Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2026 – 08:04 AM JST

PDB ID	:	8IJN / pdb_00008ijn
Title	:	Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-Bound Fully Reduced State at 100 K
Authors	:	Tsukihara, T.; Shimada, A.; Muramoto, K.
Deposited on	:	2023-02-27
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

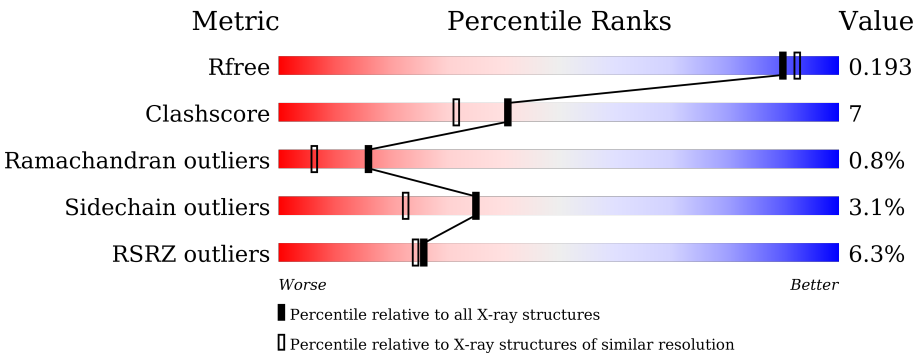
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 <=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	.% 89% 9% •
1	N	514	.% 90% 9% •
2	B	227	5% 83% 15% •
2	O	227	6% 78% 20% •
3	C	261	2% 90% 10% •
3	P	261	.% 89% 11% •

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Mol	Chain	Length	Quality of chain
4	D	147	4% 88% 9%
4	Q	147	12% 90% 8%
5	E	109	4% 91% 5%
5	R	109	4% 90% 5%
6	F	98	10% 87% 10%
6	S	98	9% 89% 7%
7	G	85	27% 76% 18%
7	T	85	24% 72% 16% 9%
8	H	85	15% 81% 8% 7%
8	U	85	18% 81% 8% 7%
9	I	73	11% 89% 10%
9	V	73	15% 86% 14%
10	J	59	8% 88% 10%
10	W	59	8% 90% 7%
11	K	56	7% 82% 5% 12%
11	X	56	12% 79% 7% 12%
12	L	47	6% 85% 13%
12	Y	47	9% 81% 13%
13	M	46	13% 72% 20% 7%
13	Z	46	15% 80% 9% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CDL	G	102	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 32780 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
			Total	C	N	O	S			
1	A	514	4072	2716	631	687	38	0	10	0
1	N	514	4072	2717	631	686	38	0	9	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1831	1191	281	341	18	0	2	0
2	O	227	1824	1185	281	340	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2116	1415	336	351	14	0	3	0
3	P	259	2110	1412	336	350	12	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

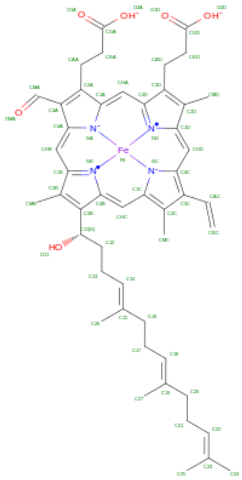
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	380	254	64	60	2	0	0	0

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

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

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

HEA



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

- Molecule 15 is NITRIC OXIDE (CCD ID: NO) (formula: NO).

NO

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

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

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

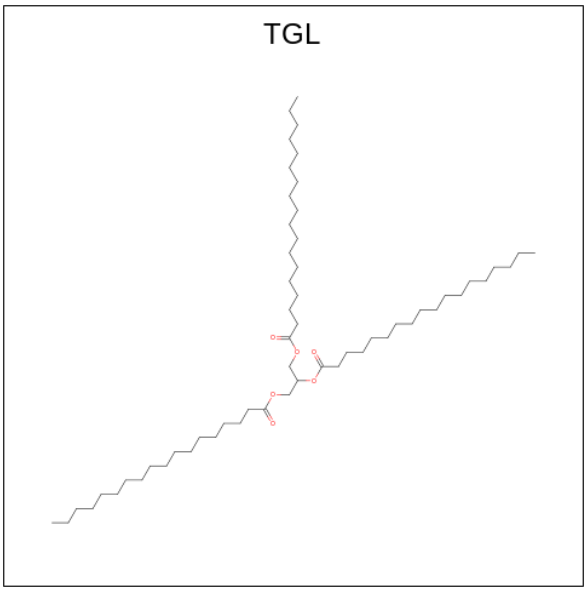
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

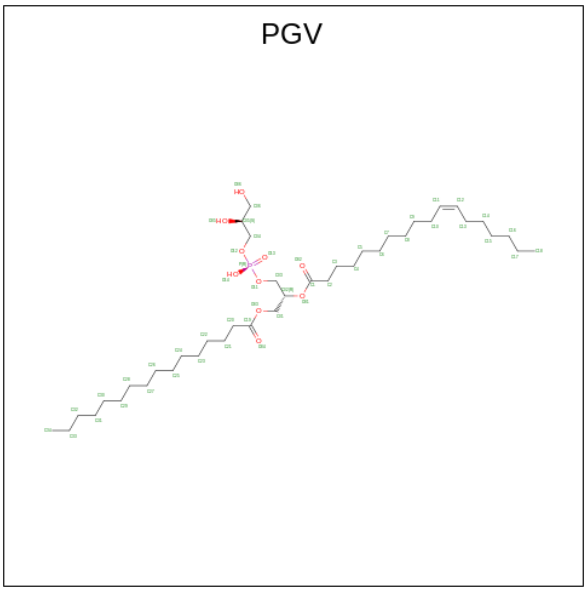
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



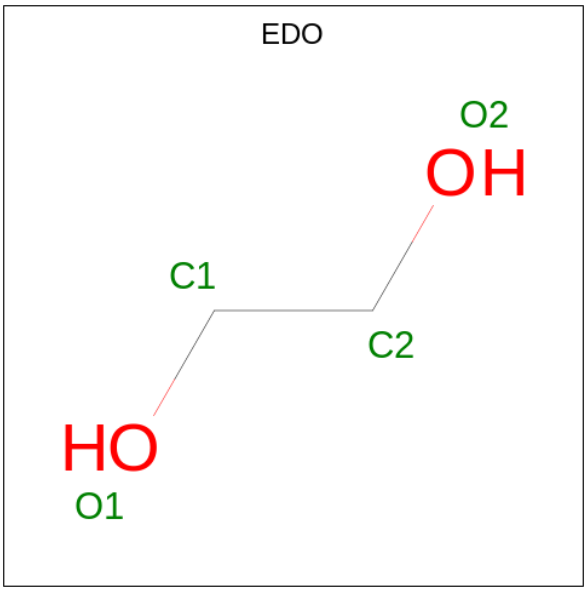
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	N	1	63	57	6	0	0
19	O	1	63	57	6	0	0
19	Q	1	63	57	6	0	0

- 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: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	A	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	C	1	51	40	10	1	0	0
			Total	C	O	P		
20	N	1	46	37	8	1	0	0
			Total	C	O	P		
20	N	1	51	40	10	1	0	0
			Total	C	O	P		
20	P	1	51	40	10	1	0	0
			Total	C	O	P		
20	P	1	51	40	10	1	0	0

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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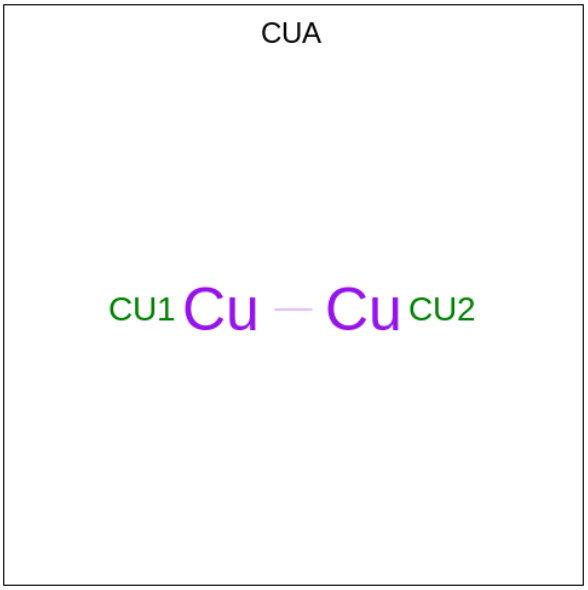
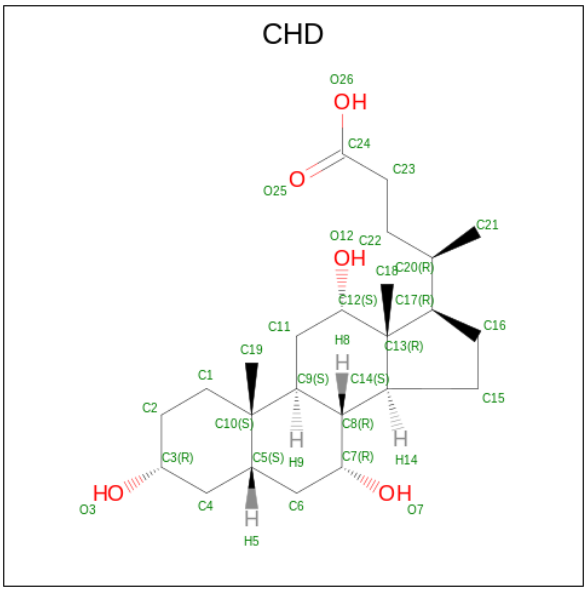
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	O	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	P	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	Q	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0
21	S	1	4	2	2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



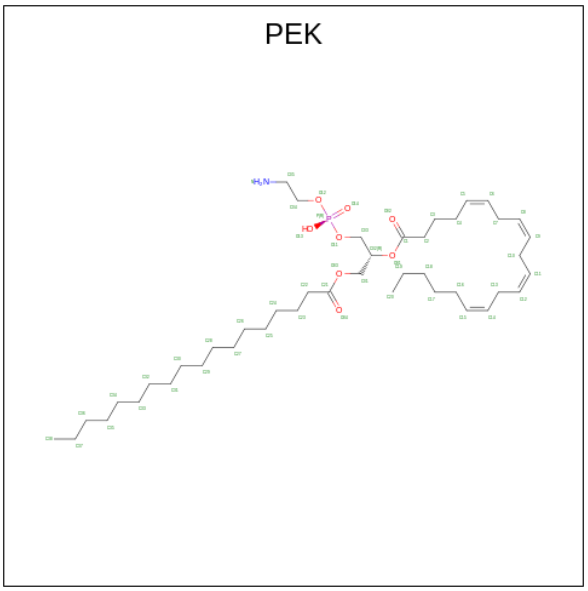
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
22	B	1	2	2	0	0
22	O	1	2	2	0	0

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



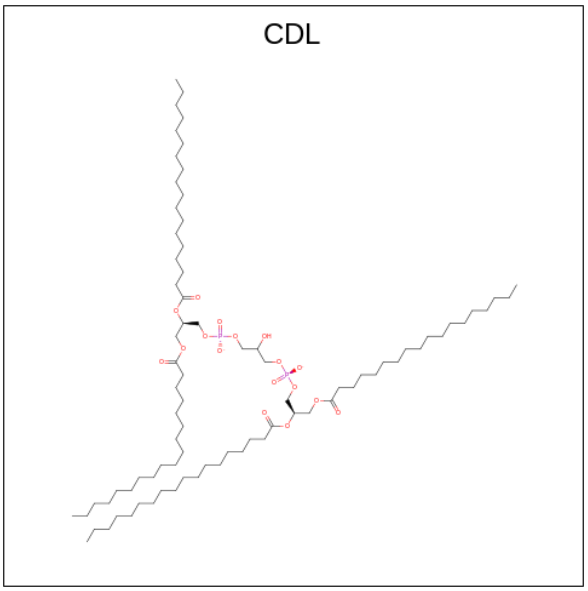
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
23	B	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	C	1	29	24	5		0	0
			Total	C	O			
23	J	1	29	24	5		0	0
			Total	C	O			
23	O	1	29	24	5		0	0
			Total	C	O			
23	P	1	29	24	5		0	0
			Total	C	O			
23	P	1	29	24	5		0	0
			Total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

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



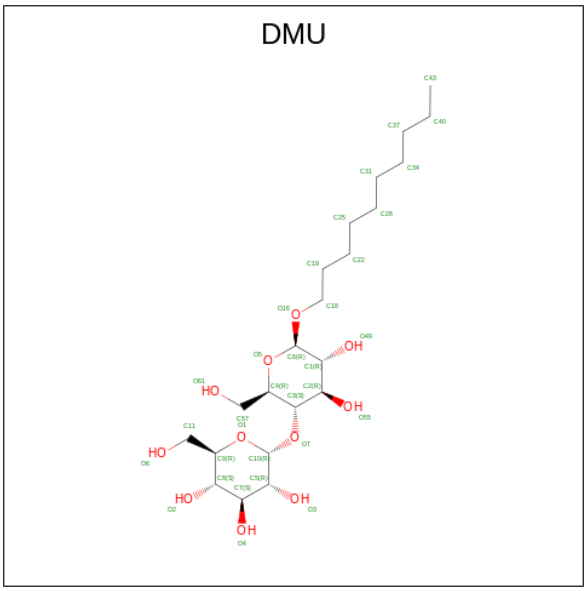
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C N O P 53 43 1 8 1	0	0
24	G	1	Total C O P 50 41 8 1	0	0
24	G	1	Total C N O P 53 43 1 8 1	0	0
24	P	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0
24	T	1	Total C N O P 53 43 1 8 1	0	0

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



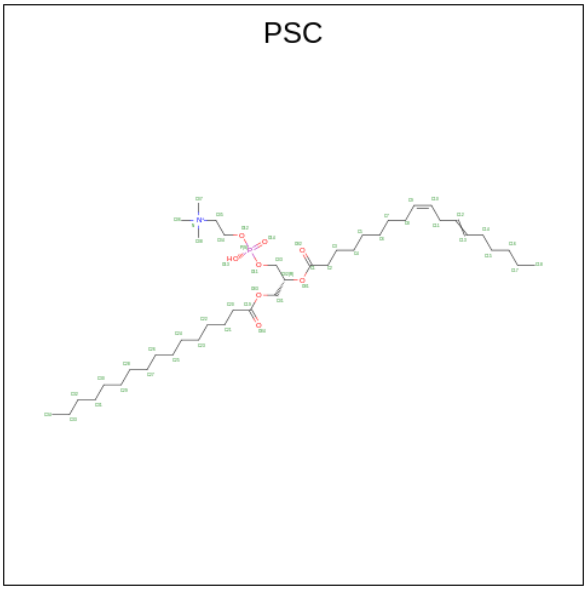
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
26	C	1	33	22	11		0	0
			Total	C	O			
26	M	1	33	22	11		0	0
			Total	C	O			
26	O	1	22	16	6		0	0
			Total	C	O			
26	P	1	33	22	11		0	0
			Total	C	O			
26	W	1	32	21	11		0	0
			Total	C	O			
26	Z	1	33	22	11		0	0

- Molecule 27 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
28	F	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
28	S	1	1	1	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	229	229	229	0	0
29	B	148	149	149	0	1
29	C	120	120	120	0	0
29	D	79	79	79	0	0
29	E	48	48	48	0	0
29	F	68	68	68	0	0
29	G	48	48	48	0	0
29	H	51	51	51	0	0
29	I	39	39	39	0	0
29	J	26	26	26	0	0
29	K	30	30	30	0	0
29	L	23	23	23	0	0
29	M	24	24	24	0	0
29	N	231	231	231	0	0
29	O	146	146	146	0	2
29	P	106	106	106	0	0
29	Q	59	59	59	0	0
29	R	55	55	55	0	0

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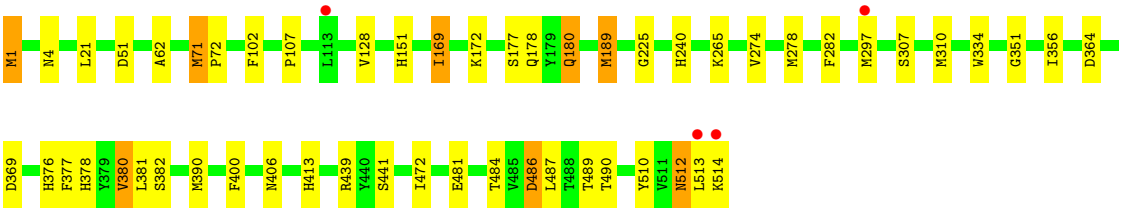
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	S	72	Total O 72 72	0	0
29	T	51	Total O 51 51	0	0
29	U	48	Total O 48 48	0	0
29	V	29	Total O 29 29	0	0
29	W	22	Total O 22 22	0	0
29	X	22	Total O 22 22	0	0
29	Y	17	Total O 17 17	0	0
29	Z	17	Total O 17 17	0	0

3 Residue-property plots (i)

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.

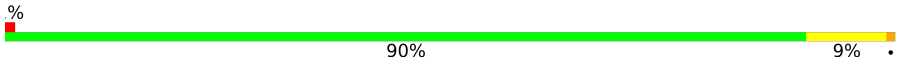
• Molecule 1: Cytochrome c oxidase subunit 1

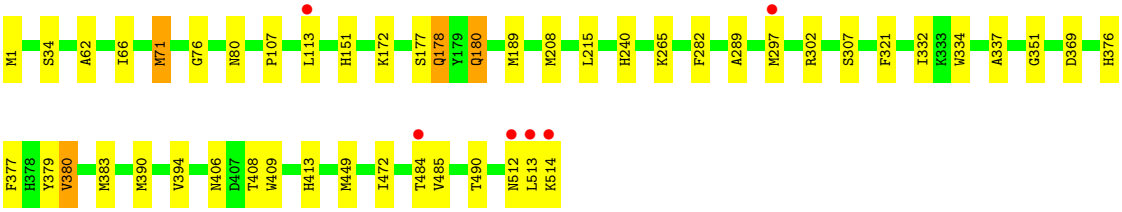
Chain A:



• Molecule 1: Cytochrome c oxidase subunit 1

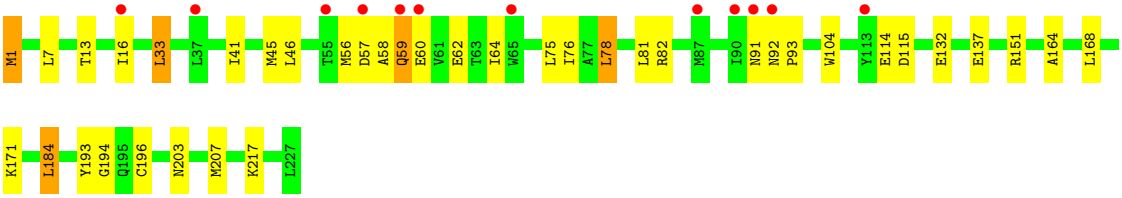
Chain N:





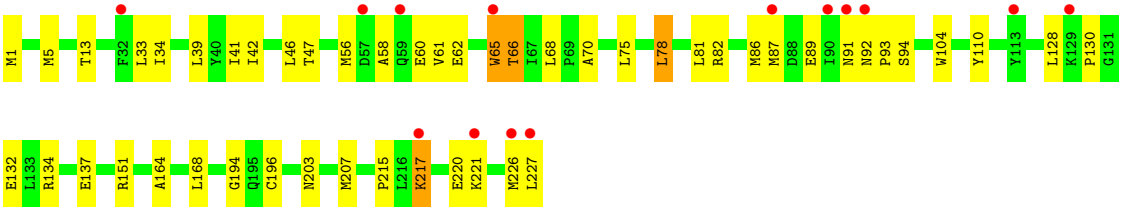
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

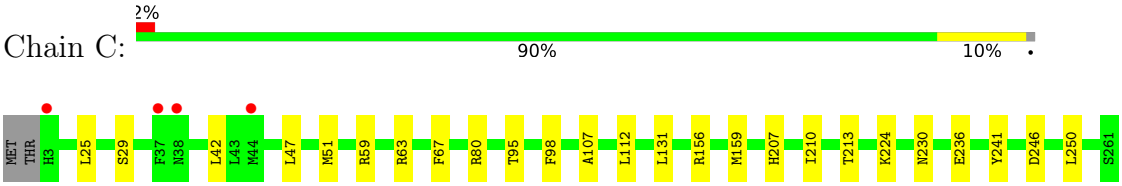


• Molecule 2: Cytochrome c oxidase subunit 2

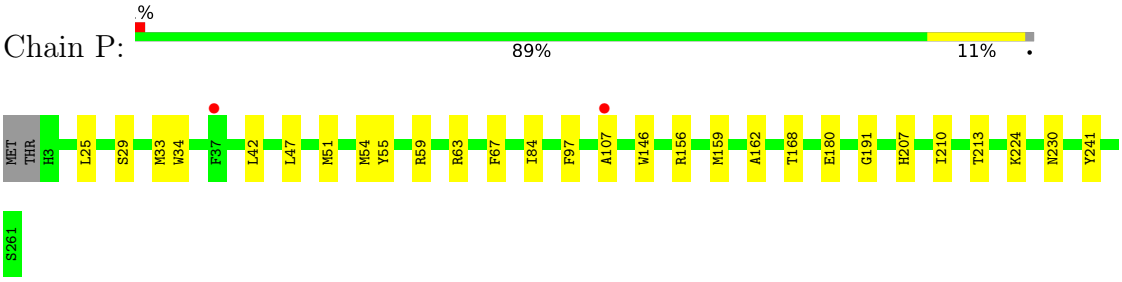
Chain O:



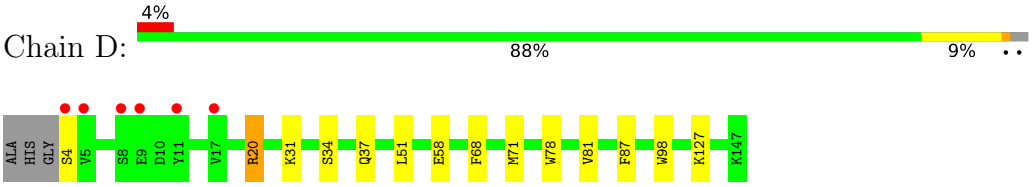
• Molecule 3: Cytochrome c oxidase subunit 3



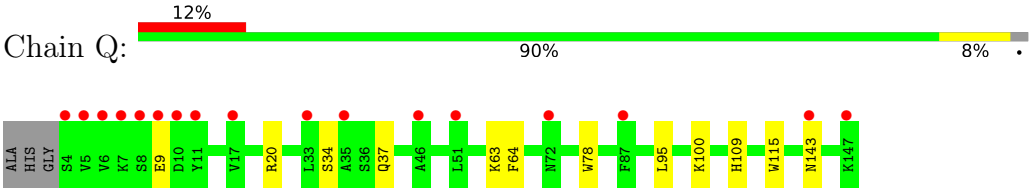
• Molecule 3: Cytochrome c oxidase subunit 3



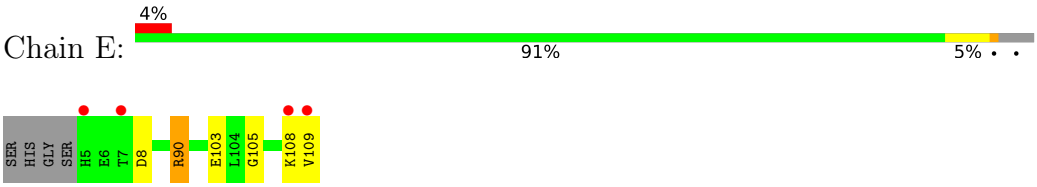
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



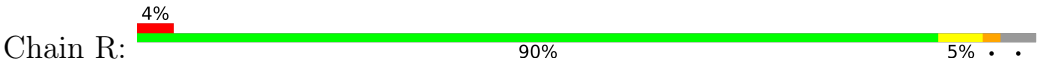
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

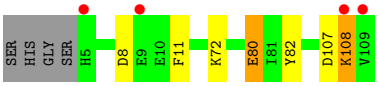


• Molecule 5: Cytochrome c oxidase subunit 5A



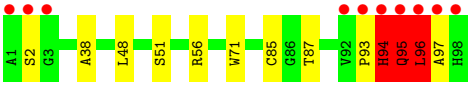
• Molecule 5: Cytochrome c oxidase subunit 5A





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

Chain F:

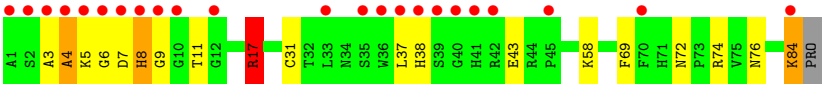


• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:

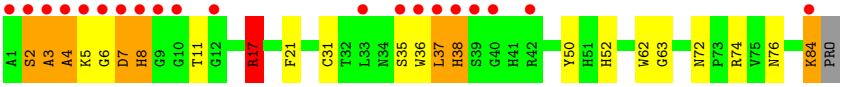
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



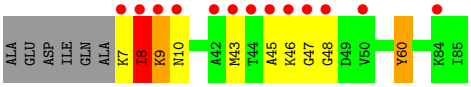
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



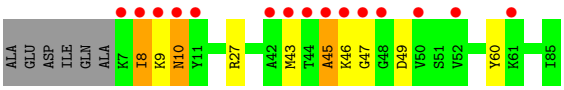
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



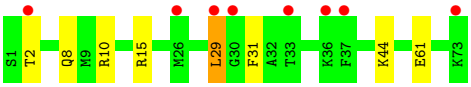
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



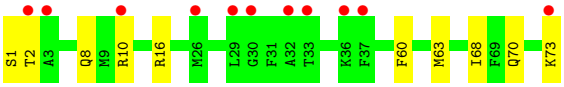
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



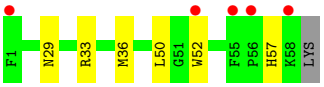
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



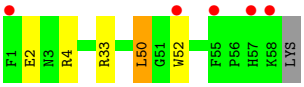
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



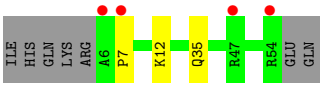
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



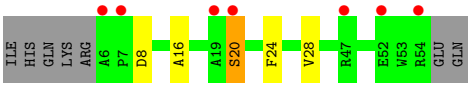
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



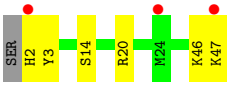
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



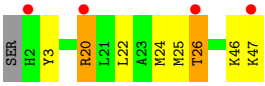
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



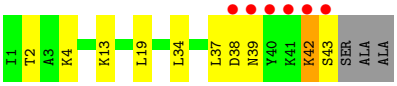
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



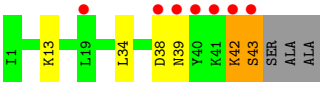
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.37 – 1.80 35.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.37-1.80) 99.6 (35.37-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.169 , 0.192 0.169 , 0.193	Depositor DCC
R_{free} test set	30652 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32780	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 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CU, NO, CUA, EDO, CHD, PGV, SAC, TGL, NA, TPO, PEK, DMU, CDL, ZN, MG, FME, PSC

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	1.08	2/4230 (0.0%)	0.92	4/5775 (0.1%)
1	N	0.90	1/4224 (0.0%)	0.85	2/5767 (0.0%)
2	B	0.96	0/1878	0.96	5/2558 (0.2%)
2	O	0.74	0/1860	0.86	1/2534 (0.0%)
3	C	0.87	0/2219	0.79	0/3033
3	P	0.80	0/2197	0.75	0/3005
4	D	0.78	0/1229	0.77	0/1658
4	Q	0.56	0/1229	0.63	0/1658
5	E	0.74	0/871	0.72	0/1182
5	R	0.59	0/871	0.67	0/1182
6	F	0.84	1/765 (0.1%)	0.87	0/1038
6	S	0.69	0/765	0.83	2/1038 (0.2%)
7	G	0.81	0/690	0.87	2/937 (0.2%)
7	T	0.73	0/690	0.85	2/937 (0.2%)
8	H	0.73	0/682	0.77	0/921
8	U	0.60	0/682	0.76	0/921
9	I	0.62	0/605	0.69	0/802
9	V	0.56	0/605	0.70	0/802
10	J	0.68	0/471	0.66	0/636
10	W	0.53	0/471	0.62	0/636
11	K	0.72	0/398	0.77	0/546
11	X	0.46	0/398	0.54	0/546
12	L	0.83	0/393	0.86	0/526
12	Y	0.63	0/393	0.64	0/526
13	M	0.81	0/345	0.71	0/470
13	Z	0.54	0/345	0.57	0/470
All	All	0.83	4/29506 (0.0%)	0.81	18/40104 (0.0%)

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

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	189	MET	CB-CG	5.52	1.69	1.52
1	A	439	ARG	CD-NE	5.46	1.53	1.46
6	F	56	ARG	CZ-NH1	5.32	1.40	1.32
1	A	512	ASN	CB-CG	-5.02	1.39	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	MET	CG-SD-CE	-11.39	75.84	100.90
1	N	71	MET	CG-SD-CE	-9.19	80.68	100.90
1	A	189	MET	CG-SD-CE	-7.36	84.72	100.90
1	A	240	HIS	CA-CB-CG	-6.87	106.93	113.80
7	T	17	ARG	NE-CZ-NH1	6.56	128.06	121.50
6	S	94	HIS	CA-C-N	6.22	133.43	121.54
6	S	94	HIS	C-N-CA	6.22	133.43	121.54
1	N	240	HIS	CA-CB-CG	-6.15	107.65	113.80
2	B	64	ILE	CA-C-N	-6.05	112.61	122.65
2	B	64	ILE	C-N-CA	-6.05	112.61	122.65
7	G	17	ARG	NE-CZ-NH2	-5.96	113.84	119.20
7	T	17	ARG	NE-CZ-NH2	-5.77	114.01	119.20
1	A	102	PHE	CA-CB-CG	-5.63	108.17	113.80
2	B	114	GLU	CA-C-N	-5.60	114.48	122.77
2	B	114	GLU	C-N-CA	-5.60	114.48	122.77
2	O	65	TRP	CA-CB-CG	5.28	123.63	113.60
7	G	17	ARG	NE-CZ-NH1	5.18	126.68	121.50
2	B	82	ARG	CG-CD-NE	-5.14	100.69	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	93	PRO	Peptide

5.2 Too-close contacts (i)

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	4072	0	4041	45	0
1	N	4072	0	4044	47	0
2	B	1831	0	1839	25	0
2	O	1824	0	1833	34	0
3	C	2116	0	2034	26	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	10	0
5	E	852	0	845	3	0
5	R	852	0	845	5	1
6	F	748	0	728	7	0
6	S	748	0	728	12	0
7	G	675	0	643	18	0
7	T	675	0	643	28	0
8	H	662	0	623	7	0
8	U	662	0	623	6	0
9	I	601	0	613	5	1
9	V	601	0	613	7	0
10	J	460	0	459	4	0
10	W	460	0	459	4	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	7	0
12	Y	380	0	380	8	0
13	M	335	0	352	6	0
13	Z	335	0	352	2	0
14	A	120	0	108	5	0
14	N	120	0	108	5	0
15	A	2	0	0	0	0
15	N	2	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	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	8	0
19	L	63	0	110	8	0
19	N	63	0	110	8	0
19	O	63	0	110	0	0
19	Q	63	0	110	9	0
20	A	102	0	152	4	0
20	C	102	0	152	9	0
20	N	97	0	145	5	0
20	P	102	0	152	6	0
21	A	16	0	24	1	0
21	B	4	0	6	0	0
21	C	4	0	6	0	0
21	F	4	0	6	0	0
21	N	24	0	36	2	0
21	O	8	0	12	0	0
21	P	8	0	12	1	0
21	Q	8	0	12	0	0
21	S	12	0	18	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	38	2	0
23	O	29	0	39	2	0
23	P	58	0	78	1	0
23	W	29	0	38	1	0
24	C	53	0	77	6	0
24	G	103	0	148	5	0
24	P	53	0	77	6	0
24	T	106	0	154	10	0
25	C	100	0	153	15	0
25	G	100	0	156	23	0
25	P	100	0	156	19	0
25	T	100	0	156	14	0
26	C	33	0	42	2	0
26	M	33	0	42	1	0
26	O	22	0	31	1	0
26	P	33	0	42	8	0
26	W	32	0	36	4	0
26	Z	33	0	42	1	0
27	E	52	0	80	12	0
27	R	52	0	80	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	229	0	0	2	0
29	B	149	0	0	3	0
29	C	120	0	0	1	0
29	D	79	0	0	1	0
29	E	48	0	0	0	0
29	F	68	0	0	1	0
29	G	48	0	0	1	0
29	H	51	0	0	0	0
29	I	39	0	0	2	0
29	J	26	0	0	0	0
29	K	30	0	0	1	0
29	L	23	0	0	0	0
29	M	24	0	0	0	0
29	N	231	0	0	4	0
29	O	146	0	0	1	0
29	P	106	0	0	2	0
29	Q	59	0	0	2	0
29	R	55	0	0	1	0
29	S	72	0	0	1	0
29	T	51	0	0	0	0
29	U	48	0	0	1	0
29	V	29	0	0	0	0
29	W	22	0	0	1	0
29	X	22	0	0	2	0
29	Y	17	0	0	1	0
29	Z	17	0	0	0	0
All	All	32780	0	31593	408	1

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 7.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CD2	6:S:95:GLN:H	1.72	1.05
21:N:614:EDO:O2	29:N:701:HOH:O	1.80	0.99
6:S:94:HIS:NE2	29:S:201:HOH:O	1.97	0.96
7:T:17:ARG:HH22	24:T:101:PEK:H041	1.27	0.96
6:S:94:HIS:HD2	6:S:95:GLN:H	1.09	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HD12	25:T:103:CDL:H351	1.53	0.88
7:G:72:ASN:H	7:G:76:ASN:HD22	1.20	0.88
7:T:72:ASN:H	7:T:76:ASN:HD22	1.22	0.87
25:G:102:CDL:H782	25:G:102:CDL:H561	1.58	0.86
1:N:406:ASN:HD21	20:N:608:PGV:H21	1.41	0.85
6:F:85:CYS:SG	6:F:87:THR:HG23	2.16	0.85
1:N:332:ILE:H	21:N:615:EDO:H12	1.41	0.84
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.59	0.82
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.44	0.82
12:L:20:ARG:NH2	19:L:101:TGL:HC32	1.96	0.80
24:P:302:PEK:H71	24:P:302:PEK:H32	1.64	0.80
25:C:305:CDL:H231	25:C:305:CDL:H661	1.64	0.80
3:P:67:PHE:HE1	25:P:305:CDL:H1	1.46	0.78
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.66	0.77
25:G:102:CDL:H511	25:G:102:CDL:H201	1.65	0.76
3:P:34:TRP:HE1	26:P:307:DMU:H29	1.51	0.75
3:C:210:ILE:HG12	20:C:303:PGV:H132	1.69	0.75
24:P:302:PEK:HN2	7:T:76:ASN:HD21	1.34	0.74
7:G:38:HIS:CE1	25:G:102:CDL:H111	2.23	0.73
29:N:867:HOH:O	2:O:87:MET:SD	2.47	0.73
25:G:102:CDL:H451	2:O:70:ALA:HB1	1.70	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.71
25:G:102:CDL:H351	2:O:81:LEU:HD12	1.72	0.71
7:G:84:LYS:H	7:G:84:LYS:HD2	1.54	0.71
6:S:52:ILE:O	6:S:94:HIS:CE1	2.43	0.71
7:G:17:ARG:HD2	29:O:429:HOH:O	1.91	0.70
19:N:607:TGL:HC32	12:Y:20:ARG:HH21	1.55	0.69
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.37	0.69
3:P:34:TRP:NE1	26:P:307:DMU:H29	2.07	0.69
6:S:94:HIS:HD2	6:S:95:GLN:N	1.89	0.68
29:B:413:HOH:O	7:T:17:ARG:HD2	1.95	0.67
25:G:102:CDL:H352	2:O:78:LEU:HD12	1.75	0.67
19:L:101:TGL:H231	19:L:101:TGL:HA92	1.75	0.67
7:T:17:ARG:NH2	24:T:101:PEK:H041	2.06	0.67
25:P:305:CDL:H341	25:P:305:CDL:H162	1.76	0.67
12:L:46:LYS:O	12:L:47:LYS:HB2	1.95	0.66
3:P:54:MET:HE3	25:P:305:CDL:H612	1.77	0.66
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.77	0.66
3:C:51[B]:MET:HE2	25:C:305:CDL:H621	1.77	0.66
13:M:39:ASN:O	13:M:43:SER:OG	2.07	0.66
4:D:20:ARG:HG3	29:D:350:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:42:ILE:HG21	19:Q:201:TGL:H231	1.78	0.65
1:N:177:SER:H	1:N:180:GLN:NE2	1.96	0.64
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.80	0.63
7:G:37:LEU:HD11	25:G:102:CDL:H361	1.79	0.63
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.63
3:P:63:ARG:HE	25:P:305:CDL:HA22	1.62	0.63
4:D:34:SER:H	4:D:37:GLN:NE2	1.96	0.63
20:A:609:PGV:H22	20:A:609:PGV:H011	1.80	0.63
7:T:5:LYS:HD2	24:T:102:PEK:H371	1.81	0.63
27:E:201:PSC:H072	9:I:10:ARG:HH21	1.64	0.62
6:F:51:SER:O	6:F:94:HIS:N	2.32	0.62
27:R:201:PSC:H071	9:V:10:ARG:HH21	1.64	0.62
27:R:201:PSC:C07	9:V:10:ARG:HH21	2.13	0.62
3:C:210:ILE:HD13	20:C:303:PGV:H301	1.81	0.62
2:O:13:THR:HB	2:O:168:LEU:HD23	1.81	0.62
3:C:224:LYS:CD	25:C:305:CDL:HB32	2.30	0.62
26:P:307:DMU:H30	7:T:62:TRP:HB3	1.80	0.62
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.62
20:A:609:PGV:H311	13:M:19:LEU:HD23	1.80	0.61
25:G:102:CDL:H531	25:G:102:CDL:H222	1.82	0.61
1:A:51:ASP:OD1	1:A:441:SER:OG	2.15	0.61
2:B:78:LEU:HD12	25:T:103:CDL:H352	1.81	0.61
1:N:472:ILE:HG21	19:N:607:TGL:HA91	1.83	0.61
19:N:607:TGL:HA62	12:Y:25:MET:HG2	1.82	0.60
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.67	0.60
1:A:472:ILE:HG21	19:L:101:TGL:HA91	1.84	0.60
1:A:377:PHE:HA	1:A:380[B]:VAL:HG22	1.84	0.60
20:C:303:PGV:H172	25:C:305:CDL:H662	1.84	0.59
4:D:78:TRP:CA	19:D:201:TGL:HB22	2.32	0.59
19:A:607:TGL:HA92	19:A:607:TGL:H252	1.84	0.59
26:W:102:DMU:O55	29:W:201:HOH:O	2.17	0.59
27:R:201:PSC:H142	27:R:201:PSC:H343	1.84	0.59
13:Z:39:ASN:O	13:Z:43:SER:OG	2.15	0.59
1:A:334:TRP:CZ3	19:D:201:TGL:HA52	2.38	0.58
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.39	0.58
1:N:151:HIS:CD2	24:P:302:PEK:H382	2.39	0.58
7:G:5:LYS:HD2	24:G:103:PEK:H371	1.84	0.58
10:W:50:LEU:HG	26:W:102:DMU:H18	1.86	0.58
2:O:66:THR:HG21	23:O:302:CHD:H3	1.86	0.58
6:S:85:CYS:SG	6:S:87:THR:HG23	2.44	0.58
12:L:2:HIS:CG	12:L:3:TYR:H	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:224:LYS:HD3	25:P:305:CDL:HB31	1.86	0.57
10:W:52:TRP:CD2	26:W:102:DMU:H1	2.29	0.57
4:D:34:SER:H	4:D:37:GLN:HE21	1.52	0.57
4:D:78:TRP:HA	19:D:201:TGL:HB22	1.86	0.57
1:A:334:TRP:CE3	19:D:201:TGL:HA31	2.40	0.57
25:G:102:CDL:H112	25:G:102:CDL:H1	1.87	0.57
20:N:608:PGV:H151	20:N:608:PGV:H321	1.85	0.56
2:B:56:MET:HA	27:E:201:PSC:H202	1.86	0.56
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.87	0.56
1:N:1:FME:HE2	12:Y:3:TYR:HE1	1.71	0.56
7:G:31:CYS:SG	25:G:102:CDL:H551	2.46	0.56
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.87	0.56
11:X:16:ALA:O	11:X:20:SER:OG	2.24	0.55
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.55
10:W:33:ARG:HG2	23:W:101:CHD:H151	1.88	0.55
2:B:41:ILE:HD13	27:E:201:PSC:C34	2.37	0.55
3:C:246:ASP:HB2	29:C:500:HOH:O	2.07	0.55
25:P:305:CDL:H242	25:P:305:CDL:H661	1.89	0.55
6:S:94:HIS:CD2	6:S:95:GLN:N	2.58	0.55
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.05	0.54
7:T:2:SER:O	24:T:102:PEK:H331	2.08	0.54
10:J:33:ARG:HG2	23:J:101:CHD:H151	1.89	0.54
26:P:307:DMU:H40	7:T:63:GLY:H	1.71	0.54
3:P:34:TRP:CE2	26:P:307:DMU:H29	2.43	0.54
27:E:201:PSC:C07	9:I:10:ARG:HH21	2.21	0.53
3:P:34:TRP:CZ2	26:P:307:DMU:H29	2.44	0.53
3:P:63:ARG:HE	25:P:305:CDL:CA2	2.22	0.53
27:E:201:PSC:O14	27:E:201:PSC:H062	2.07	0.53
1:A:514:LYS:NZ	29:A:703:HOH:O	2.41	0.53
6:F:94:HIS:O	6:F:95:GLN:HB2	2.09	0.53
25:T:103:CDL:H1	25:T:103:CDL:H111	1.91	0.53
20:C:304:PGV:H62	20:C:304:PGV:H22	1.90	0.53
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.90	0.53
12:L:20:ARG:HH22	19:L:101:TGL:HC61	1.74	0.53
7:T:31:CYS:SG	25:T:103:CDL:H551	2.49	0.53
19:A:607:TGL:H111	19:A:607:TGL:H283	1.91	0.52
3:C:224:LYS:HD3	25:C:305:CDL:HB32	1.90	0.52
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.90	0.52
3:P:67:PHE:CE1	25:P:305:CDL:H1	2.36	0.52
6:S:52:ILE:O	6:S:94:HIS:ND1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:21:PHE:CD2	24:T:101:PEK:H222	2.44	0.52
3:P:210:ILE:HG12	20:P:303:PGV:H132	1.90	0.52
20:A:609:PGV:H152	4:D:87:PHE:CZ	2.45	0.52
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.92	0.52
1:A:307:SER:HB3	25:T:103:CDL:H171	1.90	0.52
3:P:224:LYS:HD3	25:P:305:CDL:CB3	2.40	0.52
8:U:45:ALA:O	8:U:47:GLY:N	2.43	0.52
3:C:59:ARG:HA	25:C:305:CDL:H512	1.92	0.52
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.35	0.52
3:P:33:MET:HE1	3:P:42:LEU:H	1.75	0.52
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.91	0.52
1:A:278:MET:SD	7:T:5:LYS:HB3	2.50	0.52
27:E:201:PSC:H142	27:E:201:PSC:H343	1.90	0.52
2:O:89:GLU:O	2:O:91:ASN:ND2	2.43	0.52
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.46	0.51
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.40	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	2.01	0.51
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.51
20:N:608:PGV:H011	20:N:608:PGV:H22	1.91	0.51
4:Q:78:TRP:HA	19:Q:201:TGL:HB22	1.93	0.51
3:P:59:ARG:HA	25:P:305:CDL:H512	1.92	0.51
3:P:67:PHE:HE1	25:P:305:CDL:C1	2.19	0.51
3:P:168:THR:HG22	24:T:101:PEK:H14	1.92	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.51
1:A:310:MET:HE3	1:A:356:ILE:HG23	1.92	0.51
7:G:9:GLY:HA3	1:N:178:GLN:HE21	1.75	0.51
7:T:8:HIS:ND1	24:T:102:PEK:H312	2.26	0.50
2:O:39:LEU:CD1	19:Q:201:TGL:H232	2.41	0.50
29:N:863:HOH:O	4:Q:20:ARG:HG3	2.11	0.50
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.94	0.50
2:O:62:GLU:O	2:O:66:THR:HB	2.12	0.50
1:A:484:THR:HB	13:M:2:THR:OG1	2.12	0.49
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.94	0.49
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.46	0.49
3:P:47:LEU:O	3:P:51:MET:HG2	2.12	0.49
9:I:44:LYS:HE2	29:I:135:HOH:O	2.13	0.49
25:G:102:CDL:H322	25:G:102:CDL:HA62	1.94	0.49
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.93	0.49
7:T:38:HIS:HE2	25:T:103:CDL:H111	1.77	0.49
19:A:607:TGL:HC81	2:B:7:LEU:HD11	1.94	0.49
4:D:127:LYS:HD2	29:I:131:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:210:ILE:HD13	20:P:303:PGV:H301	1.95	0.49
4:Q:109:HIS:HD2	29:Q:337:HOH:O	1.95	0.49
2:O:47:THR:HB	19:Q:201:TGL:H332	1.94	0.49
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.78	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.49
4:Q:95:LEU:HD22	26:Z:101:DMU:H13	1.95	0.49
19:Q:201:TGL:HA91	19:Q:201:TGL:H242	1.94	0.49
2:B:78:LEU:CD1	25:T:103:CDL:H352	2.43	0.48
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.95	0.48
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.48
20:P:303:PGV:H172	25:P:305:CDL:H652	1.95	0.48
24:C:302:PEK:H221	7:G:69:PHE:CG	2.48	0.48
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.77	0.48
12:L:14:SER:H	19:L:101:TGL:HC31	1.79	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.48
8:H:45:ALA:O	8:H:47:GLY:N	2.45	0.48
6:S:94:HIS:O	6:S:95:GLN:HB2	2.12	0.48
3:C:213:THR:HG23	25:C:305:CDL:H771	1.95	0.48
25:G:102:CDL:C54	25:G:102:CDL:H241	2.43	0.48
1:N:1:FME:HE2	12:Y:3:TYR:CE1	2.48	0.48
25:T:103:CDL:H582	25:T:103:CDL:H552	1.53	0.48
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.12	0.48
2:O:56:MET:HA	27:R:201:PSC:H202	1.95	0.48
3:P:33:MET:HG3	26:W:102:DMU:H7	1.96	0.48
20:C:304:PGV:H161	25:T:103:CDL:H612	1.94	0.47
8:H:43:MET:HE3	8:H:48:GLY:HA3	1.95	0.47
8:H:45:ALA:C	8:H:47:GLY:H	2.21	0.47
10:J:29:ASN:HD22	10:J:29:ASN:H	1.60	0.47
11:K:7:PRO:O	11:K:12:LYS:HE3	2.13	0.47
19:Q:201:TGL:H361	9:V:16:ARG:HE	1.79	0.47
2:B:57:ASP:H	27:E:201:PSC:H202	1.78	0.47
8:H:43:MET:HE1	8:U:43:MET:HE1	1.96	0.47
21:P:308:EDO:H21	29:P:476:HOH:O	2.12	0.47
1:A:151:HIS:CD2	24:C:302:PEK:H382	2.49	0.47
19:N:607:TGL:HA92	19:N:607:TGL:H231	1.96	0.47
25:G:102:CDL:H182	1:N:307:SER:HB3	1.95	0.47
21:A:613:EDO:H21	2:B:59:GLN:HE21	1.78	0.47
19:D:201:TGL:H201	19:D:201:TGL:H231	1.60	0.47
19:N:607:TGL:H362	29:Y:117:HOH:O	2.15	0.47
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.47
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:103:CDL:H431	25:T:103:CDL:H402	1.80	0.47
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.29	0.47
1:A:274:VAL:HG12	1:A:278:MET:HE2	1.96	0.47
23:O:302:CHD:H12	23:O:302:CHD:H212	1.96	0.47
8:U:43:MET:HE3	8:U:49:ASP:N	2.29	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.47
1:N:302[B]:ARG:HH22	2:O:87:MET:HE1	1.80	0.47
7:T:7:ASP:OD1	7:T:8:HIS:N	2.48	0.47
3:C:67:PHE:HE1	25:C:305:CDL:C1	2.29	0.46
27:R:201:PSC:H063	27:R:201:PSC:H042	1.66	0.46
10:W:2:GLU:HB2	10:W:4:ARG:NH1	2.30	0.46
24:C:302:PEK:H221	7:G:69:PHE:CD2	2.51	0.46
3:P:156:ARG:HE	23:P:306:CHD:C24	2.26	0.46
19:Q:201:TGL:H351	9:V:16:ARG:HH21	1.81	0.46
3:C:95:THR:HG21	20:C:304:PGV:H302	1.98	0.46
24:C:302:PEK:H161	24:C:302:PEK:H102	1.97	0.46
1:N:513:LEU:O	1:N:514:LYS:HB2	2.16	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.98	0.46
7:G:8:HIS:CD2	24:G:103:PEK:H252	2.50	0.46
7:T:84:LYS:HD2	7:T:84:LYS:H	1.80	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
1:N:113:LEU:HD12	19:N:607:TGL:H141	1.98	0.46
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.46
24:P:302:PEK:H271	24:P:302:PEK:H6	1.98	0.46
12:L:2:HIS:CG	12:L:3:TYR:N	2.83	0.46
24:G:101:PEK:H383	25:G:102:CDL:H271	1.98	0.45
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.80	0.45
1:A:382[B]:SER:OG	14:A:601:HEA:H121	2.15	0.45
25:C:305:CDL:H401	25:C:305:CDL:H371	1.53	0.45
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	1.98	0.45
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.51	0.45
3:P:213:THR:HG23	25:P:305:CDL:H762	1.98	0.45
3:P:224:LYS:CD	25:P:305:CDL:HB31	2.45	0.45
24:P:302:PEK:H12	24:P:302:PEK:H242	1.99	0.45
4:Q:100:LYS:HE2	29:Q:332:HOH:O	2.15	0.45
25:G:102:CDL:H241	25:G:102:CDL:H542	1.99	0.45
6:S:94:HIS:CG	6:S:95:GLN:H	2.22	0.45
3:C:156:ARG:HE	23:C:306:CHD:C24	2.28	0.45
4:Q:78:TRP:CA	19:Q:201:TGL:HB22	2.46	0.45
8:U:27:ARG:HG2	29:U:143:HOH:O	2.16	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HZ	25:T:103:CDL:H761	1.81	0.45
1:N:334:TRP:CZ3	19:Q:201:TGL:HA51	2.51	0.45
9:V:73:LYS:HD2	9:V:73:LYS:HA	1.87	0.45
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.16	0.45
3:C:67:PHE:HE1	25:C:305:CDL:H1	1.82	0.45
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.99	0.45
3:P:55:TYR:CE1	25:P:305:CDL:H161	2.52	0.45
1:A:21:LEU:HD23	19:L:101:TGL:H211	1.97	0.45
1:A:484:THR:HG22	29:A:909:HOH:O	2.17	0.45
5:E:8:ASP:HA	27:E:201:PSC:H071	1.99	0.45
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.99	0.45
25:G:102:CDL:H252	25:G:102:CDL:H221	1.87	0.45
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.98	0.45
26:P:307:DMU:H36	7:T:62:TRP:HB2	1.98	0.45
2:O:227:LEU:HD23	2:O:227:LEU:HA	1.70	0.45
5:R:108:LYS:O	5:R:108:LYS:HG2	2.17	0.45
7:T:35:SER:C	7:T:37:LEU:H	2.25	0.45
11:X:8:ASP:HB3	29:X:119:HOH:O	2.17	0.45
13:Z:42:LYS:HA	13:Z:42:LYS:HD2	1.67	0.44
8:H:9:LYS:O	8:H:10:ASN:HB2	2.17	0.44
2:O:34:ILE:HA	26:O:304:DMU:H25	1.99	0.44
2:O:41:ILE:HD13	27:R:201:PSC:H342	1.99	0.44
3:C:63:ARG:HH21	25:C:305:CDL:HA22	1.82	0.44
3:C:207:HIS:HD2	3:C:241:TYR:OH	2.00	0.44
11:K:35:GLN:NE2	29:K:101:HOH:O	2.49	0.44
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.17	0.44
1:A:169:ILE:CD1	1:A:189:MET:HE1	2.47	0.44
14:A:601:HEA:HMC3	14:A:601:HEA:HBC1	1.98	0.44
25:P:305:CDL:H532	25:P:305:CDL:H561	1.74	0.44
1:N:321:PHE:CD1	2:O:65:TRP:HB2	2.53	0.44
8:U:43:MET:HE3	8:U:49:ASP:H	1.81	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.00	0.44
3:C:250:LEU:HD22	25:G:102:CDL:H662	1.99	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.85	0.44
25:P:305:CDL:H412	25:P:305:CDL:H382	1.72	0.44
26:C:307:DMU:H1	7:G:69:PHE:HZ	1.83	0.44
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.53	0.44
8:U:9:LYS:O	8:U:10:ASN:HB2	2.18	0.44
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.44
6:F:94:HIS:HE1	29:F:229:HOH:O	2.01	0.44
1:N:321:PHE:CD2	27:R:201:PSC:H341	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:102:PEK:O04	24:T:102:PEK:H242	2.17	0.44
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.99	0.44
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.18	0.43
3:C:80:ARG:NH2	3:C:236:GLU:OE1	2.47	0.43
2:B:93:PRO:HG3	2:B:151:ARG:HB2	2.00	0.43
3:C:156:ARG:NE	23:C:306:CHD:O26	2.46	0.43
4:D:98:TRP:CE2	26:M:101:DMU:H11	2.53	0.43
5:E:105:GLY:O	5:E:108:LYS:HG2	2.18	0.43
26:C:307:DMU:O1	26:C:307:DMU:H29	2.18	0.43
8:H:7:LYS:O	8:H:8:ILE:HG22	2.19	0.43
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.01	0.43
1:A:351:GLY:C	1:A:380[A]:VAL:HG13	2.44	0.43
24:C:302:PEK:H101	24:C:302:PEK:H71	1.82	0.43
3:C:47:LEU:O	3:C:51[B]:MET:HG3	2.18	0.43
13:M:42:LYS:HD2	13:M:42:LYS:HA	1.49	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.59	0.43
19:N:607:TGL:HC51	19:N:607:TGL:OC1	2.18	0.43
20:P:304:PGV:H21	20:P:304:PGV:H51	1.75	0.43
26:P:307:DMU:H40	7:T:63:GLY:N	2.33	0.43
7:T:37:LEU:HD21	25:T:103:CDL:H361	1.99	0.43
2:B:56:MET:HG2	27:E:201:PSC:H211	2.01	0.43
11:X:8:ASP:HB2	29:X:107:HOH:O	2.17	0.43
1:A:278:MET:HB3	7:T:5:LYS:HD3	2.01	0.43
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.84	0.43
23:B:302:CHD:H212	23:B:302:CHD:H12	2.01	0.42
25:G:102:CDL:H552	25:G:102:CDL:H582	1.20	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.96	0.42
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.17	0.42
24:G:103:PEK:H21	3:P:84:ILE:HG12	2.01	0.42
1:N:66:ILE:O	1:N:71:MET:HG3	2.19	0.42
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.62	0.42
3:C:131:LEU:HD21	25:G:102:CDL:HB61	2.00	0.42
20:P:304:PGV:H272	20:P:304:PGV:H241	1.87	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.42
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.68	0.42
1:A:378:HIS:HA	1:A:382[A]:SER:OG	2.19	0.42
3:C:107:ALA:HB2	20:C:304:PGV:H031	2.01	0.42
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	2.02	0.42
27:R:201:PSC:O14	29:R:301:HOH:O	2.22	0.42
11:X:24:PHE:O	11:X:28:VAL:HG12	2.20	0.42
12:Y:22:LEU:O	12:Y:26:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:MET:SD	27:E:201:PSC:H301	2.60	0.42
25:G:102:CDL:H201	25:G:102:CDL:C51	2.44	0.42
1:N:408:THR:CG2	20:N:608:PGV:H52	2.50	0.42
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.54	0.42
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.49	0.42
23:C:301:CHD:H3	25:T:103:CDL:OB3	2.20	0.42
25:C:305:CDL:H461	25:C:305:CDL:H421	2.02	0.42
1:N:380[B]:VAL:HG21	14:N:602:HEA:C3C	2.50	0.42
25:P:305:CDL:H161	25:P:305:CDL:H131	1.94	0.42
1:A:71:MET:HB3	1:A:71:MET:HE2	1.93	0.42
1:A:381[A]:LEU:HB2	14:A:602:HEA:CAC	2.50	0.42
2:B:1:FME:HCN	2:B:193:TYR:H	1.85	0.42
1:N:376:HIS:O	1:N:380[A]:VAL:HG22	2.20	0.42
25:C:305:CDL:H522	25:C:305:CDL:OB9	2.20	0.42
4:D:81:VAL:HG11	19:D:201:TGL:HB52	2.01	0.42
3:P:33:MET:CE	3:P:42:LEU:H	2.32	0.42
3:P:107:ALA:HB2	20:P:304:PGV:H031	2.02	0.42
25:C:305:CDL:H772	25:C:305:CDL:H651	2.01	0.41
25:G:102:CDL:H531	25:G:102:CDL:H241	2.02	0.41
3:P:29:SER:HB3	29:P:496:HOH:O	2.20	0.41
7:T:5:LYS:HG3	24:T:102:PEK:H383	2.01	0.41
1:A:486:ASP:HB3	1:A:487:LEU:HG	2.02	0.41
1:N:215:LEU:HD11	24:P:302:PEK:H272	2.01	0.41
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.51	0.41
3:C:98:PHE:CD2	24:T:102:PEK:H182	2.55	0.41
19:D:201:TGL:H331	19:D:201:TGL:H172	1.89	0.41
5:R:11:PHE:CG	27:R:201:PSC:H073	2.55	0.41
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.50	0.41
25:G:102:CDL:H782	25:G:102:CDL:C56	2.37	0.41
7:T:38:HIS:CE1	25:T:103:CDL:H122	2.56	0.41
5:E:90:ARG:NH2	5:E:103:GLU:OE2	2.54	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.55	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.41
5:R:8:ASP:OD1	27:R:201:PSC:H081	2.20	0.41
5:R:107:ASP:OD2	5:R:107:ASP:N	2.54	0.41
7:T:3:ALA:O	7:T:4:ALA:HB2	2.20	0.41
2:O:217:LYS:O	2:O:221:LYS:HG3	2.19	0.41
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.56	0.41
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.56	0.41
1:N:409:TRP:CZ2	20:N:608:PGV:H81	2.56	0.41
1:A:376:HIS:O	1:A:380[A]:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:102:CDL:H182	1:N:307:SER:CB	2.50	0.41
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.51	0.41
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.36	0.41
25:P:305:CDL:H652	25:P:305:CDL:H621	1.72	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.41
20:C:303:PGV:H161	20:C:303:PGV:C12	2.51	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.03	0.41
2:B:41:ILE:HG21	27:E:201:PSC:H342	2.03	0.40
29:B:413:HOH:O	7:T:17:ARG:CD	2.63	0.40
7:G:58:LYS:NZ	29:G:202:HOH:O	2.53	0.40
10:J:36:MET:HG2	23:J:101:CHD:H221	2.03	0.40
1:A:364:ASP:OD2	14:A:602:HEA:O1A	2.39	0.40
3:C:51[A]:MET:HE1	20:C:303:PGV:H141	2.03	0.40
4:D:68:PHE:HA	4:D:71:MET:HE3	2.02	0.40
29:N:813:HOH:O	3:P:191:GLY:HA3	2.21	0.40
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.56	0.40
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.56	0.40
1:A:406:ASN:HD21	20:A:609:PGV:C2	2.35	0.40
2:B:41:ILE:HD13	27:E:201:PSC:H342	2.02	0.40
9:I:29:LEU:HA	9:I:29:LEU:HD12	1.79	0.40
1:N:71:MET:HB3	1:N:71:MET:HE2	1.77	0.40
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.51	0.40
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.40
1:A:400:PHE:HB3	19:L:101:TGL:H283	2.03	0.40
2:B:16:ILE:HG13	29:B:535:HOH:O	2.20	0.40
1:N:380[B]:VAL:HG21	14:N:602:HEA:C4C	2.51	0.40
19:N:607:TGL:H211	19:N:607:TGL:HA81	1.78	0.40
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.03	0.40
1:A:489:THR:HA	6:F:71:TRP:O	2.22	0.40
2:B:13:THR:HB	2:B:168:LEU:HD23	2.03	0.40
6:F:96:LEU:HB3	6:F:97:ALA:H	1.64	0.40
7:G:8:HIS:ND1	24:G:103:PEK:H312	2.37	0.40

All (1) 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)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/514 (102%)	509 (98%)	13 (2%)	0	100	100
1	N	521/514 (101%)	509 (98%)	12 (2%)	0	100	100
2	B	227/227 (100%)	222 (98%)	4 (2%)	1 (0%)	30	19
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	14	5
3	C	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	2 (2%)	4 (4%)	2	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	0
8	U	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3528/3614 (98%)	3410 (97%)	91 (3%)	27 (1%)	16	6

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
2	O	60	GLU
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	H	8	ILE
8	H	46	LYS
8	U	10	ASN
8	U	46	LYS
6	F	96	LEU
7	G	6	GLY
7	G	8	HIS
8	U	8	ILE
8	U	45	ALA
2	B	92	ASN
7	G	3	ALA
6	S	96	LEU
7	T	3	ALA
8	H	9	LYS
7	T	6	GLY
2	O	92	ASN

5.3.2 Protein sidechains (i)

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	435/426 (102%)	427 (98%)	8 (2%)	51	43
1	N	434/426 (102%)	426 (98%)	8 (2%)	51	43
2	B	212/210 (101%)	202 (95%)	10 (5%)	23	11
2	O	210/210 (100%)	200 (95%)	10 (5%)	23	11
3	C	227/226 (100%)	225 (99%)	2 (1%)	70	67
3	P	224/226 (99%)	221 (99%)	3 (1%)	61	54
4	D	128/129 (99%)	123 (96%)	5 (4%)	28	16
4	Q	128/129 (99%)	126 (98%)	2 (2%)	55	47
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	34
5	R	92/95 (97%)	90 (98%)	2 (2%)	45	34
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	10
6	S	81/81 (100%)	78 (96%)	3 (4%)	30	18
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	26
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	26
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	4
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	9
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	38
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	28
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	9
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3062/3082 (99%)	2967 (97%)	95 (3%)	35	23

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	169	ILE
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	297	MET
1	A	369	ASP
1	A	380[A]	VAL
1	A	380[B]	VAL
1	A	486	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
2	B	184	LEU
2	B	217	LYS
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	20	ARG
4	D	31	LYS
4	D	51	LEU
4	D	58	GLU
5	E	90	ARG
5	E	109	VAL
6	F	48	LEU
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	17	ARG
7	G	43	GLU
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
9	I	61	GLU
10	J	50	LEU
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP

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Mol	Chain	Res	Type
13	M	42	LYS
1	N	178	GLN
1	N	180	GLN
1	N	369	ASP
1	N	380[A]	VAL
1	N	380[B]	VAL
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	110	TYR
2	O	217	LYS
2	O	226	MET
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	9	GLU
4	Q	143	ASN
5	R	80	GLU
5	R	108	LYS
6	S	37	LYS
6	S	80	GLN
6	S	96	LEU
7	T	2	SER
7	T	17	ARG
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	70	GLN
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	20	SER
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
1	A	512	ASN
2	B	181	GLN
3	C	3	HIS
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	119	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
7	G	34	ASN
7	G	76	ASN
8	H	31	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	170	ASN
1	N	178	GLN
1	N	180	GLN
1	N	422	ASN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN

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Mol	Chain	Res	Type
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	94	HIS
7	T	76	ASN
8	U	28	ASN
8	U	32	ASN
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.55	0	7,9,11	1.84	1 (14%)
2	FME	O	1	2	8,9,10	1.25	2 (25%)	7,9,11	4.10	2 (28%)
2	FME	B	1	2	8,9,10	2.14	3 (37%)	7,9,11	3.73	4 (57%)
1	FME	N	1	1	8,9,10	0.48	0	7,9,11	1.29	0
7	TPO	T	11	7	8,10,11	1.61	2 (25%)	10,14,16	1.34	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	SAC	I	1	9	7,8,9	0.57	0	8,9,11	0.76	0
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	1.81	2 (25%)
7	TPO	G	11	7	8,10,11	1.55	2 (25%)	10,14,16	1.37	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	4/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	5/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
9	SAC	V	1	9	-	6/7/8/10	-
7	TPO	G	11	7	-	3/9/11/13	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	4.01	1.52	1.46
2	B	1	FME	CN-N	3.66	1.45	1.33
7	T	11	TPO	P-O1P	2.94	1.60	1.50
7	G	11	TPO	P-O1P	2.94	1.60	1.50
2	O	1	FME	O1-CN	-2.54	1.15	1.22
7	T	11	TPO	P-OG1	2.40	1.63	1.59
7	G	11	TPO	P-OG1	2.08	1.63	1.59
2	B	1	FME	CG-SD	-2.06	1.70	1.81
2	O	1	FME	CG-SD	-2.03	1.70	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	FME	CA-N-CN	-10.11	107.27	122.82
2	B	1	FME	C-CA-N	7.67	123.58	109.73
2	B	1	FME	CA-N-CN	-3.91	116.80	122.82
7	G	11	TPO	CG2-CB-CA	3.73	120.52	113.16
2	B	1	FME	CG-CB-CA	-3.59	102.96	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	C-CA-N	3.52	116.08	109.73
7	T	11	TPO	CG2-CB-CA	3.45	119.98	113.16
2	O	1	FME	CG-CB-CA	-3.27	103.86	112.95
1	A	1	FME	CA-N-CN	-3.00	118.21	122.82
2	B	1	FME	O1-CN-N	-2.99	117.39	125.27
9	V	1	SAC	O-C-CA	-2.80	117.43	124.78

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	N-CA-CB-OG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
2	O	1	FME	CB-CA-N-CN
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
1	N	1	FME	CA-CB-CG-SD
9	I	1	SAC	OAC-C1A-N-CA
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	1	0
1	N	1	FME	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 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	$\#\|Z\| > 2$
21	EDO	B	303	-	3,3,3	0.73	0	2,2,2	0.55	0
14	HEA	A	602	1,15	66,67,67	1.93	20 (30%)	78,103,103	2.09	31 (39%)
21	EDO	S	103	-	3,3,3	0.55	0	2,2,2	0.55	0
22	CUA	O	301	2	0,1,1	-	-	-		
23	CHD	B	302	-	32,32,32	0.92	1 (3%)	51,51,51	1.51	11 (21%)
26	DMU	O	304	-	22,22,34	0.74	0	27,27,45	1.73	6 (22%)
20	PGV	N	609	-	50,50,50	1.05	3 (6%)	53,56,56	1.12	4 (7%)
23	CHD	P	301	-	32,32,32	1.00	2 (6%)	51,51,51	1.38	7 (13%)
21	EDO	S	102	-	3,3,3	1.09	0	2,2,2	0.62	0
20	PGV	A	608	-	50,50,50	1.02	6 (12%)	53,56,56	1.23	5 (9%)
14	HEA	N	601	1	66,67,67	1.79	18 (27%)	78,103,103	1.88	25 (32%)
20	PGV	C	303	-	50,50,50	0.89	2 (4%)	53,56,56	1.11	5 (9%)
23	CHD	O	302	-	32,32,32	1.00	1 (3%)	51,51,51	1.48	6 (11%)
21	EDO	Q	203	-	3,3,3	0.17	0	2,2,2	0.81	0
25	CDL	C	305	3	99,99,99	1.35	13 (13%)	105,111,111	1.56	13 (12%)
14	HEA	N	602	1,15	66,67,67	1.78	22 (33%)	78,103,103	1.79	24 (30%)
26	DMU	P	307	-	34,34,34	0.87	1 (2%)	45,45,45	2.03	11 (24%)
21	EDO	Q	202	-	3,3,3	0.36	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PEK	G	101	-	49,49,52	1.09	3 (6%)	53,54,57	1.32	4 (7%)
20	PGV	P	304	-	50,50,50	1.03	2 (4%)	53,56,56	1.44	6 (11%)
26	DMU	M	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.96	2 (4%)
19	TGL	O	303	-	62,62,62	1.06	3 (4%)	65,65,65	1.16	4 (6%)
21	EDO	C	308	-	3,3,3	0.34	0	2,2,2	0.92	0
23	CHD	J	101	-	32,32,32	0.70	0	51,51,51	1.83	13 (25%)
26	DMU	Z	101	-	34,34,34	0.43	0	45,45,45	0.84	1 (2%)
24	PEK	P	302	-	52,52,52	0.74	1 (1%)	55,57,57	1.67	5 (9%)
24	PEK	G	103	-	52,52,52	1.03	2 (3%)	55,57,57	1.49	5 (9%)
20	PGV	P	303	-	50,50,50	0.71	1 (2%)	53,56,56	1.13	7 (13%)
19	TGL	N	607	-	62,62,62	1.14	3 (4%)	65,65,65	1.33	11 (16%)
21	EDO	N	612	-	3,3,3	0.47	0	2,2,2	0.27	0
25	CDL	G	102	-	99,99,99	1.35	12 (12%)	105,111,111	1.49	12 (11%)
26	DMU	C	307	-	34,34,34	0.77	1 (2%)	45,45,45	1.64	10 (22%)
15	NO	A	603	14,16	0,1,1	-	-	-		
26	DMU	W	102	-	33,33,34	0.86	1 (3%)	44,44,45	2.36	17 (38%)
19	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	0.98	3 (4%)
21	EDO	A	610	-	3,3,3	1.09	0	2,2,2	0.88	0
14	HEA	A	601	1	66,67,67	1.80	19 (28%)	78,103,103	2.00	20 (25%)
21	EDO	A	611	-	3,3,3	0.92	0	2,2,2	0.70	0
21	EDO	N	610	-	3,3,3	0.79	0	2,2,2	0.50	0
21	EDO	N	615	-	3,3,3	0.64	0	2,2,2	0.27	0
21	EDO	P	309	-	3,3,3	0.79	0	2,2,2	0.39	0
23	CHD	P	306	-	32,32,32	0.64	0	51,51,51	1.25	3 (5%)
25	CDL	P	305	-	99,99,99	1.36	13 (13%)	105,111,111	1.61	14 (13%)
25	CDL	T	103	-	99,99,99	1.31	12 (12%)	105,111,111	1.48	10 (9%)
21	EDO	A	613	-	3,3,3	0.48	0	2,2,2	0.30	0
15	NO	N	603	14,16	0,1,1	-	-	-		
20	PGV	C	304	-	50,50,50	1.00	2 (4%)	53,56,56	1.46	6 (11%)
21	EDO	O	305	-	3,3,3	0.90	0	2,2,2	0.25	0
21	EDO	N	614	-	3,3,3	0.71	0	2,2,2	0.47	0
27	PSC	E	201	-	51,51,51	1.08	3 (5%)	57,59,59	1.20	4 (7%)
21	EDO	O	306	-	3,3,3	0.53	0	2,2,2	0.13	0
21	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.27	0
21	EDO	S	104	-	3,3,3	0.66	0	2,2,2	0.36	0
19	TGL	L	101	-	62,62,62	1.16	3 (4%)	65,65,65	1.67	10 (15%)
19	TGL	D	201	-	62,62,62	1.11	4 (6%)	65,65,65	1.02	4 (6%)
23	CHD	C	301	-	32,32,32	0.96	2 (6%)	51,51,51	1.61	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PEK	C	302	-	52,52,52	0.83	3 (5%)	55,57,57	1.47	10 (18%)
21	EDO	N	613	-	3,3,3	0.46	0	2,2,2	0.59	0
21	EDO	N	611	-	3,3,3	0.73	0	2,2,2	0.83	0
19	TGL	A	607	-	62,62,62	1.06	3 (4%)	65,65,65	1.14	6 (9%)
24	PEK	T	101	-	52,52,52	1.06	2 (3%)	55,57,57	1.30	5 (9%)
27	PSC	R	201	-	51,51,51	1.13	3 (5%)	57,59,59	1.20	5 (8%)
24	PEK	T	102	-	52,52,52	1.02	2 (3%)	55,57,57	1.67	6 (10%)
20	PGV	N	608	-	45,45,50	1.06	2 (4%)	49,50,56	1.53	9 (18%)
23	CHD	C	306	-	32,32,32	0.63	0	51,51,51	1.18	6 (11%)
23	CHD	W	101	-	32,32,32	0.69	0	51,51,51	1.98	14 (27%)
21	EDO	F	102	-	3,3,3	0.99	0	2,2,2	0.65	0
22	CUA	B	301	2	0,1,1	-	-	-		
20	PGV	A	609	-	50,50,50	1.00	2 (4%)	53,56,56	1.23	6 (11%)
21	EDO	P	308	-	3,3,3	0.48	0	2,2,2	0.69	0

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
21	EDO	B	303	-	-	0/1/1/1	-
14	HEA	A	602	1,15	-	5/36/76/76	-
21	EDO	S	103	-	-	0/1/1/1	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
26	DMU	O	304	-	-	6/13/33/59	0/1/1/2
20	PGV	N	609	-	-	8/55/55/55	-
23	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	S	102	-	-	0/1/1/1	-
20	PGV	A	608	-	-	8/55/55/55	-
14	HEA	N	601	1	-	7/36/76/76	-
20	PGV	C	303	-	-	6/55/55/55	-
23	CHD	O	302	-	-	2/9/74/74	0/4/4/4
21	EDO	Q	203	-	-	0/1/1/1	-
25	CDL	C	305	3	-	48/110/110/110	-
14	HEA	N	602	1,15	-	5/36/76/76	-
26	DMU	P	307	-	-	10/19/59/59	0/2/2/2
21	EDO	Q	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	G	101	-	-	25/51/51/56	-
20	PGV	P	304	-	-	18/55/55/55	-
26	DMU	M	101	-	-	6/19/59/59	0/2/2/2
19	TGL	O	303	-	-	33/65/65/65	-
21	EDO	C	308	-	-	1/1/1/1	-
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
26	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	PEK	P	302	-	-	19/56/56/56	-
24	PEK	G	103	-	-	24/56/56/56	-
20	PGV	P	303	-	-	9/55/55/55	-
19	TGL	N	607	-	-	33/65/65/65	-
21	EDO	N	612	-	-	0/1/1/1	-
25	CDL	G	102	-	-	50/110/110/110	-
26	DMU	C	307	-	-	7/19/59/59	0/2/2/2
26	DMU	W	102	-	-	5/18/58/59	0/2/2/2
19	TGL	Q	201	-	-	26/65/65/65	-
21	EDO	A	610	-	-	0/1/1/1	-
14	HEA	A	601	1	-	7/36/76/76	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	P	309	-	-	0/1/1/1	-
23	CHD	P	306	-	-	2/9/74/74	0/4/4/4
25	CDL	P	305	-	-	58/110/110/110	-
25	CDL	T	103	-	-	48/110/110/110	-
21	EDO	A	613	-	-	0/1/1/1	-
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
27	PSC	E	201	-	-	32/55/55/55	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
19	TGL	L	101	-	-	29/65/65/65	-
19	TGL	D	201	-	-	30/65/65/65	-
23	CHD	C	301	-	-	1/9/74/74	0/4/4/4
24	PEK	C	302	-	-	15/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
19	TGL	A	607	-	-	33/65/65/65	-
24	PEK	T	101	-	-	36/56/56/56	-
27	PSC	R	201	-	-	23/55/55/55	-
24	PEK	T	102	-	-	25/56/56/56	-
20	PGV	N	608	-	-	20/47/47/55	-
23	CHD	C	306	-	-	4/9/74/74	0/4/4/4
23	CHD	W	101	-	-	6/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
20	PGV	A	609	-	-	19/55/55/55	-
21	EDO	P	308	-	-	1/1/1/1	-

All (197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	607	TGL	OG2-CB1	5.33	1.49	1.34
19	L	101	TGL	OG2-CB1	5.22	1.49	1.34
24	T	101	PEK	O03-C21	5.15	1.48	1.33
20	P	304	PGV	O01-C1	5.11	1.48	1.34
14	N	601	HEA	CHA-C1A	5.07	1.48	1.38
24	G	101	PEK	O03-C21	4.82	1.47	1.33
25	C	305	CDL	OB8-CB7	4.80	1.47	1.33
24	G	103	PEK	O03-C21	4.80	1.47	1.33
19	L	101	TGL	OG3-CC1	4.80	1.47	1.33
20	A	609	PGV	O03-C19	4.78	1.47	1.33
24	G	103	PEK	O01-C1	4.76	1.47	1.34
25	G	102	CDL	OA8-CA7	4.75	1.47	1.33
24	T	102	PEK	O03-C21	4.72	1.47	1.33
25	G	102	CDL	OA6-CA5	4.66	1.47	1.34
19	N	607	TGL	OG1-CA1	4.61	1.46	1.33
25	G	102	CDL	OB6-CB5	4.60	1.47	1.34
19	A	607	TGL	OG2-CB1	4.58	1.47	1.34
19	O	303	TGL	OG3-CC1	4.57	1.46	1.33
20	N	608	PGV	O03-C19	4.56	1.46	1.33
20	C	304	PGV	O01-C1	4.54	1.47	1.34
19	A	607	TGL	OG1-CA1	4.54	1.46	1.33
25	P	305	CDL	OB8-CB7	4.53	1.46	1.33
25	P	305	CDL	OA8-CA7	4.53	1.46	1.33
19	Q	201	TGL	OG1-CA1	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	101	PEK	O01-C1	4.51	1.47	1.34
27	R	201	PSC	O01-C1	4.50	1.47	1.34
19	A	607	TGL	OG3-CC1	4.50	1.46	1.33
25	P	305	CDL	OA6-CA5	4.49	1.47	1.34
25	G	102	CDL	OB8-CB7	4.47	1.46	1.33
19	O	303	TGL	OG2-CB1	4.46	1.46	1.34
25	T	103	CDL	OA6-CA5	4.43	1.46	1.34
19	O	303	TGL	OG1-CA1	4.40	1.46	1.33
24	T	102	PEK	O01-C1	4.39	1.46	1.34
19	N	607	TGL	OG3-CC1	4.39	1.46	1.33
25	T	103	CDL	OB8-CB7	4.37	1.46	1.33
25	C	305	CDL	OA8-CA7	4.37	1.46	1.33
25	T	103	CDL	OA8-CA7	4.29	1.45	1.33
25	T	103	CDL	OB6-CB5	4.23	1.46	1.34
27	E	201	PSC	O01-C1	4.22	1.46	1.34
19	D	201	TGL	OG1-CA1	4.21	1.45	1.33
19	Q	201	TGL	OG2-CB1	4.20	1.46	1.34
20	C	304	PGV	O03-C19	4.17	1.45	1.33
19	L	101	TGL	OG1-CA1	4.16	1.45	1.33
20	N	608	PGV	O01-C1	4.14	1.46	1.34
24	T	101	PEK	O01-C1	4.14	1.46	1.34
20	A	609	PGV	O01-C1	4.12	1.45	1.34
14	N	601	HEA	C1A-C2A	-4.05	1.38	1.45
19	D	201	TGL	OG2-CB1	4.03	1.45	1.34
14	N	602	HEA	CHD-C1D	4.01	1.46	1.38
20	P	304	PGV	O03-C19	4.00	1.45	1.33
14	A	601	HEA	C1A-C2A	-3.95	1.38	1.45
27	R	201	PSC	C13-C12	3.87	1.54	1.31
14	A	602	HEA	CHA-C4D	3.85	1.48	1.39
14	A	602	HEA	C4A-NA	-3.84	1.32	1.39
19	Q	201	TGL	OG3-CC1	3.81	1.44	1.33
25	C	305	CDL	OA6-CA5	3.80	1.45	1.34
27	R	201	PSC	O03-C19	3.80	1.44	1.33
27	E	201	PSC	O03-C19	3.74	1.44	1.33
14	A	601	HEA	C4A-NA	-3.71	1.32	1.39
14	A	601	HEA	C1D-ND	-3.69	1.33	1.40
24	P	302	PEK	O03-C21	3.69	1.44	1.33
19	D	201	TGL	OB1-CB1	3.68	1.33	1.22
14	A	602	HEA	O11-C11	3.67	1.50	1.42
20	N	609	PGV	O03-C19	3.67	1.44	1.33
27	E	201	PSC	C13-C12	3.65	1.53	1.31
26	P	307	DMU	O16-C6	3.65	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4C-NC	-3.61	1.32	1.39
14	N	602	HEA	CHC-C4B	3.57	1.45	1.38
14	A	602	HEA	CHB-C4A	3.57	1.45	1.38
20	N	609	PGV	O01-C1	3.56	1.44	1.34
14	A	601	HEA	CHD-C1D	3.56	1.45	1.38
14	A	602	HEA	CHD-C1D	3.56	1.45	1.38
19	D	201	TGL	OG3-CC1	3.55	1.43	1.33
25	P	305	CDL	C59-C58	-3.54	1.31	1.51
14	A	602	HEA	C1A-C2A	-3.53	1.38	1.45
14	A	601	HEA	C4C-NC	-3.51	1.33	1.39
25	C	305	CDL	C59-C58	-3.49	1.32	1.51
25	C	305	CDL	C79-C78	-3.48	1.32	1.51
25	C	305	CDL	OB6-CB5	3.48	1.44	1.34
25	G	102	CDL	C59-C58	-3.47	1.32	1.51
14	A	602	HEA	CMC-C2C	3.46	1.58	1.50
25	P	305	CDL	C82-C81	-3.43	1.32	1.51
25	P	305	CDL	C79-C78	-3.43	1.32	1.51
25	C	305	CDL	C82-C81	-3.40	1.32	1.51
25	P	305	CDL	C19-C18	-3.40	1.32	1.51
14	N	601	HEA	C4B-NB	-3.40	1.34	1.40
25	G	102	CDL	C62-C61	-3.36	1.32	1.51
25	T	103	CDL	C59-C58	-3.33	1.32	1.51
25	P	305	CDL	C22-C21	-3.32	1.33	1.51
25	P	305	CDL	C62-C61	-3.29	1.33	1.51
25	T	103	CDL	C82-C81	-3.27	1.33	1.51
25	T	103	CDL	C62-C61	-3.26	1.33	1.51
14	N	601	HEA	C3A-C4A	-3.23	1.40	1.46
14	A	601	HEA	CHC-C4B	3.22	1.45	1.38
25	G	102	CDL	C19-C18	-3.22	1.33	1.51
25	P	305	CDL	OB6-CB5	3.21	1.43	1.34
25	C	305	CDL	C62-C61	-3.21	1.33	1.51
14	A	602	HEA	C4D-C3D	-3.20	1.39	1.45
25	G	102	CDL	C82-C81	-3.19	1.33	1.51
14	A	601	HEA	CHA-C1A	3.18	1.44	1.38
25	T	103	CDL	C39-C38	-3.15	1.33	1.51
25	T	103	CDL	C79-C78	-3.13	1.34	1.51
25	G	102	CDL	C22-C21	-3.13	1.34	1.51
14	N	602	HEA	CHA-C1A	3.13	1.44	1.38
25	C	305	CDL	C22-C21	-3.12	1.34	1.51
25	C	305	CDL	C42-C41	-3.10	1.34	1.51
14	N	601	HEA	CHC-C4B	3.08	1.44	1.38
25	C	305	CDL	C19-C18	-3.08	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	103	CDL	C22-C21	-3.08	1.34	1.51
25	G	102	CDL	C79-C78	-3.07	1.34	1.51
14	N	601	HEA	C4B-C3B	-3.04	1.39	1.44
25	P	305	CDL	C39-C38	-3.03	1.34	1.51
25	G	102	CDL	C42-C41	-3.03	1.34	1.51
25	T	103	CDL	C19-C18	-3.02	1.34	1.51
25	T	103	CDL	C42-C41	-3.02	1.34	1.51
26	W	102	DMU	O16-C6	3.01	1.45	1.40
14	N	602	HEA	C4D-C3D	-3.01	1.39	1.45
25	P	305	CDL	C42-C41	-2.99	1.34	1.51
14	N	602	HEA	CHB-C4A	2.98	1.44	1.38
25	G	102	CDL	C39-C38	-2.98	1.34	1.51
14	A	601	HEA	CHB-C1B	2.94	1.45	1.39
25	C	305	CDL	C39-C38	-2.94	1.35	1.51
14	N	602	HEA	C1A-C2A	-2.94	1.40	1.45
26	C	307	DMU	O16-C6	2.93	1.45	1.40
14	A	602	HEA	C1D-ND	-2.84	1.35	1.40
14	A	602	HEA	CHA-C1A	2.84	1.43	1.38
20	A	608	PGV	O03-C19	2.84	1.41	1.33
20	C	303	PGV	O01-C1	2.79	1.42	1.34
14	A	601	HEA	CBD-CGD	2.76	1.57	1.50
20	N	609	PGV	O01-C02	-2.76	1.39	1.46
25	C	305	CDL	PB2-OB3	2.75	1.60	1.50
24	C	302	PEK	O03-C01	-2.73	1.38	1.45
14	A	602	HEA	CHB-C1B	2.72	1.45	1.39
14	A	601	HEA	FE-NB	2.72	2.03	1.94
14	N	601	HEA	C1D-ND	-2.72	1.35	1.40
14	N	602	HEA	C4B-C3B	-2.70	1.40	1.44
14	N	602	HEA	CHD-C4C	2.68	1.45	1.39
14	N	601	HEA	FE-ND	2.68	2.03	1.94
23	P	301	CHD	C11-C9	2.65	1.58	1.53
14	A	601	HEA	FE-NC	2.65	2.04	1.95
14	N	602	HEA	CHC-C1C	2.64	1.45	1.39
14	N	601	HEA	C1B-C2B	-2.61	1.39	1.44
23	O	302	CHD	O7-C7	2.59	1.48	1.43
14	N	602	HEA	C3A-C4A	-2.58	1.41	1.46
14	A	601	HEA	CHC-C1C	2.58	1.45	1.39
14	N	601	HEA	C4D-ND	-2.56	1.33	1.38
14	A	601	HEA	C12-C13	2.56	1.61	1.53
14	N	601	HEA	CHD-C4C	2.54	1.45	1.39
14	N	601	HEA	CHC-C1C	2.53	1.45	1.39
14	A	601	HEA	FE-NA	2.53	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHA-C4D	2.52	1.45	1.39
24	C	302	PEK	O01-C1	2.50	1.41	1.34
14	A	602	HEA	CHC-C4B	2.50	1.43	1.38
14	N	602	HEA	C4A-NA	-2.47	1.35	1.39
14	A	602	HEA	C1B-NB	-2.47	1.33	1.38
14	A	602	HEA	CBA-CGA	2.46	1.56	1.50
14	N	601	HEA	O11-C11	2.44	1.48	1.42
14	N	602	HEA	FE-NB	2.40	2.02	1.94
14	N	601	HEA	CHB-C4A	2.39	1.43	1.38
14	N	602	HEA	C1D-C2D	-2.39	1.39	1.44
14	N	602	HEA	C4C-NC	-2.39	1.35	1.39
23	P	301	CHD	C18-C13	-2.38	1.50	1.54
14	N	602	HEA	C4B-NB	-2.38	1.36	1.40
20	P	303	PGV	O01-C1	2.38	1.41	1.34
20	A	608	PGV	O01-C1	2.37	1.41	1.34
20	A	608	PGV	O01-C02	-2.36	1.40	1.46
14	N	602	HEA	O11-C11	2.36	1.47	1.42
20	A	608	PGV	C01-C02	2.35	1.57	1.50
14	N	602	HEA	CHA-C4D	2.34	1.44	1.39
23	C	301	CHD	C23-C24	2.33	1.56	1.50
14	N	601	HEA	CMA-C3A	2.32	1.50	1.45
26	M	101	DMU	O16-C6	2.31	1.44	1.40
14	A	602	HEA	C1C-C2C	-2.29	1.37	1.43
14	A	601	HEA	C12-C11	-2.27	1.48	1.52
20	C	303	PGV	C03-C02	2.26	1.57	1.50
14	A	601	HEA	CAA-C2A	2.26	1.57	1.51
14	N	602	HEA	FE-ND	2.24	2.01	1.94
24	G	101	PEK	P-O12	2.23	1.63	1.54
23	C	301	CHD	C11-C9	2.23	1.57	1.53
14	A	602	HEA	C4B-C3B	-2.22	1.40	1.44
14	A	601	HEA	CBA-CGA	2.21	1.55	1.50
14	N	602	HEA	C1D-ND	-2.20	1.36	1.40
25	P	305	CDL	PB2-OB3	2.19	1.58	1.50
20	A	608	PGV	C03-C02	2.15	1.57	1.50
14	A	602	HEA	CAD-C3D	2.14	1.56	1.51
14	N	602	HEA	C1A-NA	-2.14	1.35	1.39
14	A	602	HEA	C14-C15	2.14	1.38	1.33
14	N	602	HEA	C16-C15	2.12	1.55	1.51
23	B	302	CHD	C11-C12	2.09	1.56	1.53
14	A	601	HEA	C4D-C3D	-2.07	1.41	1.45
14	N	601	HEA	FE-NB	2.06	2.01	1.94
20	A	608	PGV	O03-C01	2.05	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C1C-C2C	-2.05	1.38	1.43
14	N	601	HEA	CHA-C4D	2.04	1.43	1.39
24	C	302	PEK	C2-C1	2.04	1.56	1.50
14	N	601	HEA	CHD-C1D	2.04	1.42	1.38
14	A	602	HEA	C3C-C4C	2.00	1.47	1.42

All (397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	302	PEK	C2-C3-C4	9.28	129.78	113.23
26	P	307	DMU	C18-O16-C6	8.01	127.12	113.84
14	A	601	HEA	C13-C12-C11	-7.40	103.24	114.35
25	C	305	CDL	CB4-OB6-CB5	-6.83	100.98	117.79
25	P	305	CDL	CB4-OB6-CB5	-6.70	101.29	117.79
24	G	103	PEK	C03-C02-C01	-6.69	95.98	111.79
19	L	101	TGL	CG2-OG2-CB1	6.43	133.62	117.79
25	T	103	CDL	OA6-CA5-C11	6.42	125.33	111.50
24	T	102	PEK	O01-C1-C2	5.78	123.95	111.50
24	T	102	PEK	O03-C21-C22	5.57	129.37	111.91
19	O	303	TGL	OG2-CB1-CB2	5.44	123.23	111.50
25	T	103	CDL	OB6-CB5-C51	5.42	123.18	111.50
26	P	307	DMU	O5-C6-O16	5.37	122.69	109.97
14	N	601	HEA	C13-C12-C11	-5.31	106.37	114.35
20	C	304	PGV	O03-C19-C20	5.19	128.20	111.91
20	P	304	PGV	O01-C1-C2	5.14	122.58	111.50
23	O	302	CHD	C18-C13-C12	-5.13	103.84	109.07
26	W	102	DMU	C10-O1-C9	5.13	123.75	113.69
26	W	102	DMU	O49-C1-C6	5.07	122.37	110.05
25	G	102	CDL	OB6-CB5-C51	5.07	122.43	111.50
20	P	304	PGV	O03-C19-C20	5.02	127.66	111.91
23	P	301	CHD	C1-C2-C3	-4.98	104.08	110.47
25	G	102	CDL	OA8-CA7-C31	4.96	127.48	111.91
14	A	601	HEA	CAA-CBA-CGA	-4.95	102.95	113.60
25	G	102	CDL	OA6-CA5-C11	4.95	122.16	111.50
19	L	101	TGL	OG2-CG2-CG3	4.86	126.00	108.40
26	P	307	DMU	C10-O1-C9	4.85	123.21	113.69
24	T	102	PEK	O03-C21-O04	-4.84	111.37	123.59
24	C	302	PEK	C03-C02-C01	-4.76	100.53	111.79
27	E	201	PSC	O01-C1-C2	4.74	121.71	111.50
24	T	101	PEK	O03-C21-C22	4.65	126.50	111.91
19	A	607	TGL	OG2-CB1-CB2	4.58	121.37	111.50
20	C	304	PGV	O01-C1-C2	4.58	121.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	CHB-C4A-NA	4.56	129.37	124.44
25	T	103	CDL	OA8-CA7-C31	4.55	126.19	111.91
25	P	305	CDL	C52-C51-CB5	-4.47	97.37	113.62
24	G	101	PEK	O03-C21-C22	4.47	125.93	111.91
25	C	305	CDL	OB6-CB5-C51	4.44	121.06	111.50
26	W	102	DMU	O1-C10-C5	4.37	119.61	110.35
19	D	201	TGL	CG2-OG2-CB1	-4.37	107.04	117.79
14	A	601	HEA	C3C-C4C-NC	4.37	112.94	110.25
25	C	305	CDL	C52-C51-CB5	-4.36	97.76	113.62
25	C	305	CDL	OB8-CB7-C71	4.36	125.58	111.91
25	P	305	CDL	OA8-CA7-C31	4.34	125.54	111.91
14	A	602	HEA	C4C-CHD-C1D	-4.32	116.09	126.34
14	A	602	HEA	C4A-CHB-C1B	-4.29	116.80	126.06
24	G	103	PEK	O01-C1-C2	4.26	120.69	111.50
23	W	101	CHD	C22-C20-C17	4.26	119.09	110.28
24	G	101	PEK	O01-C1-C2	4.26	120.68	111.50
26	C	307	DMU	C10-O1-C9	4.25	122.04	113.69
23	J	101	CHD	C17-C13-C14	-4.24	95.82	100.09
23	C	306	CHD	C15-C14-C13	4.24	107.71	103.55
20	N	608	PGV	O03-C19-C20	4.24	125.20	111.91
26	W	102	DMU	O1-C9-C8	4.23	117.37	109.69
26	O	304	DMU	O5-C4-C57	4.20	116.88	106.44
23	J	101	CHD	C22-C20-C17	4.18	118.93	110.28
23	W	101	CHD	C17-C13-C14	-4.17	95.89	100.09
19	N	607	TGL	CG2-OG2-CB1	4.12	127.93	117.79
23	W	101	CHD	C14-C13-C12	4.10	111.22	107.40
14	A	601	HEA	CAD-CBD-CGD	-4.08	104.82	113.60
19	L	101	TGL	OG3-CC1-OC1	-4.07	113.33	123.59
27	R	201	PSC	O01-C1-C2	4.05	120.24	111.50
14	N	602	HEA	C4C-CHD-C1D	-4.05	116.73	126.34
23	P	306	CHD	C21-C20-C22	-4.03	104.05	110.36
23	J	101	CHD	C13-C17-C20	4.01	124.29	119.50
24	T	102	PEK	C03-C02-C01	-4.00	102.33	111.79
26	C	307	DMU	O7-C10-C5	3.99	118.45	108.10
24	T	101	PEK	O01-C1-C2	3.95	120.02	111.50
26	W	102	DMU	C7-C8-C9	3.92	117.22	110.24
14	N	601	HEA	CHA-C4D-C3D	-3.90	119.10	124.84
23	O	302	CHD	C13-C17-C20	-3.90	114.84	119.50
26	W	102	DMU	C10-O7-C3	-3.90	108.32	117.96
23	W	101	CHD	C9-C10-C5	3.89	114.05	108.58
26	W	102	DMU	C1-C2-C3	-3.87	100.86	109.68
25	P	305	CDL	OA6-CA5-C11	3.85	119.79	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	305	CDL	CA6-CA4-CA3	-3.82	102.76	111.79
19	Q	201	TGL	CG2-OG2-CB1	-3.81	108.42	117.79
26	W	102	DMU	O16-C6-C1	3.80	114.24	108.30
23	J	101	CHD	C14-C13-C12	3.78	110.92	107.40
14	A	602	HEA	C2B-C1B-NB	3.76	114.39	109.88
14	N	601	HEA	O2A-CGA-CBA	3.75	126.07	114.03
26	C	307	DMU	C2-C3-C4	-3.72	102.40	110.93
24	P	302	PEK	O01-C1-O02	-3.71	114.73	123.70
24	G	103	PEK	O03-C01-C02	3.71	119.22	108.43
14	A	601	HEA	O11-C11-C12	3.70	119.75	109.42
19	L	101	TGL	CC3-CC2-CC1	3.70	127.06	113.62
14	A	602	HEA	CHA-C1A-NA	3.69	128.44	124.44
26	O	304	DMU	C2-C3-C4	3.69	116.83	110.24
19	N	607	TGL	OG2-CB1-CB2	3.64	119.35	111.50
14	A	602	HEA	CHD-C4C-NC	3.63	130.53	123.85
23	W	101	CHD	C13-C17-C20	3.63	123.83	119.50
20	A	608	PGV	O03-C19-C20	3.63	123.29	111.91
25	P	305	CDL	OB8-CB7-C71	3.62	123.27	111.91
23	W	101	CHD	C23-C22-C20	-3.61	107.93	114.52
23	W	101	CHD	C4-C3-C2	-3.58	106.28	110.55
14	N	601	HEA	CHA-C4D-ND	3.58	128.31	124.42
14	N	601	HEA	C3C-C4C-NC	3.58	112.45	110.25
23	C	301	CHD	C21-C20-C22	-3.54	104.82	110.36
25	G	102	CDL	CA6-OA8-CA7	3.53	130.18	117.12
14	N	602	HEA	CAD-CBD-CGD	-3.50	106.06	113.60
25	G	102	CDL	OA8-CA7-OA9	-3.50	114.76	123.59
14	N	602	HEA	C13-C12-C11	-3.49	109.10	114.35
20	N	608	PGV	C01-O03-C19	3.48	130.01	117.12
25	C	305	CDL	OA6-CA5-C11	3.48	118.99	111.50
14	A	602	HEA	CHB-C1B-C2B	-3.47	119.56	124.98
20	N	608	PGV	C03-C02-C01	3.46	119.96	111.79
25	P	305	CDL	OB6-CB5-C51	3.45	118.93	111.50
20	C	303	PGV	C22-C21-C20	-3.45	100.80	113.19
23	B	302	CHD	C21-C20-C22	-3.44	104.96	110.36
23	W	101	CHD	C16-C17-C20	3.44	117.48	112.15
24	G	101	PEK	O03-C21-O04	-3.43	114.93	123.59
25	P	305	CDL	OA8-CA7-OA9	-3.42	114.97	123.59
20	A	609	PGV	C4-C3-C2	-3.41	100.94	113.19
14	A	601	HEA	O1A-CGA-CBA	-3.40	112.14	123.08
14	N	602	HEA	CHD-C1D-ND	3.40	128.57	124.37
26	P	307	DMU	O1-C10-C5	3.39	117.53	110.35
14	N	602	HEA	CHC-C1C-C2C	-3.39	117.67	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	305	CDL	OA6-CA4-CA3	3.39	120.67	108.40
14	N	601	HEA	C2D-C1D-ND	3.39	113.85	109.84
20	N	608	PGV	O01-C1-C2	3.37	118.77	111.50
23	J	101	CHD	C9-C10-C5	3.36	113.30	108.58
14	N	601	HEA	C1A-CHA-C4D	-3.35	118.82	126.06
24	C	302	PEK	O03-C01-C02	-3.35	98.68	108.43
14	N	602	HEA	C1C-CHC-C4B	-3.34	118.42	126.34
23	B	302	CHD	C13-C14-C8	-3.34	110.48	114.74
20	P	304	PGV	C21-C20-C19	-3.33	101.50	113.62
24	T	102	PEK	O01-C1-O02	-3.33	115.66	123.70
23	O	302	CHD	C14-C13-C12	3.33	110.50	107.40
20	N	609	PGV	O01-C1-O02	-3.31	115.69	123.70
23	P	301	CHD	C22-C20-C17	-3.31	103.45	110.28
19	L	101	TGL	OG3-CC1-CC2	3.28	122.19	111.91
23	C	301	CHD	C18-C13-C12	3.27	112.40	109.07
25	T	103	CDL	OA6-CA5-OA7	-3.27	115.80	123.70
20	N	608	PGV	O03-C19-O04	-3.26	115.36	123.59
14	A	601	HEA	C17-C18-C19	-3.25	119.83	127.66
19	Q	201	TGL	OG2-CB1-CB2	3.23	118.46	111.50
23	C	301	CHD	C23-C22-C20	-3.23	108.63	114.52
19	D	201	TGL	OG1-CA1-CA2	3.21	121.98	111.91
14	N	602	HEA	C4C-NC-C1C	-3.21	102.20	105.35
23	B	302	CHD	C11-C9-C10	-3.21	110.42	113.73
14	N	601	HEA	CAA-CBA-CGA	-3.19	106.73	113.60
14	A	602	HEA	C4B-NB-C1B	-3.18	101.79	105.07
25	T	103	CDL	OA8-CA7-OA9	-3.18	115.58	123.59
14	A	602	HEA	CHA-C4D-C3D	-3.16	120.20	124.84
23	B	302	CHD	C6-C5-C4	-3.15	107.56	111.19
24	T	101	PEK	O03-C21-O04	-3.14	115.66	123.59
19	A	607	TGL	OG1-CA1-CA2	3.14	121.77	111.91
25	T	103	CDL	CB4-OB6-CB5	-3.13	110.10	117.79
14	A	601	HEA	C2D-C1D-ND	3.12	113.54	109.84
24	G	101	PEK	P-O11-C03	3.12	126.88	118.30
23	O	302	CHD	C16-C17-C20	-3.12	107.32	112.15
23	J	101	CHD	C11-C9-C10	-3.11	110.52	113.73
14	A	601	HEA	CAD-C3D-C4D	3.11	130.09	124.66
20	A	608	PGV	C23-C22-C21	-3.10	98.71	114.42
23	C	301	CHD	C15-C14-C13	-3.09	100.53	103.55
14	A	602	HEA	O1D-CGD-CBD	-3.08	113.18	123.08
20	N	609	PGV	O03-C19-C20	3.07	121.55	111.91
26	C	307	DMU	O1-C10-C5	3.07	116.85	110.35
20	A	609	PGV	O03-C19-C20	3.07	121.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	O2A-CGA-CBA	3.07	123.88	114.03
24	C	302	PEK	O01-C1-O02	-3.05	116.33	123.70
23	W	101	CHD	C11-C9-C10	-3.05	110.58	113.73
20	N	608	PGV	C4-C3-C2	-3.04	102.25	113.19
20	N	608	PGV	O01-C02-C01	3.04	119.41	108.40
14	N	602	HEA	C21-C20-C19	3.03	122.95	112.98
26	W	102	DMU	C6-C1-C2	-3.03	103.69	110.00
26	O	304	DMU	C3-C2-C1	3.03	116.11	110.82
19	O	303	TGL	OG1-CA1-CA2	3.01	121.34	111.91
26	W	102	DMU	C6-O5-C4	3.01	119.59	113.69
14	N	602	HEA	CMC-C2C-C1C	3.00	129.93	125.37
23	C	301	CHD	C18-C13-C17	-2.99	106.53	111.21
14	N	601	HEA	O2D-CGD-CBD	2.99	123.62	114.03
23	C	306	CHD	C11-C9-C10	-2.99	110.65	113.73
23	C	301	CHD	C22-C20-C17	-2.97	104.14	110.28
14	A	602	HEA	C3B-C4B-NB	2.97	113.36	109.84
23	C	301	CHD	C22-C23-C24	-2.95	104.68	112.51
14	A	602	HEA	C3D-C4D-ND	2.94	113.20	110.36
20	A	609	PGV	C28-C27-C26	-2.92	99.59	114.42
19	O	303	TGL	OG3-CC1-CC2	2.92	121.08	111.91
26	M	101	DMU	C18-O16-C6	-2.92	109.00	113.84
20	P	304	PGV	O03-C19-O04	-2.89	116.29	123.59
14	A	602	HEA	C3C-C4C-NC	2.88	112.02	110.25
26	W	102	DMU	O61-C57-C4	-2.88	101.42	111.29
14	A	601	HEA	C13-C14-C15	-2.87	120.75	127.66
14	A	602	HEA	CHA-C1A-C2A	-2.86	120.30	124.94
20	A	608	PGV	O03-C19-O04	-2.86	116.37	123.59
20	C	304	PGV	C01-O03-C19	2.86	127.72	117.12
14	A	601	HEA	C2B-C1B-NB	2.86	113.31	109.88
26	C	307	DMU	O1-C9-C8	2.86	114.89	109.69
25	C	305	CDL	OB8-CB7-OB9	-2.86	116.38	123.59
24	T	102	PEK	C01-O03-C21	2.86	127.70	117.12
20	C	304	PGV	O03-C19-O04	-2.85	116.39	123.59
26	O	304	DMU	C6-O5-C4	-2.85	108.09	113.69
20	C	304	PGV	C21-C20-C19	-2.85	103.27	113.62
14	N	601	HEA	CAA-C2A-C1A	2.84	130.26	124.89
23	J	101	CHD	C4-C3-C2	-2.84	107.16	110.55
19	A	607	TGL	OG3-CC1-CC2	2.83	120.79	111.91
27	R	201	PSC	C03-C02-C01	-2.82	105.12	111.79
24	C	302	PEK	C30-C29-C28	-2.82	100.12	114.42
25	P	305	CDL	OA8-CA6-CA4	2.82	116.63	108.43
19	N	607	TGL	OG2-CG2-CG1	2.81	118.59	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	101	TGL	CA4-CA3-CA2	-2.81	103.11	113.19
14	A	602	HEA	CAD-CBD-CGD	-2.80	107.58	113.60
14	A	601	HEA	C3D-C4D-ND	2.79	113.06	110.36
14	N	602	HEA	C3C-C4C-NC	2.78	111.96	110.25
23	W	101	CHD	C1-C10-C5	2.78	111.88	107.77
25	G	102	CDL	CB4-OB6-CB5	-2.78	110.94	117.79
26	O	304	DMU	O61-C57-C4	2.77	120.78	111.29
14	A	602	HEA	C1A-CHA-C4D	-2.76	120.11	126.06
20	P	303	PGV	O03-C19-O04	-2.75	116.64	123.59
23	W	101	CHD	C6-C5-C4	-2.75	108.03	111.19
14	N	601	HEA	C1C-CHC-C4B	-2.74	119.84	126.34
23	J	101	CHD	C16-C17-C20	2.73	116.37	112.15
26	P	307	DMU	O16-C6-C1	-2.72	104.06	108.30
14	A	602	HEA	C1D-ND-C4D	-2.71	102.27	105.07
26	C	307	DMU	O5-C4-C57	2.71	113.17	106.44
27	E	201	PSC	O01-C02-C03	2.70	118.19	108.40
19	D	201	TGL	OG1-CA1-OA1	-2.69	116.80	123.59
27	E	201	PSC	O01-C1-O02	-2.69	117.20	123.70
24	P	302	PEK	C03-C02-C01	-2.68	105.44	111.79
20	P	303	PGV	O01-C1-O02	-2.68	117.23	123.70
20	N	609	PGV	O03-C19-O04	-2.67	116.86	123.59
23	W	101	CHD	C18-C13-C14	-2.66	107.04	111.21
14	N	602	HEA	C27-C19-C20	2.66	119.75	115.27
20	N	608	PGV	O14-P-O13	2.64	121.03	110.68
14	A	602	HEA	CAD-C3D-C4D	2.64	129.28	124.66
14	A	602	HEA	C2D-C1D-ND	2.64	112.97	109.84
14	A	602	HEA	C16-C15-C14	-2.63	115.80	121.12
26	W	102	DMU	O55-C2-C1	2.62	116.41	110.35
25	C	305	CDL	OA8-CA6-CA4	2.62	116.05	108.43
14	N	602	HEA	C3B-C4B-NB	2.62	112.94	109.84
14	N	601	HEA	C26-C15-C16	2.62	119.67	115.27
14	N	602	HEA	CHD-C1D-C2D	-2.61	119.47	126.73
23	P	301	CHD	C22-C23-C24	-2.61	105.59	112.51
25	P	305	CDL	OA6-CA4-CA3	2.60	117.82	108.40
20	A	608	PGV	O01-C1-O02	-2.59	117.44	123.70
19	L	101	TGL	CG3-OG3-CC1	2.58	126.66	117.12
23	P	301	CHD	C16-C17-C20	-2.57	108.16	112.15
14	A	602	HEA	O2D-CGD-O1D	2.57	129.71	123.30
14	N	602	HEA	C3C-C2C-C1C	-2.57	104.06	107.16
20	N	609	PGV	O01-C1-C2	2.57	117.03	111.50
25	G	102	CDL	C39-C38-C37	2.56	127.44	114.42
14	N	602	HEA	CHC-C1C-NC	2.54	128.51	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	302	PEK	C25-C24-C23	-2.54	101.55	114.42
25	C	305	CDL	OA8-CA7-C31	2.53	119.84	111.91
25	C	305	CDL	OA6-CA4-CA6	-2.53	99.25	108.40
14	N	602	HEA	CMD-C2D-C1D	2.53	128.89	125.04
26	W	102	DMU	O5-C4-C3	2.51	115.05	109.75
14	N	601	HEA	O1A-CGA-CBA	-2.51	115.02	123.08
26	P	307	DMU	O1-C9-C8	2.51	114.25	109.69
14	N	601	HEA	C17-C18-C19	-2.50	121.65	127.66
14	N	601	HEA	C13-C14-C15	-2.49	121.66	127.66
26	C	307	DMU	O7-C3-C4	2.49	116.26	109.45
14	A	602	HEA	C21-C20-C19	2.47	121.11	112.98
19	N	607	TGL	OG3-CC1-OC1	-2.47	117.35	123.59
19	A	607	TGL	OG1-CA1-OA1	-2.47	117.36	123.59
19	Q	201	TGL	OG1-CA1-CA2	2.47	119.64	111.91
25	C	305	CDL	C74-C73-C72	-2.46	101.93	114.42
25	T	103	CDL	OB6-CB5-OB7	-2.46	117.76	123.70
14	N	602	HEA	C2C-C1C-NC	2.45	113.82	110.08
26	W	102	DMU	C10-C5-C7	2.45	115.11	110.00
27	R	201	PSC	C21-C20-C19	-2.45	104.70	113.62
19	N	607	TGL	OG3-CC1-CC2	2.45	119.59	111.91
23	C	306	CHD	C16-C17-C13	2.43	105.94	103.55
14	A	601	HEA	CHA-C1A-C2A	-2.43	121.00	124.94
24	C	302	PEK	C01-O03-C21	2.42	126.10	117.12
23	B	302	CHD	C22-C20-C17	2.41	115.27	110.28
26	P	307	DMU	O5-C6-C1	-2.41	105.24	110.35
19	N	607	TGL	OG2-CG2-CG3	2.41	117.12	108.40
14	N	602	HEA	C2B-C1B-NB	2.41	112.76	109.88
23	O	302	CHD	C11-C9-C10	-2.39	111.26	113.73
23	O	302	CHD	C5-C4-C3	-2.39	109.25	112.76
14	A	601	HEA	CHA-C4D-C3D	-2.39	121.33	124.84
23	C	306	CHD	C1-C10-C5	2.39	111.30	107.77
19	L	101	TGL	CG3-CG2-CG1	-2.39	106.14	111.79
20	A	609	PGV	C8-C9-C10	-2.39	103.40	113.79
23	P	306	CHD	C6-C5-C4	-2.38	108.44	111.19
25	P	305	CDL	C81-C80-C79	-2.38	102.33	114.42
25	T	103	CDL	C58-C57-C56	-2.38	102.36	114.42
24	G	103	PEK	C2-C3-C4	2.37	117.46	113.23
24	C	302	PEK	C23-C22-C21	-2.37	104.99	113.62
14	A	601	HEA	C1B-C2B-C3B	-2.37	103.97	106.80
24	G	103	PEK	O03-C21-C22	2.36	119.33	111.91
25	G	102	CDL	C40-C39-C38	2.36	126.42	114.42
23	P	301	CHD	C10-C9-C8	-2.36	109.28	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C13-C14-C15	-2.36	121.97	127.66
20	P	303	PGV	C22-C21-C20	-2.36	104.72	113.19
23	J	101	CHD	C1-C10-C5	2.35	111.25	107.77
20	C	303	PGV	C21-C20-C19	-2.35	105.09	113.62
26	O	304	DMU	C18-O16-C6	2.34	117.73	113.84
25	G	102	CDL	CB6-CB4-CB3	-2.34	106.25	111.79
25	C	305	CDL	OB4-PB2-OB3	2.34	123.79	112.24
14	N	602	HEA	O1A-CGA-CBA	-2.33	115.61	123.08
25	G	102	CDL	C58-C57-C56	-2.32	102.62	114.42
14	A	602	HEA	C2C-C1C-NC	2.32	113.62	110.08
20	C	303	PGV	O03-C01-C02	-2.32	101.67	108.43
14	N	602	HEA	CAA-C2A-C1A	2.32	129.28	124.89
23	J	101	CHD	C23-C22-C20	-2.32	110.29	114.52
14	A	602	HEA	CHD-C4C-C3C	-2.31	117.43	127.71
26	C	307	DMU	O16-C6-C1	2.31	111.90	108.30
23	B	302	CHD	C19-C10-C5	-2.30	106.45	110.36
25	P	305	CDL	OB4-PB2-OB3	2.29	123.58	112.24
23	B	302	CHD	C9-C11-C12	-2.29	111.27	114.30
20	P	303	PGV	C21-C20-C19	-2.29	105.28	113.62
26	C	307	DMU	O61-C57-C4	2.28	119.13	111.29
26	P	307	DMU	O5-C4-C57	2.28	112.11	106.44
23	W	101	CHD	C4-C5-C10	2.28	115.08	112.66
23	B	302	CHD	O26-C24-C23	2.28	121.34	114.03
23	C	301	CHD	O12-C12-C13	-2.27	107.18	111.03
25	P	305	CDL	C42-C41-C40	2.27	125.95	114.42
19	L	101	TGL	CA3-CA2-CA1	-2.27	105.37	113.62
26	W	102	DMU	C8-C7-C5	2.27	114.78	110.82
14	A	601	HEA	CBD-CAD-C3D	-2.26	106.34	112.63
23	B	302	CHD	C5-C4-C3	-2.26	109.45	112.76
14	N	601	HEA	C3D-C4D-ND	2.25	112.54	110.36
23	P	301	CHD	C23-C22-C20	-2.25	110.40	114.52
24	C	302	PEK	C3-C2-C1	-2.25	105.43	113.62
23	P	301	CHD	C21-C20-C22	-2.25	106.83	110.36
20	C	304	PGV	O04-C19-C20	-2.25	114.95	123.73
23	J	101	CHD	C18-C13-C14	-2.25	107.69	111.21
25	C	305	CDL	C81-C80-C79	-2.24	103.03	114.42
19	A	607	TGL	CG3-CG2-CG1	-2.24	106.49	111.79
14	A	602	HEA	CBD-CAD-C3D	2.24	118.85	112.63
14	A	602	HEA	CHD-C1D-C2D	-2.24	120.52	126.73
24	T	101	PEK	C01-O03-C21	2.23	125.39	117.12
14	N	601	HEA	C2B-C1B-NB	2.23	112.56	109.88
24	C	302	PEK	C32-C31-C30	-2.23	103.10	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	302	PEK	O02-C1-C2	2.23	132.42	123.73
14	N	602	HEA	CHC-C4B-C3B	-2.22	120.08	125.80
14	A	602	HEA	CAA-CBA-CGA	-2.22	108.82	113.60
14	A	602	HEA	CMB-C2B-C3B	-2.20	126.14	130.34
26	M	101	DMU	C10-O7-C3	-2.20	112.52	117.96
19	D	201	TGL	CB3-CB2-CB1	2.20	121.61	113.62
23	J	101	CHD	C21-C20-C17	-2.19	109.56	112.92
26	W	102	DMU	O5-C6-C1	-2.19	105.71	110.35
23	C	301	CHD	C19-C10-C1	-2.19	104.73	108.26
14	N	601	HEA	CHC-C4B-NB	2.18	127.06	124.37
19	N	607	TGL	CA3-CA2-CA1	-2.18	105.69	113.62
23	J	101	CHD	C6-C5-C4	-2.16	108.70	111.19
14	A	601	HEA	C1D-ND-C4D	-2.15	102.85	105.07
19	N	607	TGL	CG3-OG3-CC1	2.15	125.08	117.12
20	P	303	PGV	O14-P-O13	2.15	122.87	112.24
19	N	607	TGL	OG1-CA1-CA2	2.13	118.61	111.91
14	N	601	HEA	CHC-C1C-C2C	-2.13	121.21	127.24
14	A	602	HEA	CMB-C2B-C1B	2.13	128.29	125.04
14	N	601	HEA	CAD-C3D-C2D	2.13	131.85	127.88
23	C	301	CHD	C17-C13-C14	2.13	102.24	100.09
14	N	601	HEA	C3B-C4B-NB	2.12	112.36	109.84
25	T	103	CDL	OA8-CA6-CA4	-2.12	102.26	108.43
20	A	608	PGV	C7-C6-C5	-2.11	103.72	114.42
20	A	609	PGV	C01-O03-C19	2.11	124.93	117.12
14	N	601	HEA	CHD-C1D-C2D	-2.11	120.87	126.73
25	T	103	CDL	CB6-CB4-CB3	-2.10	106.83	111.79
26	P	307	DMU	C8-C7-C5	-2.09	107.17	110.82
26	P	307	DMU	O7-C10-C5	2.09	113.51	108.10
14	A	602	HEA	O1A-CGA-CBA	-2.09	116.38	123.08
19	N	607	TGL	CG1-OG1-CA1	2.08	124.84	117.12
27	E	201	PSC	C14-C13-C12	-2.08	108.76	124.73
14	A	601	HEA	CHA-C1A-NA	2.08	126.69	124.44
23	B	302	CHD	C18-C13-C17	-2.08	107.96	111.21
24	P	302	PEK	O11-P-O14	-2.08	100.95	109.07
23	C	306	CHD	C5-C4-C3	-2.08	109.71	112.76
25	G	102	CDL	OA6-CA5-OA7	-2.08	118.68	123.70
23	C	306	CHD	C19-C10-C1	-2.07	104.92	108.26
26	C	307	DMU	C18-O16-C6	2.07	117.28	113.84
20	N	608	PGV	O03-C01-C02	-2.07	102.40	108.43
14	N	602	HEA	C4B-NB-C1B	-2.07	102.94	105.07
25	G	102	CDL	O1-C1-CA2	-2.06	102.32	109.56
23	B	302	CHD	C2-C1-C10	-2.06	109.24	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	303	PGV	O03-C19-O04	-2.06	118.38	123.59
14	N	602	HEA	CHC-C4B-NB	2.06	126.92	124.37
26	W	102	DMU	C2-C3-C4	-2.06	106.21	110.93
20	P	303	PGV	O03-C01-C02	-2.05	102.46	108.43
19	A	607	TGL	OG3-CC1-OC1	-2.05	118.42	123.59
19	L	101	TGL	OG3-CG3-CG2	-2.05	102.47	108.43
20	A	609	PGV	O03-C19-O04	-2.05	118.42	123.59
19	N	607	TGL	CC3-CC2-CC1	2.05	121.07	113.62
14	N	601	HEA	CAD-CBD-CGD	-2.04	109.21	113.60
25	P	305	CDL	C55-C54-C53	-2.04	104.06	114.42
20	C	303	PGV	O01-C1-C2	2.04	115.89	111.50
20	P	304	PGV	O04-C19-C20	-2.03	115.80	123.73
23	P	306	CHD	C11-C9-C10	-2.03	111.63	113.73
27	R	201	PSC	O01-C1-O02	-2.03	118.80	123.70
24	T	101	PEK	C3-C2-C1	-2.03	106.24	113.62
27	R	201	PSC	O13-P-O14	2.03	122.27	112.24
14	N	602	HEA	CHD-C4C-NC	2.03	127.58	123.85
14	N	601	HEA	CHC-C4B-C3B	-2.03	120.58	125.80
20	P	303	PGV	C27-C26-C25	-2.02	104.16	114.42
20	P	304	PGV	O14-P-O13	2.02	122.21	112.24
26	Z	101	DMU	C11-C9-C8	-2.02	108.28	113.00
23	W	101	CHD	C19-C10-C5	-2.01	106.95	110.36
19	O	303	TGL	CG3-CG2-CG1	-2.01	107.03	111.79
24	P	302	PEK	O03-C01-C02	-2.01	102.59	108.43
14	N	601	HEA	OMA-CMA-C3A	-2.01	121.15	125.69
14	A	601	HEA	C20-C21-C22	-2.00	105.30	111.88
23	C	301	CHD	O26-C24-O25	-2.00	118.31	123.30
26	P	307	DMU	O1-C9-C11	2.00	111.41	106.44

There are no chirality outliers.

All (781) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	601	HEA	C2A-C3A-CMA-OMA
19	A	607	TGL	OG1-CG1-CG2-OG2
19	N	607	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C03-O11-P-O13
20	A	609	PGV	C04-O12-P-O11
20	A	609	PGV	C2-C1-O01-C02
20	A	609	PGV	O04-C19-O03-C01
20	A	609	PGV	C20-C19-O03-C01
20	C	304	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
20	C	304	PGV	C04-O12-P-O13
20	C	304	PGV	C10-C11-C12-C13
20	N	608	PGV	C03-O11-P-O12
20	N	608	PGV	C03-O11-P-O13
20	N	608	PGV	C03-O11-P-O14
20	N	608	PGV	O02-C1-O01-C02
20	N	608	PGV	C2-C1-O01-C02
20	N	608	PGV	O04-C19-O03-C01
20	N	608	PGV	C20-C19-O03-C01
20	P	304	PGV	C04-O12-P-O13
20	P	304	PGV	C2-C1-O01-C02
24	G	101	PEK	C13-C14-C15-C16
24	G	103	PEK	C11-C12-C13-C14
24	G	103	PEK	C12-C13-C14-C15
24	T	101	PEK	C04-O12-P-O13
24	T	101	PEK	C5-C6-C7-C8
24	T	102	PEK	C03-O11-P-O13
24	T	102	PEK	O03-C01-C02-O01
24	T	102	PEK	O12-C04-C05-N
24	T	102	PEK	O04-C21-O03-C01
24	T	102	PEK	C11-C10-C9-C8
25	C	305	CDL	C11-CA5-OA6-CA4
25	C	305	CDL	CB2-OB2-PB2-OB4
25	C	305	CDL	OB5-CB3-CB4-OB6
25	G	102	CDL	CA2-OA2-PA1-OA3
25	G	102	CDL	CB2-OB2-PB2-OB5
25	G	102	CDL	CB3-OB5-PB2-OB4
25	P	305	CDL	CA2-C1-CB2-OB2
25	P	305	CDL	C11-CA5-OA6-CA4
25	P	305	CDL	CB3-OB5-PB2-OB2
25	T	103	CDL	CA2-OA2-PA1-OA3
25	T	103	CDL	OA7-CA5-OA6-CA4
25	T	103	CDL	CB2-OB2-PB2-OB5
25	T	103	CDL	CB3-OB5-PB2-OB4
26	C	307	DMU	O5-C6-O16-C18
26	P	307	DMU	O5-C6-O16-C18
27	E	201	PSC	C03-O11-P-O13
27	E	201	PSC	C04-O12-P-O11
27	E	201	PSC	C04-O12-P-O13
27	E	201	PSC	C04-O12-P-O14
27	E	201	PSC	O12-C04-C05-N
27	R	201	PSC	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
27	R	201	PSC	O12-C04-C05-N
25	C	305	CDL	OA9-CA7-OA8-CA6
25	G	102	CDL	OA9-CA7-OA8-CA6
20	C	304	PGV	C20-C19-O03-C01
25	C	305	CDL	C31-CA7-OA8-CA6
25	G	102	CDL	C31-CA7-OA8-CA6
20	C	304	PGV	O04-C19-O03-C01
20	A	609	PGV	O02-C1-O01-C02
20	P	304	PGV	O02-C1-O01-C02
25	C	305	CDL	OA7-CA5-OA6-CA4
25	P	305	CDL	OA7-CA5-OA6-CA4
27	E	201	PSC	O02-C1-O01-C02
19	Q	201	TGL	CC2-CC1-OG3-CG3
24	T	101	PEK	C22-C21-O03-C01
26	O	304	DMU	O5-C4-C57-O61
25	T	103	CDL	C11-CA5-OA6-CA4
20	P	304	PGV	C20-C19-O03-C01
24	T	102	PEK	C22-C21-O03-C01
25	T	103	CDL	C31-CA7-OA8-CA6
20	C	303	PGV	C10-C11-C12-C13
20	P	303	PGV	C10-C11-C12-C13
24	G	103	PEK	C4-C5-C6-C7
24	P	302	PEK	C4-C5-C6-C7
24	P	302	PEK	C10-C11-C12-C13
24	T	101	PEK	C7-C8-C9-C10
24	T	101	PEK	C10-C11-C12-C13
24	T	102	PEK	C4-C5-C6-C7
27	R	201	PSC	C11-C12-C13-C14
25	C	305	CDL	C80-C81-C82-C83
19	N	607	TGL	OB1-CB1-OG2-CG2
20	P	304	PGV	O04-C19-O03-C01
24	T	101	PEK	O04-C21-O03-C01
25	T	103	CDL	OA9-CA7-OA8-CA6
20	A	609	PGV	O12-C04-C05-O05
25	C	305	CDL	O1-C1-CA2-OA2
25	C	305	CDL	O1-C1-CB2-OB2
25	P	305	CDL	O1-C1-CB2-OB2
24	G	103	PEK	C22-C21-O03-C01
19	Q	201	TGL	CB9-C10-C11-C12
19	Q	201	TGL	OC1-CC1-OG3-CG3
24	G	103	PEK	O04-C21-O03-C01
26	W	102	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
26	O	304	DMU	C3-C4-C57-O61
25	P	305	CDL	C51-CB5-OB6-CB4
27	E	201	PSC	C2-C1-O01-C02
19	D	201	TGL	C13-C14-C29-C30
25	P	305	CDL	C20-C21-C22-C23
25	T	103	CDL	C60-C61-C62-C63
25	C	305	CDL	C37-C38-C39-C40
26	P	307	DMU	O6-C11-C9-O1
19	L	101	TGL	CC1-CC2-CC3-CC4
23	P	306	CHD	C17-C20-C22-C23
19	D	201	TGL	CC2-CC1-OG3-CG3
25	P	305	CDL	C31-CA7-OA8-CA6
25	P	305	CDL	OA9-CA7-OA8-CA6
26	P	307	DMU	O5-C4-C57-O61
23	W	101	CHD	C13-C17-C20-C22
20	A	609	PGV	C4-C5-C6-C7
25	G	102	CDL	C37-C38-C39-C40
19	D	201	TGL	OC1-CC1-OG3-CG3
26	W	102	DMU	C3-C4-C57-O61
20	A	609	PGV	O12-C04-C05-C06
25	C	305	CDL	CB2-C1-CA2-OA2
25	C	305	CDL	CA2-C1-CB2-OB2
25	P	305	CDL	CB2-C1-CA2-OA2
23	P	306	CHD	C21-C20-C22-C23
24	G	101	PEK	O04-C21-O03-C01
19	L	101	TGL	CA2-CA1-OG1-CG1
24	G	101	PEK	C22-C21-O03-C01
23	J	101	CHD	C13-C17-C20-C21
23	W	101	CHD	C13-C17-C20-C21
25	G	102	CDL	C55-C56-C57-C58
25	T	103	CDL	C40-C41-C42-C43
26	Z	101	DMU	C19-C22-C25-C28
26	C	307	DMU	C3-C4-C57-O61
19	A	607	TGL	CA1-CA2-CA3-CA4
24	T	101	PEK	C1-C2-C3-C4
26	C	307	DMU	C1-C6-O16-C18
23	J	101	CHD	C13-C17-C20-C22
19	O	303	TGL	CB1-CB2-CB3-CB4
19	L	101	TGL	OA1-CA1-OG1-CG1
19	Q	201	TGL	C13-C14-C29-C30
19	N	607	TGL	CC2-CC3-CC4-CC5
19	O	303	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
24	G	101	PEK	C1-C2-C3-C4
24	G	101	PEK	C10-C11-C12-C13
24	T	101	PEK	C13-C14-C15-C16
24	T	102	PEK	C13-C14-C15-C16
26	C	307	DMU	O5-C4-C57-O61
19	D	201	TGL	CB1-CB2-CB3-CB4
20	A	609	PGV	C19-C20-C21-C22
19	A	607	TGL	CA9-C20-C21-C22
23	C	306	CHD	C17-C20-C22-C23
25	P	305	CDL	C38-C39-C40-C41
23	C	306	CHD	C21-C20-C22-C23
19	N	607	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB1-CB2-CB3-CB4
25	P	305	CDL	CB7-C71-C72-C73
27	R	201	PSC	C1-C2-C3-C4
19	L	101	TGL	CC3-CC4-CC5-CC6
26	P	307	DMU	C3-C4-C57-O61
25	P	305	CDL	C60-C61-C62-C63
25	P	305	CDL	O1-C1-CA2-OA2
25	P	305	CDL	OB7-CB5-OB6-CB4
19	N	607	TGL	CA2-CA1-OG1-CG1
20	P	304	PGV	C10-C11-C12-C13
24	C	302	PEK	C13-C14-C15-C16
24	G	101	PEK	C4-C5-C6-C7
27	E	201	PSC	C11-C10-C9-C8
26	C	307	DMU	O16-C18-C19-C22
27	R	201	PSC	C22-C23-C24-C25
19	N	607	TGL	OA1-CA1-OG1-CG1
25	C	305	CDL	C51-CB5-OB6-CB4
25	G	102	CDL	C15-C16-C17-C18
20	A	609	PGV	C03-O11-P-O12
20	P	304	PGV	C04-O12-P-O11
24	T	101	PEK	C04-O12-P-O11
24	T	102	PEK	C03-O11-P-O12
25	C	305	CDL	CA3-OA5-PA1-OA2
25	C	305	CDL	CB3-OB5-PB2-OB2
25	G	102	CDL	CA2-OA2-PA1-OA5
25	G	102	CDL	CA3-OA5-PA1-OA2
25	G	102	CDL	CB3-OB5-PB2-OB2
25	P	305	CDL	CA2-OA2-PA1-OA5
25	P	305	CDL	CA3-OA5-PA1-OA2
25	P	305	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	CA2-OA2-PA1-OA5
25	T	103	CDL	CB3-OB5-PB2-OB2
27	E	201	PSC	C03-O11-P-O12
27	R	201	PSC	C04-O12-P-O11
24	T	101	PEK	C34-C35-C36-C37
25	C	305	CDL	OB7-CB5-OB6-CB4
27	E	201	PSC	C04-C05-N-C06
27	E	201	PSC	C04-C05-N-C08
23	W	101	CHD	C16-C17-C20-C21
19	Q	201	TGL	CA9-C20-C21-C22
23	W	101	CHD	C16-C17-C20-C22
19	O	303	TGL	C11-C12-C13-C14
19	D	201	TGL	C11-C10-CB9-CB8
20	C	304	PGV	C30-C31-C32-C33
19	Q	201	TGL	C16-C17-C18-C19
24	C	302	PEK	C26-C27-C28-C29
25	C	305	CDL	C77-C78-C79-C80
25	G	102	CDL	C79-C80-C81-C82
25	P	305	CDL	C57-C58-C59-C60
25	P	305	CDL	C73-C74-C75-C76
27	E	201	PSC	C03-C02-O01-C1
19	O	303	TGL	CA2-CA3-CA4-CA5
19	O	303	TGL	CA5-CA6-CA7-CA8
19	L	101	TGL	CA3-CA4-CA5-CA6
25	P	305	CDL	C82-C83-C84-C85
25	T	103	CDL	O1-C1-CB2-OB2
20	N	608	PGV	C23-C24-C25-C26
25	G	102	CDL	C77-C78-C79-C80
25	P	305	CDL	C41-C42-C43-C44
20	P	304	PGV	C1-C2-C3-C4
26	W	102	DMU	C1-C6-O16-C18
19	N	607	TGL	C22-C23-C24-C25
19	L	101	TGL	C23-C24-C25-C26
19	N	607	TGL	CC5-CC6-CC7-CC8
19	Q	201	TGL	C20-C21-C22-C23
25	C	305	CDL	C36-C37-C38-C39
26	M	101	DMU	C19-C22-C25-C28
27	R	201	PSC	C29-C30-C31-C32
20	C	303	PGV	C7-C8-C9-C10
20	C	304	PGV	O02-C1-O01-C02
19	D	201	TGL	C23-C24-C25-C26
19	O	303	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
19	Q	201	TGL	C21-C20-CA9-CA8
20	N	609	PGV	C30-C31-C32-C33
20	P	303	PGV	C13-C14-C15-C16
25	G	102	CDL	C20-C21-C22-C23
24	G	103	PEK	C15-C16-C17-C18
19	A	607	TGL	CB1-CB2-CB3-CB4
19	D	201	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	CC6-CC7-CC8-CC9
19	N	607	TGL	C12-C13-C14-C29
19	Q	201	TGL	C17-C18-C19-C33
24	G	101	PEK	C25-C26-C27-C28
25	P	305	CDL	C71-C72-C73-C74
25	P	305	CDL	C74-C75-C76-C77
27	E	201	PSC	C04-C05-N-C07
26	W	102	DMU	O5-C6-O16-C18
25	T	103	CDL	C79-C80-C81-C82
25	G	102	CDL	C56-C57-C58-C59
25	P	305	CDL	C76-C77-C78-C79
25	T	103	CDL	C17-C18-C19-C20
26	O	304	DMU	O16-C18-C19-C22
26	Z	101	DMU	C25-C28-C31-C34
25	G	102	CDL	CB7-C71-C72-C73
19	A	607	TGL	CA5-CA6-CA7-CA8
23	J	101	CHD	C16-C17-C20-C21
19	L	101	TGL	CC2-CC3-CC4-CC5
19	O	303	TGL	CB4-CB5-CB6-CB7
19	L	101	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	C11-C12-C13-C14
19	N	607	TGL	CA9-C20-C21-C22
25	P	305	CDL	C19-C20-C21-C22
19	A	607	TGL	CB4-CB5-CB6-CB7
25	T	103	CDL	C57-C58-C59-C60
24	T	102	PEK	C10-C11-C12-C13
25	T	103	CDL	C82-C83-C84-C85
19	L	101	TGL	CA9-C20-C21-C22
25	C	305	CDL	C61-C62-C63-C64
20	C	304	PGV	C2-C1-O01-C02
19	O	303	TGL	C13-C14-C29-C30
25	C	305	CDL	C38-C39-C40-C41
19	L	101	TGL	C11-C10-CB9-CB8
19	L	101	TGL	C21-C22-C23-C24
19	N	607	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
19	O	303	TGL	CA3-CA4-CA5-CA6
24	G	103	PEK	C25-C26-C27-C28
20	N	608	PGV	C22-C23-C24-C25
20	P	303	PGV	C7-C8-C9-C10
25	T	103	CDL	C55-C56-C57-C58
26	W	102	DMU	C22-C25-C28-C31
25	T	103	CDL	C77-C78-C79-C80
24	T	101	PEK	C33-C34-C35-C36
24	P	302	PEK	C24-C25-C26-C27
21	C	308	EDO	O1-C1-C2-O2
19	L	101	TGL	C19-C33-C34-C35
19	O	303	TGL	CB2-CB1-OG2-CG2
19	Q	201	TGL	CC2-CC3-CC4-CC5
19	D	201	TGL	CC1-CC2-CC3-CC4
19	Q	201	TGL	CC1-CC2-CC3-CC4
19	L	101	TGL	C25-C26-C27-C28
19	O	303	TGL	CA9-C20-C21-C22
19	D	201	TGL	CA2-CA3-CA4-CA5
24	G	101	PEK	C22-C23-C24-C25
24	P	302	PEK	C7-C8-C9-C10
19	Q	201	TGL	C18-C19-C33-C34
19	A	607	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
24	G	101	PEK	O02-C1-O01-C02
25	G	102	CDL	OB7-CB5-OB6-CB4
19	A	607	TGL	CA4-CA5-CA6-CA7
19	A	607	TGL	C20-C21-C22-C23
25	C	305	CDL	C41-C42-C43-C44
25	T	103	CDL	C56-C57-C58-C59
19	Q	201	TGL	C11-C10-CB9-CB8
27	E	201	PSC	C20-C21-C22-C23
26	P	307	DMU	O6-C11-C9-C8
19	D	201	TGL	CA6-CA7-CA8-CA9
19	L	101	TGL	C12-C13-C14-C29
19	L	101	TGL	C18-C19-C33-C34
19	O	303	TGL	C15-C16-C17-C18
20	P	303	PGV	C14-C15-C16-C17
24	T	102	PEK	C30-C31-C32-C33
19	A	607	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CB2-CB1-OG2-CG2
24	G	101	PEK	C2-C1-O01-C02
24	T	101	PEK	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	G	102	CDL	C51-CB5-OB6-CB4
25	T	103	CDL	C51-CB5-OB6-CB4
20	C	304	PGV	O01-C02-C03-O11
25	G	102	CDL	C17-C18-C19-C20
19	O	303	TGL	OB1-CB1-OG2-CG2
24	T	101	PEK	O02-C1-O01-C02
25	T	103	CDL	OB7-CB5-OB6-CB4
26	O	304	DMU	C1-C6-O16-C18
19	O	303	TGL	OG1-CG1-CG2-OG2
25	P	305	CDL	C59-C60-C61-C62
25	T	103	CDL	C20-C21-C22-C23
19	L	101	TGL	C22-C23-C24-C25
25	T	103	CDL	C62-C63-C64-C65
24	P	302	PEK	C2-C3-C4-C5
14	N	601	HEA	C26-C15-C16-C17
19	L	101	TGL	CC4-CC5-CC6-CC7
24	T	101	PEK	C24-C25-C26-C27
19	Q	201	TGL	CA6-CA7-CA8-CA9
25	G	102	CDL	C43-C44-C45-C46
20	N	609	PGV	C29-C30-C31-C32
25	G	102	CDL	OA7-CA5-OA6-CA4
25	G	102	CDL	C11-CA5-OA6-CA4
20	A	608	PGV	C29-C30-C31-C32
25	C	305	CDL	CB2-OB2-PB2-OB5
20	N	608	PGV	C01-C02-C03-O11
19	L	101	TGL	CA2-CA3-CA4-CA5
27	E	201	PSC	C1-C2-C3-C4
25	G	102	CDL	C13-C14-C15-C16
19	N	607	TGL	C11-C12-C13-C14
24	P	302	PEK	C15-C16-C17-C18
24	T	102	PEK	C15-C16-C17-C18
25	G	102	CDL	CA7-C31-C32-C33
19	A	607	TGL	CA6-CA7-CA8-CA9
19	A	607	TGL	CB3-CB4-CB5-CB6
19	O	303	TGL	CC7-CC8-CC9-C15
20	A	608	PGV	C7-C8-C9-C10
25	T	103	CDL	C39-C40-C41-C42
19	A	607	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	CG1-CG2-CG3-OG3
19	N	607	TGL	OG1-CG1-CG2-CG3
24	G	103	PEK	O03-C01-C02-C03
24	T	102	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C37-C38-C39-C40
25	T	103	CDL	CA3-CA4-CA6-OA8
27	R	201	PSC	C20-C19-O03-C01
19	N	607	TGL	C29-C30-C31-C32
26	O	304	DMU	C34-C37-C40-C43
20	P	303	PGV	C15-C16-C17-C18
25	P	305	CDL	C39-C40-C41-C42
25	T	103	CDL	C32-C33-C34-C35
25	T	103	CDL	C58-C59-C60-C61
19	L	101	TGL	OG1-CA1-CA2-CA3
25	T	103	CDL	C32-C31-CA7-OA8
24	C	302	PEK	O04-C21-O03-C01
19	D	201	TGL	C21-C20-CA9-CA8
19	O	303	TGL	C16-C17-C18-C19
24	P	302	PEK	C27-C28-C29-C30
25	T	103	CDL	C24-C25-C26-C27
20	C	304	PGV	C11-C10-C9-C8
19	D	201	TGL	C17-C18-C19-C33
25	G	102	CDL	C19-C20-C21-C22
19	N	607	TGL	CA5-CA6-CA7-CA8
24	C	302	PEK	C25-C26-C27-C28
25	C	305	CDL	CA5-C11-C12-C13
25	G	102	CDL	C53-C54-C55-C56
19	L	101	TGL	CG3-CG2-OG2-CB1
19	D	201	TGL	CB2-CB3-CB4-CB5
19	O	303	TGL	CB3-CB4-CB5-CB6
24	C	302	PEK	C10-C11-C12-C13
24	P	302	PEK	C13-C14-C15-C16
27	E	201	PSC	O01-C1-C2-C3
25	G	102	CDL	C58-C59-C60-C61
25	P	305	CDL	C58-C59-C60-C61
19	N	607	TGL	OG1-CA1-CA2-CA3
25	G	102	CDL	C82-C83-C84-C85
27	E	201	PSC	C28-C29-C30-C31
26	Z	101	DMU	C18-C19-C22-C25
25	T	103	CDL	C80-C81-C82-C83
19	N	607	TGL	C11-C10-CB9-CB8
24	G	103	PEK	C16-C17-C18-C19
25	C	305	CDL	C57-C58-C59-C60
24	C	302	PEK	C22-C21-O03-C01
23	C	306	CHD	C20-C22-C23-C24
19	Q	201	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
24	C	302	PEK	C4-C5-C6-C7
24	G	103	PEK	C13-C14-C15-C16
25	P	305	CDL	C75-C76-C77-C78
24	P	302	PEK	C3-C4-C5-C6
20	C	304	PGV	C01-C02-C03-O11
24	T	101	PEK	C01-C02-C03-O11
25	C	305	CDL	OA5-CA3-CA4-CA6
25	C	305	CDL	C63-C64-C65-C66
20	A	608	PGV	C26-C27-C28-C29
24	G	101	PEK	C31-C32-C33-C34
25	C	305	CDL	C58-C59-C60-C61
19	A	607	TGL	CC2-CC1-OG3-CG3
19	O	303	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	C02-C03-O11-P
24	T	101	PEK	C29-C30-C31-C32
19	A	607	TGL	C18-C19-C33-C34
19	O	303	TGL	OG1-CG1-CG2-CG3
20	A	609	PGV	O03-C01-C02-C03
25	G	102	CDL	CA3-CA4-CA6-OA8
20	A	608	PGV	C31-C32-C33-C34
24	T	101	PEK	C4-C5-C6-C7
19	Q	201	TGL	C12-C13-C14-C29
24	P	302	PEK	C16-C17-C18-C19
20	P	304	PGV	C3-C4-C5-C6
24	G	103	PEK	C33-C34-C35-C36
25	C	305	CDL	C59-C60-C61-C62
14	A	601	HEA	C2A-C3A-CMA-OMA
24	C	302	PEK	C9-C10-C11-C12
24	G	101	PEK	C5-C6-C7-C8
24	G	101	PEK	C6-C7-C8-C9
24	G	101	PEK	C11-C10-C9-C8
24	G	101	PEK	C9-C10-C11-C12
24	G	101	PEK	C11-C12-C13-C14
24	G	101	PEK	C12-C13-C14-C15
24	G	103	PEK	C5-C6-C7-C8
24	G	103	PEK	C6-C7-C8-C9
24	G	103	PEK	C11-C10-C9-C8
24	G	103	PEK	C9-C10-C11-C12
24	P	302	PEK	C9-C10-C11-C12
24	T	101	PEK	C6-C7-C8-C9
24	T	101	PEK	C11-C10-C9-C8
24	T	101	PEK	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	T	101	PEK	C11-C12-C13-C14
24	T	102	PEK	C5-C6-C7-C8
24	T	102	PEK	C9-C10-C11-C12
24	T	102	PEK	C11-C12-C13-C14
24	T	102	PEK	C12-C13-C14-C15
27	E	201	PSC	C9-C10-C11-C12
27	E	201	PSC	C10-C11-C12-C13
27	R	201	PSC	C9-C10-C11-C12
27	R	201	PSC	C10-C11-C12-C13
19	N	607	TGL	C19-C33-C34-C35
26	P	307	DMU	C22-C25-C28-C31
19	A	607	TGL	C16-C17-C18-C19
24	T	101	PEK	C22-C23-C24-C25
25	C	305	CDL	C60-C61-C62-C63
25	C	305	CDL	OA5-CA3-CA4-OA6
25	T	103	CDL	OA5-CA3-CA4-OA6
27	E	201	PSC	C21-C22-C23-C24
19	N	607	TGL	CB4-CB5-CB6-CB7
19	N	607	TGL	CC4-CC5-CC6-CC7
19	O	303	TGL	C11-C10-CB9-CB8
27	R	201	PSC	O04-C19-O03-C01
19	D	201	TGL	OG2-CG2-CG3-OG3
20	A	609	PGV	O03-C01-C02-O01
24	G	103	PEK	O03-C01-C02-O01
25	G	102	CDL	OA6-CA4-CA6-OA8
25	P	305	CDL	OA6-CA4-CA6-OA8
25	T	103	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	CB5-CB6-CB7-CB8
19	Q	201	TGL	C15-C16-C17-C18
27	R	201	PSC	C11-C10-C9-C8
19	A	607	TGL	CA2-CA3-CA4-CA5
20	N	609	PGV	C5-C6-C7-C8
19	D	201	TGL	CA5-CA6-CA7-CA8
19	O	303	TGL	CB6-CB7-CB8-CB9
27	E	201	PSC	C27-C28-C29-C30
20	P	303	PGV	C02-C03-O11-P
25	P	305	CDL	CA4-CA3-OA5-PA1
24	C	302	PEK	C28-C29-C30-C31
24	G	103	PEK	C30-C31-C32-C33
26	M	101	DMU	C28-C31-C34-C37
27	E	201	PSC	C24-C25-C26-C27
25	G	102	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	C21-C20-CA9-CA8
20	P	304	PGV	C30-C31-C32-C33
20	A	609	PGV	C01-C02-C03-O11
24	G	101	PEK	C01-C02-C03-O11
25	C	305	CDL	OB5-CB3-CB4-CB6
25	P	305	CDL	OA5-CA3-CA4-CA6
19	O	303	TGL	C20-C21-C22-C23
19	Q	201	TGL	C23-C24-C25-C26
25	C	305	CDL	C43-C44-C45-C46
19	A	607	TGL	C11-C10-CB9-CB8
25	C	305	CDL	C14-C15-C16-C17
27	E	201	PSC	C20-C19-O03-C01
19	N	607	TGL	C17-C18-C19-C33
19	N	607	TGL	C15-C16-C17-C18
19	O	303	TGL	CA6-CA7-CA8-CA9
24	T	101	PEK	O03-C01-C02-C03
25	G	102	CDL	C1-CB2-OB2-PB2
25	T	103	CDL	C1-CB2-OB2-PB2
20	N	608	PGV	O01-C02-C03-O11
24	G	101	PEK	O01-C02-C03-O11
24	T	101	PEK	O01-C02-C03-O11
26	P	307	DMU	C25-C28-C31-C34
25	G	102	CDL	C39-C40-C41-C42
26	M	101	DMU	O6-C11-C9-C8
19	A	607	TGL	OC1-CC1-OG3-CG3
19	O	303	TGL	OC1-CC1-OG3-CG3
26	Z	101	DMU	C34-C37-C40-C43
19	A	607	TGL	OG2-CG2-CG3-OG3
19	L	101	TGL	OG1-CG1-CG2-OG2
19	N	607	TGL	OG1-CG1-CG2-OG2
19	O	303	TGL	OG2-CG2-CG3-OG3
19	Q	201	TGL	OG2-CG2-CG3-OG3
25	G	102	CDL	OB6-CB4-CB6-OB8
25	T	103	CDL	OA6-CA4-CA6-OA8
20	A	608	PGV	C5-C6-C7-C8
24	T	102	PEK	C31-C32-C33-C34
25	G	102	CDL	C74-C75-C76-C77
26	Z	101	DMU	O6-C11-C9-O1
25	T	103	CDL	C22-C23-C24-C25
25	G	102	CDL	C32-C31-CA7-OA8
25	G	102	CDL	C40-C41-C42-C43
20	N	608	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C63-C64-C65-C66
24	G	103	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O12
19	A	607	TGL	C13-C14-C29-C30
24	T	102	PEK	C22-C23-C24-C25
20	P	304	PGV	C26-C27-C28-C29
20	N	608	PGV	C02-C03-O11-P
25	C	305	CDL	CA4-CA3-OA5-PA1
19	N	607	TGL	C18-C19-C33-C34
25	P	305	CDL	C36-C37-C38-C39
20	A	609	PGV	C03-O11-P-O14
20	A	609	PGV	C04-O12-P-O13
20	C	304	PGV	C04-O12-P-O14
20	P	304	PGV	C04-O12-P-O14
24	T	101	PEK	C03-O11-P-O13
24	T	101	PEK	C04-O12-P-O14
24	T	102	PEK	C03-O11-P-O14
25	C	305	CDL	CA3-OA5-PA1-OA3
25	C	305	CDL	CB2-OB2-PB2-OB3
25	C	305	CDL	CB3-OB5-PB2-OB3
25	G	102	CDL	CA2-OA2-PA1-OA4
25	G	102	CDL	CA3-OA5-PA1-OA3
25	G	102	CDL	CB2-OB2-PB2-OB4
25	P	305	CDL	CA2-OA2-PA1-OA4
25	P	305	CDL	CA3-OA5-PA1-OA3
25	P	305	CDL	CB2-OB2-PB2-OB3
25	P	305	CDL	CB3-OB5-PB2-OB4
25	T	103	CDL	CA2-OA2-PA1-OA4
25	T	103	CDL	CB2-OB2-PB2-OB4
25	C	305	CDL	CB7-C71-C72-C73
25	G	102	CDL	CA5-C11-C12-C13
27	R	201	PSC	C20-C21-C22-C23
26	M	101	DMU	C25-C28-C31-C34
24	G	103	PEK	C7-C8-C9-C10
24	C	302	PEK	C2-C3-C4-C5
25	P	305	CDL	OA5-CA3-CA4-OA6
19	D	201	TGL	CB9-C10-C11-C12
25	P	305	CDL	C78-C79-C80-C81
27	E	201	PSC	C26-C27-C28-C29
27	R	201	PSC	C04-C05-N-C06
20	N	608	PGV	C5-C6-C7-C8
24	G	103	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	CB7-C71-C72-C73
14	N	601	HEA	C4A-C3A-CMA-OMA
19	A	607	TGL	CG1-CG2-CG3-OG3
19	L	101	TGL	OG1-CG1-CG2-CG3
19	O	303	TGL	CG1-CG2-CG3-OG3
19	Q	201	TGL	CG1-CG2-CG3-OG3
25	P	305	CDL	C34-C35-C36-C37
25	P	305	CDL	OB6-CB4-CB6-OB8
20	C	303	PGV	C02-C03-O11-P
14	N	601	HEA	C14-C15-C16-C17
25	P	305	CDL	C32-C31-CA7-OA8
27	R	201	PSC	O01-C1-C2-C3
25	G	102	CDL	C54-C55-C56-C57
25	C	305	CDL	C15-C16-C17-C18
27	E	201	PSC	O04-C19-O03-C01
19	A	607	TGL	CB7-CB8-CB9-C10
19	D	201	TGL	C20-C21-C22-C23
20	A	609	PGV	C10-C11-C12-C13
19	N	607	TGL	C25-C26-C27-C28
25	P	305	CDL	C16-C17-C18-C19
19	O	303	TGL	C21-C22-C23-C24
19	L	101	TGL	CB4-CB5-CB6-CB7
19	N	607	TGL	CG1-CG2-OG2-CB1
25	T	103	CDL	CA2-C1-CB2-OB2
24	T	102	PEK	O02-C1-O01-C02
20	P	304	PGV	C02-C03-O11-P
20	A	609	PGV	O01-C02-C03-O11
21	P	308	EDO	O1-C1-C2-O2
25	G	102	CDL	C44-C45-C46-C47
24	G	101	PEK	C28-C29-C30-C31
25	C	305	CDL	C56-C57-C58-C59
25	G	102	CDL	C80-C81-C82-C83
25	C	305	CDL	CA2-OA2-PA1-OA5
25	T	103	CDL	CA3-OA5-PA1-OA2
27	R	201	PSC	C03-O11-P-O12
25	P	305	CDL	C17-C18-C19-C20
19	N	607	TGL	CG2-CG1-OG1-CA1
25	G	102	CDL	CB3-CB4-CB6-OB8
19	D	201	TGL	CA7-CA8-CA9-C20
27	R	201	PSC	C12-C13-C14-C15
19	A	607	TGL	CC7-CC8-CC9-C15
26	M	101	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	OA1-CA1-CA2-CA3
25	P	305	CDL	C80-C81-C82-C83
25	T	103	CDL	CB4-CB3-OB5-PB2
20	C	304	PGV	C3-C4-C5-C6
20	C	303	PGV	C9-C10-C11-C12
24	P	302	PEK	C22-C23-C24-C25
20	N	609	PGV	C7-C8-C9-C10
20	N	608	PGV	C10-C11-C12-C13
20	N	609	PGV	C10-C11-C12-C13
19	D	201	TGL	C15-C16-C17-C18
19	D	201	TGL	C12-C13-C14-C29
23	W	101	CHD	C22-C23-C24-O26
19	L	101	TGL	CA7-CA8-CA9-C20
25	C	305	CDL	C23-C24-C25-C26
25	T	103	CDL	OA5-CA3-CA4-CA6
14	A	602	HEA	CAA-CBA-CGA-O1A
25	G	102	CDL	C57-C58-C59-C60
27	R	201	PSC	C2-C3-C4-C5
19	N	607	TGL	OA1-CA1-CA2-CA3
23	O	302	CHD	C22-C23-C24-O25
25	C	305	CDL	C82-C83-C84-C85
26	P	307	DMU	C1-C6-O16-C18
23	B	302	CHD	C22-C23-C24-O25
24	T	101	PEK	O03-C01-C02-O01
25	C	305	CDL	OB6-CB4-CB6-OB8
20	C	303	PGV	C13-C14-C15-C16
23	W	101	CHD	C22-C23-C24-O25
20	P	303	PGV	C9-C10-C11-C12
26	C	307	DMU	C19-C18-O16-C6
14	N	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O1A
24	T	101	PEK	C27-C28-C29-C30
19	O	303	TGL	CC2-CC3-CC4-CC5
25	C	305	CDL	C53-C54-C55-C56
25	C	305	CDL	C72-C73-C74-C75
19	D	201	TGL	CA9-C20-C21-C22
25	T	103	CDL	C43-C44-C45-C46
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	601	HEA	CAD-CBD-CGD-O2D
20	C	303	PGV	C31-C32-C33-C34
19	N	607	TGL	CC6-CC7-CC8-CC9
26	C	307	DMU	C2-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAA-CBA-CGA-O2A
23	J	101	CHD	C22-C23-C24-O25
23	O	302	CHD	C22-C23-C24-O26
14	N	602	HEA	C2A-C3A-CMA-OMA
24	C	302	PEK	C5-C6-C7-C8
24	P	302	PEK	C5-C6-C7-C8
24	T	101	PEK	C12-C13-C14-C15
24	G	101	PEK	C23-C24-C25-C26
14	A	601	HEA	C26-C15-C16-C17
19	O	303	TGL	CA4-CA5-CA6-CA7
14	A	602	HEA	CAA-CBA-CGA-O2A
14	A	602	HEA	CAD-CBD-CGD-O1D
19	A	607	TGL	C15-C16-C17-C18
19	O	303	TGL	C17-C18-C19-C33
25	C	305	CDL	C34-C35-C36-C37
23	B	302	CHD	C22-C23-C24-O26
27	E	201	PSC	C2-C3-C4-C5
14	N	602	HEA	CAD-CBD-CGD-O2D
24	C	302	PEK	C7-C8-C9-C10
14	N	602	HEA	CAD-CBD-CGD-O1D
19	A	607	TGL	C21-C22-C23-C24
19	D	201	TGL	C33-C34-C35-C36
25	P	305	CDL	C43-C44-C45-C46
19	A	607	TGL	C19-C33-C34-C35
25	P	305	CDL	CB3-CB4-CB6-OB8
21	Q	202	EDO	O1-C1-C2-O2
26	P	307	DMU	C5-C10-O7-C3
26	P	307	DMU	O16-C18-C19-C22
20	N	609	PGV	O03-C19-C20-C21
24	P	302	PEK	C22-C21-O03-C01
14	A	602	HEA	CAD-CBD-CGD-O2D
23	J	101	CHD	C22-C23-C24-O26
25	T	103	CDL	C54-C55-C56-C57
20	N	609	PGV	C9-C10-C11-C12
27	E	201	PSC	C12-C13-C14-C15
25	G	102	CDL	C32-C31-CA7-OA9
19	Q	201	TGL	CC6-CC7-CC8-CC9
19	L	101	TGL	OG2-CB1-CB2-CB3
19	N	607	TGL	OG2-CB1-CB2-CB3
25	P	305	CDL	C72-C73-C74-C75
19	A	607	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
27	R	201	PSC	C5-C6-C7-C8
20	A	608	PGV	C9-C10-C11-C12
20	N	608	PGV	C9-C10-C11-C12
24	G	101	PEK	C03-O11-P-O13
14	A	602	HEA	C26-C15-C16-C17
25	T	103	CDL	C53-C54-C55-C56
19	A	607	TGL	CC5-CC6-CC7-CC8
24	C	302	PEK	C14-C15-C16-C17
24	G	101	PEK	C3-C4-C5-C6
24	G	103	PEK	C3-C4-C5-C6
24	T	102	PEK	C3-C4-C5-C6
27	R	201	PSC	C7-C8-C9-C10
19	A	607	TGL	CC3-CC4-CC5-CC6
26	O	304	DMU	C31-C34-C37-C40
23	C	301	CHD	C22-C23-C24-O25
25	C	305	CDL	CB3-CB4-CB6-OB8
25	G	102	CDL	CB4-CB3-OB5-PB2
25	T	103	CDL	CB3-CB4-CB6-OB8
23	P	301	CHD	C22-C23-C24-O25
24	P	302	PEK	O03-C21-C22-C23
27	E	201	PSC	O02-C1-C2-C3
24	G	101	PEK	O01-C1-C2-C3
25	P	305	CDL	C32-C31-CA7-OA9
24	G	103	PEK	C14-C15-C16-C17
24	T	101	PEK	C3-C4-C5-C6
19	D	201	TGL	C16-C17-C18-C19
24	P	302	PEK	O01-C1-C2-C3
25	P	305	CDL	C21-C22-C23-C24
19	D	201	TGL	C24-C25-C26-C27
24	P	302	PEK	O04-C21-O03-C01
20	P	303	PGV	C24-C25-C26-C27
20	C	304	PGV	C9-C10-C11-C12
20	N	608	PGV	C11-C12-C13-C14
19	D	201	TGL	OG2-CB1-CB2-CB3
25	G	102	CDL	C62-C63-C64-C65
20	P	304	PGV	C14-C15-C16-C17
24	T	102	PEK	C2-C1-O01-C02
24	T	101	PEK	O01-C1-C2-C3
20	N	609	PGV	C11-C12-C13-C14
20	N	608	PGV	O03-C19-C20-C21
19	N	607	TGL	C10-C11-C12-C13
27	E	201	PSC	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
25	P	305	CDL	C23-C24-C25-C26
20	C	304	PGV	C31-C32-C33-C34
24	T	101	PEK	C26-C27-C28-C29
27	E	201	PSC	C23-C24-C25-C26
24	T	102	PEK	C26-C27-C28-C29
27	R	201	PSC	C04-C05-N-C07
24	P	302	PEK	O04-C21-C22-C23
25	G	102	CDL	C11-C12-C13-C14
24	G	101	PEK	O02-C1-C2-C3
19	Q	201	TGL	C16-C15-CC9-CC8
25	P	305	CDL	C14-C15-C16-C17
27	E	201	PSC	C7-C8-C9-C10
20	N	608	PGV	O04-C19-C20-C21
25	T	103	CDL	C32-C31-CA7-OA9
19	O	303	TGL	C21-C20-CA9-CA8
20	N	608	PGV	C11-C10-C9-C8
25	P	305	CDL	C61-C62-C63-C64
24	T	102	PEK	C33-C34-C35-C36
14	N	601	HEA	CAA-CBA-CGA-O1A
19	N	607	TGL	CB3-CB4-CB5-CB6
19	A	607	TGL	OG1-CA1-CA2-CA3
14	A	601	HEA	C14-C15-C16-C17
24	G	103	PEK	C03-O11-P-O13
24	G	103	PEK	C03-O11-P-O14
24	T	101	PEK	C03-O11-P-O14
25	T	103	CDL	CA3-OA5-PA1-OA3
20	P	304	PGV	C15-C16-C17-C18
20	P	304	PGV	C28-C29-C30-C31
24	C	302	PEK	O12-C04-C05-N
21	N	614	EDO	O1-C1-C2-O2
23	C	306	CHD	C22-C23-C24-O25
23	P	301	CHD	C22-C23-C24-O26
24	P	302	PEK	O02-C1-C2-C3
25	P	305	CDL	CA3-CA4-OA6-CA5
27	E	201	PSC	C05-C04-O12-P
27	R	201	PSC	C05-C04-O12-P
20	P	303	PGV	C31-C32-C33-C34
19	O	303	TGL	OG1-CA1-CA2-CA3
20	P	304	PGV	O12-C04-C05-O05
19	L	101	TGL	C24-C25-C26-C27
20	A	608	PGV	C11-C12-C13-C14
24	T	101	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	CAA-CBA-CGA-O1A
20	P	304	PGV	O01-C1-C2-C3
14	A	601	HEA	CAA-CBA-CGA-O2A
24	T	101	PEK	O02-C1-C2-C3
25	P	305	CDL	OB5-CB3-CB4-OB6
19	A	607	TGL	OA1-CA1-CA2-CA3
26	M	101	DMU	O6-C11-C9-O1
19	D	201	TGL	OG3-CC1-CC2-CC3
20	A	608	PGV	O03-C19-C20-C21
19	O	303	TGL	C22-C23-C24-C25
24	C	302	PEK	O02-C1-C2-C3
27	R	201	PSC	O02-C1-C2-C3
19	Q	201	TGL	OG1-CA1-CA2-CA3
19	Q	201	TGL	OG2-CB1-CB2-CB3
19	Q	201	TGL	CA3-CA4-CA5-CA6
19	N	607	TGL	C24-C25-C26-C27

There are no ring outliers.

44 monomers are involved in 216 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	602	HEA	2	0
23	B	302	CHD	1	0
26	O	304	DMU	1	0
14	N	601	HEA	3	0
20	C	303	PGV	5	0
23	O	302	CHD	2	0
25	C	305	CDL	15	0
14	N	602	HEA	2	0
26	P	307	DMU	8	0
24	G	101	PEK	1	0
20	P	304	PGV	3	0
26	M	101	DMU	1	0
23	J	101	CHD	2	0
26	Z	101	DMU	1	0
24	P	302	PEK	6	0
24	G	103	PEK	4	0
20	P	303	PGV	3	0
19	N	607	TGL	8	0
25	G	102	CDL	23	0
26	C	307	DMU	2	0
26	W	102	DMU	4	0

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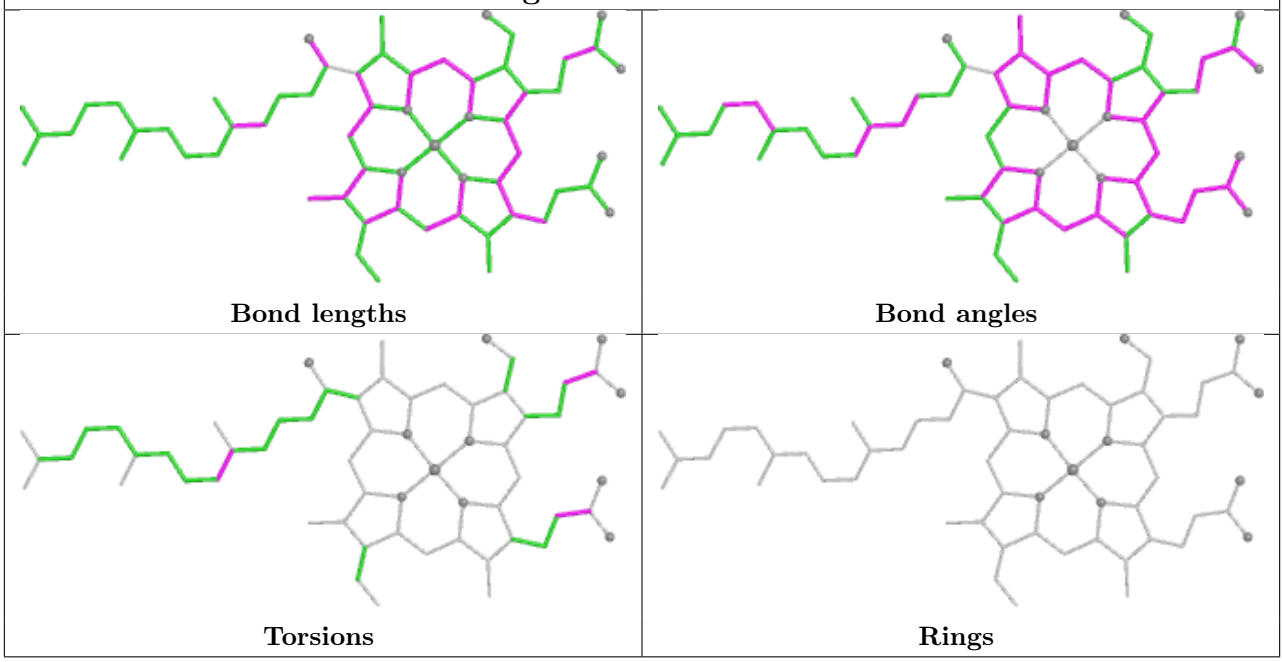
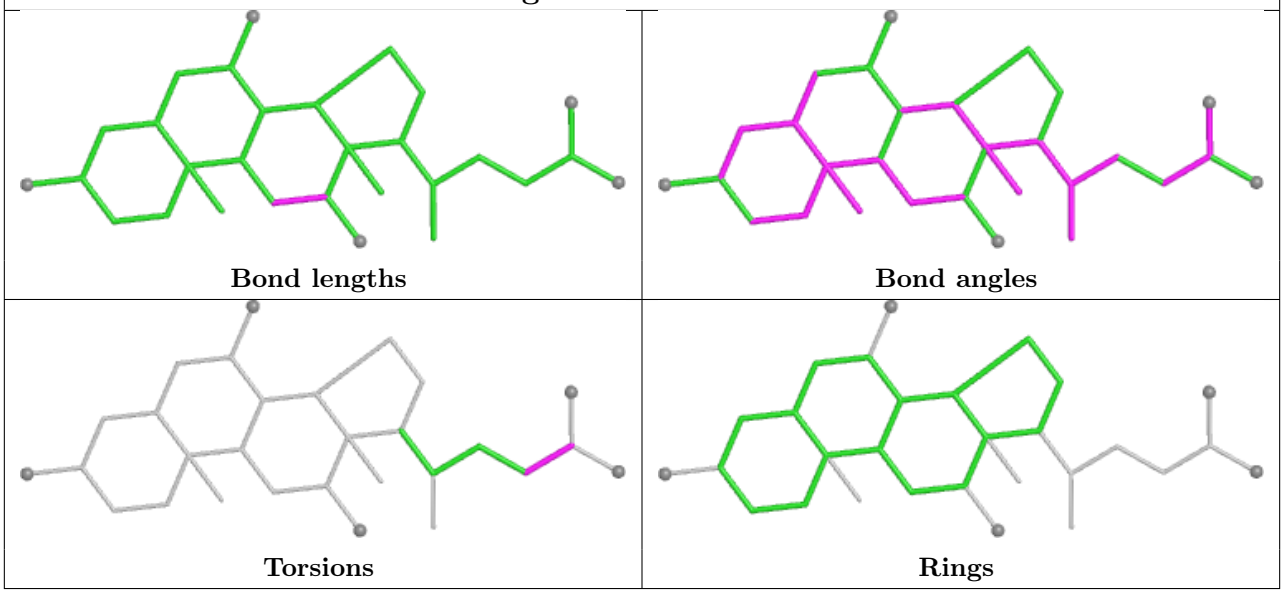
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Q	201	TGL	9	0
14	A	601	HEA	3	0
21	N	615	EDO	1	0
23	P	306	CHD	1	0
25	P	305	CDL	19	0
25	T	103	CDL	14	0
21	A	613	EDO	1	0
20	C	304	PGV	4	0
21	N	614	EDO	1	0
27	E	201	PSC	12	0
19	L	101	TGL	8	0
19	D	201	TGL	8	0
23	C	301	CHD	1	0
24	C	302	PEK	6	0
19	A	607	TGL	3	0
24	T	101	PEK	4	0
27	R	201	PSC	10	0
24	T	102	PEK	6	0
20	N	608	PGV	5	0
23	C	306	CHD	2	0
23	W	101	CHD	1	0
20	A	609	PGV	4	0
21	P	308	EDO	1	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 then 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.

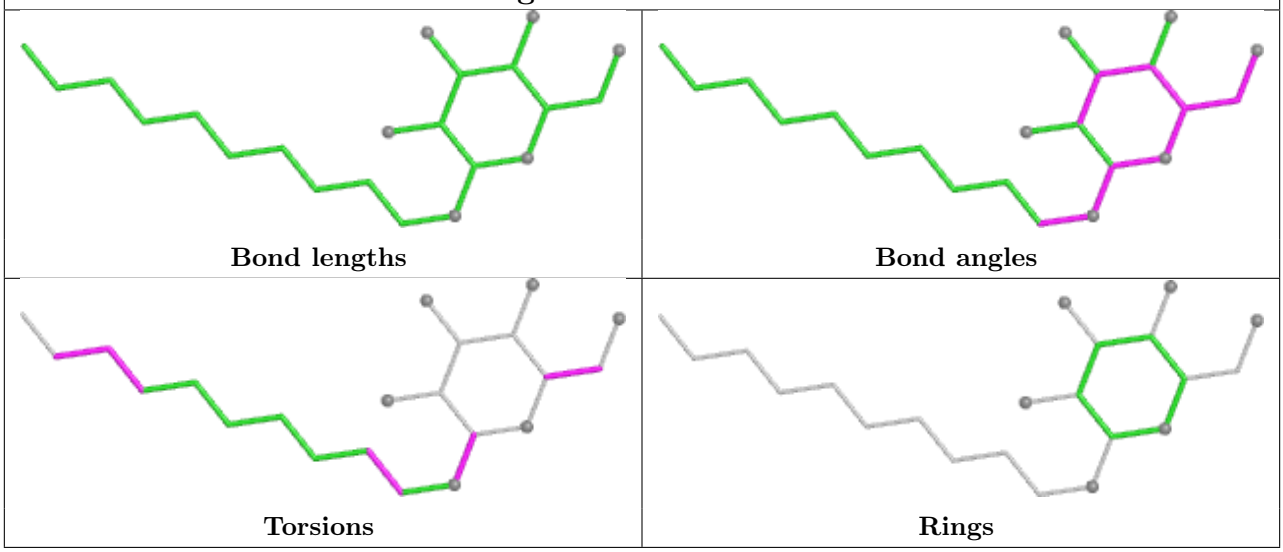
Ligand HEA A 602



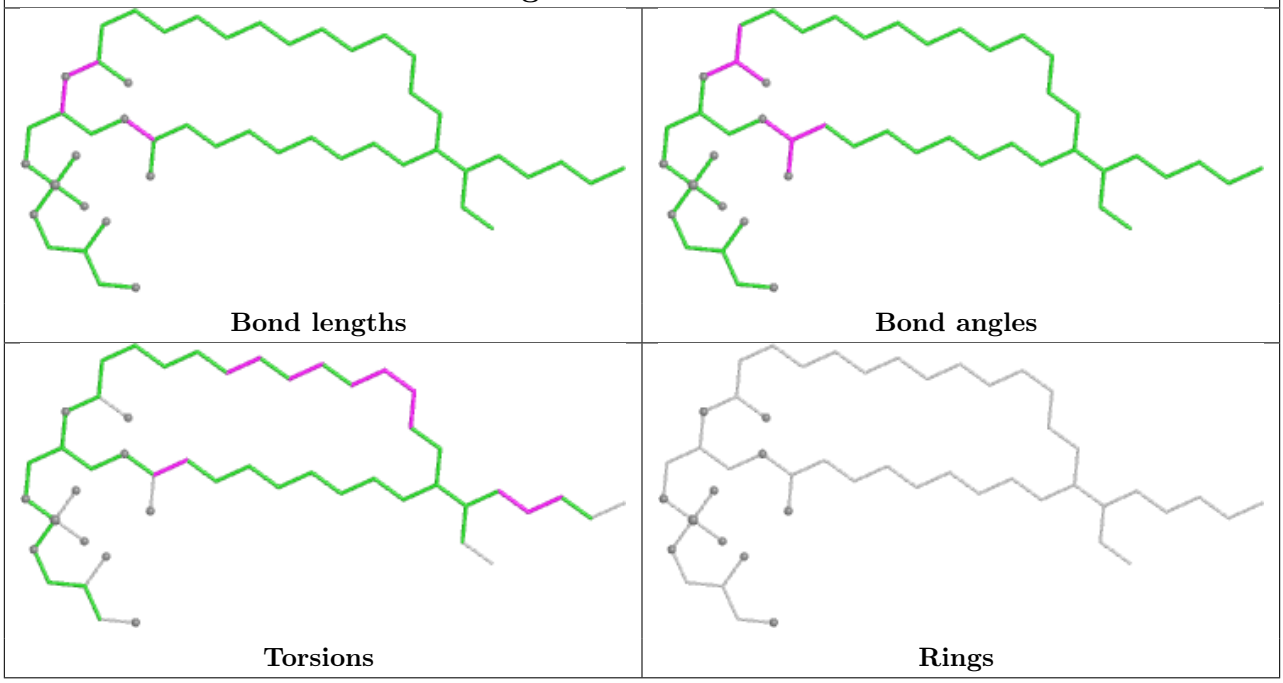
Ligand CHD B 302



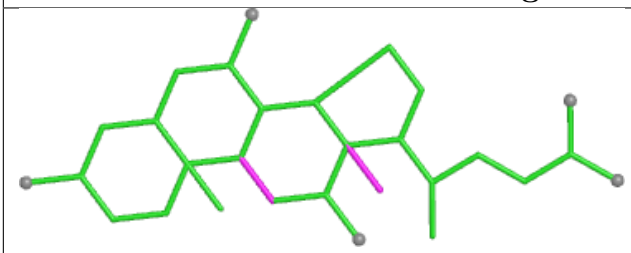
Ligand DMU O 304



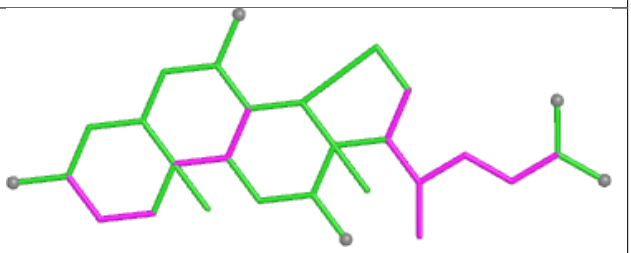
Ligand PGV N 609



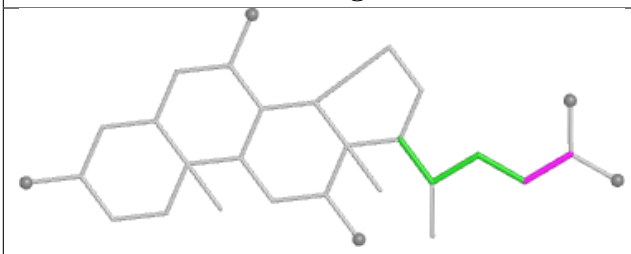
Ligand CHD P 301



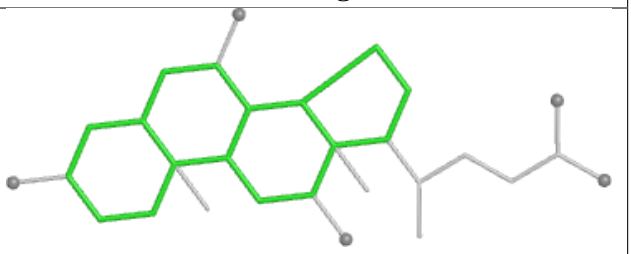
Bond lengths



Bond angles

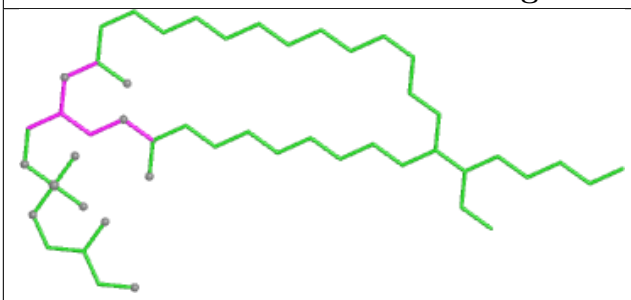


Torsions

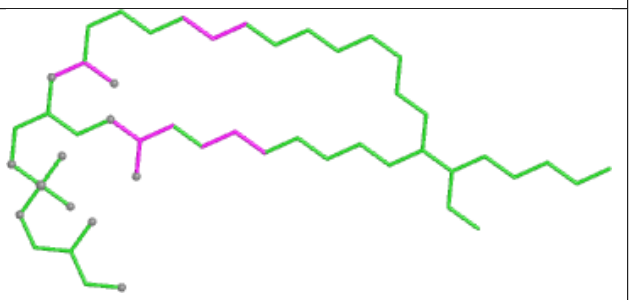


Rings

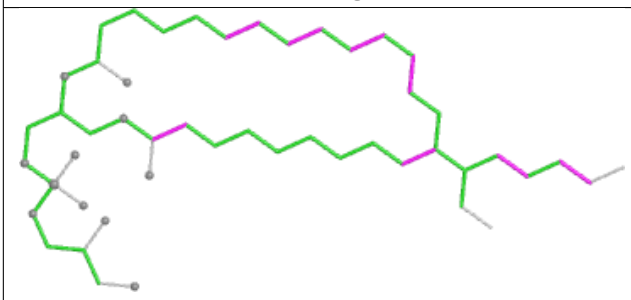
Ligand PGV A 608



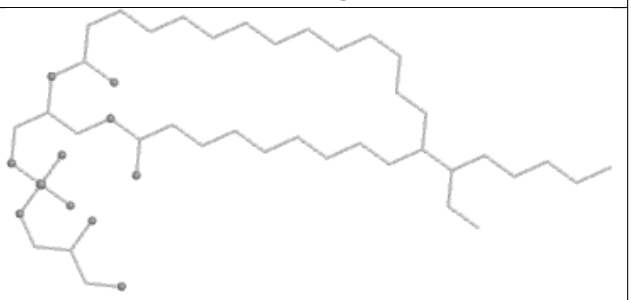
Bond lengths



Bond angles

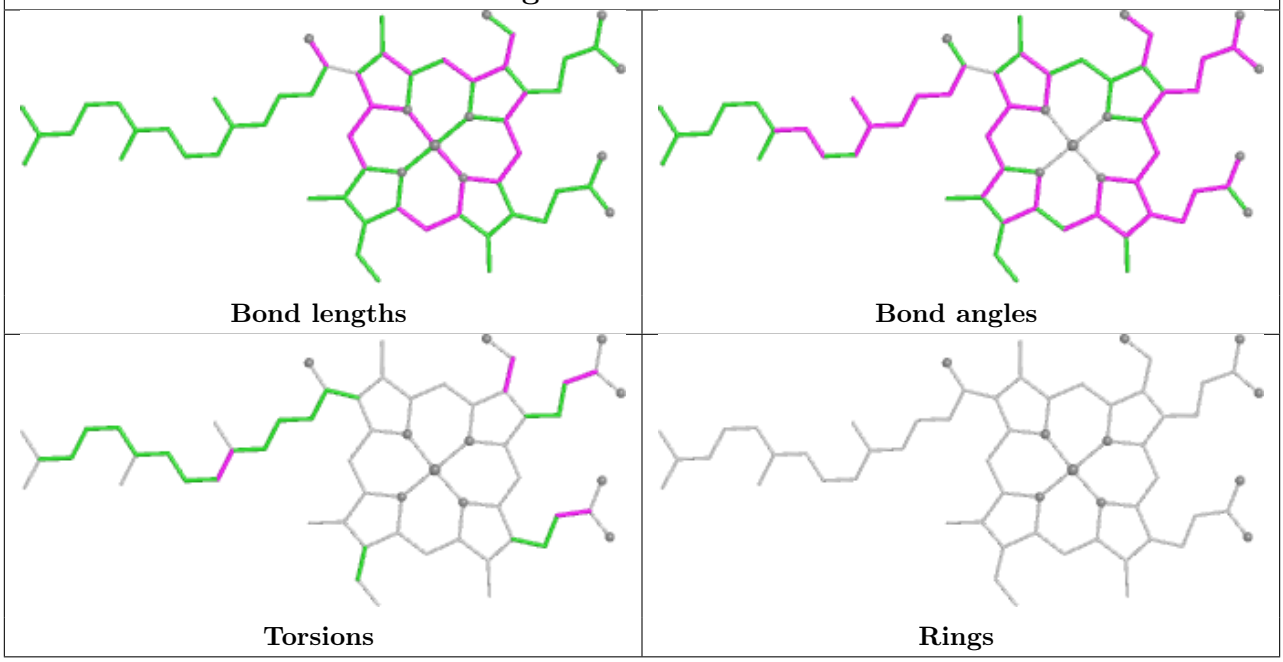


Torsions

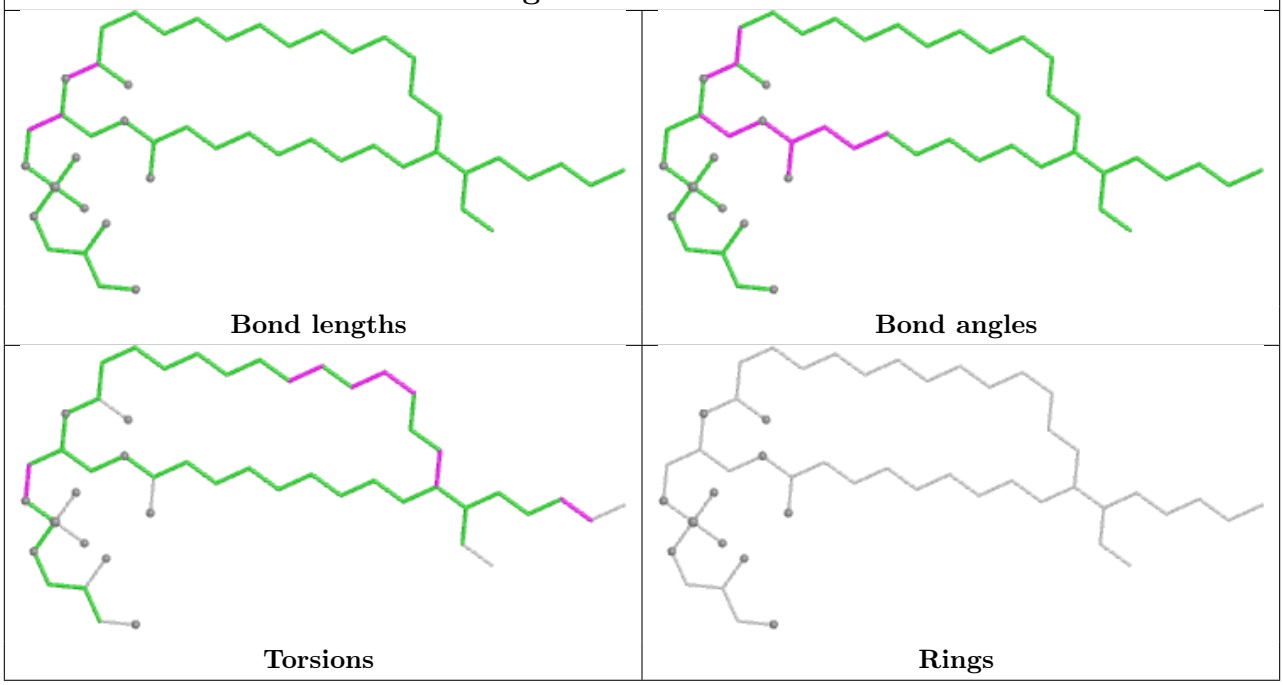


Rings

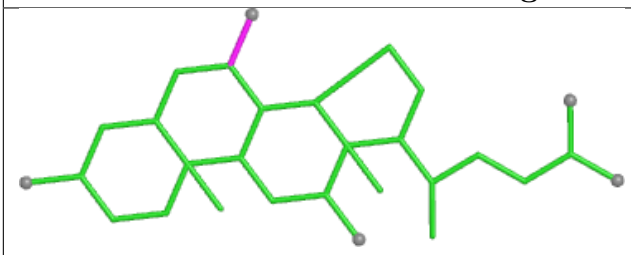
Ligand HEA N 601



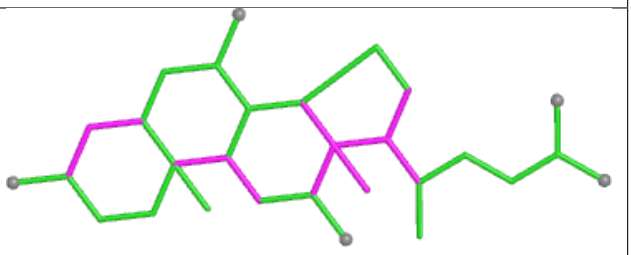
Ligand PGV C 303



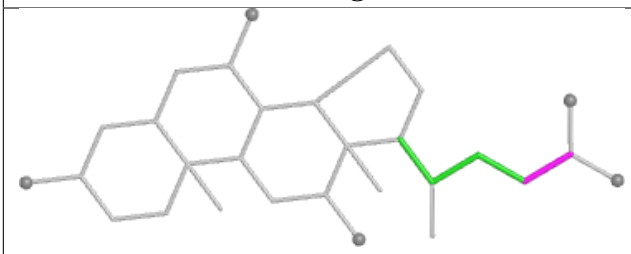
Ligand CHD O 302



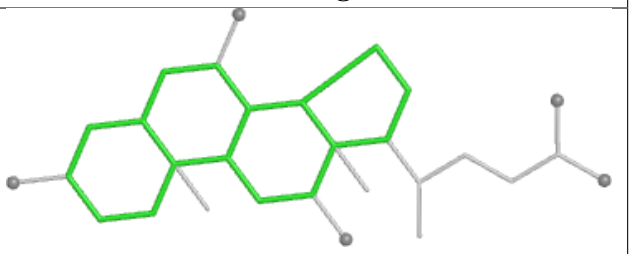
Bond lengths



Bond angles

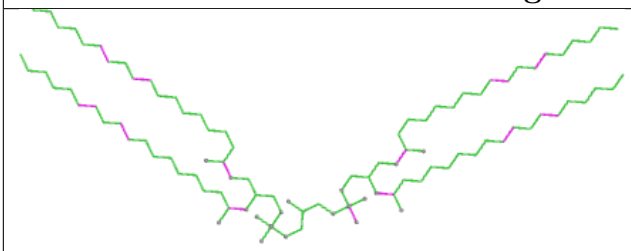


Torsions

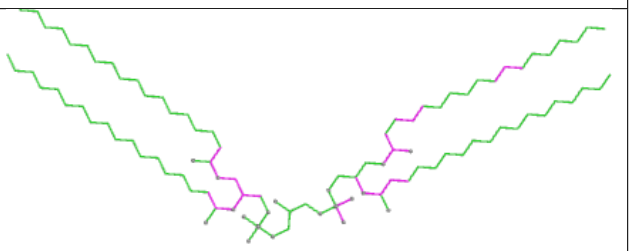


Rings

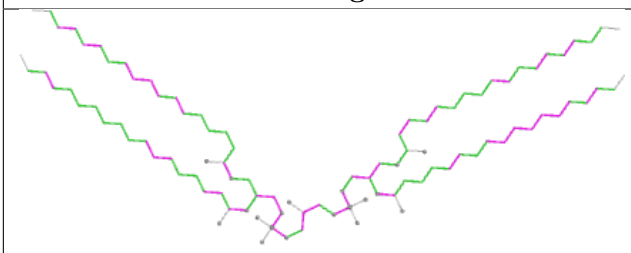
Ligand CDL C 305



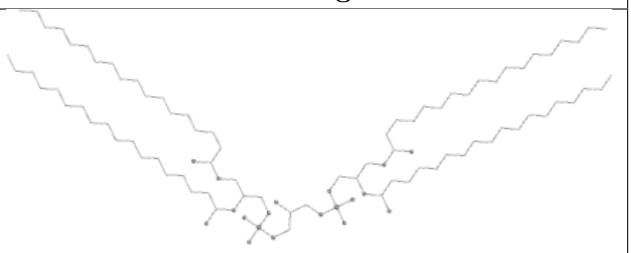
Bond lengths



Bond angles

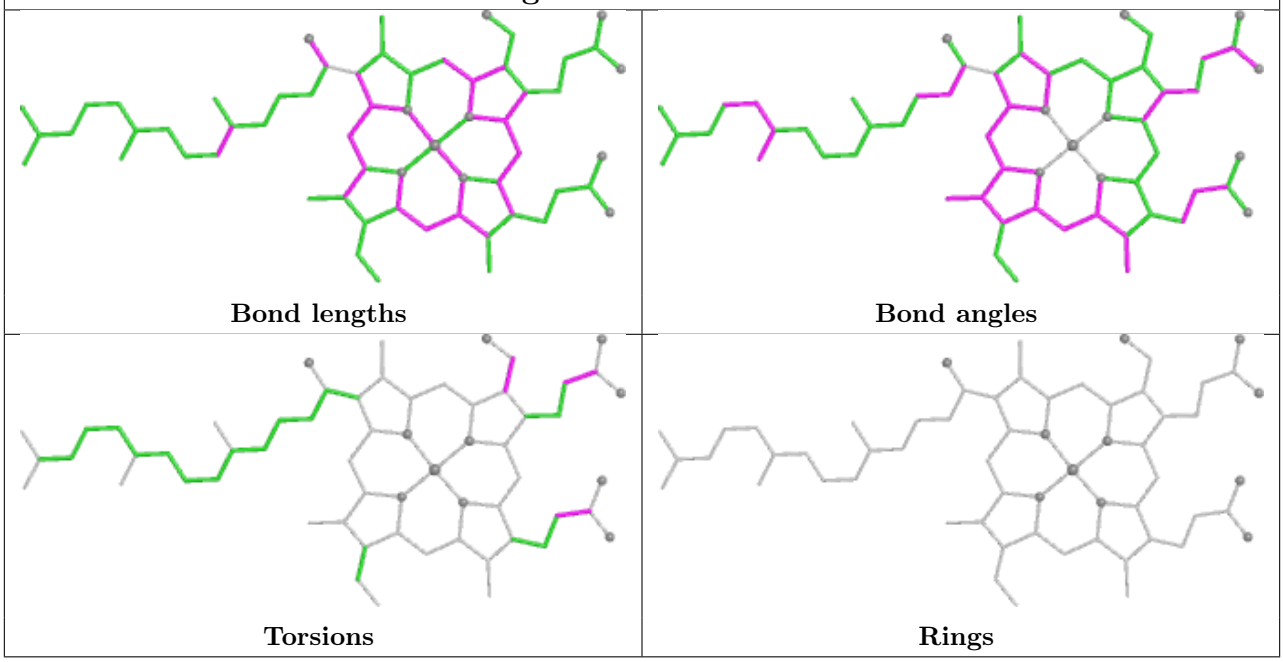


Torsions

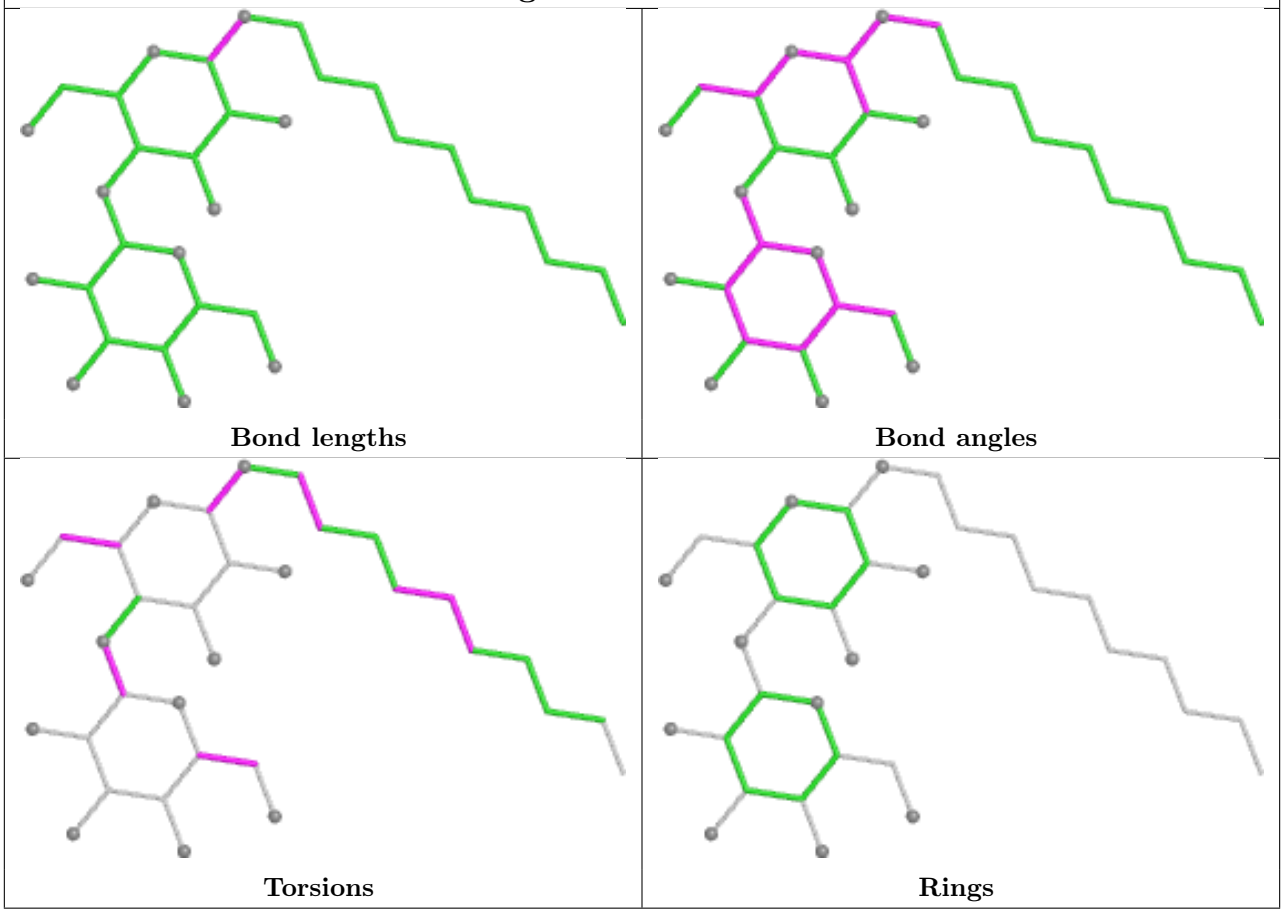


Rings

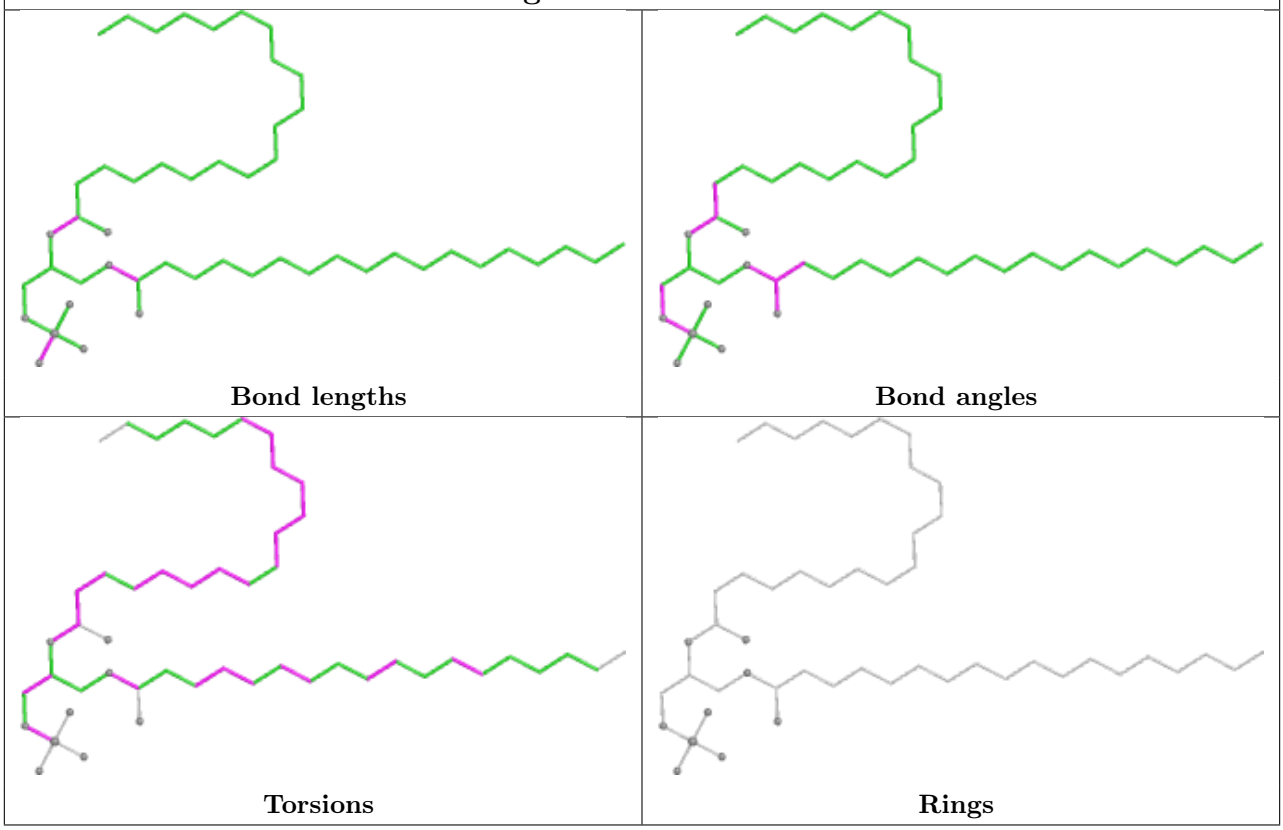
Ligand HEA N 602



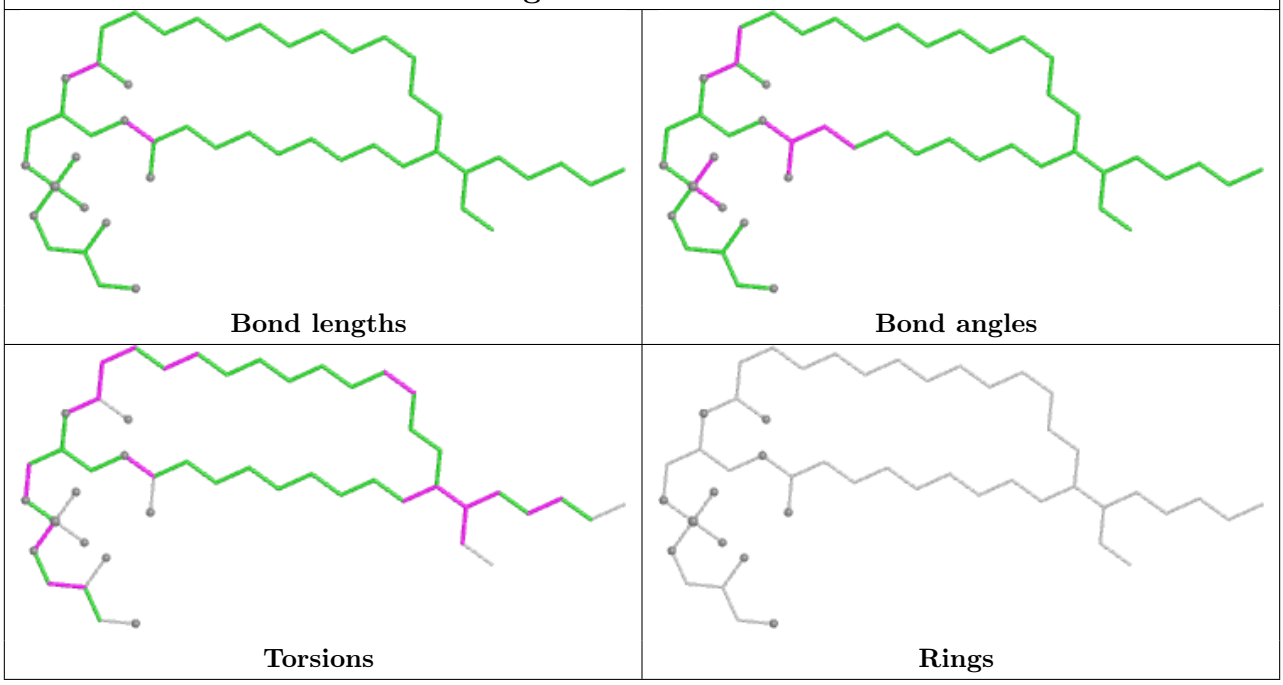
Ligand DMU P 307



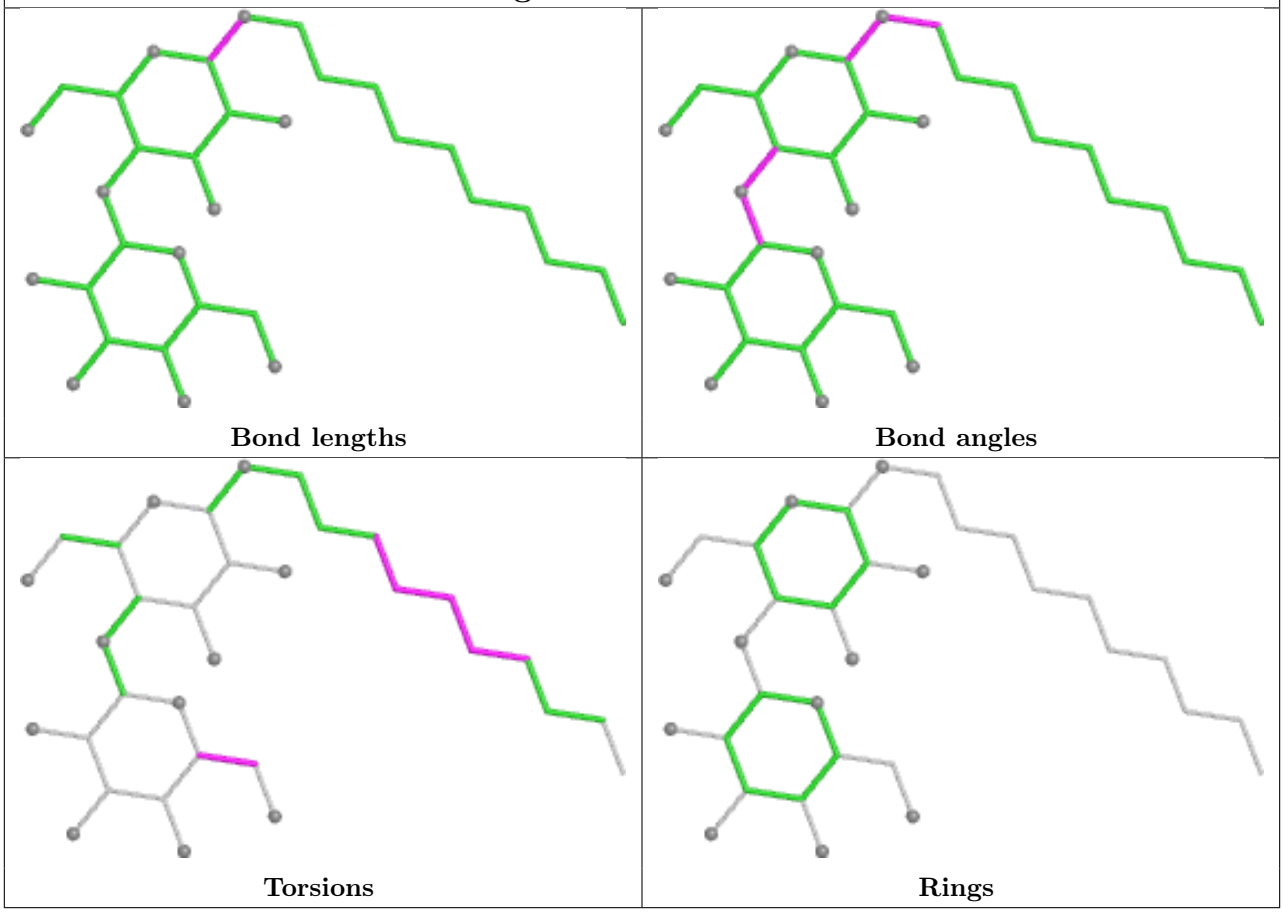
Ligand PEK G 101



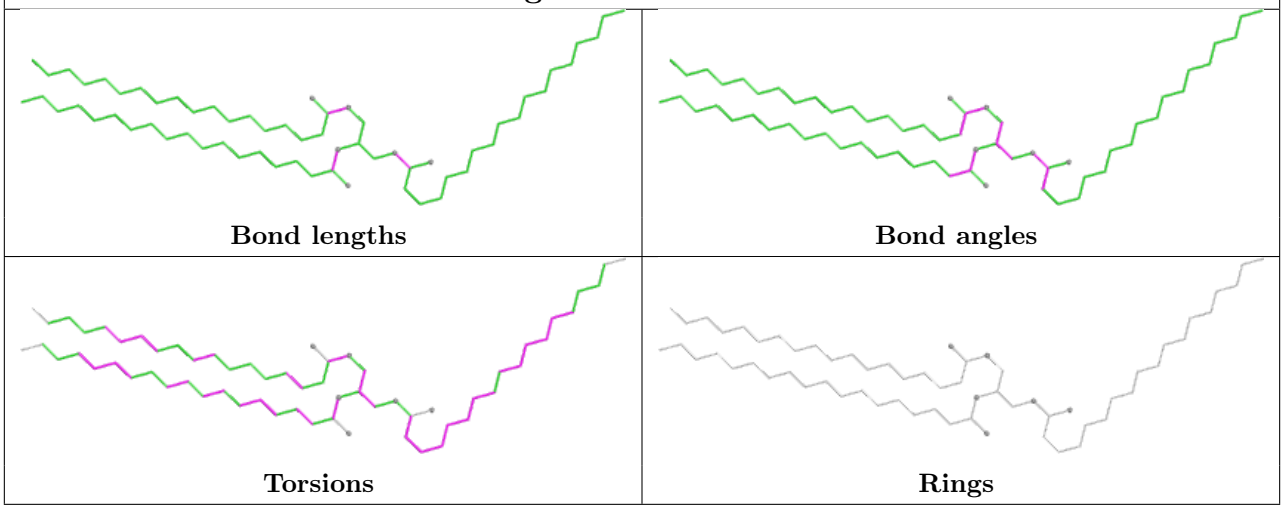
Ligand PGV P 304



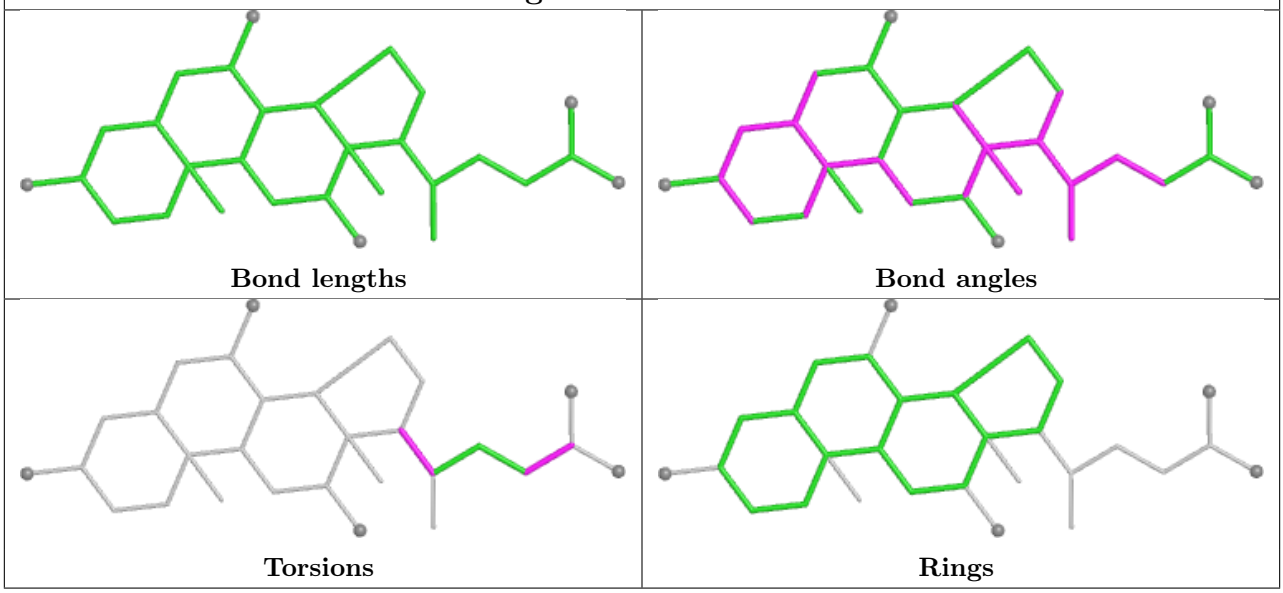
Ligand DMU M 101



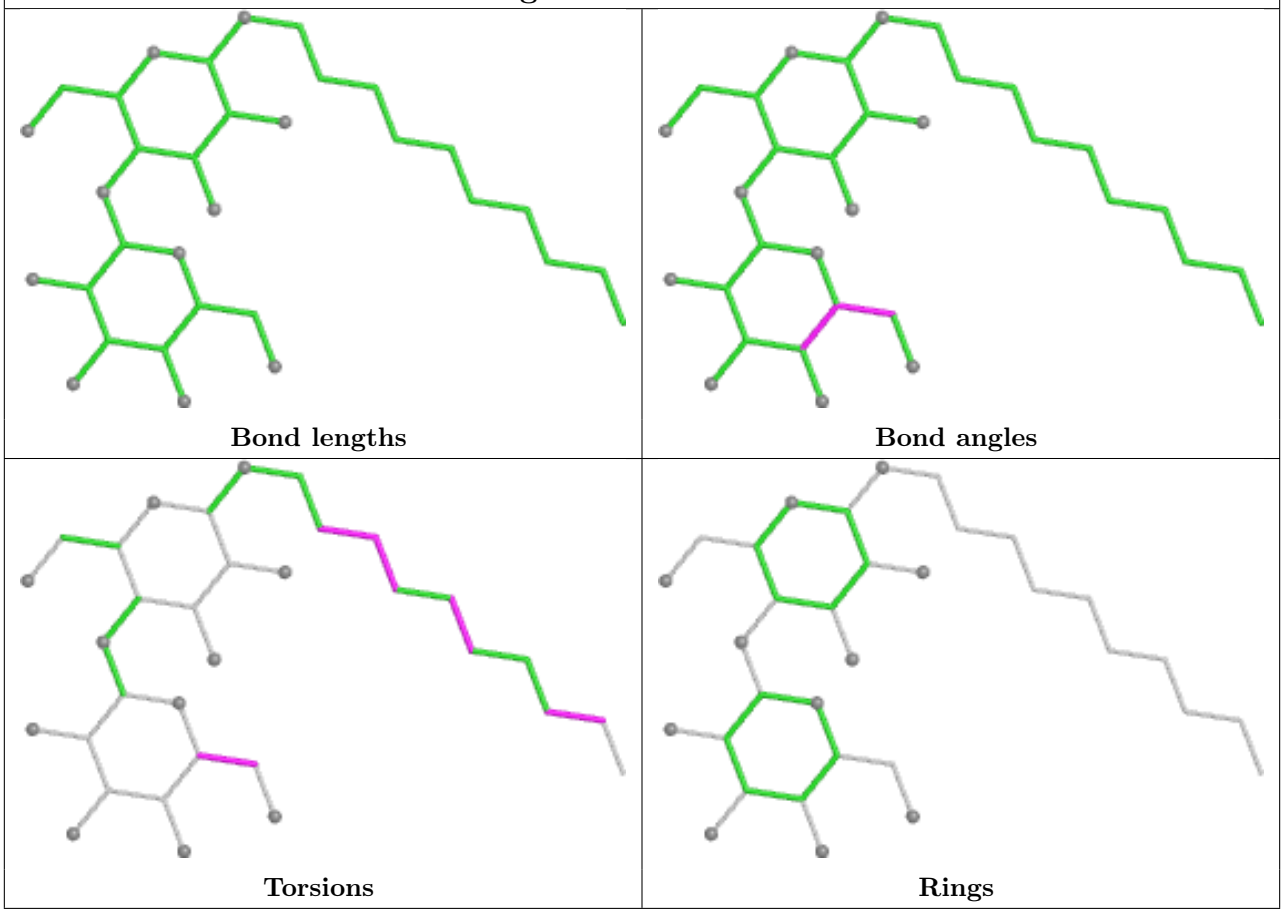
Ligand TGL O 303



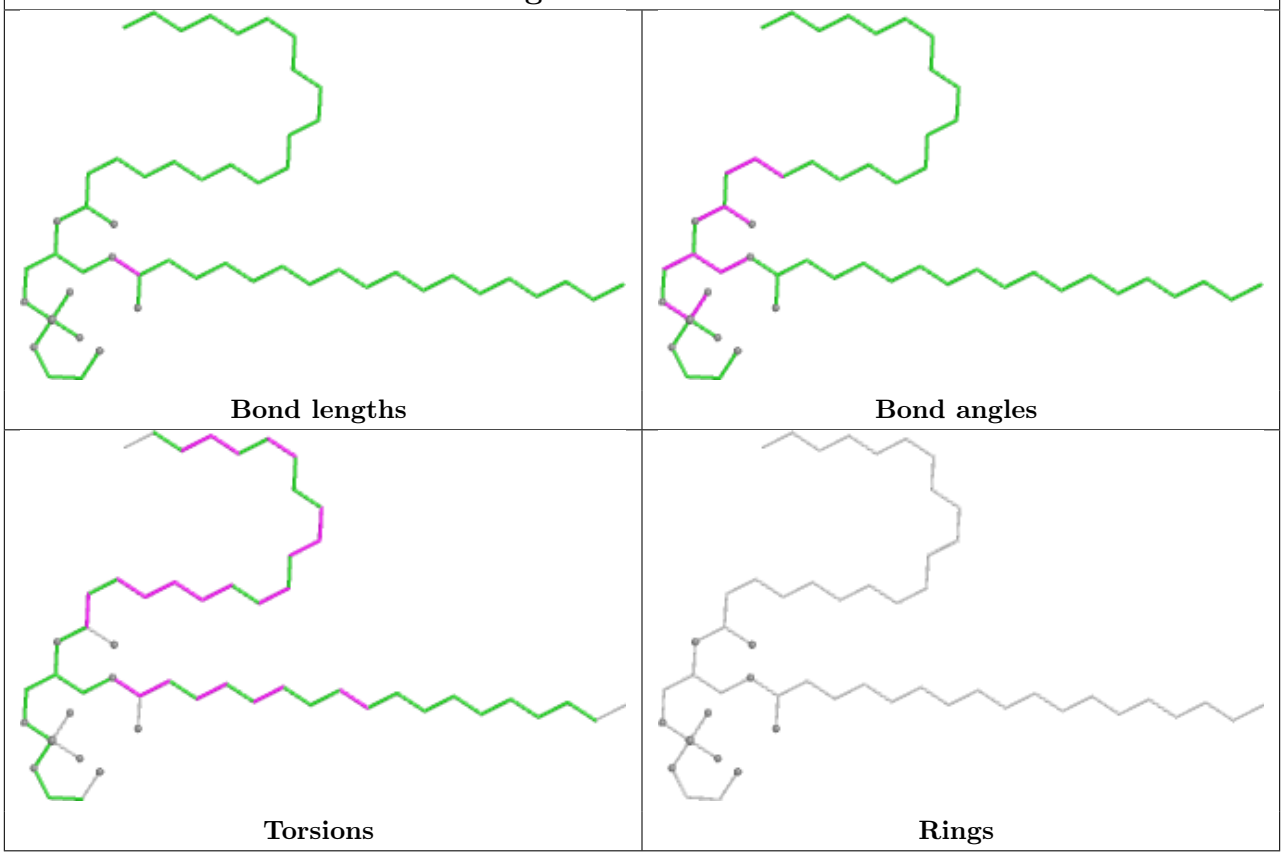
Ligand CHD J 101



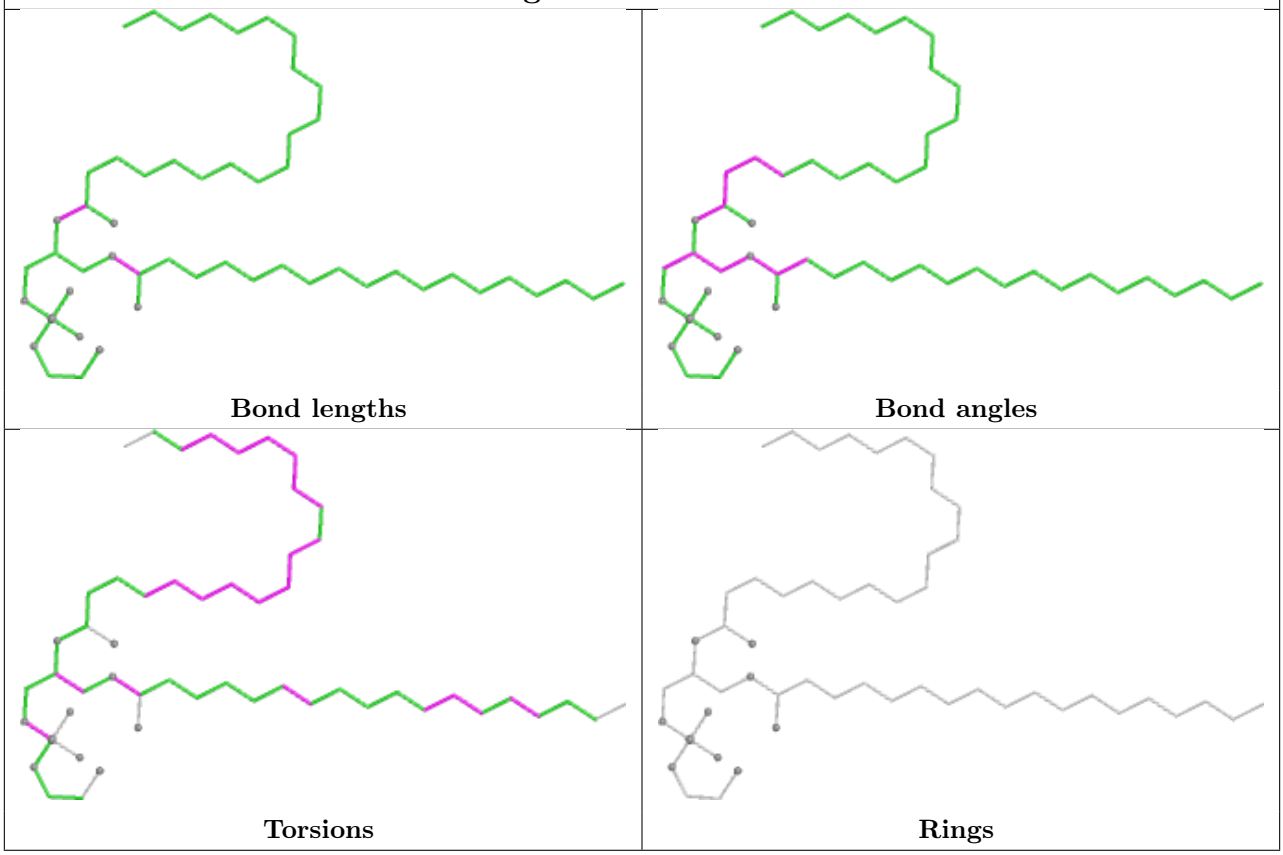
Ligand DMU Z 101



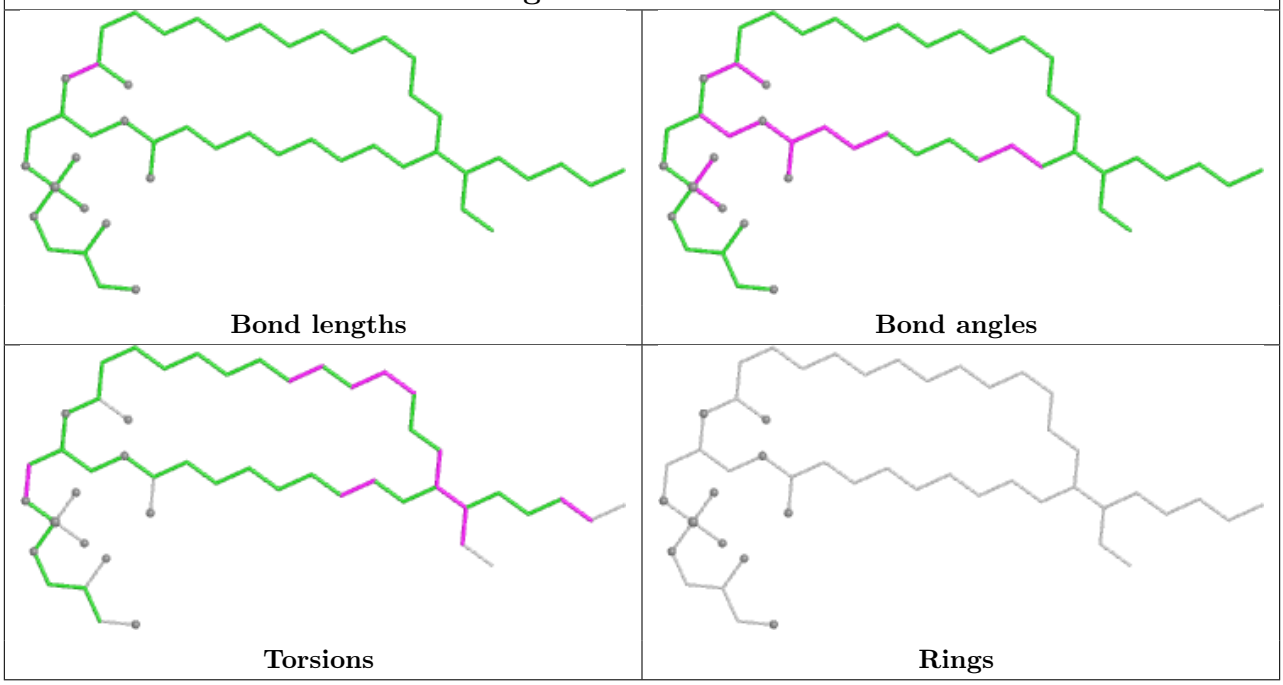
Ligand PEK P 302



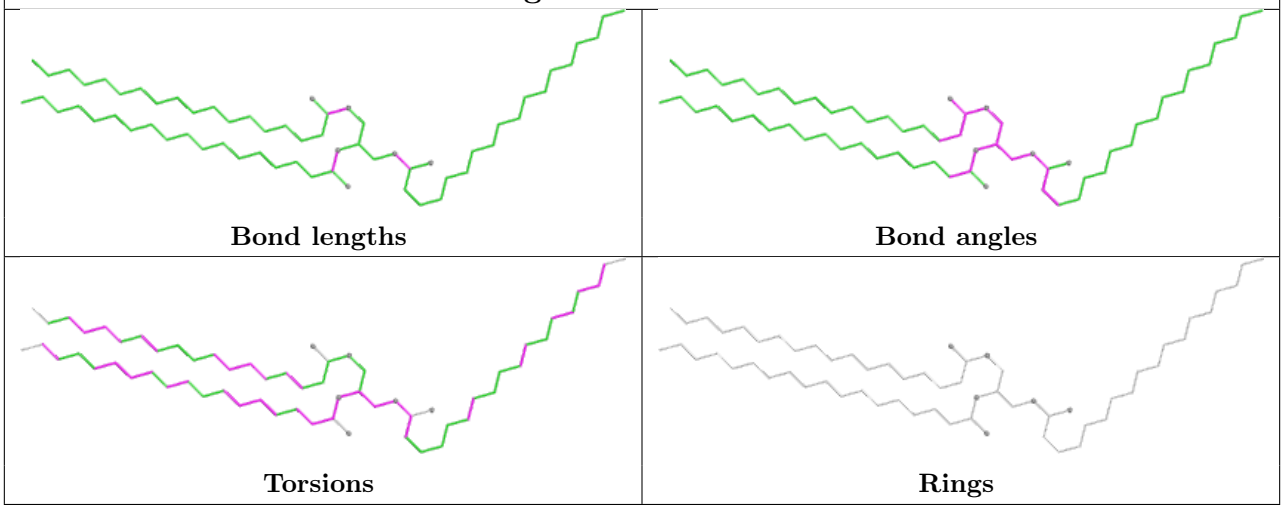
Ligand PEK G 103



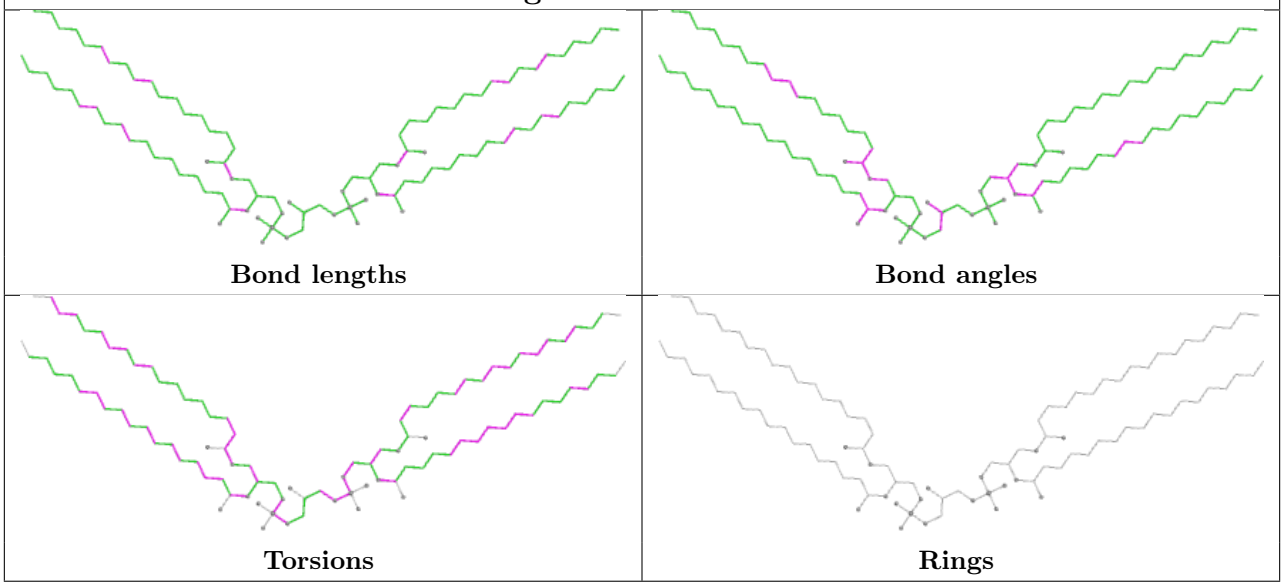
Ligand PGV P 303



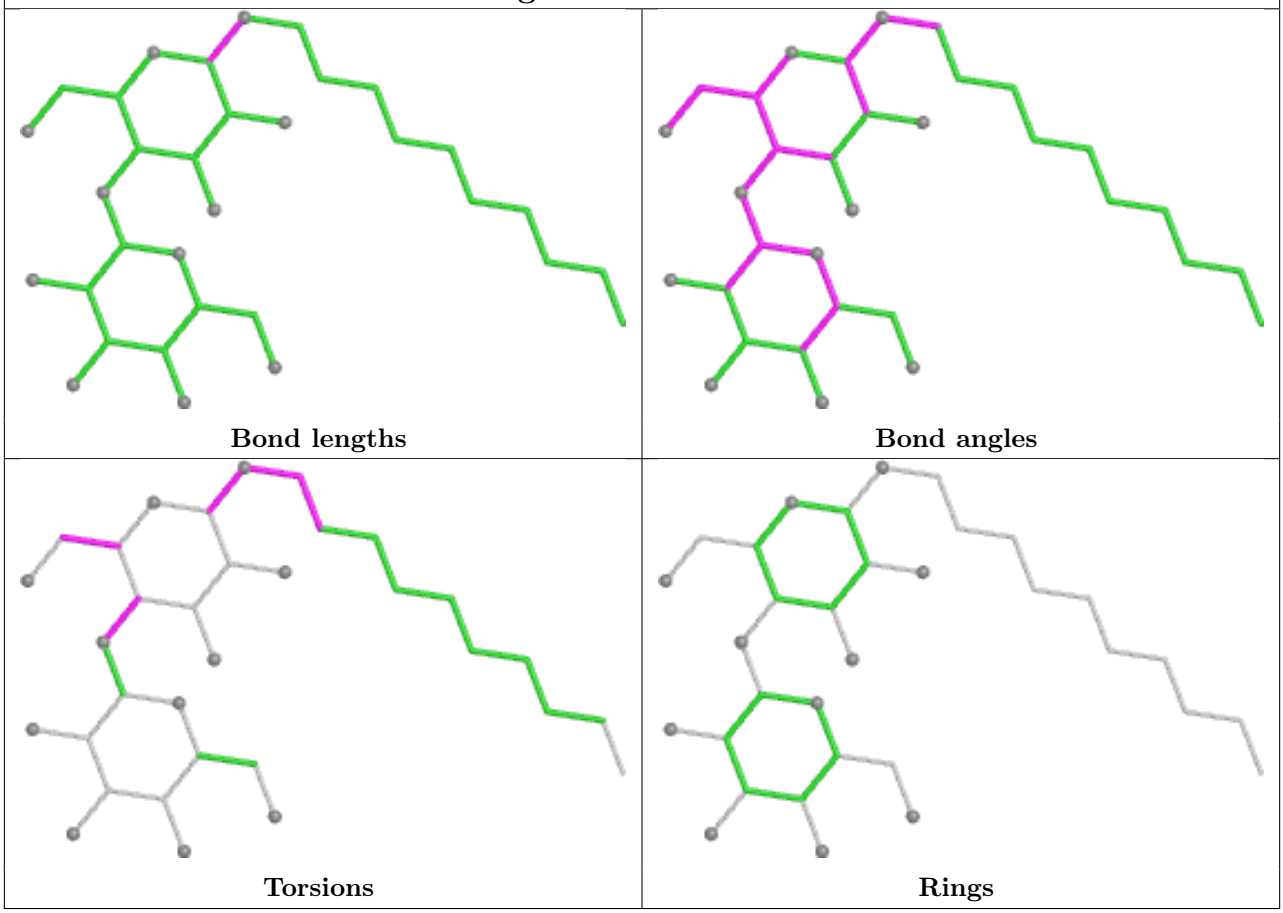
Ligand TGL N 607



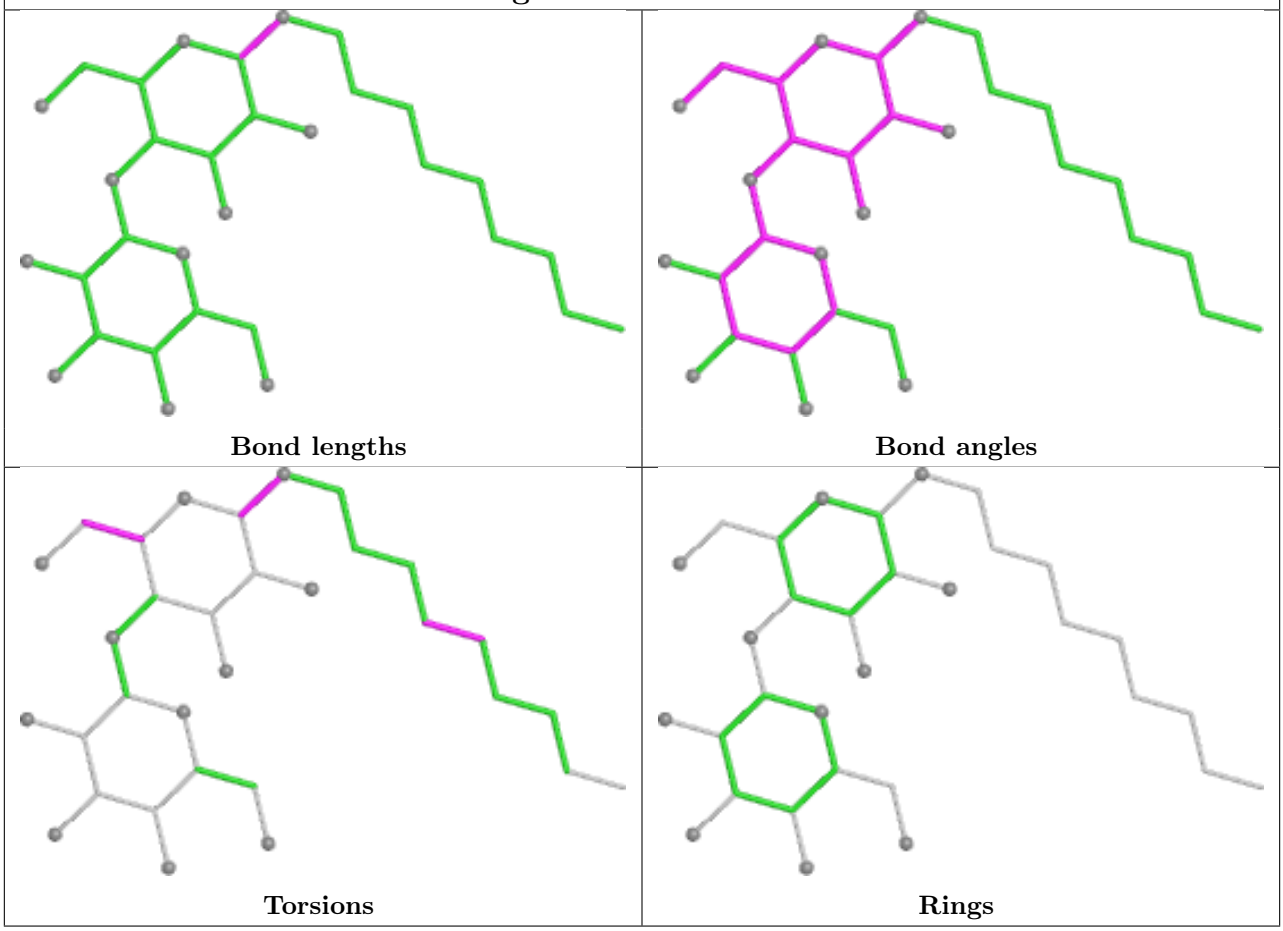
Ligand CDL G 102



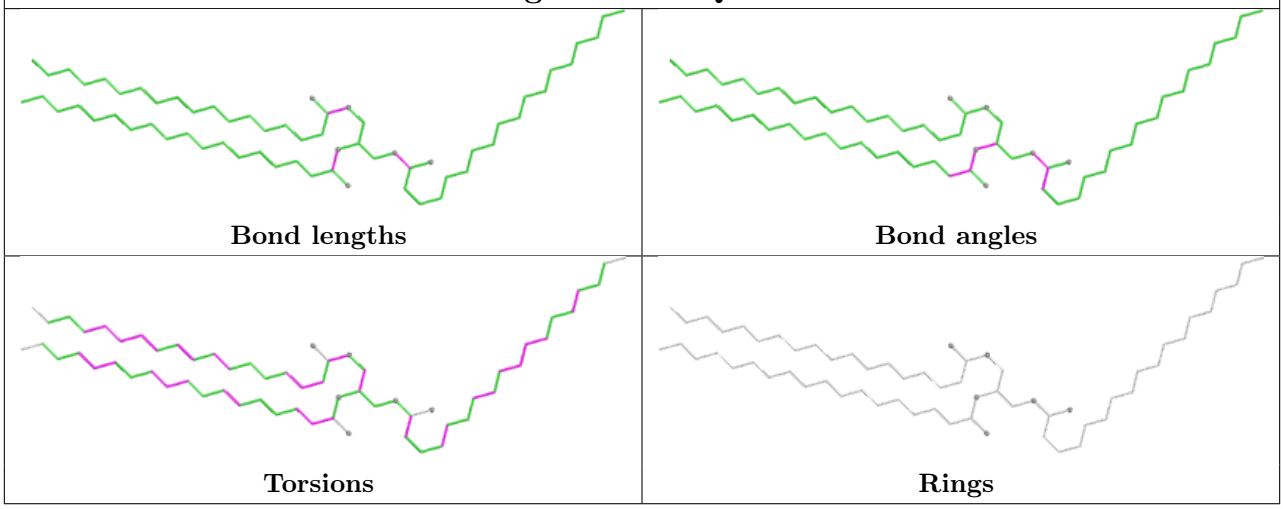
Ligand DMU C 307



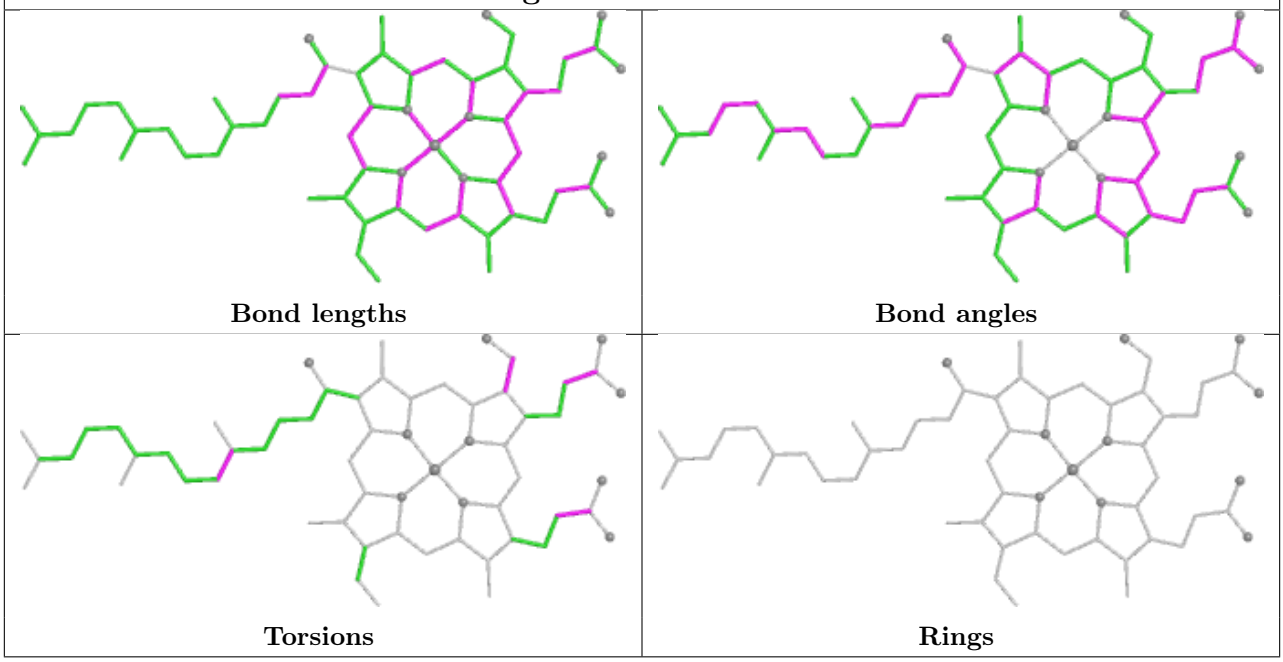
Ligand DMU W 102



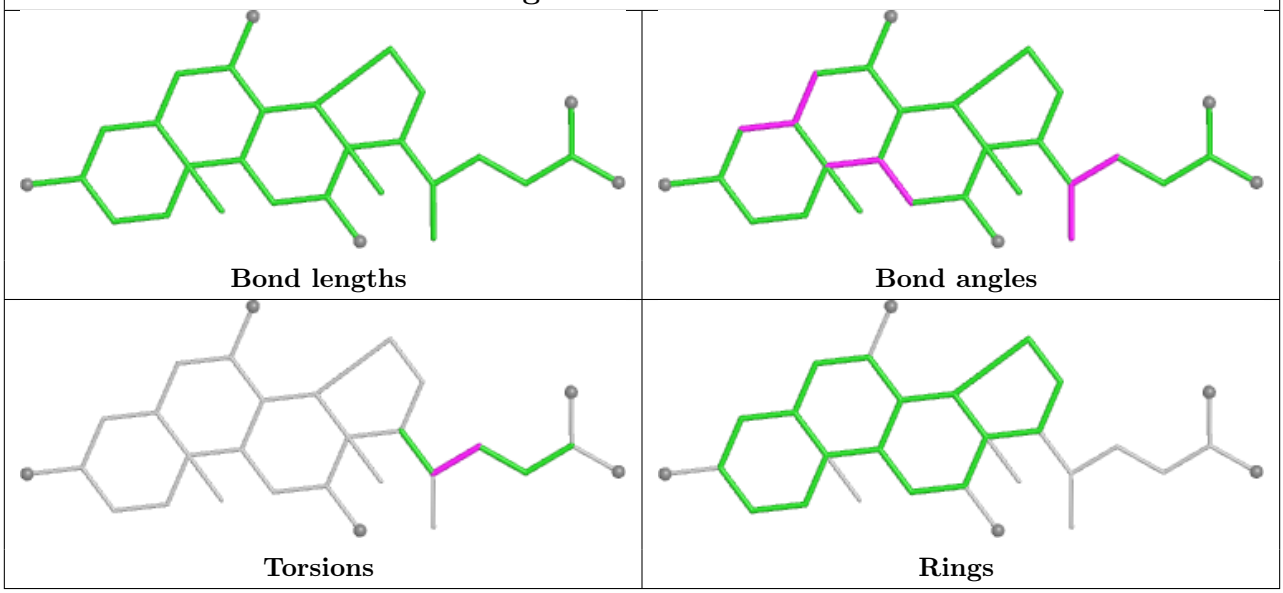
Ligand TGL Q 201



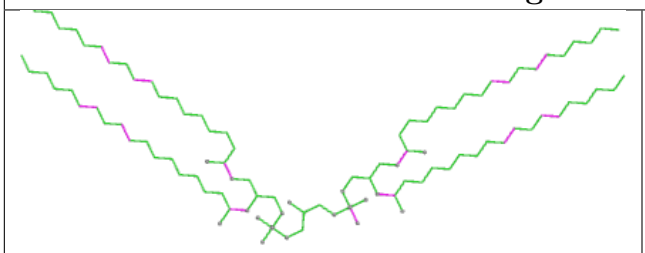
Ligand HEA A 601



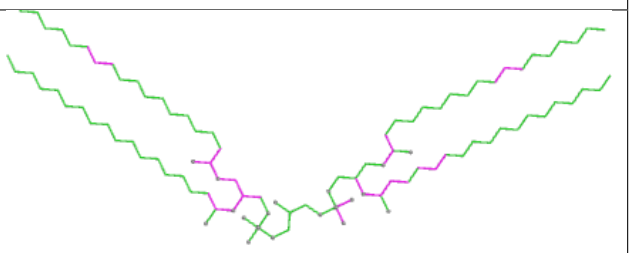
Ligand CHD P 306



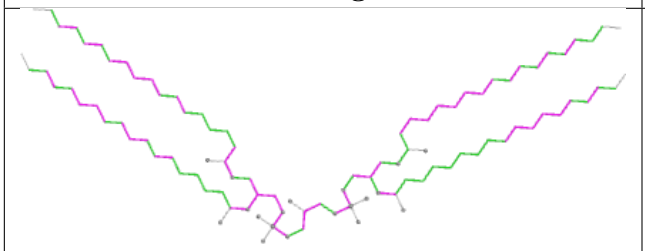
Ligand CDL P 305



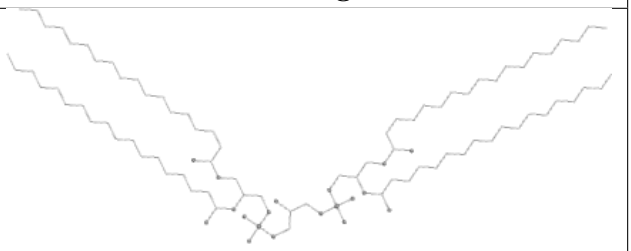
Bond lengths



Bond angles

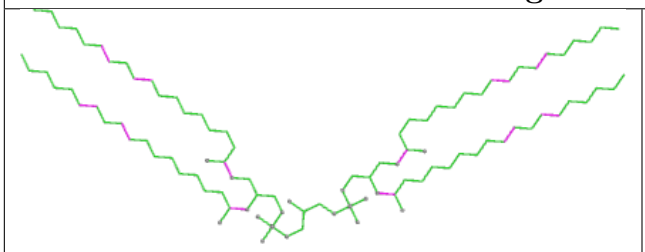


Torsions

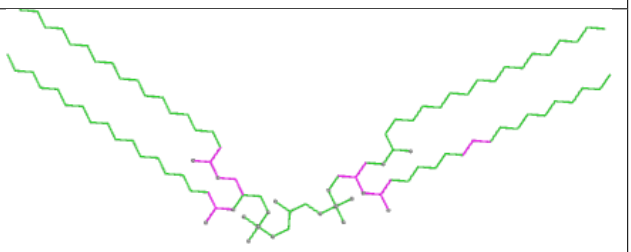


Rings

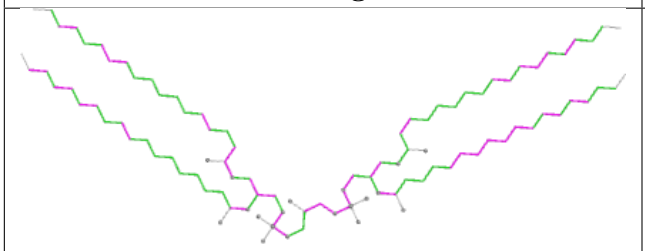
Ligand CDL T 103



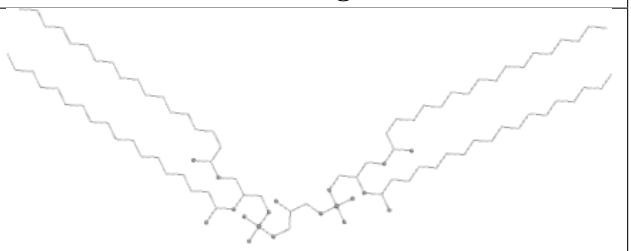
Bond lengths



Bond angles

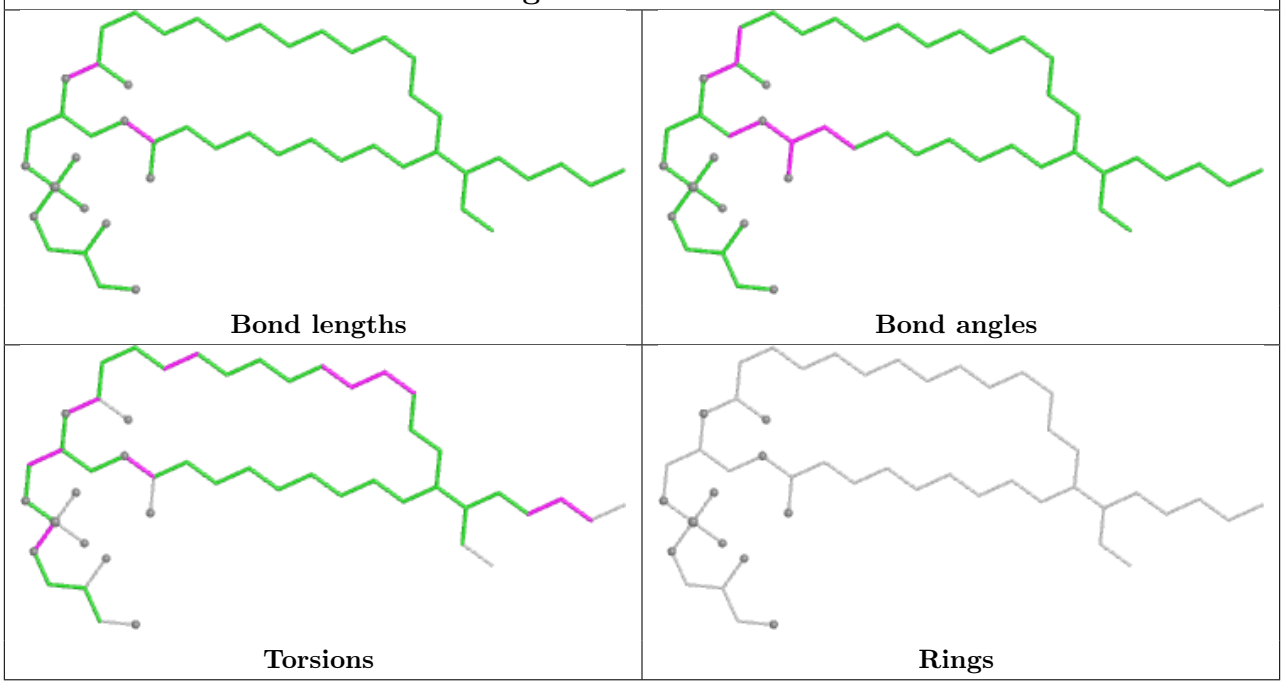


Torsions

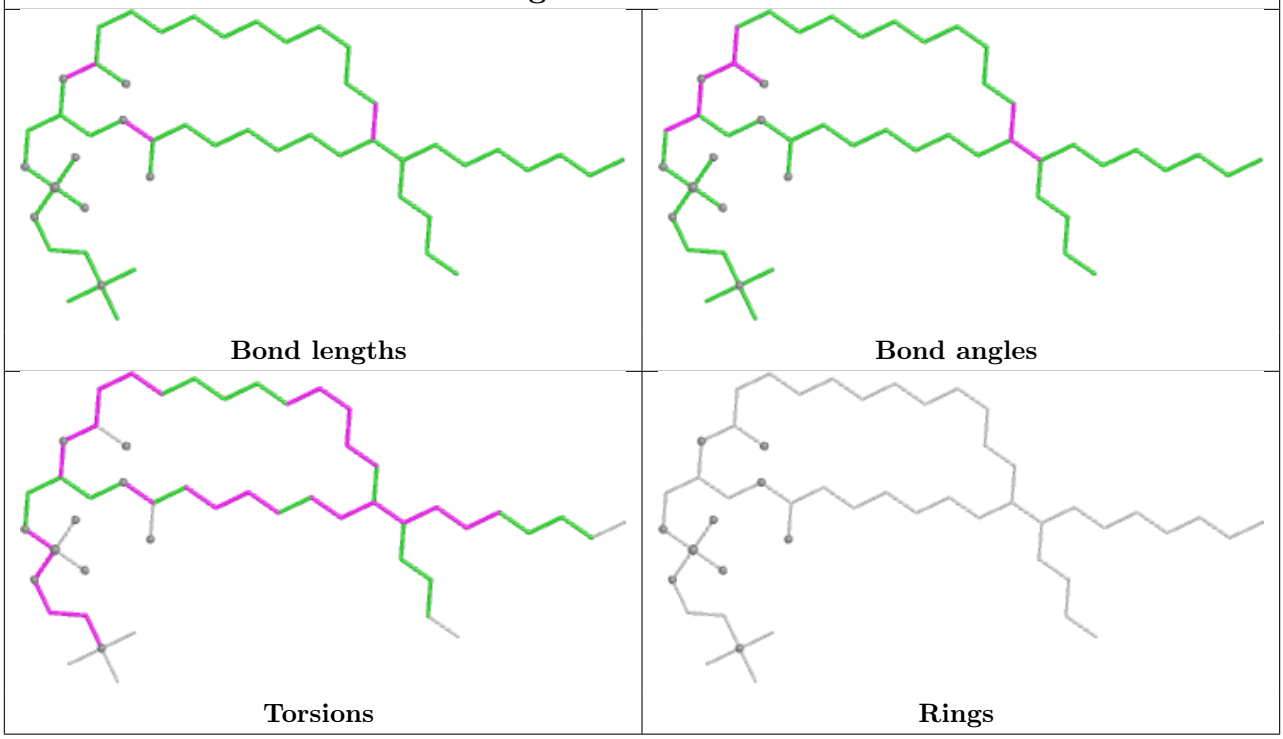


Rings

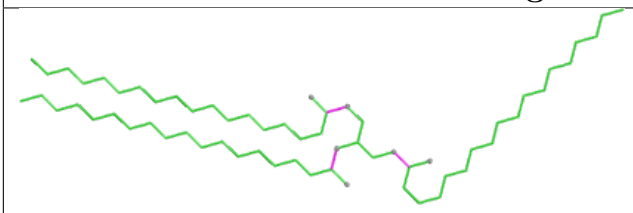
Ligand PGV C 304



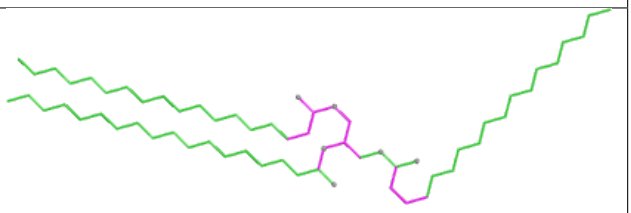
Ligand PSC E 201



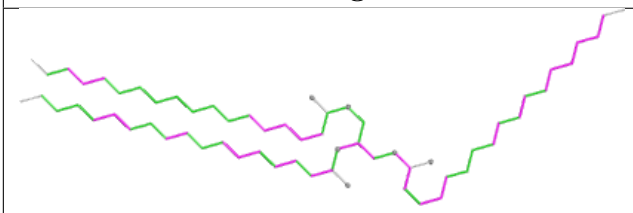
Ligand TGL L 101



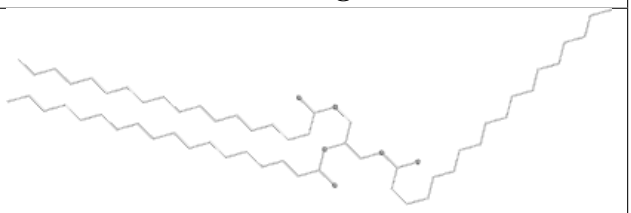
Bond lengths



Bond angles

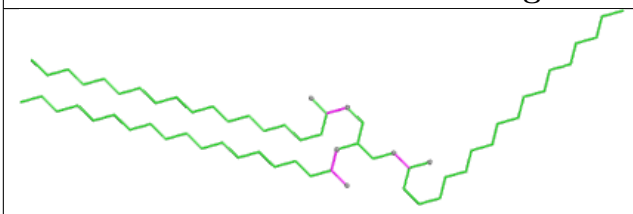


Torsions

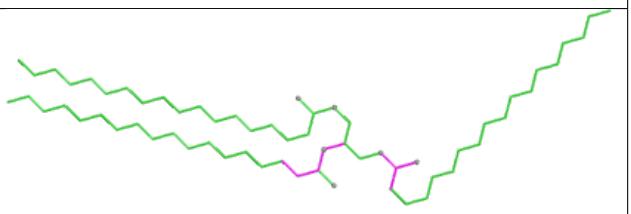


Rings

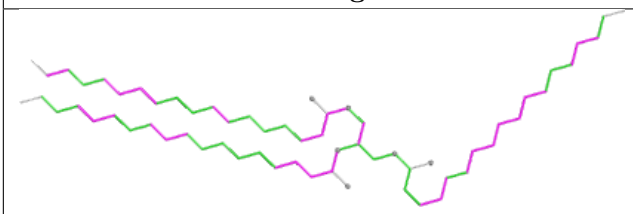
Ligand TGL D 201



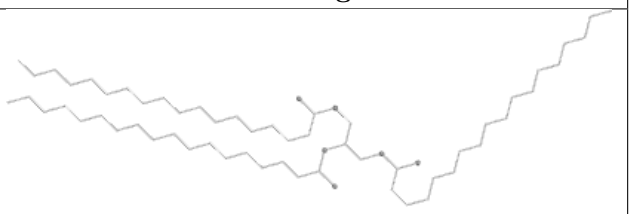
Bond lengths



Bond angles

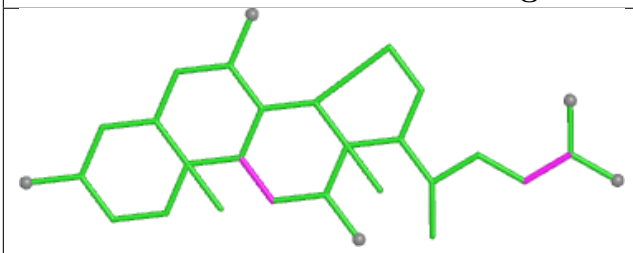


Torsions

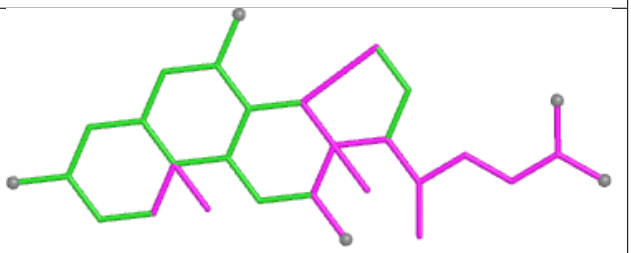


Rings

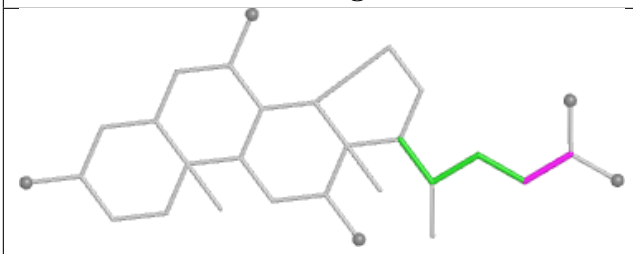
Ligand CHD C 301



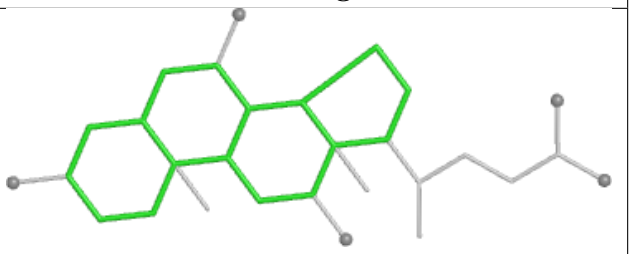
Bond lengths



Bond angles

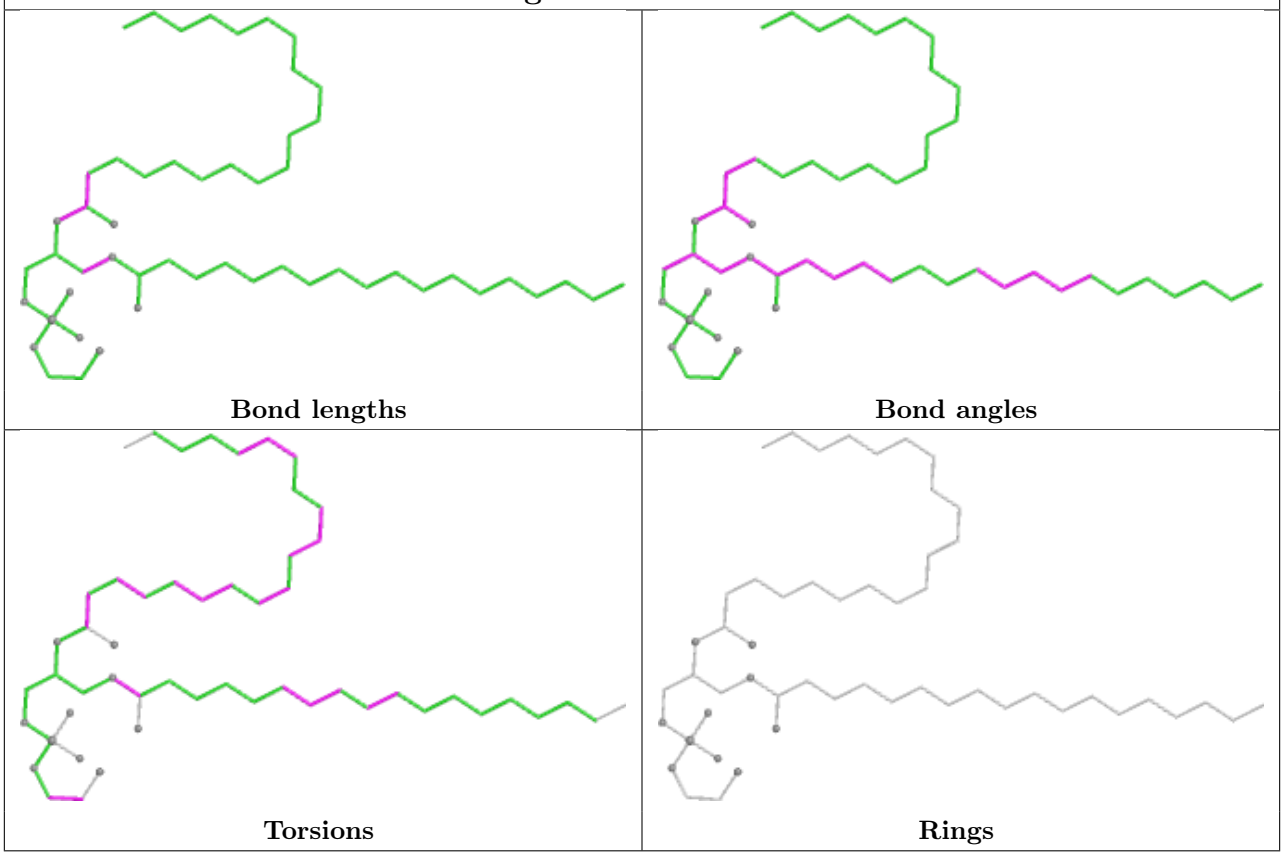


Torsions

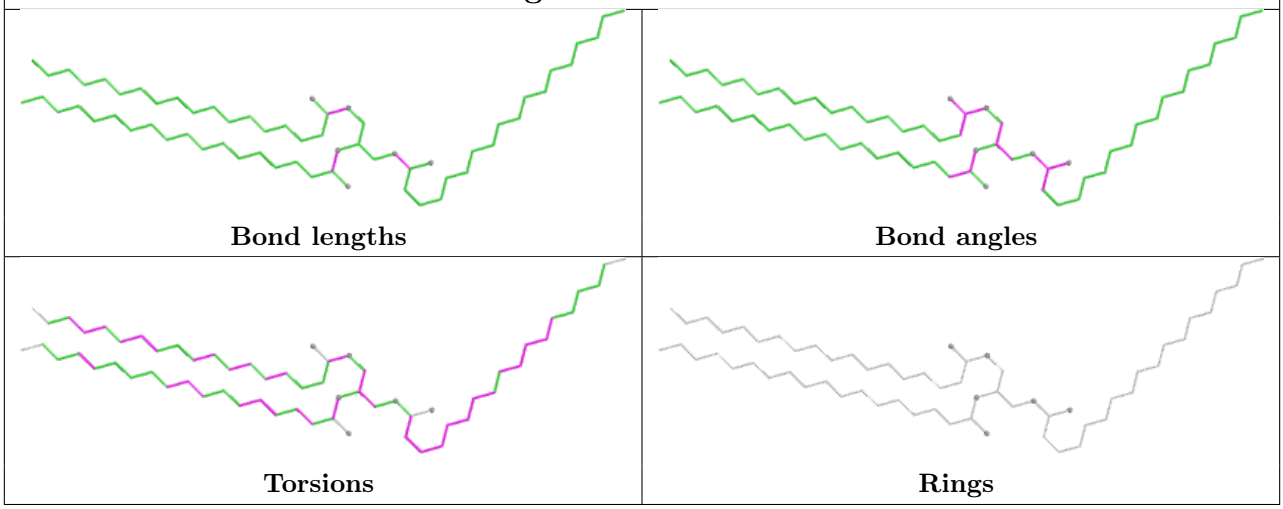


Rings

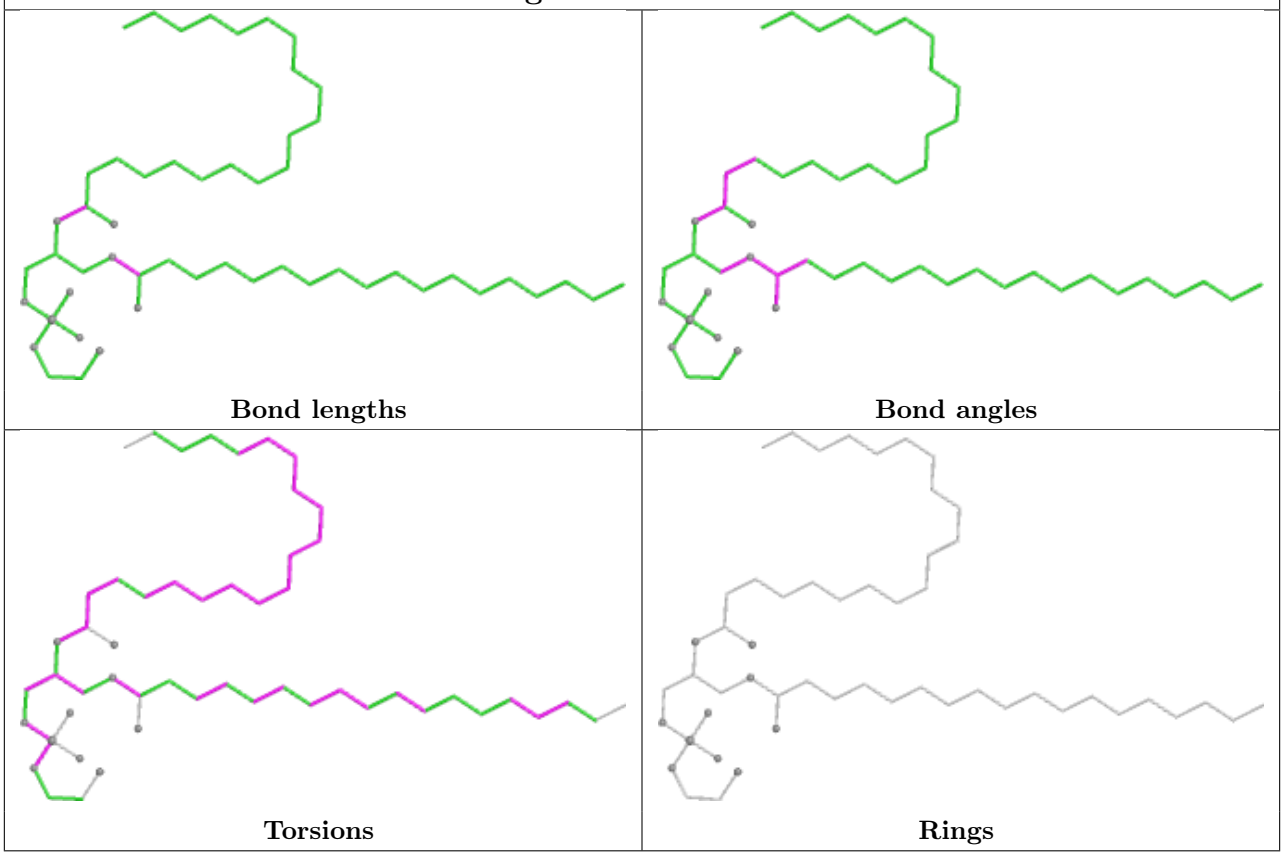
Ligand PEK C 302



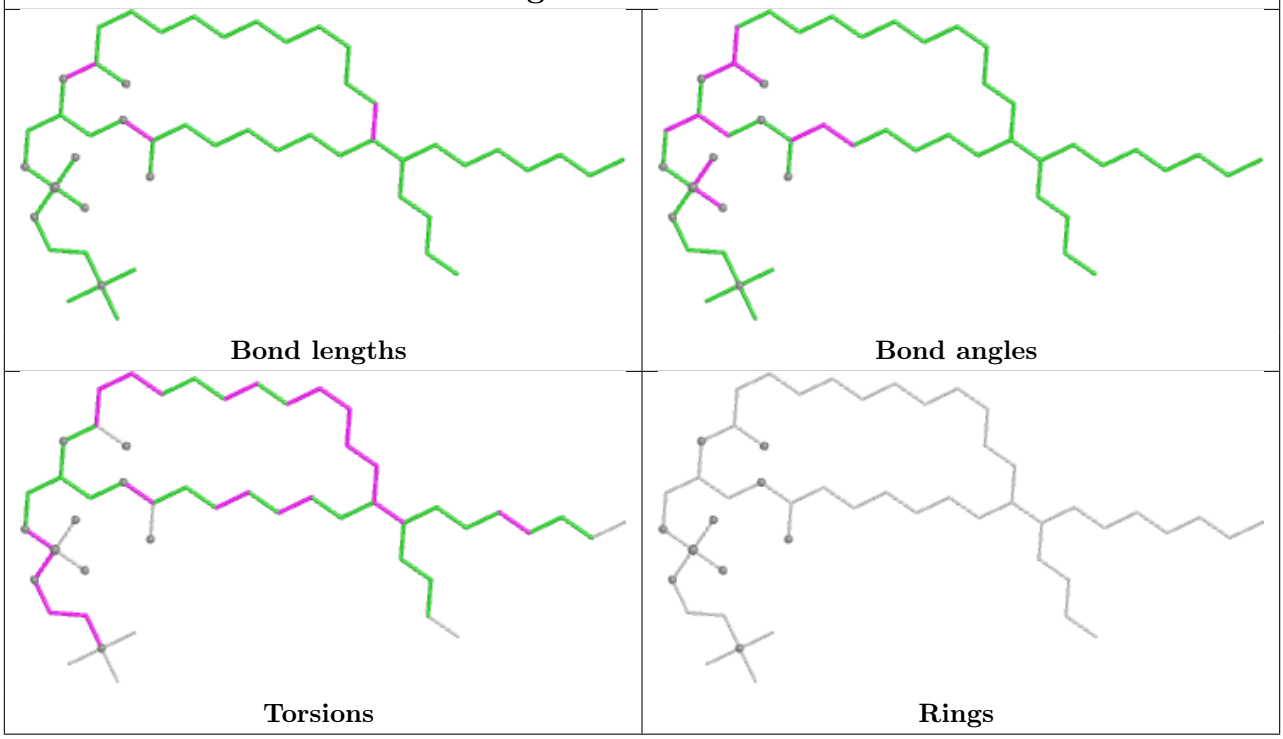
Ligand TGL A 607



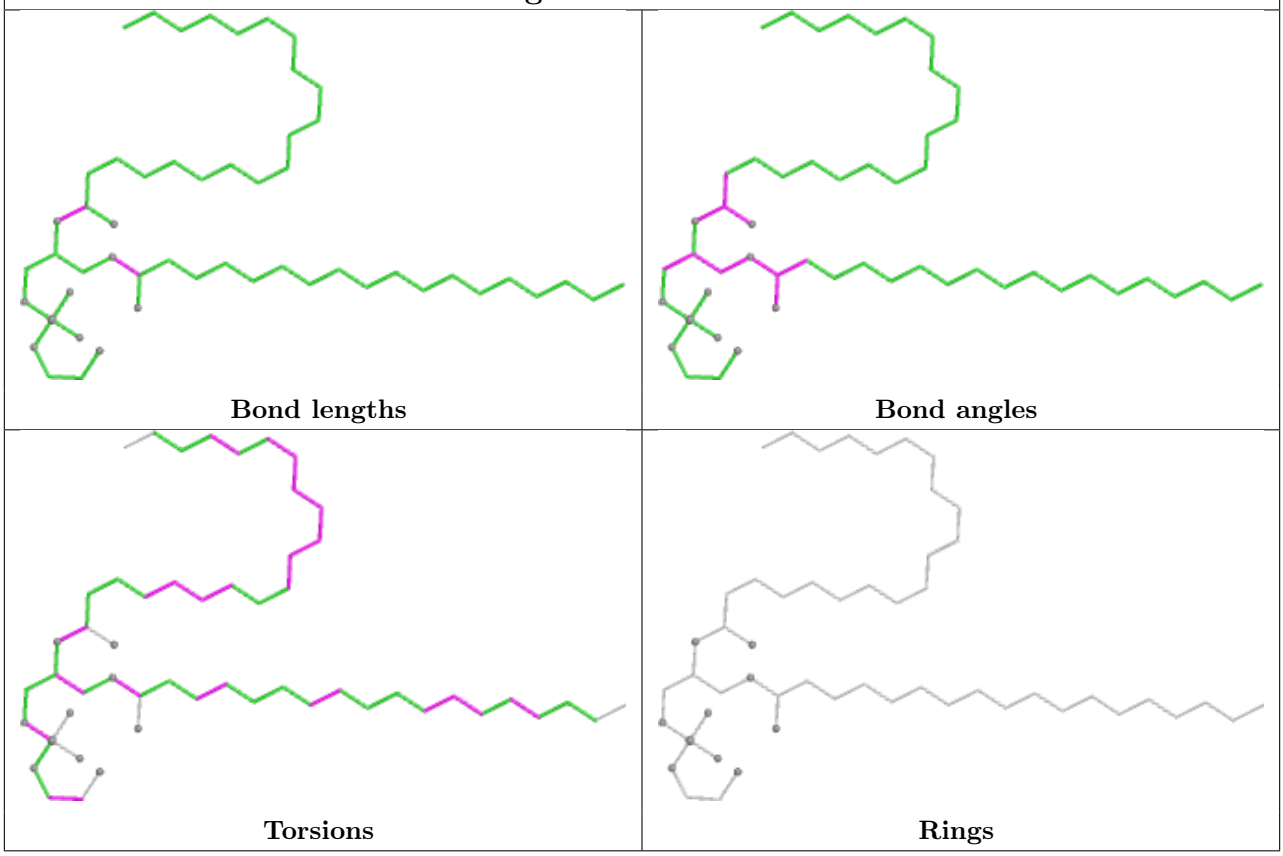
Ligand PEK T 101



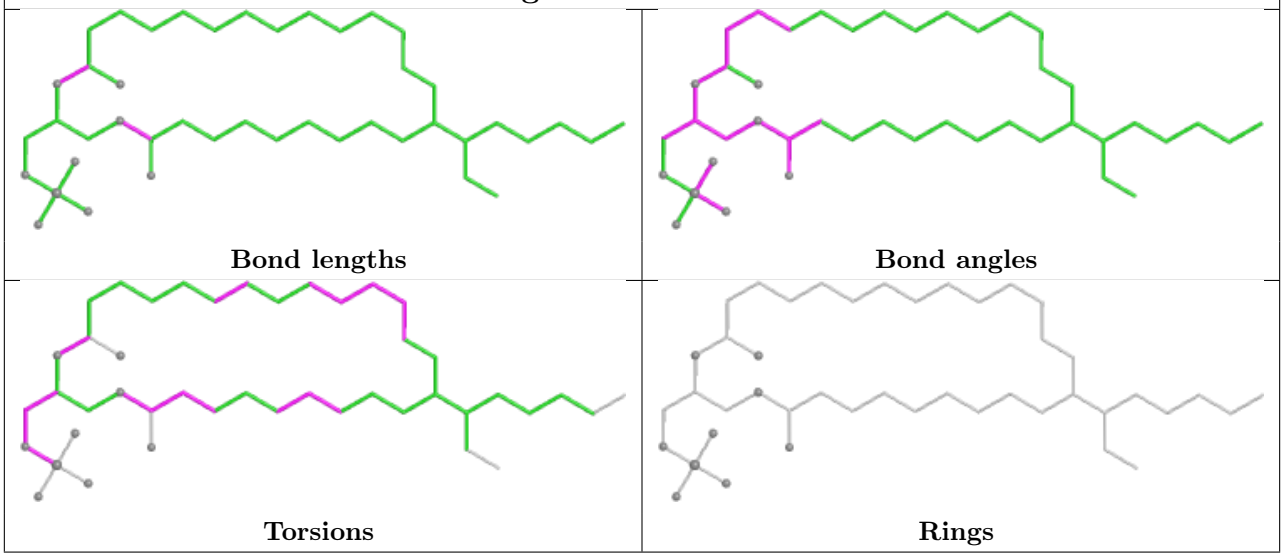
Ligand PSC R 201

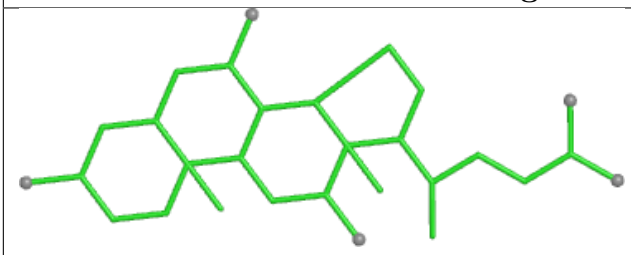
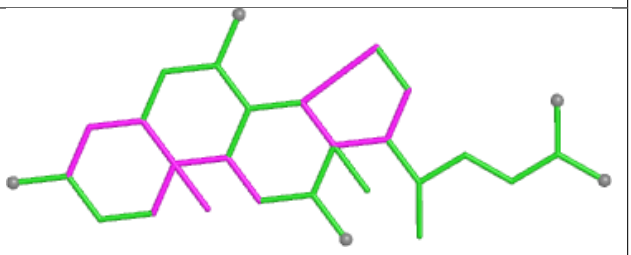
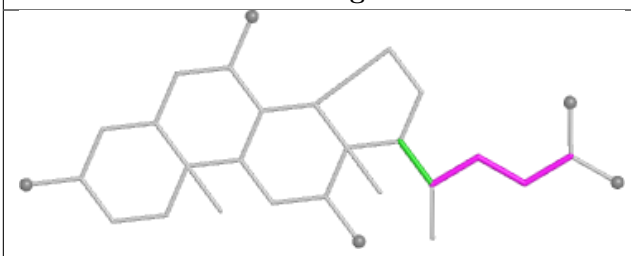
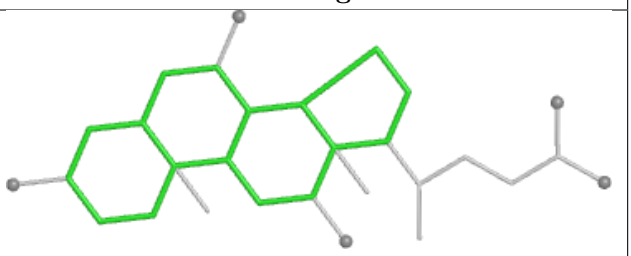


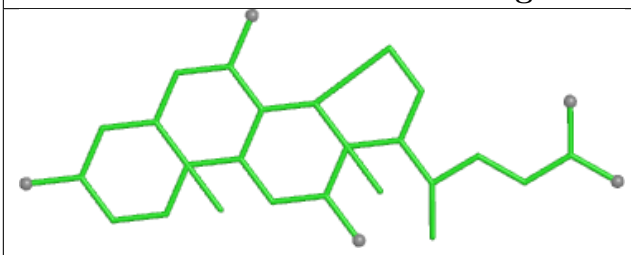
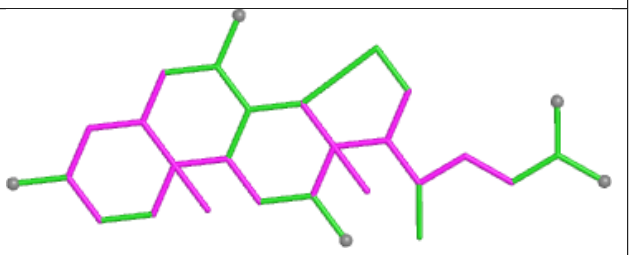
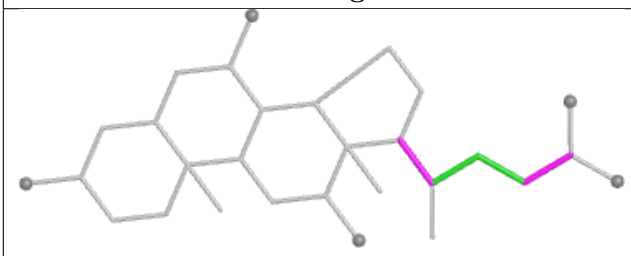
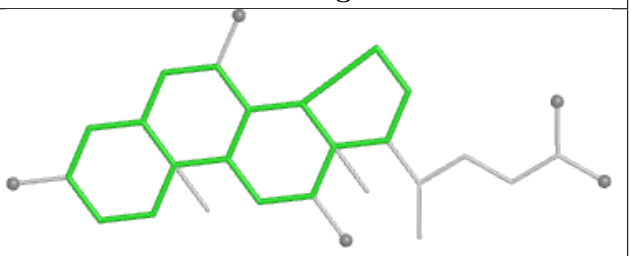
Ligand PEK T 102

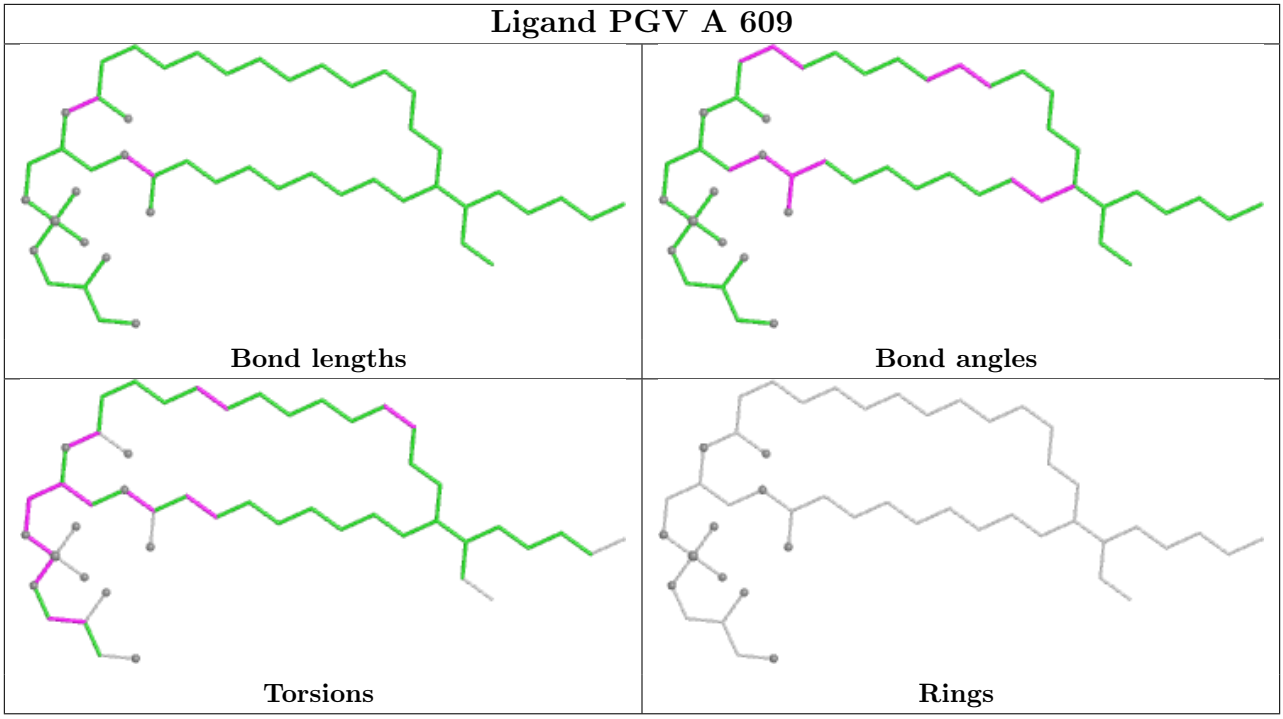


Ligand PGV N 608



Ligand CHD C 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHD W 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.59	4 (0%)	82	83	11, 25, 34, 79	10 (1%)
1	N	513/514 (99%)	-0.43	6 (1%)	76	77	14, 30, 40, 78	9 (1%)
2	B	226/227 (99%)	-0.03	12 (5%)	32	31	22, 32, 55, 85	2 (0%)
2	O	226/227 (99%)	0.29	14 (6%)	26	25	27, 38, 72, 110	0
3	C	259/261 (99%)	-0.31	4 (1%)	72	72	22, 29, 42, 77	3 (1%)
3	P	259/261 (99%)	-0.25	2 (0%)	82	83	25, 31, 47, 70	0
4	D	144/147 (97%)	0.32	6 (4%)	40	40	29, 39, 57, 86	0
4	Q	144/147 (97%)	0.88	17 (11%)	9	7	35, 48, 83, 162	0
5	E	105/109 (96%)	0.10	4 (3%)	44	44	32, 39, 69, 134	0
5	R	105/109 (96%)	0.30	4 (3%)	44	44	34, 46, 73, 145	0
6	F	98/98 (100%)	0.61	10 (10%)	12	10	26, 37, 120, 152	0
6	S	98/98 (100%)	0.79	9 (9%)	14	12	26, 39, 118, 159	0
7	G	83/85 (97%)	1.20	23 (27%)	1	1	26, 37, 109, 152	0
7	T	83/85 (97%)	1.21	20 (24%)	2	1	27, 41, 112, 149	0
8	H	79/85 (92%)	0.77	13 (16%)	4	3	28, 40, 91, 135	0
8	U	79/85 (92%)	1.05	15 (18%)	3	2	33, 44, 115, 144	0
9	I	72/73 (98%)	0.71	8 (11%)	10	8	32, 45, 68, 77	0
9	V	72/73 (98%)	1.06	11 (15%)	5	4	33, 51, 74, 128	0
10	J	58/59 (98%)	0.41	5 (8%)	16	14	29, 38, 68, 127	0
10	W	58/59 (98%)	0.57	5 (8%)	16	14	33, 44, 76, 146	0
11	K	49/56 (87%)	0.57	4 (8%)	17	15	32, 41, 62, 71	0
11	X	49/56 (87%)	0.90	7 (14%)	6	5	40, 51, 75, 93	0
12	L	46/47 (97%)	0.12	3 (6%)	25	23	26, 32, 54, 94	0
12	Y	46/47 (97%)	0.44	4 (8%)	16	14	33, 41, 68, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	0.51	6 (13%)	6	5	29, 34, 76, 123	0
13	Z	43/46 (93%)	0.81	7 (16%)	4	3	37, 45, 98, 153	0
All	All	3550/3614 (98%)	0.12	223 (6%)	26	24	11, 34, 70, 162	24 (0%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	22.1
6	S	97	ALA	11.4
4	Q	6	VAL	11.0
6	F	1	ALA	10.2
7	T	3	ALA	9.4
8	U	8	ILE	9.4
6	S	94	HIS	8.7
2	O	227	LEU	8.7
7	G	36	TRP	8.7
6	F	96	LEU	8.6
8	H	8	ILE	8.3
7	G	7	ASP	7.9
4	Q	4	SER	7.8
7	G	2	SER	7.5
7	T	36	TRP	7.5
8	H	47	GLY	7.5
7	G	9	GLY	6.9
6	F	97	ALA	6.9
6	S	98	HIS	6.8
7	T	2	SER	6.7
7	G	3	ALA	6.6
4	Q	5	VAL	6.5
2	B	59	GLN	6.3
5	R	109	VAL	6.0
7	T	84	LYS	6.0
9	V	2	THR	5.9
4	Q	8	SER	5.9
7	T	5	LYS	5.8
7	G	5	LYS	5.7
6	S	96	LEU	5.7
9	I	37	PHE	5.6
7	T	9	GLY	5.6
6	S	95	GLN	5.5
2	O	59	GLN	5.4

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Mol	Chain	Res	Type	RSRZ
7	G	10	GLY	5.4
7	G	8	HIS	5.3
2	B	113	TYR	5.3
2	O	113	TYR	5.2
6	F	94	HIS	5.2
7	T	8	HIS	5.2
7	T	4	ALA	5.2
6	S	3	GLY	5.1
8	U	47	GLY	5.1
8	U	45	ALA	5.1
7	G	4	ALA	4.9
4	Q	9	GLU	4.9
12	L	47	LYS	4.9
13	M	43	SER	4.8
2	O	65	TRP	4.8
2	O	226	MET	4.8
1	N	484	THR	4.8
8	U	48	GLY	4.8
8	H	7	LYS	4.7
9	V	36	LYS	4.6
7	G	1	ALA	4.6
7	T	1	ALA	4.6
7	T	7	ASP	4.6
7	G	37	LEU	4.5
8	U	44	THR	4.5
4	Q	7	LYS	4.4
6	F	2	SER	4.4
7	T	37	LEU	4.4
8	H	48	GLY	4.3
9	V	3	ALA	4.3
2	B	90	ILE	4.3
6	S	2	SER	4.3
9	V	37	PHE	4.2
11	X	6	ALA	4.2
12	L	2	HIS	4.2
1	N	113	LEU	4.2
7	T	10	GLY	4.2
11	K	6	ALA	4.2
10	W	52	TRP	4.1
10	W	58	LYS	4.1
5	R	5	HIS	4.1
8	H	9	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
11	X	7	PRO	4.0
4	D	4	SER	4.0
10	W	57	HIS	3.9
2	B	92	ASN	3.9
13	Z	43	SER	3.9
7	G	84	LYS	3.9
6	F	95	GLN	3.9
5	E	109	VAL	3.9
1	A	113	LEU	3.9
7	T	38	HIS	3.9
7	G	6	GLY	3.8
8	U	7	LYS	3.8
6	F	3	GLY	3.8
2	B	65	TRP	3.8
12	Y	47	LYS	3.8
13	Z	42	LYS	3.8
8	U	50	VAL	3.8
10	J	1	PHE	3.7
2	O	90	ILE	3.7
8	U	61	LYS	3.7
10	J	58	LYS	3.7
11	K	7	PRO	3.6
2	B	87	MET	3.6
8	U	9	LYS	3.6
4	Q	51	LEU	3.6
13	Z	41	LYS	3.6
13	M	40	TYR	3.5
11	X	47	ARG	3.5
10	J	56	PRO	3.5
7	T	40	GLY	3.5
6	S	93	PRO	3.5
7	G	41	HIS	3.5
7	G	39	SER	3.4
9	V	33	THR	3.4
1	A	514	LYS	3.4
13	M	42	LYS	3.4
3	C	3	HIS	3.4
6	F	98	HIS	3.4
12	Y	2	HIS	3.4
12	Y	20	ARG	3.4
8	U	43	MET	3.4
13	Z	38	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
7	T	39	SER	3.3
5	E	5	HIS	3.3
8	H	10	ASN	3.3
4	D	11	TYR	3.3
1	A	297	MET	3.2
8	U	46	LYS	3.2
9	V	29	LEU	3.2
2	O	129	LYS	3.2
9	V	30	GLY	3.2
2	B	91	ASN	3.2
13	Z	39	ASN	3.2
8	H	46	LYS	3.2
2	O	32	PHE	3.2
4	Q	33	LEU	3.1
7	G	38	HIS	3.1
7	G	12	GLY	3.1
7	G	33	LEU	3.1
4	Q	11	TYR	3.0
4	Q	46	ALA	3.0
2	B	16	ILE	3.0
4	Q	17	VAL	2.9
4	Q	10	ASP	2.9
9	V	73	LYS	2.9
7	T	42	ARG	2.9
13	Z	40	TYR	2.9
4	Q	143	ASN	2.9
7	T	35	SER	2.9
1	N	513	LEU	2.9
3	C	37	PHE	2.8
3	P	37	PHE	2.8
9	I	36	LYS	2.8
9	V	26	MET	2.8
7	T	12	GLY	2.8
11	K	47	ARG	2.7
11	K	54	ARG	2.7
9	I	33	THR	2.7
8	H	50	VAL	2.7
1	N	512	ASN	2.7
8	U	42	ALA	2.7
7	G	40	GLY	2.7
4	Q	72	ASN	2.7
2	B	60	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	8	SER	2.7
4	Q	35	ALA	2.6
9	I	73	LYS	2.6
13	M	41	LYS	2.6
9	I	29	LEU	2.6
2	O	221	LYS	2.6
5	E	7	THR	2.6
8	U	10	ASN	2.6
10	W	1	PHE	2.6
8	H	45	ALA	2.6
13	M	39	ASN	2.6
2	O	91	ASN	2.5
2	O	217	LYS	2.5
9	I	30	GLY	2.5
2	O	57	ASP	2.5
4	Q	147	LYS	2.5
13	Z	19	LEU	2.4
1	N	514	LYS	2.4
8	H	44	THR	2.4
7	T	6	GLY	2.4
9	I	26	MET	2.4
10	J	55	PHE	2.4
7	G	35	SER	2.4
10	W	55	PHE	2.4
8	H	42	ALA	2.4
11	X	19	ALA	2.4
2	O	92	ASN	2.4
4	D	5	VAL	2.4
1	N	297[A]	MET	2.4
9	V	10	ARG	2.3
3	C	44	MET	2.3
6	F	92	VAL	2.3
8	U	52	VAL	2.3
3	C	38	ASN	2.3
2	O	87	MET	2.3
4	Q	87	PHE	2.2
6	F	93	PRO	2.2
7	G	45	PRO	2.2
5	E	108	LYS	2.2
7	G	42	ARG	2.2
9	I	2	THR	2.2
7	T	33	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	57	ASP	2.2
11	X	52	GLU	2.2
11	X	20	SER	2.2
7	G	70	PHE	2.2
5	R	9	GLU	2.2
12	L	24	MET	2.1
4	D	9	GLU	2.1
4	D	17	VAL	2.1
8	H	43	MET	2.1
3	P	107	ALA	2.1
10	J	52	TRP	2.1
1	A	513	LEU	2.1
11	X	54	ARG	2.1
2	B	55	THR	2.1
9	V	32	ALA	2.1
5	R	108	LYS	2.0
2	B	37	LEU	2.0
13	M	38	ASP	2.0
8	H	84	LYS	2.0
12	Y	26	THR	2.0
8	U	11	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SAC	V	1	9/10	0.31	0.23	147,152,161,162	0
7	TPO	G	11	11/12	0.57	0.38	90,120,150,166	0
7	TPO	T	11	11/12	0.65	0.30	103,113,156,158	0
9	SAC	I	1	9/10	0.68	0.23	65,84,106,118	0
1	FME	N	1	10/11	0.91	0.14	40,54,91,104	0
1	FME	A	1	10/11	0.94	0.12	36,39,76,103	0
2	FME	B	1	10/11	0.97	0.10	17,34,75,76	0
2	FME	O	1	10/11	0.97	0.09	30,39,45,76	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PEK	G	103	53/53	0.71	0.26	46,95,133,145	0
26	DMU	P	307	33/33	0.71	0.21	60,110,126,129	0
20	PGV	P	304	51/51	0.72	0.24	43,78,120,149	0
23	CHD	J	101	29/29	0.72	0.23	73,104,110,113	0
24	PEK	T	102	53/53	0.73	0.25	47,94,128,138	0
23	CHD	W	101	29/29	0.73	0.22	81,107,119,120	0
26	DMU	C	307	33/33	0.74	0.21	58,102,122,124	0
25	CDL	T	103	100/100	0.74	0.23	52,88,125,150	0
20	PGV	N	608	46/51	0.75	0.25	40,83,127,143	0
24	PEK	T	101	53/53	0.75	0.24	40,80,124,154	0
24	PEK	G	101	50/53	0.75	0.24	46,82,118,145	0
26	DMU	W	102	32/33	0.75	0.21	50,80,104,115	0
19	TGL	D	201	63/63	0.76	0.24	41,71,103,117	0
19	TGL	Q	201	63/63	0.76	0.25	49,77,107,112	0
25	CDL	G	102	100/100	0.77	0.23	46,88,122,152	0
20	PGV	C	304	51/51	0.78	0.25	44,88,114,150	0
20	PGV	A	609	51/51	0.78	0.25	43,77,132,157	0
27	PSC	R	201	52/52	0.78	0.27	44,94,141,175	0
25	CDL	P	305	100/100	0.79	0.24	41,90,124,138	0
19	TGL	A	607	63/63	0.79	0.23	47,73,96,105	0
25	CDL	C	305	100/100	0.80	0.23	41,86,116,128	0
19	TGL	O	303	63/63	0.80	0.21	52,76,99,106	0
19	TGL	L	101	63/63	0.80	0.23	33,63,97,113	0
19	TGL	N	607	63/63	0.80	0.25	45,69,101,121	0
21	EDO	N	615	4/4	0.81	0.24	46,68,84,87	0
27	PSC	E	201	52/52	0.81	0.27	42,95,144,175	0
21	EDO	S	103	4/4	0.81	0.26	40,50,56,68	0
21	EDO	Q	203	4/4	0.82	0.22	41,46,57,69	0
21	EDO	P	308	4/4	0.84	0.18	53,62,69,87	0
26	DMU	O	304	22/33	0.86	0.15	43,69,95,113	0
21	EDO	N	610	4/4	0.87	0.20	39,45,49,55	0
23	CHD	C	306	29/29	0.87	0.13	42,54,66,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	DMU	Z	101	33/33	0.89	0.14	46,58,88,96	0
21	EDO	Q	202	4/4	0.90	0.14	35,43,43,59	0
23	CHD	P	306	29/29	0.90	0.12	46,57,72,86	0
21	EDO	A	613	4/4	0.90	0.15	34,42,61,62	0
21	EDO	O	306	4/4	0.91	0.16	43,43,53,53	0
26	DMU	M	101	33/33	0.92	0.11	36,48,66,80	0
21	EDO	A	611	4/4	0.93	0.13	29,30,33,47	0
21	EDO	N	613	4/4	0.93	0.12	40,47,52,58	0
21	EDO	N	612	4/4	0.94	0.14	33,47,64,72	0
24	PEK	P	302	53/53	0.94	0.15	31,53,96,104	0
24	PEK	C	302	53/53	0.94	0.13	26,46,92,97	0
21	EDO	P	309	4/4	0.94	0.12	37,41,42,53	0
20	PGV	P	303	51/51	0.95	0.12	24,36,88,99	0
20	PGV	N	609	51/51	0.96	0.11	23,35,75,81	0
21	EDO	A	612	4/4	0.96	0.14	31,38,51,57	0
21	EDO	N	611	4/4	0.96	0.08	31,32,32,40	0
21	EDO	O	305	4/4	0.96	0.08	32,33,36,36	0
21	EDO	N	614	4/4	0.97	0.07	26,33,35,37	0
21	EDO	S	104	4/4	0.97	0.08	40,40,47,58	0
23	CHD	C	301	29/29	0.97	0.06	24,29,35,38	0
20	PGV	C	303	51/51	0.97	0.10	20,33,83,93	0
21	EDO	C	308	4/4	0.97	0.09	34,40,48,56	0
23	CHD	O	302	29/29	0.97	0.06	24,28,36,41	0
23	CHD	P	301	29/29	0.97	0.06	24,31,35,37	0
20	PGV	A	608	51/51	0.97	0.10	20,31,73,85	0
21	EDO	S	102	4/4	0.97	0.07	26,27,29,30	0
18	NA	N	606	1/1	0.98	0.09	34,34,34,34	0
14	HEA	N	601	60/60	0.98	0.06	21,27,44,47	0
21	EDO	B	303	4/4	0.98	0.05	27,27,29,31	0
15	NO	A	603	2/2	0.98	0.06	20,20,20,25	0
21	EDO	F	102	4/4	0.98	0.05	25,25,26,27	0
21	EDO	A	610	4/4	0.98	0.07	24,24,26,29	0
23	CHD	B	302	29/29	0.98	0.05	24,28,35,40	0
18	NA	A	606	1/1	0.98	0.10	29,29,29,29	0
14	HEA	A	601	60/60	0.99	0.05	16,22,37,41	0
14	HEA	N	602	60/60	0.99	0.05	21,25,31,37	0
14	HEA	A	602	60/60	0.99	0.05	17,21,28,34	0
15	NO	N	603	2/2	0.99	0.04	26,26,26,27	0
16	CU	A	604	1/1	1.00	0.01	22,22,22,22	0
16	CU	N	604	1/1	1.00	0.01	24,24,24,24	0
22	CUA	B	301	2/2	1.00	0.01	23,23,23,23	0
22	CUA	O	301	2/2	1.00	0.02	28,28,28,28	0

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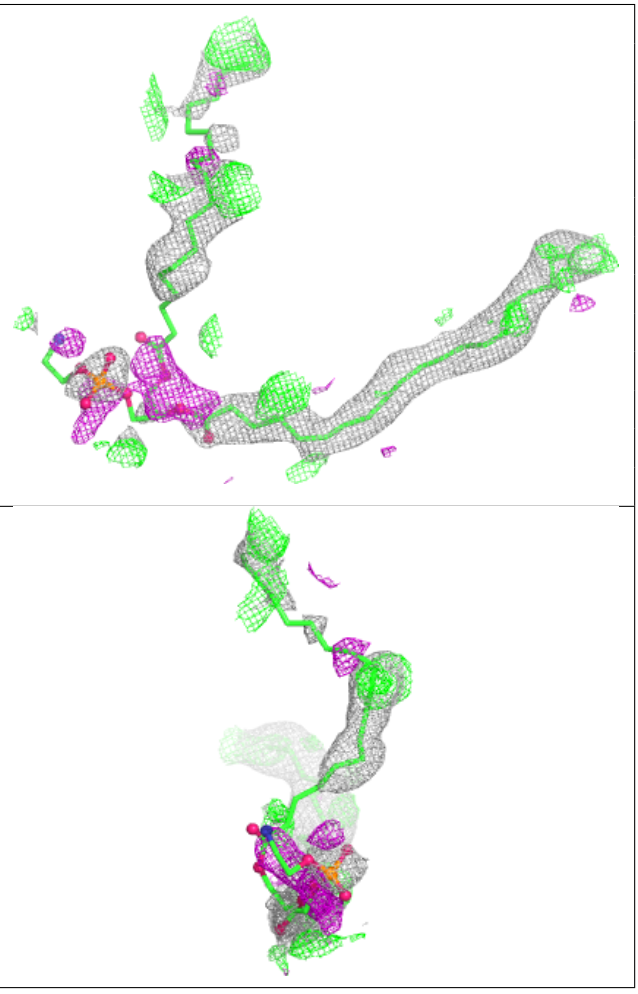
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	MG	A	605	1/1	1.00	0.05	19,19,19,19	0
17	MG	N	605	1/1	1.00	0.07	24,24,24,24	0
28	ZN	F	101	1/1	1.00	0.04	29,29,29,29	0
28	ZN	S	101	1/1	1.00	0.03	31,31,31,31	0

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

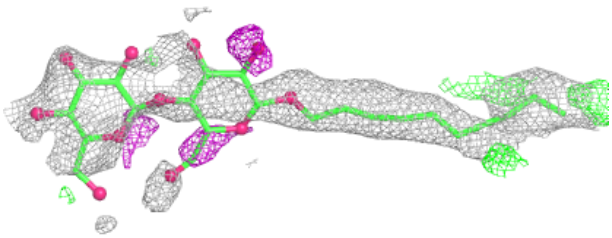
Electron density around PEK G 103:

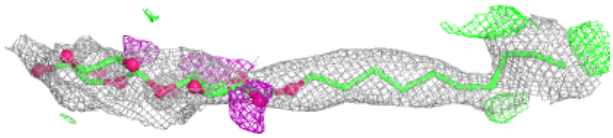
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

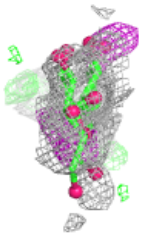


Electron density around DMU P 307:

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

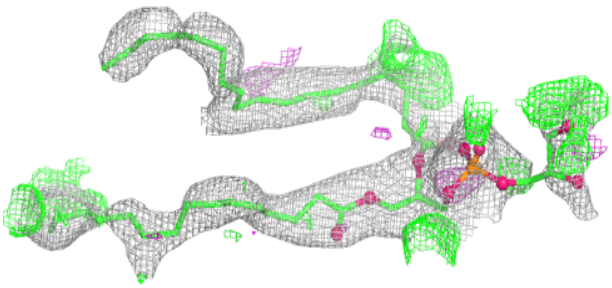


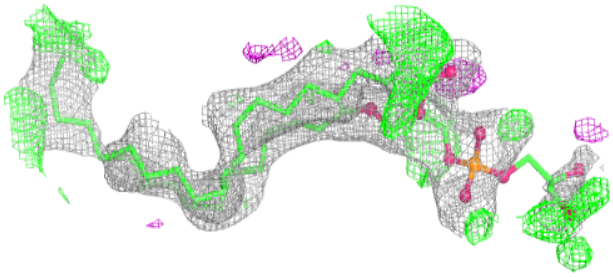


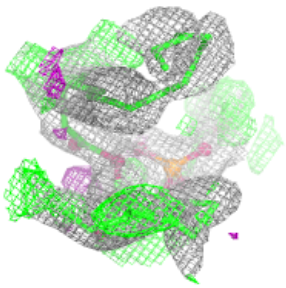


Electron density around PGV P 304:

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

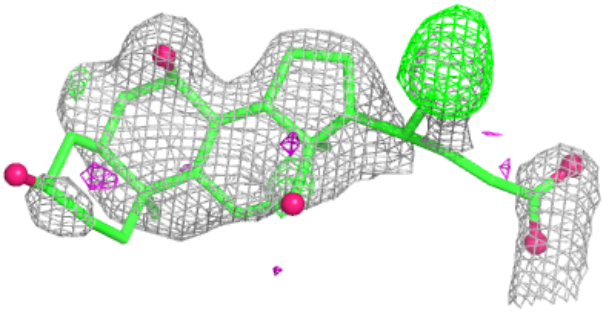


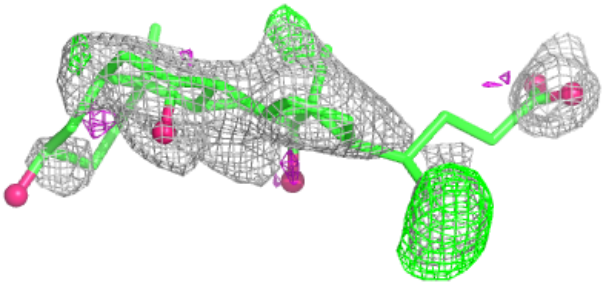


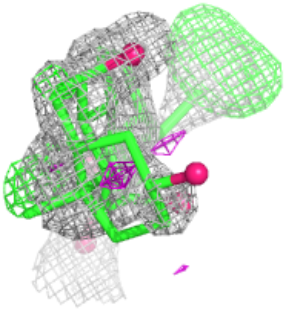


Electron density around CHD J 101:

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

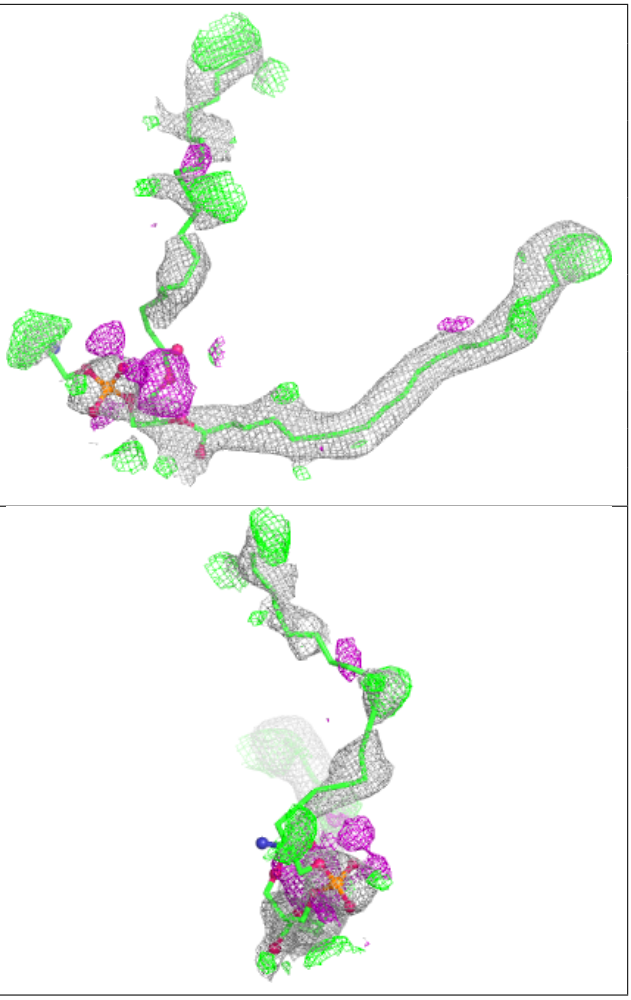






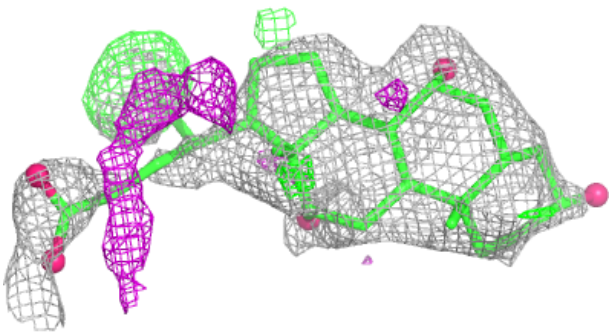
Electron density around PEK T 102:

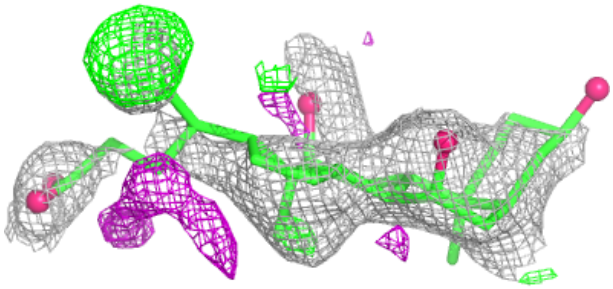
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

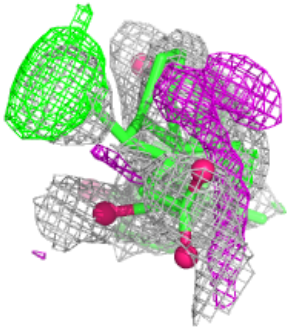


Electron density around CHD W 101:

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

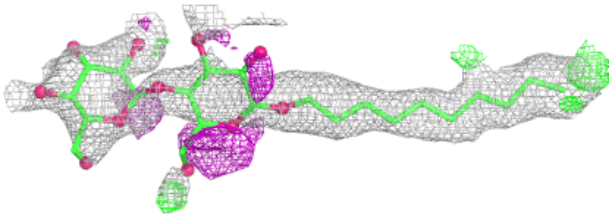


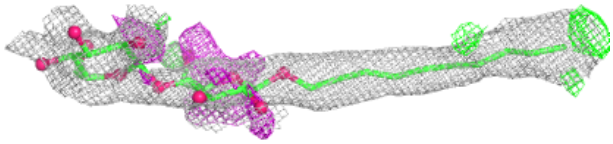


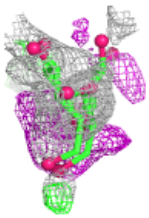


Electron density around DMU C 307:

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

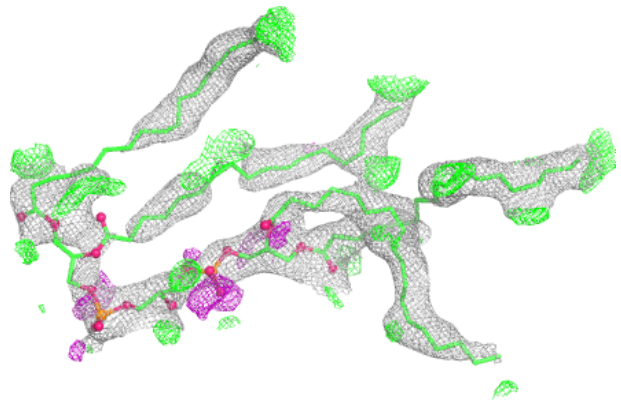


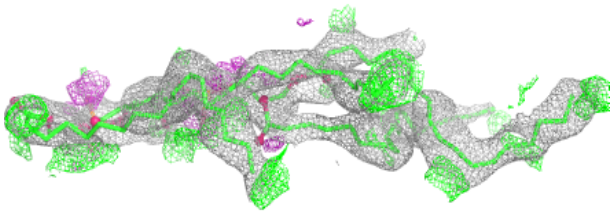


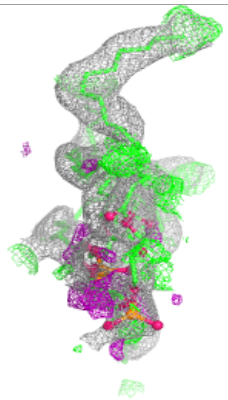


Electron density around CDL T 103:

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

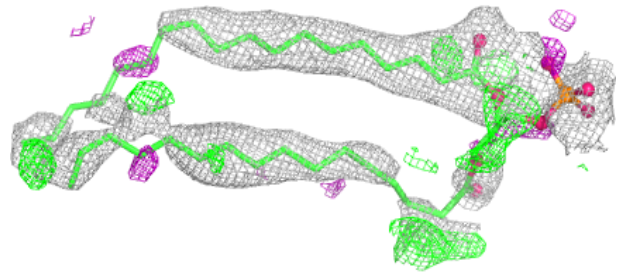


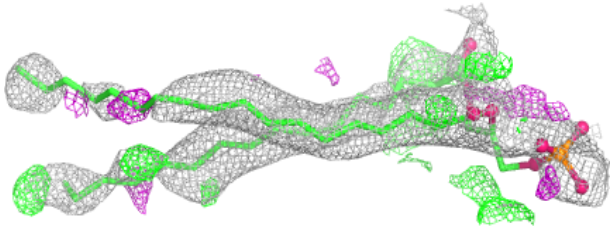


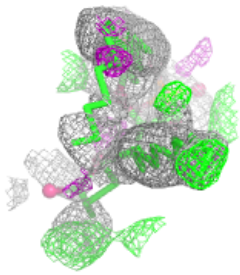


Electron density around PGV N 608:

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

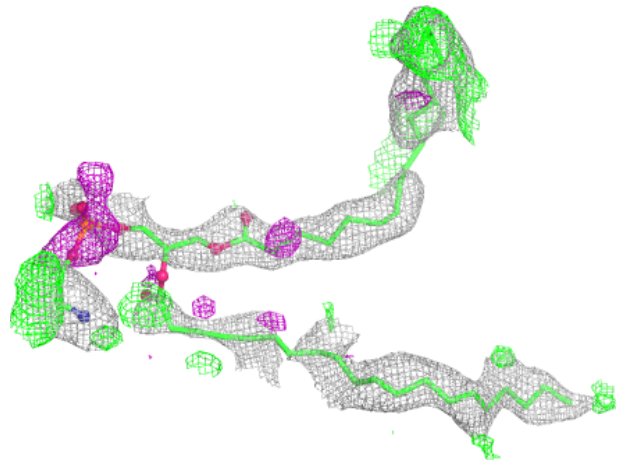


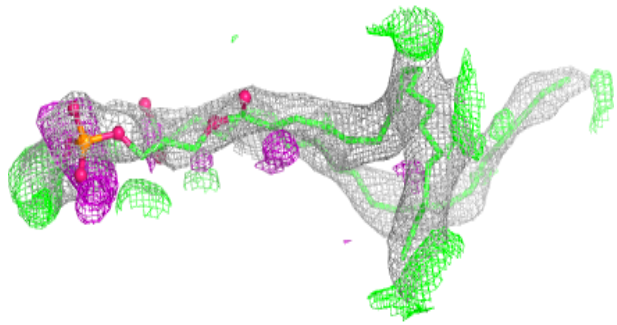


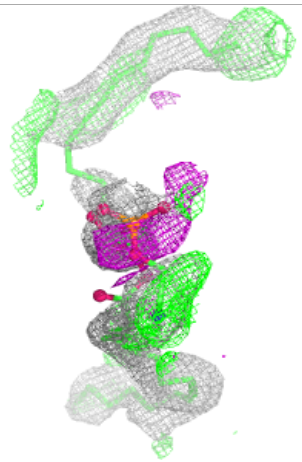


Electron density around PEK T 101:

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

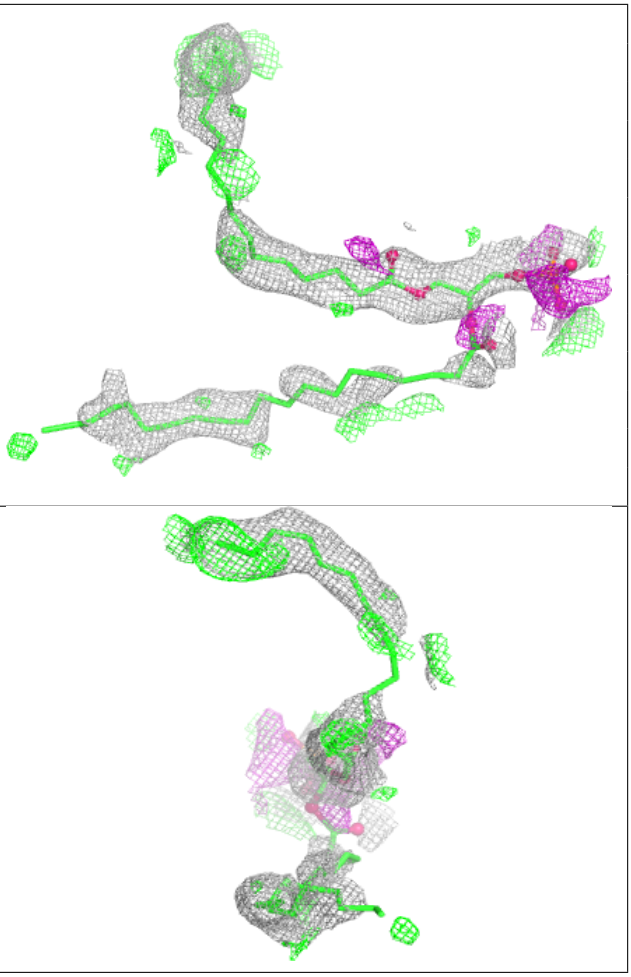






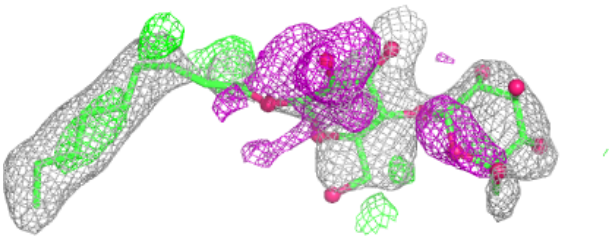
Electron density around PEK G 101:

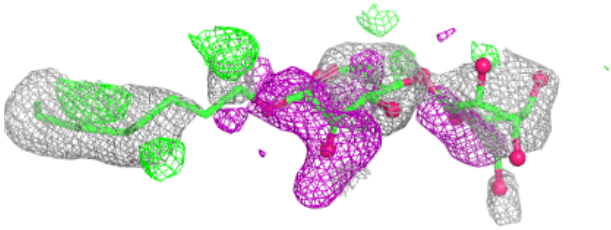
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

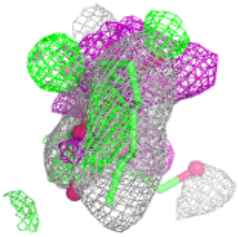


Electron density around DMU W 102:

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

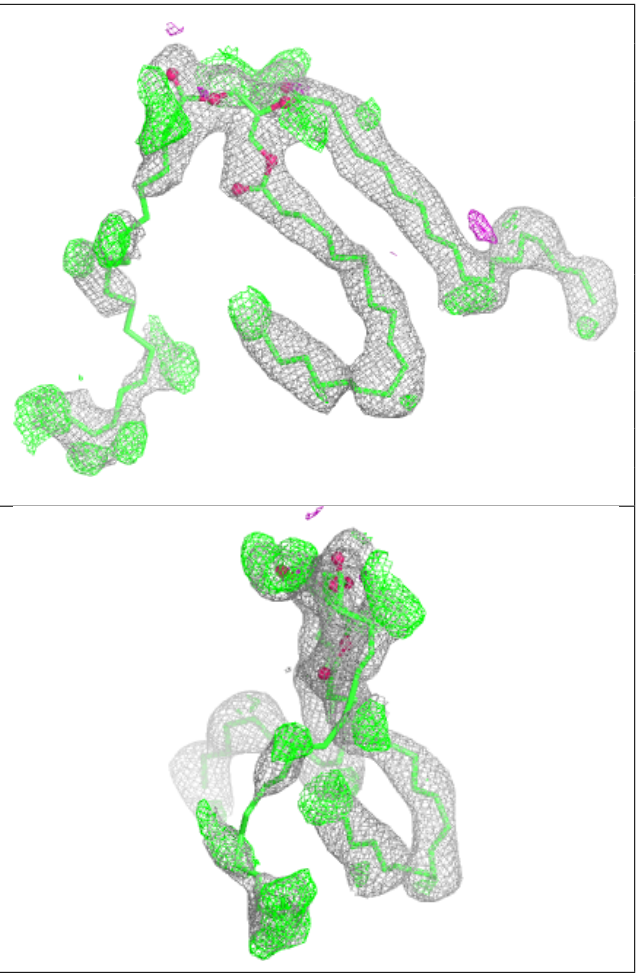






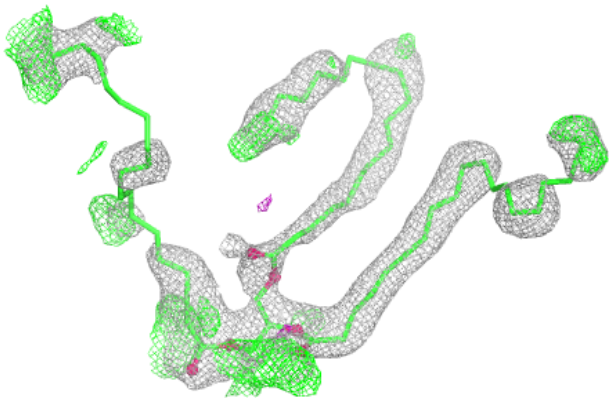
Electron density around TGL D 201:

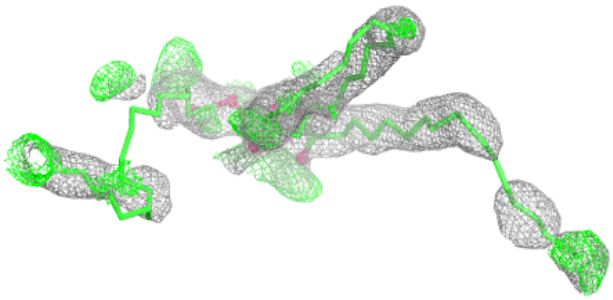
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

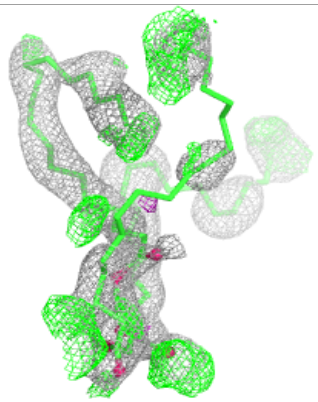


Electron density around TGL Q 201:

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

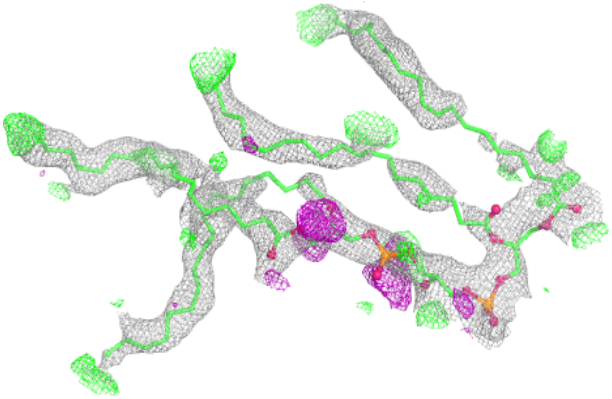


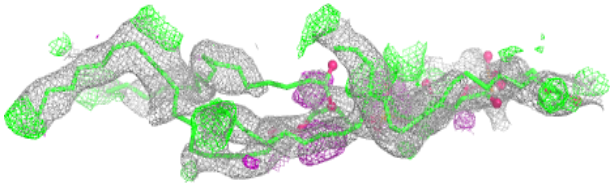


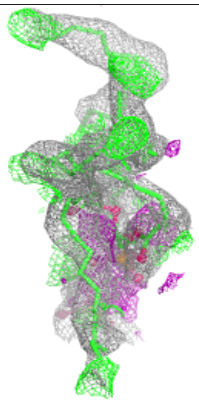


Electron density around CDL G 102:

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

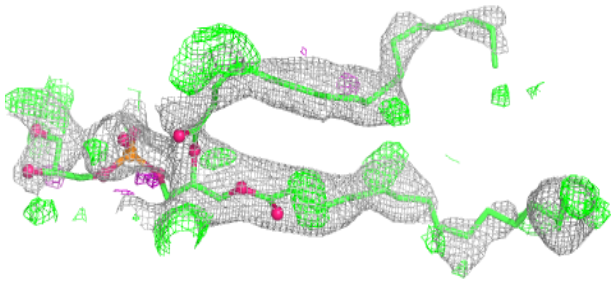


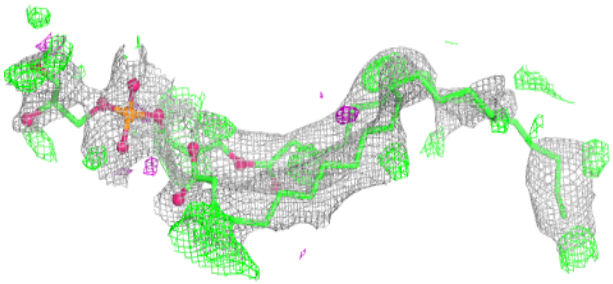


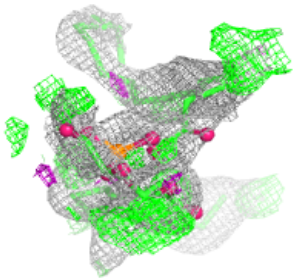


Electron density around PGV C 304:

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

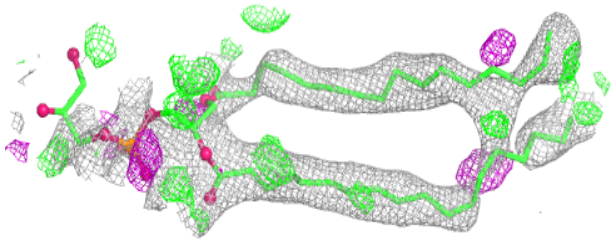


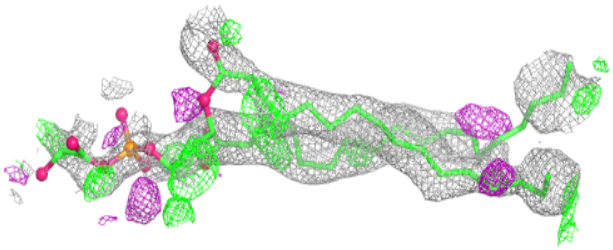


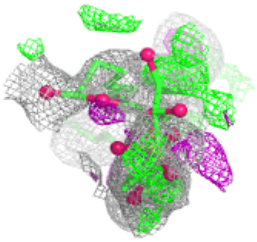


Electron density around PGV A 609:

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

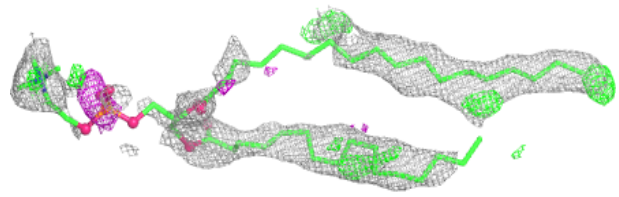


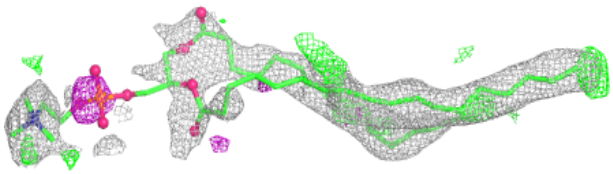


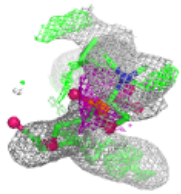


Electron density around PSC R 201:

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

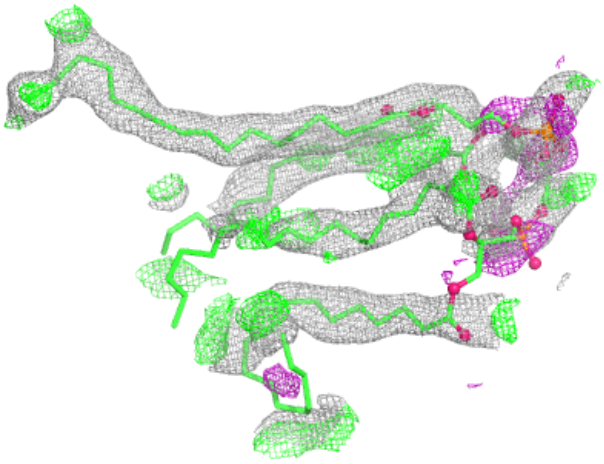


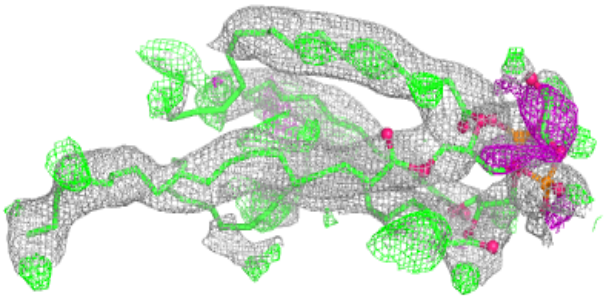


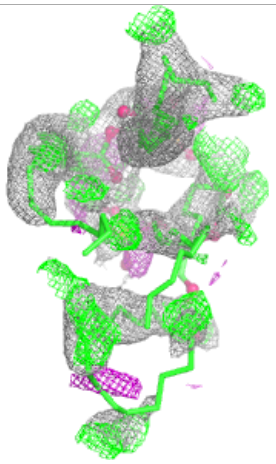


Electron density around CDL P 305:

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

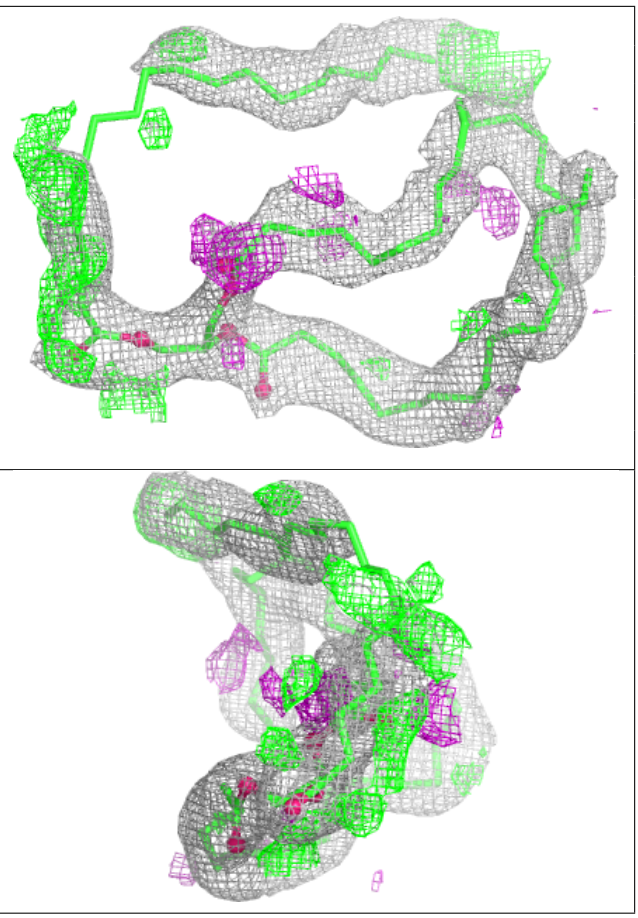






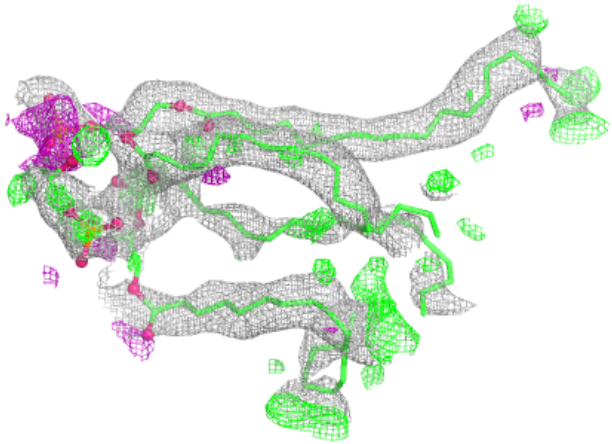
Electron density around TGL A 607:

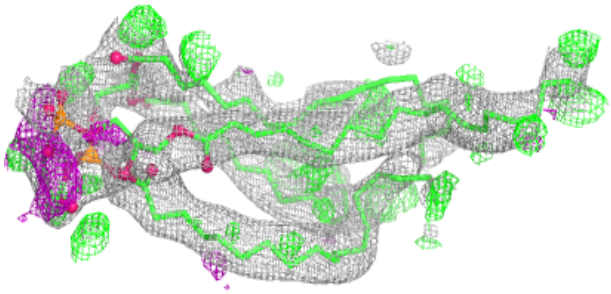
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

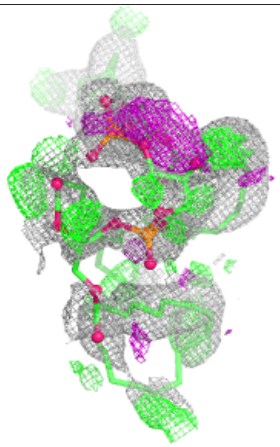


Electron density around CDL C 305:

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

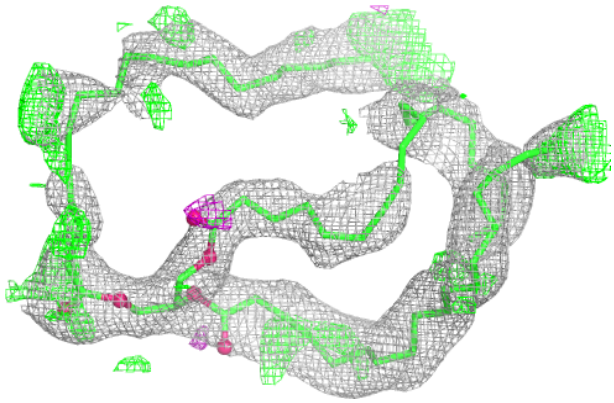


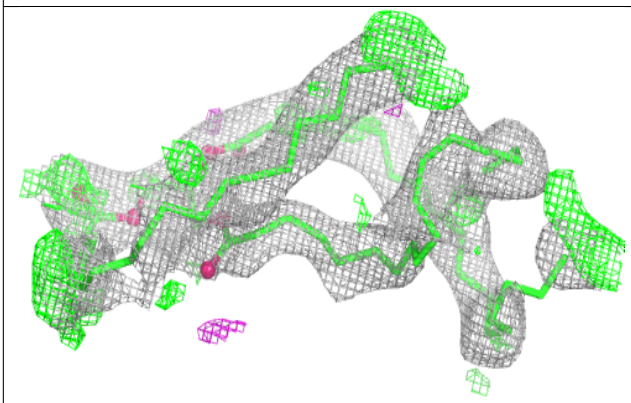


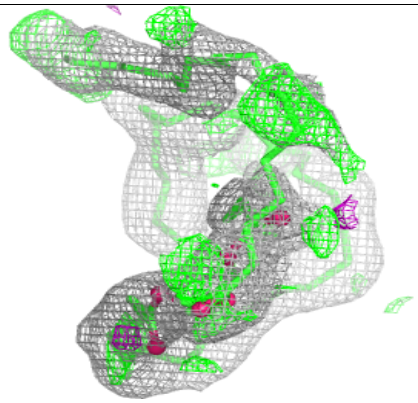


Electron density around TGL O 303:

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

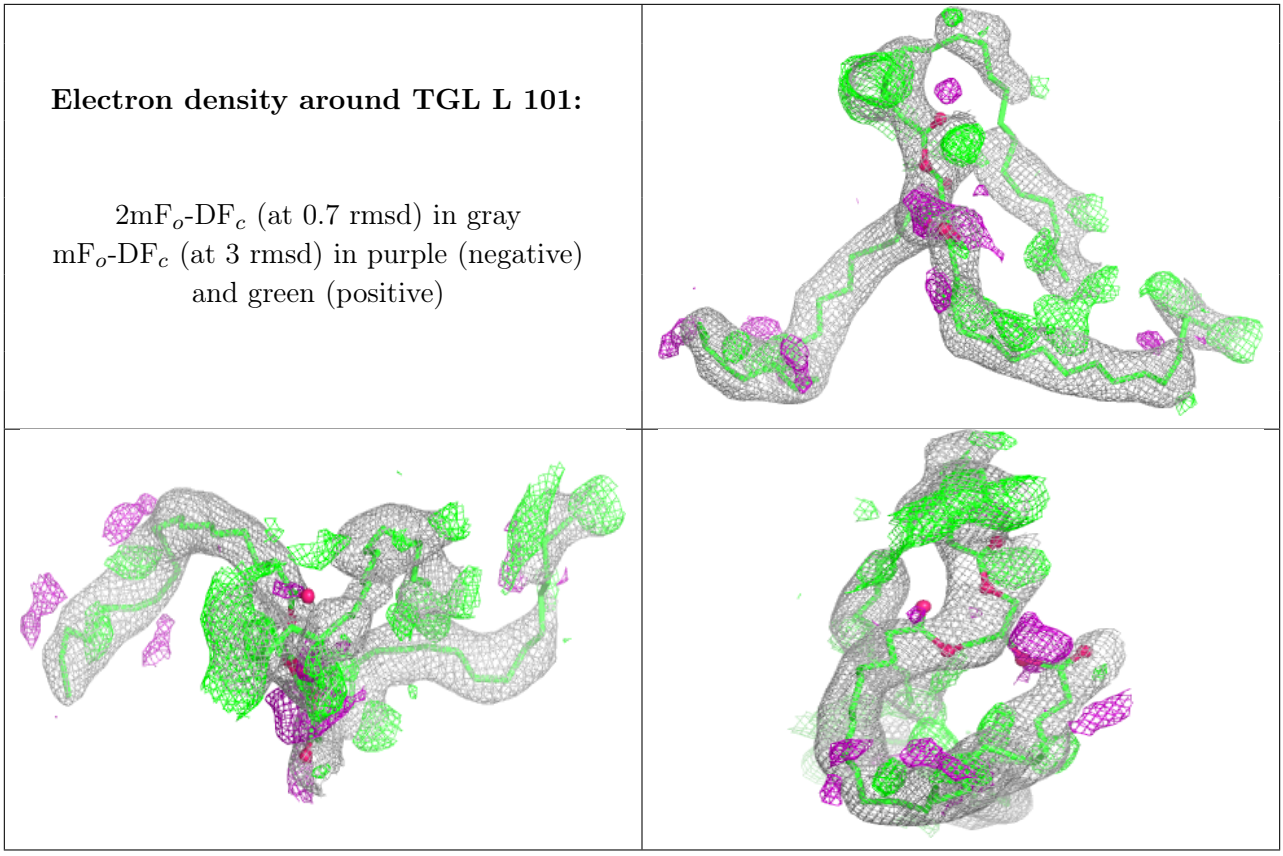






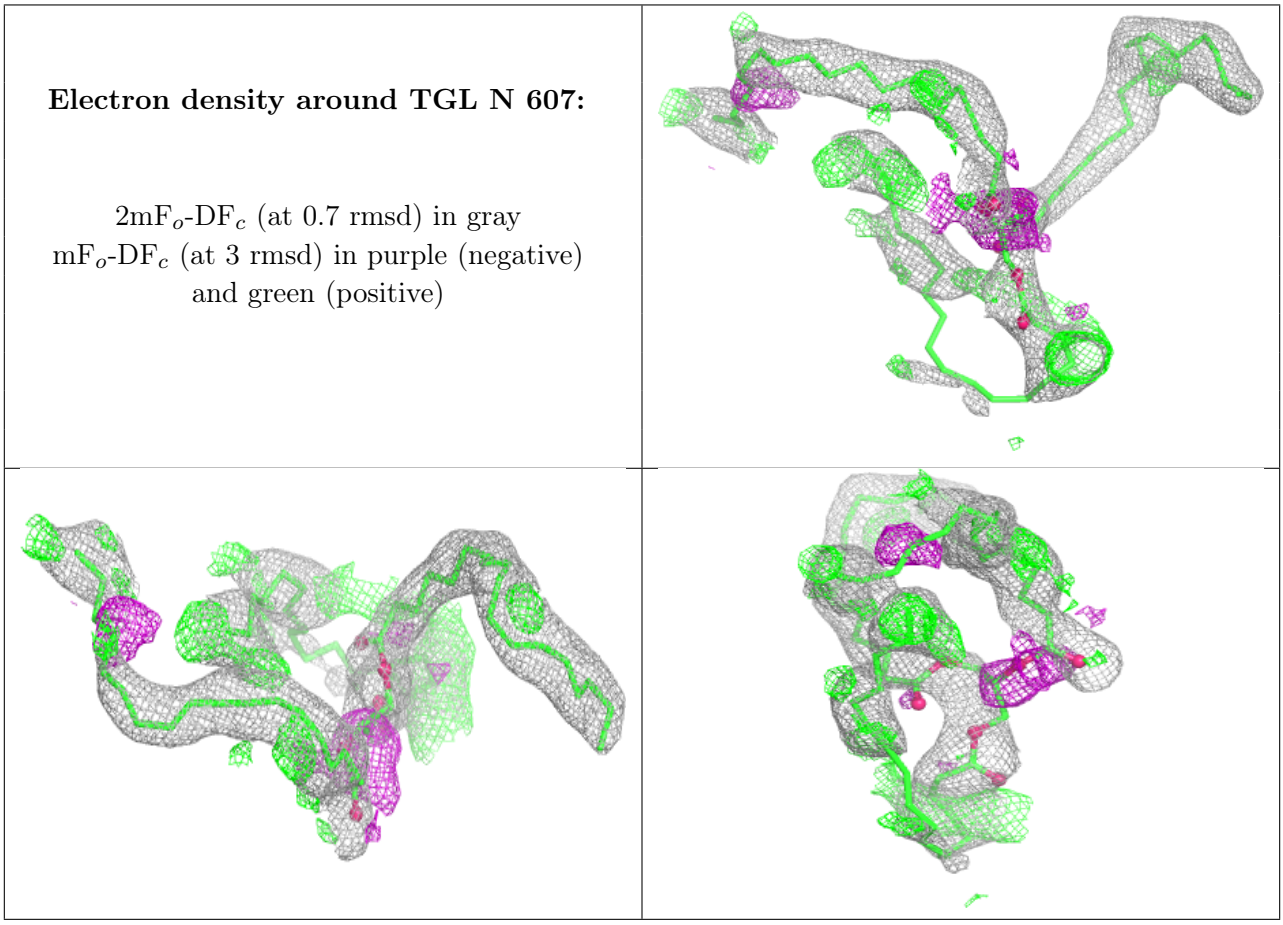
Electron density around TGL L 101:

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



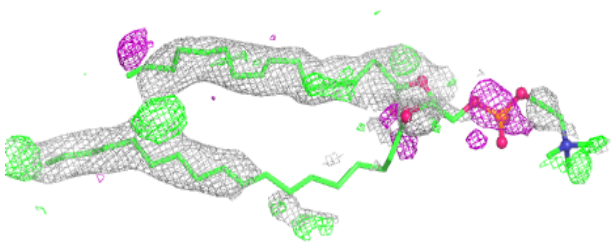
Electron density around TGL N 607:

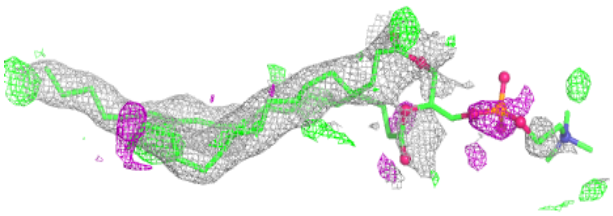
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

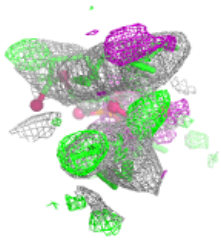


Electron density around PSC E 201:

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

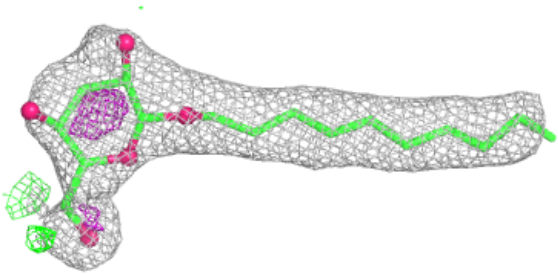


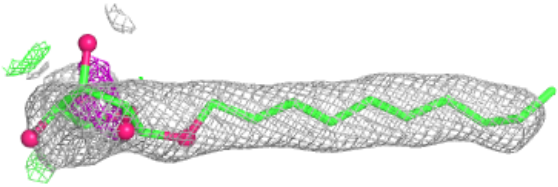


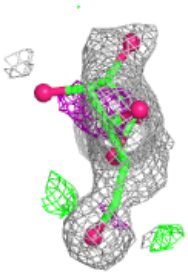


Electron density around DMU O 304:

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

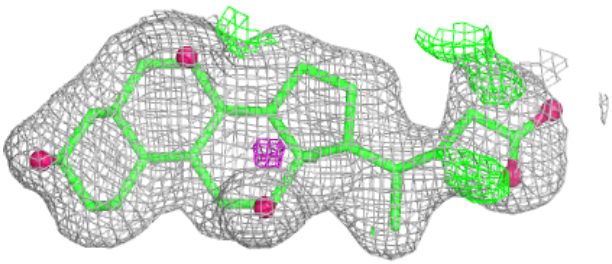


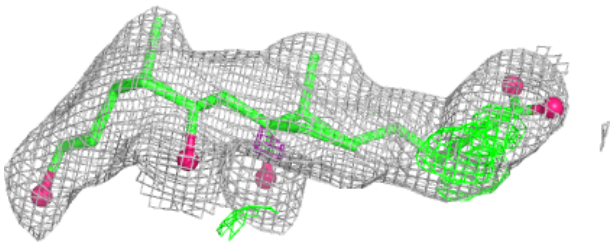


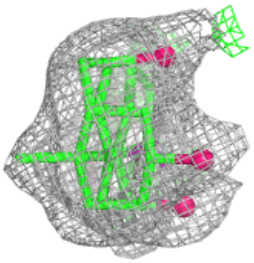


Electron density around CHD C 306:

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

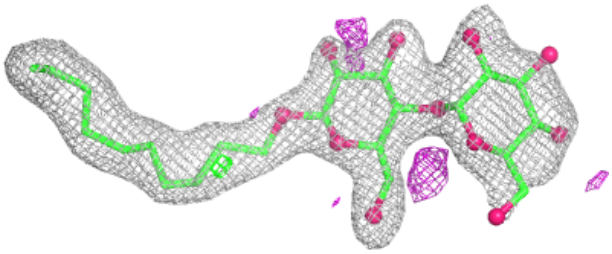


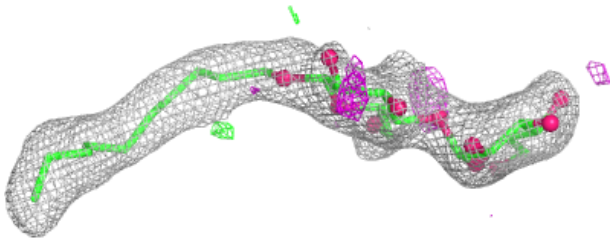


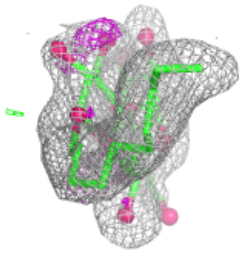


Electron density around DMU Z 101:

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

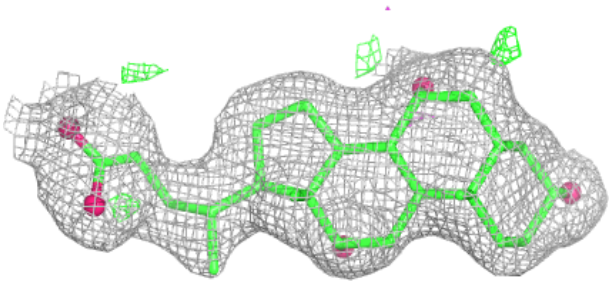


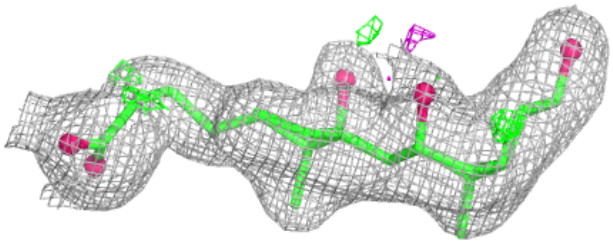


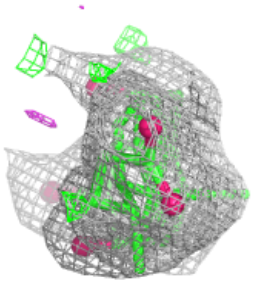


Electron density around CHD P 306:

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

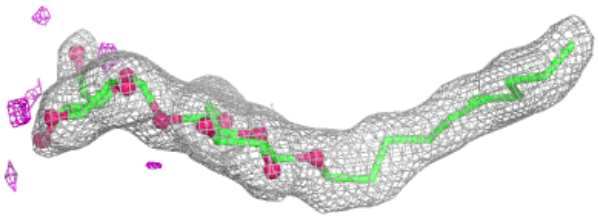


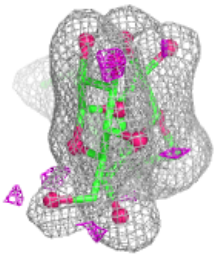




Electron density around DMU M 101:

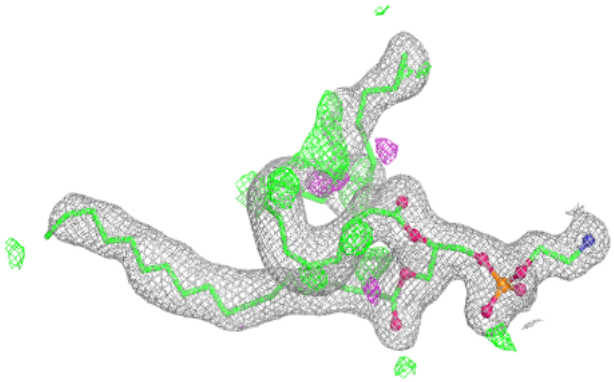
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

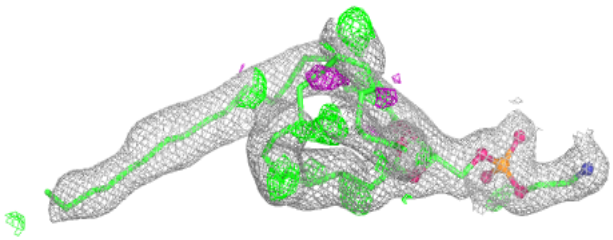


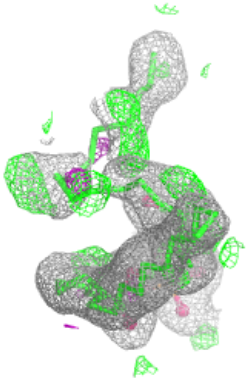


Electron density around PEK P 302:

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

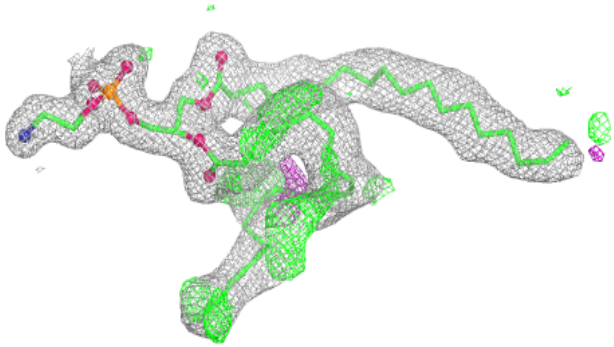


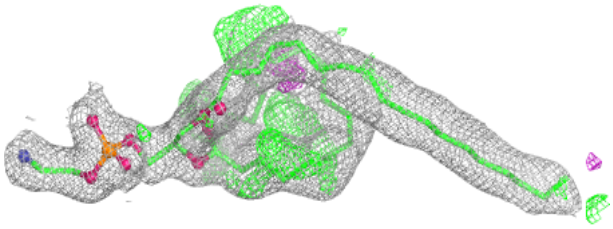




Electron density around PEK C 302:

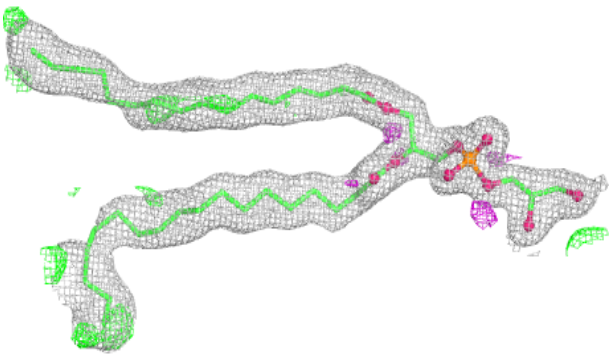
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

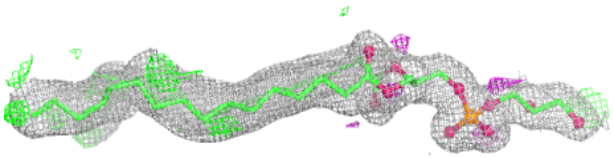


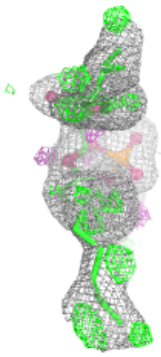


Electron density around PGV P 303:

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

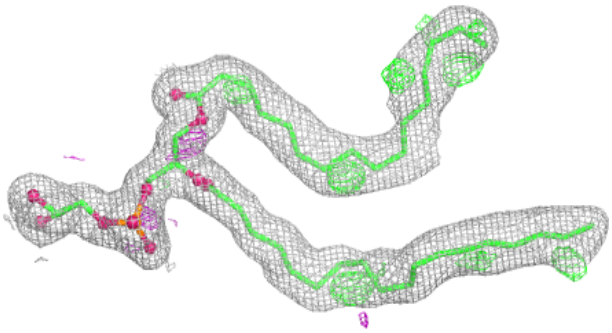


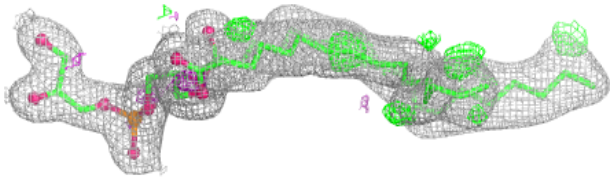


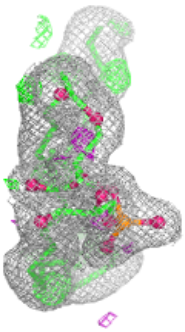


Electron density around PGV N 609:

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

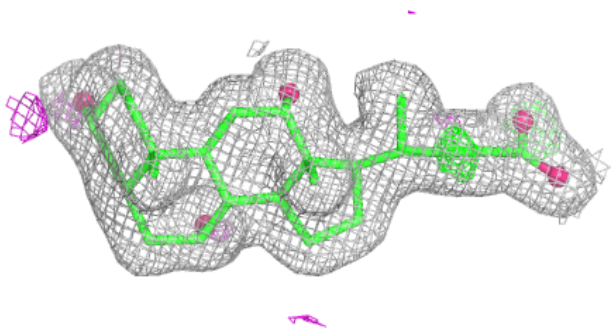


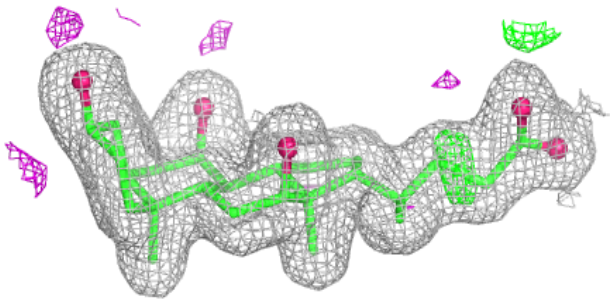


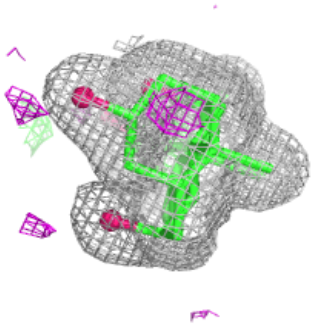


Electron density around CHD C 301:

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

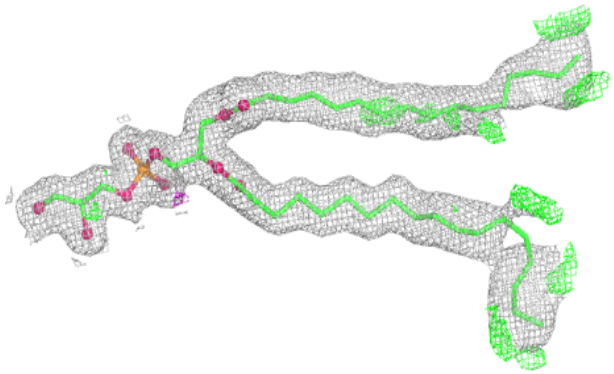


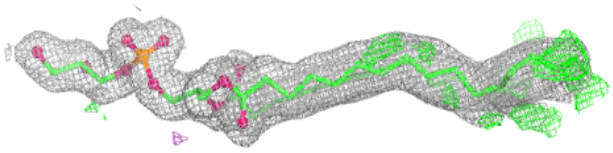


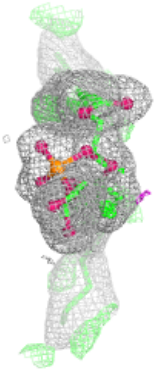


Electron density around PGV C 303:

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

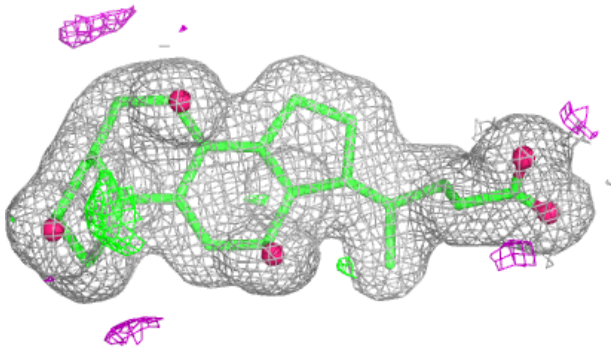


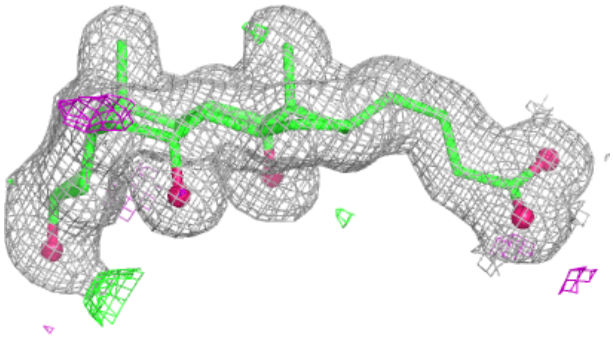


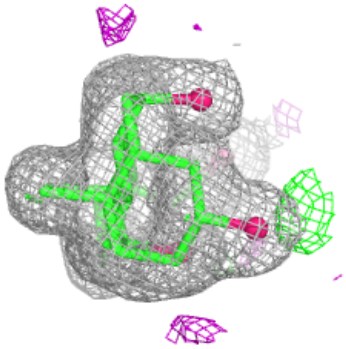


Electron density around CHD O 302:

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

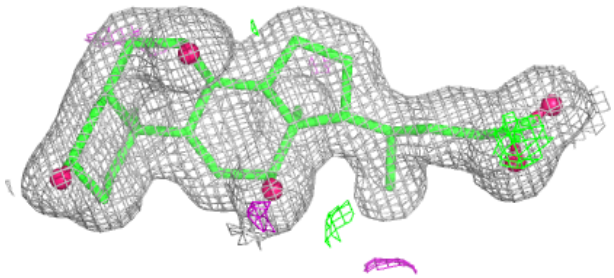


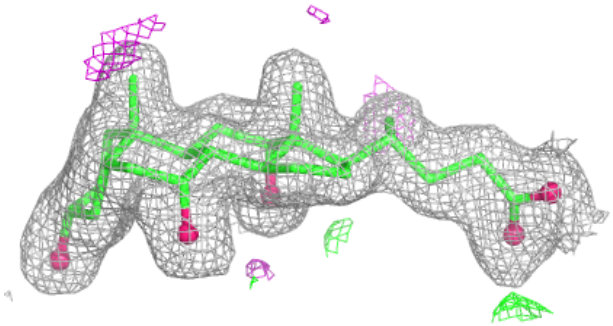


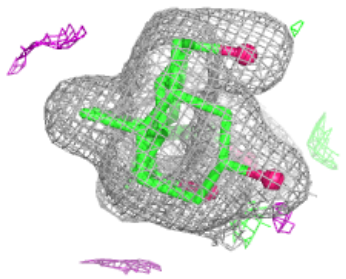


Electron density around CHD P 301:

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

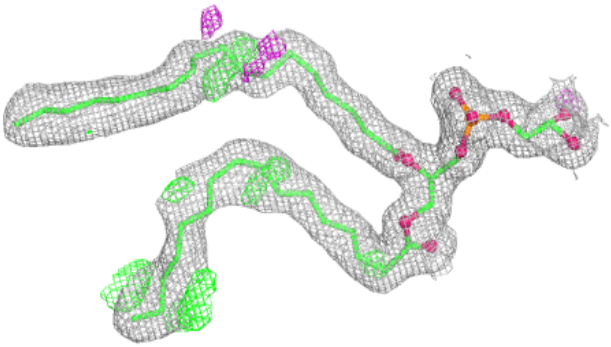


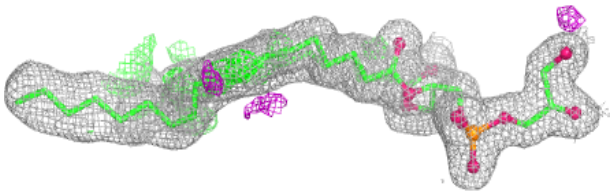


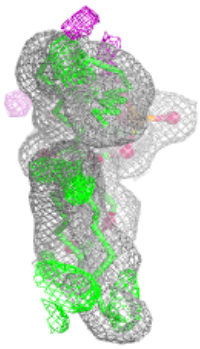


Electron density around PGV A 608:

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

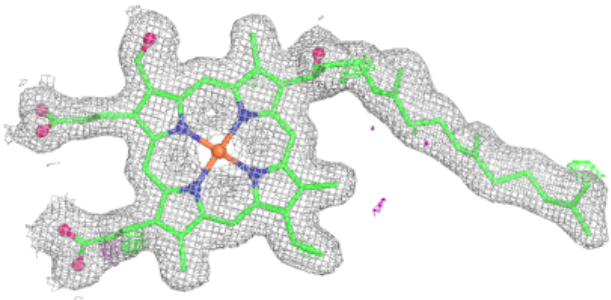


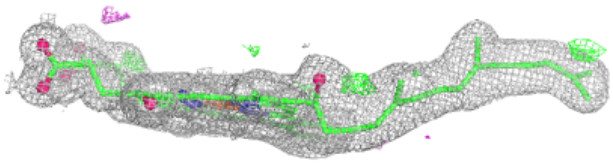


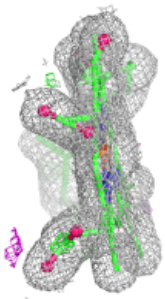


Electron density around HEA N 601:

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

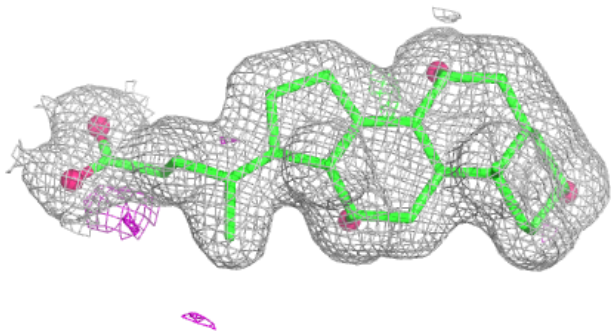


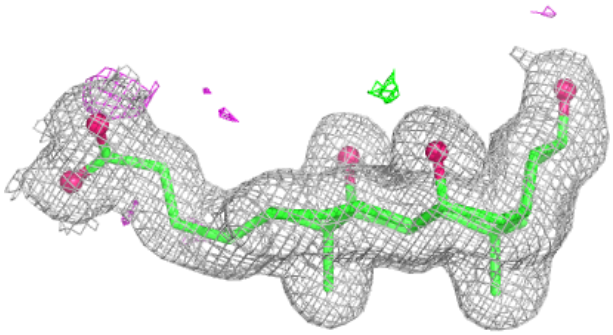


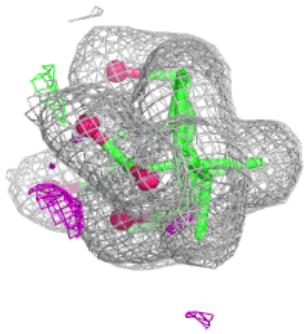


Electron density around CHD B 302:

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

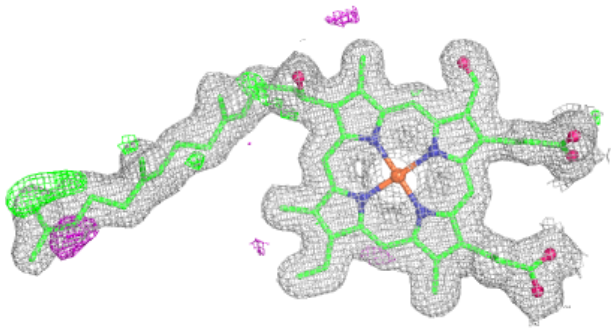


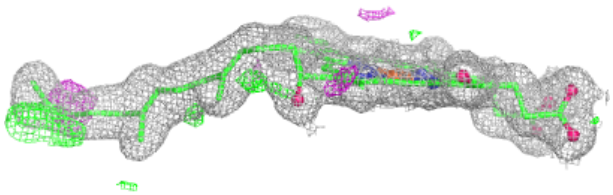


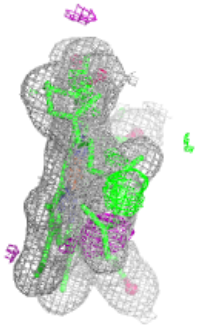


Electron density around HEA A 601:

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

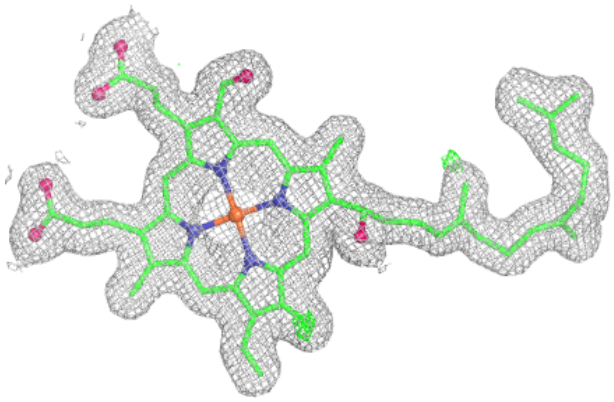


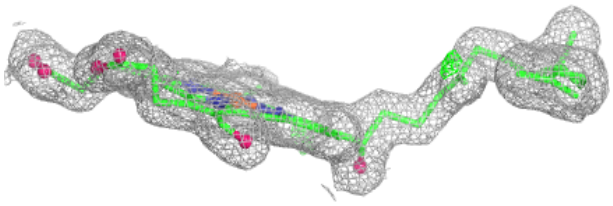


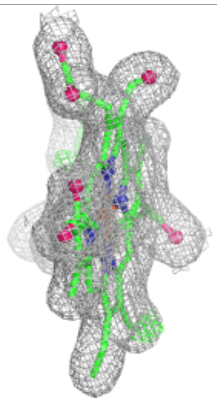


Electron density around HEA N 602:

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

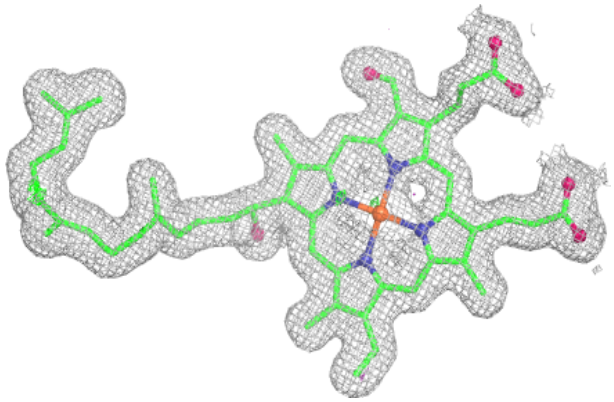


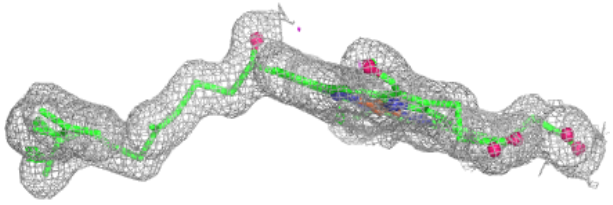


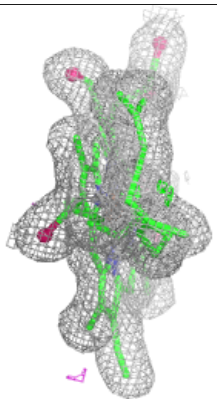


Electron density around HEA A 602:

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







6.5 Other polymers (i)

There are no such residues in this entry.