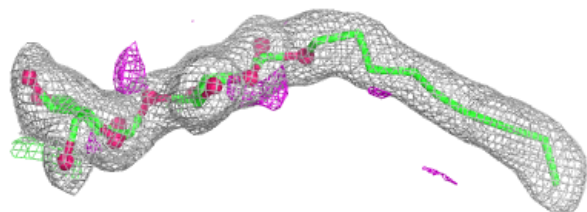
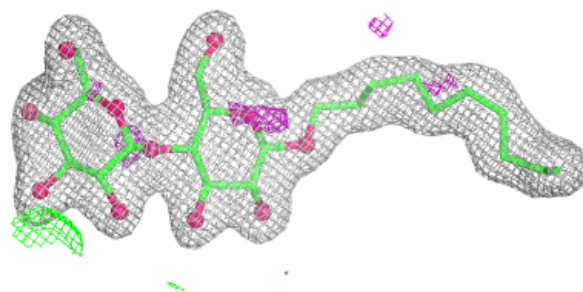


Electron density around DMU Z 101:

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

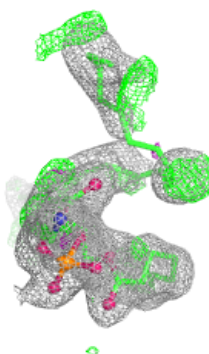
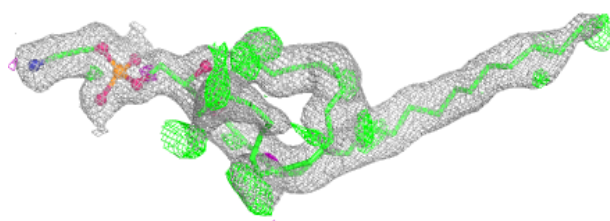
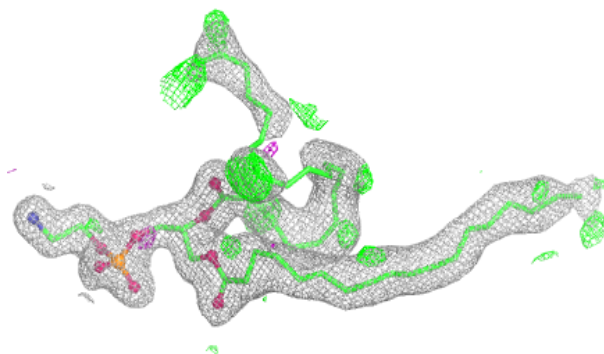
**Electron density around DMU M 101:**

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

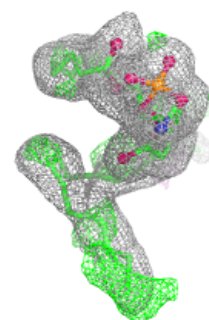
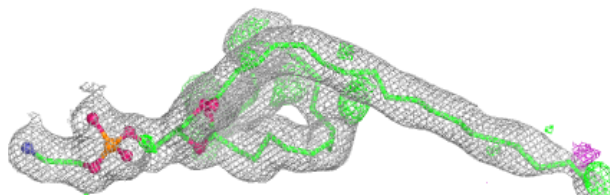
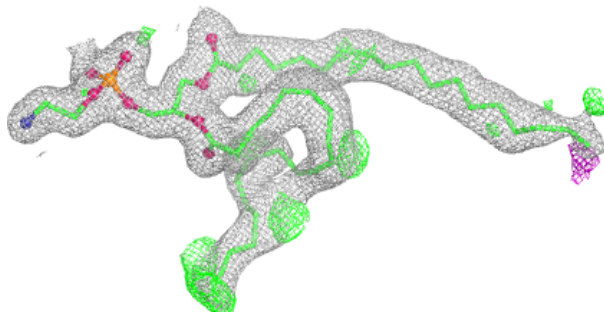


Electron density around PEK T 101:

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

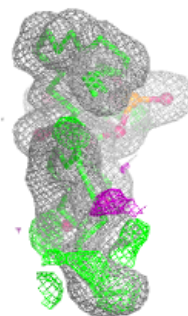
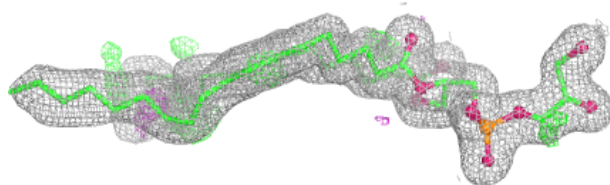
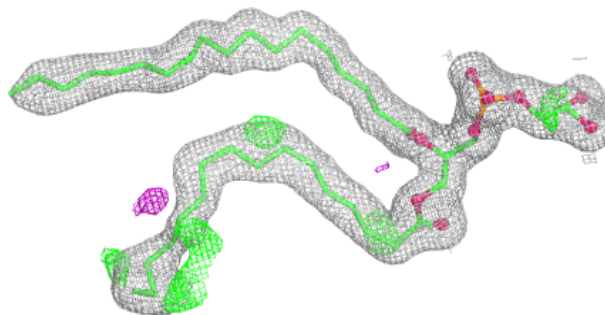
**Electron density around PEK G 101:**

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

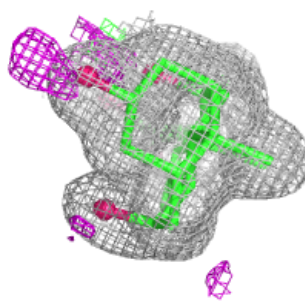
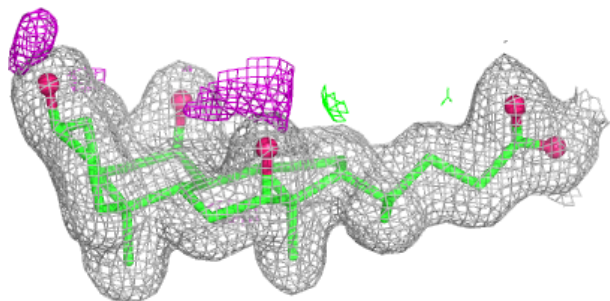
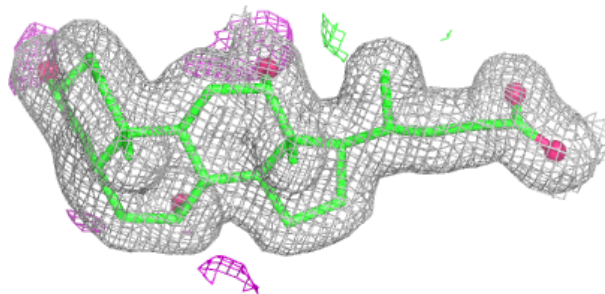


Electron density around PGV A 609:

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

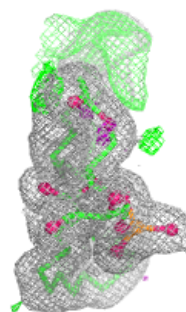
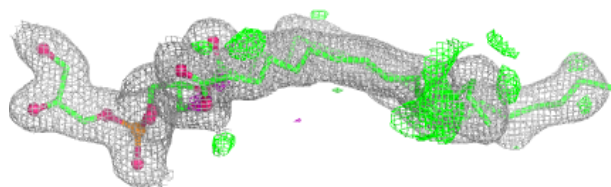
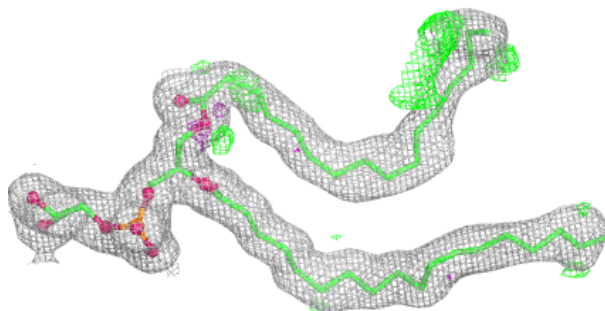
**Electron density around CHD C 301:**

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

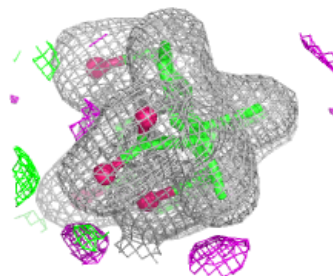
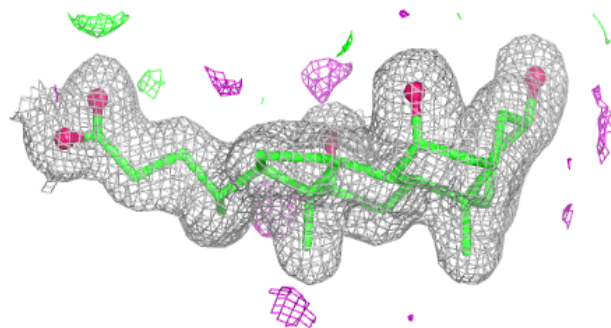
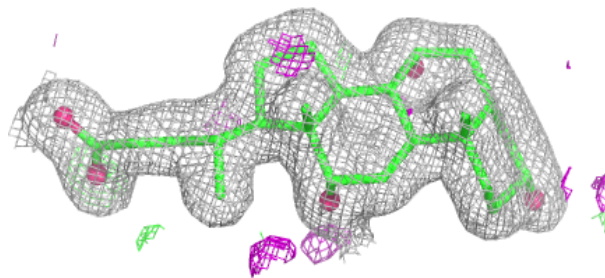


Electron density around PGV N 610:

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

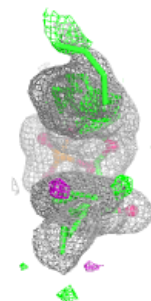
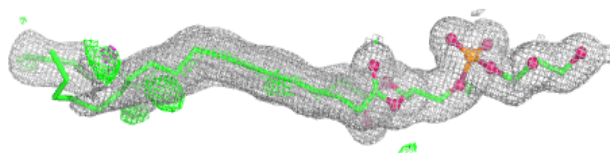
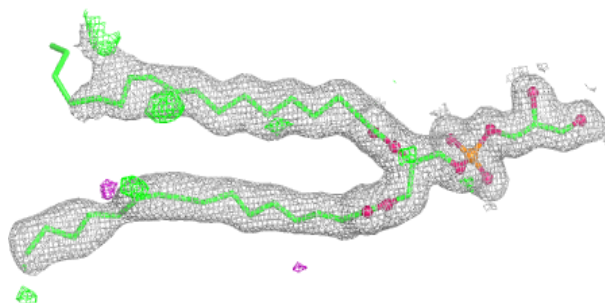
**Electron density around CHD P 301:**

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

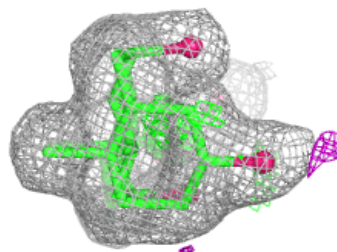
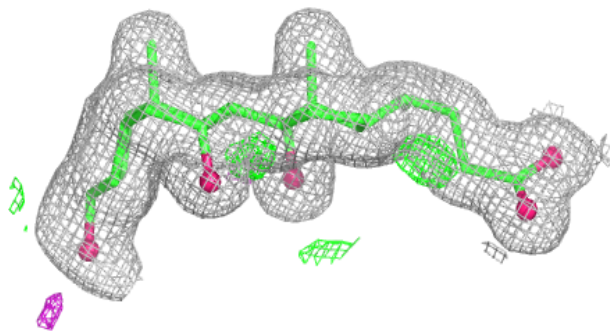
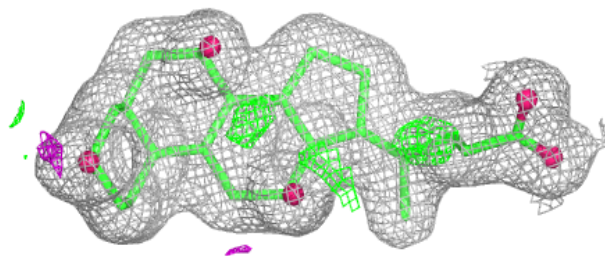


Electron density around PGV C 304:

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

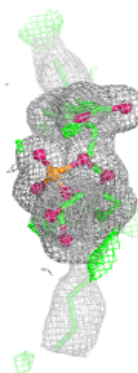
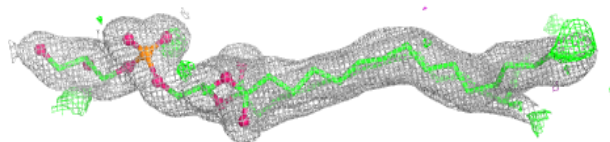
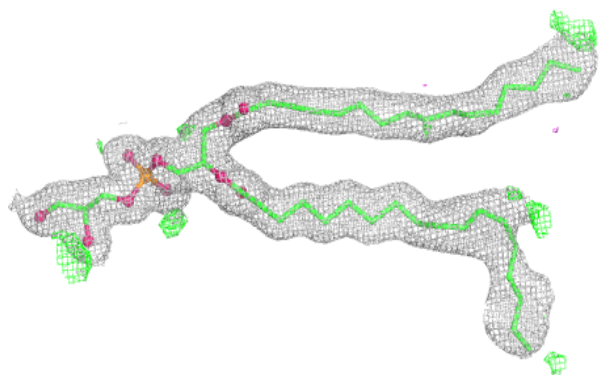
**Electron density around CHD B 301:**

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

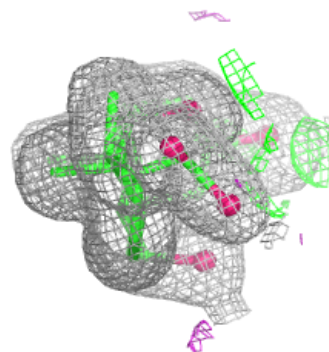
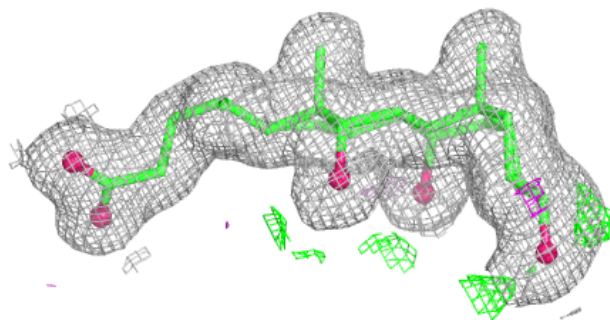
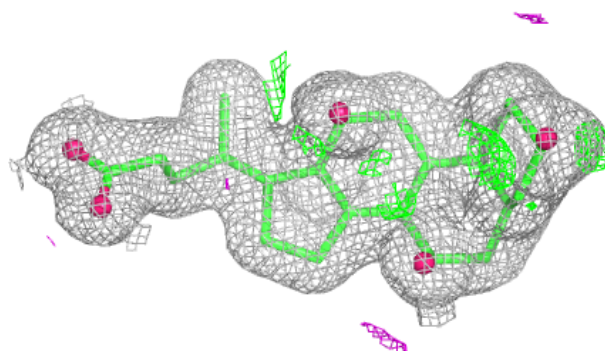


Electron density around PGV P 304:

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

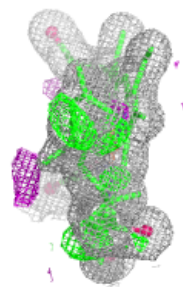
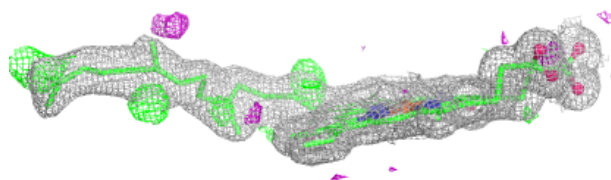
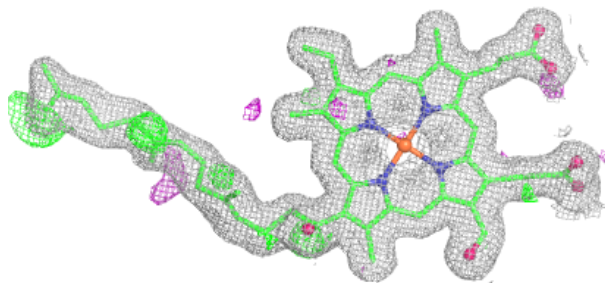
**Electron density around CHD G 102:**

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

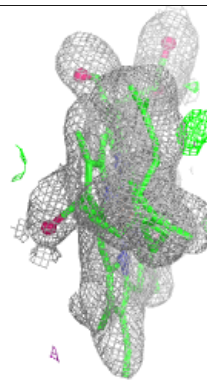
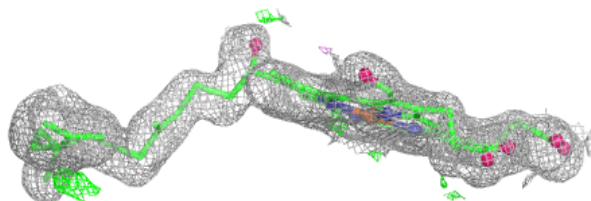
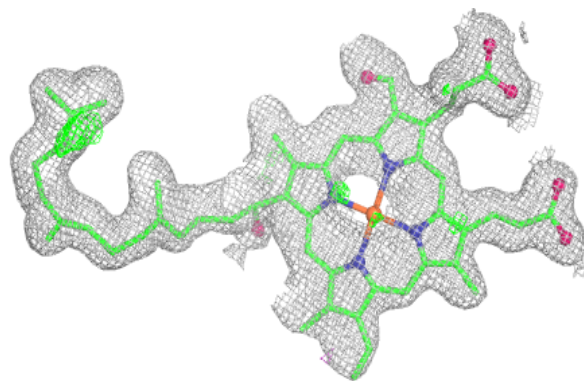


Electron density around HEA A 601:

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

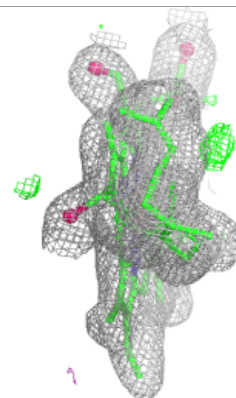
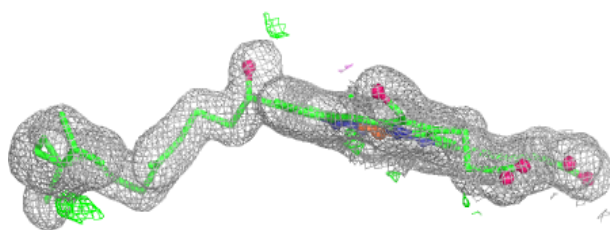
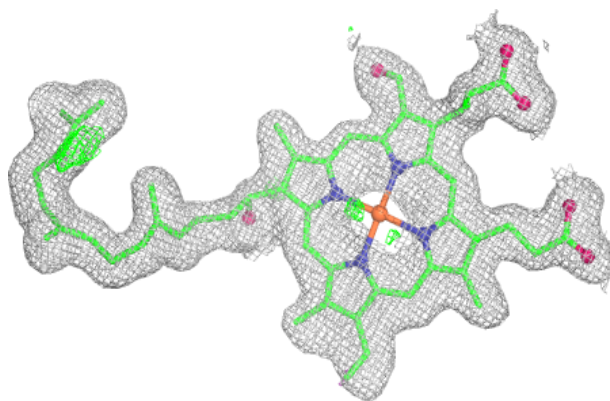
**Electron density around HEA A 602 (A):**

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

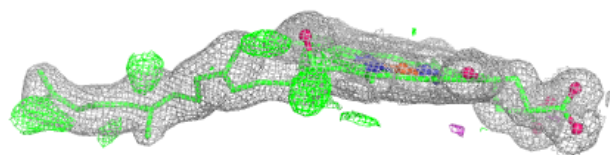
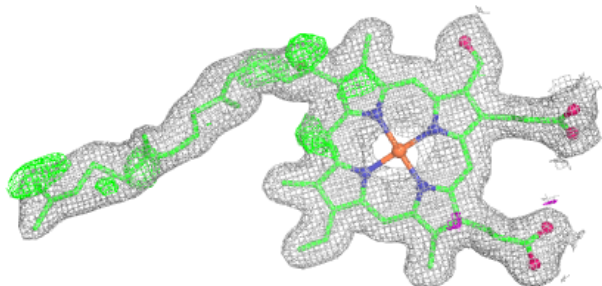


Electron density around HEA A 602 (B):

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

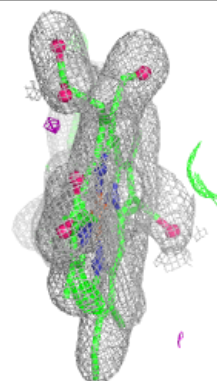
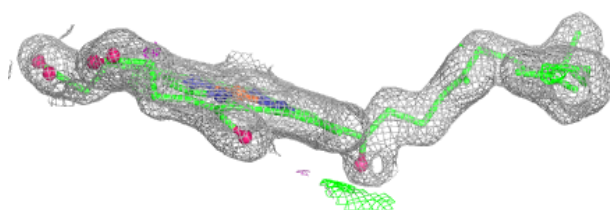
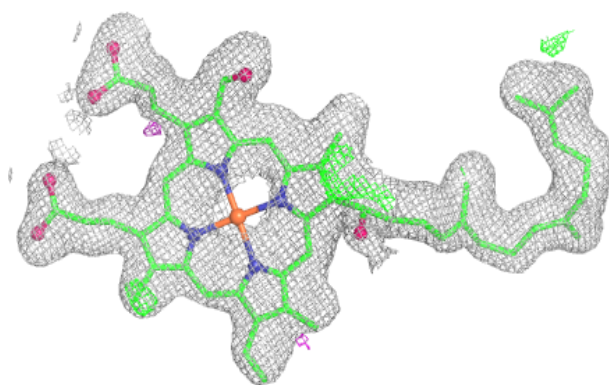
**Electron density around HEA N 602:**

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

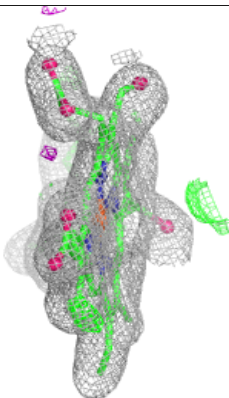
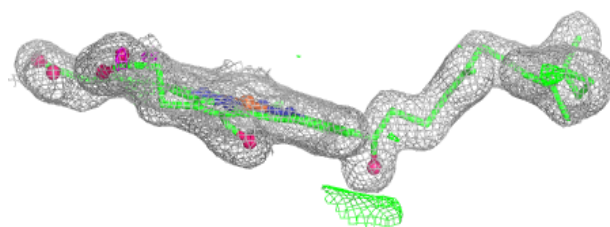
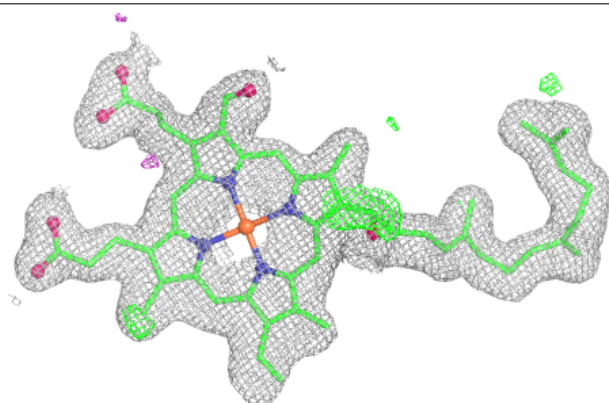


Electron density around HEA N 603 (A):

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

**Electron density around HEA N 603 (B):**

$2mF_o-DF_c$ (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.