Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 12:10 PM JST

PDB ID	:	5X19
Title	:	CO bound cytochrome c oxidase at 100 micro sec after pump laser irradiation to release CO from O2 reduction center
Authors	:	Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on	:	2017-01-25
Resolution	:	2.20 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:

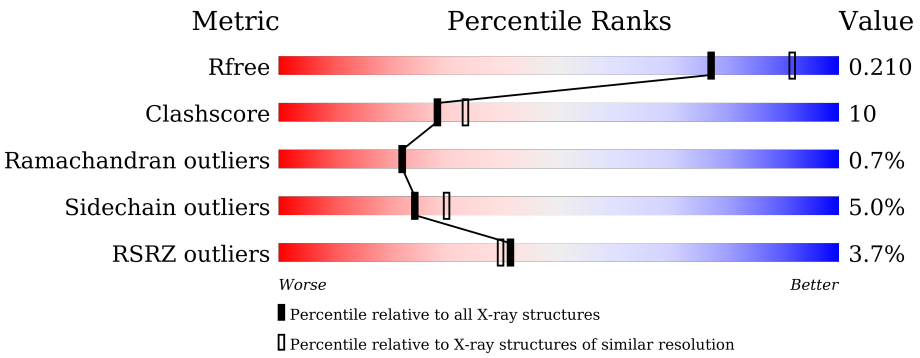
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	85% 14% •
1	N	514	% 81% 18% •
2	B	227	% 77% 22% •

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	O	227	3% 74% 22%
3	C	261	84% 15%
3	P	261	2% 88% 11%
4	D	147	% 84% 12%
4	Q	147	11% 79% 17%
5	E	109	2% 85% 11%
5	R	109	6% 73% 19%
6	F	98	10% 67% 24% 5%
6	S	98	6% 76% 20%
7	G	85	18% 66% 26% 5%
7	T	85	12% 62% 28% 8%
8	H	85	5% 71% 18% 7%
8	U	85	6% 76% 15% 7%
9	I	73	4% 81% 14% 5%
9	V	73	7% 79% 19%
10	J	59	8% 88% 7%
10	W	59	5% 76% 19%
11	K	56	9% 68% 20% 12%
11	X	56	14% 70% 16% 12%
12	L	47	66% 28%
12	Y	47	6% 72% 23%
13	M	46	2% 74% 17% 7%
13	Z	46	9% 72% 22% 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
18	CMO	N	606	-	-	X	-
21	EDO	A	612	-	-	X	-
21	EDO	A	613	-	-	X	-
21	EDO	C	310	-	-	-	X
21	EDO	N	610	-	-	-	X
21	EDO	T	105	-	-	X	-
25	UNX	P	302	-	-	-	X
26	CDL	T	104	-	-	X	-
27	PEK	G	103	-	-	-	X
27	PEK	T	102	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 32242 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	4068	2718	628	686	36	0	7	0
1	N	514	4027	2691	623	678	35	0	0	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	1824	1185	281	340	18	0	0	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	2110	1412	336	350	12	0	0	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, mitochondrial.

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	609	398	107	100	4	0	1	0
9	V	73	617	406	107	100	4	0	2	0

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

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.

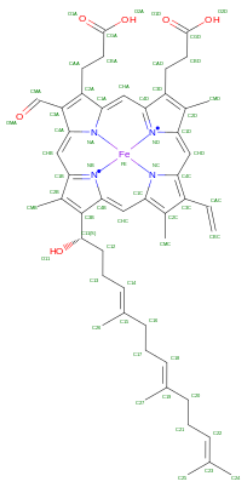
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	380	254	64	60	2	0	0	0

- 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 (three-letter code: 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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

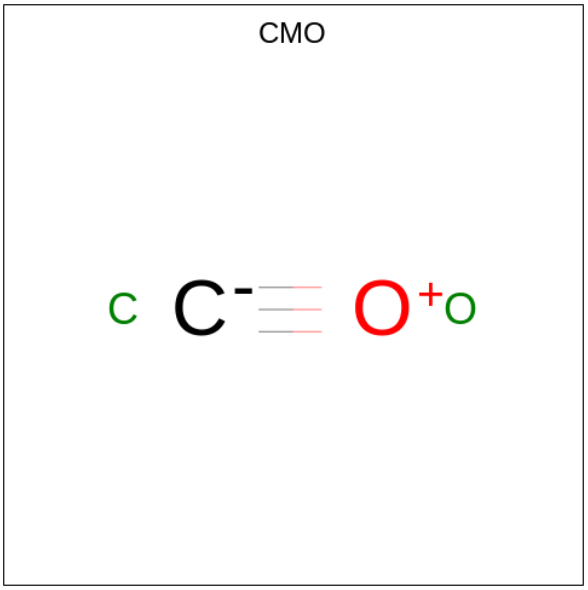
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

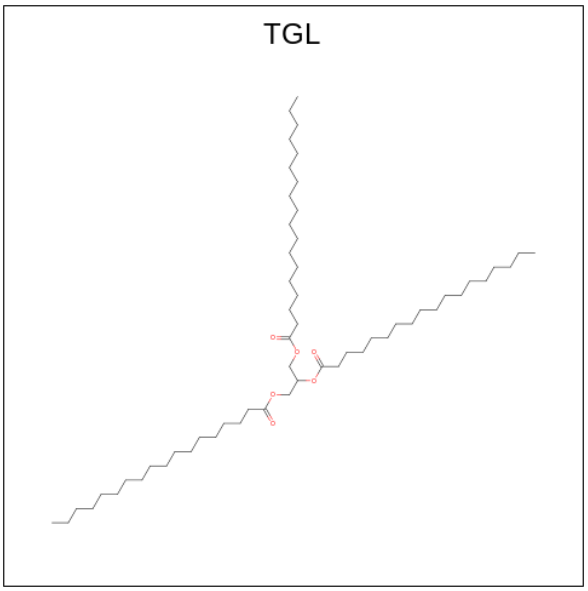
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
17	A	1	1	1	0	0
			Total	Na		
17	N	1	1	1	0	0

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



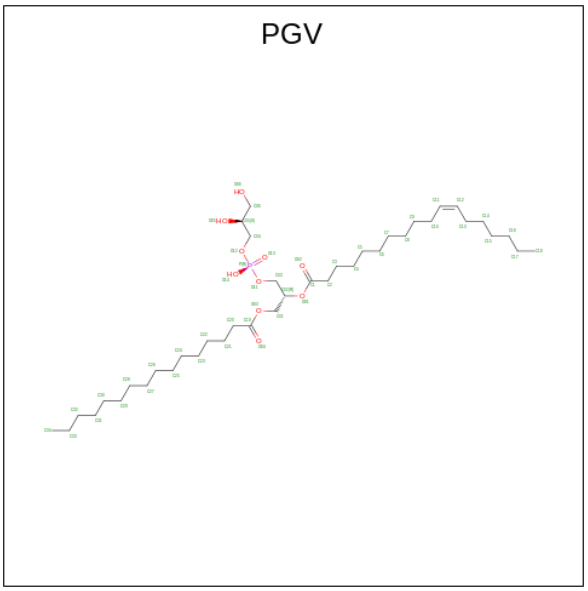
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	A	1	2	1	1	0	0
			Total	C	O		
18	N	1	2	1	1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



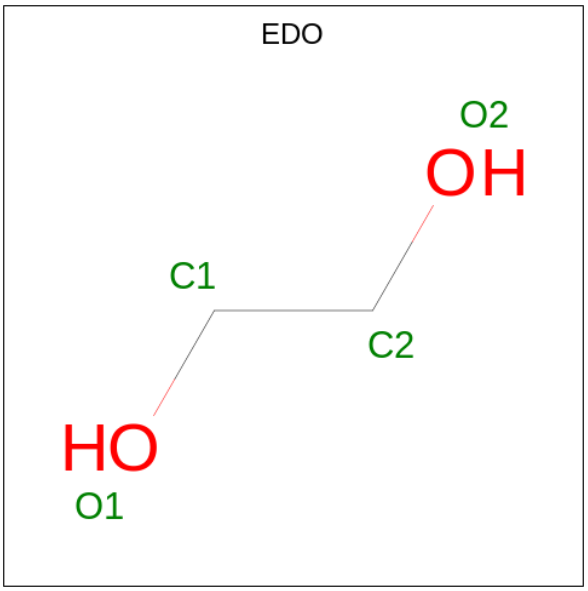
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	D	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	O	1	63	57	6	0	0
19	Q	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: 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	51	40	10	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 (three-letter code: 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	B	1	4	2	2	0	0
			Total	C	O		
21	C	1	4	2	2	0	0
			Total	C	O		
21	C	1	4	2	2	0	0
			Total	C	O		
21	C	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	F	1	4	2	2	0	0
			Total	C	O		
21	G	1	4	2	2	0	0
			Total	C	O		
21	H	1	4	2	2	0	0

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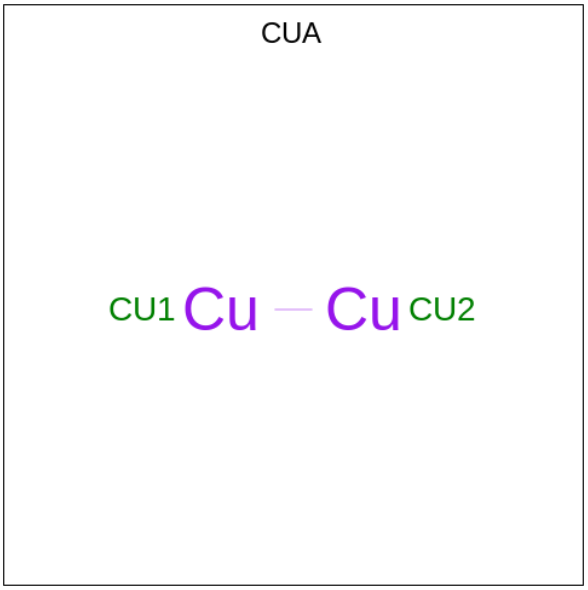
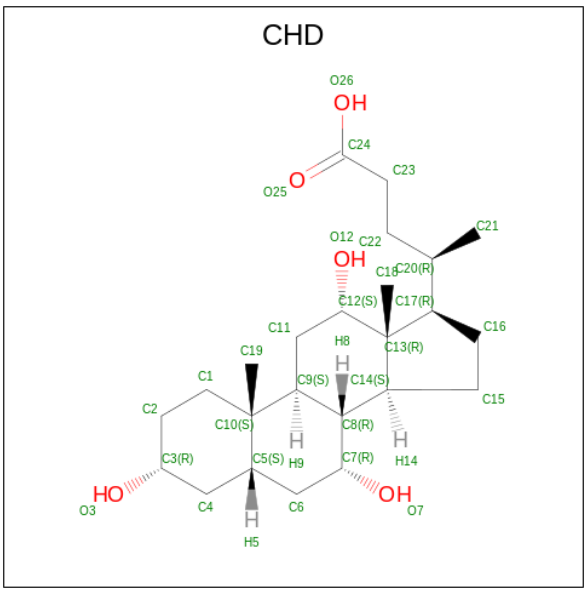
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
21	K	1	4	2	2	0	0
			Total	C	O		
21	K	1	4	2	2	0	0
			Total	C	O		
21	L	1	4	2	2	0	0
			Total	C	O		
21	N	1	4	2	2	0	0
			Total	C	O		
21	N	1	4	2	2	0	0
			Total	C	O		
21	O	1	4	2	2	0	0
			Total	C	O		
21	P	1	4	2	2	0	0
			Total	C	O		
21	P	1	4	2	2	0	0
			Total	C	O		
21	T	1	4	2	2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



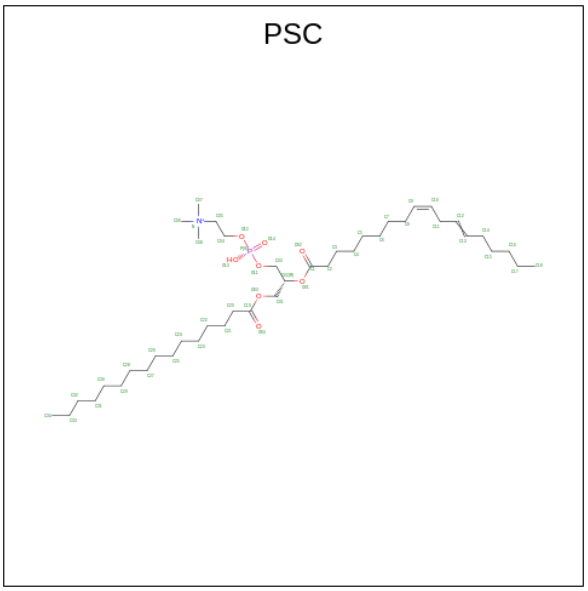
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
22	B	1	2	2	0	0
			Total	Cu		
22	O	1	2	2	0	0

- Molecule 23 is CHOLIC ACID (three-letter code: 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
23	C	1	29	24	5	0	0
23	C	1	29	24	5	0	0
23	G	1	29	24	5	0	0
23	J	1	29	24	5	0	0
23	P	1	29	24	5	0	0
23	P	1	29	24	5	0	0
23	W	1	29	24	5	0	0

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

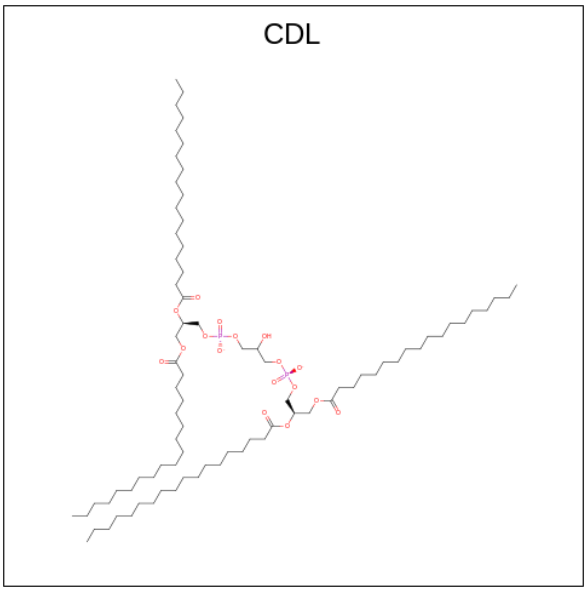


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
24	B	1	52	42	1	8	1	0	0
			Total	C	N	O	P		
24	O	1	52	42	1	8	1	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

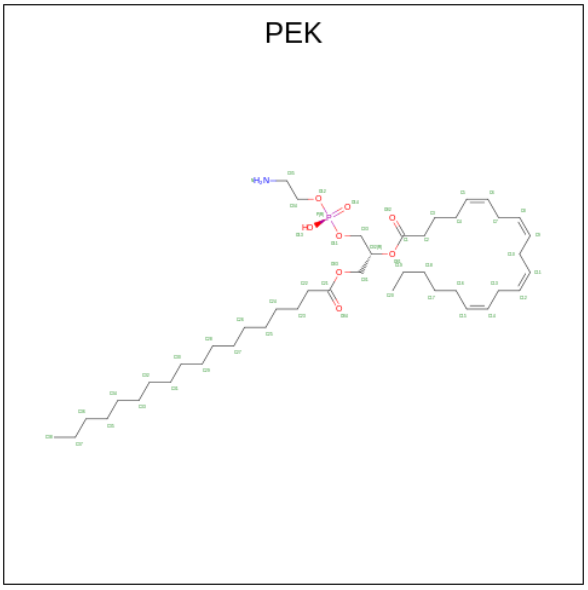
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
25	C	1	1	1	0	0
			Total	X		
25	P	1	1	1	0	0

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



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

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).

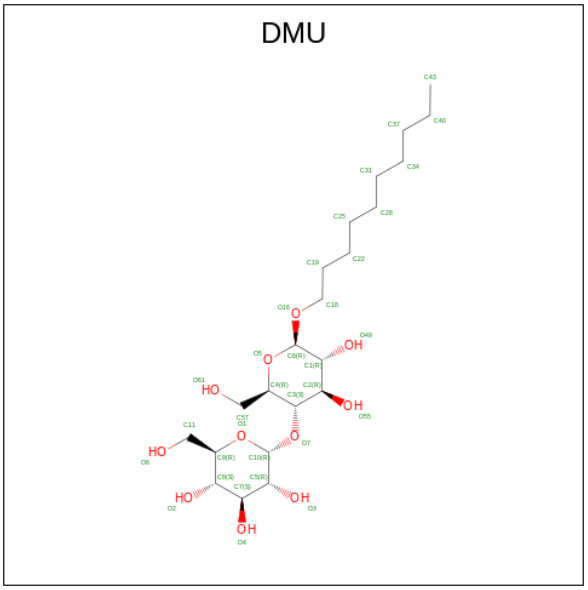


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
27	C	1	53	43	1	8	1	0	0
27	G	1	53	43	1	8	1	0	0
27	G	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0
27	T	1	53	43	1	8	1	0	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
30	A	191	191	191	0	0
30	B	120	121	121	0	1
30	C	83	83	83	0	0
30	D	89	89	89	0	0
30	E	45	45	45	0	0
30	F	49	49	49	0	0
30	G	40	40	40	0	0
30	H	37	37	37	0	0
30	I	19	19	19	0	0
30	J	19	19	19	0	0
30	K	27	27	27	0	0
30	L	27	27	27	0	0
30	M	18	18	18	0	0
30	N	169	169	169	0	0
30	O	100	101	101	0	1
30	P	91	91	91	0	0
30	Q	38	38	38	0	0
30	R	40	40	40	0	0

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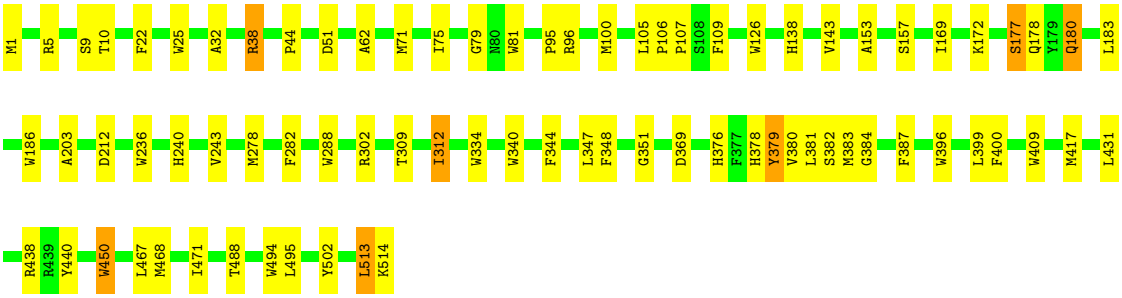
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	S	55	Total O 55 55	0	0
30	T	45	Total O 45 45	0	0
30	U	27	Total O 27 27	0	0
30	V	23	Total O 23 23	0	0
30	W	23	Total O 23 23	0	0
30	X	16	Total O 16 16	0	0
30	Y	18	Total O 18 18	0	0
30	Z	4	Total O 4 4	0	0

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.

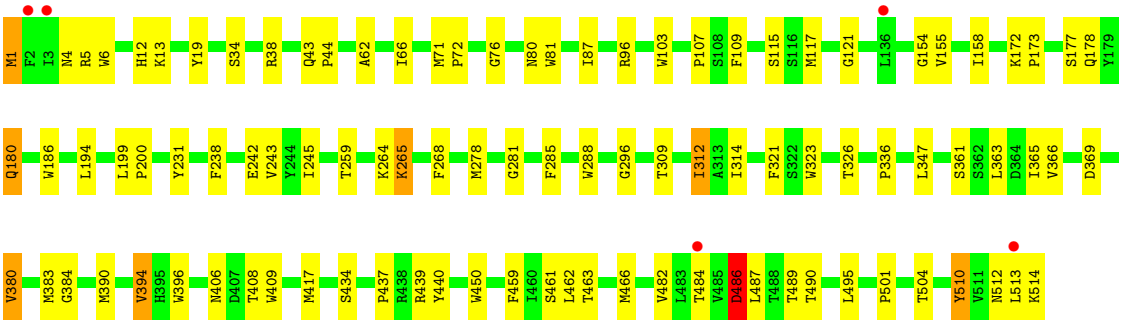
• Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



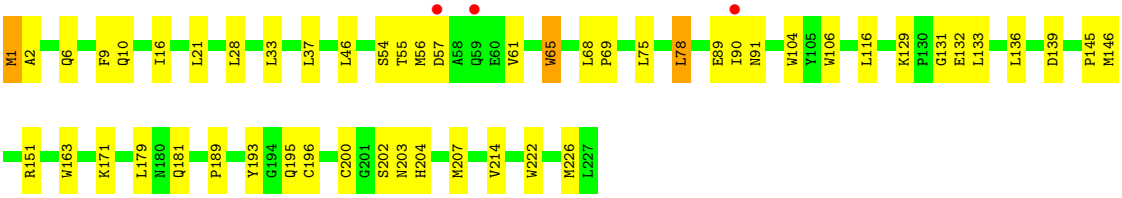
• Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



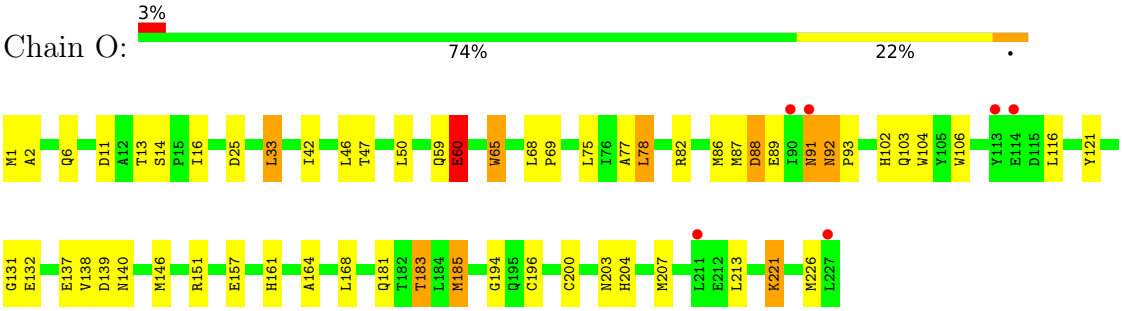
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



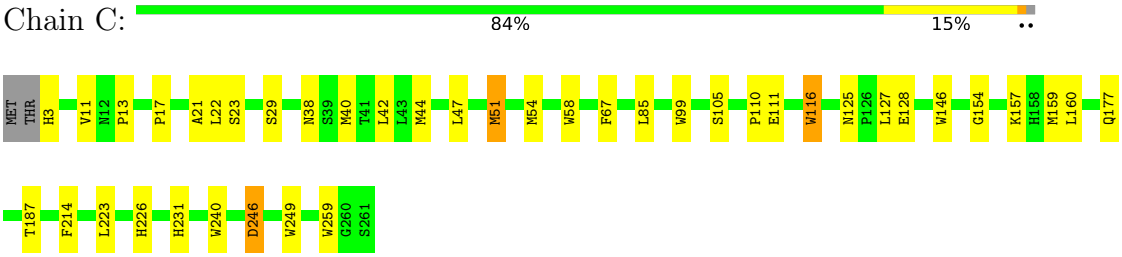
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:



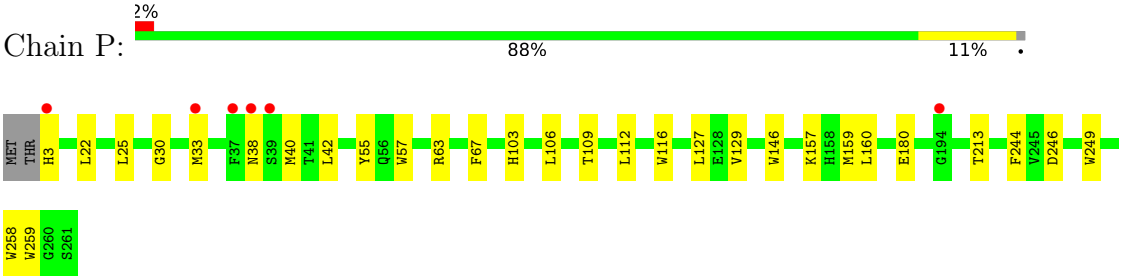
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



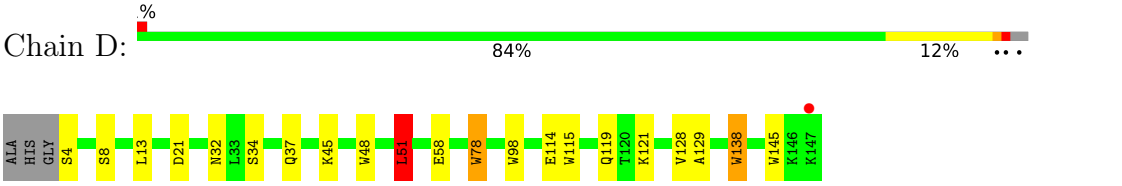
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



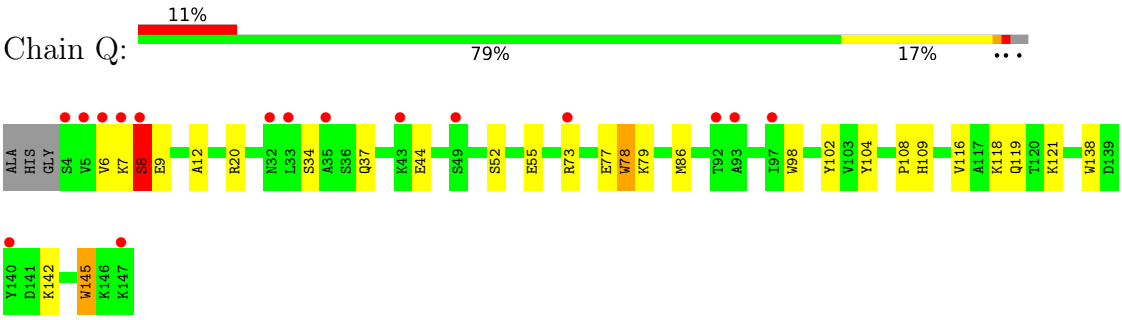
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



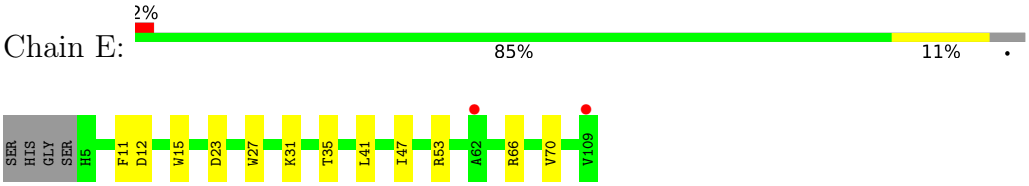
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



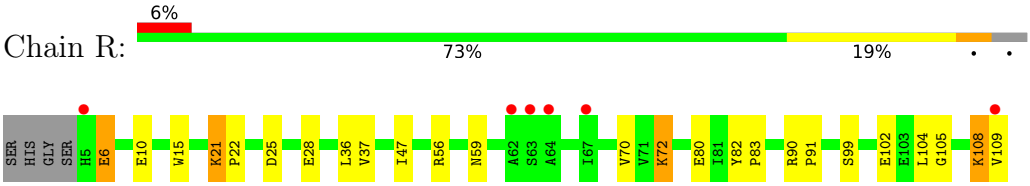
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



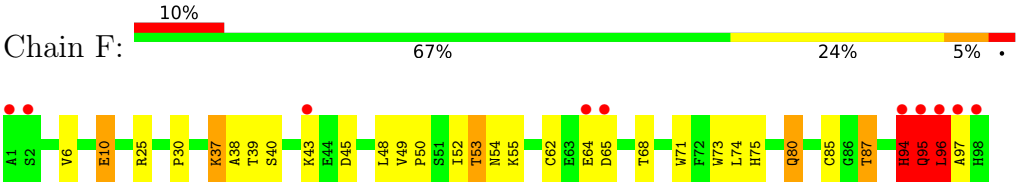
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



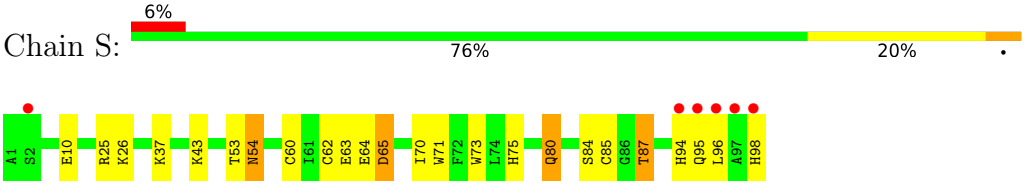
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



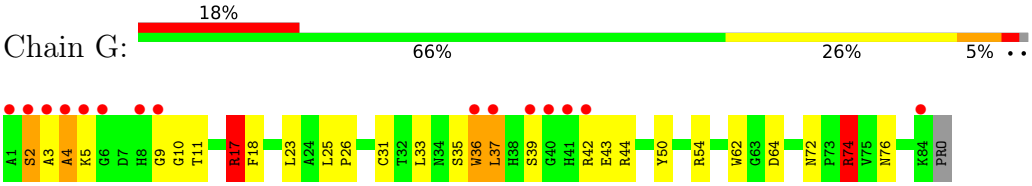
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



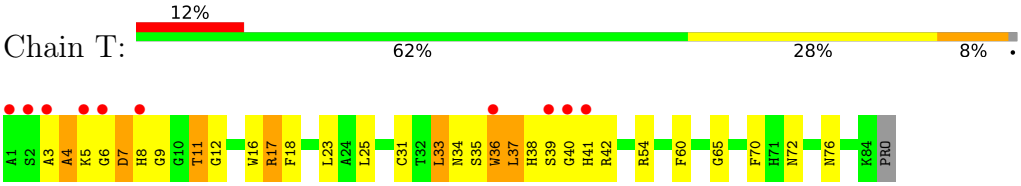
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



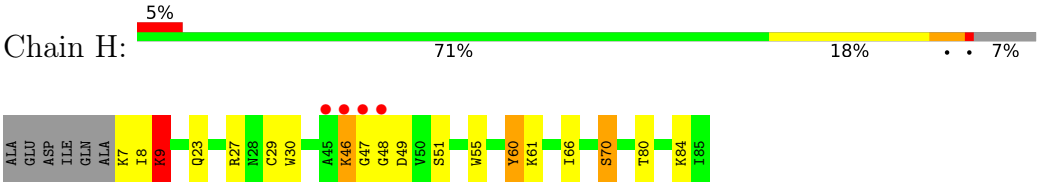
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



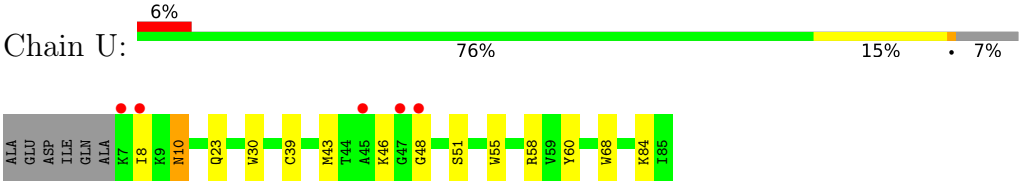
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



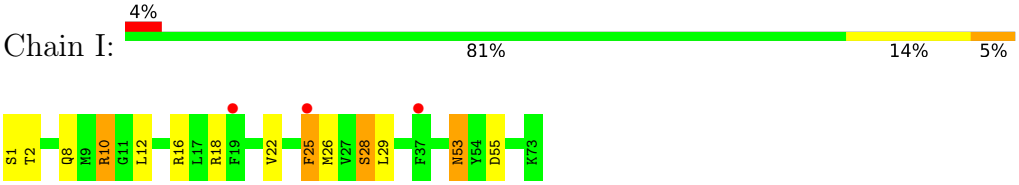
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



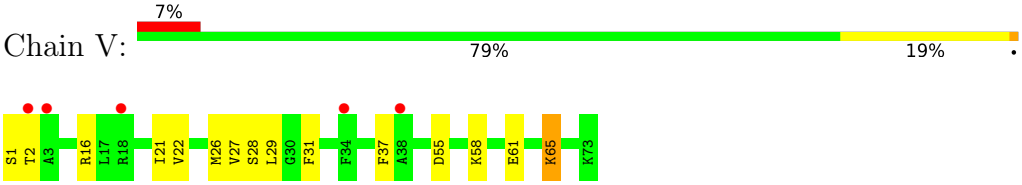
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



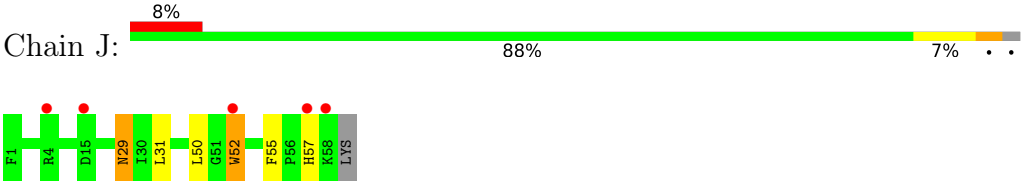
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



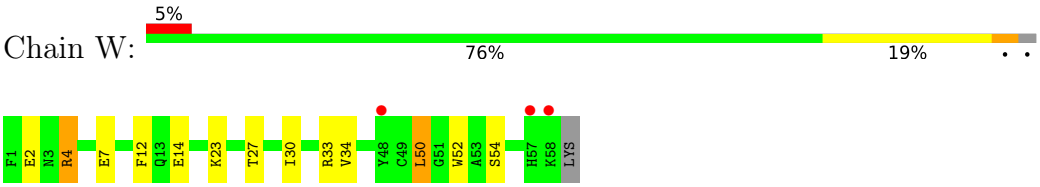
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



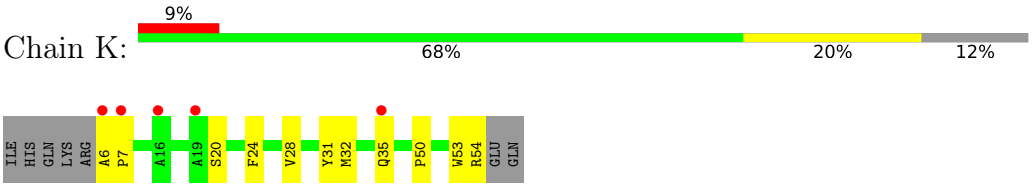
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



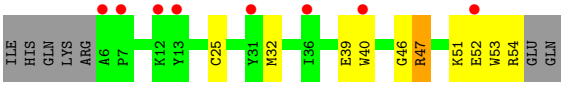
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



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

Chain X:

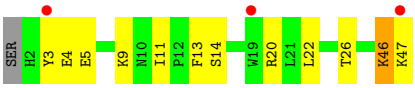


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

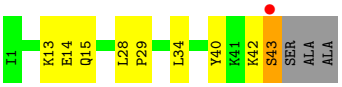
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

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	185.03Å 208.85Å 178.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-2.20) 96.9 (24.99-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.173 , 0.210 0.173 , 0.210	Depositor DCC
R_{free} test set	17156 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32242	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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: UNX, PSC, TGL, FME, HEA, CUA, CMO, CU, MG, ZN, TPO, CHD, SAC, DMU, PEK, PGV, CDL, EDO, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.05	12/4205 (0.3%)	0.95	5/5744 (0.1%)
1	N	1.02	9/4156 (0.2%)	0.92	4/5678 (0.1%)
2	B	0.94	3/1860 (0.2%)	0.96	4/2534 (0.2%)
2	O	0.83	2/1860 (0.1%)	0.91	2/2534 (0.1%)
3	C	1.06	5/2197 (0.2%)	0.92	1/3005 (0.0%)
3	P	1.01	4/2197 (0.2%)	0.87	1/3005 (0.0%)
4	D	0.94	5/1229 (0.4%)	0.88	2/1658 (0.1%)
4	Q	0.78	3/1229 (0.2%)	0.80	2/1658 (0.1%)
5	E	0.82	2/871 (0.2%)	0.94	2/1182 (0.2%)
5	R	0.72	1/871 (0.1%)	0.79	0/1182
6	F	0.86	2/765 (0.3%)	0.89	0/1038
6	S	0.80	0/765	0.89	1/1038 (0.1%)
7	G	0.97	2/690 (0.3%)	0.99	5/937 (0.5%)
7	T	0.90	1/690 (0.1%)	0.86	0/937
8	H	0.88	1/682 (0.1%)	0.88	0/921
8	U	0.84	3/682 (0.4%)	0.81	0/921
9	I	0.76	0/617	0.93	2/818 (0.2%)
9	V	0.70	0/629	0.83	1/834 (0.1%)
10	J	0.80	1/471 (0.2%)	0.84	0/636
10	W	0.71	1/471 (0.2%)	0.75	0/636
11	K	0.93	1/398 (0.3%)	0.75	0/546
11	X	0.85	2/398 (0.5%)	0.80	0/546
12	L	0.88	0/393	0.84	0/526
12	Y	0.77	0/393	0.76	0/526
13	M	0.85	0/345	0.82	0/470
13	Z	0.76	0/345	0.74	0/470
All	All	0.93	60/29409 (0.2%)	0.89	32/39980 (0.1%)

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
8	H	0	1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	TRP	CD2-CE2	7.66	1.50	1.41
2	B	65	TRP	CD2-CE2	7.41	1.50	1.41
1	N	323	TRP	CD2-CE2	7.36	1.50	1.41
3	C	240	TRP	CD2-CE2	7.11	1.49	1.41
1	N	81	TRP	CD2-CE2	7.05	1.49	1.41
3	P	116	TRP	CD2-CE2	7.03	1.49	1.41
3	C	259	TRP	CD2-CE2	6.67	1.49	1.41
3	C	249	TRP	CD2-CE2	6.47	1.49	1.41
5	E	27	TRP	CD2-CE2	6.29	1.49	1.41
7	G	36	TRP	CD2-CE2	6.22	1.48	1.41
4	D	78	TRP	CD2-CE2	6.10	1.48	1.41
3	C	58	TRP	CD2-CE2	6.09	1.48	1.41
2	B	163	TRP	CD2-CE2	6.02	1.48	1.41
1	A	409	TRP	CD2-CE2	5.79	1.48	1.41
2	O	106	TRP	CD2-CE2	5.78	1.48	1.41
1	N	186	TRP	CD2-CE2	5.75	1.48	1.41
4	D	98	TRP	CD2-CE2	5.75	1.48	1.41
7	T	36	TRP	CD2-CE2	5.74	1.48	1.41
1	A	340	TRP	CD2-CE2	5.71	1.48	1.41
2	O	65	TRP	CD2-CE2	5.69	1.48	1.41
2	B	106	TRP	CD2-CE2	5.67	1.48	1.41
8	U	68	TRP	CD2-CE2	5.62	1.48	1.41
10	W	52	TRP	CD2-CE2	5.57	1.48	1.41
11	K	53	TRP	CD2-CE2	5.55	1.48	1.41
10	J	52	TRP	CD2-CE2	5.54	1.48	1.41
11	X	53	TRP	CD2-CE2	5.54	1.48	1.41
3	P	258	TRP	CD2-CE2	5.53	1.48	1.41
4	D	115	TRP	CD2-CE2	5.52	1.48	1.41
4	Q	138	TRP	CD2-CE2	5.50	1.48	1.41
8	U	55	TRP	CD2-CE2	5.48	1.48	1.41
1	A	25	TRP	CD2-CE2	5.46	1.48	1.41
1	A	186	TRP	CD2-CE2	5.46	1.48	1.41
6	F	73	TRP	CD2-CE2	5.46	1.48	1.41
1	A	396	TRP	CD2-CE2	5.42	1.47	1.41
8	U	30	TRP	CD2-CE2	5.41	1.47	1.41
5	R	15	TRP	CD2-CE2	5.38	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	409	TRP	CD2-CE2	5.37	1.47	1.41
1	N	396	TRP	CD2-CE2	5.37	1.47	1.41
4	Q	78	TRP	CD2-CE2	5.37	1.47	1.41
8	H	55	TRP	CD2-CE2	5.35	1.47	1.41
1	N	288	TRP	CD2-CE2	5.33	1.47	1.41
4	Q	145	TRP	CD2-CE2	5.31	1.47	1.41
3	C	116	TRP	CD2-CE2	5.31	1.47	1.41
1	A	450	TRP	CD2-CE2	5.28	1.47	1.41
6	F	71	TRP	CD2-CE2	5.27	1.47	1.41
4	D	145	TRP	CD2-CE2	5.24	1.47	1.41
1	N	450	TRP	CD2-CE2	5.22	1.47	1.41
1	A	236	TRP	CD2-CE2	5.19	1.47	1.41
1	N	6	TRP	CD2-CE2	5.19	1.47	1.41
3	P	249	TRP	CD2-CE2	5.18	1.47	1.41
11	X	40	TRP	CD2-CE2	5.14	1.47	1.41
1	A	126	TRP	CD2-CE2	5.12	1.47	1.41
5	E	15	TRP	CD2-CE2	5.10	1.47	1.41
1	A	288	TRP	CD2-CE2	5.10	1.47	1.41
3	P	57	TRP	CD2-CE2	5.09	1.47	1.41
7	G	62	TRP	CD2-CE2	5.08	1.47	1.41
1	A	376	HIS	CG-CD2	5.06	1.44	1.35
1	N	231	TYR	CE1-CZ	5.05	1.45	1.38
1	A	379	TYR	CE1-CZ	5.04	1.45	1.38
4	D	138	TRP	CD2-CE2	5.04	1.47	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	246	ASP	CB-CG-OD1	-8.98	110.22	118.30
9	I	10	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	71	MET	CG-SD-CE	-7.57	88.08	100.20
1	N	96	ARG	NE-CZ-NH2	-7.12	116.74	120.30
5	E	53	ARG	NE-CZ-NH1	6.43	123.52	120.30
4	D	21	ASP	CB-CG-OD1	6.35	124.01	118.30
7	G	37	LEU	CA-CB-CG	6.26	129.70	115.30
2	B	65	TRP	CB-CA-C	6.17	122.73	110.40
5	E	66	ARG	NE-CZ-NH2	-6.06	117.27	120.30
2	O	11	ASP	CB-CG-OD1	6.00	123.70	118.30
2	O	11	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	438	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	N	312	ILE	CG1-CB-CG2	-5.94	98.34	111.40
2	B	139	ASP	CB-CG-OD1	5.87	123.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	380	VAL	CB-CA-C	5.75	122.32	111.40
7	G	17	ARG	NE-CZ-NH2	-5.71	117.45	120.30
4	Q	20	ARG	NE-CZ-NH2	-5.70	117.45	120.30
7	G	64	ASP	CB-CG-OD2	-5.58	113.28	118.30
9	I	55	ASP	CB-CG-OD1	5.54	123.28	118.30
3	P	63	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	96	ARG	NE-CZ-NH2	-5.40	117.60	120.30
7	G	64	ASP	CB-CG-OD1	5.33	123.10	118.30
2	B	116	LEU	CB-CG-CD1	-5.32	101.95	111.00
9	V	16	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	212	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	438	ARG	CB-CA-C	-5.22	99.96	110.40
6	S	65	ASP	CB-CG-OD1	5.18	122.97	118.30
1	N	486	ASP	CB-CG-OD1	-5.17	113.64	118.30
4	Q	20	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	B	179	LEU	CA-CB-CG	5.08	126.98	115.30
7	G	74	ARG	NE-CZ-NH2	-5.06	117.77	120.30
4	D	51	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	LYS	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	4068	0	4048	86	0
1	N	4027	0	4001	90	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	48	0
3	C	2110	0	2027	41	0
3	P	2110	0	2027	18	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	852	0	845	4	0
5	R	852	0	845	13	0
6	F	748	0	728	24	0
6	S	748	0	728	17	0
7	G	675	0	643	23	0
7	T	675	0	643	29	0
8	H	662	0	623	9	0
8	U	662	0	623	7	0
9	I	609	0	622	11	0
9	V	617	0	631	7	0
10	J	460	0	459	3	0
10	W	460	0	459	13	0
11	K	384	0	366	5	0
11	X	384	0	366	7	0
12	L	380	0	380	20	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	0
14	A	120	0	108	13	0
14	N	120	0	108	11	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	2	0
19	A	63	0	110	3	0
19	D	63	0	110	5	0
19	L	63	0	110	9	0
19	O	63	0	110	7	0
19	Q	63	0	110	5	0
19	Y	63	0	110	3	0
20	A	102	0	152	5	0
20	C	102	0	152	4	0
20	N	102	0	152	6	0
20	P	102	0	152	3	0
21	A	16	0	24	19	0
21	B	8	0	12	1	0
21	C	16	0	24	2	0
21	F	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	G	4	0	6	0	0
21	H	4	0	6	2	0
21	K	8	0	12	0	0
21	L	4	0	6	0	0
21	N	8	0	12	3	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	T	4	0	6	4	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	5	0
23	G	29	0	39	1	0
23	J	29	0	38	0	0
23	P	58	0	78	6	0
23	W	29	0	38	9	0
24	B	52	0	80	4	0
24	O	52	0	80	5	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	6	0
26	G	100	0	156	6	0
26	P	100	0	156	7	0
26	T	100	0	156	21	0
27	C	53	0	77	3	0
27	G	106	0	154	6	0
27	T	159	0	231	13	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	0	0
29	Z	33	0	42	2	0
30	A	191	0	0	17	0
30	B	121	0	0	5	0
30	C	83	0	0	16	0
30	D	89	0	0	1	0
30	E	45	0	0	2	0
30	F	49	0	0	2	0
30	G	40	0	0	6	0
30	H	37	0	0	1	0
30	I	19	0	0	0	0
30	J	19	0	0	1	0
30	K	27	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	L	27	0	0	6	0
30	M	18	0	0	0	0
30	N	169	0	0	22	0
30	O	101	0	0	21	0
30	P	91	0	0	7	0
30	Q	38	0	0	8	0
30	R	40	0	0	0	0
30	S	55	0	0	5	0
30	T	45	0	0	3	0
30	U	27	0	0	0	0
30	V	23	0	0	1	0
30	W	23	0	0	4	0
30	X	16	0	0	1	0
30	Y	18	0	0	3	0
30	Z	4	0	0	0	0
All	All	32242	0	31442	611	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (611) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HE1	30:A:867:HOH:O	1.15	1.25
1:N:312:ILE:HB	30:N:844:HOH:O	1.31	1.23
7:G:50:TYR:HA	30:G:208:HOH:O	1.07	1.23
30:A:704:HOH:O	3:C:17:PRO:HB3	1.34	1.21
3:P:246:ASP:HB2	30:P:464:HOH:O	1.35	1.20
1:N:259:THR:HA	30:N:740:HOH:O	1.39	1.20
3:C:160:LEU:HB3	30:C:459:HOH:O	1.43	1.16
3:C:99:TRP:CD1	30:C:408:HOH:O	1.98	1.15
12:L:24:MET:HG3	30:L:224:HOH:O	1.47	1.14
21:A:613:EDO:H21	30:A:762:HOH:O	0.97	1.13
2:O:69:PRO:HB2	30:O:455:HOH:O	1.49	1.13
3:C:21:ALA:HB2	30:C:448:HOH:O	1.49	1.11
1:N:434:SER:HB3	30:O:409:HOH:O	1.51	1.10
2:O:161:HIS:HE1	30:O:478:HOH:O	1.31	1.09
1:A:100:MET:HA	30:A:704:HOH:O	1.52	1.09
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.33	1.08
2:O:200:CYS:HB3	30:O:404:HOH:O	1.53	1.08
30:G:208:HOH:O	8:H:80:THR:HB	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:85:CYS:SG	6:S:87:THR:HG23	1.94	1.06
2:O:161:HIS:CE1	30:O:478:HOH:O	2.06	1.04
4:D:114:GLU:HG3	30:K:209:HOH:O	1.59	1.03
3:C:51:MET:HA	30:C:444:HOH:O	1.61	1.01
1:A:62:ALA:HA	30:A:846:HOH:O	1.58	1.01
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.43	0.99
30:A:855:HOH:O	19:D:201:TGL:HB21	1.65	0.97
7:T:5:LYS:HD2	27:T:102:PEK:H383	1.42	0.96
9:I:53:ASN:HD22	9:I:53:ASN:H	1.13	0.96
3:C:160:LEU:CB	30:C:459:HOH:O	2.02	0.95
1:A:502:TYR:OH	21:A:612:EDO:H22	1.68	0.94
1:A:347[A]:LEU:HD13	1:A:383[A]:MET:SD	2.09	0.92
30:A:704:HOH:O	3:C:17:PRO:CB	2.02	0.90
1:A:106:PRO:HA	30:A:867:HOH:O	1.72	0.89
1:A:347[B]:LEU:HD22	1:A:383[B]:MET:SD	2.12	0.89
1:A:153:ALA:O	21:A:613:EDO:H11	1.72	0.89
6:F:68:THR:HG23	21:F:103:EDO:H12	1.54	0.88
1:A:347[B]:LEU:HD21	1:A:383[B]:MET:HB3	1.52	0.88
20:C:307:PGV:H211	30:C:408:HOH:O	1.75	0.87
30:C:439:HOH:O	21:H:101:EDO:H11	1.74	0.87
1:N:265:LYS:HD2	1:N:265:LYS:H	1.38	0.87
7:T:37:LEU:O	7:T:38:HIS:HD2	1.57	0.87
6:S:75:HIS:H	6:S:80:GLN:HE22	1.22	0.86
12:Y:46:LYS:HA	30:Y:210:HOH:O	1.73	0.86
1:A:138:HIS:HB2	30:A:710:HOH:O	1.73	0.86
1:A:143:VAL:HG21	30:A:710:HOH:O	1.75	0.86
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.86
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.58	0.86
1:A:138:HIS:CB	30:A:710:HOH:O	2.24	0.85
19:L:101:TGL:OC1	19:L:101:TGL:HC41	1.74	0.85
8:H:49:ASP:HB3	30:H:218:HOH:O	1.76	0.85
27:T:103:PEK:H381	30:T:235:HOH:O	1.76	0.84
3:C:146:TRP:HE1	21:C:311:EDO:H12	1.43	0.83
1:N:326:THR:HG22	30:N:740:HOH:O	1.76	0.83
6:F:85:CYS:SG	6:F:87:THR:HG23	2.19	0.82
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.22	0.82
6:S:94:HIS:O	6:S:96:LEU:HD13	1.79	0.82
4:Q:9:GLU:O	4:Q:9:GLU:HG2	1.80	0.82
11:K:6:ALA:HB1	11:K:7:PRO:HD2	1.60	0.82
4:Q:109:HIS:HD2	30:Q:314:HOH:O	1.62	0.82
4:Q:116:VAL:HG13	30:Q:302:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:PHE:HA	30:E:209:HOH:O	1.81	0.81
1:A:243:VAL:HG21	18:A:606:CMO:C	2.11	0.81
1:N:312:ILE:CB	30:N:844:HOH:O	2.01	0.80
1:A:347[B]:LEU:CD2	1:A:383[B]:MET:HB3	2.10	0.80
2:B:90:ILE:HA	30:B:444:HOH:O	1.80	0.80
1:A:513:LEU:O	1:A:514:LYS:HB2	1.81	0.79
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.65	0.79
2:O:13:THR:HB	2:O:168:LEU:HD23	1.65	0.79
30:N:784:HOH:O	19:Q:201:TGL:HB32	1.82	0.79
3:P:160:LEU:HD13	23:P:305:CHD:H181	1.66	0.78
7:T:72:ASN:H	7:T:76:ASN:HD22	1.32	0.78
12:L:32:GLY:HA3	30:L:201:HOH:O	1.82	0.78
26:T:104:CDL:H151	26:T:104:CDL:OB4	1.83	0.78
10:W:7:GLU:HB3	30:W:207:HOH:O	1.82	0.77
10:W:14:GLU:HG2	30:W:210:HOH:O	1.83	0.77
3:C:99:TRP:HD1	30:C:408:HOH:O	1.49	0.77
1:N:326:THR:CG2	30:N:740:HOH:O	2.29	0.76
26:T:104:CDL:H121	26:T:104:CDL:H371	1.67	0.76
26:T:104:CDL:H273	30:T:235:HOH:O	1.84	0.76
21:A:612:EDO:H12	3:C:13:PRO:HG3	1.67	0.76
12:Y:20:ARG:HD2	30:Y:205:HOH:O	1.86	0.75
2:B:129:LYS:O	2:B:132:GLU:HB2	1.86	0.75
30:G:207:HOH:O	1:N:178:GLN:CB	2.33	0.75
11:X:47:ARG:HB3	11:X:47:ARG:NH1	2.01	0.75
20:A:608:PGV:H61	3:C:54:MET:HG2	1.68	0.74
1:A:100:MET:CA	30:A:704:HOH:O	2.19	0.74
1:N:314:ILE:HG12	30:O:455:HOH:O	1.86	0.74
9:I:53:ASN:HD22	9:I:53:ASN:N	1.83	0.74
6:S:10:GLU:HB2	30:S:224:HOH:O	1.86	0.74
23:P:305:CHD:H162	23:P:305:CHD:H232	1.69	0.73
6:F:75:HIS:H	6:F:80:GLN:HE22	1.36	0.73
7:T:12:GLY:HA3	30:T:225:HOH:O	1.87	0.73
9:V:61:GLU:HG3	9:V:65:LYS:NZ	2.04	0.73
4:D:34:SER:H	4:D:37:GLN:HE21	1.37	0.73
9:I:53:ASN:H	9:I:53:ASN:ND2	1.86	0.72
8:U:10:ASN:H	8:U:10:ASN:HD22	1.37	0.72
1:A:278:MET:HE2	21:T:105:EDO:O1	1.90	0.72
4:Q:109:HIS:CD2	30:Q:314:HOH:O	2.38	0.71
4:D:34:SER:H	4:D:37:GLN:NE2	1.89	0.71
26:T:104:CDL:H161	26:T:104:CDL:H421	1.71	0.71
6:F:64:GLU:O	6:F:65:ASP:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:3:TYR:HA	30:Y:208:HOH:O	1.91	0.70
4:Q:102:TYR:HD1	13:Z:35:TYR:CE2	2.10	0.70
11:X:47:ARG:HB3	11:X:47:ARG:CZ	2.22	0.70
1:N:383:MET:C	30:N:701:HOH:O	2.29	0.70
12:Y:14:SER:O	12:Y:20:ARG:NH2	2.25	0.69
30:G:207:HOH:O	1:N:178:GLN:HB3	1.90	0.69
4:Q:102:TYR:CD1	13:Z:35:TYR:HE2	2.09	0.69
1:A:502:TYR:OH	21:A:612:EDO:C2	2.40	0.69
12:Y:46:LYS:O	12:Y:47:LYS:HB2	1.92	0.69
1:A:157:SER:OG	21:A:613:EDO:H22	1.93	0.69
2:O:183:THR:CG2	30:O:408:HOH:O	2.40	0.69
23:W:101:CHD:H3	30:W:209:HOH:O	1.93	0.69
2:O:33:LEU:HD23	9:V:28:SER:HB3	1.75	0.68
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.24	0.68
6:F:10:GLU:OE1	6:F:25:ARG:NH1	2.26	0.68
6:S:85:CYS:SG	6:S:87:THR:CG2	2.79	0.68
12:L:20:ARG:NH2	19:L:101:TGL:HC32	2.08	0.68
23:W:101:CHD:O12	23:W:101:CHD:H222	1.93	0.68
1:A:10:THR:H	21:A:612:EDO:C2	2.07	0.68
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.40	0.68
20:A:609:PGV:H222	13:M:15:GLN:HE22	1.59	0.67
1:N:487:LEU:HD13	30:N:717:HOH:O	1.93	0.67
9:V:61:GLU:HG3	9:V:65:LYS:HZ1	1.57	0.67
11:K:24:PHE:O	11:K:28:VAL:HG12	1.95	0.67
1:A:157:SER:OG	21:A:613:EDO:C2	2.43	0.67
1:A:502:TYR:OH	21:A:612:EDO:H11	1.95	0.66
4:Q:98:TRP:CZ3	29:Z:101:DMU:H15	2.31	0.66
2:O:88:ASP:HB3	30:O:469:HOH:O	1.95	0.66
12:L:24:MET:HE3	30:L:222:HOH:O	1.96	0.66
4:Q:119:GLN:HB2	30:Q:305:HOH:O	1.96	0.66
6:F:85:CYS:SG	6:F:87:THR:CG2	2.83	0.65
4:Q:102:TYR:CD1	13:Z:35:TYR:CE2	2.82	0.65
10:J:55:PHE:HB2	30:J:208:HOH:O	1.95	0.65
12:L:20:ARG:HH22	19:L:101:TGL:HC52	1.62	0.65
30:B:431:HOH:O	7:T:17:ARG:HD2	1.96	0.65
5:R:56:ARG:NH2	5:R:59:ASN:OD1	2.27	0.65
6:F:30:PRO:O	6:F:96:LEU:HD23	1.97	0.65
12:L:46:LYS:O	12:L:47:LYS:HB2	1.97	0.65
20:P:303:PGV:H172	26:P:304:CDL:H611	1.77	0.65
26:C:303:CDL:H522	26:C:303:CDL:HB62	1.78	0.64
27:T:101:PEK:H32	27:T:101:PEK:H71	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:307:PGV:C21	30:C:408:HOH:O	2.40	0.64
30:G:207:HOH:O	1:N:178:GLN:HB2	1.96	0.64
2:O:200:CYS:HB2	30:O:478:HOH:O	1.97	0.64
1:A:100:MET:HG3	30:C:448:HOH:O	1.96	0.64
8:U:10:ASN:H	8:U:10:ASN:ND2	1.95	0.64
21:A:612:EDO:H11	12:L:3:TYR:HE2	1.62	0.64
7:T:37:LEU:O	7:T:38:HIS:CD2	2.45	0.64
23:P:306:CHD:H12	23:P:306:CHD:H212	1.80	0.64
27:T:102:PEK:H381	26:T:104:CDL:C87	2.27	0.63
14:A:601:HEA:CHD	30:A:846:HOH:O	2.46	0.63
2:O:221:LYS:NZ	30:O:401:HOH:O	2.31	0.63
26:T:104:CDL:H211	26:T:104:CDL:CB5	2.28	0.63
3:C:111:GLU:HG3	21:H:101:EDO:O1	1.98	0.62
2:O:2:ALA:HA	2:O:6:GLN:OE1	1.98	0.62
2:O:161:HIS:HA	30:O:404:HOH:O	1.99	0.62
7:T:5:LYS:HD2	27:T:102:PEK:C38	2.23	0.62
7:T:76:ASN:HD21	27:T:101:PEK:HN2	1.47	0.62
26:T:104:CDL:H522	26:T:104:CDL:H712	1.82	0.62
6:F:95:GLN:HG3	6:F:96:LEU:N	2.15	0.62
24:O:303:PSC:H211	24:O:303:PSC:C01	2.30	0.62
2:B:33:LEU:CD1	9:I:28:SER:HB3	2.29	0.61
27:C:306:PEK:H5	27:C:306:PEK:H221	1.82	0.61
1:N:312:ILE:CG2	30:N:844:HOH:O	2.42	0.61
2:O:91:ASN:ND2	30:O:402:HOH:O	2.33	0.61
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.83	0.61
20:A:609:PGV:H222	13:M:15:GLN:NE2	2.14	0.61
1:A:10:THR:H	21:A:612:EDO:H21	1.66	0.61
1:N:296:GLY:HA2	8:U:23:GLN:NE2	2.15	0.61
8:U:10:ASN:HD22	8:U:10:ASN:N	1.96	0.61
24:O:303:PSC:H231	24:O:303:PSC:H011	1.83	0.60
4:Q:98:TRP:CE3	29:Z:101:DMU:H15	2.36	0.60
6:F:95:GLN:O	6:F:97:ALA:N	2.33	0.60
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.00	0.60
1:A:105:LEU:HD21	21:A:613:EDO:H12	1.82	0.60
4:D:78:TRP:HA	19:D:201:TGL:HB42	1.83	0.60
1:N:199:LEU:N	1:N:200:PRO:CD	2.64	0.60
1:A:95:PRO:HG2	3:C:11:VAL:HG23	1.83	0.60
3:C:67:PHE:HE2	26:C:303:CDL:H1	1.66	0.60
2:O:33:LEU:CD2	9:V:28:SER:HB3	2.32	0.60
2:O:131:GLY:HA2	30:Q:305:HOH:O	2.02	0.59
6:S:10:GLU:CB	30:S:224:HOH:O	2.47	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HA	21:A:612:EDO:H21	1.84	0.59
1:A:177:SER:H	1:A:180:GLN:NE2	2.01	0.59
6:F:94:HIS:O	6:F:96:LEU:HD12	2.02	0.59
11:K:6:ALA:HB1	11:K:7:PRO:CD	2.33	0.59
12:L:22:LEU:O	12:L:26:THR:HB	2.01	0.59
7:T:3:ALA:HB1	27:T:102:PEK:H331	1.83	0.59
2:B:89:GLU:O	2:B:91:ASN:OD1	2.21	0.59
1:N:1:FME:HCN	1:N:4:ASN:H	1.68	0.59
1:A:513:LEU:O	1:A:514:LYS:CB	2.49	0.59
24:B:303:PSC:H062	9:I:10:ARG:HE	1.65	0.59
1:N:383:MET:CA	30:N:701:HOH:O	2.51	0.59
3:C:160:LEU:HD13	23:C:304:CHD:H181	1.85	0.58
1:A:138:HIS:HB3	30:A:710:HOH:O	1.96	0.58
12:L:32:GLY:CA	30:L:201:HOH:O	2.46	0.58
7:T:3:ALA:CB	27:T:102:PEK:H331	2.32	0.58
1:N:406:ASN:HD21	20:N:607:PGV:H22	1.68	0.58
1:N:265:LYS:HD2	1:N:265:LYS:N	2.16	0.58
1:A:383[A]:MET:HA	1:A:387:PHE:CD1	2.39	0.58
4:Q:9:GLU:O	4:Q:9:GLU:CG	2.52	0.58
1:A:95:PRO:HG2	3:C:11:VAL:CG2	2.34	0.57
10:J:29:ASN:HD22	10:J:29:ASN:H	1.51	0.57
20:N:607:PGV:H02	20:N:607:PGV:H042	1.85	0.57
1:N:365:ILE:HB	30:N:705:HOH:O	2.04	0.57
7:G:18:PHE:CE1	1:N:278:MET:HE3	2.39	0.57
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.85	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.03	0.57
1:N:103:TRP:O	1:N:107:PRO:HD2	2.05	0.57
1:N:243:VAL:HG21	18:N:606:CMO:O	2.04	0.57
26:P:304:CDL:H341	26:P:304:CDL:H171	1.87	0.56
3:C:3:HIS:HA	30:C:458:HOH:O	2.04	0.56
9:I:53:ASN:N	9:I:53:ASN:ND2	2.48	0.56
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.40	0.56
2:B:1:FME:HA	21:B:304:EDO:H22	1.87	0.56
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.41	0.56
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.41	0.56
2:O:139:ASP:OD1	2:O:140:ASN:N	2.38	0.56
1:N:417:MET:HE3	30:N:841:HOH:O	2.05	0.55
2:O:59:GLN:C	2:O:60:GLU:HG3	2.27	0.55
19:A:607:TGL:H341	19:A:607:TGL:H211	1.88	0.55
3:C:154:GLY:HA2	6:F:6:VAL:HB	1.87	0.55
24:O:303:PSC:H211	24:O:303:PSC:H011	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:6:GLU:HB2	5:R:10:GLU:OE2	2.05	0.55
14:N:602:HEA:C1D	18:N:606:CMO:O	2.55	0.55
4:Q:145:TRP:CD1	11:X:46:GLY:HA2	2.41	0.55
26:T:104:CDL:HB22	26:T:104:CDL:H131	1.89	0.55
9:V:22:VAL:O	9:V:26:MET:HG2	2.07	0.55
7:G:31:CYS:SG	26:G:102:CDL:H522	2.47	0.55
5:R:72:LYS:NZ	5:R:102:GLU:OE2	2.39	0.55
3:C:157:LYS:HD3	27:C:306:PEK:H052	1.89	0.55
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.89	0.55
3:C:146:TRP:NE1	21:C:311:EDO:H12	2.19	0.54
7:T:38:HIS:NE2	26:T:104:CDL:H122	2.23	0.54
12:L:20:ARG:HH22	19:L:101:TGL:HC32	1.71	0.54
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
10:W:33:ARG:HG2	23:W:101:CHD:H181	1.88	0.54
1:A:502:TYR:OH	21:A:612:EDO:C1	2.55	0.54
2:O:89:GLU:HB3	30:O:433:HOH:O	2.06	0.54
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.90	0.54
7:T:38:HIS:CE1	26:T:104:CDL:HA21	2.43	0.54
4:Q:116:VAL:HA	30:Q:306:HOH:O	2.08	0.54
19:O:302:TGL:C28	19:O:302:TGL:HB92	2.38	0.54
12:L:19:TRP:HZ2	13:M:14:GLU:HG2	1.72	0.53
27:T:102:PEK:H381	26:T:104:CDL:H871	1.88	0.53
1:A:172:LYS:HB2	30:A:788:HOH:O	2.07	0.53
14:A:602:HEA:HBC1	14:A:602:HEA:CMC	2.20	0.53
7:G:5:LYS:HB2	27:G:103:PEK:H351	1.90	0.53
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.91	0.53
1:A:400:PHE:HB3	19:L:101:TGL:H283	1.90	0.53
4:D:34:SER:N	4:D:37:GLN:HE21	2.07	0.53
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.73	0.53
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.44	0.53
1:N:177:SER:H	1:N:180:GLN:HE22	1.55	0.53
6:S:54:ASN:HD22	6:S:54:ASN:C	2.12	0.53
14:A:602:HEA:HMC1	14:A:602:HEA:CBC	2.19	0.53
7:G:4:ALA:C	7:G:5:LYS:HG3	2.30	0.53
3:P:38:ASN:HA	30:P:405:HOH:O	2.08	0.53
20:C:307:PGV:H41	30:P:469:HOH:O	2.09	0.52
2:O:102:HIS:HE1	2:O:157:GLU:OE2	1.92	0.52
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.05	0.52
10:W:33:ARG:CZ	23:W:101:CHD:H162	2.39	0.52
1:A:157:SER:HG	21:A:613:EDO:C1	2.23	0.52
1:N:390:MET:HA	1:N:390:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:THR:HB	19:Q:201:TGL:H182	1.91	0.52
2:O:103:GLN:HG2	30:O:478:HOH:O	2.10	0.52
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.74	0.52
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.23	0.52
3:C:47:LEU:O	3:C:51:MET:HG2	2.10	0.52
26:G:102:CDL:H712	26:G:102:CDL:H512	1.91	0.52
2:O:200:CYS:CB	30:O:404:HOH:O	2.31	0.52
1:N:513:LEU:O	1:N:514:LYS:HB2	2.09	0.52
2:O:151:ARG:HE	2:O:181:GLN:NE2	2.08	0.52
26:T:104:CDL:H522	26:T:104:CDL:H231	1.91	0.52
21:A:612:EDO:H11	12:L:3:TYR:CE2	2.45	0.52
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.44	0.52
10:J:52:TRP:O	10:J:57:HIS:HE1	1.92	0.52
12:L:19:TRP:CZ2	13:M:14:GLU:HG2	2.45	0.52
3:C:54:MET:CE	30:C:444:HOH:O	2.58	0.51
19:D:201:TGL:H362	9:I:16:ARG:HE	1.76	0.51
1:A:378:HIS:O	1:A:382[B]:SER:HB2	2.10	0.51
23:C:305:CHD:H152	20:C:307:PGV:H102	1.93	0.51
1:N:155:VAL:HG21	20:N:608:PGV:H142	1.91	0.51
1:N:384:GLY:N	30:N:701:HOH:O	2.42	0.51
1:N:408:THR:HB	20:N:607:PGV:H21	1.92	0.51
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.57	0.51
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.91	0.51
20:A:609:PGV:H221	20:A:609:PGV:H012	1.91	0.51
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.92	0.51
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.11	0.51
1:A:22:PHE:HA	19:L:101:TGL:HB71	1.92	0.51
1:N:484:THR:HG22	21:N:610:EDO:C1	2.41	0.51
2:O:91:ASN:N	30:O:403:HOH:O	2.43	0.51
1:N:484:THR:HG22	21:N:610:EDO:O1	2.11	0.51
9:I:25:PHE:CD1	9:I:25:PHE:C	2.84	0.51
2:O:69:PRO:HG2	30:O:416:HOH:O	2.11	0.51
5:R:99:SER:HB2	5:R:104:LEU:HD21	1.93	0.51
1:A:381[B]:LEU:HB2	14:A:602:HEA:HAC	1.93	0.51
26:P:304:CDL:HA4	26:P:304:CDL:H121	1.92	0.51
8:H:60:TYR:CD1	8:H:60:TYR:C	2.84	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.93	0.50
2:B:54:SER:HB2	30:B:473:HOH:O	2.11	0.50
26:T:104:CDL:H111	26:T:104:CDL:HA22	1.93	0.50
23:B:302:CHD:H212	23:B:302:CHD:H12	1.93	0.50
1:N:514:LYS:NZ	6:S:60:CYS:SG	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:HIS:CE1	26:C:303:CDL:HB32	2.46	0.50
7:G:17:ARG:HD2	30:G:220:HOH:O	2.10	0.50
5:R:105:GLY:O	5:R:108:LYS:HD3	2.12	0.50
6:S:10:GLU:OE2	6:S:25:ARG:NH2	2.45	0.50
20:N:607:PGV:H292	13:Z:16:ALA:HA	1.94	0.50
6:S:64:GLU:O	6:S:65:ASP:HB2	2.11	0.50
3:C:54:MET:HE2	30:C:444:HOH:O	2.12	0.49
7:G:3:ALA:O	7:G:4:ALA:HB2	2.12	0.49
4:Q:44:GLU:O	4:Q:44:GLU:HG2	2.12	0.49
1:A:282:PHE:HA	7:T:4:ALA:CB	2.42	0.49
3:C:160:LEU:HB2	30:C:459:HOH:O	1.88	0.49
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.93	0.49
7:T:38:HIS:HE1	26:T:104:CDL:HA21	1.77	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.49
23:G:104:CHD:H12	23:G:104:CHD:H212	1.93	0.49
1:N:487:LEU:CD1	30:N:717:HOH:O	2.58	0.49
2:O:131:GLY:CA	30:Q:305:HOH:O	2.58	0.49
4:Q:142:LYS:HD3	30:Q:325:HOH:O	2.13	0.49
6:S:37:LYS:NZ	30:S:201:HOH:O	2.41	0.49
1:A:38:ARG:HD2	14:A:601:HEA:OMA	2.12	0.49
7:G:18:PHE:CZ	1:N:278:MET:CE	2.95	0.49
8:H:46:LYS:O	8:H:48:GLY:N	2.45	0.49
2:O:13:THR:HB	2:O:168:LEU:CD2	2.40	0.49
1:A:157:SER:OG	21:A:613:EDO:C1	2.61	0.49
1:A:502:TYR:HH	21:A:612:EDO:H22	1.77	0.49
14:N:601:HEA:CHD	30:N:759:HOH:O	2.60	0.49
20:N:607:PGV:H02	20:N:607:PGV:C04	2.43	0.49
1:N:437:PRO:HG2	1:N:440:TYR:CZ	2.47	0.49
2:O:60:GLU:HG2	30:O:485:HOH:O	2.12	0.49
3:P:213:THR:HG23	26:P:304:CDL:H771	1.94	0.49
20:P:301:PGV:H011	30:P:472:HOH:O	2.11	0.49
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.94	0.49
6:F:53:THR:HB	6:F:54:ASN:H	1.49	0.48
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.09	0.48
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.12	0.48
2:O:14:SER:HB3	2:O:185:MET:O	2.13	0.48
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.95	0.48
2:O:16:ILE:HD12	2:O:87:MET:HG2	1.94	0.48
7:T:60:PHE:O	7:T:65:GLY:HA2	2.13	0.48
1:A:347[B]:LEU:HD12	1:A:348:PHE:N	2.28	0.48
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:MET:HB2	26:C:303:CDL:H381	1.95	0.48
12:L:47:LYS:HE2	13:M:43:SER:OG	2.13	0.48
3:C:40:MET:O	3:C:44:MET:HG2	2.14	0.48
26:C:303:CDL:H352	30:C:478:HOH:O	2.14	0.48
9:I:22:VAL:O	9:I:26:MET:HG2	2.14	0.48
5:R:72:LYS:HB2	5:R:82:TYR:CD1	2.48	0.48
26:C:303:CDL:H673	30:C:481:HOH:O	2.14	0.48
1:N:484:THR:HG22	21:N:610:EDO:H12	1.96	0.48
9:V:27:VAL:O	9:V:31[B]:PHE:HD2	1.96	0.48
1:N:5:ARG:HA	30:N:709:HOH:O	2.14	0.47
20:P:301:PGV:H031	30:P:472:HOH:O	2.14	0.47
2:B:9:PHE:HB2	2:B:21:LEU:HD21	1.96	0.47
23:C:304:CHD:H12	23:C:304:CHD:H212	1.94	0.47
7:G:4:ALA:HB1	1:N:281:GLY:HA3	1.96	0.47
1:A:278:MET:CE	21:T:105:EDO:O1	2.59	0.47
2:B:56:MET:HA	24:B:303:PSC:H232	1.97	0.47
7:G:23:LEU:C	7:G:26:PRO:HD2	2.34	0.47
1:N:19:TYR:CG	1:N:76:GLY:HA3	2.49	0.47
1:N:461:SER:HB2	30:N:814:HOH:O	2.14	0.47
7:G:72:ASN:N	7:G:76:ASN:HD22	2.01	0.47
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.43	0.47
2:O:146:MET:HA	2:O:213:LEU:HD12	1.96	0.47
7:T:37:LEU:C	7:T:38:HIS:HD2	2.15	0.47
1:A:380[A]:VAL:O	1:A:384[A]:GLY:HA3	2.14	0.47
12:L:41:ARG:HG3	13:M:40:TYR:CE2	2.50	0.47
1:N:117:MET:HB3	10:W:54:SER:OG	2.14	0.47
1:N:390:MET:HA	1:N:390:MET:HE3	1.97	0.47
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.12	0.47
11:K:31:TYR:CD1	11:K:35:GLN:HG3	2.49	0.47
12:L:14:SER:H	19:L:101:TGL:HC31	1.80	0.47
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.61	0.47
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.95	0.47
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.97	0.47
14:N:602:HEA:H243	2:O:69:PRO:HB3	1.97	0.47
19:A:607:TGL:H222	19:A:607:TGL:C36	2.45	0.47
4:D:78:TRP:HB3	19:D:201:TGL:HB31	1.97	0.47
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.97	0.47
1:N:154:GLY:O	1:N:158:ILE:HG13	2.15	0.46
23:W:101:CHD:H21	23:W:101:CHD:H9	1.90	0.46
6:F:40:SER:OG	6:F:45:ASP:HB3	2.15	0.46
10:W:33:ARG:NE	23:W:101:CHD:H212	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.64	0.46
1:N:336:PRO:HB2	1:N:394:VAL:HG21	1.97	0.46
1:A:347[B]:LEU:CD2	1:A:383[B]:MET:CB	2.90	0.46
3:C:29:SER:HB3	3:C:42:LEU:CD1	2.39	0.46
1:N:312:ILE:HG22	1:N:312:ILE:O	2.15	0.46
1:N:321:PHE:CZ	24:O:303:PSC:H161	2.51	0.46
8:H:66:ILE:O	8:H:70:SER:HB3	2.16	0.46
1:N:43:GLN:HB2	1:N:44:PRO:CD	2.46	0.46
19:O:302:TGL:HB92	19:O:302:TGL:H283	1.97	0.46
6:F:10:GLU:HB2	30:F:229:HOH:O	2.16	0.46
7:T:70:PHE:HB2	27:T:101:PEK:H041	1.98	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.76	0.46
4:D:128:VAL:O	4:D:129:ALA:C	2.53	0.46
5:R:80:GLU:H	5:R:80:GLU:CD	2.19	0.46
1:A:169:ILE:N	1:A:169:ILE:HD13	2.27	0.45
1:N:439:ARG:O	2:O:204:HIS:HD2	1.99	0.45
1:A:351:GLY:HA3	1:A:380[B]:VAL:HB	1.98	0.45
6:F:95:GLN:C	6:F:97:ALA:H	2.19	0.45
24:O:303:PSC:H252	24:O:303:PSC:H21	1.99	0.45
7:T:7:ASP:O	7:T:9:GLY:N	2.47	0.45
1:A:282:PHE:HE2	26:T:104:CDL:H262	1.81	0.45
1:A:347[B]:LEU:HD13	1:A:379:TYR:O	2.16	0.45
7:G:18:PHE:CE1	1:N:278:MET:CE	2.99	0.45
1:N:501:PRO:HA	12:Y:5:GLU:OE2	2.16	0.45
19:O:302:TGL:H281	19:O:302:TGL:CB9	2.46	0.45
6:S:64:GLU:HG3	30:S:243:HOH:O	2.17	0.45
2:B:222:TRP:CE2	2:B:226:MET:HG3	2.52	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.98	0.45
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.99	0.45
2:O:25:ASP:HA	30:O:427:HOH:O	2.17	0.45
6:S:25:ARG:HD3	30:S:244:HOH:O	2.15	0.45
8:U:10:ASN:ND2	8:U:10:ASN:N	2.60	0.45
11:X:39:GLU:HB3	30:X:106:HOH:O	2.16	0.45
2:B:1:FME:CE	2:B:133:LEU:HD13	2.47	0.45
1:N:486:ASP:HB2	30:N:804:HOH:O	2.16	0.45
26:P:304:CDL:H641	26:P:304:CDL:H271	1.99	0.45
1:A:51:ASP:HB2	2:B:202:SER:O	2.17	0.45
1:A:312:ILE:HG22	1:A:312:ILE:O	2.17	0.45
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.89	0.45
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:264:LYS:HE2	30:O:413:HOH:O	2.16	0.45
1:N:347:LEU:HD13	1:N:383:MET:SD	2.57	0.45
19:O:302:TGL:HA71	19:O:302:TGL:H202	1.57	0.45
7:T:37:LEU:C	7:T:38:HIS:CD2	2.91	0.45
1:A:468:MET:HG3	30:A:873:HOH:O	2.17	0.44
4:D:32:ASN:ND2	30:D:301:HOH:O	2.29	0.44
1:N:87:ILE:O	1:N:173:PRO:HD3	2.17	0.44
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.81	0.44
3:P:106:LEU:HA	3:P:106:LEU:HD23	1.71	0.44
3:P:109:THR:O	3:P:112:LEU:HB2	2.17	0.44
26:T:104:CDL:H231	26:T:104:CDL:H511	1.99	0.44
1:N:115:SER:O	1:N:121:GLY:HA2	2.17	0.44
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.52	0.44
1:A:240:HIS:CD2	1:A:240:HIS:C	2.91	0.44
19:O:302:TGL:H162	19:O:302:TGL:HC81	1.68	0.44
1:A:75:ILE:O	1:A:79:GLY:HA3	2.17	0.44
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.99	0.44
6:F:39:THR:HG23	21:F:102:EDO:H12	1.98	0.44
4:Q:7:LYS:O	4:Q:8:SER:HB2	2.17	0.44
12:Y:4:GLU:HB3	12:Y:9:LYS:HB3	1.99	0.44
3:C:231:HIS:HB2	30:F:211:HOH:O	2.17	0.44
6:F:62:CYS:HB3	6:F:85:CYS:HB3	1.99	0.44
7:G:2:SER:HA	27:G:103:PEK:H331	2.00	0.44
26:G:102:CDL:H852	27:G:103:PEK:H372	1.99	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
19:O:302:TGL:HB92	19:O:302:TGL:H281	2.00	0.44
7:G:3:ALA:O	7:G:4:ALA:CB	2.66	0.44
14:N:601:HEA:HHC	14:N:601:HEA:H11	1.85	0.44
2:O:102:HIS:CE1	2:O:157:GLU:OE2	2.71	0.44
6:S:70:ILE:HG13	6:S:84:SER:HB3	1.98	0.44
1:A:177:SER:HB3	1:A:180:GLN:HE22	1.83	0.44
10:W:12:PHE:O	10:W:23:LYS:HE2	2.16	0.44
8:H:46:LYS:O	8:H:46:LYS:HD3	2.18	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.80	0.44
1:N:12:HIS:CE1	1:N:13:LYS:HG2	2.53	0.43
2:O:59:GLN:O	2:O:60:GLU:HG3	2.17	0.43
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.33	0.43
3:P:103:HIS:ND1	23:P:306:CHD:O26	2.51	0.43
19:Q:201:TGL:HB51	19:Q:201:TGL:HA21	2.00	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLN:HG3	6:F:96:LEU:H	1.82	0.43
6:F:95:GLN:CG	6:F:96:LEU:N	2.80	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
4:Q:77:GLU:OE2	19:Q:201:TGL:HB21	2.18	0.43
1:A:203:ALA:HB1	27:G:101:PEK:H383	2.00	0.43
12:L:2:HIS:CG	12:L:3:TYR:H	2.36	0.43
3:P:55:TYR:HA	26:P:304:CDL:H552	2.00	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	1.99	0.43
7:G:25:LEU:HD23	7:G:25:LEU:HA	1.83	0.43
12:L:32:GLY:N	30:L:201:HOH:O	2.51	0.43
1:N:466:MET:HG2	13:Z:26:PHE:CG	2.54	0.43
10:W:30:ILE:O	10:W:34:VAL:HG23	2.18	0.43
1:N:309:THR:CG2	14:N:602:HEA:HMB2	2.48	0.43
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.83	0.43
3:P:67:PHE:HE2	26:P:304:CDL:H1	1.83	0.43
9:V:55:ASP:HA	30:V:110:HOH:O	2.18	0.43
1:A:302:ARG:NH2	8:H:23:GLN:HE21	2.17	0.43
1:A:381[B]:LEU:HD13	14:A:602:HEA:HBC2	2.01	0.43
3:P:259:TRP:HB2	30:P:481:HOH:O	2.17	0.43
10:W:33:ARG:CZ	23:W:101:CHD:H212	2.49	0.43
10:W:33:ARG:HD3	30:W:208:HOH:O	2.18	0.43
1:A:467:LEU:O	1:A:471:ILE:HG13	2.19	0.43
2:B:146:MET:SD	2:B:189:PRO:HB3	2.59	0.43
1:N:501:PRO:HD2	1:N:504:THR:CG2	2.49	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.96	0.43
3:P:30:GLY:HA2	3:P:42:LEU:HB3	2.00	0.43
23:P:305:CHD:H232	23:P:305:CHD:C16	2.46	0.43
7:T:3:ALA:O	7:T:4:ALA:HB2	2.19	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.54	0.42
30:E:239:HOH:O	9:I:12:LEU:HD12	2.19	0.42
2:O:116:LEU:HD11	2:O:226:MET:HG2	2.01	0.42
3:P:129:VAL:HG11	3:P:180:GLU:CG	2.49	0.42
4:Q:86:MET:O	11:X:25:CYS:HB2	2.19	0.42
1:A:106:PRO:N	1:A:107:PRO:HD2	2.33	0.42
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.01	0.42
20:A:609:PGV:H02	20:A:609:PGV:O14	2.18	0.42
1:N:463:THR:HA	1:N:466:MET:HE2	2.01	0.42
1:N:510:TYR:C	1:N:510:TYR:CD1	2.91	0.42
19:Y:101:TGL:H222	19:Y:101:TGL:HA92	1.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:LEU:HD21	23:C:304:CHD:H183	2.01	0.42
27:C:306:PEK:H032	7:G:17:ARG:NH2	2.34	0.42
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.55	0.42
10:W:2:GLU:OE1	10:W:4:ARG:NH2	2.52	0.42
14:A:601:HEA:H271	14:A:601:HEA:H212	1.80	0.42
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.64	0.42
26:G:102:CDL:H392	2:O:78:LEU:HD12	2.00	0.42
4:Q:78:TRP:N	19:Q:201:TGL:HB22	2.33	0.42
1:A:5:ARG:HA	21:A:612:EDO:O1	2.19	0.42
1:A:344:PHE:CD2	1:A:384[A]:GLY:O	2.73	0.42
3:C:187:THR:HG22	27:G:101:PEK:H051	2.00	0.42
6:F:37:LYS:HA	6:F:37:LYS:HD2	1.70	0.42
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	2.01	0.42
2:O:50:LEU:HD23	2:O:50:LEU:HA	1.89	0.42
10:W:50:LEU:O	10:W:50:LEU:HD22	2.20	0.42
1:N:366:VAL:N	30:N:705:HOH:O	2.52	0.42
3:P:157:LYS:NZ	27:T:103:PEK:H051	2.34	0.42
7:T:11:TPO:O	7:T:11:TPO:CG2	2.68	0.42
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.54	0.42
1:A:495:LEU:HD12	1:A:495:LEU:HA	1.82	0.42
1:N:459:PHE:O	1:N:462:LEU:HB3	2.20	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.42
26:G:102:CDL:H431	2:O:77:ALA:HB3	2.00	0.42
26:T:104:CDL:H231	26:T:104:CDL:C51	2.49	0.42
12:Y:22:LEU:O	12:Y:26:THR:HB	2.20	0.42
2:B:145:PRO:HA	2:B:214:VAL:O	2.19	0.42
6:F:49:VAL:HA	6:F:50:PRO:HD3	1.89	0.42
1:N:43:GLN:HG2	4:Q:104:TYR:CE1	2.55	0.42
14:N:602:HEA:HHA	14:N:602:HEA:HAD2	1.80	0.42
4:Q:121:LYS:HG2	11:X:52:GLU:HA	2.02	0.42
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.42
3:P:33:MET:HG2	30:P:473:HOH:O	2.20	0.42
8:U:58:ARG:HA	8:U:58:ARG:HD2	1.82	0.42
3:C:125:ASN:HB3	3:C:128:GLU:HG3	2.01	0.41
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.87	0.41
7:T:23:LEU:HB2	21:T:105:EDO:H12	2.02	0.41
2:B:68:LEU:CB	2:B:69:PRO:HD3	2.50	0.41
14:N:601:HEA:HHD	30:N:759:HOH:O	2.19	0.41
27:T:102:PEK:H381	26:T:104:CDL:H872	1.99	0.41
1:A:344:PHE:HD2	1:A:384[A]:GLY:O	2.03	0.41
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:ARG:HD2	7:G:74:ARG:O	2.20	0.41
12:L:25:MET:HG2	19:L:101:TGL:HA61	2.02	0.41
3:C:105:SER:HA	3:C:116:TRP:CE3	2.56	0.41
5:E:23:ASP:OD1	5:E:23:ASP:N	2.38	0.41
6:F:52:ILE:HG23	6:F:96:LEU:HD13	2.02	0.41
7:G:9:GLY:O	1:N:177:SER:HA	2.21	0.41
2:B:131:GLY:HA2	4:D:119:GLN:HA	2.03	0.41
4:Q:102:TYR:CE1	13:Z:35:TYR:HE2	2.38	0.41
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.18	0.41
19:Y:101:TGL:H321	19:Y:101:TGL:H362	2.01	0.41
2:B:10:GLN:HB3	30:B:487:HOH:O	2.20	0.41
26:G:102:CDL:H521	26:G:102:CDL:H242	2.02	0.41
2:B:129:LYS:HE3	30:B:471:HOH:O	2.21	0.41
5:R:36:LEU:HD21	5:R:47:ILE:HG21	2.02	0.41
7:T:33:LEU:O	7:T:34:ASN:C	2.58	0.41
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.55	0.41
19:Y:101:TGL:HC22	19:Y:101:TGL:HC52	1.93	0.41
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.21	0.41
19:A:607:TGL:H222	19:A:607:TGL:H362	2.02	0.41
2:B:37:LEU:HB2	9:I:28:SER:OG	2.21	0.41
24:B:303:PSC:H212	24:B:303:PSC:H02	2.02	0.41
3:C:85:LEU:HD21	27:T:102:PEK:H281	2.03	0.41
19:D:201:TGL:HA62	19:D:201:TGL:HB82	2.03	0.41
5:E:31:LYS:HE2	5:E:35:THR:OG1	2.21	0.41
7:G:18:PHE:HE1	1:N:278:MET:HE3	1.86	0.41
1:N:66:ILE:HG13	30:N:759:HOH:O	2.21	0.41
1:N:268:PHE:CD1	1:N:268:PHE:C	2.94	0.41
19:O:302:TGL:C28	19:O:302:TGL:CB9	2.99	0.41
26:T:104:CDL:H252	26:T:104:CDL:H761	2.01	0.41
23:W:101:CHD:H151	23:W:101:CHD:O7	2.20	0.41
1:A:282:PHE:HZ	26:T:104:CDL:H752	1.86	0.41
2:B:171:LYS:HB2	2:B:171:LYS:HE3	1.92	0.41
1:A:344:PHE:HD2	1:A:384[B]:GLY:O	2.04	0.40
2:B:28:LEU:HD12	2:B:28:LEU:HA	1.89	0.40
2:O:121:TYR:O	2:O:138:VAL:HA	2.20	0.40
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.02	0.40
5:R:21:LYS:HA	5:R:22:PRO:HD3	1.94	0.40
7:T:31:CYS:SG	26:T:104:CDL:H512	2.61	0.40
1:A:22:PHE:CE1	30:A:867:HOH:O	2.07	0.40
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.95	0.40
1:N:62:ALA:HA	30:N:759:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:18:PHE:HE1	21:T:105:EDO:HO1	1.69	0.40
23:C:304:CHD:H112	23:C:304:CHD:H12A	1.95	0.40
4:D:13:LEU:HD23	4:D:13:LEU:HA	1.93	0.40
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.02	0.40
19:L:101:TGL:HC21	30:L:224:HOH:O	2.21	0.40
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.40
1:N:172:LYS:HB2	1:N:172:LYS:HE2	1.87	0.40
1:N:265:LYS:HD2	30:O:483:HOH:O	2.21	0.40
2:O:42:ILE:O	2:O:46:LEU:HG	2.21	0.40
2:B:200:CYS:SG	2:B:204:HIS:HA	2.61	0.40
7:G:10:GLY:HA3	1:N:177:SER:HB2	2.03	0.40
4:Q:118:LYS:HG2	11:X:51:LYS:HB3	2.03	0.40
10:W:33:ARG:NH2	23:W:101:CHD:H212	2.37	0.40
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.83	0.40
2:B:1:FME:HB2	2:B:1:FME:HCN	1.76	0.40
24:B:303:PSC:H241	24:B:303:PSC:H21	2.03	0.40
4:D:48:TRP:HA	4:D:51:LEU:HD22	2.04	0.40
23:P:306:CHD:H12	23:P:306:CHD:C21	2.47	0.40
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.88	0.40

There are no symmetry-related clashes.

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	519/514 (101%)	503 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	217 (96%)	6 (3%)	2 (1%)	17	16
3	C	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	4 (3%)	1 (1%)	22	22
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	2
6	S	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3	1
7	T	81/85 (95%)	69 (85%)	5 (6%)	7 (9%)	1	0
8	H	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	5	3
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	1
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	73/73 (100%)	71 (97%)	1 (1%)	1 (1%)	11	8
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	42 (89%)	5 (11%)	0	100	100
12	L	44/47 (94%)	44 (100%)	0	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3374 (96%)	117 (3%)	23 (1%)	22	22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	39	SER
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
9	V	2	THR

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Mol	Chain	Res	Type
8	H	47	GLY
2	O	60	GLU
4	Q	8	SER
7	T	40	GLY
7	T	41	HIS
8	U	48	GLY
7	G	43	GLU
2	O	92	ASN
8	U	51	SER
3	C	38	ASN
6	F	95	GLN
8	H	8	ILE
8	U	8	ILE
7	T	6	GLY

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	432/426 (101%)	423 (98%)	9 (2%)	53	67
1	N	426/426 (100%)	413 (97%)	13 (3%)	40	51
2	B	210/210 (100%)	204 (97%)	6 (3%)	42	54
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	28
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	57
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	65
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	33
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	51
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	65
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	26
6	F	81/81 (100%)	71 (88%)	10 (12%)	4	4
6	S	81/81 (100%)	72 (89%)	9 (11%)	6	5
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	6
8	H	71/75 (95%)	61 (86%)	10 (14%)	3	2
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	25
9	I	58/57 (102%)	51 (88%)	7 (12%)	5	4
9	V	59/57 (104%)	53 (90%)	6 (10%)	7	6
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	21
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	21
11	K	39/46 (85%)	36 (92%)	3 (8%)	13	13
11	X	39/46 (85%)	36 (92%)	3 (8%)	13	13
12	L	39/40 (98%)	36 (92%)	3 (8%)	13	13
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	58
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	6
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3049/3082 (99%)	2896 (95%)	153 (5%)	24	30

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	44	PRO
1	A	109	PHE
1	A	177	SER
1	A	180	GLN
1	A	312	ILE
1	A	369	ASP
1	A	417	MET
1	A	513	LEU
2	B	55	THR
2	B	57	ASP
2	B	61	VAL
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
3	C	23	SER
3	C	51	MET
3	C	127	LEU
3	C	159	MET

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Mol	Chain	Res	Type
3	C	214	PHE
3	C	246	ASP
4	D	4	SER
4	D	8	SER
4	D	45	LYS
4	D	51	LEU
4	D	58	GLU
4	D	121	LYS
5	E	41	LEU
5	E	70	VAL
6	F	10	GLU
6	F	37	LYS
6	F	43	LYS
6	F	48	LEU
6	F	53	THR
6	F	80	GLN
6	F	87	THR
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	17	ARG
7	G	33	LEU
7	G	35	SER
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
7	G	74	ARG
8	H	7	LYS
8	H	9	LYS
8	H	27	ARG
8	H	29	CYS
8	H	46	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
8	H	70	SER
8	H	84	LYS
9	I	2	THR
9	I	8	GLN
9	I	18	ARG

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Mol	Chain	Res	Type
9	I	25	PHE
9	I	28	SER
9	I	29	LEU
9	I	53	ASN
10	J	29	ASN
10	J	31	LEU
10	J	50	LEU
11	K	20	SER
11	K	32	MET
11	K	54	ARG
12	L	5	GLU
12	L	26	THR
12	L	47	LYS
13	M	13	LYS
13	M	34	LEU
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	238	PHE
1	N	265	LYS
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	380	VAL
1	N	394	VAL
1	N	486	ASP
1	N	495	LEU
1	N	510	TYR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	88	ASP
2	O	91	ASN
2	O	183	THR
2	O	185	MET
2	O	221	LYS
3	P	3	HIS

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Mol	Chain	Res	Type
3	P	40	MET
3	P	127	LEU
3	P	159	MET
3	P	244	PHE
4	Q	6	VAL
4	Q	8	SER
4	Q	73	ARG
4	Q	108	PRO
5	R	6	GLU
5	R	21	LYS
5	R	72	LYS
5	R	108	LYS
5	R	109	VAL
6	S	26	LYS
6	S	43	LYS
6	S	53	THR
6	S	54	ASN
6	S	63	GLU
6	S	80	GLN
6	S	87	THR
6	S	95	GLN
6	S	98	HIS
7	T	17	ARG
7	T	33	LEU
7	T	35	SER
7	T	36	TRP
7	T	37	LEU
7	T	42	ARG
7	T	54	ARG
8	U	10	ASN
8	U	46	LYS
8	U	60	TYR
8	U	84	LYS
9	V	21	ILE
9	V	29	LEU
9	V	37[A]	PHE
9	V	37[B]	PHE
9	V	58	LYS
9	V	65	LYS
10	W	4	ARG
10	W	27	THR
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	32	MET
11	X	47	ARG
11	X	54	ARG
12	Y	46	LYS
13	Z	19	LEU
13	Z	34	LEU
13	Z	37	LEU
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	328	HIS
1	A	512	ASN
2	B	10	GLN
2	B	24	HIS
2	B	52	HIS
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
6	F	80	GLN
7	G	34	ASN
7	G	76	ASN
8	H	23	GLN
9	I	53	ASN
10	J	29	ASN
10	J	57	HIS
13	M	39	ASN
1	N	178	GLN
1	N	180	GLN
1	N	328	HIS
1	N	512	ASN
2	O	10	GLN

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Mol	Chain	Res	Type
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	68	GLN
4	Q	29	HIS
4	Q	37	GLN
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	8	HIS
7	T	34	ASN
7	T	38	HIS
7	T	76	ASN
8	U	10	ASN
8	U	23	GLN
11	X	35	GLN
13	Z	39	ASN

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	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	1.12	0	7,9,11	5.86	2 (28%)
1	FME	N	1	1	8,9,10	0.47	0	7,9,11	3.11	3 (42%)
1	FME	A	1	1	8,9,10	0.97	0	7,9,11	5.70	4 (57%)
9	SAC	V	1	9	7,8,9	1.74	1 (14%)	8,9,11	1.68	2 (25%)

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	1.54	1 (14%)	8,9,11	1.05	0
2	FME	O	1	2	8,9,10	1.07	1 (12%)	7,9,11	4.24	3 (42%)
7	TPO	G	11	7	8,10,11	1.72	2 (25%)	10,14,16	0.94	0
7	TPO	T	11	7	8,10,11	1.53	2 (25%)	10,14,16	1.10	1 (10%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.34	1.52	1.46
9	I	1	SAC	CA-N	3.81	1.51	1.46
7	G	11	TPO	P-O1P	2.85	1.59	1.50
7	T	11	TPO	P-O1P	2.78	1.59	1.50
7	G	11	TPO	P-OG1	2.52	1.64	1.59
7	T	11	TPO	P-OG1	2.06	1.63	1.59
2	O	1	FME	CA-N	2.00	1.49	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CA-N-CN	-14.94	99.85	122.82
1	A	1	FME	CA-N-CN	-13.87	101.50	122.82
2	O	1	FME	CA-N-CN	-10.10	107.28	122.82
1	N	1	FME	CA-N-CN	-7.45	111.36	122.82
2	O	1	FME	C-CA-N	3.84	116.67	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	1	SAC	C-CA-N	3.52	116.09	109.73
1	A	1	FME	O1-CN-N	3.41	134.25	125.27
2	B	1	FME	C-CA-N	3.26	115.62	109.73
1	A	1	FME	CG-CB-CA	-3.04	104.52	112.95
1	A	1	FME	CE-SD-CG	2.65	109.49	100.40
1	N	1	FME	O-C-CA	-2.33	118.67	124.78
7	T	11	TPO	O3P-P-OG1	2.18	115.74	105.99
9	V	1	SAC	CA-N-C1A	2.17	127.14	123.15
2	O	1	FME	CG-CB-CA	-2.12	107.07	112.95
1	N	1	FME	C-CA-N	-2.08	105.98	109.73

There are no chirality outliers.

All (29) 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-OG1
7	G	11	TPO	CG2-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O3P
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
2	B	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C-CA-N-C1A
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	CB-CG-SD-CE
2	B	1	FME	CB-CA-N-CN
2	O	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	3	0
1	N	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 67 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CHD	B	302	-	32,32,32	0.75	0	51,51,51	1.45	11 (21%)
19	TGL	Q	201	-	62,62,62	1.14	3 (4%)	65,65,65	1.05	5 (7%)
21	EDO	F	102	-	3,3,3	0.54	0	2,2,2	0.12	0
27	PEK	T	102	-	52,52,52	1.12	2 (3%)	55,57,57	0.98	5 (9%)
14	HEA	A	602	1	57,67,67	1.56	10 (17%)	61,103,103	1.98	18 (29%)
21	EDO	C	309	-	3,3,3	0.52	0	2,2,2	0.22	0
20	PGV	A	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.45	4 (7%)
21	EDO	G	105	-	3,3,3	0.42	0	2,2,2	0.56	0
23	CHD	G	104	-	32,32,32	1.16	2 (6%)	51,51,51	1.51	10 (19%)
21	EDO	A	611	-	3,3,3	0.39	0	2,2,2	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.23	9 (8%)
21	EDO	C	310	-	3,3,3	0.57	0	2,2,2	0.35	0
21	EDO	K	102	-	3,3,3	0.47	0	2,2,2	0.30	0
20	PGV	N	607	-	50,50,50	1.04	2 (4%)	53,56,56	1.11	5 (9%)
21	EDO	K	101	-	3,3,3	0.52	0	2,2,2	0.29	0
14	HEA	A	601	1	57,67,67	1.63	12 (21%)	61,103,103	1.61	11 (18%)
21	EDO	C	311	-	3,3,3	0.73	0	2,2,2	0.41	0
18	CMO	N	606	-	0,1,1	-	-	-		
23	CHD	J	101	-	32,32,32	0.79	0	51,51,51	1.86	9 (17%)
26	CDL	T	104	-	99,99,99	1.37	12 (12%)	105,111,111	1.16	5 (4%)
21	EDO	O	304	-	3,3,3	0.40	0	2,2,2	0.69	0
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.43	8 (12%)
23	CHD	W	101	-	32,32,32	0.89	0	51,51,51	4.04	25 (49%)
23	CHD	C	305	-	32,32,32	0.87	1 (3%)	51,51,51	1.66	11 (21%)
22	CUA	B	301	2	0,1,1	-	-	-		
24	PSC	B	303	-	51,51,51	1.20	3 (5%)	57,59,59	1.13	4 (7%)
21	EDO	A	613	-	3,3,3	0.57	0	2,2,2	0.07	0
21	EDO	N	610	-	3,3,3	0.41	0	2,2,2	0.19	0
20	PGV	C	302	-	50,50,50	0.88	2 (4%)	53,56,56	0.95	4 (7%)
21	EDO	P	307	-	3,3,3	0.54	0	2,2,2	0.17	0
21	EDO	T	105	-	3,3,3	0.48	0	2,2,2	0.25	0
18	CMO	A	606	15	0,1,1	-	-	-		
19	TGL	D	201	-	62,62,62	1.30	3 (4%)	65,65,65	1.07	6 (9%)
20	PGV	P	303	-	50,50,50	0.86	3 (6%)	53,56,56	1.17	7 (13%)
23	CHD	P	306	-	32,32,32	0.83	0	51,51,51	1.61	11 (21%)
19	TGL	A	607	-	62,62,62	1.19	4 (6%)	65,65,65	1.69	8 (12%)
29	DMU	Z	101	-	34,34,34	0.49	0	45,45,45	0.85	2 (4%)
21	EDO	A	612	-	3,3,3	0.47	0	2,2,2	0.35	0
29	DMU	M	101	-	34,34,34	0.46	0	45,45,45	0.94	1 (2%)
20	PGV	P	301	-	50,50,50	1.07	2 (4%)	53,56,56	1.11	4 (7%)
19	TGL	Y	101	-	62,62,62	1.14	3 (4%)	65,65,65	1.24	6 (9%)
21	EDO	C	308	-	3,3,3	0.41	0	2,2,2	0.38	0
21	EDO	H	101	-	3,3,3	0.53	0	2,2,2	0.20	0
27	PEK	T	101	-	52,52,52	0.90	3 (5%)	55,57,57	1.01	3 (5%)
26	CDL	P	304	-	99,99,99	1.42	12 (12%)	105,111,111	1.27	7 (6%)
14	HEA	N	602	1	57,67,67	1.61	14 (24%)	61,103,103	1.88	16 (26%)
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.29	0
21	EDO	N	609	-	3,3,3	0.41	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	PSC	O	303	-	51,51,51	1.19	3 (5%)	57,59,59	1.05	4 (7%)
26	CDL	G	102	-	99,99,99	1.43	12 (12%)	105,111,111	1.21	9 (8%)
21	EDO	B	304	-	3,3,3	0.35	0	2,2,2	0.63	0
20	PGV	N	608	-	50,50,50	0.87	2 (4%)	53,56,56	1.08	4 (7%)
23	CHD	C	304	-	32,32,32	0.56	0	51,51,51	1.94	16 (31%)
20	PGV	A	609	-	50,50,50	1.04	2 (4%)	53,56,56	1.17	7 (13%)
23	CHD	P	305	-	32,32,32	0.60	0	51,51,51	1.73	13 (25%)
21	EDO	P	308	-	3,3,3	0.59	0	2,2,2	0.16	0
27	PEK	C	306	-	52,52,52	1.18	3 (5%)	55,57,57	1.17	5 (9%)
21	EDO	F	103	-	3,3,3	0.53	0	2,2,2	0.41	0
27	PEK	G	103	-	52,52,52	1.17	2 (3%)	55,57,57	1.07	5 (9%)
21	EDO	B	305	-	3,3,3	0.52	0	2,2,2	0.85	0
14	HEA	N	601	1	57,67,67	1.58	12 (21%)	61,103,103	1.32	8 (13%)
19	TGL	O	302	-	62,62,62	1.12	3 (4%)	65,65,65	1.24	7 (10%)
20	PGV	C	307	-	50,50,50	1.04	2 (4%)	53,56,56	0.92	3 (5%)
21	EDO	L	102	-	3,3,3	0.41	0	2,2,2	0.31	0
27	PEK	T	103	-	52,52,52	1.13	2 (3%)	55,57,57	0.94	2 (3%)
22	CUA	O	301	2,30	0,1,1	-	-	-		
27	PEK	G	101	-	52,52,52	0.87	3 (5%)	55,57,57	1.37	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	B	302	-	-	3/9/74/74	0/4/4/4
19	TGL	Q	201	-	-	35/65/65/65	-
21	EDO	F	102	-	-	0/1/1/1	-
27	PEK	T	102	-	-	29/56/56/56	-
14	HEA	A	602	1	-	2/32/76/76	-
21	EDO	C	309	-	-	0/1/1/1	-
20	PGV	A	608	-	-	15/55/55/55	-
21	EDO	G	105	-	-	0/1/1/1	-
23	CHD	G	104	-	-	3/9/74/74	0/4/4/4
21	EDO	A	611	-	-	1/1/1/1	-
26	CDL	C	303	-	-	58/110/110/110	-
21	EDO	C	310	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	K	102	-	-	1/1/1/1	-
20	PGV	N	607	-	-	28/55/55/55	-
21	EDO	K	101	-	-	1/1/1/1	-
14	HEA	A	601	1	-	3/32/76/76	-
21	EDO	C	311	-	-	0/1/1/1	-
23	CHD	J	101	-	-	8/9/74/74	0/4/4/4
26	CDL	T	104	-	-	61/110/110/110	-
21	EDO	O	304	-	-	1/1/1/1	-
19	TGL	L	101	-	-	39/65/65/65	-
23	CHD	W	101	-	-	7/9/74/74	0/4/4/4
23	CHD	C	305	-	-	2/9/74/74	0/4/4/4
24	PSC	B	303	-	-	38/55/55/55	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
20	PGV	C	302	-	-	10/55/55/55	-
21	EDO	P	307	-	-	0/1/1/1	-
21	EDO	T	105	-	-	1/1/1/1	-
19	TGL	D	201	-	-	37/65/65/65	-
20	PGV	P	303	-	-	20/55/55/55	-
23	CHD	P	306	-	-	1/9/74/74	0/4/4/4
19	TGL	A	607	-	-	42/65/65/65	-
29	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
21	EDO	A	612	-	-	1/1/1/1	-
29	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	PGV	P	301	-	-	25/55/55/55	-
19	TGL	Y	101	-	-	43/65/65/65	-
21	EDO	C	308	-	-	1/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-
27	PEK	T	101	-	-	23/56/56/56	-
26	CDL	P	304	-	-	64/110/110/110	-
14	HEA	N	602	1	-	7/32/76/76	-
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	N	609	-	-	0/1/1/1	-
24	PSC	O	303	-	-	34/55/55/55	-
26	CDL	G	102	-	-	66/110/110/110	-
21	EDO	B	304	-	-	1/1/1/1	-
20	PGV	N	608	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	C	304	-	-	2/9/74/74	0/4/4/4
20	PGV	A	609	-	-	38/55/55/55	-
23	CHD	P	305	-	-	2/9/74/74	1/4/4/4
21	EDO	P	308	-	-	1/1/1/1	-
27	PEK	C	306	-	-	30/56/56/56	-
21	EDO	F	103	-	-	0/1/1/1	-
27	PEK	G	103	-	-	28/56/56/56	-
21	EDO	B	305	-	-	1/1/1/1	-
14	HEA	N	601	1	-	4/32/76/76	-
19	TGL	O	302	-	-	36/65/65/65	-
20	PGV	C	307	-	-	28/55/55/55	-
21	EDO	L	102	-	-	1/1/1/1	-
27	PEK	T	103	-	-	31/56/56/56	-
27	PEK	G	101	-	-	19/56/56/56	-

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.61	1.50	1.34
19	D	201	TGL	OG2-CB1	5.59	1.50	1.34
26	P	304	CDL	OA6-CA5	5.57	1.50	1.34
19	A	607	TGL	OG2-CB1	5.52	1.49	1.34
26	G	102	CDL	OB8-CB7	5.49	1.49	1.33
26	G	102	CDL	OB6-CB5	5.46	1.49	1.34
27	C	306	PEK	O01-C1	5.33	1.49	1.34
19	Y	101	TGL	OG2-CB1	5.26	1.49	1.34
27	G	103	PEK	O03-C21	5.21	1.48	1.33
27	T	103	PEK	O01-C1	5.15	1.48	1.34
19	D	201	TGL	OG1-CA1	5.14	1.48	1.33
27	C	306	PEK	O03-C21	5.14	1.48	1.33
20	C	307	PGV	O01-C1	5.12	1.48	1.34
24	B	303	PSC	O03-C19	5.06	1.48	1.33
26	T	104	CDL	OB6-CB5	5.05	1.48	1.34
19	D	201	TGL	OG3-CC1	4.98	1.47	1.33
27	T	102	PEK	O03-C21	4.97	1.47	1.33
19	Q	201	TGL	OG1-CA1	4.96	1.47	1.33
26	C	303	CDL	OB8-CB7	4.96	1.47	1.33
19	A	607	TGL	OG1-CA1	4.95	1.47	1.33
26	T	104	CDL	OB8-CB7	4.89	1.47	1.33
20	P	301	PGV	O03-C19	4.88	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	103	PEK	O03-C21	4.86	1.47	1.33
26	P	304	CDL	OA8-CA7	4.86	1.47	1.33
26	C	303	CDL	OB6-CB5	4.85	1.48	1.34
19	O	302	TGL	OG2-CB1	4.85	1.48	1.34
24	O	303	PSC	O01-C1	4.83	1.47	1.34
19	L	101	TGL	OG3-CC1	4.82	1.47	1.33
24	O	303	PSC	O03-C19	4.77	1.47	1.33
26	C	303	CDL	OA8-CA7	4.74	1.47	1.33
26	T	104	CDL	OA8-CA7	4.74	1.47	1.33
19	O	302	TGL	OG1-CA1	4.73	1.47	1.33
26	C	303	CDL	OA6-CA5	4.73	1.47	1.34
27	G	103	PEK	O01-C1	4.72	1.47	1.34
26	P	304	CDL	OB6-CB5	4.68	1.47	1.34
19	Y	101	TGL	OG3-CC1	4.68	1.47	1.33
26	P	304	CDL	OB8-CB7	4.67	1.47	1.33
20	N	607	PGV	O03-C19	4.66	1.47	1.33
19	L	101	TGL	OG1-CA1	4.66	1.47	1.33
26	G	102	CDL	OA6-CA5	4.56	1.47	1.34
20	P	301	PGV	O01-C1	4.56	1.47	1.34
19	Q	201	TGL	OG2-CB1	4.55	1.47	1.34
14	N	602	HEA	C1D-ND	-4.51	1.32	1.40
26	G	102	CDL	OA8-CA7	4.49	1.46	1.33
14	N	602	HEA	C4D-C3D	-4.48	1.37	1.45
20	A	609	PGV	O03-C19	4.47	1.46	1.33
20	A	609	PGV	O01-C1	4.45	1.46	1.34
27	T	102	PEK	O01-C1	4.45	1.46	1.34
24	B	303	PSC	O01-C1	4.44	1.46	1.34
19	O	302	TGL	OG3-CC1	4.39	1.46	1.33
19	Y	101	TGL	OG1-CA1	4.37	1.46	1.33
19	Q	201	TGL	OG3-CC1	4.35	1.46	1.33
20	N	607	PGV	O01-C1	4.23	1.46	1.34
26	T	104	CDL	OA6-CA5	4.17	1.46	1.34
20	C	302	PGV	O03-C19	4.06	1.45	1.33
20	C	307	PGV	O03-C19	4.03	1.45	1.33
14	A	601	HEA	CHC-C4B	3.87	1.44	1.35
14	A	601	HEA	CHD-C1D	3.75	1.44	1.35
14	A	601	HEA	C1D-ND	-3.74	1.33	1.40
14	A	601	HEA	C4D-C3D	-3.69	1.38	1.45
14	A	602	HEA	CHD-C1D	3.66	1.44	1.35
14	N	601	HEA	CHD-C1D	3.65	1.44	1.35
14	A	602	HEA	C4B-NB	-3.65	1.34	1.40
24	O	303	PSC	C13-C12	3.62	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	101	PEK	O03-C21	3.60	1.43	1.33
20	P	303	PGV	O01-C1	3.58	1.44	1.34
19	A	607	TGL	OG3-CC1	3.57	1.43	1.33
24	B	303	PSC	C13-C12	3.56	1.52	1.31
20	A	608	PGV	O03-C19	3.56	1.43	1.33
20	N	608	PGV	O01-C1	3.52	1.44	1.34
20	N	608	PGV	O03-C19	3.46	1.43	1.33
14	N	601	HEA	C1D-ND	-3.45	1.34	1.40
14	N	601	HEA	C4B-C3B	-3.38	1.38	1.44
27	T	101	PEK	O01-C1	3.38	1.43	1.34
27	G	101	PEK	O03-C21	3.36	1.43	1.33
14	A	601	HEA	C4B-NB	-3.36	1.34	1.40
14	A	602	HEA	CHC-C4B	3.32	1.43	1.35
26	T	104	CDL	C79-C78	-3.28	1.33	1.51
27	G	101	PEK	O01-C1	3.28	1.43	1.34
14	N	601	HEA	CHC-C4B	3.27	1.43	1.35
26	C	303	CDL	C59-C58	-3.19	1.33	1.51
14	A	602	HEA	CAA-C2A	3.16	1.57	1.52
26	C	303	CDL	C62-C61	-3.15	1.33	1.51
26	P	304	CDL	C22-C21	-3.14	1.33	1.51
26	P	304	CDL	C79-C78	-3.13	1.34	1.51
26	T	104	CDL	C19-C18	-3.12	1.34	1.51
26	G	102	CDL	C39-C38	-3.12	1.34	1.51
26	G	102	CDL	C19-C18	-3.09	1.34	1.51
26	P	304	CDL	C59-C58	-3.08	1.34	1.51
26	G	102	CDL	C79-C78	-3.07	1.34	1.51
26	P	304	CDL	C39-C38	-3.06	1.34	1.51
26	P	304	CDL	C19-C18	-3.06	1.34	1.51
14	N	602	HEA	FE-ND	3.05	2.12	1.96
20	P	303	PGV	O03-C19	3.05	1.42	1.33
26	T	104	CDL	C59-C58	-3.04	1.34	1.51
26	T	104	CDL	C22-C21	-3.03	1.34	1.51
26	C	303	CDL	C79-C78	-3.03	1.34	1.51
26	P	304	CDL	C62-C61	-3.03	1.34	1.51
26	G	102	CDL	C59-C58	-3.02	1.34	1.51
26	T	104	CDL	C39-C38	-3.02	1.34	1.51
26	C	303	CDL	C82-C81	-3.01	1.34	1.51
20	A	608	PGV	O01-C1	3.00	1.42	1.34
26	G	102	CDL	C82-C81	-3.00	1.34	1.51
26	C	303	CDL	C19-C18	-2.98	1.34	1.51
26	T	104	CDL	C62-C61	-2.98	1.34	1.51
26	P	304	CDL	C82-C81	-2.98	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	303	CDL	C22-C21	-2.97	1.34	1.51
26	C	303	CDL	C39-C38	-2.97	1.34	1.51
26	P	304	CDL	C42-C41	-2.96	1.35	1.51
26	G	102	CDL	C42-C41	-2.95	1.35	1.51
26	G	102	CDL	C62-C61	-2.95	1.35	1.51
14	N	601	HEA	C4B-NB	-2.95	1.35	1.40
26	T	104	CDL	C42-C41	-2.94	1.35	1.51
26	C	303	CDL	C42-C41	-2.94	1.35	1.51
26	T	104	CDL	C82-C81	-2.92	1.35	1.51
26	G	102	CDL	C22-C21	-2.91	1.35	1.51
14	A	602	HEA	C1D-ND	-2.91	1.35	1.40
14	A	602	HEA	C1B-NB	-2.76	1.33	1.38
14	N	602	HEA	CHD-C1D	2.71	1.41	1.35
14	N	602	HEA	C12-C11	2.69	1.57	1.52
14	N	601	HEA	FE-ND	2.69	2.10	1.96
27	G	101	PEK	O03-C01	-2.65	1.39	1.45
27	T	101	PEK	O01-C02	-2.59	1.40	1.46
14	N	602	HEA	C18-C19	2.59	1.39	1.33
14	N	601	HEA	FE-NB	2.57	2.09	1.96
14	N	601	HEA	C4D-C3D	-2.54	1.40	1.45
14	A	601	HEA	FE-NB	2.52	2.09	1.96
19	A	607	TGL	OC1-CC1	-2.50	1.15	1.22
14	A	602	HEA	FE-ND	2.50	2.09	1.96
14	N	602	HEA	C3B-C2B	2.49	1.40	1.34
14	A	601	HEA	FE-ND	2.48	2.09	1.96
14	N	601	HEA	C4D-ND	-2.48	1.33	1.38
14	A	602	HEA	C4D-ND	-2.46	1.33	1.38
23	G	104	CHD	C13-C17	-2.44	1.51	1.55
14	A	601	HEA	C4B-C3B	-2.44	1.40	1.44
14	A	601	HEA	C1D-C2D	-2.43	1.39	1.44
14	N	602	HEA	O11-C11	2.40	1.48	1.42
14	A	601	HEA	C3B-C2B	2.38	1.40	1.34
14	N	601	HEA	C1D-C2D	-2.34	1.40	1.44
14	N	602	HEA	C14-C15	2.31	1.38	1.33
20	C	302	PGV	O01-C1	2.29	1.40	1.34
14	N	601	HEA	C3B-C2B	2.29	1.39	1.34
14	A	602	HEA	C3A-CMA	2.27	1.51	1.46
14	N	602	HEA	CHC-C4B	2.26	1.40	1.35
23	G	104	CHD	O7-C7	2.24	1.48	1.43
20	P	303	PGV	O03-C01	-2.19	1.40	1.45
14	N	602	HEA	C4C-CHD	2.19	1.47	1.41
14	N	601	HEA	O1D-CGD	2.17	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	O1A-CGA	2.15	1.29	1.22
27	C	306	PEK	C01-C02	2.14	1.57	1.50
14	A	601	HEA	C4D-ND	-2.10	1.34	1.38
14	A	601	HEA	C1C-CHC	2.07	1.46	1.41
14	N	602	HEA	C4B-NB	-2.03	1.36	1.40
14	A	602	HEA	C4B-C3B	-2.02	1.41	1.44
23	C	305	CHD	C4-C3	2.01	1.55	1.51
14	N	602	HEA	C3A-CMA	2.00	1.51	1.46

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	101	CHD	C14-C8-C9	-13.54	91.13	109.71
23	W	101	CHD	C18-C13-C12	-9.16	99.74	109.07
23	W	101	CHD	C14-C13-C12	9.14	115.91	107.40
23	W	101	CHD	C10-C9-C8	8.27	120.70	111.82
19	A	607	TGL	OG2-CB1-CB2	8.22	129.22	111.50
23	W	101	CHD	C17-C13-C14	-6.97	93.07	100.09
19	L	101	TGL	OG2-CB1-CB2	6.52	125.54	111.50
23	W	101	CHD	C6-C7-C8	6.09	117.98	111.48
20	A	608	PGV	O03-C19-C20	5.97	130.64	111.91
23	J	101	CHD	C13-C17-C20	5.97	126.62	119.50
19	Y	101	TGL	OG2-CB1-CB2	5.68	123.75	111.50
23	W	101	CHD	C13-C17-C20	5.65	126.24	119.50
26	P	304	CDL	OA6-CA5-C11	5.63	123.64	111.50
19	A	607	TGL	CG3-CG2-CG1	-5.50	98.79	111.79
23	W	101	CHD	C14-C8-C7	5.47	119.06	111.81
20	A	608	PGV	O03-C19-O04	-5.36	110.05	123.59
14	A	602	HEA	CMD-C2D-C1D	5.36	133.20	125.04
14	A	602	HEA	C27-C19-C20	5.33	124.24	115.27
23	W	101	CHD	C17-C13-C12	5.28	122.49	117.67
19	O	302	TGL	OG2-CB1-CB2	5.25	122.83	111.50
23	J	101	CHD	C17-C13-C14	-5.21	94.84	100.09
14	N	602	HEA	CAD-CBD-CGD	-5.17	102.47	113.60
23	W	101	CHD	C9-C11-C12	-5.16	107.48	114.30
20	P	301	PGV	O01-C1-C2	5.10	122.49	111.50
23	W	101	CHD	C15-C14-C8	5.03	125.37	118.33
26	G	102	CDL	OB6-CB5-C51	5.01	122.29	111.50
23	W	101	CHD	C9-C8-C7	5.00	117.86	111.88
20	N	607	PGV	O01-C1-C2	4.98	122.23	111.50
23	P	306	CHD	C15-C14-C13	4.94	108.40	103.55
27	G	101	PEK	O01-C1-C2	4.93	122.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	303	CDL	OA6-CA5-C11	4.84	121.94	111.50
14	N	602	HEA	CMB-C2B-C1B	4.84	132.41	125.04
23	W	101	CHD	C11-C9-C10	4.57	118.44	113.73
14	A	602	HEA	CAD-CBD-CGD	-4.55	103.81	113.60
26	T	104	CDL	OB6-CB5-C51	4.53	121.27	111.50
27	C	306	PEK	O01-C1-C2	4.49	121.18	111.50
26	P	304	CDL	OB6-CB5-C51	4.44	121.08	111.50
23	W	101	CHD	C11-C12-C13	4.44	115.80	111.24
14	A	601	HEA	C13-C12-C11	-4.39	107.75	114.35
24	B	303	PSC	O01-C1-C2	4.34	120.86	111.50
27	G	103	PEK	O01-C1-C2	4.29	120.74	111.50
23	C	305	CHD	C23-C22-C20	-4.28	106.69	114.52
19	L	101	TGL	OG3-CC1-CC2	4.27	125.30	111.91
19	A	607	TGL	OG3-CC1-OC1	-4.25	112.87	123.59
23	C	304	CHD	C15-C14-C13	4.21	107.68	103.55
27	T	103	PEK	O01-C1-C2	4.20	120.56	111.50
23	C	305	CHD	C21-C20-C22	-4.14	103.88	110.36
23	P	305	CHD	C14-C13-C12	4.14	111.25	107.40
23	G	104	CHD	C4-C5-C10	-4.08	108.32	112.66
27	T	102	PEK	O01-C1-C2	4.03	120.18	111.50
20	A	609	PGV	O01-C1-C2	4.01	120.13	111.50
26	C	303	CDL	OB6-CB5-C51	4.00	120.11	111.50
27	G	101	PEK	C01-O03-C21	3.94	131.70	117.12
26	G	102	CDL	OA6-CA5-C11	3.93	119.97	111.50
14	N	602	HEA	CAD-C3D-C2D	3.92	135.17	127.88
27	T	101	PEK	O03-C01-C02	-3.90	97.07	108.43
23	P	305	CHD	C9-C10-C5	3.90	114.05	108.58
14	N	602	HEA	C25-C23-C24	3.89	123.20	114.60
14	A	601	HEA	C26-C15-C16	3.87	121.78	115.27
14	N	601	HEA	C3C-C4C-NC	3.87	114.21	109.21
14	N	602	HEA	CHC-C4B-NB	3.87	129.16	124.38
19	O	302	TGL	OG3-CC1-CC2	3.83	123.94	111.91
26	T	104	CDL	OA6-CA5-C11	3.83	119.75	111.50
19	A	607	TGL	OG3-CC1-CC2	3.79	123.79	111.91
23	W	101	CHD	C16-C17-C13	3.78	107.26	103.55
24	O	303	PSC	O03-C19-C20	3.77	123.74	111.91
23	J	101	CHD	C17-C13-C12	3.76	121.10	117.67
19	Q	201	TGL	OG2-CB1-CB2	3.75	119.57	111.50
14	A	602	HEA	C26-C15-C16	3.73	121.54	115.27
19	D	201	TGL	OG3-CC1-CC2	3.72	123.57	111.91
23	B	302	CHD	C15-C14-C13	3.70	107.18	103.55
20	A	609	PGV	O03-C19-C20	3.68	123.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	101	TGL	OG3-CC1-CC2	3.68	123.45	111.91
26	C	303	CDL	OB8-CB7-C71	3.64	123.35	111.91
23	W	101	CHD	C22-C23-C24	-3.62	102.90	112.51
23	P	306	CHD	C17-C13-C14	-3.59	96.48	100.09
14	A	601	HEA	C21-C22-C23	3.58	139.98	127.75
14	A	601	HEA	C21-C20-C19	-3.57	101.23	112.98
26	P	304	CDL	OB8-CB7-C71	3.55	123.04	111.91
27	G	101	PEK	O01-C1-O02	-3.52	115.20	123.70
23	C	304	CHD	C10-C9-C8	3.50	115.58	111.82
23	C	304	CHD	C13-C14-C8	-3.44	110.34	114.74
26	T	104	CDL	OB8-CB7-C71	3.43	122.66	111.91
27	C	306	PEK	O03-C01-C02	3.42	118.40	108.43
24	O	303	PSC	O01-C1-C2	3.38	118.78	111.50
23	C	304	CHD	C6-C5-C4	-3.37	107.31	111.19
20	C	307	PGV	O01-C1-C2	3.36	118.74	111.50
23	P	305	CHD	C1-C10-C9	-3.36	106.08	111.35
14	A	602	HEA	C13-C12-C11	-3.33	109.35	114.35
20	N	608	PGV	O03-C19-C20	3.32	122.33	111.91
20	P	301	PGV	O03-C19-C20	3.31	122.31	111.91
23	P	306	CHD	C5-C6-C7	-3.31	110.81	114.46
14	N	602	HEA	CMB-C2B-C3B	-3.29	124.06	130.34
23	C	304	CHD	C1-C10-C5	3.29	112.64	107.77
14	A	602	HEA	C1D-C2D-C3D	-3.28	103.50	106.96
23	P	305	CHD	C15-C14-C13	3.28	106.77	103.55
20	N	608	PGV	O01-C1-C2	3.27	118.56	111.50
26	G	102	CDL	OB8-CB7-C71	3.26	122.13	111.91
19	O	302	TGL	OG1-CA1-CA2	3.25	122.10	111.91
23	C	304	CHD	C11-C9-C10	-3.23	110.40	113.73
23	W	101	CHD	C1-C10-C9	-3.22	106.29	111.35
26	G	102	CDL	OA8-CA7-C31	3.20	121.95	111.91
24	B	303	PSC	O03-C19-C20	3.19	121.92	111.91
26	P	304	CDL	OB8-CB7-OB9	-3.19	115.55	123.59
19	L	101	TGL	CG2-OG2-CB1	3.17	125.60	117.79
19	A	607	TGL	OG1-CA1-CA2	3.17	121.85	111.91
26	P	304	CDL	OA8-CA7-C31	3.16	121.81	111.91
23	C	304	CHD	C6-C5-C10	3.14	115.99	112.66
14	N	602	HEA	C20-C19-C18	-3.13	114.78	121.12
14	A	602	HEA	CMB-C2B-C1B	3.12	129.79	125.04
20	P	303	PGV	C03-C02-C01	-3.10	104.45	111.79
20	N	608	PGV	O03-C19-O04	-3.09	115.78	123.59
23	P	305	CHD	C6-C5-C10	3.09	115.94	112.66
26	C	303	CDL	OA8-CA7-C31	3.07	121.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	302	CHD	C6-C5-C4	-3.04	107.69	111.19
14	A	601	HEA	C26-C15-C14	-3.04	115.89	123.68
19	D	201	TGL	CG1-OG1-CA1	3.03	128.35	117.12
19	Y	101	TGL	OG3-CC1-OC1	-3.02	115.98	123.59
20	P	303	PGV	O01-C1-C2	3.01	118.00	111.50
23	J	101	CHD	C22-C20-C17	2.98	116.45	110.28
23	G	104	CHD	C13-C17-C20	-2.98	115.94	119.50
19	A	607	TGL	OB1-CB1-CB2	-2.97	112.14	123.73
23	W	101	CHD	C16-C15-C14	-2.96	99.27	105.13
19	Q	201	TGL	OG3-CC1-CC2	2.95	121.17	111.91
14	A	601	HEA	CHA-C4D-C3D	-2.95	120.50	124.84
23	C	304	CHD	C4-C5-C10	2.95	115.79	112.66
23	P	305	CHD	C10-C9-C8	2.94	114.97	111.82
14	N	601	HEA	C1D-C2D-C3D	-2.92	103.89	106.96
23	W	101	CHD	C5-C6-C7	2.92	117.68	114.46
27	C	306	PEK	O03-C21-C22	2.92	121.06	111.91
14	A	602	HEA	C27-C19-C18	-2.90	116.23	123.68
23	C	305	CHD	C6-C5-C10	2.90	115.73	112.66
29	M	101	DMU	O1-C9-C11	2.89	113.63	106.44
23	C	304	CHD	C9-C10-C5	2.89	112.64	108.58
19	Q	201	TGL	OG1-CA1-CA2	2.89	120.97	111.91
23	W	101	CHD	C23-C22-C20	-2.89	109.25	114.52
20	A	609	PGV	O03-C19-O04	-2.88	116.33	123.59
23	P	306	CHD	C1-C10-C5	2.87	112.01	107.77
23	C	304	CHD	C15-C14-C8	2.84	122.31	118.33
23	C	304	CHD	C2-C1-C10	2.83	117.64	112.78
23	C	305	CHD	O25-C24-C23	-2.83	113.99	123.08
20	C	307	PGV	O03-C19-C20	2.82	120.75	111.91
27	T	102	PEK	O03-C21-C22	2.82	120.75	111.91
20	P	303	PGV	O03-C19-O04	-2.81	116.49	123.59
19	Q	201	TGL	CG2-OG2-CB1	-2.81	110.87	117.79
23	G	104	CHD	O12-C12-C13	-2.81	106.28	111.03
14	A	602	HEA	CHC-C4B-NB	2.81	127.85	124.38
23	P	306	CHD	C18-C13-C14	2.81	115.61	111.21
14	N	601	HEA	C4B-NB-C1B	2.80	107.96	105.07
19	D	201	TGL	OG2-CB1-CB2	2.79	117.52	111.50
23	P	305	CHD	C11-C9-C10	-2.79	110.85	113.73
20	N	608	PGV	O01-C1-O02	-2.77	117.01	123.70
23	C	304	CHD	C16-C17-C20	2.76	116.42	112.15
14	N	602	HEA	C25-C23-C22	-2.75	114.69	122.65
19	O	302	TGL	CG3-CG2-CG1	-2.75	105.29	111.79
14	N	602	HEA	C1B-C2B-C3B	-2.75	103.52	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	305	CHD	O26-C24-C23	2.74	122.83	114.03
19	A	607	TGL	OG2-CG2-CG3	2.73	118.29	108.40
27	G	103	PEK	O03-C01-C02	2.73	116.38	108.43
14	N	601	HEA	C17-C18-C19	-2.73	121.10	127.66
23	C	305	CHD	C19-C10-C1	-2.72	103.87	108.26
23	J	101	CHD	C6-C7-C8	2.72	114.39	111.48
23	G	104	CHD	O26-C24-C23	2.72	122.77	114.03
27	T	103	PEK	O03-C21-C22	2.71	120.42	111.91
14	N	602	HEA	O11-C11-C12	2.71	116.98	109.42
27	G	103	PEK	O03-C21-C22	2.69	120.36	111.91
19	Q	201	TGL	OG3-CC1-OC1	-2.69	116.81	123.59
14	N	601	HEA	C4D-CHA-C1A	2.68	126.10	122.56
20	C	302	PGV	O03-C19-O04	-2.67	116.84	123.59
26	G	102	CDL	CB4-OB6-CB5	2.66	124.34	117.79
14	A	602	HEA	CBD-CAD-C3D	2.66	120.00	112.63
26	T	104	CDL	OA8-CA7-C31	2.65	120.22	111.91
19	D	201	TGL	CG3-OG3-CC1	2.64	126.89	117.12
23	W	101	CHD	C4-C5-C10	2.63	115.44	112.66
23	W	101	CHD	C21-C20-C17	2.58	116.87	112.92
20	P	303	PGV	C04-C05-C06	-2.58	102.51	111.67
23	B	302	CHD	O26-C24-C23	2.57	122.30	114.03
23	B	302	CHD	C6-C7-C8	2.56	114.22	111.48
14	A	602	HEA	C3C-C4C-NC	2.55	112.50	109.21
20	P	303	PGV	O03-C19-C20	2.54	119.87	111.91
27	G	103	PEK	O01-C1-O02	-2.54	117.57	123.70
19	Y	101	TGL	OG2-CB1-OB1	-2.53	117.59	123.70
20	N	607	PGV	O03-C01-C02	2.52	115.78	108.43
19	Y	101	TGL	OG1-CA1-CA2	2.52	119.83	111.91
24	B	303	PSC	O01-C1-O02	-2.50	117.65	123.70
14	N	602	HEA	CAD-C3D-C4D	-2.50	120.29	124.66
14	A	602	HEA	C25-C23-C24	2.50	120.12	114.60
23	J	101	CHD	C1-C10-C5	2.50	111.46	107.77
23	B	302	CHD	C19-C10-C5	-2.50	106.13	110.36
23	G	104	CHD	O3-C3-C4	-2.49	104.90	109.85
19	D	201	TGL	OG3-CC1-OC1	-2.48	117.32	123.59
26	P	304	CDL	OB6-CB5-OB7	-2.48	117.72	123.70
19	L	101	TGL	CA4-CA3-CA2	-2.48	104.29	113.19
26	C	303	CDL	OB8-CB7-OB9	-2.47	117.35	123.59
19	L	101	TGL	OG2-CB1-OB1	-2.45	117.78	123.70
14	N	601	HEA	C2D-C1D-ND	2.44	112.73	109.84
23	P	305	CHD	C4-C3-C2	2.44	113.46	110.55
27	T	101	PEK	O01-C1-C2	2.43	116.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	304	CHD	C16-C17-C13	2.43	105.93	103.55
14	N	602	HEA	C13-C12-C11	-2.43	110.70	114.35
23	J	101	CHD	C6-C5-C10	2.42	115.23	112.66
23	G	104	CHD	C13-C14-C8	-2.42	111.65	114.74
14	A	602	HEA	CMB-C2B-C3B	-2.42	125.73	130.34
23	C	305	CHD	C15-C14-C13	2.41	105.92	103.55
23	P	305	CHD	C1-C10-C5	2.41	111.34	107.77
20	A	608	PGV	O03-C01-C02	2.40	115.41	108.43
27	T	101	PEK	C01-O03-C21	2.40	125.99	117.12
23	P	306	CHD	C11-C9-C8	2.39	114.38	110.88
14	N	601	HEA	CHC-C4B-NB	2.39	127.33	124.38
14	A	602	HEA	CAD-C3D-C4D	2.39	128.83	124.66
23	P	306	CHD	C5-C4-C3	-2.38	109.26	112.76
23	P	305	CHD	C14-C8-C9	-2.38	106.44	109.71
23	B	302	CHD	C13-C14-C8	-2.37	111.71	114.74
23	P	306	CHD	C19-C10-C5	-2.37	106.35	110.36
20	P	303	PGV	O14-P-O13	2.37	123.94	112.24
14	A	601	HEA	C3C-C4C-NC	2.36	112.27	109.21
20	P	301	PGV	C01-O03-C19	2.36	125.85	117.12
26	G	102	CDL	CB6-OB8-CB7	2.36	125.85	117.12
23	C	304	CHD	C9-C8-C7	2.36	114.69	111.88
20	A	609	PGV	C02-O01-C1	2.35	123.59	117.79
19	O	302	TGL	OG3-CG3-CG2	2.35	115.26	108.43
24	O	303	PSC	O03-C01-C02	2.35	115.26	108.43
23	B	302	CHD	C13-C17-C20	-2.35	116.69	119.50
20	P	303	PGV	C22-C21-C20	-2.35	104.76	113.19
19	D	201	TGL	OG1-CA1-CA2	2.33	119.21	111.91
23	B	302	CHD	C11-C9-C10	2.33	116.13	113.73
23	G	104	CHD	O7-C7-C6	2.32	115.71	109.94
19	O	302	TGL	OG2-CB1-OB1	-2.32	118.10	123.70
14	A	601	HEA	CHA-C4D-ND	2.32	126.95	124.43
23	P	306	CHD	C19-C10-C1	-2.31	104.54	108.26
26	C	303	CDL	OA6-CA5-OA7	-2.31	118.12	123.70
23	J	101	CHD	C14-C13-C12	2.31	109.55	107.40
14	N	602	HEA	C2B-C1B-NB	2.31	112.65	109.88
23	P	305	CHD	C18-C13-C12	-2.30	106.72	109.07
23	G	104	CHD	C2-C1-C10	2.29	116.72	112.78
26	G	102	CDL	OB8-CB6-CB4	2.29	115.09	108.43
23	P	306	CHD	C14-C8-C7	2.28	114.83	111.81
20	C	302	PGV	O03-C19-C20	2.28	119.06	111.91
20	P	301	PGV	O01-C1-O02	-2.28	118.20	123.70
19	Y	101	TGL	OG3-CG3-CG2	2.27	115.05	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	609	PGV	C6-C5-C4	-2.27	102.89	114.42
19	L	101	TGL	OG1-CA1-CA2	2.26	119.01	111.91
19	L	101	TGL	OG3-CG3-CG2	2.26	115.01	108.43
23	B	302	CHD	C11-C9-C8	2.26	114.18	110.88
26	G	102	CDL	OA8-CA7-OA9	-2.26	117.90	123.59
14	N	602	HEA	CHC-C4B-C3B	-2.24	120.02	125.80
14	A	602	HEA	C2D-C1D-ND	2.24	112.49	109.84
20	C	307	PGV	C01-O03-C19	2.23	125.38	117.12
23	P	306	CHD	C6-C5-C4	2.21	113.74	111.19
26	T	104	CDL	CA6-OA8-CA7	2.21	125.30	117.12
23	B	302	CHD	C4-C3-C2	-2.21	107.92	110.55
20	N	607	PGV	C03-C02-C01	-2.21	106.57	111.79
20	N	607	PGV	O03-C19-C20	2.20	118.82	111.91
26	C	303	CDL	CB6-OB8-CB7	2.20	125.27	117.12
23	W	101	CHD	C22-C20-C17	2.20	114.83	110.28
23	G	104	CHD	C15-C14-C8	-2.20	115.26	118.33
14	A	601	HEA	O2D-CGD-O1D	-2.19	117.83	123.30
27	G	101	PEK	C3-C2-C1	-2.19	105.66	113.62
27	T	102	PEK	O01-C1-O02	-2.18	118.42	123.70
27	T	102	PEK	O03-C21-O04	-2.18	118.10	123.59
26	P	304	CDL	OA8-CA7-OA9	-2.17	118.11	123.59
14	N	602	HEA	CHA-C4D-C3D	-2.16	121.66	124.84
23	J	101	CHD	C13-C14-C8	2.16	117.50	114.74
14	A	602	HEA	C21-C20-C19	2.16	120.09	112.98
23	P	305	CHD	C6-C5-C4	-2.16	108.70	111.19
14	A	602	HEA	O2A-CGA-CBA	2.16	120.96	114.03
27	C	306	PEK	O01-C02-C01	2.16	116.21	108.40
23	W	101	CHD	O3-C3-C4	2.16	114.14	109.85
26	C	303	CDL	OB8-CB6-CB4	2.15	114.70	108.43
26	G	102	CDL	OB6-CB5-OB7	-2.15	118.51	123.70
19	L	101	TGL	OG3-CC1-OC1	-2.15	118.17	123.59
14	N	602	HEA	CMC-C2C-C3C	2.14	128.69	124.68
24	O	303	PSC	O03-C19-O04	-2.14	118.19	123.59
27	C	306	PEK	O03-C21-O04	-2.13	118.23	123.59
27	G	103	PEK	O01-C02-C01	2.12	116.07	108.40
19	A	607	TGL	OG2-CB1-OB1	-2.10	118.62	123.70
23	C	305	CHD	C17-C13-C12	2.10	119.58	117.67
19	O	302	TGL	OG3-CC1-OC1	-2.10	118.29	123.59
14	A	601	HEA	CAA-CBA-CGA	-2.10	107.87	113.76
23	W	101	CHD	C18-C13-C17	2.10	114.49	111.21
23	P	305	CHD	C15-C14-C8	2.08	121.24	118.33
14	A	601	HEA	C3D-C4D-ND	2.07	112.36	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	304	CHD	C19-C10-C9	-2.07	108.33	111.18
29	Z	101	DMU	O49-C1-C6	-2.07	105.02	110.05
26	C	303	CDL	OA8-CA7-OA9	-2.06	118.38	123.59
29	Z	101	DMU	O1-C9-C11	2.06	111.56	106.44
23	C	305	CHD	C18-C13-C14	2.06	114.43	111.21
23	G	104	CHD	C11-C9-C8	2.05	113.88	110.88
20	A	609	PGV	O01-C02-C03	2.05	115.83	108.40
24	B	303	PSC	O01-C02-C01	2.05	115.82	108.40
20	C	302	PGV	O01-C1-O02	-2.04	118.76	123.70
23	C	305	CHD	C14-C13-C12	-2.04	105.50	107.40
20	A	609	PGV	C4-C3-C2	-2.04	105.86	113.19
14	A	602	HEA	C1B-C2B-C3B	-2.04	104.36	106.80
20	C	302	PGV	O01-C1-C2	2.04	115.89	111.50
20	N	607	PGV	O01-C1-O02	-2.04	118.78	123.70
23	C	304	CHD	C19-C10-C1	-2.03	104.99	108.26
23	B	302	CHD	C16-C17-C13	2.03	105.54	103.55
23	C	305	CHD	C5-C6-C7	-2.02	112.23	114.46
14	N	601	HEA	CAA-CBA-CGA	-2.02	108.10	113.76
27	T	102	PEK	C01-O03-C21	2.02	124.59	117.12
20	A	608	PGV	C5-C4-C3	-2.01	104.22	114.42

There are no chirality outliers.

All (959) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	OB1-CB1-OG2-CG2
19	L	101	TGL	CB2-CB1-OG2-CG2
19	L	101	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	CC2-CC1-OG3-CG3
19	Q	201	TGL	OC1-CC1-OG3-CG3
19	Y	101	TGL	CB2-CB1-OG2-CG2
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	609	PGV	C02-C03-O11-P
20	A	609	PGV	O02-C1-O01-C02
20	A	609	PGV	C2-C1-O01-C02
20	C	307	PGV	C03-O11-P-O12
20	C	307	PGV	C03-O11-P-O13
20	C	307	PGV	C03-O11-P-O14
20	C	307	PGV	O12-C04-C05-C06
20	C	307	PGV	C04-C05-C06-O06
20	N	607	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	C02-C03-O11-P
20	N	607	PGV	O12-C04-C05-C06
20	N	607	PGV	C2-C1-O01-C02
20	P	301	PGV	C04-O12-P-O11
20	P	301	PGV	C2-C1-O01-C02
23	W	101	CHD	C13-C17-C20-C22
24	B	303	PSC	C04-O12-P-O14
24	B	303	PSC	C2-C1-O01-C02
24	O	303	PSC	C03-O11-P-O13
24	O	303	PSC	C04-O12-P-O11
24	O	303	PSC	C04-O12-P-O13
24	O	303	PSC	C04-O12-P-O14
24	O	303	PSC	O12-C04-C05-N
24	O	303	PSC	C11-C12-C13-C14
26	C	303	CDL	CA2-C1-CB2-OB2
26	C	303	CDL	CA2-OA2-PA1-OA3
26	C	303	CDL	CA2-OA2-PA1-OA4
26	C	303	CDL	C11-CA5-OA6-CA4
26	C	303	CDL	C51-CB5-OB6-CB4
26	G	102	CDL	O1-C1-CA2-OA2
26	G	102	CDL	CA2-OA2-PA1-OA3
26	G	102	CDL	CA2-OA2-PA1-OA4
26	G	102	CDL	C11-CA5-OA6-CA4
26	G	102	CDL	OB7-CB5-OB6-CB4
26	G	102	CDL	C51-CB5-OB6-CB4
26	P	304	CDL	CA2-OA2-PA1-OA3
26	P	304	CDL	CA2-OA2-PA1-OA4
26	P	304	CDL	CA2-OA2-PA1-OA5
26	P	304	CDL	CA3-OA5-PA1-OA3
26	P	304	CDL	CA3-OA5-PA1-OA4
26	P	304	CDL	OA7-CA5-OA6-CA4
26	P	304	CDL	C11-CA5-OA6-CA4
26	P	304	CDL	CB3-OB5-PB2-OB4
26	T	104	CDL	CA2-C1-CB2-OB2
26	T	104	CDL	CA2-OA2-PA1-OA3
26	T	104	CDL	CA2-OA2-PA1-OA4
26	T	104	CDL	C11-CA5-OA6-CA4
26	T	104	CDL	CB3-OB5-PB2-OB2
26	T	104	CDL	CB3-OB5-PB2-OB3
27	C	306	PEK	C03-O11-P-O14
27	C	306	PEK	C04-O12-P-O14
27	C	306	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
27	G	103	PEK	C04-O12-P-O13
27	G	103	PEK	C04-O12-P-O14
27	G	103	PEK	O12-C04-C05-N
27	G	103	PEK	C2-C1-O01-C02
27	T	101	PEK	C13-C14-C15-C16
27	T	102	PEK	C03-O11-P-O13
27	T	102	PEK	C12-C13-C14-C15
27	T	103	PEK	O03-C01-C02-O01
27	T	103	PEK	C5-C6-C7-C8
27	T	103	PEK	C9-C10-C11-C12
19	D	201	TGL	OC1-CC1-OG3-CG3
24	O	303	PSC	O04-C19-O03-C01
24	O	303	PSC	C20-C19-O03-C01
19	O	302	TGL	OC1-CC1-OG3-CG3
20	A	609	PGV	O04-C19-O03-C01
20	N	607	PGV	O04-C19-O03-C01
24	B	303	PSC	O04-C19-O03-C01
26	T	104	CDL	OA9-CA7-OA8-CA6
27	T	102	PEK	O04-C21-O03-C01
20	N	607	PGV	O02-C1-O01-C02
20	P	301	PGV	O02-C1-O01-C02
26	C	303	CDL	OA7-CA5-OA6-CA4
26	C	303	CDL	OB7-CB5-OB6-CB4
27	G	103	PEK	O02-C1-O01-C02
19	A	607	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	CC2-CC1-OG3-CG3
19	O	302	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	C20-C19-O03-C01
26	T	104	CDL	C31-CA7-OA8-CA6
19	A	607	TGL	CA2-CA1-OG1-CG1
20	N	607	PGV	C20-C19-O03-C01
24	B	303	PSC	C20-C19-O03-C01
26	C	303	CDL	C71-CB7-OB8-CB6
27	T	102	PEK	C22-C21-O03-C01
20	C	307	PGV	C10-C11-C12-C13
27	G	101	PEK	C4-C5-C6-C7
27	G	101	PEK	C7-C8-C9-C10
27	G	101	PEK	C13-C14-C15-C16
24	B	303	PSC	O02-C1-O01-C02
26	G	102	CDL	OA7-CA5-OA6-CA4
26	T	104	CDL	OA7-CA5-OA6-CA4
26	C	303	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
24	B	303	PSC	C04-C05-N-C08
20	N	607	PGV	O12-C04-C05-O05
26	G	102	CDL	O1-C1-CB2-OB2
26	P	304	CDL	O1-C1-CA2-OA2
24	O	303	PSC	C24-C25-C26-C27
19	A	607	TGL	OC1-CC1-OG3-CG3
19	Q	201	TGL	CB2-CB1-OG2-CG2
20	A	608	PGV	C26-C27-C28-C29
19	A	607	TGL	OA1-CA1-OG1-CG1
19	Y	101	TGL	CA9-C20-C21-C22
26	G	102	CDL	C78-C79-C80-C81
23	J	101	CHD	C17-C20-C22-C23
19	O	302	TGL	CA7-CA8-CA9-C20
23	J	101	CHD	C21-C20-C22-C23
23	P	305	CHD	C21-C20-C22-C23
20	A	609	PGV	C20-C21-C22-C23
19	L	101	TGL	CA2-CA1-OG1-CG1
23	P	305	CHD	C17-C20-C22-C23
20	A	609	PGV	C10-C11-C12-C13
19	A	607	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	O12-C04-C05-C06
26	C	303	CDL	CB2-C1-CA2-OA2
26	G	102	CDL	CB2-C1-CA2-OA2
26	P	304	CDL	CB2-C1-CA2-OA2
26	G	102	CDL	C31-CA7-OA8-CA6
29	M	101	DMU	O6-C11-C9-O1
29	M	101	DMU	O6-C11-C9-C8
20	C	307	PGV	O12-C04-C05-O05
26	C	303	CDL	O1-C1-CB2-OB2
26	T	104	CDL	O1-C1-CB2-OB2
19	Q	201	TGL	OB1-CB1-OG2-CG2
26	P	304	CDL	C51-CB5-OB6-CB4
23	J	101	CHD	C13-C17-C20-C22
26	C	303	CDL	CA5-C11-C12-C13
26	G	102	CDL	OA9-CA7-OA8-CA6
19	L	101	TGL	CB1-CB2-CB3-CB4
20	P	303	PGV	C1-C2-C3-C4
27	C	306	PEK	C4-C5-C6-C7
27	C	306	PEK	C10-C11-C12-C13
26	C	303	CDL	C59-C60-C61-C62
20	A	609	PGV	O05-C05-C06-O06
19	D	201	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CC1-CC2-CC3-CC4
19	Y	101	TGL	CA1-CA2-CA3-CA4
20	N	607	PGV	C19-C20-C21-C22
24	B	303	PSC	C1-C2-C3-C4
26	P	304	CDL	CB7-C71-C72-C73
27	G	103	PEK	C21-C22-C23-C24
19	O	302	TGL	CA2-CA1-OG1-CG1
27	G	101	PEK	C22-C21-O03-C01
26	P	304	CDL	C1-CA2-OA2-PA1
23	W	101	CHD	C16-C17-C20-C22
19	L	101	TGL	OA1-CA1-OG1-CG1
27	G	101	PEK	O04-C21-O03-C01
26	T	104	CDL	CA7-C31-C32-C33
26	C	303	CDL	O1-C1-CA2-OA2
26	P	304	CDL	OB7-CB5-OB6-CB4
23	W	101	CHD	C16-C17-C20-C21
23	J	101	CHD	C13-C17-C20-C21
19	L	101	TGL	CC1-CC2-CC3-CC4
19	Y	101	TGL	CB1-CB2-CB3-CB4
20	N	608	PGV	C10-C11-C12-C13
20	P	303	PGV	C10-C11-C12-C13
24	B	303	PSC	C11-C10-C9-C8
27	T	103	PEK	C13-C14-C15-C16
20	A	609	PGV	C04-O12-P-O11
20	P	301	PGV	C03-O11-P-O12
24	B	303	PSC	C03-O11-P-O12
24	O	303	PSC	C03-O11-P-O12
26	C	303	CDL	CA2-OA2-PA1-OA5
26	C	303	CDL	CA3-OA5-PA1-OA2
26	G	102	CDL	CA2-OA2-PA1-OA5
26	G	102	CDL	CB3-OB5-PB2-OB2
26	P	304	CDL	CA3-OA5-PA1-OA2
26	T	104	CDL	CA2-OA2-PA1-OA5
27	G	103	PEK	C04-O12-P-O11
27	T	102	PEK	C03-O11-P-O12
27	T	103	PEK	C04-O12-P-O11
26	T	104	CDL	C71-CB7-OB8-CB6
26	G	102	CDL	CA2-C1-CB2-OB2
19	A	607	TGL	OB1-CB1-OG2-CG2
24	B	303	PSC	C04-C05-N-C06
19	Y	101	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
20	A	608	PGV	C4-C5-C6-C7
26	T	104	CDL	C79-C80-C81-C82
27	T	103	PEK	C34-C35-C36-C37
29	Z	101	DMU	C31-C34-C37-C40
19	L	101	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	CB9-C10-C11-C12
19	Y	101	TGL	C11-C12-C13-C14
19	Y	101	TGL	C23-C24-C25-C26
20	C	307	PGV	C24-C25-C26-C27
24	B	303	PSC	C4-C5-C6-C7
24	B	303	PSC	C26-C27-C28-C29
26	P	304	CDL	C60-C61-C62-C63
29	Z	101	DMU	C19-C22-C25-C28
19	A	607	TGL	C20-C21-C22-C23
19	Q	201	TGL	CA6-CA7-CA8-CA9
19	Y	101	TGL	CB6-CB7-CB8-CB9
20	A	609	PGV	C14-C15-C16-C17
26	C	303	CDL	C80-C81-C82-C83
26	G	102	CDL	C55-C56-C57-C58
20	N	607	PGV	C03-C02-O01-C1
27	G	103	PEK	C01-C02-O01-C1
26	T	104	CDL	OB7-CB5-OB6-CB4
26	G	102	CDL	CA5-C11-C12-C13
19	D	201	TGL	CB3-CB4-CB5-CB6
19	Y	101	TGL	CB3-CB4-CB5-CB6
19	Y	101	TGL	C21-C22-C23-C24
20	P	303	PGV	C7-C8-C9-C10
24	O	303	PSC	C20-C21-C22-C23
26	G	102	CDL	C59-C60-C61-C62
26	G	102	CDL	C77-C78-C79-C80
26	T	104	CDL	C19-C20-C21-C22
26	T	104	CDL	C32-C33-C34-C35
20	A	608	PGV	C10-C11-C12-C13
27	G	103	PEK	C4-C5-C6-C7
27	G	103	PEK	C10-C11-C12-C13
19	L	101	TGL	CB7-CB8-CB9-C10
20	C	307	PGV	C2-C3-C4-C5
26	T	104	CDL	C51-C52-C53-C54
26	T	104	CDL	C53-C54-C55-C56
27	C	306	PEK	C23-C24-C25-C26
20	A	609	PGV	O12-C04-C05-O05

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CA6-CA7-CA8-CA9
19	D	201	TGL	C18-C19-C33-C34
19	Y	101	TGL	C19-C33-C34-C35
20	C	302	PGV	C1-C2-C3-C4
27	C	306	PEK	O03-C01-C02-O01
19	L	101	TGL	CB5-CB6-CB7-CB8
19	O	302	TGL	CB2-CB3-CB4-CB5
19	Y	101	TGL	CA5-CA6-CA7-CA8
20	P	301	PGV	C26-C27-C28-C29
26	G	102	CDL	C71-C72-C73-C74
27	G	103	PEK	C30-C31-C32-C33
29	M	101	DMU	O16-C18-C19-C22
19	O	302	TGL	OA1-CA1-OG1-CG1
23	W	101	CHD	C17-C20-C22-C23
19	Y	101	TGL	CB2-CB3-CB4-CB5
19	Y	101	TGL	C11-C10-CB9-CB8
19	Y	101	TGL	C13-C14-C29-C30
20	N	608	PGV	C28-C29-C30-C31
24	O	303	PSC	C21-C22-C23-C24
24	O	303	PSC	C23-C24-C25-C26
26	G	102	CDL	C33-C34-C35-C36
26	P	304	CDL	C31-C32-C33-C34
19	A	607	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	C11-C12-C13-C14
19	Q	201	TGL	CC2-CC3-CC4-CC5
19	Y	101	TGL	C10-C11-C12-C13
19	Y	101	TGL	CC5-CC6-CC7-CC8
20	N	607	PGV	C22-C23-C24-C25
20	P	303	PGV	C24-C25-C26-C27
26	C	303	CDL	C52-C53-C54-C55
27	G	101	PEK	C30-C31-C32-C33
27	G	103	PEK	C25-C26-C27-C28
26	T	104	CDL	OB9-CB7-OB8-CB6
19	A	607	TGL	C12-C13-C14-C29
19	L	101	TGL	C18-C19-C33-C34
19	Y	101	TGL	CB4-CB5-CB6-CB7
26	T	104	CDL	C33-C34-C35-C36
20	A	609	PGV	C04-C05-C06-O06
23	J	101	CHD	C16-C17-C20-C21
19	D	201	TGL	C10-C11-C12-C13
19	D	201	TGL	C16-C17-C18-C19
19	Q	201	TGL	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
20	C	302	PGV	C7-C8-C9-C10
20	P	303	PGV	C25-C26-C27-C28
20	A	609	PGV	C12-C13-C14-C15
27	T	101	PEK	C1-C2-C3-C4
19	A	607	TGL	C11-C12-C13-C14
19	D	201	TGL	C16-C15-CC9-CC8
19	L	101	TGL	C16-C15-CC9-CC8
19	O	302	TGL	CA2-CA3-CA4-CA5
19	O	302	TGL	C13-C14-C29-C30
19	Q	201	TGL	CA2-CA3-CA4-CA5
19	Y	101	TGL	CA6-CA7-CA8-CA9
20	A	609	PGV	C4-C5-C6-C7
20	A	609	PGV	C24-C25-C26-C27
20	A	609	PGV	C29-C30-C31-C32
20	C	307	PGV	C23-C24-C25-C26
24	B	303	PSC	C3-C4-C5-C6
24	O	303	PSC	C3-C4-C5-C6
24	O	303	PSC	C4-C5-C6-C7
26	C	303	CDL	C36-C37-C38-C39
26	G	102	CDL	C75-C76-C77-C78
26	P	304	CDL	C55-C56-C57-C58
26	P	304	CDL	C73-C74-C75-C76
26	T	104	CDL	C37-C38-C39-C40
26	T	104	CDL	C39-C40-C41-C42
24	B	303	PSC	C04-C05-N-C07
19	A	607	TGL	C22-C23-C24-C25
19	O	302	TGL	CB9-C10-C11-C12
20	C	307	PGV	C20-C21-C22-C23
20	N	608	PGV	C30-C31-C32-C33
26	C	303	CDL	C42-C43-C44-C45
27	C	306	PEK	C25-C26-C27-C28
27	T	102	PEK	O12-C04-C05-N
19	A	607	TGL	CC4-CC5-CC6-CC7
20	C	302	PGV	C23-C24-C25-C26
20	P	301	PGV	C22-C23-C24-C25
27	G	101	PEK	C24-C25-C26-C27
29	M	101	DMU	C25-C28-C31-C34
26	G	102	CDL	CA7-C31-C32-C33
24	B	303	PSC	C27-C28-C29-C30
26	G	102	CDL	C83-C84-C85-C86
27	T	102	PEK	C30-C31-C32-C33
27	C	306	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	CA5-CA6-CA7-CA8
27	C	306	PEK	C16-C17-C18-C19
19	A	607	TGL	CB6-CB7-CB8-CB9
19	L	101	TGL	C22-C23-C24-C25
19	Q	201	TGL	C16-C15-CC9-CC8
26	P	304	CDL	C83-C84-C85-C86
26	T	104	CDL	C35-C36-C37-C38
27	T	103	PEK	C27-C28-C29-C30
19	A	607	TGL	CB9-C10-C11-C12
19	O	302	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	CC7-CC8-CC9-C15
20	P	303	PGV	C14-C15-C16-C17
26	G	102	CDL	C51-C52-C53-C54
26	P	304	CDL	C16-C17-C18-C19
26	P	304	CDL	C63-C64-C65-C66
26	G	102	CDL	CA3-CA4-CA6-OA8
27	G	103	PEK	C7-C8-C9-C10
27	T	101	PEK	C10-C11-C12-C13
20	N	608	PGV	C26-C27-C28-C29
19	A	607	TGL	CA2-CA3-CA4-CA5
19	Y	101	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	CC4-CC5-CC6-CC7
26	G	102	CDL	C12-C13-C14-C15
19	O	302	TGL	CB2-CB1-OG2-CG2
26	T	104	CDL	C51-CB5-OB6-CB4
20	A	608	PGV	C22-C23-C24-C25
26	G	102	CDL	C74-C75-C76-C77
27	T	101	PEK	C23-C24-C25-C26
19	L	101	TGL	CC3-CC4-CC5-CC6
19	Y	101	TGL	CB7-CB8-CB9-C10
20	C	307	PGV	C3-C4-C5-C6
20	C	307	PGV	C30-C31-C32-C33
26	G	102	CDL	C21-C22-C23-C24
26	G	102	CDL	C60-C61-C62-C63
26	G	102	CDL	C63-C64-C65-C66
20	N	608	PGV	C11-C10-C9-C8
24	B	303	PSC	C13-C14-C15-C16
24	O	303	PSC	C13-C14-C15-C16
27	T	103	PEK	C2-C3-C4-C5
27	T	103	PEK	C15-C16-C17-C18
19	D	201	TGL	CB2-CB3-CB4-CB5
19	O	302	TGL	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	C21-C22-C23-C24
24	O	303	PSC	C5-C6-C7-C8
19	Y	101	TGL	OA1-CA1-OG1-CG1
19	L	101	TGL	CB2-CB3-CB4-CB5
26	C	303	CDL	C40-C41-C42-C43
26	C	303	CDL	C60-C61-C62-C63
26	G	102	CDL	C72-C73-C74-C75
27	G	103	PEK	C22-C23-C24-C25
27	T	101	PEK	C34-C35-C36-C37
27	C	306	PEK	O02-C1-O01-C02
19	A	607	TGL	CC3-CC4-CC5-CC6
19	A	607	TGL	CC5-CC6-CC7-CC8
19	O	302	TGL	CB4-CB5-CB6-CB7
26	G	102	CDL	C1-CB2-OB2-PB2
19	D	201	TGL	C17-C18-C19-C33
19	O	302	TGL	CA3-CA4-CA5-CA6
20	N	607	PGV	C20-C21-C22-C23
26	P	304	CDL	C82-C83-C84-C85
26	T	104	CDL	C59-C60-C61-C62
27	C	306	PEK	C33-C34-C35-C36
20	C	307	PGV	C1-C2-C3-C4
21	A	612	EDO	O1-C1-C2-O2
21	A	613	EDO	O1-C1-C2-O2
21	B	304	EDO	O1-C1-C2-O2
21	T	105	EDO	O1-C1-C2-O2
19	Q	201	TGL	C13-C14-C29-C30
19	Y	101	TGL	C20-C21-C22-C23
20	P	301	PGV	C6-C7-C8-C9
26	G	102	CDL	C71-CB7-OB8-CB6
20	C	307	PGV	C27-C28-C29-C30
26	P	304	CDL	C13-C14-C15-C16
19	O	302	TGL	CC5-CC6-CC7-CC8
20	A	609	PGV	C2-C3-C4-C5
26	G	102	CDL	C57-C58-C59-C60
19	A	607	TGL	C18-C19-C33-C34
26	C	303	CDL	C61-C62-C63-C64
26	G	102	CDL	C11-C12-C13-C14
27	G	101	PEK	C10-C11-C12-C13
27	C	306	PEK	O04-C21-O03-C01
19	Y	101	TGL	CC9-C15-C16-C17
24	B	303	PSC	C24-C25-C26-C27
26	C	303	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
27	T	103	PEK	C16-C17-C18-C19
27	T	103	PEK	C23-C24-C25-C26
20	A	608	PGV	C12-C13-C14-C15
27	G	101	PEK	C15-C16-C17-C18
27	T	102	PEK	C2-C3-C4-C5
19	A	607	TGL	C11-C10-CB9-CB8
19	L	101	TGL	C12-C13-C14-C29
20	A	609	PGV	C13-C14-C15-C16
26	P	304	CDL	C56-C57-C58-C59
19	L	101	TGL	CA7-CA8-CA9-C20
19	L	101	TGL	CB3-CB4-CB5-CB6
19	L	101	TGL	CC6-CC7-CC8-CC9
19	O	302	TGL	C12-C13-C14-C29
26	G	102	CDL	C13-C14-C15-C16
26	P	304	CDL	C41-C42-C43-C44
19	O	302	TGL	CB7-CB8-CB9-C10
20	N	608	PGV	C29-C30-C31-C32
27	C	306	PEK	C26-C27-C28-C29
26	T	104	CDL	C58-C59-C60-C61
23	C	305	CHD	C16-C17-C20-C22
19	A	607	TGL	C19-C33-C34-C35
19	D	201	TGL	CC6-CC7-CC8-CC9
20	A	609	PGV	C26-C27-C28-C29
20	P	303	PGV	C27-C28-C29-C30
26	C	303	CDL	C76-C77-C78-C79
26	G	102	CDL	C58-C59-C60-C61
26	T	104	CDL	C63-C64-C65-C66
19	A	607	TGL	CA1-CA2-CA3-CA4
20	A	609	PGV	C19-C20-C21-C22
24	O	303	PSC	C2-C1-O01-C02
27	C	306	PEK	C2-C1-O01-C02
19	L	101	TGL	CA4-CA5-CA6-CA7
20	C	302	PGV	C14-C15-C16-C17
27	T	103	PEK	C30-C31-C32-C33
27	T	102	PEK	C32-C33-C34-C35
19	O	302	TGL	OB1-CB1-OG2-CG2
24	O	303	PSC	O02-C1-O01-C02
19	O	302	TGL	CB6-CB7-CB8-CB9
26	P	304	CDL	C52-C53-C54-C55
26	P	304	CDL	C61-C62-C63-C64
20	P	301	PGV	O03-C01-C02-O01
19	A	607	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
26	C	303	CDL	C23-C24-C25-C26
26	G	102	CDL	C23-C24-C25-C26
27	G	101	PEK	C23-C24-C25-C26
26	C	303	CDL	C77-C78-C79-C80
26	P	304	CDL	C79-C80-C81-C82
27	G	103	PEK	C33-C34-C35-C36
20	P	301	PGV	C12-C13-C14-C15
19	D	201	TGL	CA2-CA3-CA4-CA5
19	Y	101	TGL	C16-C15-CC9-CC8
20	P	301	PGV	C30-C31-C32-C33
24	B	303	PSC	C23-C24-C25-C26
26	T	104	CDL	C62-C63-C64-C65
24	O	303	PSC	C28-C29-C30-C31
26	C	303	CDL	C75-C76-C77-C78
26	G	102	CDL	C35-C36-C37-C38
20	C	302	PGV	C10-C11-C12-C13
19	D	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	CA3-CA4-CA5-CA6
19	Q	201	TGL	CB7-CB8-CB9-C10
26	C	303	CDL	C17-C18-C19-C20
26	G	102	CDL	C52-C53-C54-C55
27	G	101	PEK	C34-C35-C36-C37
27	G	103	PEK	C31-C32-C33-C34
19	O	302	TGL	C21-C20-CA9-CA8
20	A	609	PGV	C25-C26-C27-C28
26	C	303	CDL	C11-C12-C13-C14
24	B	303	PSC	C04-O12-P-O11
26	P	304	CDL	CB3-OB5-PB2-OB2
19	O	302	TGL	C16-C17-C18-C19
27	T	103	PEK	C25-C26-C27-C28
19	O	302	TGL	CA1-CA2-CA3-CA4
24	B	303	PSC	C02-C03-O11-P
20	A	609	PGV	C01-C02-C03-O11
26	C	303	CDL	OA5-CA3-CA4-CA6
27	T	103	PEK	C01-C02-C03-O11
19	A	607	TGL	C13-C14-C29-C30
19	A	607	TGL	C23-C24-C25-C26
20	P	303	PGV	C29-C30-C31-C32
19	Q	201	TGL	C21-C20-CA9-CA8
20	A	608	PGV	C14-C15-C16-C17
20	A	609	PGV	C7-C8-C9-C10
20	N	607	PGV	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	Z	101	DMU	C3-C4-C57-O61
23	W	101	CHD	C13-C17-C20-C21
19	A	607	TGL	C21-C20-CA9-CA8
19	D	201	TGL	CC5-CC6-CC7-CC8
19	Q	201	TGL	C23-C24-C25-C26
27	C	306	PEK	C15-C16-C17-C18
19	Q	201	TGL	C19-C33-C34-C35
20	C	307	PGV	C21-C22-C23-C24
26	G	102	CDL	C16-C17-C18-C19
27	T	102	PEK	C25-C26-C27-C28
19	A	607	TGL	CB4-CB5-CB6-CB7
20	C	302	PGV	C22-C23-C24-C25
26	G	102	CDL	OB9-CB7-OB8-CB6
19	D	201	TGL	CA7-CA8-CA9-C20
27	G	101	PEK	C25-C26-C27-C28
19	D	201	TGL	OG1-CG1-CG2-CG3
19	Y	101	TGL	OG1-CG1-CG2-CG3
20	C	307	PGV	O03-C01-C02-C03
20	N	607	PGV	C27-C28-C29-C30
20	P	301	PGV	O03-C01-C02-C03
26	P	304	CDL	CA3-CA4-CA6-OA8
27	C	306	PEK	O03-C01-C02-C03
27	T	102	PEK	C4-C5-C6-C7
19	Q	201	TGL	CC4-CC5-CC6-CC7
26	T	104	CDL	C72-C73-C74-C75
19	Q	201	TGL	CA9-C20-C21-C22
26	C	303	CDL	C84-C85-C86-C87
26	G	102	CDL	C19-C20-C21-C22
27	T	102	PEK	C35-C36-C37-C38
29	M	101	DMU	C28-C31-C34-C37
19	O	302	TGL	C25-C26-C27-C28
26	G	102	CDL	C39-C40-C41-C42
26	P	304	CDL	C84-C85-C86-C87
26	T	104	CDL	C55-C56-C57-C58
27	T	103	PEK	C17-C18-C19-C20
19	A	607	TGL	C29-C30-C31-C32
19	D	201	TGL	C21-C22-C23-C24
20	A	608	PGV	C31-C32-C33-C34
26	P	304	CDL	C24-C25-C26-C27
19	Q	201	TGL	CC6-CC7-CC8-CC9
26	C	303	CDL	C37-C38-C39-C40
20	A	608	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
20	C	307	PGV	C12-C13-C14-C15
20	P	303	PGV	C12-C13-C14-C15
19	D	201	TGL	CB4-CB5-CB6-CB7
26	C	303	CDL	C33-C34-C35-C36
20	C	307	PGV	C4-C5-C6-C7
26	P	304	CDL	C35-C36-C37-C38
19	Q	201	TGL	CA1-CA2-CA3-CA4
26	C	303	CDL	C74-C75-C76-C77
26	P	304	CDL	C37-C38-C39-C40
20	A	609	PGV	C03-C02-O01-C1
24	O	303	PSC	C01-C02-O01-C1
26	P	304	CDL	C77-C78-C79-C80
19	Q	201	TGL	C20-C21-C22-C23
26	C	303	CDL	C18-C19-C20-C21
26	T	104	CDL	C81-C82-C83-C84
27	G	103	PEK	O01-C02-C03-O11
21	K	102	EDO	O1-C1-C2-O2
21	P	308	EDO	O1-C1-C2-O2
26	C	303	CDL	C62-C63-C64-C65
20	P	301	PGV	C31-C32-C33-C34
26	G	102	CDL	C44-C45-C46-C47
29	Z	101	DMU	O16-C18-C19-C22
20	C	307	PGV	O03-C01-C02-O01
19	O	302	TGL	C20-C21-C22-C23
24	O	303	PSC	C22-C23-C24-C25
27	T	101	PEK	C25-C26-C27-C28
26	T	104	CDL	C40-C41-C42-C43
19	L	101	TGL	C21-C20-CA9-CA8
20	A	608	PGV	C23-C24-C25-C26
26	C	303	CDL	C35-C36-C37-C38
19	O	302	TGL	C11-C12-C13-C14
19	Q	201	TGL	CA5-CA6-CA7-CA8
24	O	303	PSC	C31-C32-C33-C34
26	T	104	CDL	C24-C25-C26-C27
19	O	302	TGL	C29-C30-C31-C32
27	T	101	PEK	C4-C5-C6-C7
19	A	607	TGL	CB5-CB6-CB7-CB8
26	G	102	CDL	C17-C18-C19-C20
14	N	602	HEA	C4D-C3D-CAD-CBD
26	P	304	CDL	C80-C81-C82-C83
26	P	304	CDL	OA5-CA3-CA4-CA6
23	G	104	CHD	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
20	A	609	PGV	C22-C23-C24-C25
20	N	607	PGV	C29-C30-C31-C32
20	P	301	PGV	C13-C14-C15-C16
26	T	104	CDL	C14-C15-C16-C17
19	L	101	TGL	C13-C14-C29-C30
26	G	102	CDL	C43-C44-C45-C46
19	Q	201	TGL	C10-C11-C12-C13
20	A	608	PGV	O03-C19-C20-C21
20	C	302	PGV	C25-C26-C27-C28
20	C	307	PGV	C02-C03-O11-P
26	C	303	CDL	C78-C79-C80-C81
26	P	304	CDL	C14-C15-C16-C17
19	O	302	TGL	CC4-CC5-CC6-CC7
19	A	607	TGL	C25-C26-C27-C28
19	O	302	TGL	CC6-CC7-CC8-CC9
19	L	101	TGL	OG1-CG1-CG2-CG3
26	C	303	CDL	CB3-CB4-CB6-OB8
26	P	304	CDL	CB3-CB4-CB6-OB8
26	T	104	CDL	CA3-CA4-CA6-OA8
19	Q	201	TGL	C24-C25-C26-C27
20	P	301	PGV	C25-C26-C27-C28
19	Y	101	TGL	CC1-CC2-CC3-CC4
26	P	304	CDL	CA5-C11-C12-C13
24	O	303	PSC	C11-C10-C9-C8
19	A	607	TGL	C33-C34-C35-C36
19	D	201	TGL	CA3-CA4-CA5-CA6
26	P	304	CDL	C59-C60-C61-C62
27	G	101	PEK	C32-C33-C34-C35
19	D	201	TGL	CB5-CB6-CB7-CB8
19	Q	201	TGL	C15-C16-C17-C18
24	B	303	PSC	C10-C11-C12-C13
24	O	303	PSC	C9-C10-C11-C12
24	O	303	PSC	C10-C11-C12-C13
27	C	306	PEK	C5-C6-C7-C8
27	C	306	PEK	C6-C7-C8-C9
27	C	306	PEK	C11-C10-C9-C8
27	G	103	PEK	C11-C10-C9-C8
27	G	103	PEK	C9-C10-C11-C12
27	G	103	PEK	C12-C13-C14-C15
27	T	101	PEK	C11-C10-C9-C8
27	T	102	PEK	C9-C10-C11-C12
27	T	103	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	T	103	PEK	C11-C10-C9-C8
27	T	103	PEK	C12-C13-C14-C15
27	G	101	PEK	C33-C34-C35-C36
27	T	101	PEK	C17-C18-C19-C20
19	O	302	TGL	CC7-CC8-CC9-C15
19	Q	201	TGL	CC5-CC6-CC7-CC8
20	C	307	PGV	C14-C15-C16-C17
26	P	304	CDL	C22-C23-C24-C25
20	P	301	PGV	O01-C02-C03-O11
27	T	102	PEK	O01-C02-C03-O11
19	A	607	TGL	CB1-CB2-CB3-CB4
19	Q	201	TGL	CB3-CB4-CB5-CB6
26	T	104	CDL	C22-C23-C24-C25
19	O	302	TGL	C16-C15-CC9-CC8
20	P	303	PGV	C31-C32-C33-C34
27	G	101	PEK	C26-C27-C28-C29
19	Y	101	TGL	OG1-CG1-CG2-OG2
20	A	609	PGV	O03-C01-C02-O01
24	B	303	PSC	O03-C01-C02-O01
14	N	602	HEA	C2D-C3D-CAD-CBD
20	A	609	PGV	C31-C32-C33-C34
26	G	102	CDL	C15-C16-C17-C18
27	T	103	PEK	O02-C1-O01-C02
26	T	104	CDL	C41-C42-C43-C44
27	G	103	PEK	C34-C35-C36-C37
23	B	302	CHD	C17-C20-C22-C23
19	Y	101	TGL	CB5-CB6-CB7-CB8
26	G	102	CDL	C62-C63-C64-C65
20	P	301	PGV	C02-C03-O11-P
20	P	303	PGV	C02-C03-O11-P
26	P	304	CDL	CA4-CA3-OA5-PA1
26	P	304	CDL	C1-CB2-OB2-PB2
29	M	101	DMU	C19-C22-C25-C28
26	G	102	CDL	CB5-C51-C52-C53
20	P	303	PGV	C13-C14-C15-C16
21	K	101	EDO	O1-C1-C2-O2
21	L	102	EDO	O1-C1-C2-O2
21	O	304	EDO	O1-C1-C2-O2
19	L	101	TGL	CA9-C20-C21-C22
20	N	608	PGV	C31-C32-C33-C34
20	P	301	PGV	C3-C4-C5-C6
26	T	104	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	CC3-CC4-CC5-CC6
26	P	304	CDL	C34-C35-C36-C37
19	L	101	TGL	C17-C18-C19-C33
27	G	101	PEK	C16-C17-C18-C19
20	N	607	PGV	C01-C02-C03-O11
20	P	301	PGV	C01-C02-C03-O11
24	B	303	PSC	C01-C02-C03-O11
27	G	103	PEK	C01-C02-C03-O11
27	T	102	PEK	C01-C02-C03-O11
19	A	607	TGL	C24-C25-C26-C27
27	G	103	PEK	C27-C28-C29-C30
20	N	607	PGV	C23-C24-C25-C26
19	Q	201	TGL	CB4-CB5-CB6-CB7
26	P	304	CDL	C51-C52-C53-C54
29	M	101	DMU	C22-C25-C28-C31
26	T	104	CDL	C71-C72-C73-C74
20	N	608	PGV	C19-C20-C21-C22
20	A	608	PGV	C30-C31-C32-C33
20	P	301	PGV	C4-C5-C6-C7
19	D	201	TGL	C13-C14-C29-C30
27	T	103	PEK	C26-C27-C28-C29
27	T	103	PEK	C28-C29-C30-C31
24	O	303	PSC	C6-C7-C8-C9
19	Y	101	TGL	CG1-CG2-CG3-OG3
20	N	607	PGV	O03-C01-C02-C03
24	O	303	PSC	O03-C01-C02-C03
26	C	303	CDL	CA3-CA4-CA6-OA8
26	T	104	CDL	C1-CB2-OB2-PB2
27	T	103	PEK	O03-C01-C02-C03
27	T	103	PEK	C2-C1-O01-C02
20	A	609	PGV	O01-C02-C03-O11
20	N	607	PGV	O01-C02-C03-O11
27	T	103	PEK	O01-C02-C03-O11
26	C	303	CDL	C58-C59-C60-C61
19	D	201	TGL	OG1-CG1-CG2-OG2
19	Y	101	TGL	OG2-CG2-CG3-OG3
24	O	303	PSC	O03-C01-C02-O01
26	C	303	CDL	OB6-CB4-CB6-OB8
27	T	102	PEK	O03-C01-C02-O01
19	L	101	TGL	C20-C21-C22-C23
27	C	306	PEK	C34-C35-C36-C37
27	T	102	PEK	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	C12-C13-C14-C15
27	T	101	PEK	C15-C16-C17-C18
24	B	303	PSC	C15-C16-C17-C18
26	C	303	CDL	CB4-CB6-OB8-CB7
19	D	201	TGL	CC9-C15-C16-C17
24	B	303	PSC	C31-C32-C33-C34
27	T	101	PEK	C7-C8-C9-C10
27	G	103	PEK	C3-C4-C5-C6
19	A	607	TGL	CA4-CA5-CA6-CA7
27	C	306	PEK	C30-C31-C32-C33
26	T	104	CDL	CB2-OB2-PB2-OB5
27	C	306	PEK	C03-O11-P-O12
27	G	103	PEK	C03-O11-P-O12
26	C	303	CDL	C32-C33-C34-C35
20	C	302	PGV	C02-C03-O11-P
26	C	303	CDL	C1-CA2-OA2-PA1
27	T	102	PEK	C02-C03-O11-P
20	P	303	PGV	C28-C29-C30-C31
20	A	609	PGV	C04-O12-P-O13
20	P	301	PGV	C03-O11-P-O13
20	P	303	PGV	C04-O12-P-O14
24	B	303	PSC	C03-O11-P-O14
24	B	303	PSC	C04-O12-P-O13
26	C	303	CDL	CA3-OA5-PA1-OA3
26	G	102	CDL	CB2-OB2-PB2-OB4
26	G	102	CDL	CB3-OB5-PB2-OB3
26	P	304	CDL	CB3-OB5-PB2-OB3
27	T	103	PEK	C04-O12-P-O13
21	C	308	EDO	O1-C1-C2-O2
24	O	303	PSC	C15-C16-C17-C18
27	T	101	PEK	C27-C28-C29-C30
19	O	302	TGL	CA5-CA6-CA7-CA8
20	N	608	PGV	C5-C6-C7-C8
27	G	101	PEK	C21-C22-C23-C24
26	G	102	CDL	CB7-C71-C72-C73
19	Y	101	TGL	C17-C18-C19-C33
27	G	103	PEK	C28-C29-C30-C31
24	B	303	PSC	O01-C02-C03-O11
26	C	303	CDL	OA5-CA3-CA4-OA6
19	Y	101	TGL	CA2-CA3-CA4-CA5
19	L	101	TGL	CA2-CA3-CA4-CA5
24	B	303	PSC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
20	N	608	PGV	O03-C19-C20-C21
19	Y	101	TGL	C22-C23-C24-C25
20	A	609	PGV	O03-C01-C02-C03
26	C	303	CDL	C31-C32-C33-C34
26	G	102	CDL	OA6-CA4-CA6-OA8
26	P	304	CDL	OA6-CA4-CA6-OA8
26	P	304	CDL	OB6-CB4-CB6-OB8
26	T	104	CDL	OA6-CA4-CA6-OA8
19	D	201	TGL	CB7-CB8-CB9-C10
19	D	201	TGL	C14-C29-C30-C31
20	N	607	PGV	C31-C32-C33-C34
26	P	304	CDL	C78-C79-C80-C81
26	C	303	CDL	CA4-CA3-OA5-PA1
26	P	304	CDL	C39-C40-C41-C42
26	P	304	CDL	C74-C75-C76-C77
26	P	304	CDL	C72-C73-C74-C75
19	D	201	TGL	CA4-CA5-CA6-CA7
19	L	101	TGL	C10-C11-C12-C13
27	C	306	PEK	C28-C29-C30-C31
26	G	102	CDL	C64-C65-C66-C67
20	N	608	PGV	C27-C28-C29-C30
20	A	608	PGV	C24-C25-C26-C27
24	O	303	PSC	O03-C19-C20-C21
20	P	303	PGV	C4-C5-C6-C7
20	P	301	PGV	C23-C24-C25-C26
26	P	304	CDL	C57-C58-C59-C60
27	T	102	PEK	O02-C1-O01-C02
27	T	101	PEK	C35-C36-C37-C38
19	D	201	TGL	CA9-C20-C21-C22
24	O	303	PSC	C02-C03-O11-P
20	P	301	PGV	C27-C28-C29-C30
20	A	608	PGV	C21-C22-C23-C24
21	A	611	EDO	O1-C1-C2-O2
21	B	305	EDO	O1-C1-C2-O2
27	T	102	PEK	C31-C32-C33-C34
27	T	103	PEK	C29-C30-C31-C32
19	L	101	TGL	CA5-CA6-CA7-CA8
20	N	608	PGV	C9-C10-C11-C12
26	G	102	CDL	C81-C82-C83-C84
19	L	101	TGL	OG1-CG1-CG2-OG2
20	A	609	PGV	C03-O11-P-O12
20	C	307	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
20	N	607	PGV	C04-O12-P-O11
26	C	303	CDL	CB2-OB2-PB2-OB5
26	G	102	CDL	CA3-OA5-PA1-OA2
26	T	104	CDL	CA3-OA5-PA1-OA2
27	C	306	PEK	C04-O12-P-O11
19	L	101	TGL	C29-C30-C31-C32
19	A	607	TGL	OG1-CG1-CG2-CG3
24	B	303	PSC	O03-C01-C02-C03
27	T	101	PEK	C32-C33-C34-C35
26	P	304	CDL	C40-C41-C42-C43
26	T	104	CDL	C75-C76-C77-C78
26	T	104	CDL	C77-C78-C79-C80
19	A	607	TGL	C14-C29-C30-C31
20	C	302	PGV	C05-C04-O12-P
20	A	608	PGV	C11-C12-C13-C14
14	A	601	HEA	CAD-CBD-CGD-O1D
26	P	304	CDL	C12-C13-C14-C15
20	C	307	PGV	O05-C05-C06-O06
19	D	201	TGL	CB9-C10-C11-C12
19	D	201	TGL	C19-C33-C34-C35
26	G	102	CDL	C54-C55-C56-C57
26	G	102	CDL	C79-C80-C81-C82
23	J	101	CHD	C22-C23-C24-O25
27	C	306	PEK	C1-C2-C3-C4
23	C	304	CHD	C22-C23-C24-O25
19	Y	101	TGL	CA7-CA8-CA9-C20
26	P	304	CDL	C43-C44-C45-C46
26	P	304	CDL	OB9-CB7-OB8-CB6
19	O	302	TGL	C22-C23-C24-C25
20	P	303	PGV	C15-C16-C17-C18
27	T	101	PEK	C3-C4-C5-C6
20	A	608	PGV	C29-C30-C31-C32
26	C	303	CDL	C63-C64-C65-C66
26	G	102	CDL	OB6-CB4-CB6-OB8
26	P	304	CDL	C71-CB7-OB8-CB6
19	O	302	TGL	C15-C16-C17-C18
20	P	303	PGV	C05-C04-O12-P
23	B	302	CHD	C22-C23-C24-O26
23	G	104	CHD	C22-C23-C24-O26
19	A	607	TGL	CC7-CC8-CC9-C15
27	T	102	PEK	C27-C28-C29-C30
20	A	609	PGV	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	T	102	PEK	C24-C25-C26-C27
24	B	303	PSC	C20-C21-C22-C23
20	C	307	PGV	C11-C10-C9-C8
20	P	303	PGV	C22-C23-C24-C25
23	B	302	CHD	C22-C23-C24-O25
23	J	101	CHD	C16-C17-C20-C22
27	T	101	PEK	O03-C01-C02-C03
14	N	601	HEA	CAD-CBD-CGD-O2D
23	G	104	CHD	C22-C23-C24-O25
27	T	102	PEK	C33-C34-C35-C36
23	C	304	CHD	C22-C23-C24-O26
26	T	104	CDL	C31-C32-C33-C34
27	C	306	PEK	C31-C32-C33-C34
24	B	303	PSC	C9-C10-C11-C12
27	G	101	PEK	C6-C7-C8-C9
27	T	103	PEK	C11-C12-C13-C14
26	T	104	CDL	C44-C45-C46-C47
19	A	607	TGL	C17-C18-C19-C33
19	D	201	TGL	CC7-CC8-CC9-C15
27	T	101	PEK	C26-C27-C28-C29
20	N	607	PGV	C11-C12-C13-C14
20	A	609	PGV	C3-C4-C5-C6
14	N	601	HEA	CAD-CBD-CGD-O1D
27	T	102	PEK	C34-C35-C36-C37
27	T	101	PEK	C30-C31-C32-C33
14	N	602	HEA	CAD-CBD-CGD-O1D
19	L	101	TGL	C14-C29-C30-C31
19	D	201	TGL	CB6-CB7-CB8-CB9
19	Q	201	TGL	CB5-CB6-CB7-CB8
19	L	101	TGL	OG1-CA1-CA2-CA3
26	P	304	CDL	C75-C76-C77-C78
23	J	101	CHD	C22-C23-C24-O26
20	C	307	PGV	C15-C16-C17-C18
20	N	608	PGV	C13-C14-C15-C16
14	N	602	HEA	CAD-CBD-CGD-O2D
26	T	104	CDL	C15-C16-C17-C18
20	N	607	PGV	C11-C10-C9-C8
19	D	201	TGL	C21-C20-CA9-CA8
19	L	101	TGL	CC5-CC6-CC7-CC8
26	T	104	CDL	C52-C51-CB5-OB6
19	L	101	TGL	CG1-CG2-CG3-OG3
19	Y	101	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
27	T	103	PEK	C4-C5-C6-C7
26	T	104	CDL	C18-C19-C20-C21
27	T	103	PEK	C14-C15-C16-C17
26	G	102	CDL	OA5-CA3-CA4-OA6
26	C	303	CDL	C39-C40-C41-C42
19	A	607	TGL	CA7-CA8-CA9-C20
27	T	103	PEK	C31-C32-C33-C34
19	Q	201	TGL	C18-C19-C33-C34
14	A	602	HEA	CAD-CBD-CGD-O2D
27	T	101	PEK	O03-C01-C02-O01
14	A	602	HEA	CAD-CBD-CGD-O1D
27	T	101	PEK	O04-C21-O03-C01
26	C	303	CDL	C22-C23-C24-C25
19	O	302	TGL	OG3-CC1-CC2-CC3
20	A	609	PGV	O01-C1-C2-C3
20	N	607	PGV	O03-C19-C20-C21
20	P	301	PGV	O01-C1-C2-C3
23	C	305	CHD	C13-C17-C20-C22
27	C	306	PEK	C13-C14-C15-C16
26	T	104	CDL	C21-C22-C23-C24
14	A	601	HEA	CAD-CBD-CGD-O2D
27	T	102	PEK	O01-C1-C2-C3
29	Z	101	DMU	O5-C4-C57-O61
20	N	607	PGV	C24-C25-C26-C27
23	W	101	CHD	C22-C23-C24-O26
24	B	303	PSC	C01-C02-O01-C1
26	P	304	CDL	CB5-C51-C52-C53
19	O	302	TGL	C24-C25-C26-C27
14	N	602	HEA	C26-C15-C16-C17
19	L	101	TGL	CA3-CA4-CA5-CA6
24	B	303	PSC	O03-C19-C20-C21
20	N	608	PGV	C22-C23-C24-C25
19	A	607	TGL	OG3-CC1-CC2-CC3
19	Q	201	TGL	OG1-CA1-CA2-CA3
26	G	102	CDL	C12-C11-CA5-OA6
24	O	303	PSC	C7-C8-C9-C10
19	L	101	TGL	CC4-CC5-CC6-CC7
19	Q	201	TGL	CB9-C10-C11-C12
19	L	101	TGL	C24-C25-C26-C27
26	T	104	CDL	OB6-CB4-CB6-OB8
19	L	101	TGL	C25-C26-C27-C28
24	B	303	PSC	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OG1-CA1-CA2-CA3
26	T	104	CDL	C72-C71-CB7-OB8
27	T	101	PEK	O01-C1-C2-C3
20	C	302	PGV	C27-C28-C29-C30
20	P	303	PGV	C9-C10-C11-C12
24	O	303	PSC	C12-C13-C14-C15
27	T	103	PEK	C3-C4-C5-C6
26	C	303	CDL	CB7-C71-C72-C73
19	A	607	TGL	OC1-CC1-CC2-CC3
23	W	101	CHD	C22-C23-C24-O25
19	Q	201	TGL	OA1-CA1-CA2-CA3
26	P	304	CDL	OA5-CA3-CA4-OA6
20	A	609	PGV	C21-C22-C23-C24
20	P	301	PGV	C11-C12-C13-C14
26	T	104	CDL	C74-C75-C76-C77
19	O	302	TGL	OC1-CC1-CC2-CC3
20	P	301	PGV	O02-C1-C2-C3
24	B	303	PSC	O04-C19-C20-C21
26	G	102	CDL	C12-C11-CA5-OA7
19	Q	201	TGL	OG1-CG1-CG2-CG3
20	N	607	PGV	O04-C19-C20-C21
27	T	101	PEK	C22-C21-O03-C01
20	A	609	PGV	C05-C04-O12-P
20	C	307	PGV	C04-O12-P-O13
26	G	102	CDL	CB2-OB2-PB2-OB3
26	T	104	CDL	CA3-OA5-PA1-OA3
26	T	104	CDL	C73-C74-C75-C76
27	T	102	PEK	O02-C1-C2-C3
26	T	104	CDL	C60-C61-C62-C63
27	G	103	PEK	C15-C16-C17-C18
19	D	201	TGL	OA1-CA1-CA2-CA3
26	T	104	CDL	C72-C71-CB7-OB9
20	P	303	PGV	C30-C31-C32-C33
23	P	306	CHD	C22-C23-C24-O26
26	P	304	CDL	C17-C18-C19-C20
14	N	602	HEA	C14-C15-C16-C17
24	B	303	PSC	C05-C04-O12-P
27	G	101	PEK	C05-C04-O12-P
20	A	609	PGV	O02-C1-C2-C3
26	C	303	CDL	C43-C44-C45-C46
27	T	101	PEK	O02-C1-C2-C3
27	C	306	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	C	306	PEK	C24-C25-C26-C27
26	T	104	CDL	C12-C11-CA5-OA6
24	B	303	PSC	C22-C23-C24-C25
27	T	102	PEK	O03-C21-C22-C23
20	C	307	PGV	C7-C8-C9-C10
26	C	303	CDL	C24-C25-C26-C27
14	A	601	HEA	CAA-CBA-CGA-O1A
26	C	303	CDL	C52-C51-CB5-OB6
19	Y	101	TGL	OG2-CB1-CB2-CB3
27	G	103	PEK	O03-C21-C22-C23
14	N	601	HEA	CAA-CBA-CGA-O1A
14	N	602	HEA	CAA-CBA-CGA-O1A
19	Y	101	TGL	C25-C26-C27-C28
27	T	102	PEK	C17-C18-C19-C20
26	T	104	CDL	C12-C11-CA5-OA7
27	T	102	PEK	O04-C21-C22-C23
26	G	102	CDL	C76-C77-C78-C79
14	N	601	HEA	CAA-CBA-CGA-O2A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	P	305	CHD	C1-C10-C2-C3-C4-C5

48 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	302	CHD	1	0
19	Q	201	TGL	5	0
21	F	102	EDO	1	0
27	T	102	PEK	8	0
14	A	602	HEA	8	0
20	A	608	PGV	1	0
23	G	104	CHD	1	0
26	C	303	CDL	6	0
20	N	607	PGV	5	0
14	A	601	HEA	5	0
21	C	311	EDO	2	0
18	N	606	CMO	2	0
26	T	104	CDL	21	0
19	L	101	TGL	9	0
23	W	101	CHD	9	0

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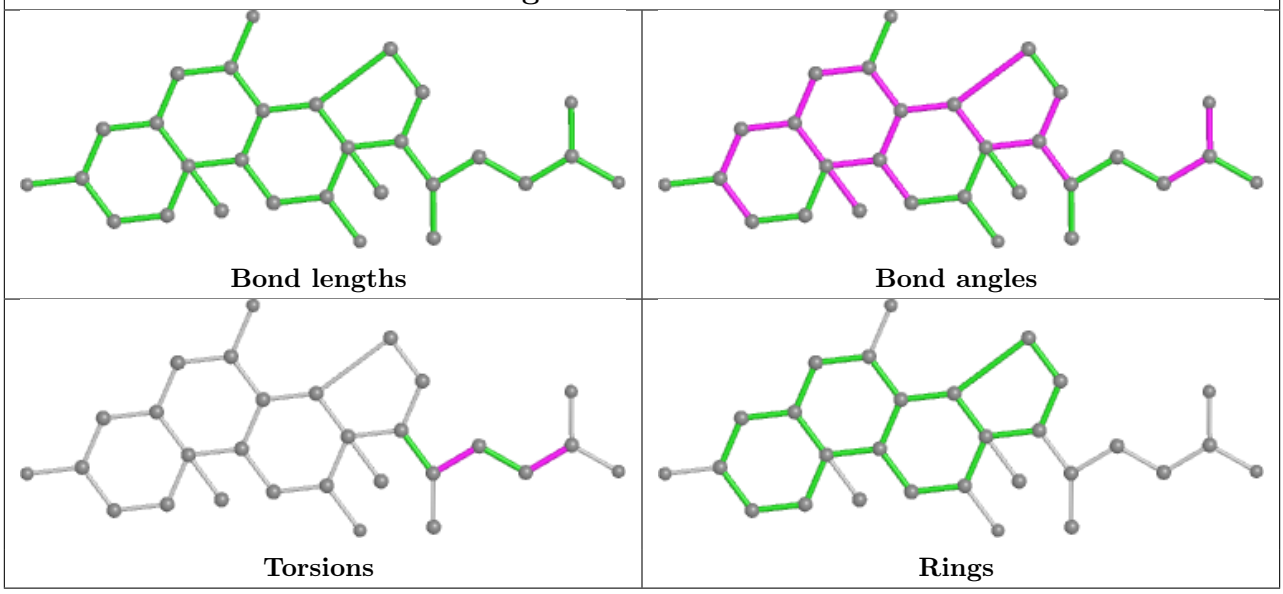
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	305	CHD	1	0
24	B	303	PSC	4	0
21	A	613	EDO	7	0
21	N	610	EDO	3	0
21	T	105	EDO	4	0
18	A	606	CMO	1	0
19	D	201	TGL	5	0
20	P	303	PGV	1	0
23	P	306	CHD	3	0
19	A	607	TGL	3	0
29	Z	101	DMU	2	0
21	A	612	EDO	12	0
20	P	301	PGV	2	0
19	Y	101	TGL	3	0
21	H	101	EDO	2	0
27	T	101	PEK	3	0
26	P	304	CDL	7	0
14	N	602	HEA	5	0
24	O	303	PSC	5	0
26	G	102	CDL	6	0
21	B	304	EDO	1	0
20	N	608	PGV	1	0
23	C	304	CHD	4	0
20	A	609	PGV	4	0
23	P	305	CHD	3	0
27	C	306	PEK	3	0
21	F	103	EDO	1	0
27	G	103	PEK	3	0
14	N	601	HEA	6	0
19	O	302	TGL	7	0
20	C	307	PGV	4	0
27	T	103	PEK	2	0
27	G	101	PEK	3	0

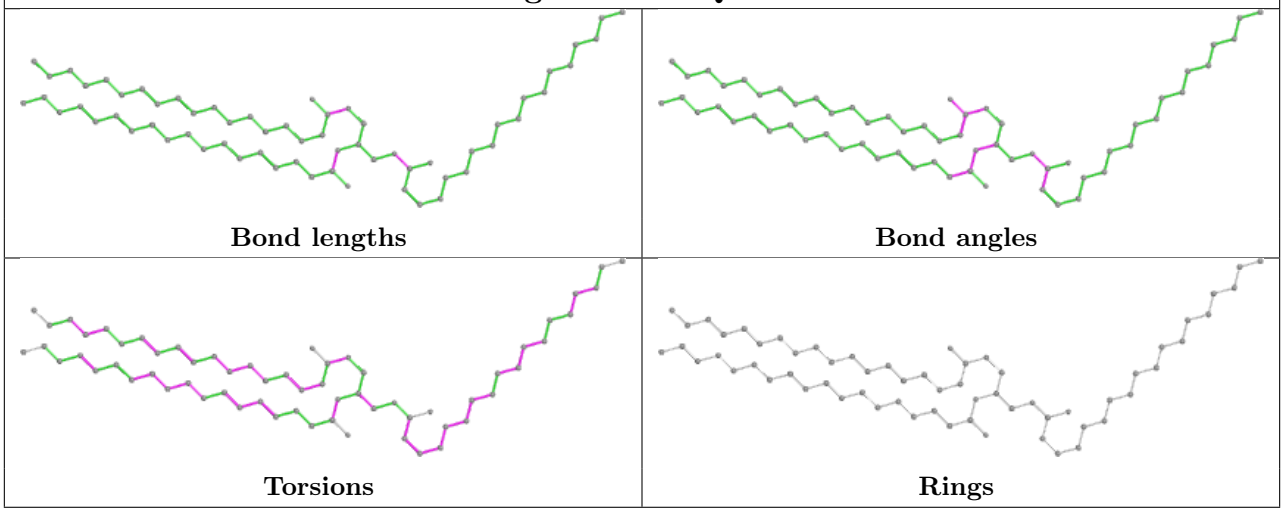
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

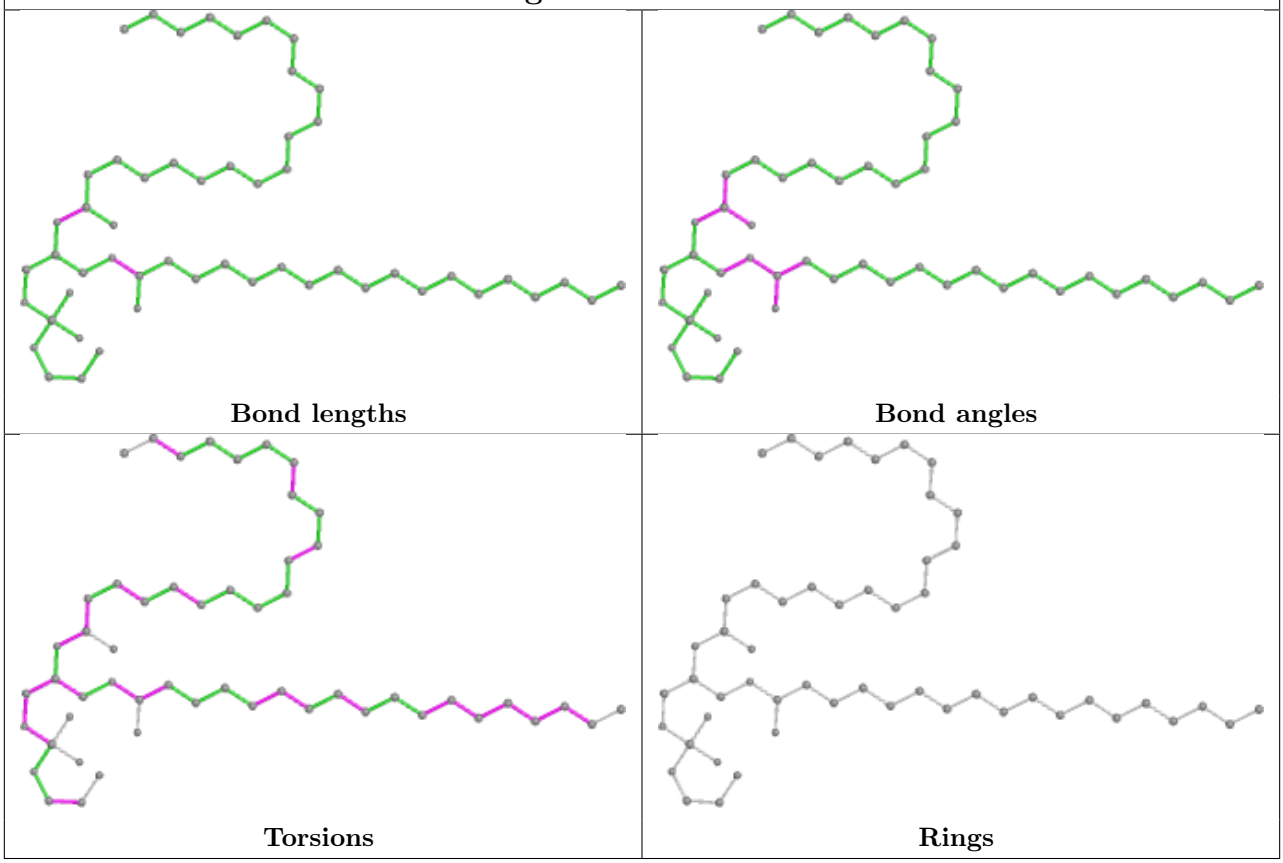
Ligand CHD B 302



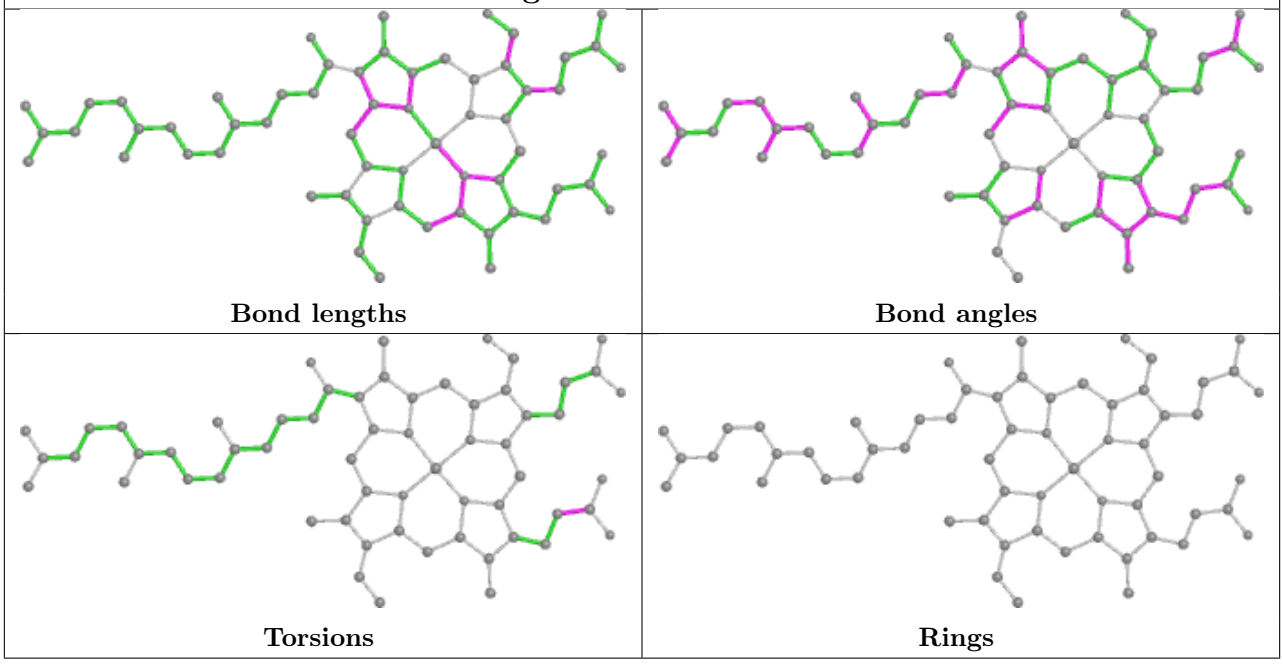
Ligand TGL Q 201



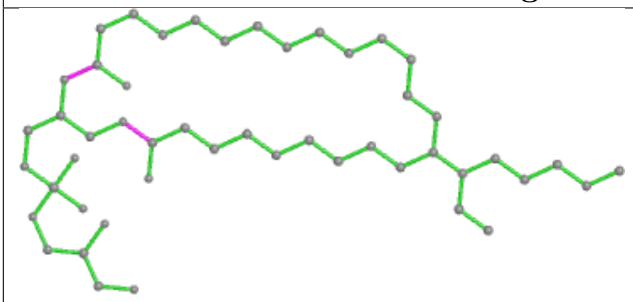
Ligand PEK T 102



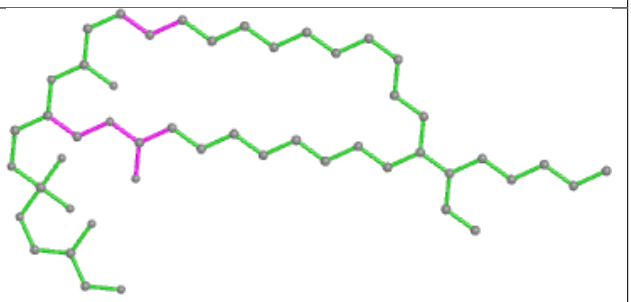
Ligand HEA A 602



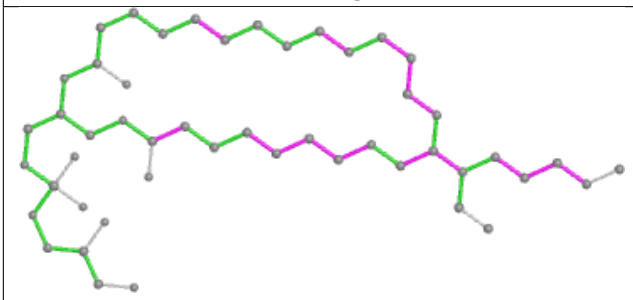
Ligand PGV A 608



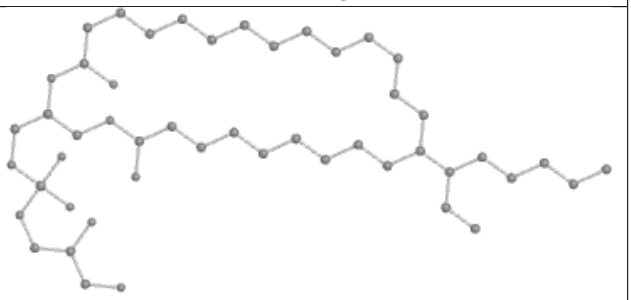
Bond lengths



Bond angles

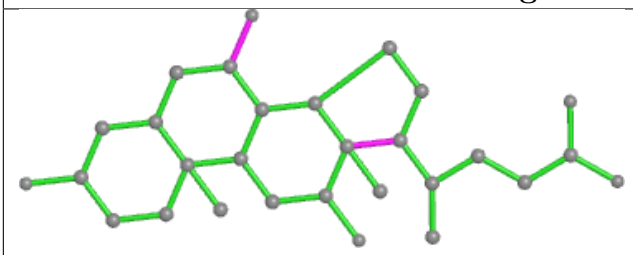


Torsions

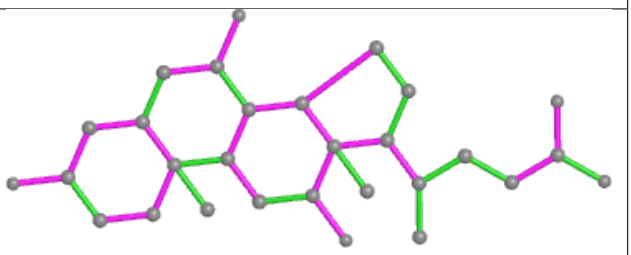


Rings

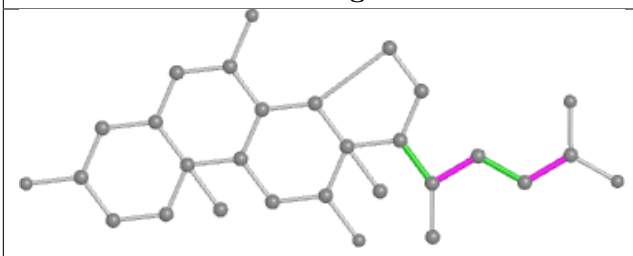
Ligand CHD G 104



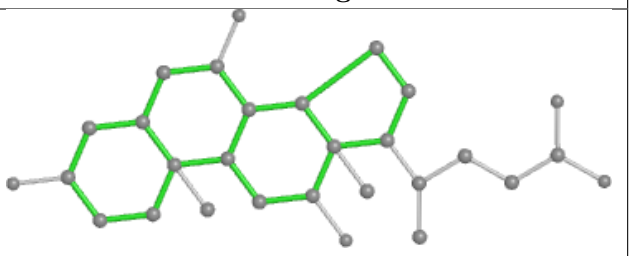
Bond lengths



Bond angles

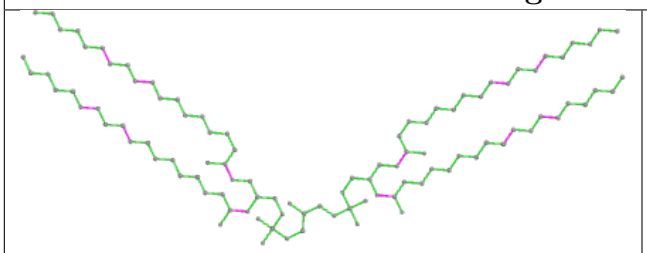


Torsions

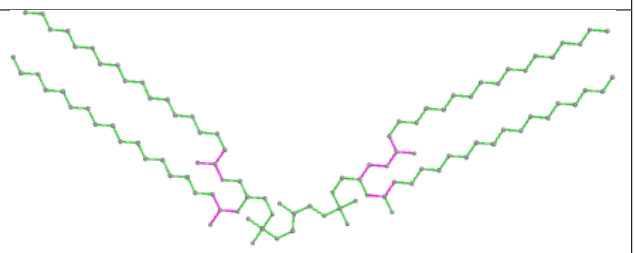


Rings

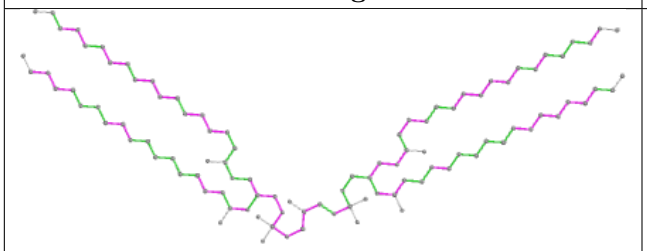
Ligand CDL C 303



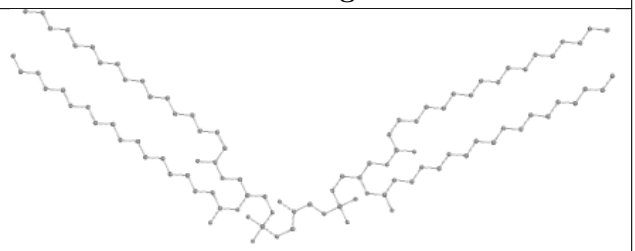
Bond lengths



Bond angles

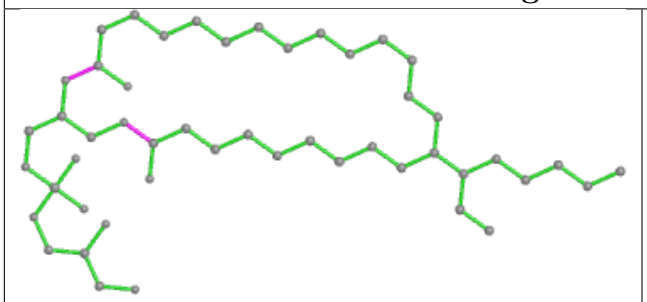


Torsions



Rings

Ligand PGV N 607



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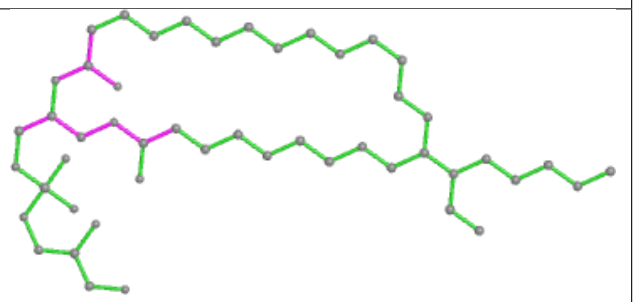
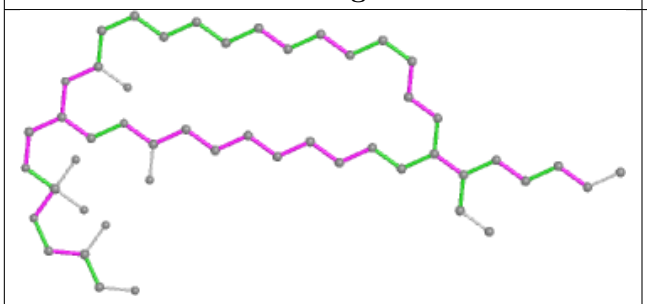


Bond angles



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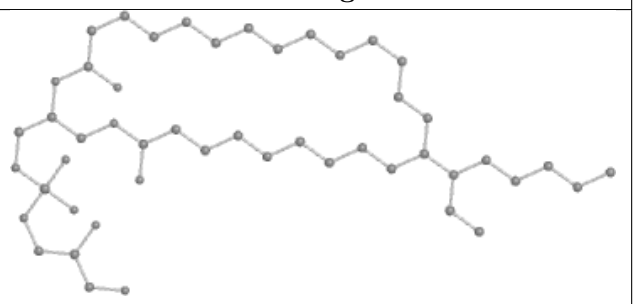
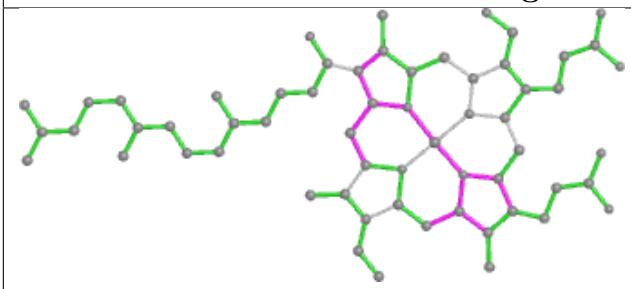


Rings

Ligand HEA A 601



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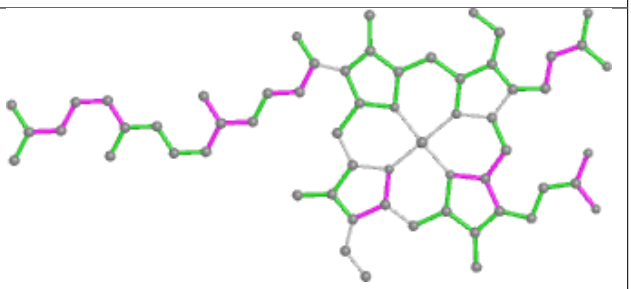
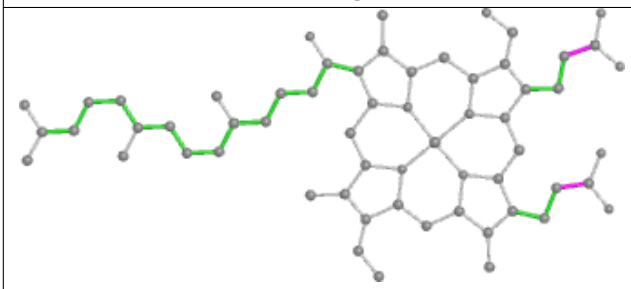


Bond angles



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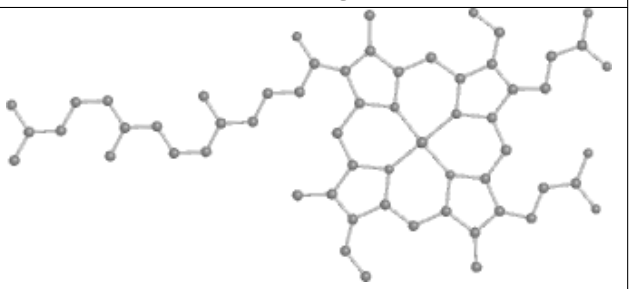
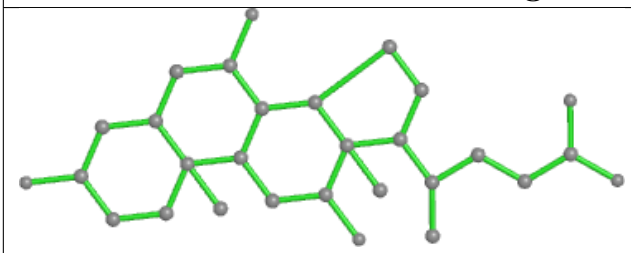
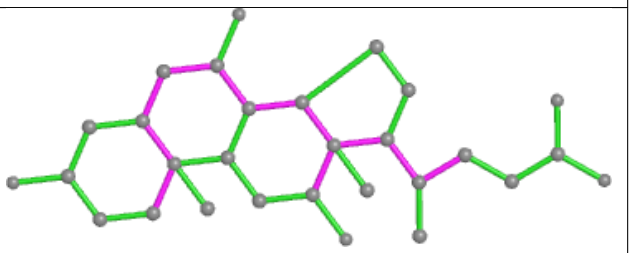


Rings

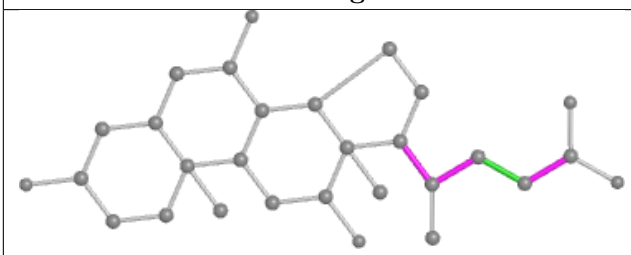
Ligand CHD J 101



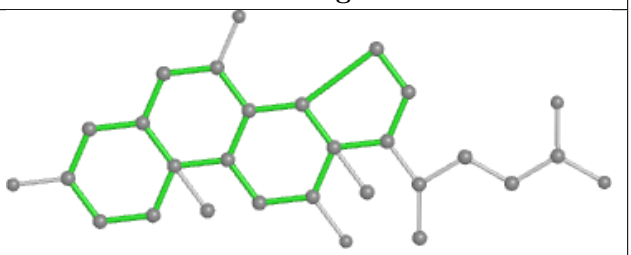
Bond lengths



Bond angles

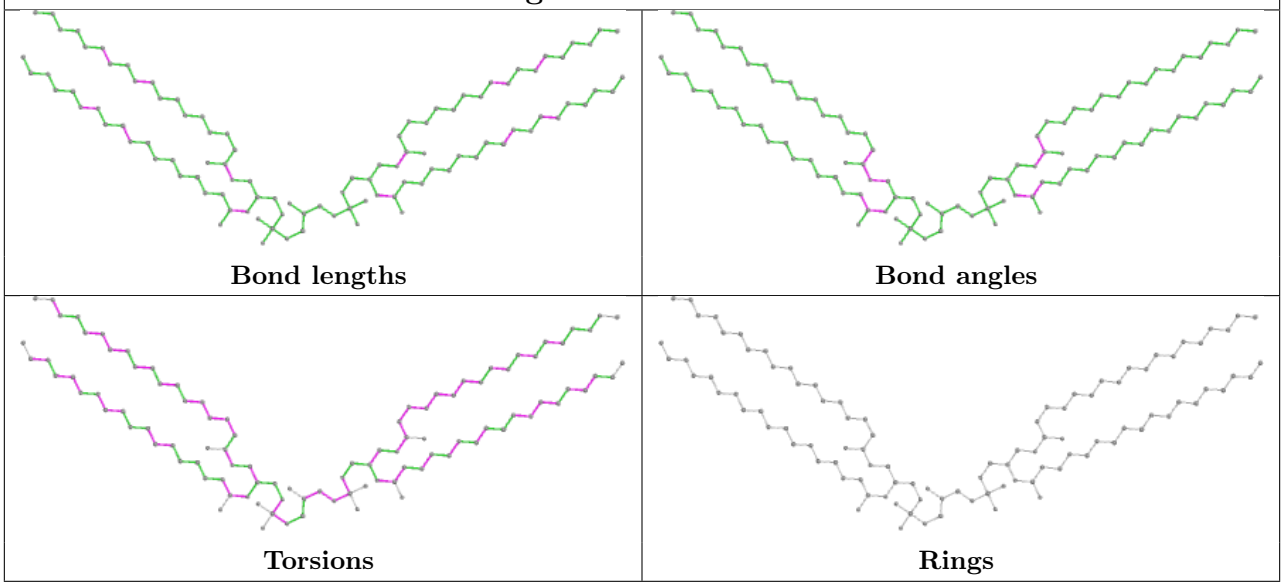


Torsions

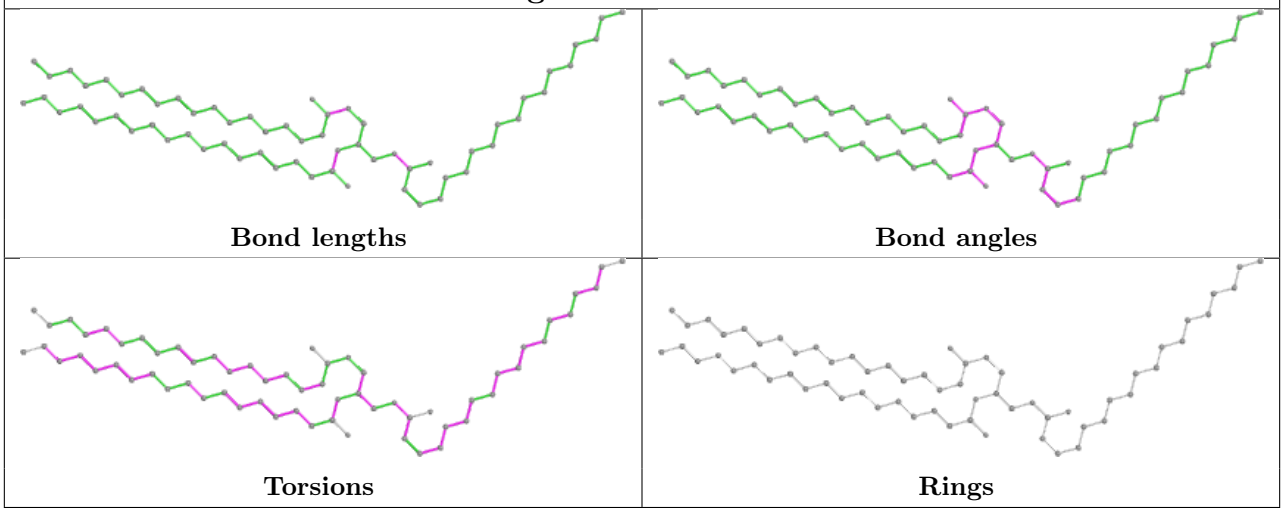


Rings

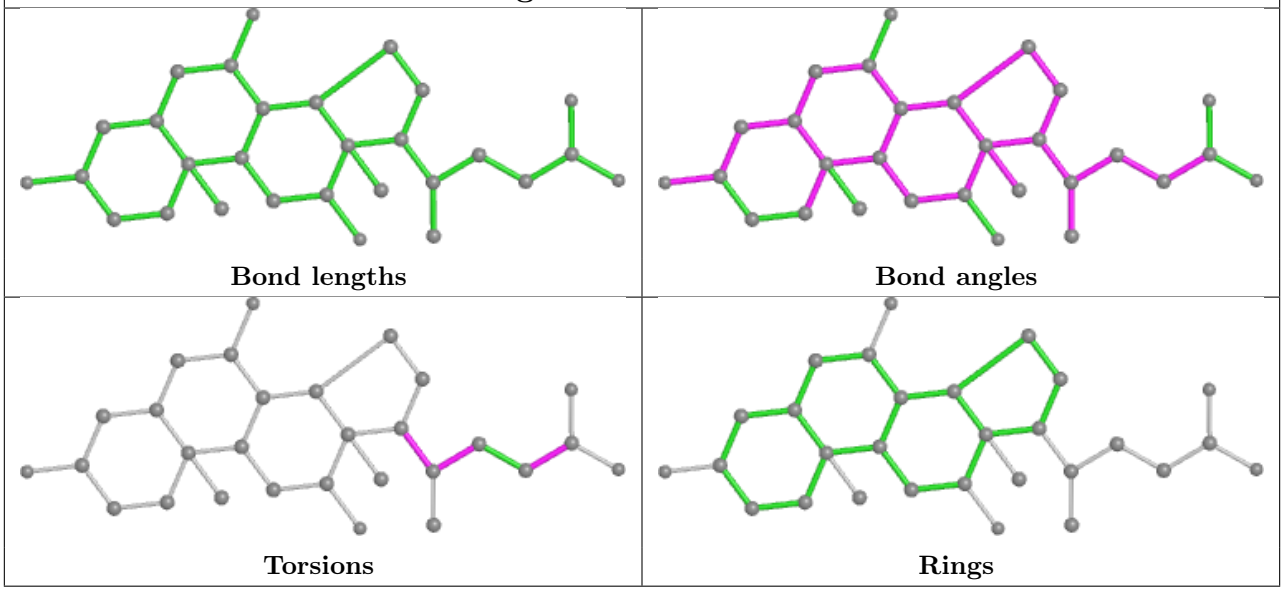
Ligand CDL T 104



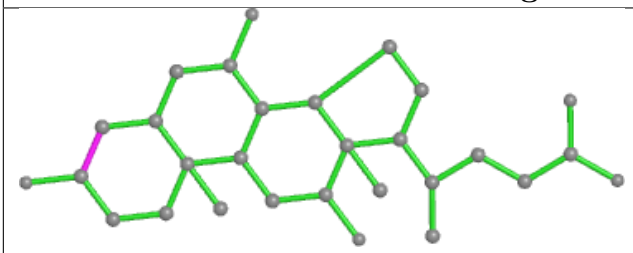
Ligand TGL L 101



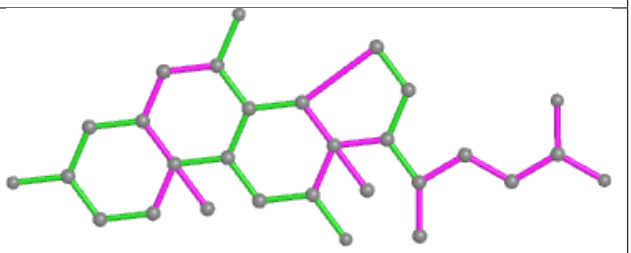
Ligand CHD W 101



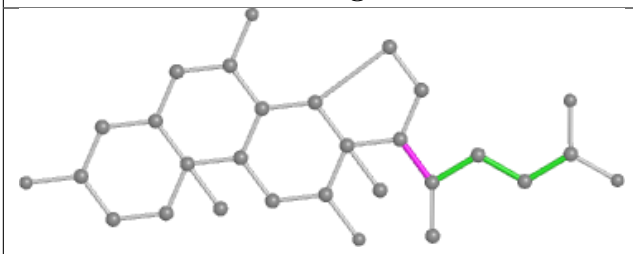
Ligand CHD C 305



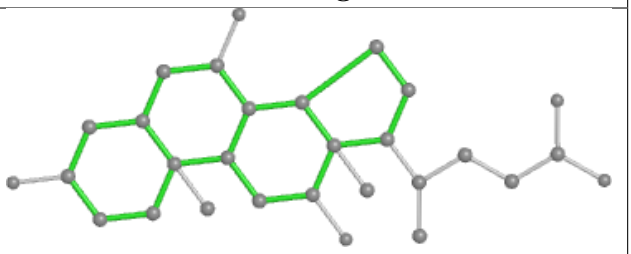
Bond lengths



Bond angles

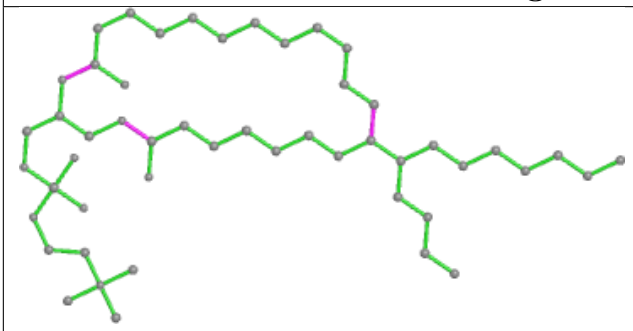


Torsions



Rings

Ligand PSC B 303



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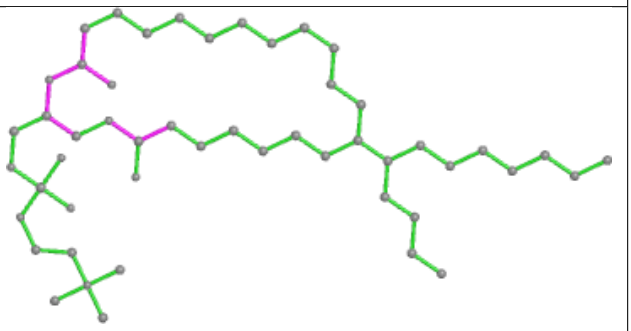
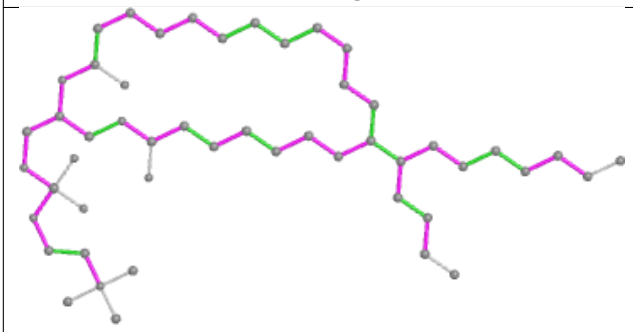


Bond angles



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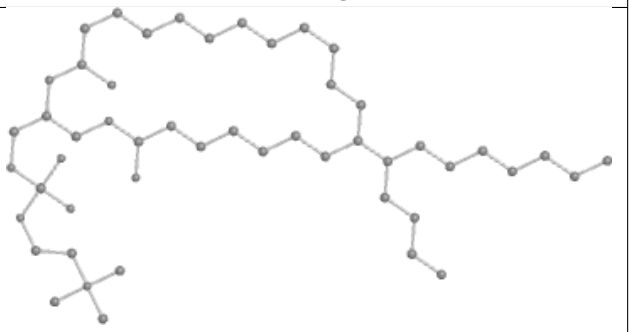
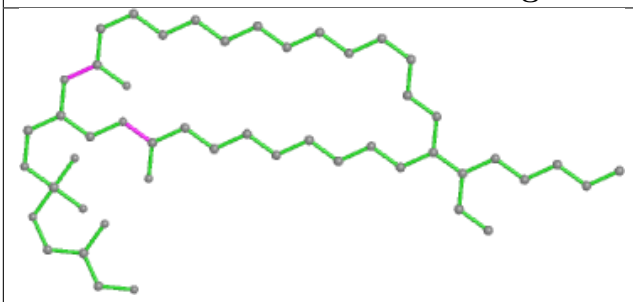


Rings

Ligand PGV C 302



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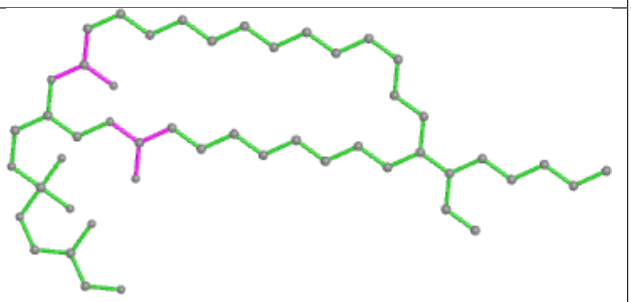
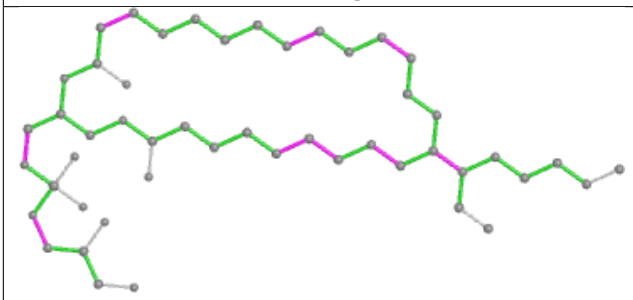
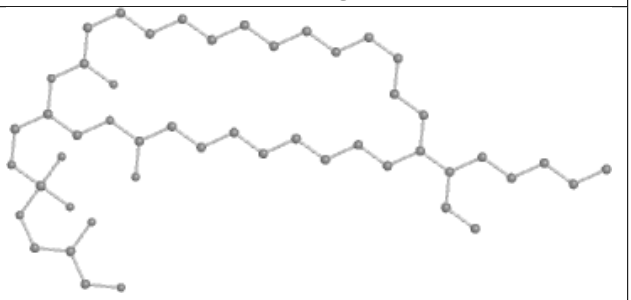


Bond angles

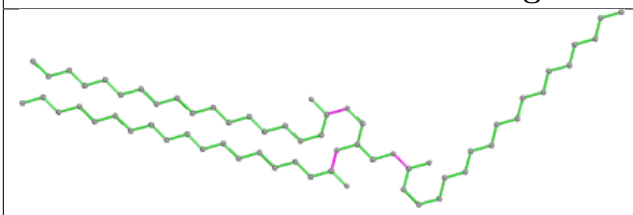


Torsions



Rings

Ligand TGL D 201



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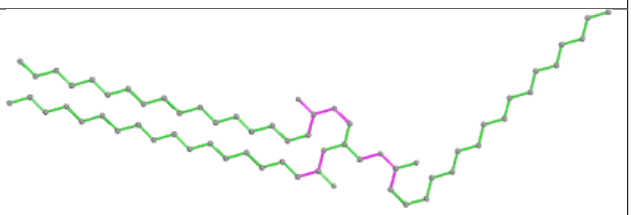
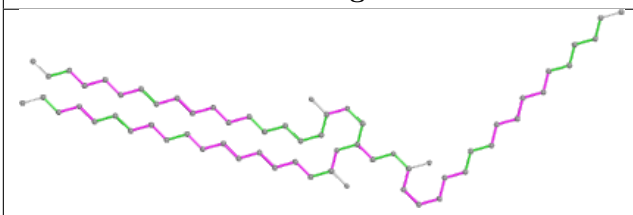
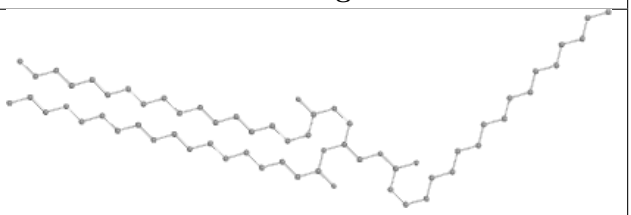


Bond angles

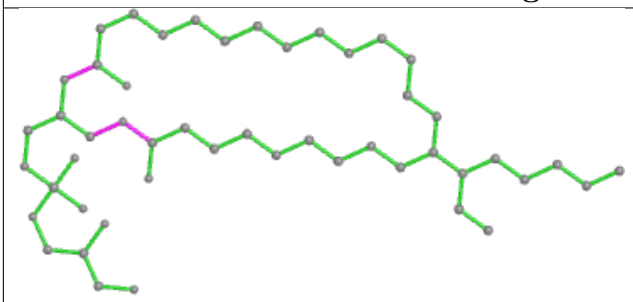


Torsions



Rings

Ligand PGV P 303



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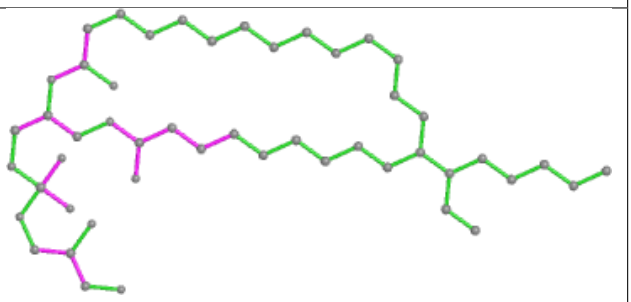
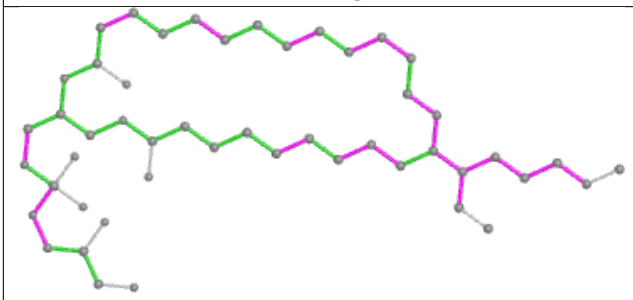
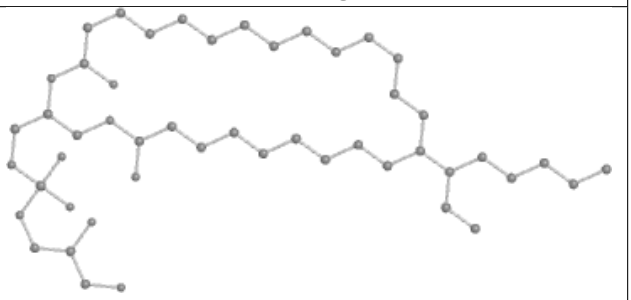


Bond angles

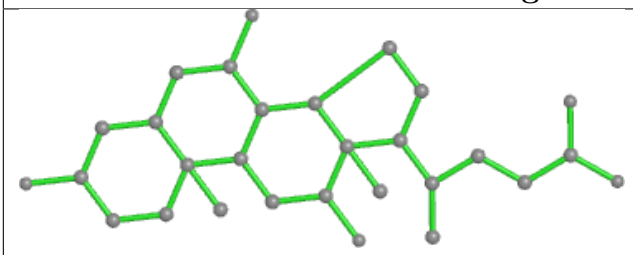


Torsions

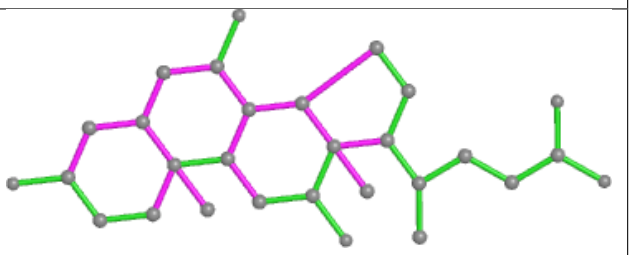


Rings

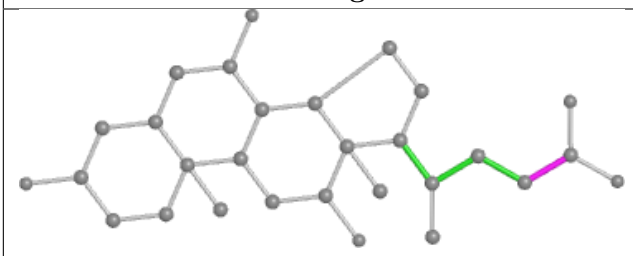
Ligand CHD P 306



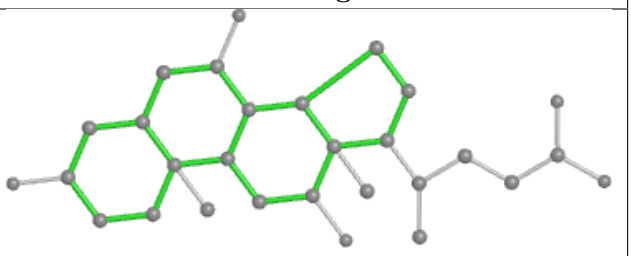
Bond lengths



Bond angles

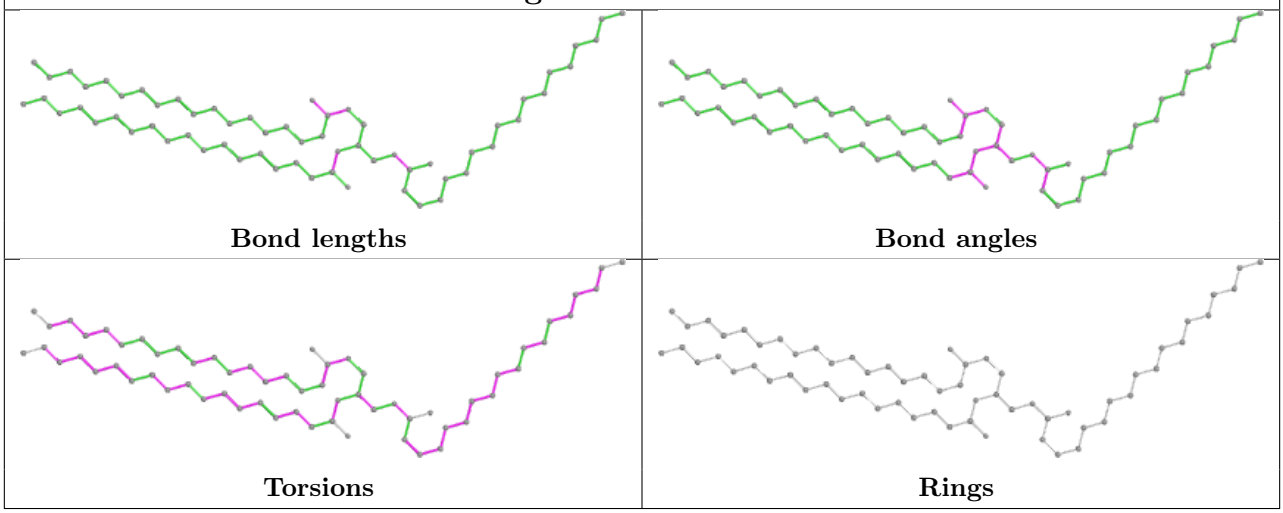


Torsions

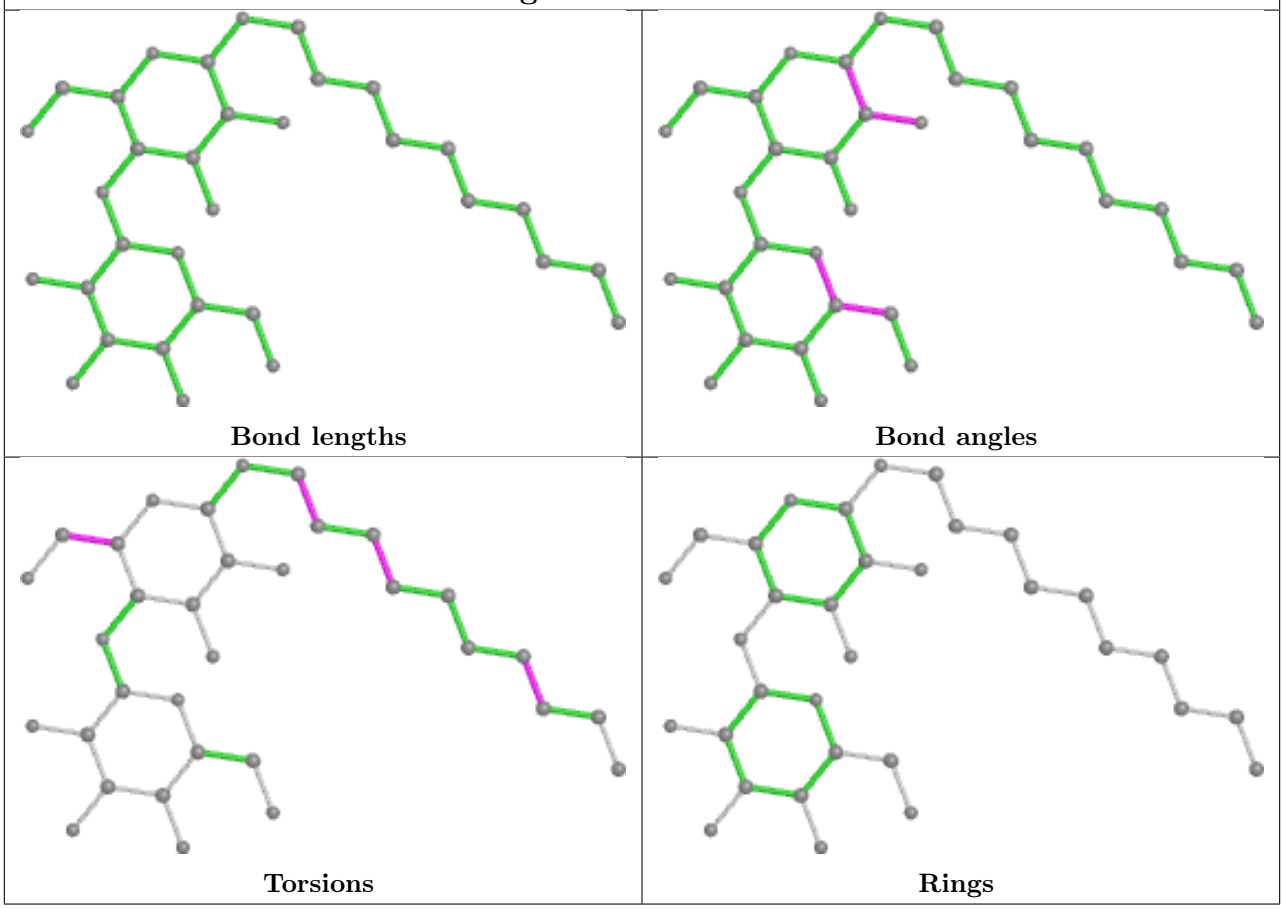


Rings

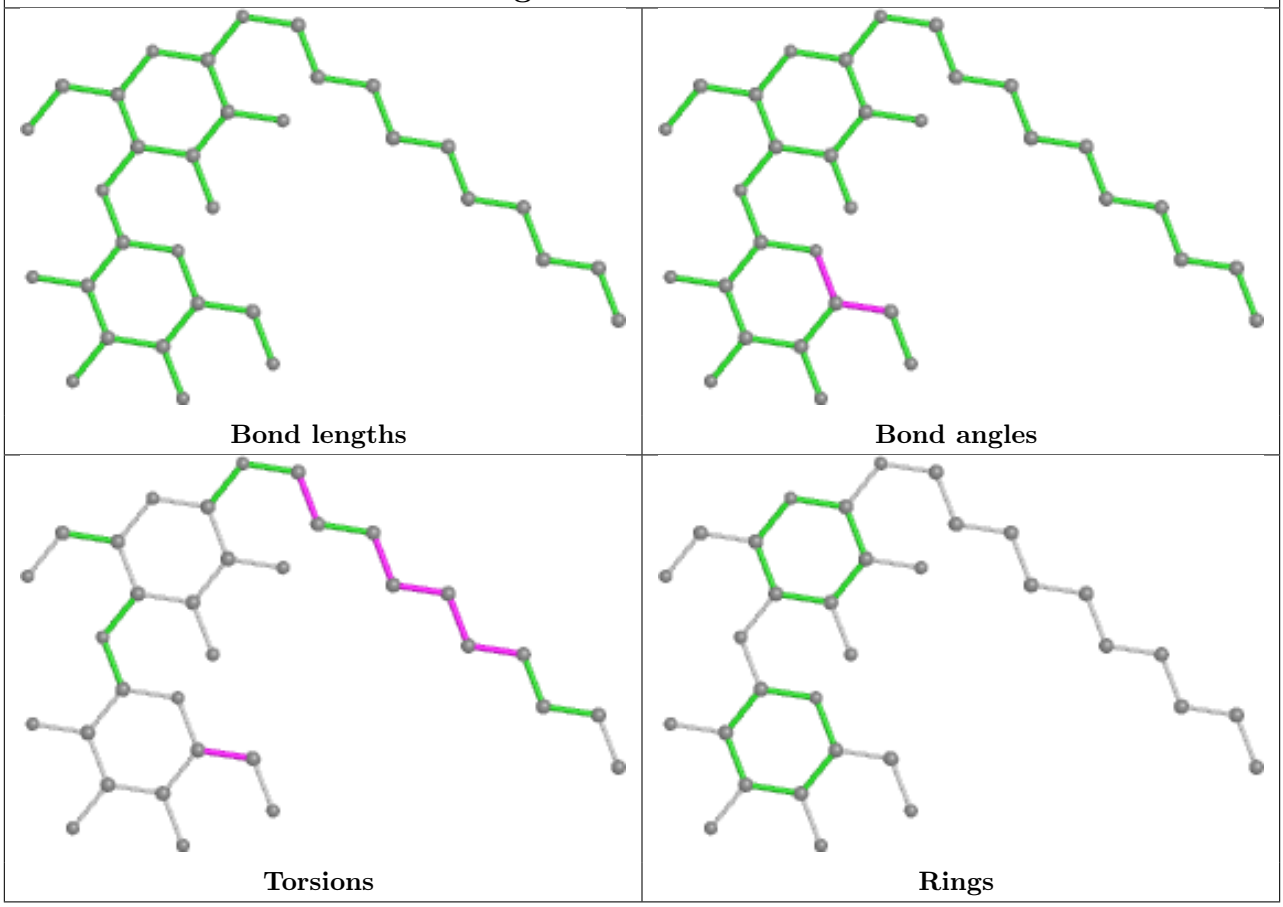
Ligand TGL A 607



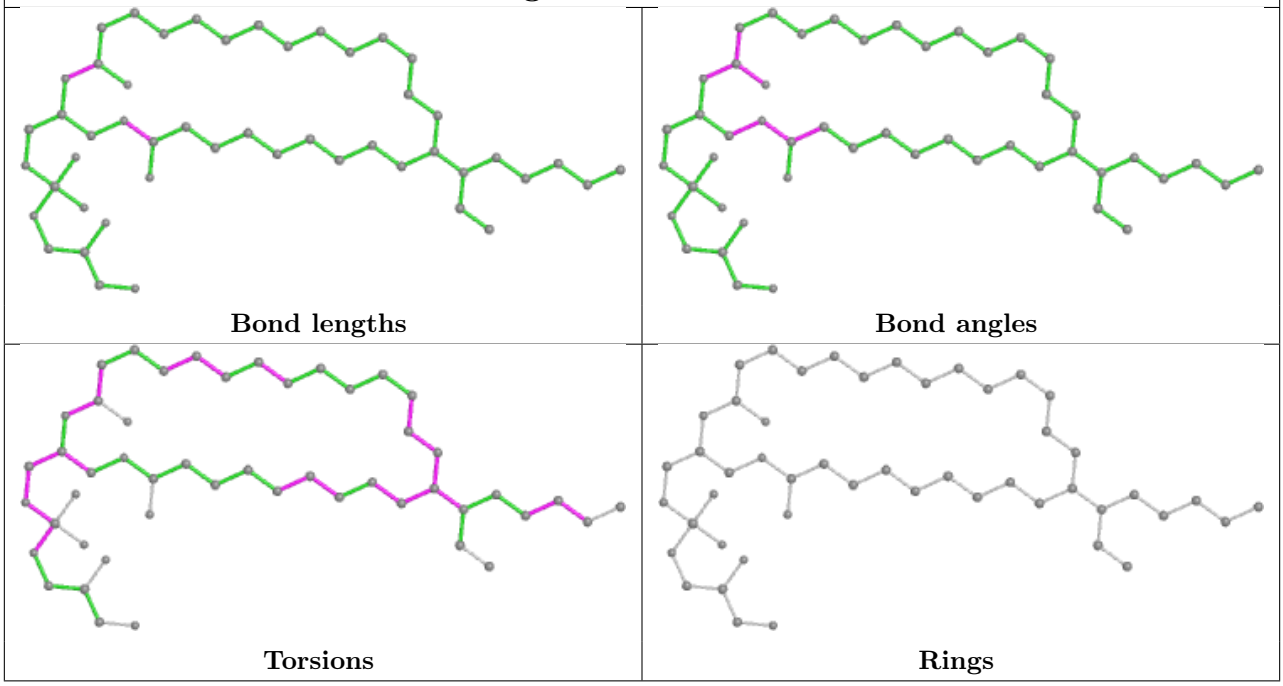
Ligand DMU Z 101



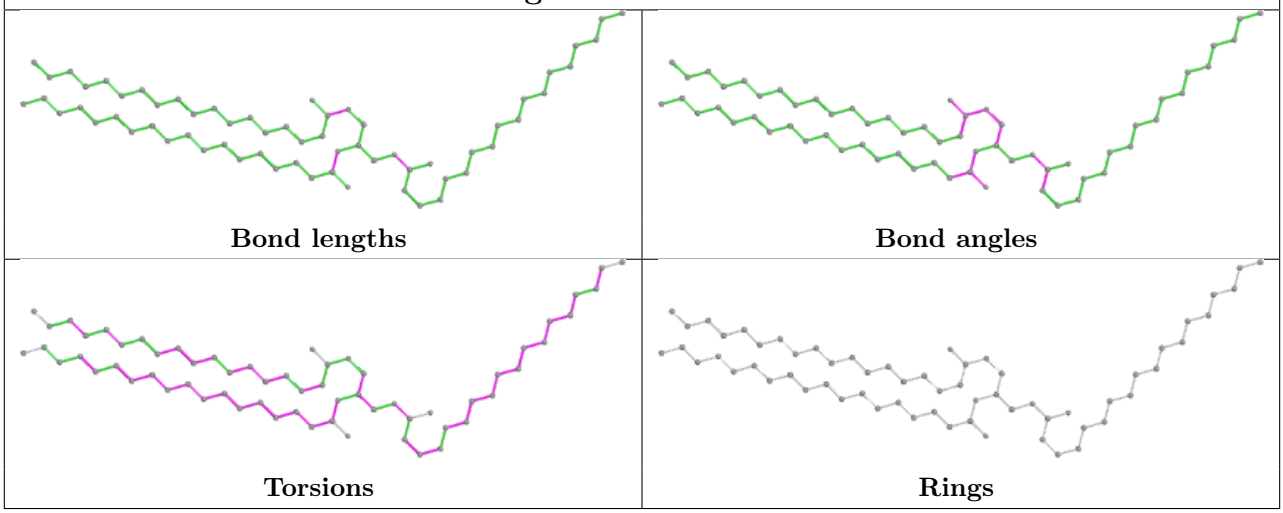
Ligand DMU M 101



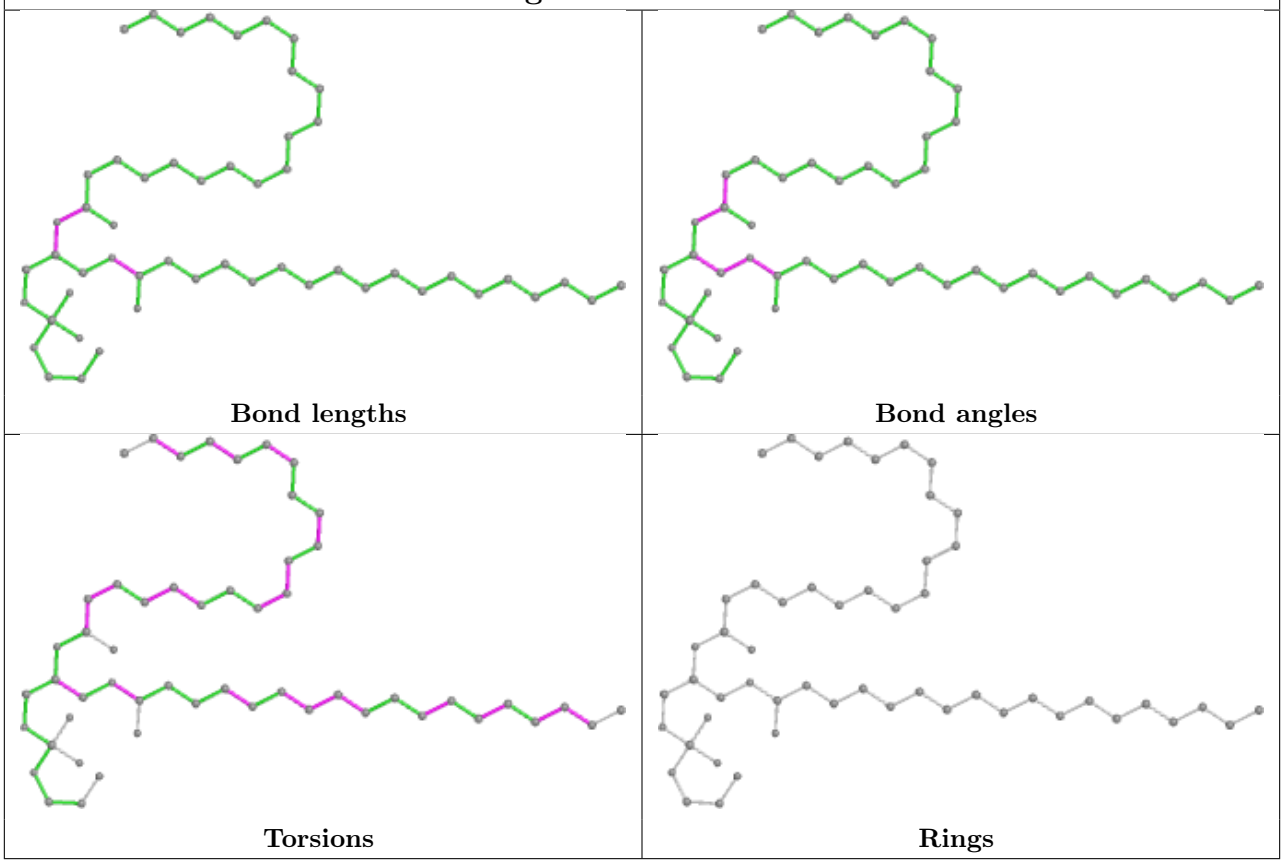
Ligand PGV P 301



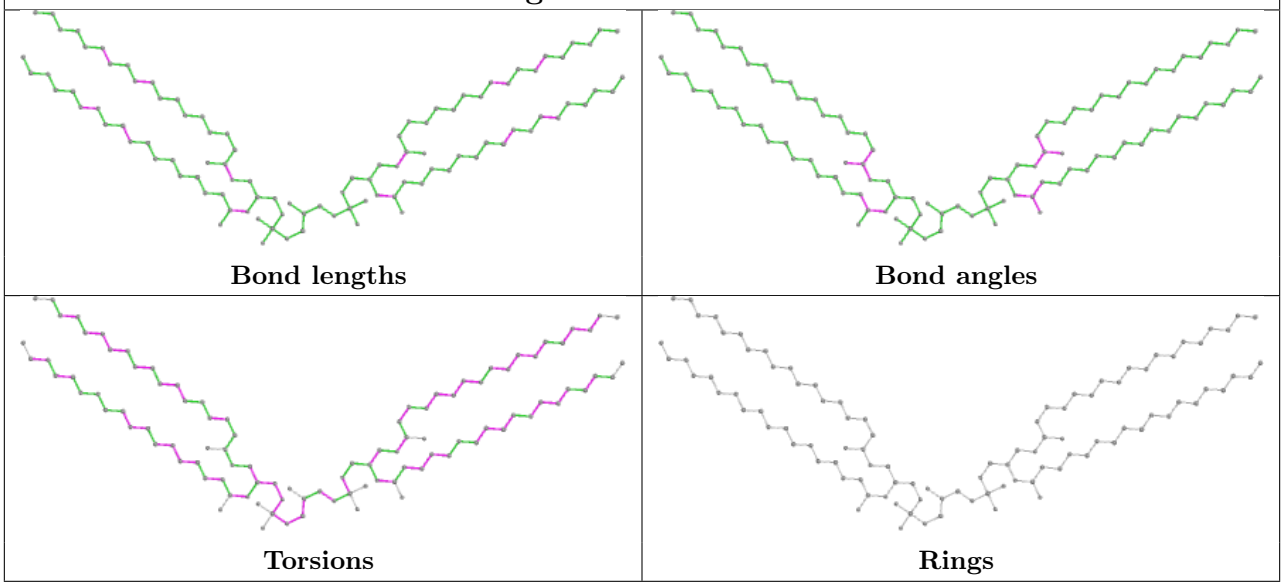
Ligand TGL Y 101



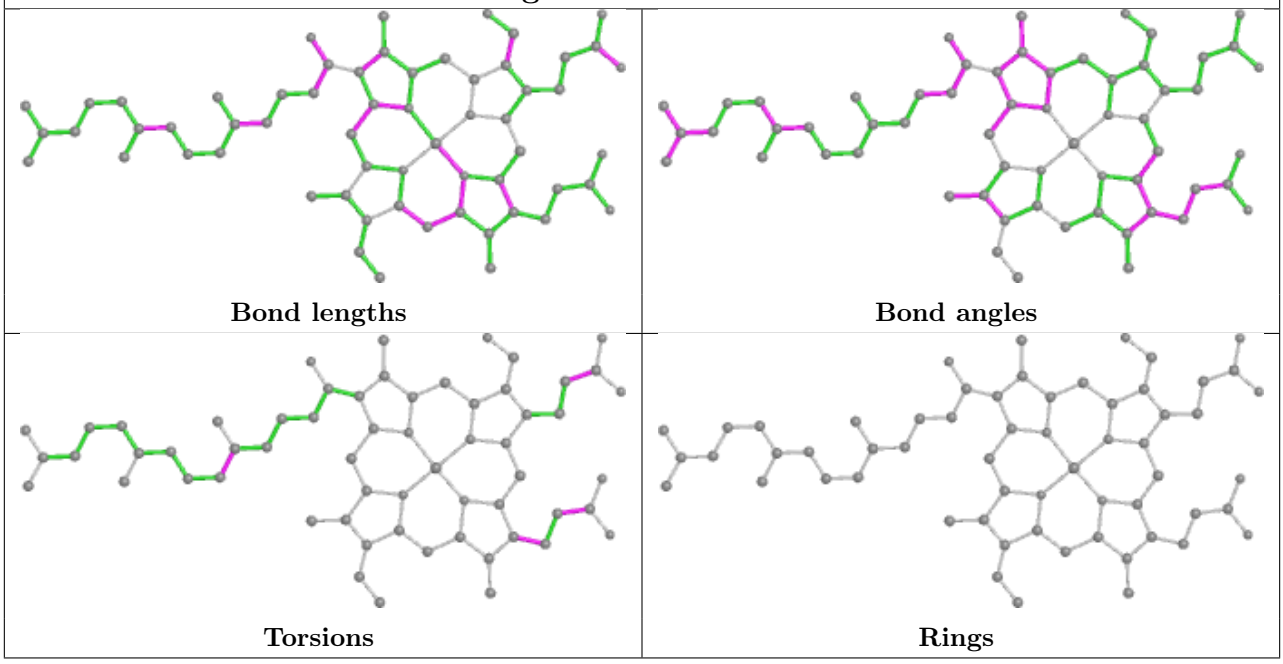
Ligand PEK T 101



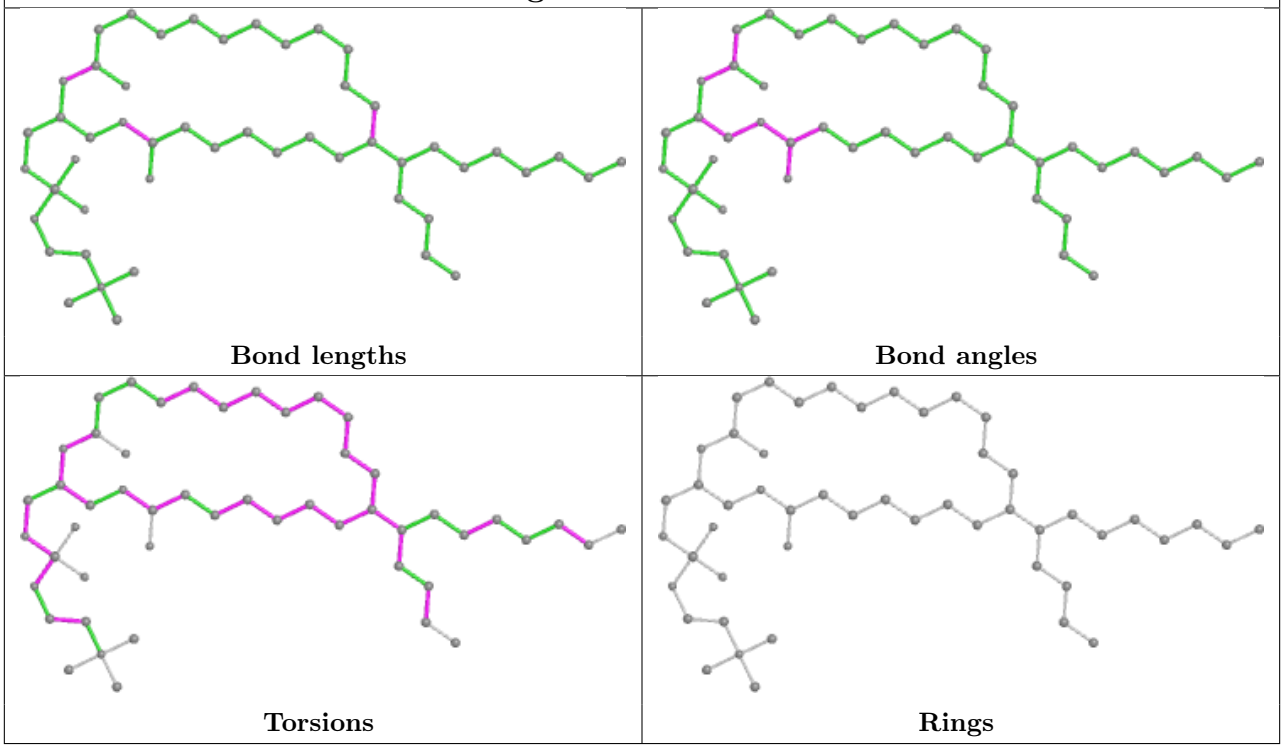
Ligand CDL P 304



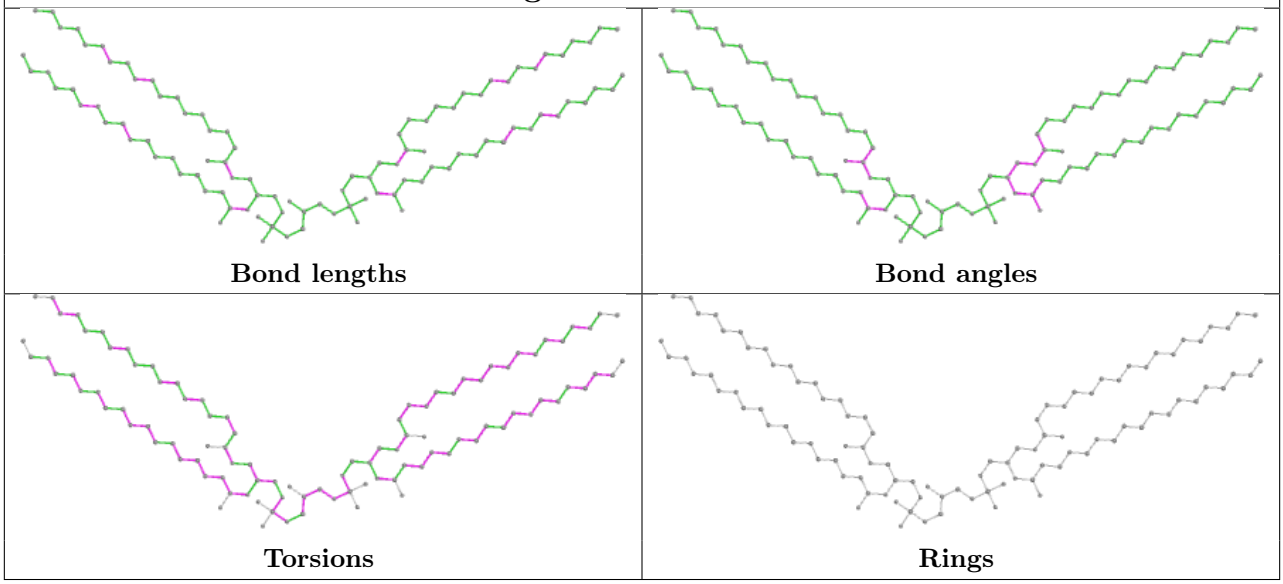
Ligand HEA N 602



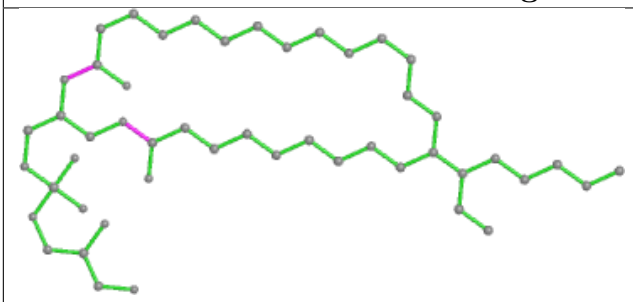
Ligand PSC O 303



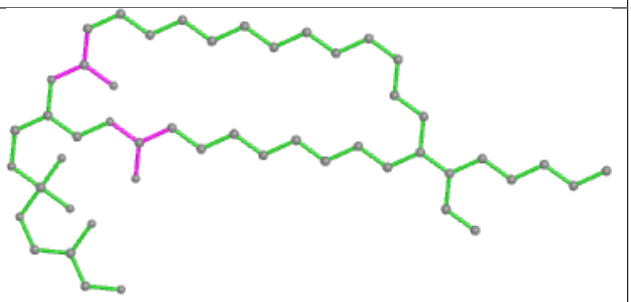
Ligand CDL G 102



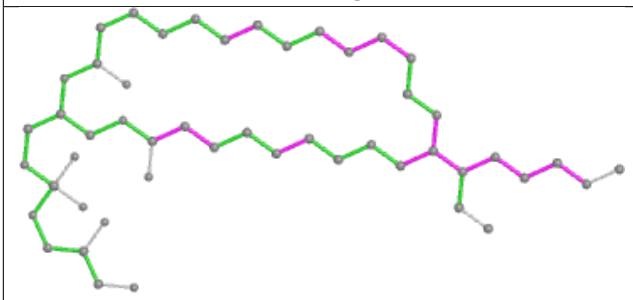
Ligand PGV N 608



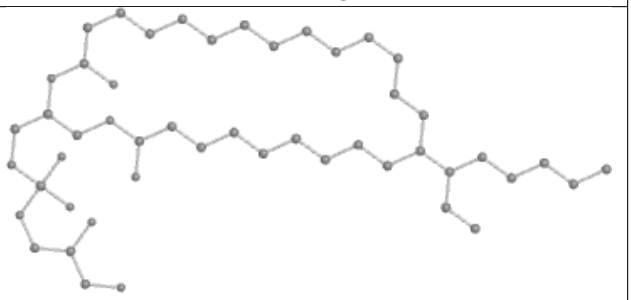
Bond lengths



Bond angles

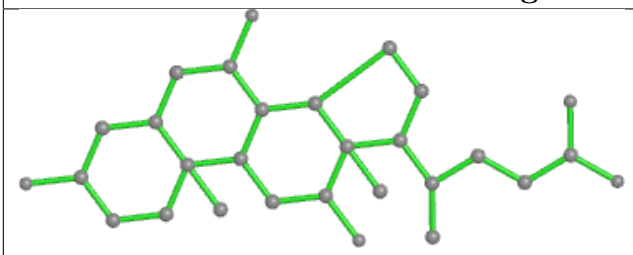


Torsions

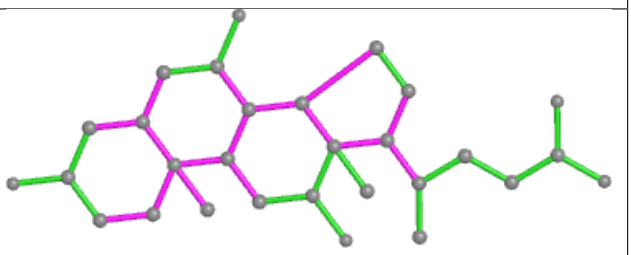


Rings

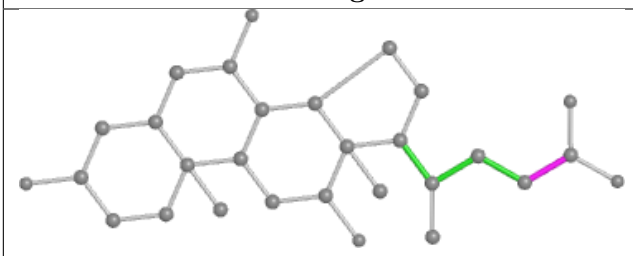
Ligand CHD C 304



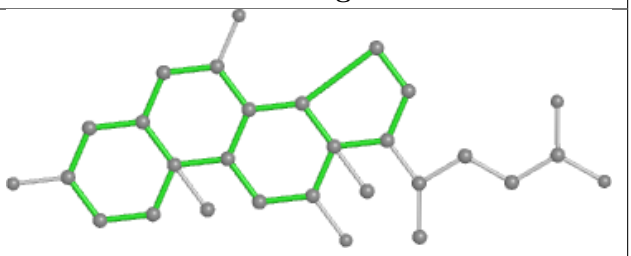
Bond lengths



Bond angles

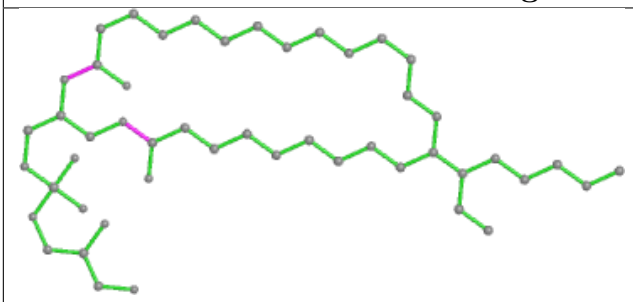


Torsions

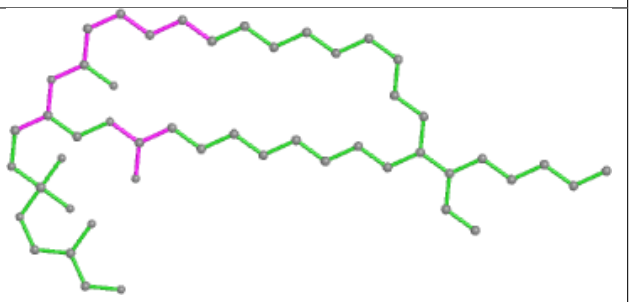


Rings

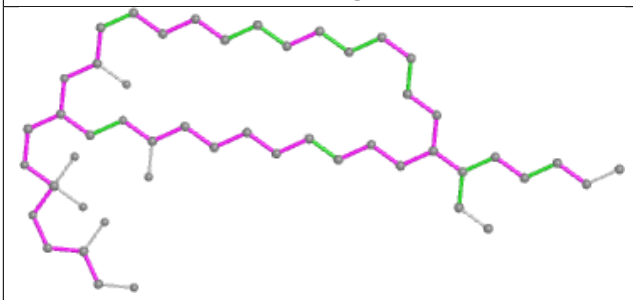
Ligand PGV A 609



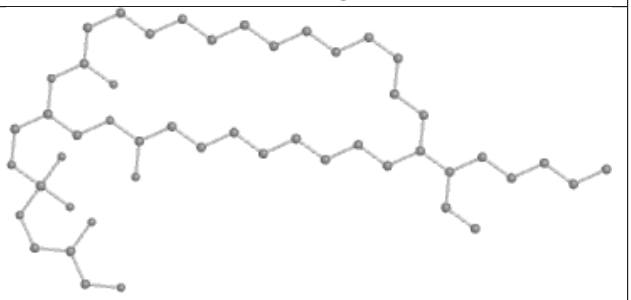
Bond lengths



Bond angles

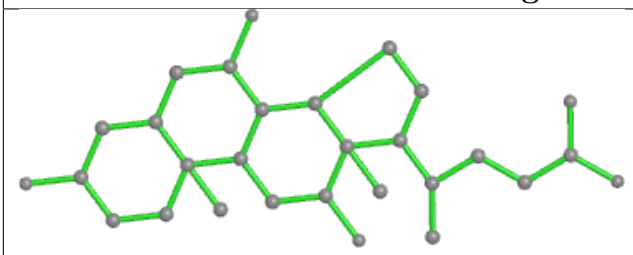


Torsions

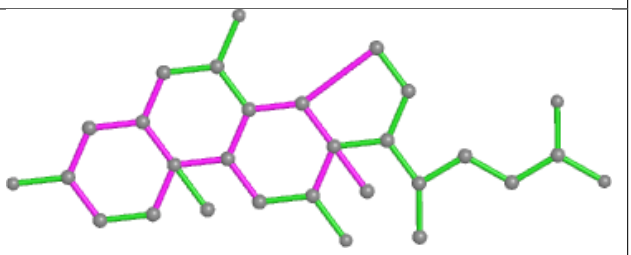


Rings

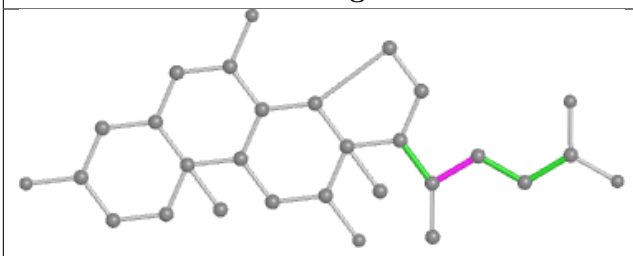
Ligand CHD P 305



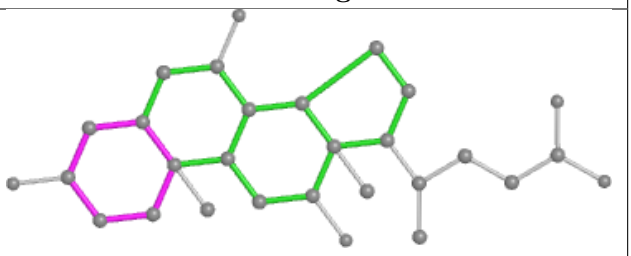
Bond lengths



Bond angles

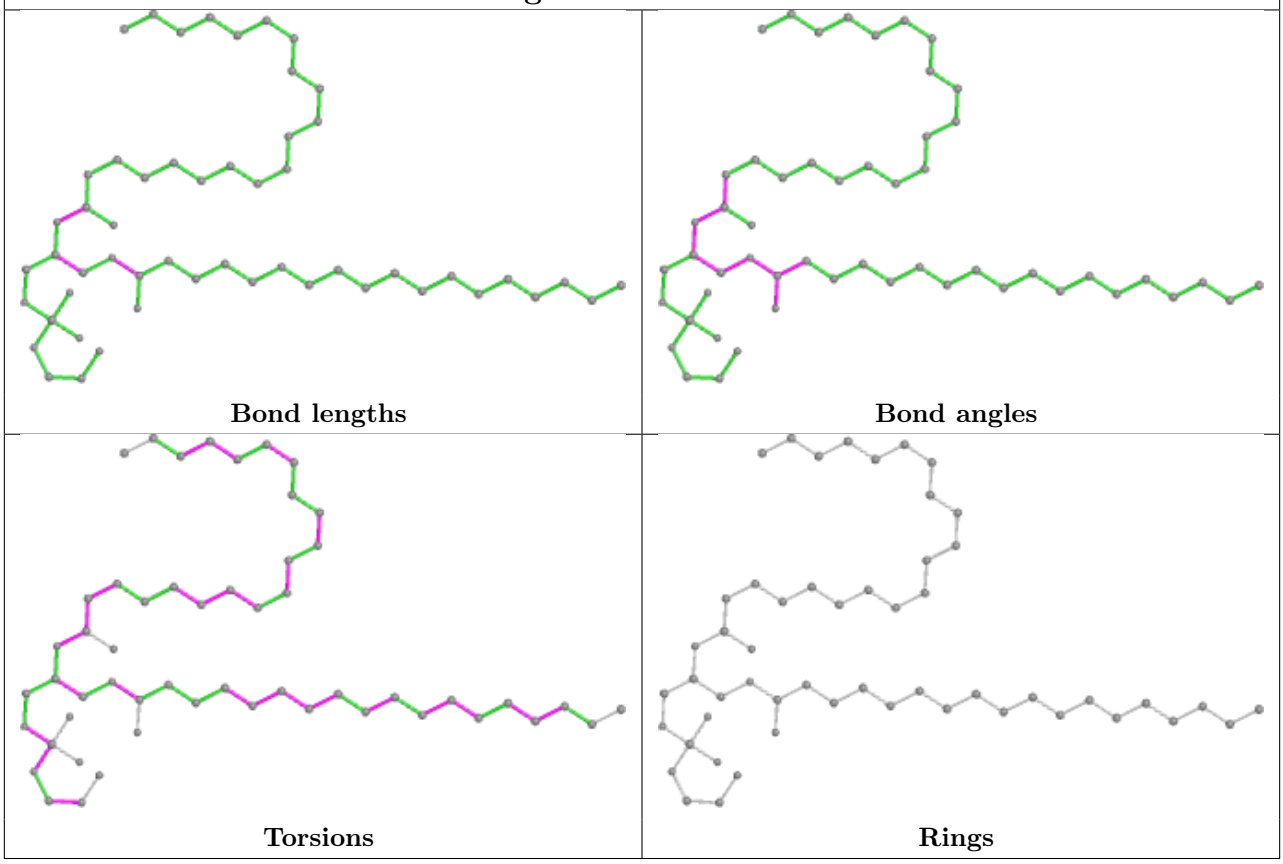


Torsions

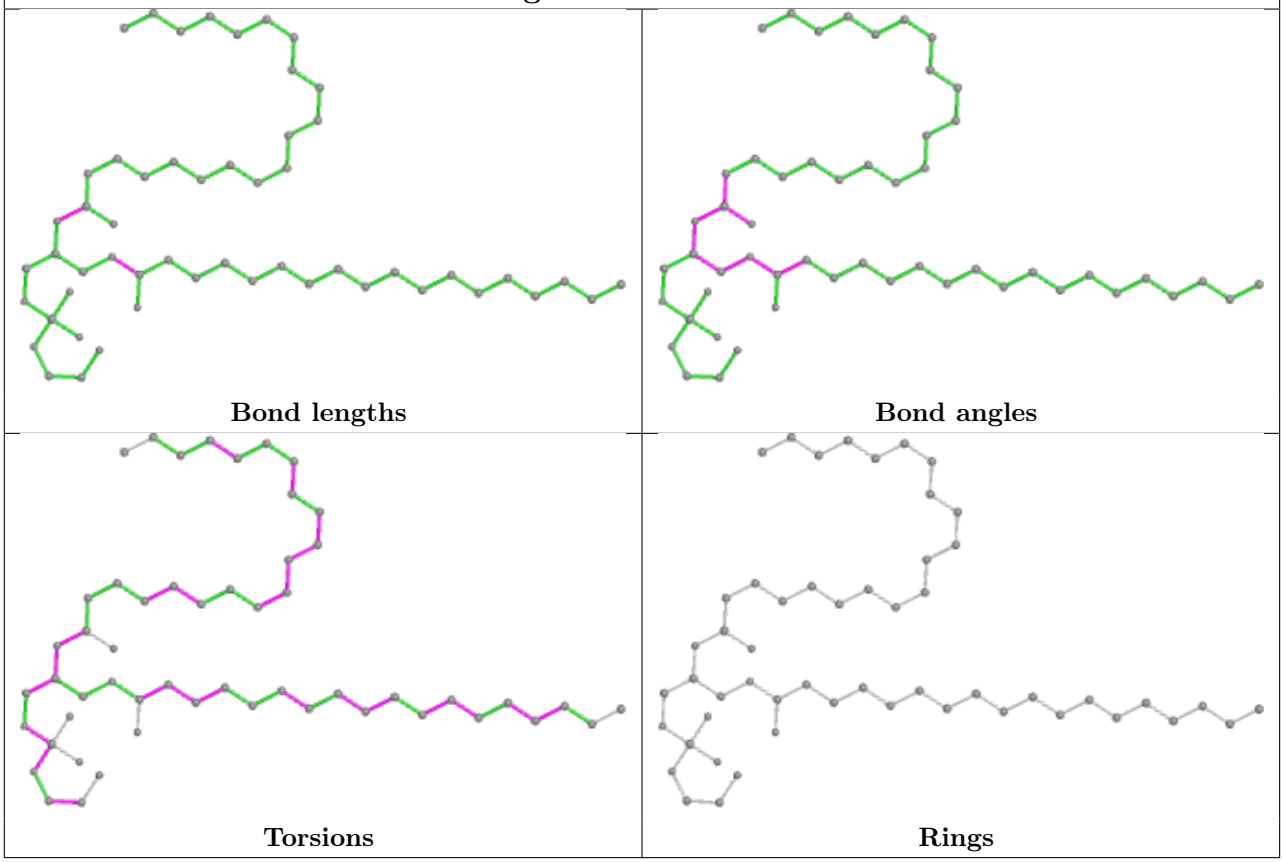


Rings

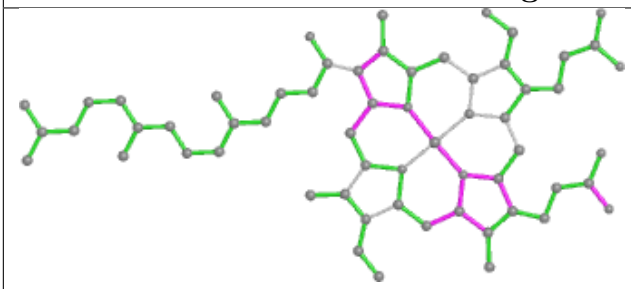
Ligand PEK C 306



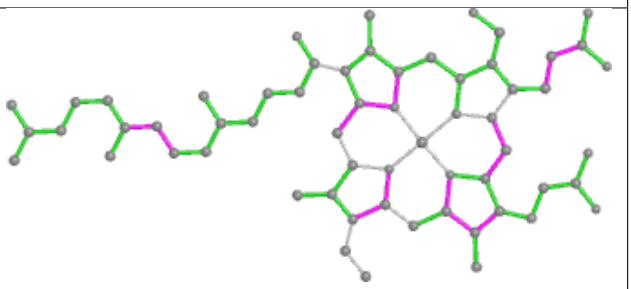
Ligand PEK G 103



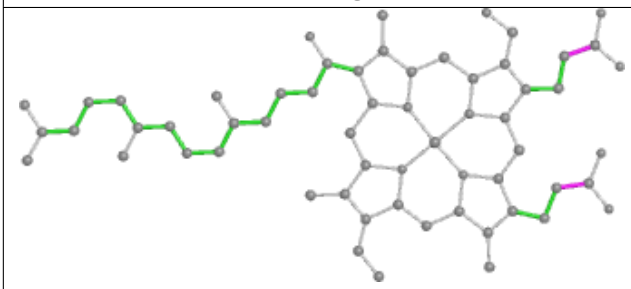
Ligand HEA N 601



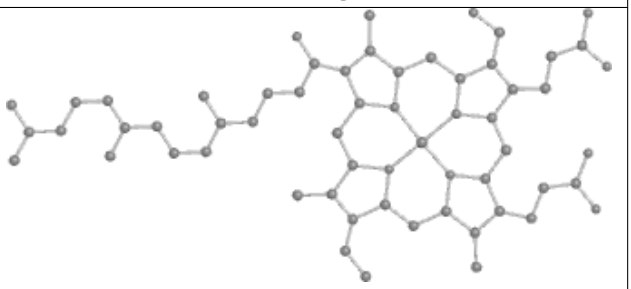
Bond lengths



Bond angles

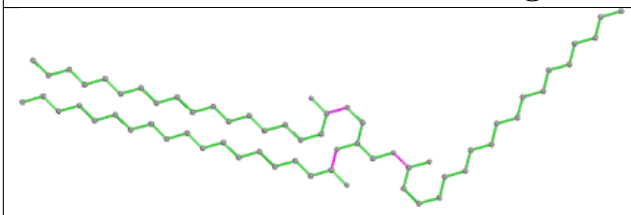


Torsions

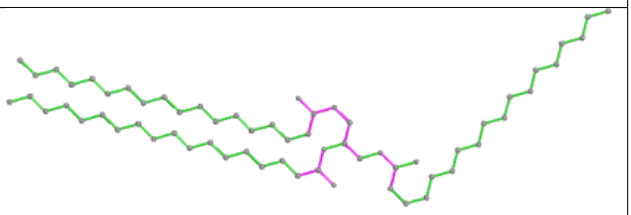


Rings

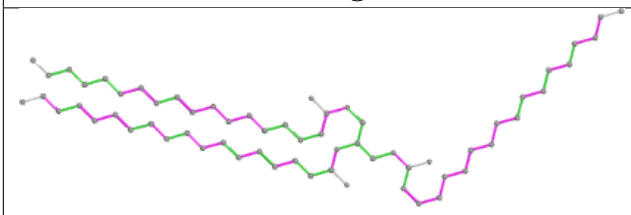
Ligand TGL O 302



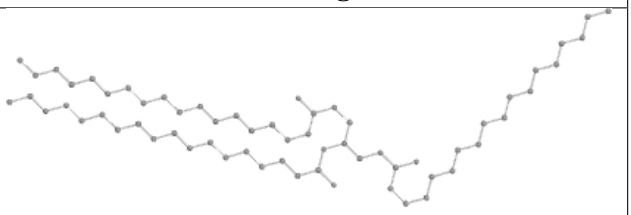
Bond lengths



Bond angles

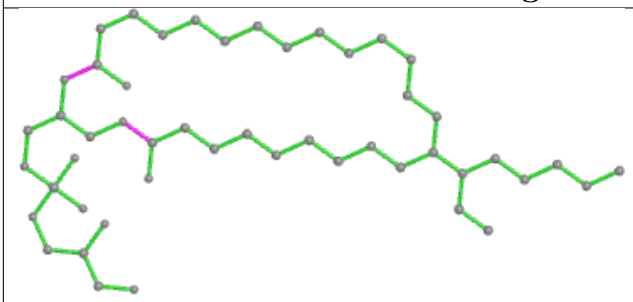


Torsions

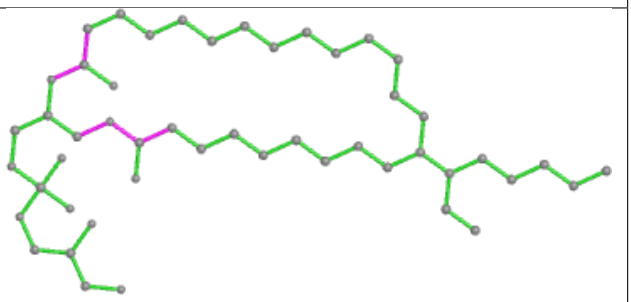


Rings

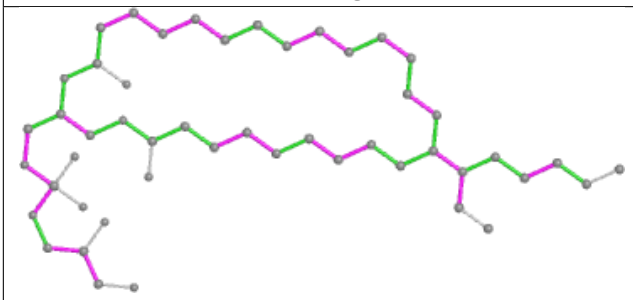
Ligand PGV C 307



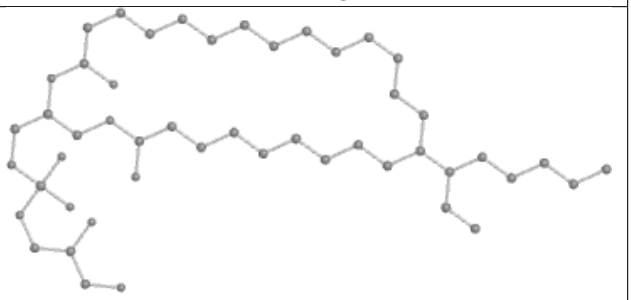
Bond lengths



Bond angles

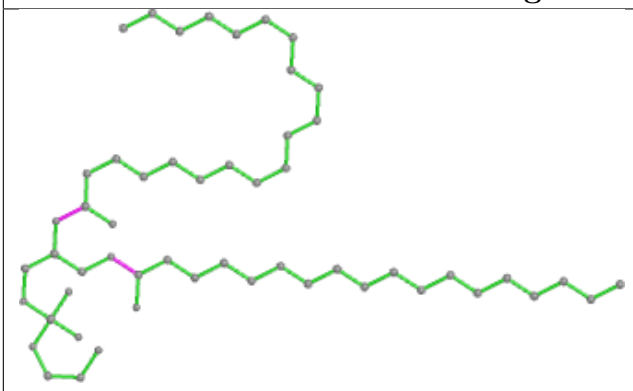


Torsions

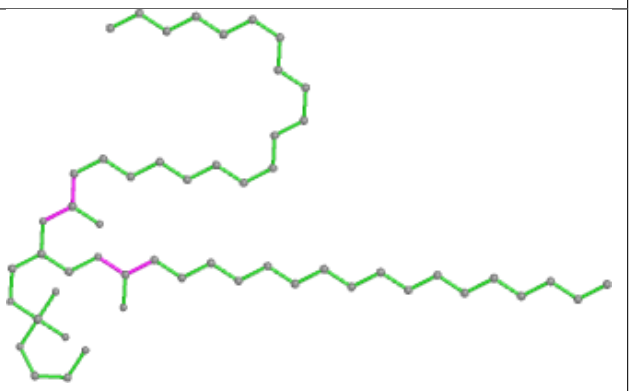


Rings

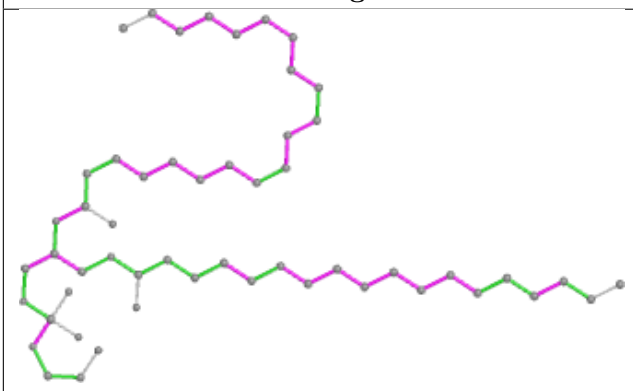
Ligand PEK T 103



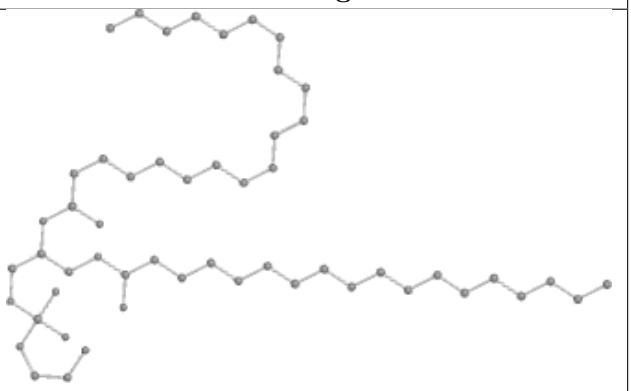
Bond lengths



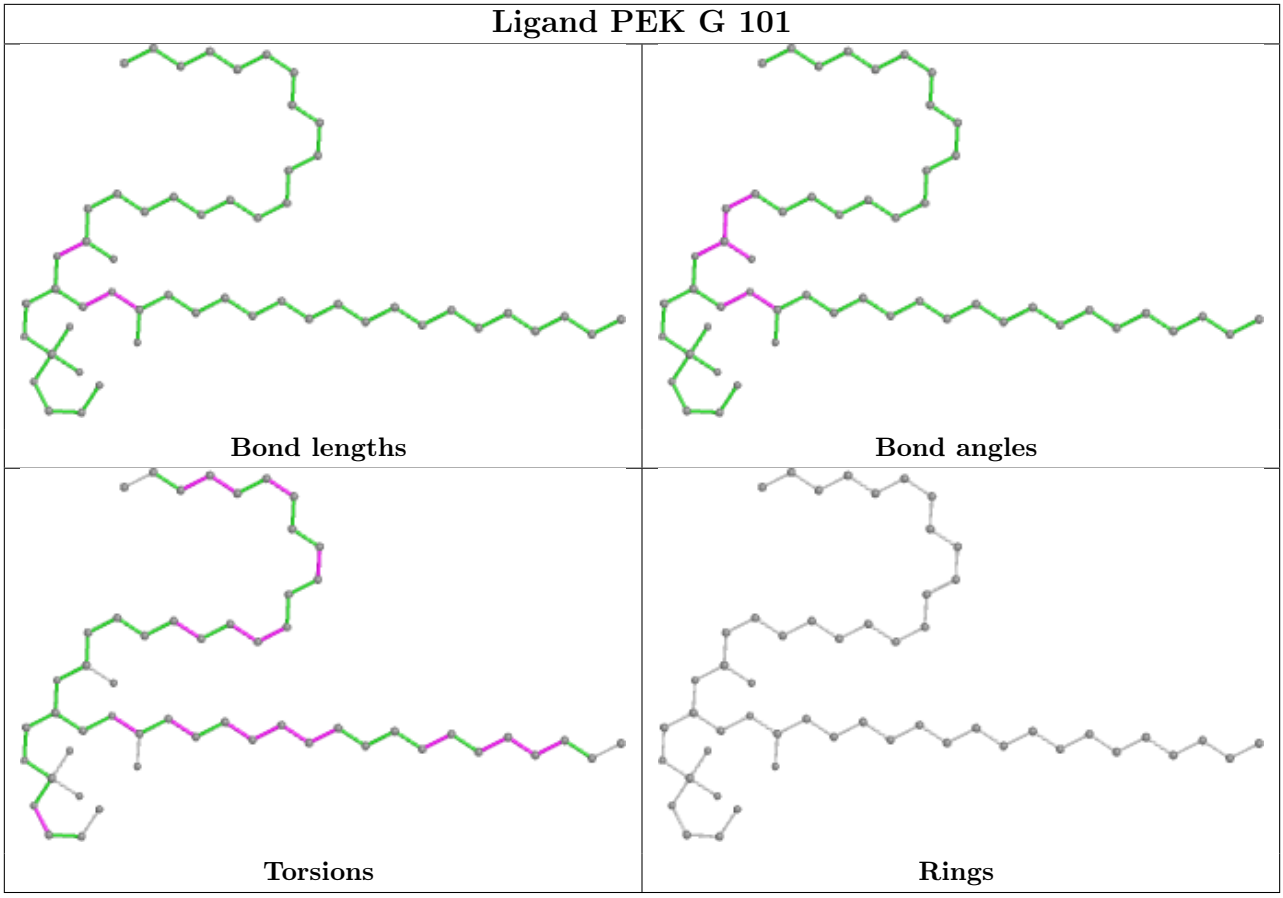
Bond angles



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%)	-0.71	0	100	100	39, 47, 59, 90	0
1	N	513/514 (99%)	-0.71	5 (0%)	82	81	43, 55, 71, 103	0
2	B	226/227 (99%)	-0.74	3 (1%)	77	75	43, 54, 82, 118	0
2	O	226/227 (99%)	-0.48	6 (2%)	54	52	51, 64, 98, 140	0
3	C	259/261 (99%)	-0.55	0	100	100	44, 51, 69, 123	0
3	P	259/261 (99%)	-0.41	6 (2%)	60	58	46, 56, 75, 129	0
4	D	144/147 (97%)	-0.52	1 (0%)	87	86	49, 59, 87, 126	0
4	Q	144/147 (97%)	0.43	16 (11%)	5	4	60, 81, 126, 157	0
5	E	105/109 (96%)	-0.31	2 (1%)	66	65	49, 59, 88, 147	0
5	R	105/109 (96%)	-0.00	6 (5%)	23	22	56, 73, 104, 142	0
6	F	98/98 (100%)	-0.27	10 (10%)	6	6	47, 61, 138, 155	0
6	S	98/98 (100%)	-0.06	6 (6%)	21	20	51, 70, 140, 158	0
7	G	83/85 (97%)	0.62	15 (18%)	1	1	49, 62, 150, 157	0
7	T	83/85 (97%)	0.54	10 (12%)	4	3	49, 68, 143, 154	0
8	H	79/85 (92%)	-0.16	4 (5%)	28	26	49, 64, 129, 144	0
8	U	79/85 (92%)	-0.14	5 (6%)	20	19	56, 71, 143, 153	0
9	I	72/73 (98%)	-0.39	3 (4%)	36	34	53, 66, 96, 118	0
9	V	72/73 (98%)	-0.31	5 (6%)	16	15	50, 77, 105, 140	0
10	J	58/59 (98%)	0.06	5 (8%)	10	9	52, 64, 98, 150	0
10	W	58/59 (98%)	-0.17	3 (5%)	27	26	59, 76, 110, 157	0
11	K	49/56 (87%)	-0.08	5 (10%)	6	6	57, 67, 88, 105	0
11	X	49/56 (87%)	0.33	8 (16%)	1	1	69, 80, 109, 122	0
12	L	46/47 (97%)	-0.84	0	100	100	47, 55, 75, 109	0
12	Y	46/47 (97%)	-0.35	3 (6%)	18	17	57, 72, 98, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.41	1 (2%) 60 58	51, 57, 89, 130	0
13	Z	43/46 (93%)	-0.13	4 (9%) 8 7	66, 78, 113, 150	0
All	All	3550/3614 (98%)	-0.39	132 (3%) 41 39	39, 59, 103, 158	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.4
7	T	3	ALA	12.1
7	G	1	ALA	11.1
7	G	2	SER	10.3
4	Q	6	VAL	9.9
6	S	96	LEU	9.6
7	G	5	LYS	9.4
10	J	58	LYS	9.2
7	T	40	GLY	8.9
6	S	98	HIS	8.7
4	Q	4	SER	8.7
4	Q	5	VAL	8.3
6	F	98	HIS	8.3
7	G	3	ALA	7.9
7	G	41	HIS	7.8
7	T	39	SER	7.3
4	Q	7	LYS	7.3
7	T	1	ALA	6.6
4	Q	8	SER	6.3
7	T	2	SER	6.3
7	T	8	HIS	6.2
7	G	40	GLY	6.2
7	T	41	HIS	6.0
5	R	109	VAL	5.8
6	F	97	ALA	5.8
7	G	84	LYS	5.8
7	T	5	LYS	5.5
8	H	48	GLY	5.3
9	V	2	THR	5.3
13	Z	42	LYS	5.3
7	G	42	ARG	5.2
8	H	45	ALA	5.1
7	G	6	GLY	5.1
6	S	95	GLN	5.0

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Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	6	ALA	5.0
1	N	513	LEU	4.9
8	U	48	GLY	4.8
11	X	13	TYR	4.7
2	O	90	ILE	4.6
8	H	47	GLY	4.6
6	F	1	ALA	4.5
5	R	5	HIS	4.4
11	X	7	PRO	4.4
4	Q	147	LYS	4.4
7	G	39	SER	4.2
3	P	38	ASN	4.1
10	J	57	HIS	3.9
4	Q	140	TYR	3.8
7	G	8	HIS	3.8
6	S	2	SER	3.8
11	X	12	LYS	3.8
8	U	47	GLY	3.7
5	E	109	VAL	3.7
11	K	7	PRO	3.6
2	O	227	LEU	3.6
4	Q	35	ALA	3.6
5	R	64	ALA	3.6
7	G	4	ALA	3.6
9	I	25	PHE	3.5
8	U	8	ILE	3.5
1	N	2	PHE	3.5
9	V	3	ALA	3.5
3	P	37	PHE	3.4
7	G	37	LEU	3.4
13	Z	43	SER	3.4
1	N	484	THR	3.3
12	Y	3	TYR	3.3
5	R	62	ALA	3.3
6	F	65	ASP	3.3
12	Y	47	LYS	3.3
6	F	64	GLU	3.2
11	X	6	ALA	3.2
3	P	3	HIS	3.1
4	Q	73	ARG	3.1
10	W	48	TYR	3.1
2	O	113	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
6	F	96	LEU	3.0
9	I	19	PHE	3.0
1	N	136	LEU	2.9
10	W	58	LYS	2.9
8	U	45	ALA	2.9
6	F	2	SER	2.9
9	V	34	PHE	2.9
11	X	31	TYR	2.8
7	T	36	TRP	2.8
4	Q	43	LYS	2.8
10	J	52	TRP	2.7
4	Q	33	LEU	2.7
4	Q	97	ILE	2.7
7	G	36	TRP	2.7
5	R	63	SER	2.6
2	O	211	LEU	2.6
4	Q	49	SER	2.5
11	K	19	ALA	2.5
10	J	4	ARG	2.5
6	F	95	GLN	2.5
9	I	37[A]	PHE	2.5
12	Y	19	TRP	2.5
2	B	57	ASP	2.5
11	K	16	ALA	2.4
4	Q	32	ASN	2.4
9	V	38	ALA	2.4
13	Z	41	LYS	2.4
3	P	33	MET	2.4
8	H	46	LYS	2.4
10	W	57	HIS	2.4
11	X	40	TRP	2.3
9	V	18	ARG	2.3
2	O	91	ASN	2.3
2	B	90	ILE	2.3
11	X	36	ILE	2.3
6	S	94	HIS	2.3
4	Q	92	THR	2.2
7	G	9	GLY	2.2
11	X	52	GLU	2.2
5	E	62	ALA	2.2
1	N	3	ILE	2.2
8	U	7	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	43	LYS	2.2
6	F	94	HIS	2.2
13	Z	32	TRP	2.2
4	D	147	LYS	2.1
11	K	35	GLN	2.2
4	Q	93	ALA	2.1
10	J	15	ASP	2.1
2	O	114	GLU	2.1
5	R	67	ILE	2.1
7	T	6	GLY	2.1
13	M	43	SER	2.1
3	P	39	SER	2.1
3	P	194	GLY	2.1
2	B	59	GLN	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	0.58	0.59	134,154,162,162	0
9	SAC	I	1	9/10	0.73	0.27	108,138,147,149	0
7	TPO	G	11	11/12	0.74	0.13	105,144,154,158	0
7	TPO	T	11	11/12	0.77	0.24	100,127,155,158	0
1	FME	A	1	10/11	0.96	0.28	58,69,114,141	0
2	FME	O	1	10/11	0.98	0.15	62,65,74,76	0
2	FME	B	1	10/11	0.98	0.08	51,56,62,76	0
1	FME	N	1	10/11	0.98	0.48	77,90,144,145	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
27	PEK	T	102	53/53	0.50	0.51	74,133,150,150	0
21	EDO	C	310	4/4	0.57	0.84	146,146,149,149	0
25	UNX	P	302	1/1	0.58	0.71	20,20,20,20	1
23	CHD	W	101	29/29	0.61	0.35	108,149,150,150	0
27	PEK	C	306	53/53	0.61	0.30	68,138,150,150	0
24	PSC	O	303	52/52	0.61	0.33	72,134,150,150	0
26	CDL	G	102	100/100	0.63	0.37	99,145,150,150	0
26	CDL	T	104	100/100	0.63	0.33	83,136,150,150	0
26	CDL	P	304	100/100	0.67	0.27	70,139,150,150	0
19	TGL	Y	101	63/63	0.68	0.35	78,127,150,150	0
19	TGL	D	201	63/63	0.68	0.29	68,117,150,150	0
21	EDO	P	307	4/4	0.68	0.30	92,96,107,115	0
21	EDO	P	308	4/4	0.68	0.22	89,95,98,99	0
21	EDO	K	101	4/4	0.69	0.16	87,91,96,105	0
27	PEK	G	103	53/53	0.70	0.47	84,136,150,150	0
24	PSC	B	303	52/52	0.70	0.27	73,142,150,150	0
20	PGV	A	609	51/51	0.72	0.30	62,112,152,160	0
19	TGL	Q	201	63/63	0.75	0.23	76,124,150,150	0
20	PGV	N	607	51/51	0.75	0.39	66,140,150,150	0
21	EDO	N	610	4/4	0.75	0.91	125,132,135,138	0
26	CDL	C	303	100/100	0.77	0.24	56,121,153,157	0
27	PEK	T	103	53/53	0.77	0.26	67,132,150,150	0
19	TGL	A	607	63/63	0.78	0.24	50,96,139,151	0
21	EDO	H	101	4/4	0.78	0.33	111,112,118,127	0
19	TGL	O	302	63/63	0.78	0.21	67,115,150,150	0
19	TGL	L	101	63/63	0.79	0.26	67,106,149,150	0
20	PGV	C	307	51/51	0.80	0.26	61,126,150,150	0
20	PGV	P	301	51/51	0.81	0.21	73,119,150,150	0
21	EDO	F	103	4/4	0.82	0.55	71,125,128,147	0
21	EDO	B	305	4/4	0.82	0.32	84,86,91,94	0
29	DMU	Z	101	33/33	0.83	0.30	95,106,138,147	0
23	CHD	J	101	29/29	0.84	0.33	90,142,150,150	0
21	EDO	A	611	4/4	0.84	0.16	81,82,106,109	0
25	UNX	C	301	1/1	0.85	0.75	17,17,17,17	1
21	EDO	G	105	4/4	0.87	0.17	74,78,88,97	0
21	EDO	A	613	4/4	0.88	0.47	96,116,120,122	0
18	CMO	N	606	2/2	0.89	0.12	47,47,47,50	2
23	CHD	P	305	29/29	0.89	0.21	82,131,147,148	0
21	EDO	C	309	4/4	0.89	0.25	80,86,89,95	0
29	DMU	M	101	33/33	0.89	0.23	61,78,111,115	0
23	CHD	C	304	29/29	0.89	0.27	89,104,112,113	0

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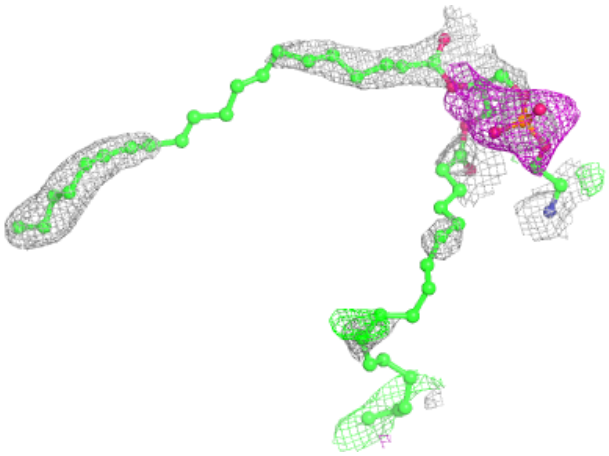
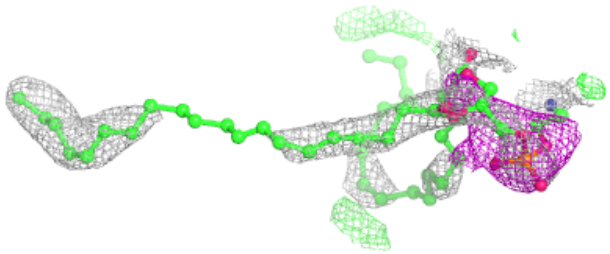
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	EDO	C	308	4/4	0.91	0.22	89,93,96,106	0
21	EDO	T	105	4/4	0.91	0.22	121,130,135,136	0
21	EDO	F	102	4/4	0.92	0.17	82,82,101,101	0
21	EDO	K	102	4/4	0.92	0.60	89,96,101,112	0
21	EDO	L	102	4/4	0.93	0.16	83,86,90,95	0
21	EDO	N	609	4/4	0.93	0.09	88,91,100,108	0
21	EDO	A	612	4/4	0.94	0.28	62,76,80,93	0
20	PGV	P	303	51/51	0.94	0.22	53,65,143,148	0
21	EDO	C	311	4/4	0.95	0.12	60,77,78,84	0
27	PEK	T	101	53/53	0.95	0.18	62,77,149,150	0
21	EDO	O	304	4/4	0.96	0.18	68,70,73,77	0
27	PEK	G	101	53/53	0.96	0.15	50,67,123,137	0
23	CHD	P	306	29/29	0.97	0.10	52,60,64,66	0
20	PGV	C	302	51/51	0.97	0.13	46,57,107,115	0
23	CHD	C	305	29/29	0.97	0.09	48,56,63,68	0
23	CHD	G	104	29/29	0.97	0.11	42,51,59,66	0
20	PGV	A	608	51/51	0.97	0.12	43,65,86,105	0
21	EDO	B	304	4/4	0.97	0.14	64,66,67,75	0
18	CMO	A	606	2/2	0.98	0.25	33,33,33,35	2
20	PGV	N	608	51/51	0.98	0.13	50,71,101,113	0
14	HEA	A	601	60/60	0.98	0.09	38,44,59,72	0
23	CHD	B	302	29/29	0.98	0.09	49,57,63,73	0
14	HEA	A	602	60/60	0.98	0.08	37,44,53,64	0
21	EDO	A	610	4/4	0.98	0.08	54,63,68,71	0
14	HEA	N	601	60/60	0.98	0.11	48,57,76,84	0
16	MG	N	604	1/1	0.98	0.03	52,52,52,52	0
17	NA	N	605	1/1	0.98	0.05	65,65,65,65	0
14	HEA	N	602	60/60	0.99	0.08	40,49,58,65	0
28	ZN	S	101	1/1	0.99	0.03	64,64,64,64	0
22	CUA	B	301	2/2	0.99	0.07	48,48,48,50	0
22	CUA	O	301	2/2	0.99	0.03	56,56,56,59	0
17	NA	A	605	1/1	1.00	0.10	53,53,53,53	0
28	ZN	F	101	1/1	1.00	0.05	57,57,57,57	0
15	CU	N	603	1/1	1.00	0.05	51,51,51,51	0
16	MG	A	604	1/1	1.00	0.02	41,41,41,41	0
15	CU	A	603	1/1	1.00	0.04	45,45,45,45	0

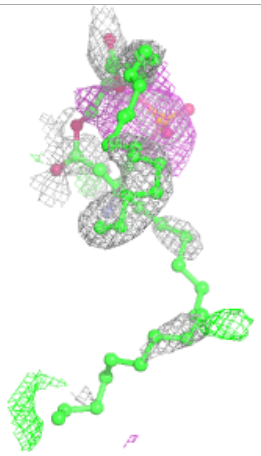
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEK 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)

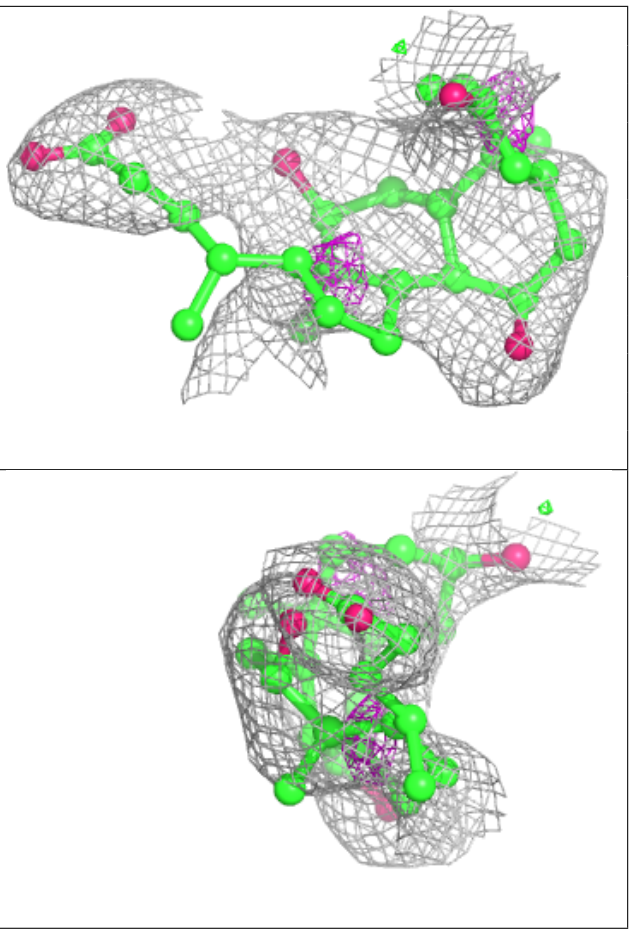


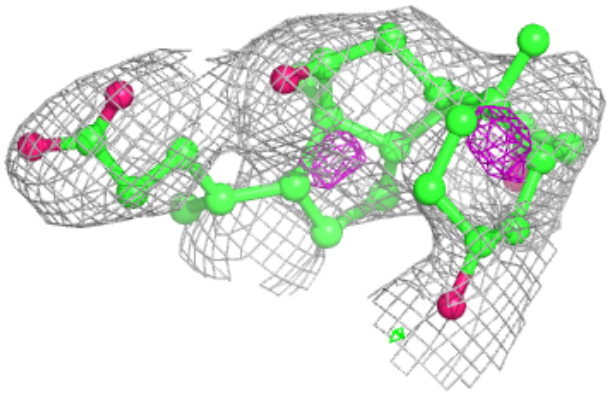




Electron density around CHD W 101:

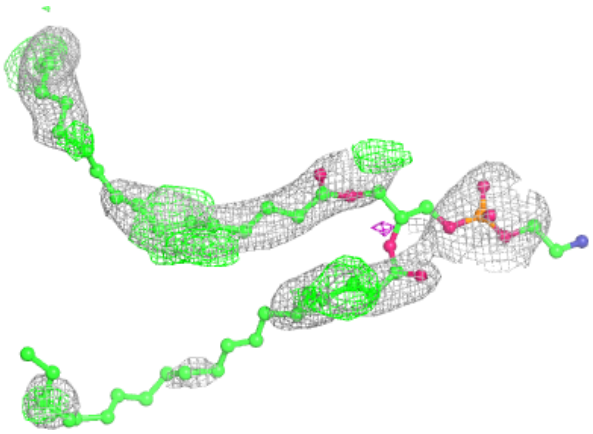
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

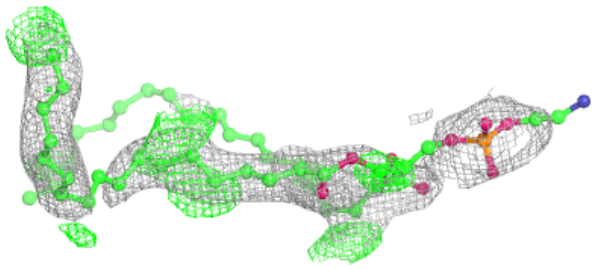


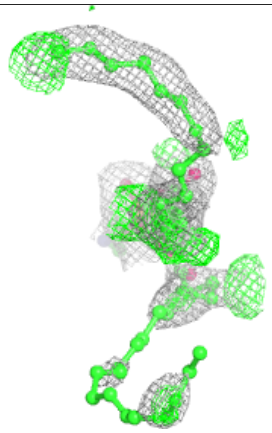


Electron density around PEK C 306:

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

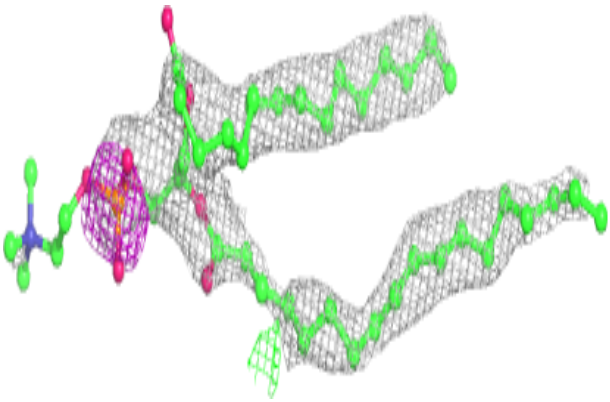


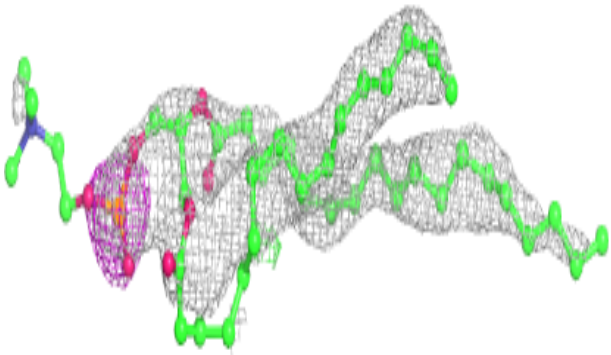


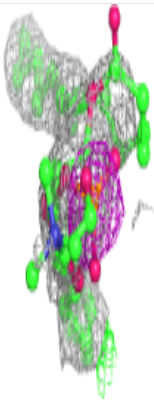


Electron density around PSC O 303:

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

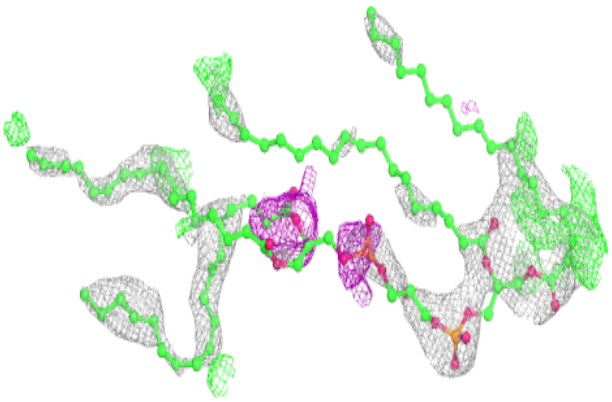


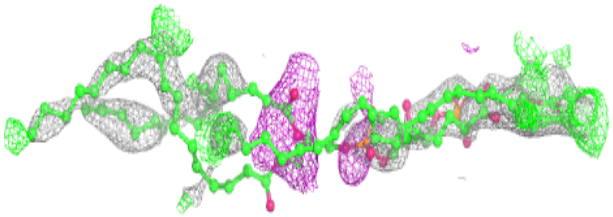


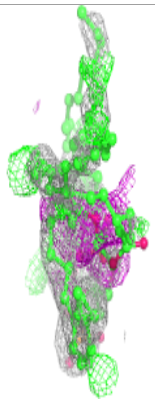


Electron density around CDL G 102:

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

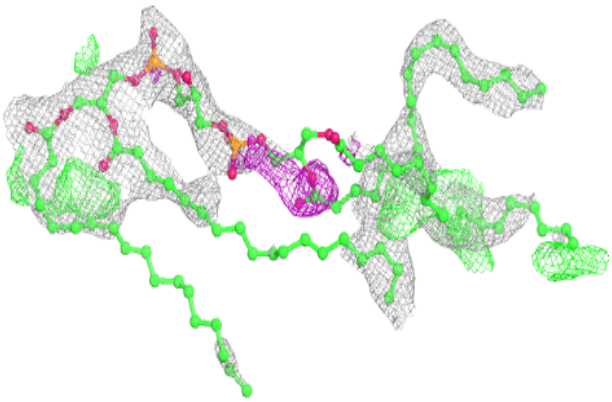


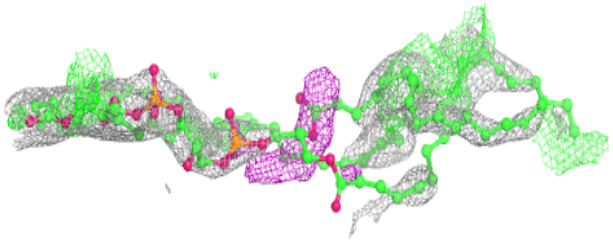


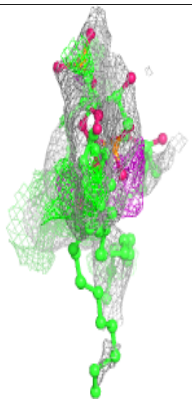


Electron density around CDL T 104:

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

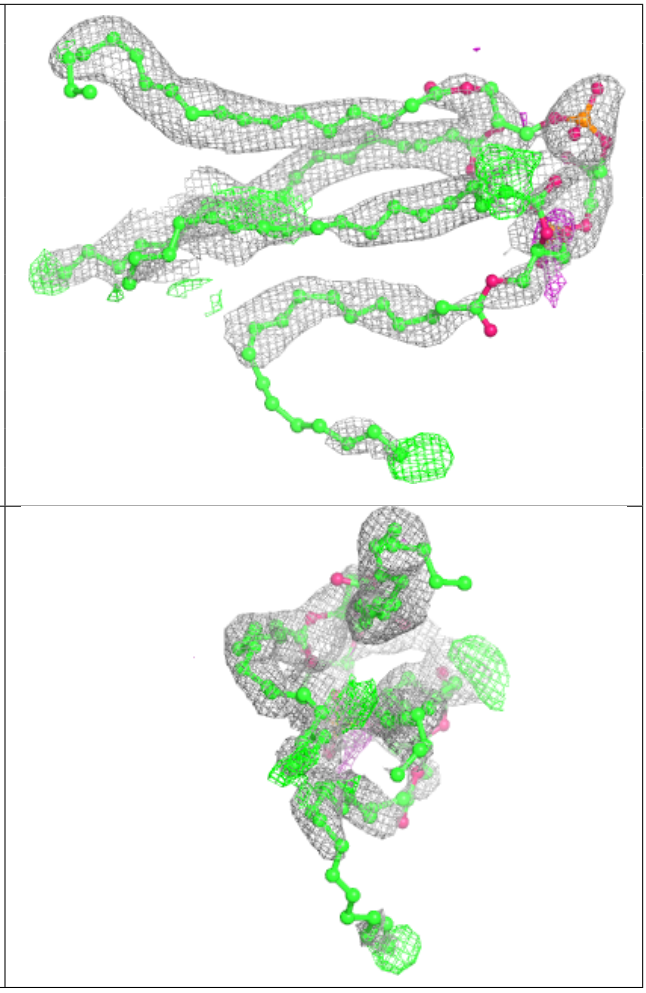






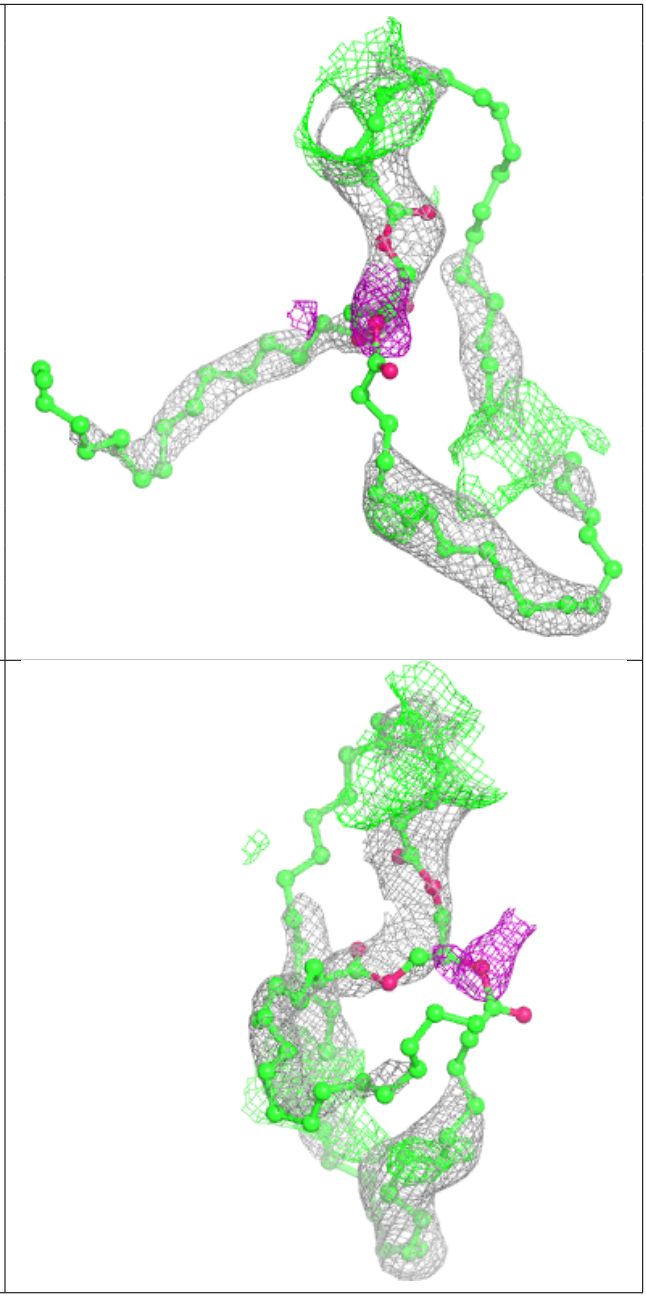
Electron density around CDL P 304:

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



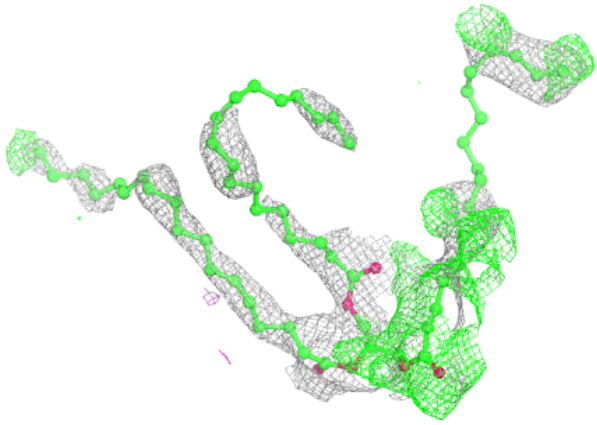
Electron density around TGL Y 101:

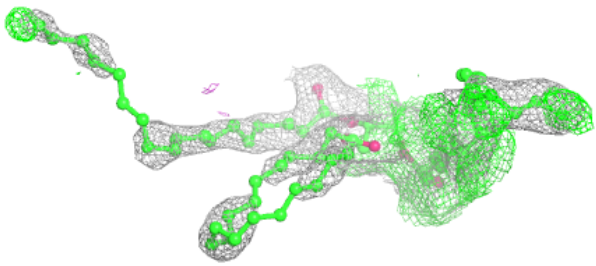
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

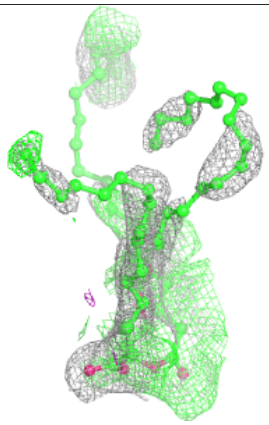


Electron density around TGL D 201:

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

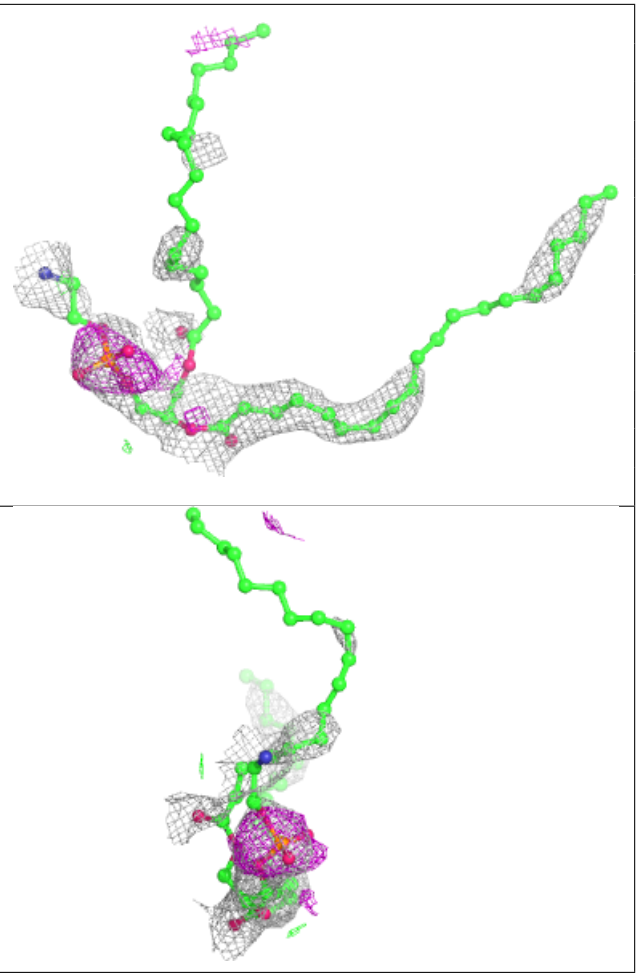






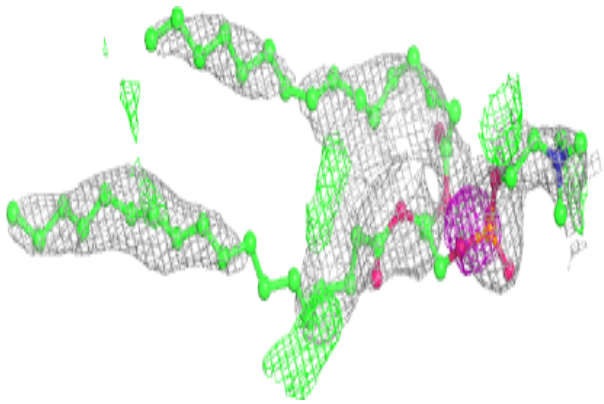
Electron density around PEK G 103:

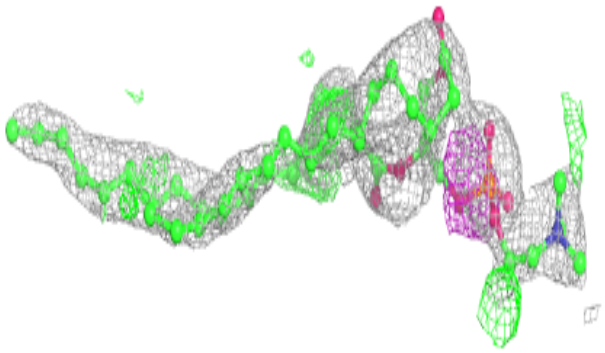
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

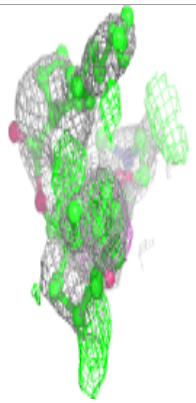


Electron density around PSC B 303:

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

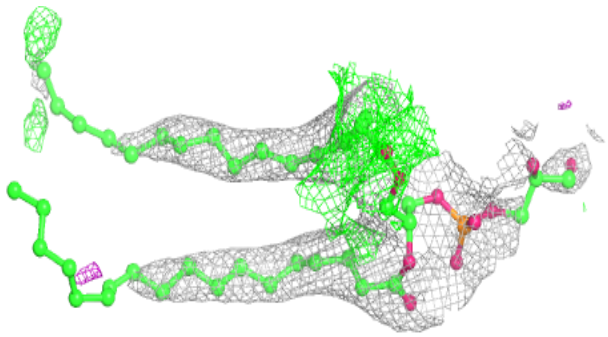


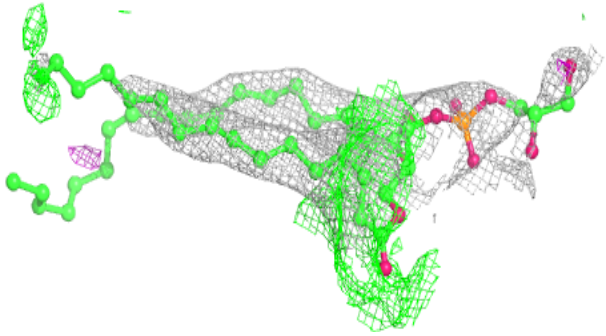


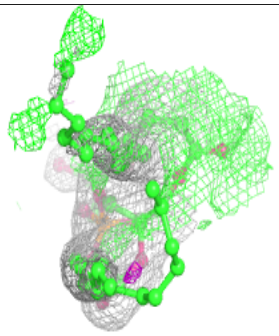


Electron density around PGV A 609:

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

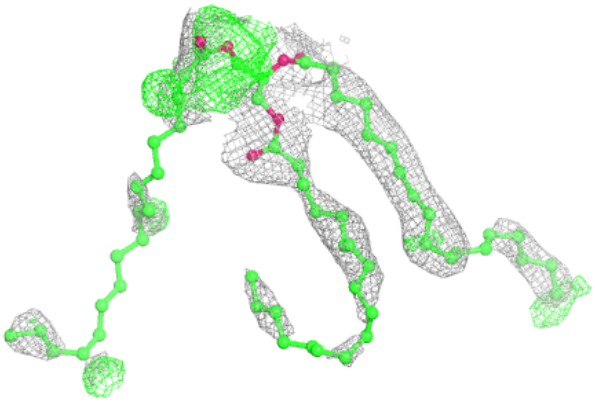


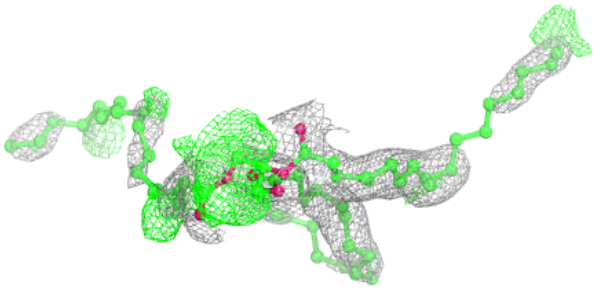


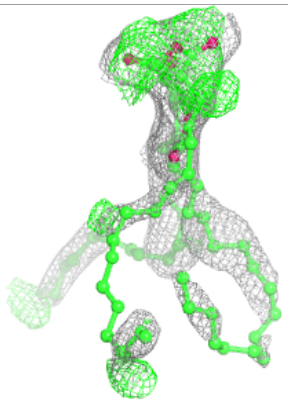


Electron density around TGL Q 201:

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

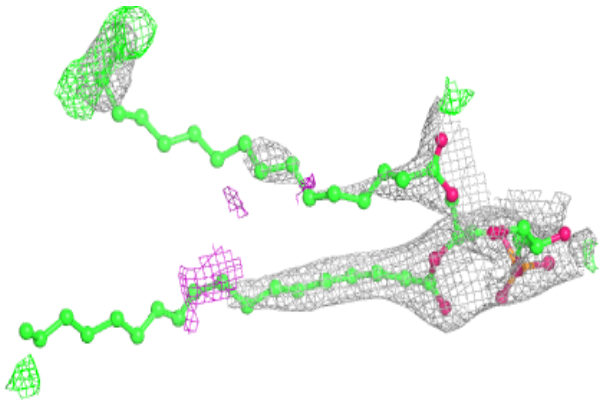


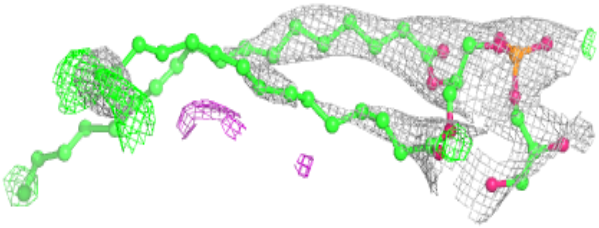


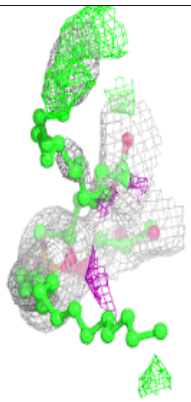


Electron density around PGV N 607:

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

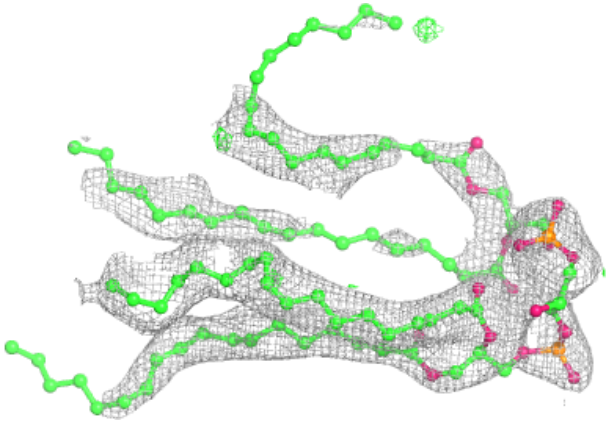


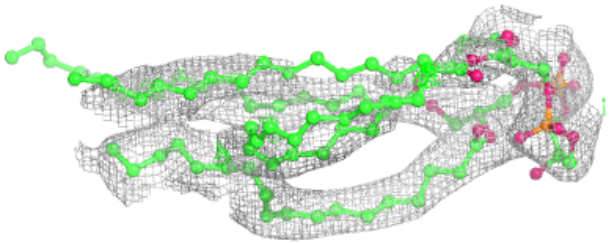


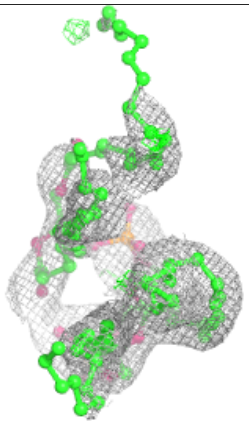


Electron density around CDL C 303:

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

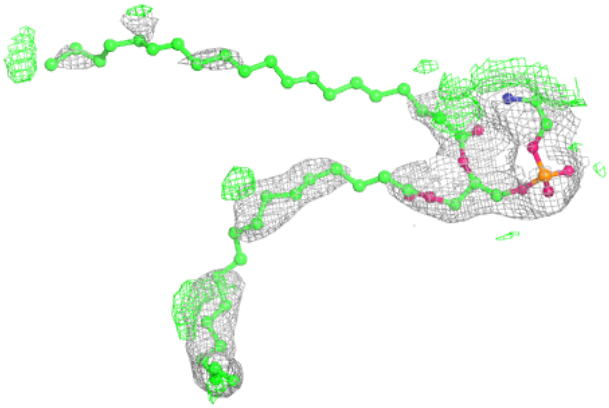


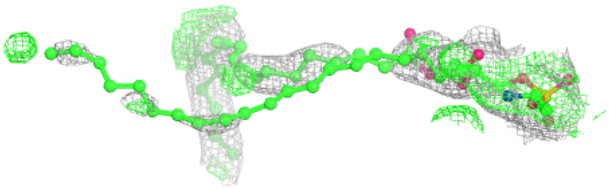


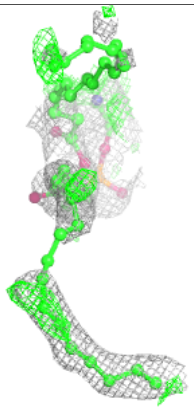


Electron density around PEK T 103:

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

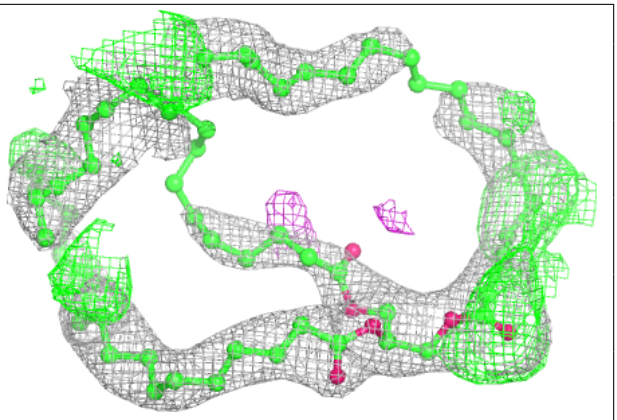


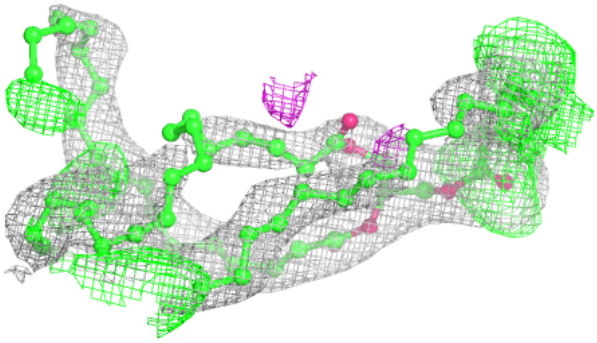


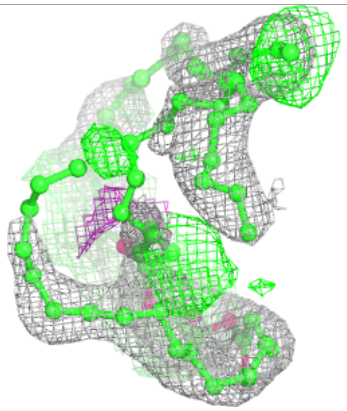


Electron density around TGL A 607:

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

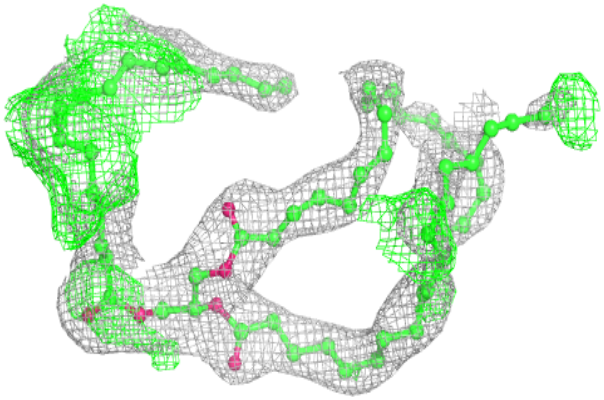


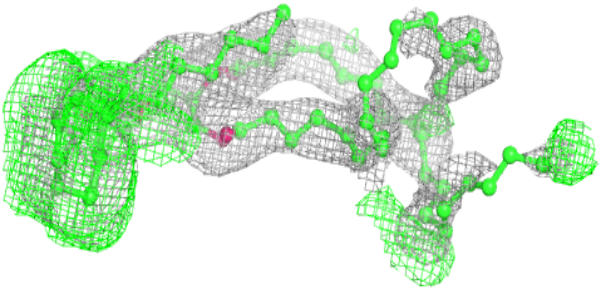


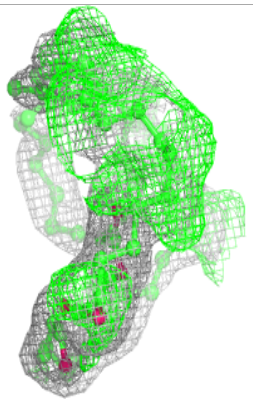


Electron density around TGL O 302:

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

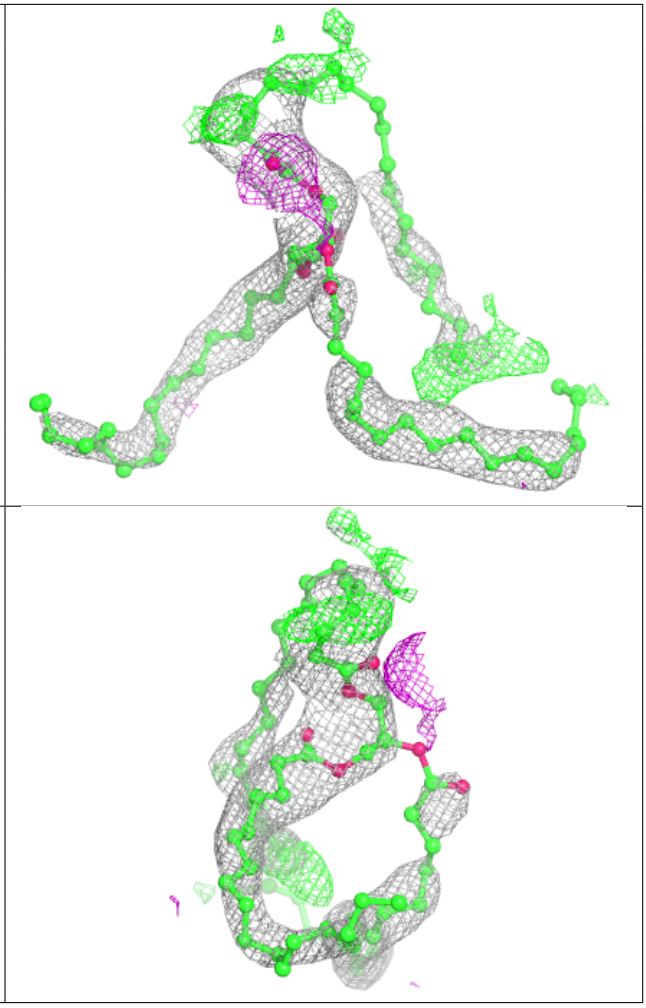






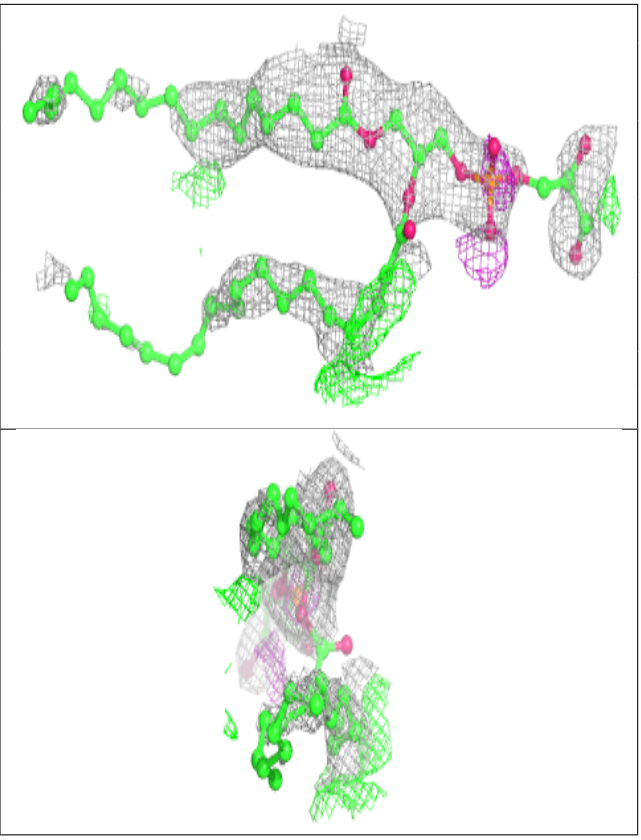
Electron density around TGL L 101:

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



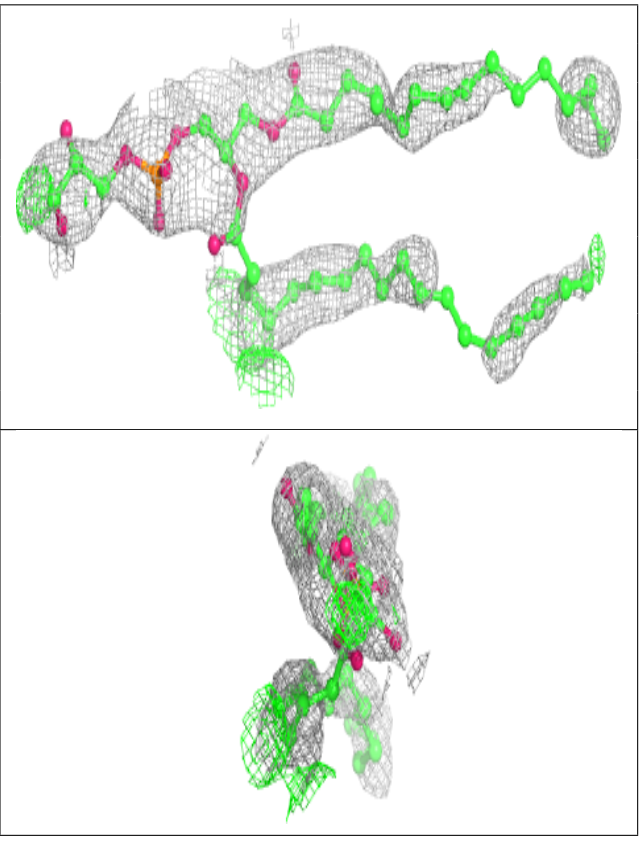
Electron density around PGV C 307:

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



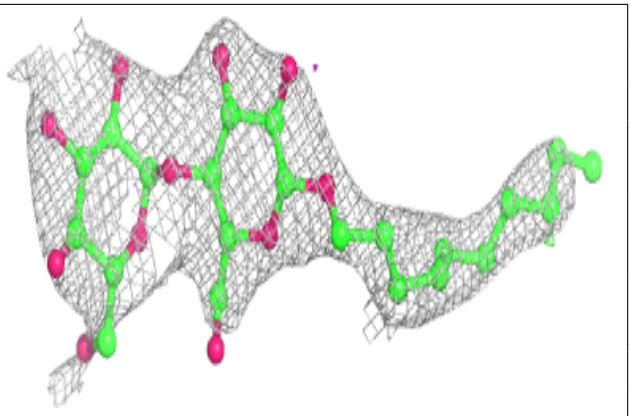
Electron density around PGV P 301:

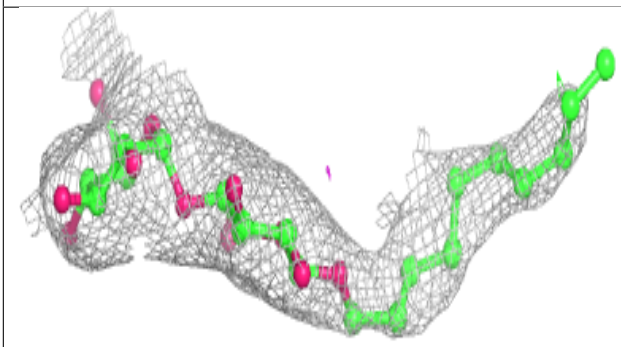
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

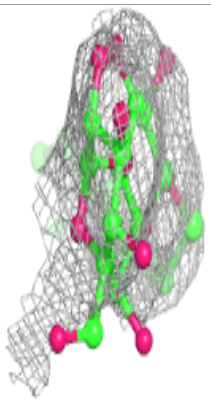


Electron density around DMU Z 101:

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

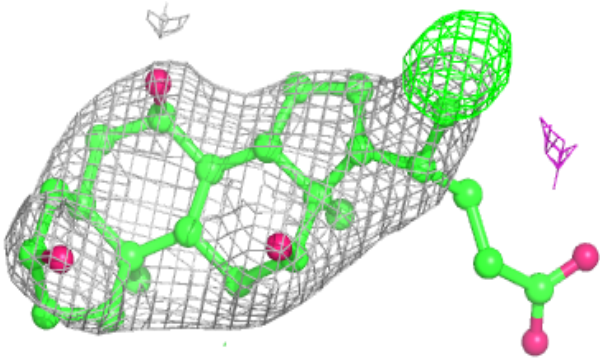


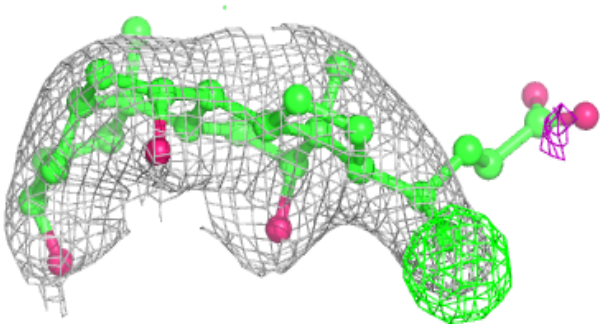


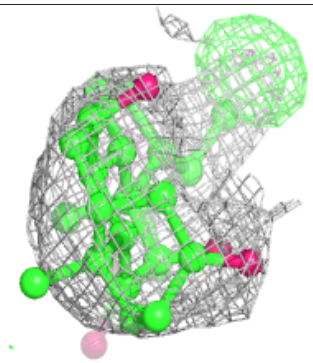


Electron density around CHD J 101:

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

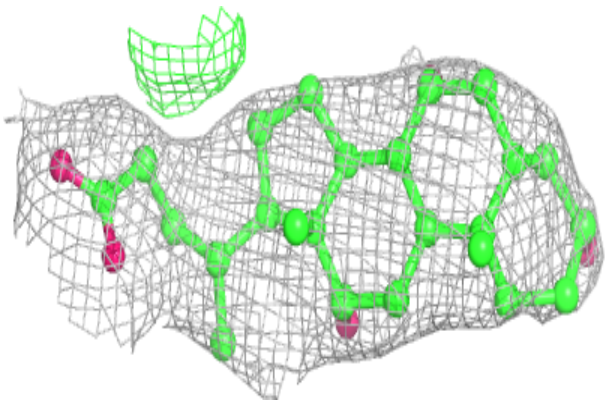


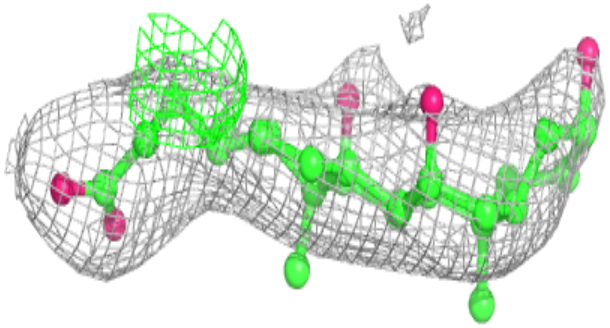


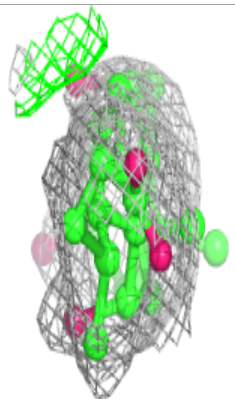


Electron density around CHD P 305:

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

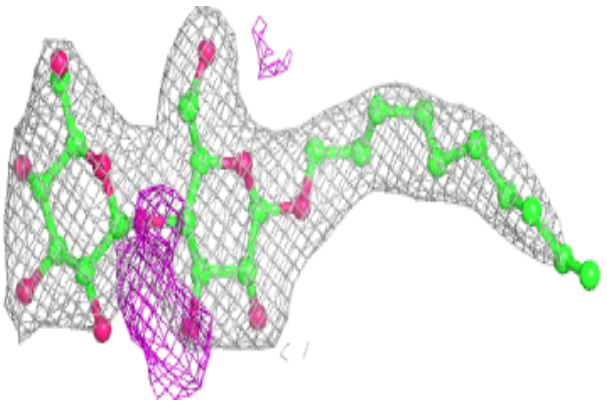


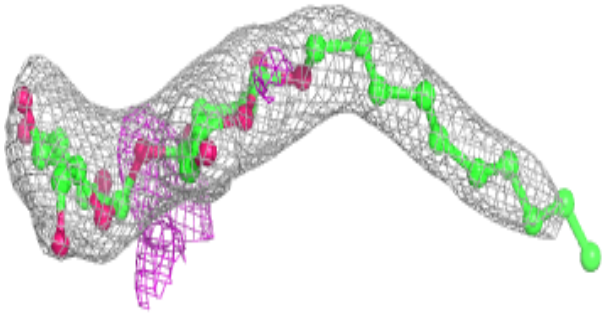


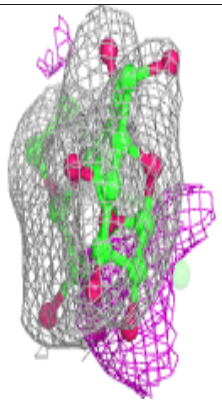


Electron density around DMU M 101:

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

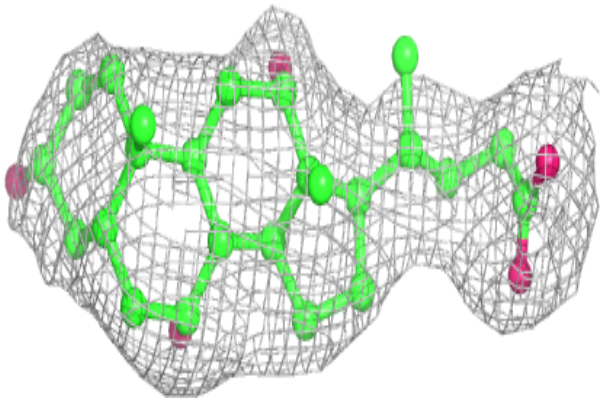


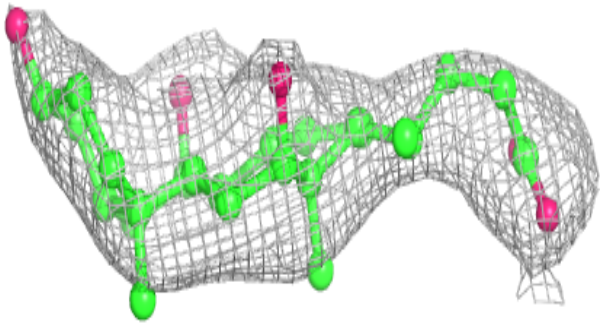


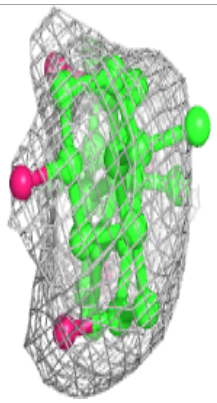


Electron density around CHD C 304:

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

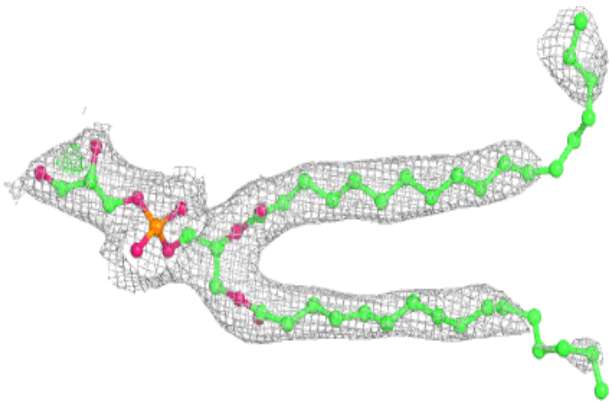


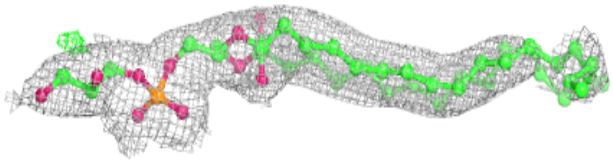


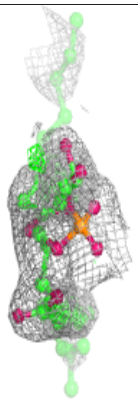


Electron density around PGV P 303:

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

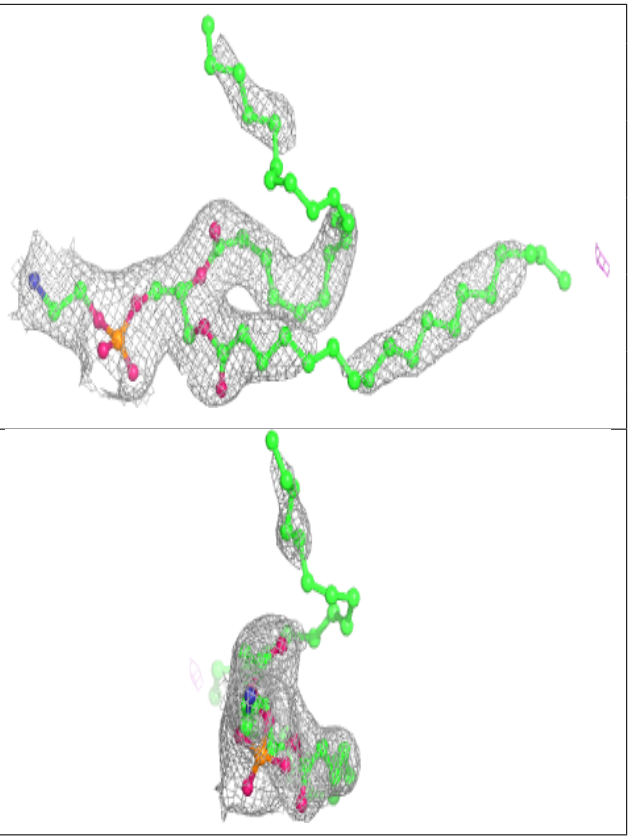


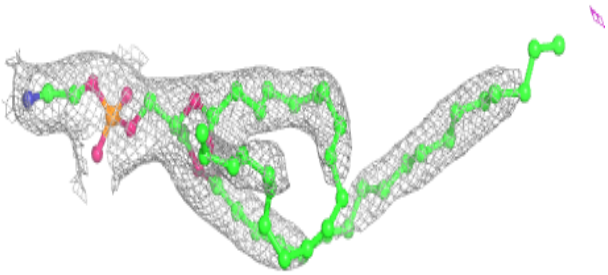




Electron density around PEK T 101:

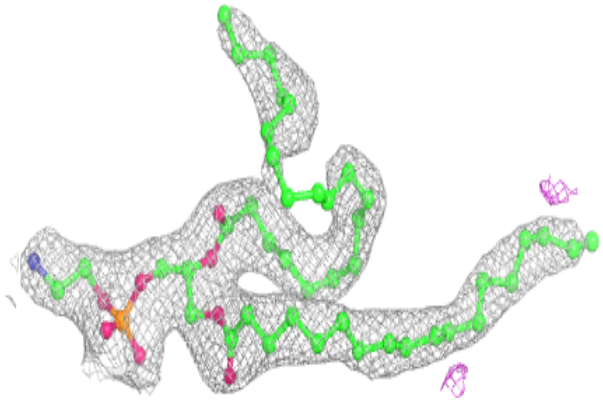
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

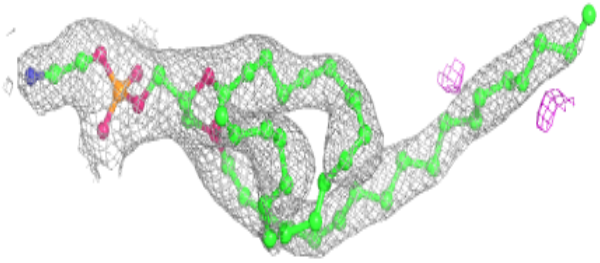


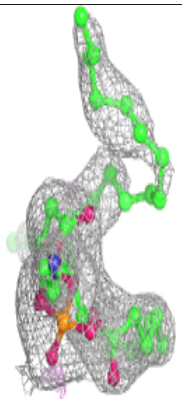


Electron density around PEK G 101:

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

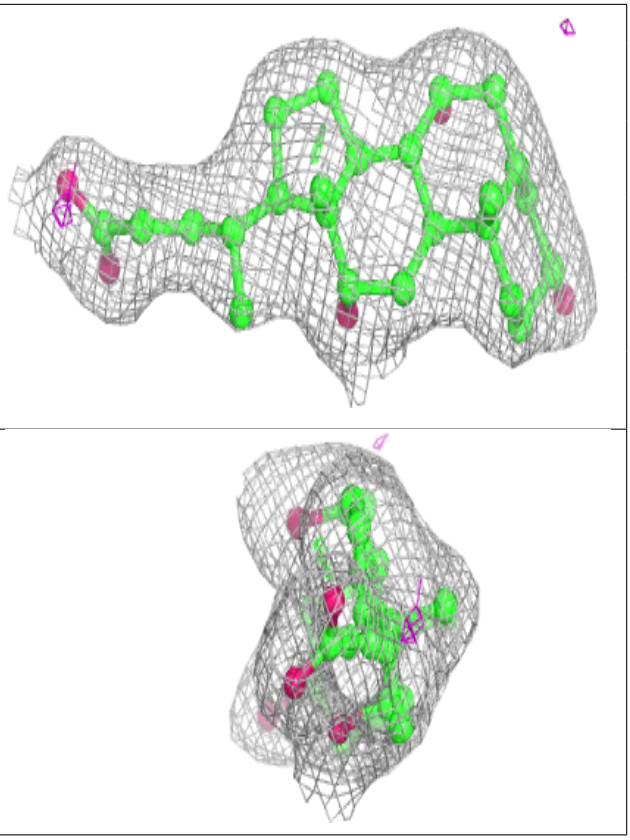






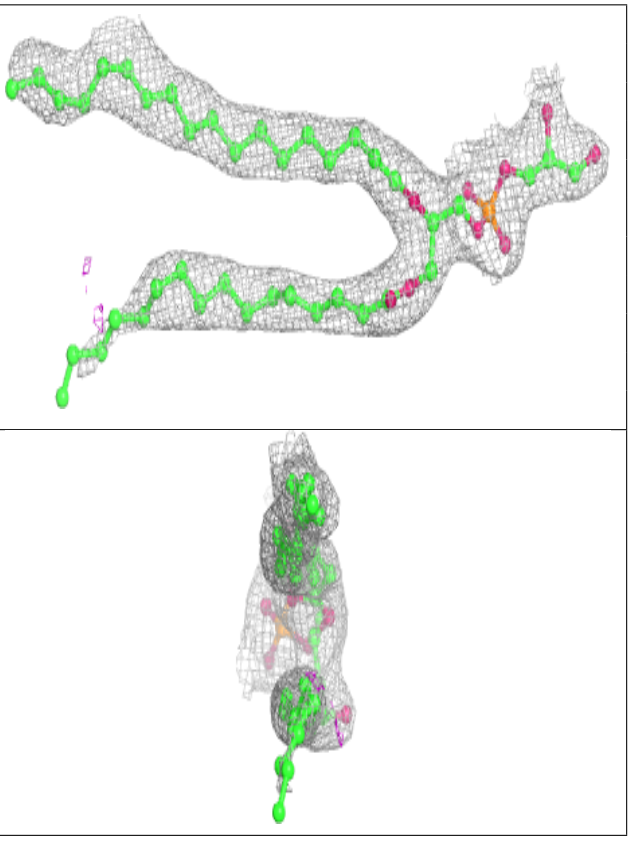
Electron density around CHD P 306:

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



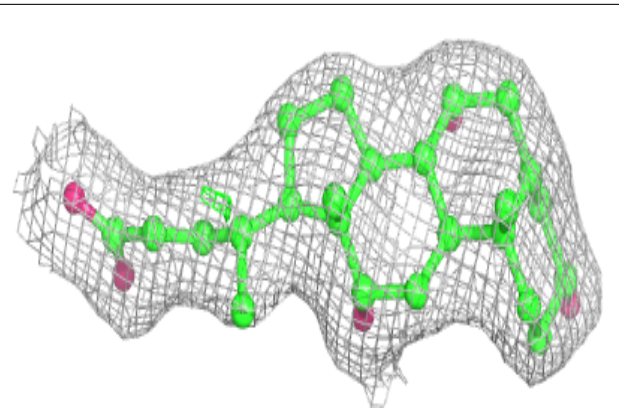
Electron density around PGV C 302:

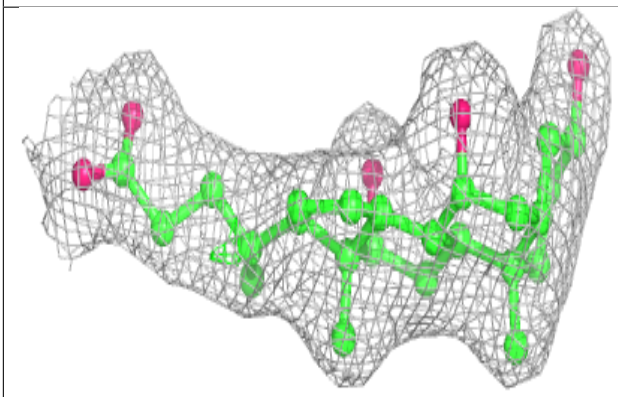
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

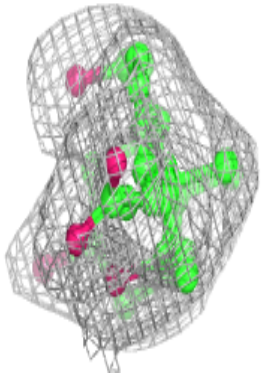


Electron density around CHD C 305:

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

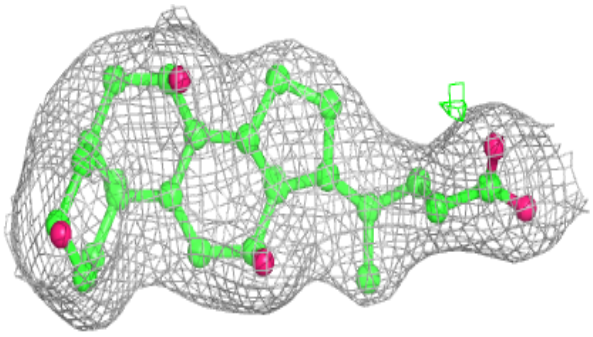


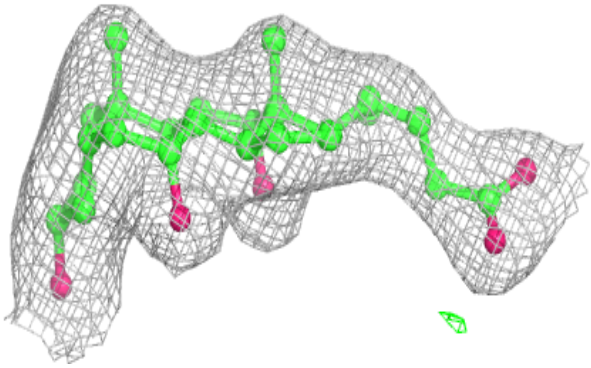


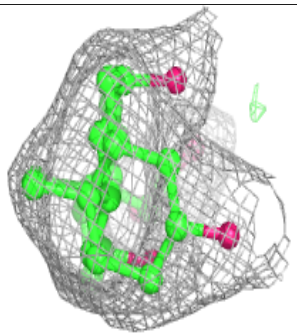


Electron density around CHD G 104:

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

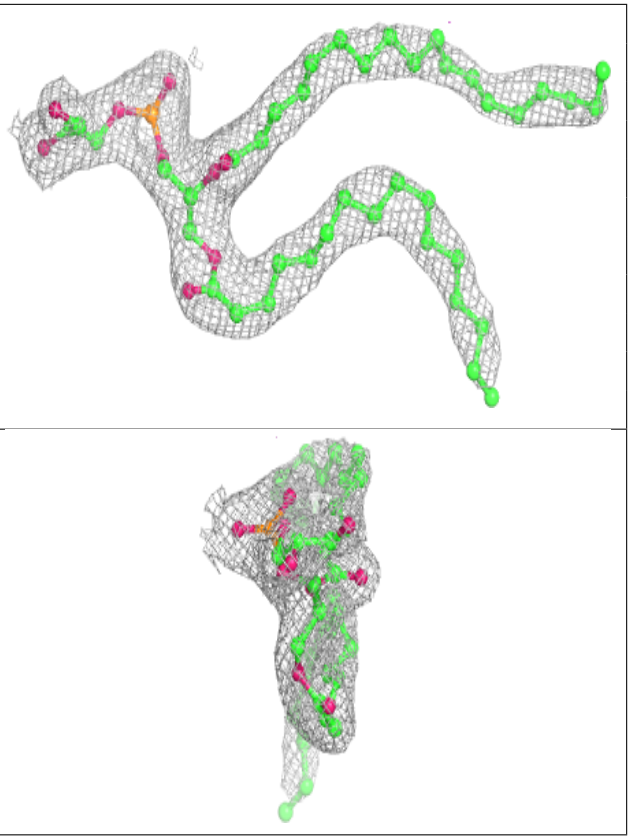


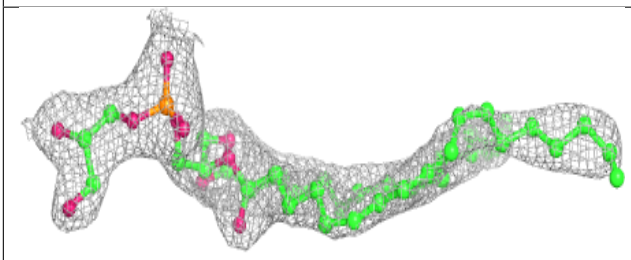




Electron density around PGV A 608:

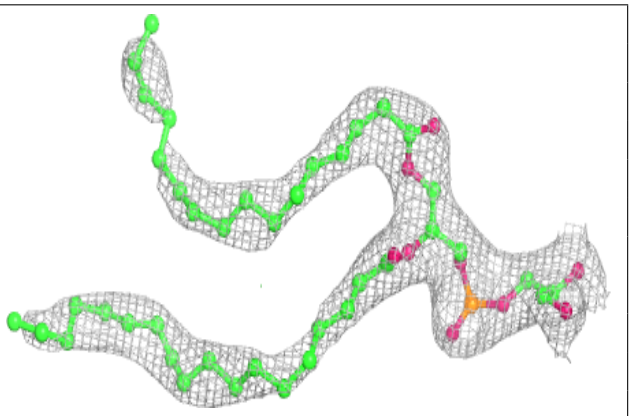
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

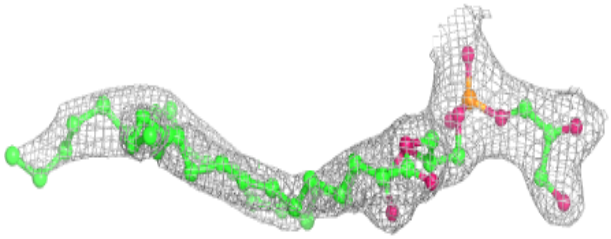


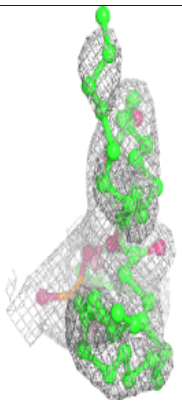


Electron density around PGV N 608:

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

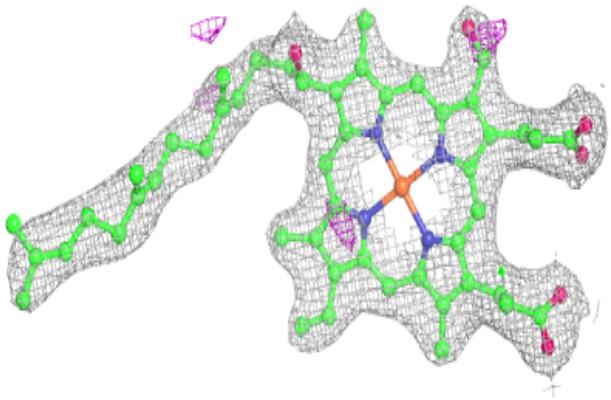


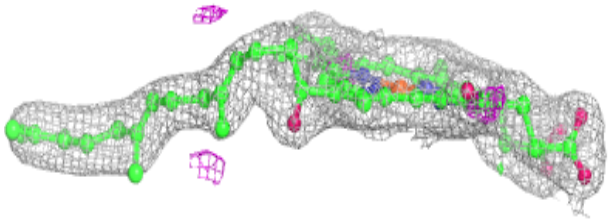


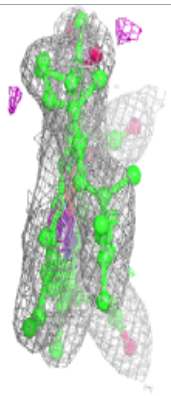


Electron density around HEA A 601:

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

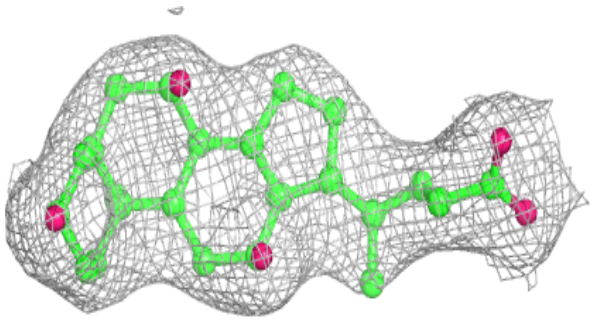


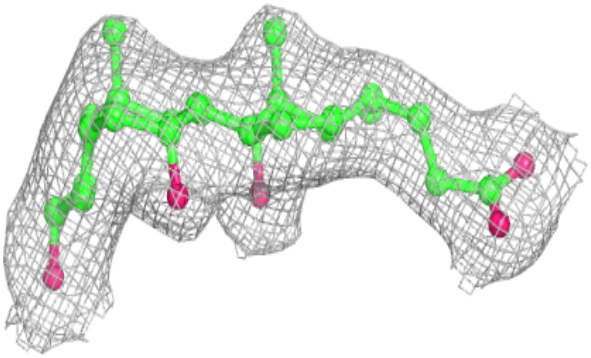


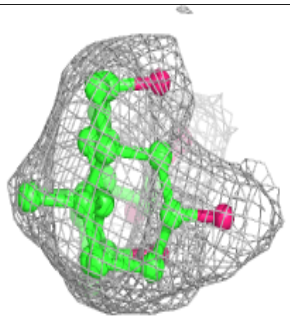


Electron density around CHD B 302:

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

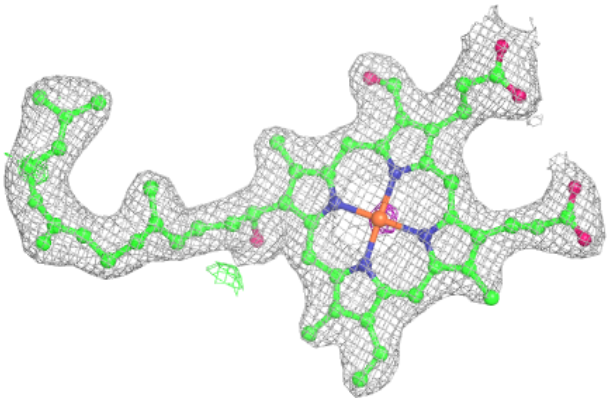


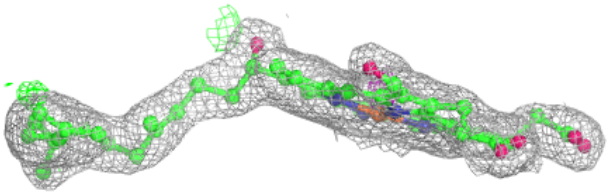


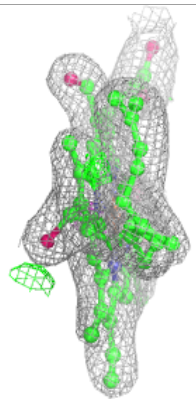


Electron density around HEA A 602:

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

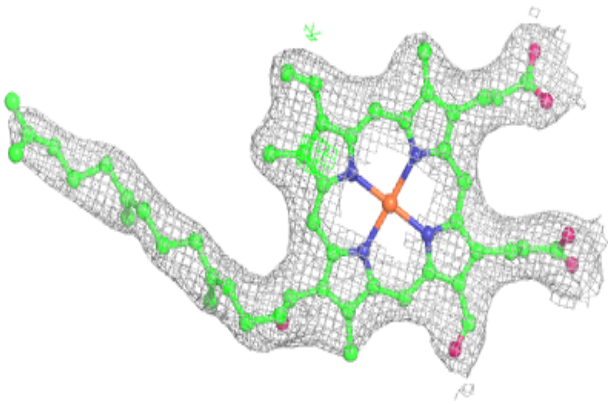


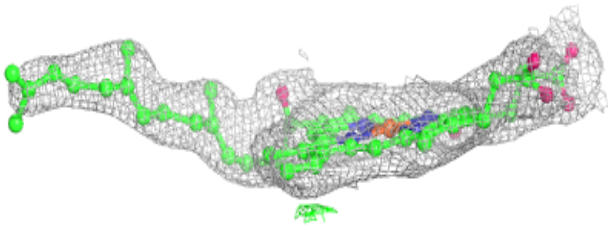


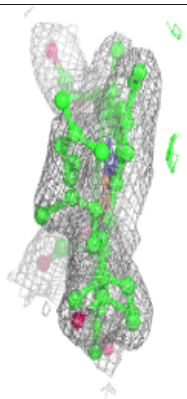


Electron density around HEA N 601:

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

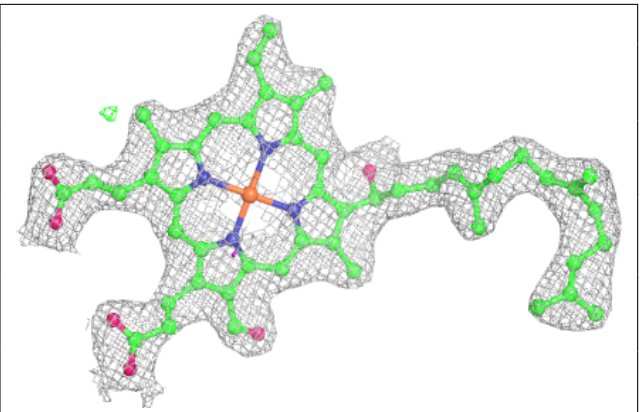


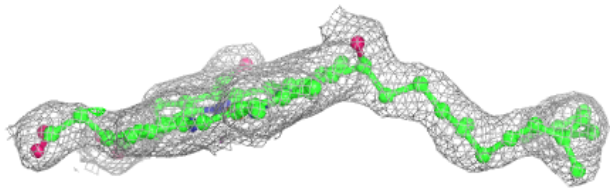


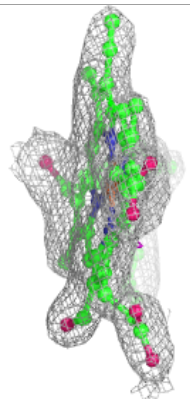


Electron density around HEA N 602:

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







6.5 Other polymers (i)

There are no such residues in this entry.