wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 04:56 am BST

PDB ID	:	2Y69 / pdb_00002y69
Title	:	Bovine heart cytochrome c oxidase re-refined with molecular oxygen
Authors	:	Kaila, V.R.I.; Oksanen, E.; Goldman, A.; Verkhovsky, M.I.; Sundholm, D.; Wikstrom, M.
Deposited on	:	2011-01-20
Resolution	:	1.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

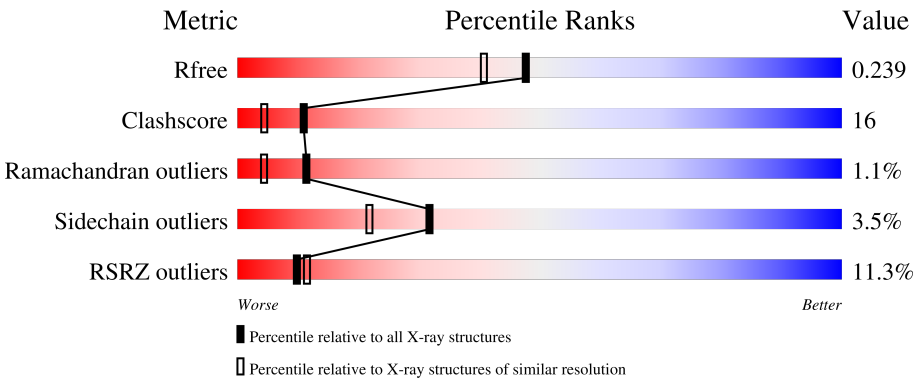
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	4% 79% 20% •
2	B	227	6% 78% 19% •
2	O	227	13% 71% 25% •
3	C	261	2% 88% 11% •

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Mol	Chain	Length	Quality of chain
3	P	261	4% 85% 14%
4	D	169	9% 69% 16% 15%
4	Q	169	30% 51% 30% 15%
5	E	152	3% 63% 6% 32%
5	R	152	6% 52% 15% 32%
6	F	129	11% 53% 15% 28%
6	S	129	12% 52% 16% 28%
7	G	97	25% 53% 25% 8% 13%
7	T	97	25% 58% 19% 8% 13%
8	H	86	12% 66% 13% 8% 13%
8	U	86	20% 60% 21% 5% 13%
9	I	74	23% 73% 19%
9	V	74	39% 68% 22% 7%
10	J	80	11% 62% 6% 29%
10	W	80	19% 64% 8% 29%
11	K	80	6% 55% 5% 39%
11	X	80	25% 32% 25% 39%
12	L	63	5% 56% 16% 27%
12	Y	63	17% 43% 27% 27%
13	M	70	11% 49% 9% 39%
13	Z	70	17% 36% 21% 40%

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
23	DMU	M	1044	X	-	-	-
23	DMU	Z	1043	X	-	-	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 30116 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	513	4017	2685	622	676	34	0	0	0
1	N	513	4017	2685	622	676	34	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	1822	1184	281	339	18	0	0	0
2	O	226	1814	1179	280	338	17	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.

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

- Molecule 5 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	104	842	538	141	161	2	0	0	0
5	R	104	842	538	141	161	2	0	0	0

- Molecule 6 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	93	717	447	127	138	5	0	0	0
6	S	93	717	447	127	138	5	0	0	0

- Molecule 7 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 6A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
7	G	84	671	428	128	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 VIB ISOFORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	75	628	395	114	114	5	0	0	0
8	U	75	628	395	114	114	5	0	0	0

- Molecule 9 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	71	585	381	105	95	4	0	0	0
9	V	71	585	381	105	95	4	0	0	0

- Molecule 10 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	57	451	291	76	81	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	W	57	451	291	76	81	3	0	0	0

- Molecule 11 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 7B.

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.

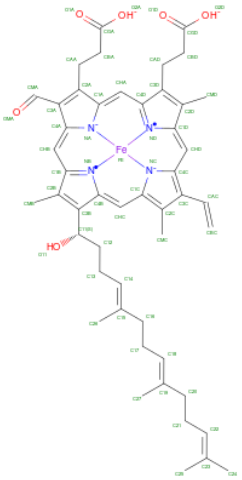
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	380	254	64	60	2	0	0	0
			Total	C	N	O	S			
12	Y	46	380	254	64	60	2	0	0	0

- Molecule 13 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 8H.

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	42	329	220	52	57	0	0	0

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

HEA

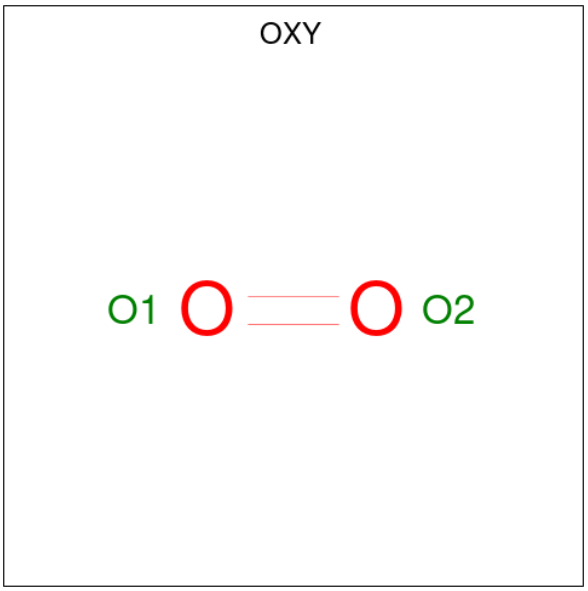


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
14	N	1	60	49	1	4	6	0	0

- Molecule 15 is COPPER (II) ION (CCD ID: 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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).

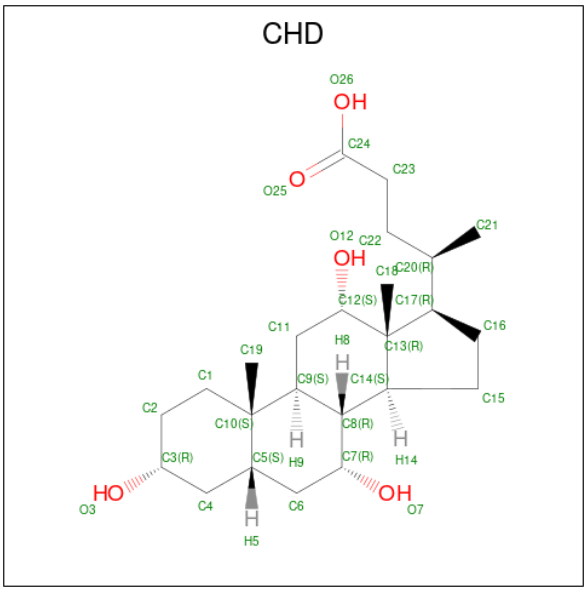


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 2 2	0	0
16	N	1	Total O 2 2	0	0

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

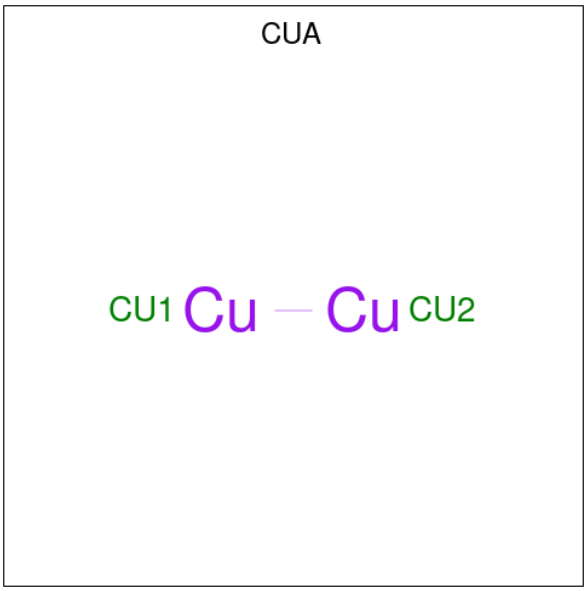
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



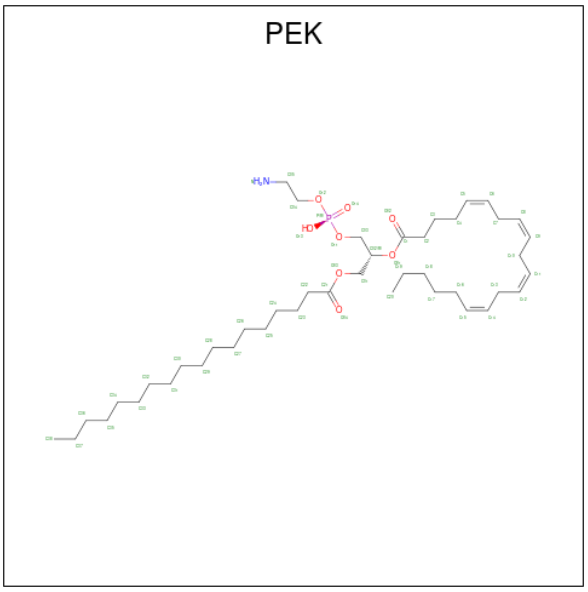
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
18	A	1	29	24	5	0	0
			Total	C	O		
18	C	1	29	24	5	0	0
			Total	C	O		
18	G	1	29	24	5	0	0
			Total	C	O		
18	N	1	29	24	5	0	0
			Total	C	O		
18	P	1	29	24	5	0	0
			Total	C	O		
18	T	1	29	24	5	0	0

- Molecule 19 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

- Molecule 20 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

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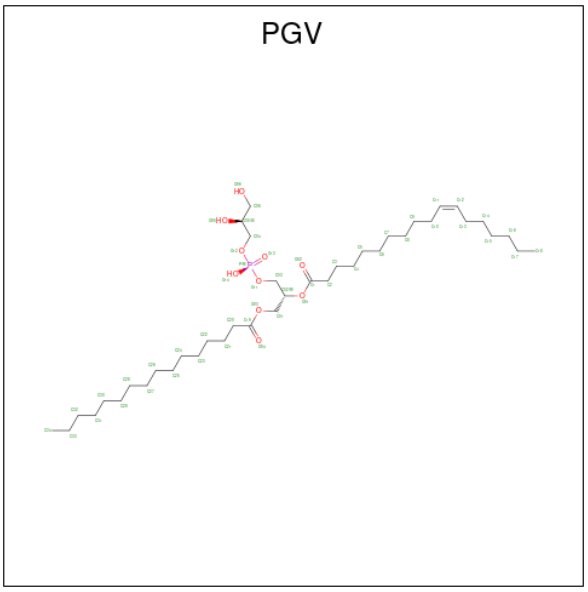
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
20	P	1	53	43	1	8	1	0	0

- Molecule 21 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).

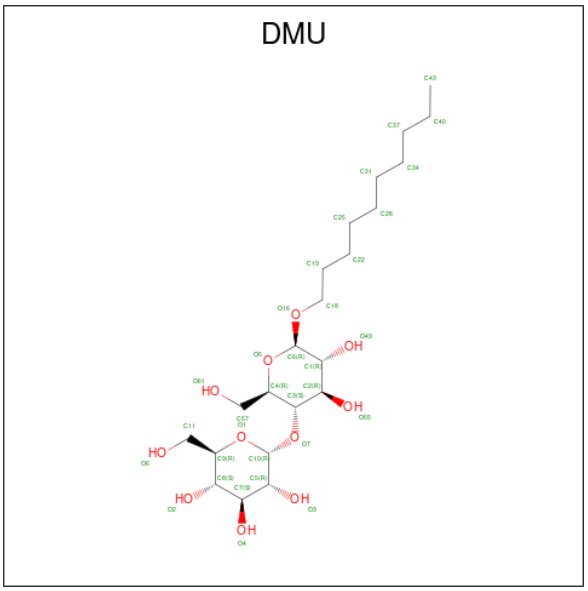


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
21	C	1	51	40	10	1	0	0
			Total	C	O	P		
21	C	1	51	40	10	1	0	0
			Total	C	O	P		
21	P	1	51	40	10	1	0	0
			Total	C	O	P		
21	P	1	51	40	10	1	0	0

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
24	A	114	114	114	0	0
24	B	102	102	102	0	0
24	C	85	85	85	0	0
24	D	43	43	43	0	0
24	F	45	45	45	0	0
24	G	41	41	41	0	0
24	H	49	49	49	0	0
24	I	20	20	20	0	0
24	J	26	26	26	0	0
24	K	10	10	10	0	0

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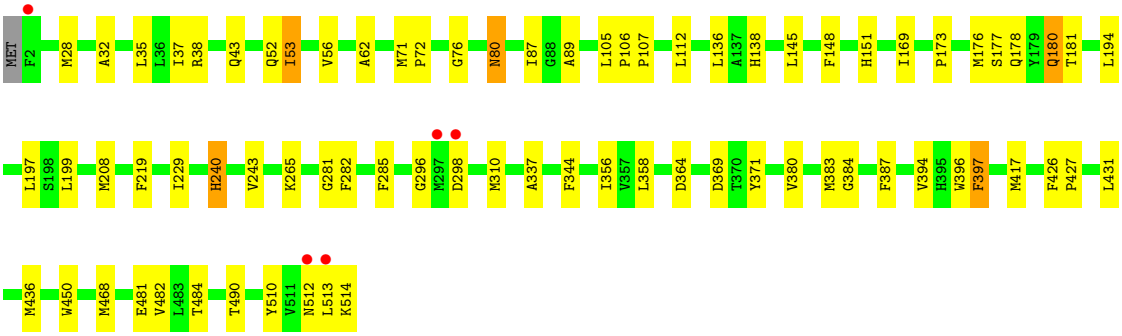
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
24	L	11	11	11	0	0
			Total	O		
24	M	10	10	10	0	0
			Total	O		
24	N	118	118	118	0	0
			Total	O		
24	O	88	88	88	0	0
			Total	O		
24	P	17	17	17	0	0
			Total	O		
24	Q	54	54	54	0	0
			Total	O		
24	R	56	56	56	0	0
			Total	O		
24	S	46	46	46	0	0
			Total	O		
24	T	30	30	30	0	0
			Total	O		
24	U	32	32	32	0	0
			Total	O		
24	V	23	23	23	0	0
			Total	O		
24	X	12	12	12	0	0
			Total	O		
24	Y	6	6	6	0	0
			Total	O		
24	Z	10	10	10	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.

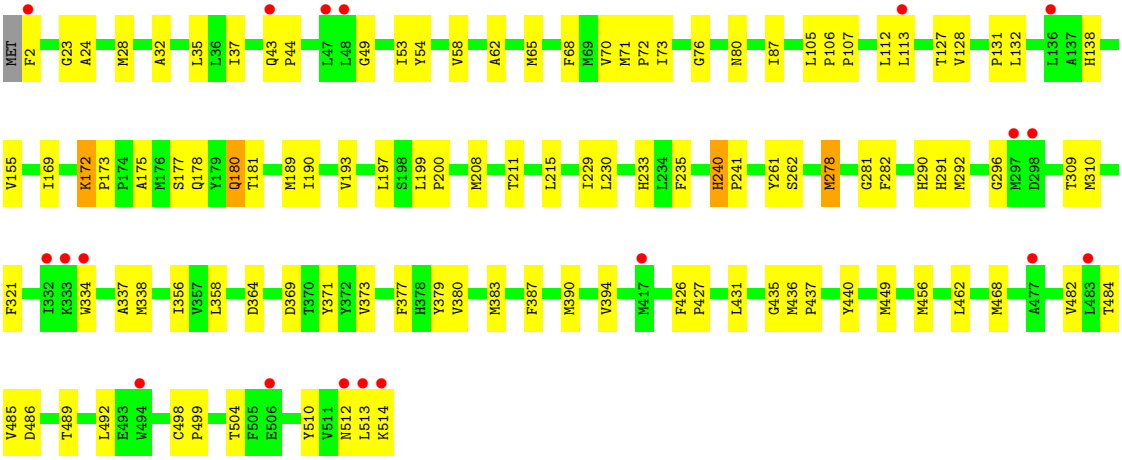
• Molecule 1: CYTOCHROME C OXIDASE SUBUNIT 1

Chain A:



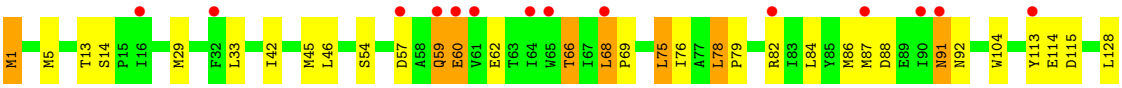
• Molecule 1: CYTOCHROME C OXIDASE SUBUNIT 1

Chain N:



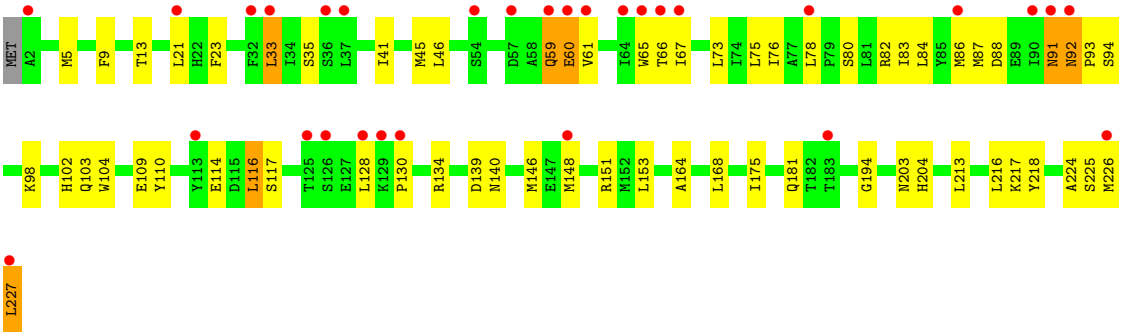
• Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2

Chain B:



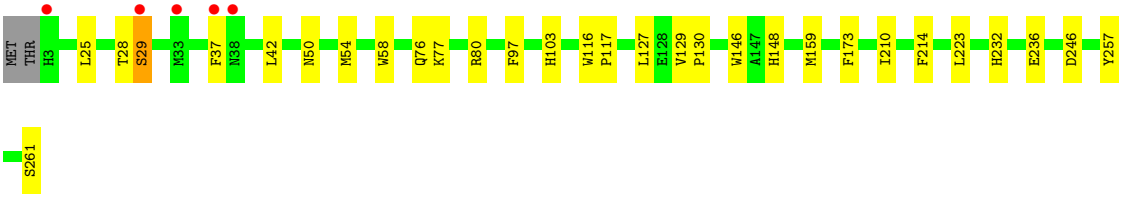
• Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2

Chain O:



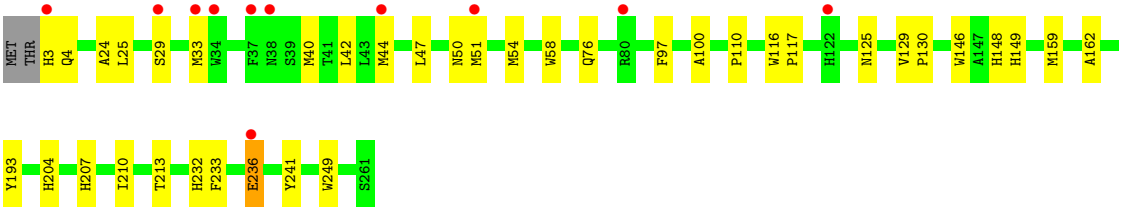
• Molecule 3: CYTOCHROME C OXIDASE SUBUNIT 3

Chain C:



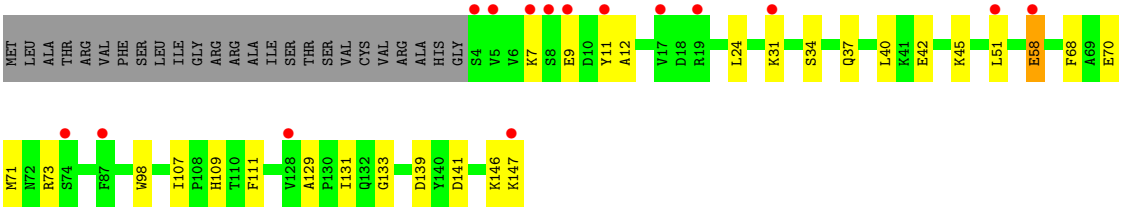
• Molecule 3: CYTOCHROME C OXIDASE SUBUNIT 3

Chain P:



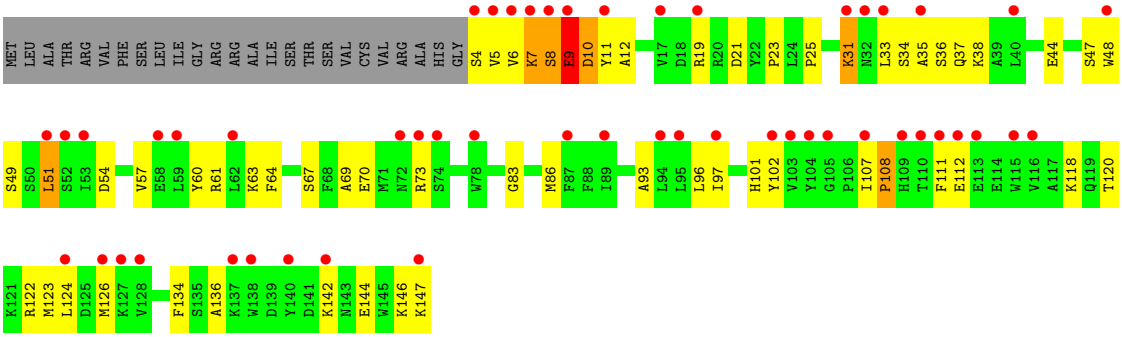
• Molecule 4: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1

Chain D:



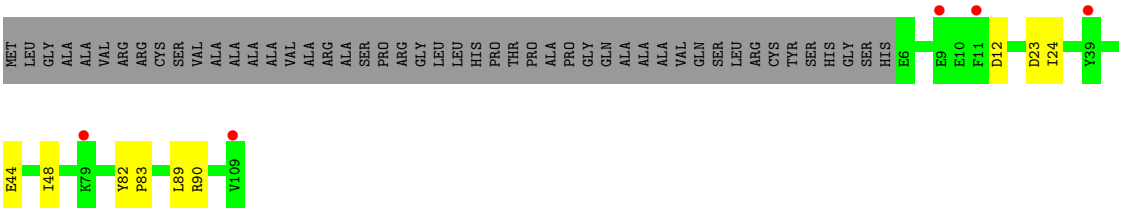
• Molecule 4: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1

Chain Q:



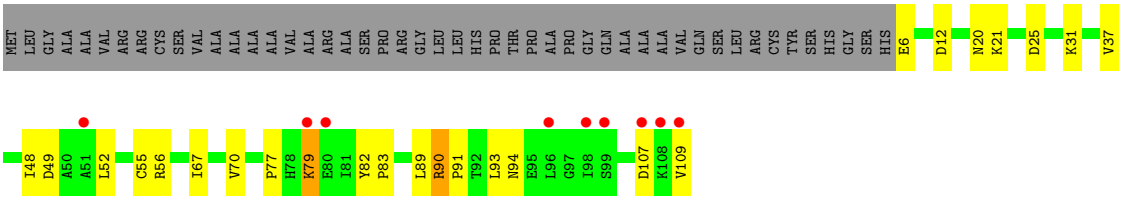
• Molecule 5: CYTOCHROME C OXIDASE SUBUNIT 5A

Chain E:



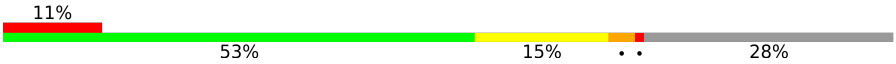
• Molecule 5: CYTOCHROME C OXIDASE SUBUNIT 5A

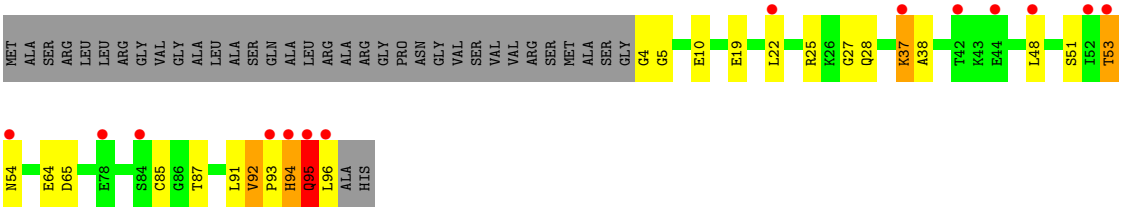
Chain R:



• Molecule 6: CYTOCHROME C OXIDASE SUBUNIT 5B

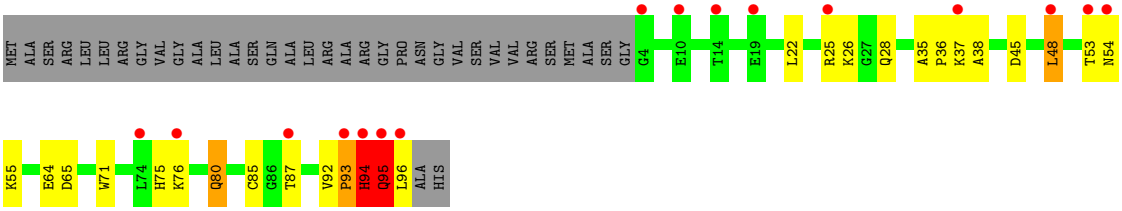
Chain F:





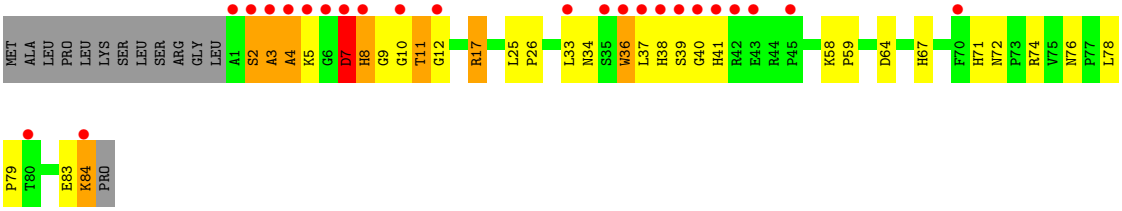
• Molecule 6: CYTOCHROME C OXIDASE SUBUNIT 5B

Chain S:



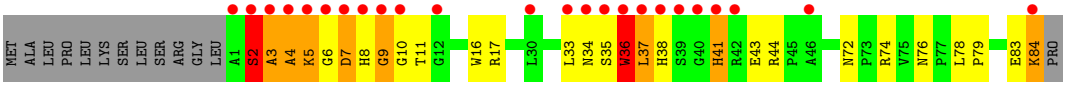
• Molecule 7: CYTOCHROME C OXIDASE POLYPEPTIDE 6A2

Chain G:



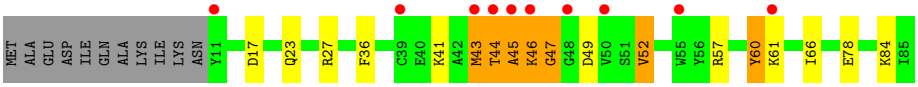
• Molecule 7: CYTOCHROME C OXIDASE POLYPEPTIDE 6A2

Chain T:



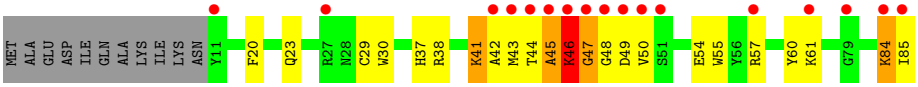
• Molecule 8: CYTOCHROME C OXIDASE SUBUNIT VIB ISOFORM 1

Chain H:



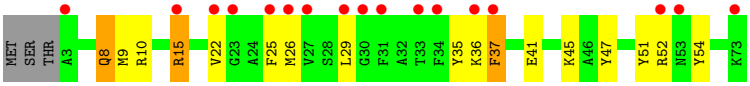
• Molecule 8: CYTOCHROME C OXIDASE SUBUNIT VIB ISOFORM 1

Chain U:



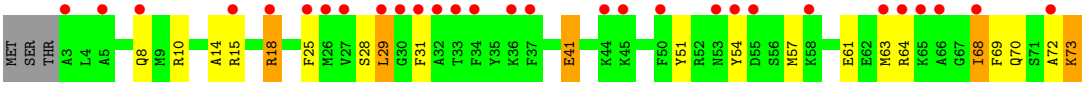
• Molecule 9: CYTOCHROME C OXIDASE POLYPEPTIDE VIC

Chain I:



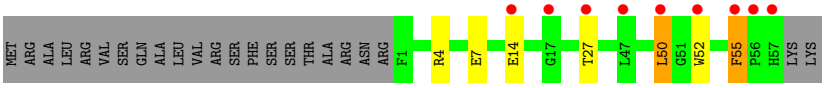
• Molecule 9: CYTOCHROME C OXIDASE POLYPEPTIDE VIC

Chain V:



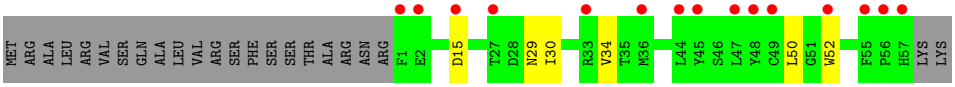
• Molecule 10: CYTOCHROME C OXIDASE POLYPEPTIDE 7A1

Chain J:



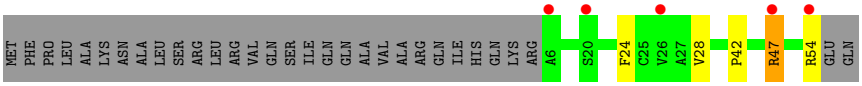
• Molecule 10: CYTOCHROME C OXIDASE POLYPEPTIDE 7A1

Chain W:



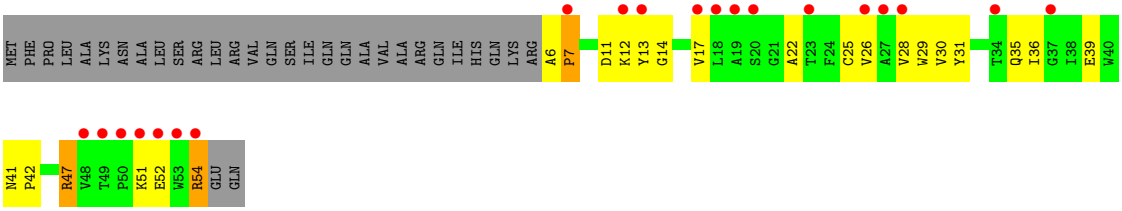
• Molecule 11: CYTOCHROME C OXIDASE POLYPEPTIDE 7B

Chain K:



• Molecule 11: CYTOCHROME C OXIDASE POLYPEPTIDE 7B

Chain X:

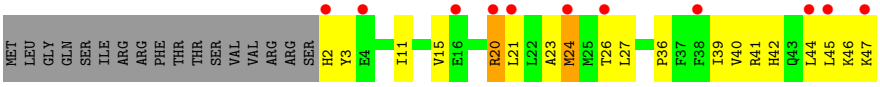


• Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 7C

Chain L:

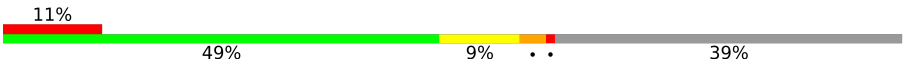
• Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 7C

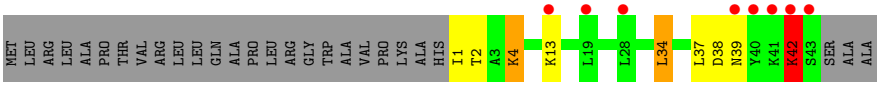
Chain Y:



• Molecule 13: CYTOCHROME C OXIDASE POLYPEPTIDE 8H

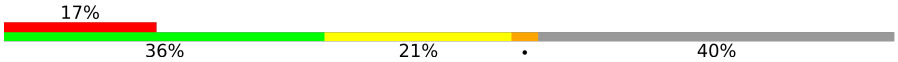
Chain M:

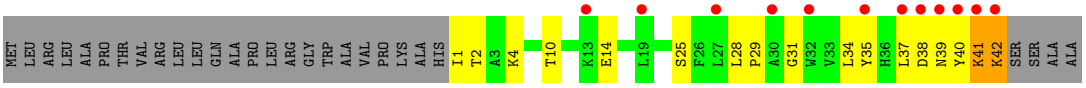




• Molecule 13: CYTOCHROME C OXIDASE POLYPEPTIDE 8H

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	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.15 – 1.95 64.15 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.15-1.95) 96.4 (64.15-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.245 0.209 , 0.239	Depositor DCC
R_{free} test set	16433 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30116	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: OXY, TPO, ZN, CUA, PGV, MG, DMU, CHD, HEA, PEK, CU

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	0.91	0/4156	1.02	11/5678 (0.2%)
1	N	0.76	0/4156	0.93	8/5678 (0.1%)
2	B	0.81	0/1868	0.95	1/2544 (0.0%)
2	O	0.63	0/1860	0.89	1/2534 (0.0%)
3	C	0.72	0/2197	0.84	0/3005
3	P	0.74	1/2197 (0.0%)	0.84	3/3005 (0.1%)
4	D	0.74	0/1229	0.91	2/1658 (0.1%)
4	Q	0.48	0/1229	0.77	0/1658
5	E	0.72	0/860	0.83	0/1167
5	R	0.57	0/860	0.86	0/1167
6	F	0.76	0/733	1.05	2/996 (0.2%)
6	S	0.70	0/733	1.01	1/996 (0.1%)
7	G	0.60	0/686	0.82	0/933
7	T	0.60	0/690	0.91	1/937 (0.1%)
8	H	0.66	0/648	0.85	0/877
8	U	0.53	0/648	0.87	2/877 (0.2%)
9	I	0.65	0/598	0.78	0/792
9	V	0.51	0/598	0.73	0/792
10	J	0.58	0/462	0.84	2/625 (0.3%)
10	W	0.55	0/462	0.83	0/625
11	K	0.73	0/398	0.89	0/546
11	X	0.48	0/398	0.85	1/546 (0.2%)
12	L	0.71	0/393	0.91	2/526 (0.4%)
12	Y	0.56	0/393	0.79	0/526
13	M	0.73	0/345	0.87	0/470
13	Z	0.52	0/339	0.83	0/462
All	All	0.72	1/29136 (0.0%)	0.90	37/39620 (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
6	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	236	GLU	CB-CG	6.01	1.70	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	92	VAL	CA-C-N	9.03	129.08	119.78
6	F	92	VAL	C-N-CA	9.03	129.08	119.78
1	N	240	HIS	N-CA-CB	7.21	117.24	110.39
1	A	105	LEU	CA-C-N	-6.99	113.18	120.38
1	A	105	LEU	C-N-CA	-6.99	113.18	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4017	0	3990	85	0
1	N	4017	0	3990	102	0
2	B	1822	0	1834	57	0
2	O	1814	0	1822	53	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	22	0
4	Q	1195	0	1183	115	0
5	E	842	0	838	5	0
5	R	842	0	838	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	717	0	700	34	0
6	S	717	0	700	46	0
7	G	671	0	633	56	0
7	T	675	0	644	49	0
8	H	628	0	578	21	0
8	U	628	0	580	33	0
9	I	585	0	597	37	0
9	V	585	0	597	57	0
10	J	451	0	446	11	0
10	W	451	0	446	8	1
11	K	384	0	366	3	0
11	X	384	0	366	34	1
12	L	380	0	380	15	0
12	Y	380	0	380	34	0
13	M	335	0	351	20	0
13	Z	329	0	347	34	0
14	A	120	0	108	18	0
14	N	120	0	108	22	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	2	0	0	0	0
16	N	2	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	29	0	39	1	0
18	C	29	0	39	2	0
18	G	29	0	39	1	0
18	N	29	0	39	2	0
18	P	29	0	39	1	0
18	T	29	0	39	1	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	C	53	0	77	10	0
20	P	53	0	77	13	0
21	C	102	0	152	6	0
21	P	102	0	152	11	0
22	F	1	0	0	0	0
22	S	1	0	0	0	0
23	M	33	0	40	2	0
23	Z	33	0	40	9	0
24	A	114	0	0	11	0
24	B	102	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	C	85	0	0	2	0
24	D	43	0	0	6	0
24	F	45	0	0	15	0
24	G	41	0	0	7	0
24	H	49	0	0	11	0
24	I	20	0	0	3	0
24	J	26	0	0	5	0
24	K	10	0	0	0	0
24	L	11	0	0	1	0
24	M	10	0	0	1	0
24	N	118	0	0	1	0
24	O	88	0	0	3	0
24	P	17	0	0	0	0
24	Q	54	0	0	28	0
24	R	56	0	0	16	0
24	S	46	0	0	6	0
24	T	30	0	0	1	0
24	U	32	0	0	4	0
24	V	23	0	0	8	0
24	X	12	0	0	3	0
24	Y	6	0	0	5	0
24	Z	10	0	0	5	0
All	All	30116	0	28831	955	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 955 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)
9:V:18:ARG:HH11	9:V:18:ARG:CB	1.09	1.59
13:M:42:LYS:O	13:M:42:LYS:CE	1.66	1.40
9:V:18:ARG:NH1	9:V:18:ARG:HB3	1.07	1.38
7:G:37:LEU:HD23	7:G:38:HIS:CE1	1.59	1.38
4:Q:4:SER:HB2	24:Q:2001:HOH:O	1.18	1.36

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:15:ASP:OD2	11:X:52:GLU:OE1[2_685]	2.16	0.04

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	511/514 (99%)	497 (97%)	13 (2%)	1 (0%)	43	36
1	N	511/514 (99%)	496 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	30	21
2	O	224/227 (99%)	209 (93%)	13 (6%)	2 (1%)	14	6
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/169 (84%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/169 (84%)	126 (89%)	13 (9%)	3 (2%)	5	1
5	E	102/152 (67%)	101 (99%)	1 (1%)	0	100	100
5	R	102/152 (67%)	101 (99%)	1 (1%)	0	100	100
6	F	91/129 (70%)	87 (96%)	2 (2%)	2 (2%)	5	1
6	S	91/129 (70%)	87 (96%)	2 (2%)	2 (2%)	5	1
7	G	81/97 (84%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/97 (84%)	65 (80%)	6 (7%)	10 (12%)	0	0
8	H	73/86 (85%)	68 (93%)	0	5 (7%)	1	0
8	U	73/86 (85%)	66 (90%)	4 (6%)	3 (4%)	2	0
9	I	69/74 (93%)	66 (96%)	3 (4%)	0	100	100
9	V	69/74 (93%)	64 (93%)	5 (7%)	0	100	100
10	J	55/80 (69%)	55 (100%)	0	0	100	100
10	W	55/80 (69%)	55 (100%)	0	0	100	100
11	K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	X	47/80 (59%)	42 (89%)	4 (8%)	1 (2%)	5	1
12	L	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
13	M	41/70 (59%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	40/70 (57%)	35 (88%)	4 (10%)	1 (2%)	4	1
All	All	3474/4004 (87%)	3314 (95%)	123 (4%)	37 (1%)	11	4

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	GLN
6	F	95	GLN
7	G	3	ALA
7	G	8	HIS
8	H	43	MET

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	426/427 (100%)	420 (99%)	6 (1%)	59	56
1	N	426/427 (100%)	418 (98%)	8 (2%)	50	45
2	B	211/211 (100%)	200 (95%)	11 (5%)	21	9
2	O	210/211 (100%)	198 (94%)	12 (6%)	18	8
3	C	224/226 (99%)	219 (98%)	5 (2%)	45	40
3	P	224/226 (99%)	223 (100%)	1 (0%)	84	85
4	D	128/148 (86%)	126 (98%)	2 (2%)	55	52
4	Q	128/148 (86%)	123 (96%)	5 (4%)	28	18
5	E	91/123 (74%)	90 (99%)	1 (1%)	65	64
5	R	91/123 (74%)	89 (98%)	2 (2%)	45	40
6	F	79/103 (77%)	75 (95%)	4 (5%)	21	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	79/103 (77%)	75 (95%)	4 (5%)	21	10
7	G	66/78 (85%)	60 (91%)	6 (9%)	9	2
7	T	67/78 (86%)	63 (94%)	4 (6%)	17	7
8	H	67/76 (88%)	65 (97%)	2 (3%)	36	27
8	U	67/76 (88%)	62 (92%)	5 (8%)	12	4
9	I	56/59 (95%)	53 (95%)	3 (5%)	20	9
9	V	56/59 (95%)	51 (91%)	5 (9%)	9	2
10	J	48/68 (71%)	47 (98%)	1 (2%)	47	41
10	W	48/68 (71%)	47 (98%)	1 (2%)	47	41
11	K	39/66 (59%)	37 (95%)	2 (5%)	21	10
11	X	39/66 (59%)	35 (90%)	4 (10%)	7	1
12	L	39/55 (71%)	37 (95%)	2 (5%)	21	10
12	Y	39/55 (71%)	36 (92%)	3 (8%)	12	3
13	M	37/57 (65%)	33 (89%)	4 (11%)	6	1
13	Z	36/57 (63%)	34 (94%)	2 (6%)	19	8
All	All	3021/3394 (89%)	2916 (96%)	105 (4%)	32	22

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	33	LEU
4	Q	9	GLU
11	X	54	ARG
2	O	60	GLU
2	O	110	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
10	W	29	ASN
3	P	68	GLN
9	V	53	ASN
6	S	95	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
7	TPO	T	11	7	8,10,11	0.70	0	10,14,16	1.19	0
7	TPO	G	11	7	8,10,11	0.73	0	10,14,16	1.27	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
7	TPO	T	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	11	TPO	P-OG1-CB	-2.30	116.27	123.21

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	5	0
7	G	11	TPO	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
18	CHD	G	1085	-	32,32,32	0.80	0	51,51,51	1.23	5 (9%)
21	PGV	P	1264	-	50,50,50	0.88	3 (6%)	53,56,56	0.97	4 (7%)
16	OXY	N	1515	14,15	1,1,1	0.59	0	-		
18	CHD	P	1265	-	32,32,32	0.75	0	51,51,51	1.38	11 (21%)
23	DMU	Z	1043	-	34,34,34	1.39	1 (2%)	45,45,45	1.88	7 (15%)
21	PGV	C	1263	-	50,50,50	0.90	2 (4%)	53,56,56	1.08	3 (5%)
23	DMU	M	1044	-	34,34,34	1.39	1 (2%)	45,45,45	2.07	9 (20%)
18	CHD	T	1085	-	32,32,32	0.67	0	51,51,51	1.43	5 (9%)
14	HEA	N	515	1	66,67,67	1.57	10 (15%)	78,103,103	2.23	25 (32%)
19	CUA	O	228	2	0,1,1	-	-	-		
14	HEA	A	516	1,16	66,67,67	1.40	8 (12%)	78,103,103	2.24	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	PGV	P	1263	-	50,50,50	0.90	2 (4%)	53,56,56	1.21	5 (9%)
18	CHD	C	1265	-	32,32,32	0.82	1 (3%)	51,51,51	1.21	5 (9%)
14	HEA	N	516	1,16	66,67,67	1.27	8 (12%)	78,103,103	2.19	25 (32%)
20	PEK	C	1262	-	52,52,52	0.85	2 (3%)	55,57,57	0.94	4 (7%)
16	OXY	A	1515	14,15	1,1,1	0.69	0	-		
18	CHD	N	1517	-	32,32,32	0.78	1 (3%)	51,51,51	1.10	4 (7%)
14	HEA	A	515	1	66,67,67	1.53	10 (15%)	78,103,103	2.28	26 (33%)
21	PGV	C	1264	-	50,50,50	0.91	2 (4%)	53,56,56	0.94	4 (7%)
20	PEK	P	1262	-	52,52,52	0.87	2 (3%)	55,57,57	0.99	4 (7%)
18	CHD	A	1517	-	32,32,32	0.82	1 (3%)	51,51,51	1.28	6 (11%)
19	CUA	B	228	2	0,1,1	-	-	-		

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
18	CHD	T	1085	-	-	2/9/74/74	0/4/4/4
18	CHD	G	1085	-	-	2/9/74/74	0/4/4/4
21	PGV	P	1264	-	-	16/55/55/55	-
18	CHD	A	1517	-	-	2/9/74/74	0/4/4/4
18	CHD	P	1265	-	-	2/9/74/74	0/4/4/4
14	HEA	A	515	1	-	7/36/76/76	-
23	DMU	Z	1043	-	4/4/10/10	11/19/59/59	0/2/2/2
21	PGV	P	1263	-	-	13/55/55/55	-
18	CHD	C	1265	-	-	2/9/74/74	0/4/4/4
21	PGV	C	1263	-	-	16/55/55/55	-
21	PGV	C	1264	-	-	17/55/55/55	-
14	HEA	N	516	1,16	-	7/36/76/76	-
20	PEK	C	1262	-	-	19/56/56/56	-
20	PEK	P	1262	-	-	20/56/56/56	-
18	CHD	N	1517	-	-	0/9/74/74	0/4/4/4
14	HEA	N	515	1	-	11/36/76/76	-
14	HEA	A	516	1,16	-	8/36/76/76	-
23	DMU	M	1044	-	4/4/10/10	10/19/59/59	0/2/2/2

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	1044	DMU	C3-C4	-7.75	1.32	1.52
23	Z	1043	DMU	C3-C4	-7.71	1.32	1.52
14	N	515	HEA	C3B-C2B	4.43	1.44	1.34
14	N	515	HEA	C3A-C2A	4.40	1.46	1.36
21	C	1263	PGV	O03-C19	4.18	1.45	1.33

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	515	HEA	C3A-C2A-C1A	-7.96	99.48	107.08
14	A	516	HEA	C3A-C2A-C1A	-7.86	99.57	107.08
14	A	515	HEA	C3A-C2A-C1A	-7.25	100.15	107.08
14	N	516	HEA	C3A-C2A-C1A	-6.79	100.59	107.08
23	Z	1043	DMU	O5-C4-C57	6.67	123.03	106.44

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	M	1044	DMU	C3
23	M	1044	DMU	C5
23	M	1044	DMU	C4
23	M	1044	DMU	C2
23	Z	1043	DMU	C3

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	515	HEA	C2A-C3A-CMA-OMA
14	A	515	HEA	C4A-C3A-CMA-OMA
14	A	515	HEA	C14-C15-C16-C17
14	A	515	HEA	C26-C15-C16-C17
14	A	515	HEA	C16-C17-C18-C19

There are no ring outliers.

18 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	1085	CHD	1	0
21	P	1264	PGV	7	0
18	P	1265	CHD	1	0
23	Z	1043	DMU	9	0

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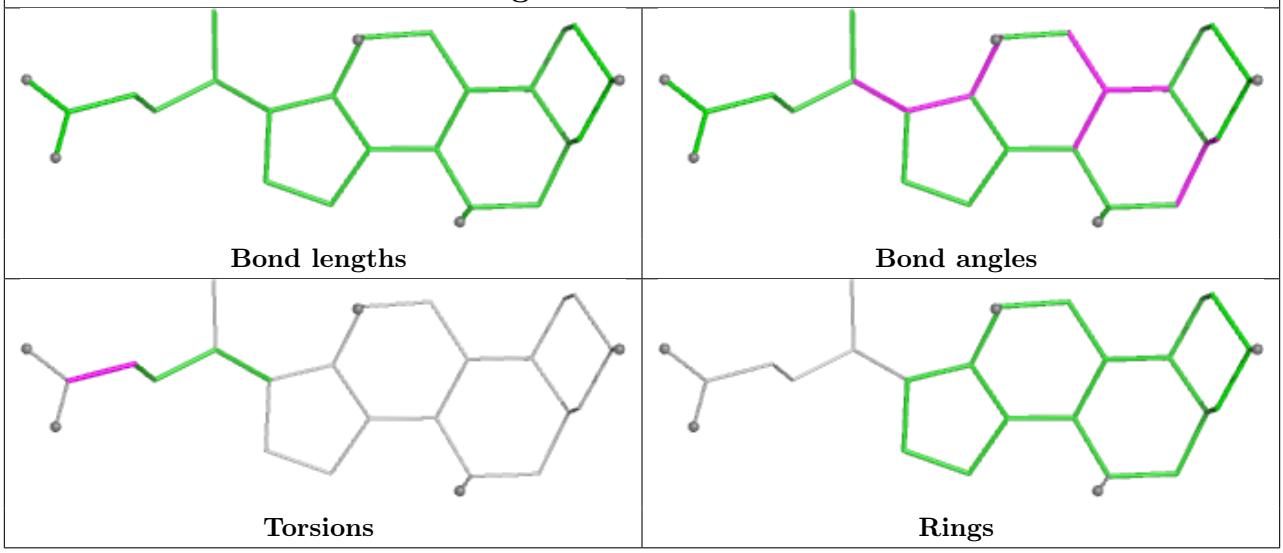
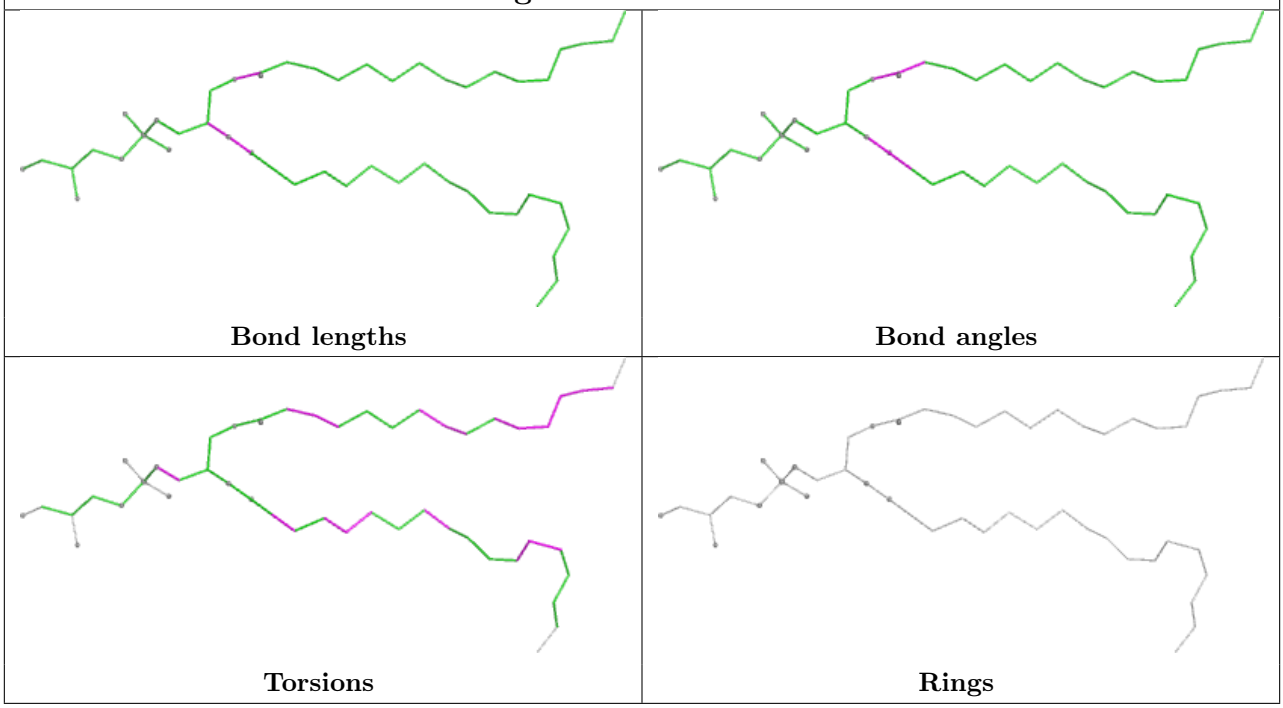
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	1263	PGV	1	0
23	M	1044	DMU	2	0
18	T	1085	CHD	1	0
14	N	515	HEA	18	0
14	A	516	HEA	3	0
21	P	1263	PGV	4	0
18	C	1265	CHD	2	0
14	N	516	HEA	4	0
20	C	1262	PEK	10	0
18	N	1517	CHD	2	0
14	A	515	HEA	15	0
21	C	1264	PGV	5	0
20	P	1262	PEK	13	0
18	A	1517	CHD	1	0

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

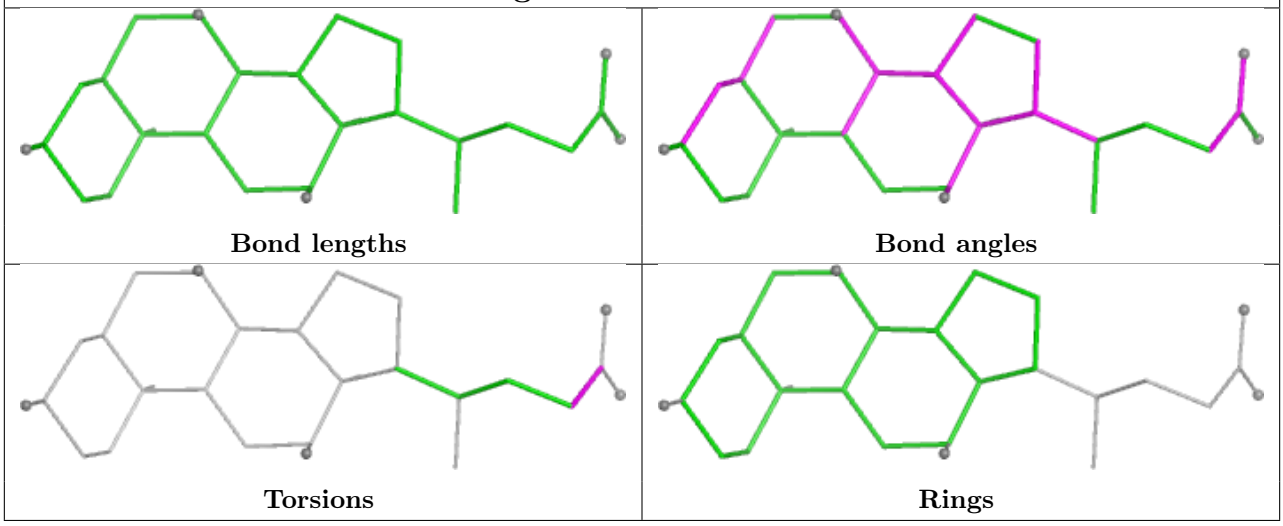
Ligand CHD G 1085



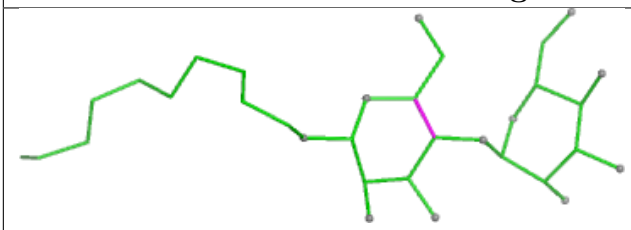
Ligand PGV P 1264



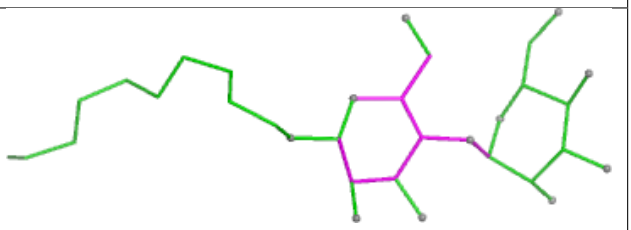
Ligand CHD P 1265



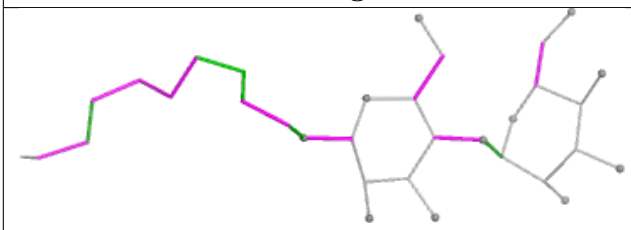
Ligand DMU Z 1043



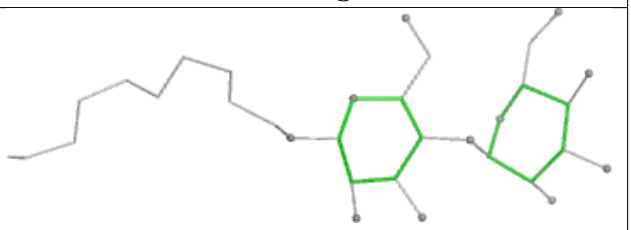
Bond lengths



Bond angles

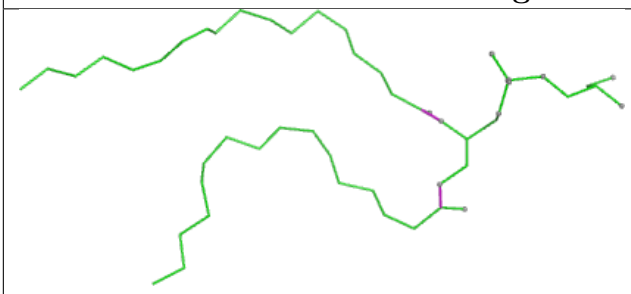


Torsions



Rings

Ligand PGV C 1263



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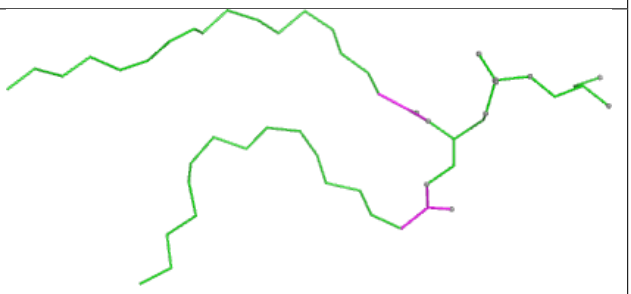

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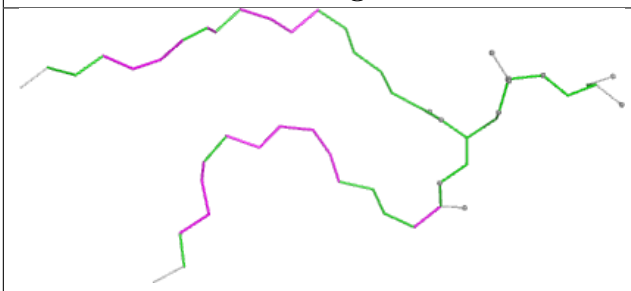

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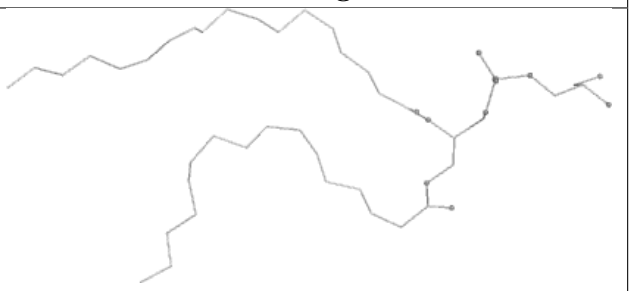
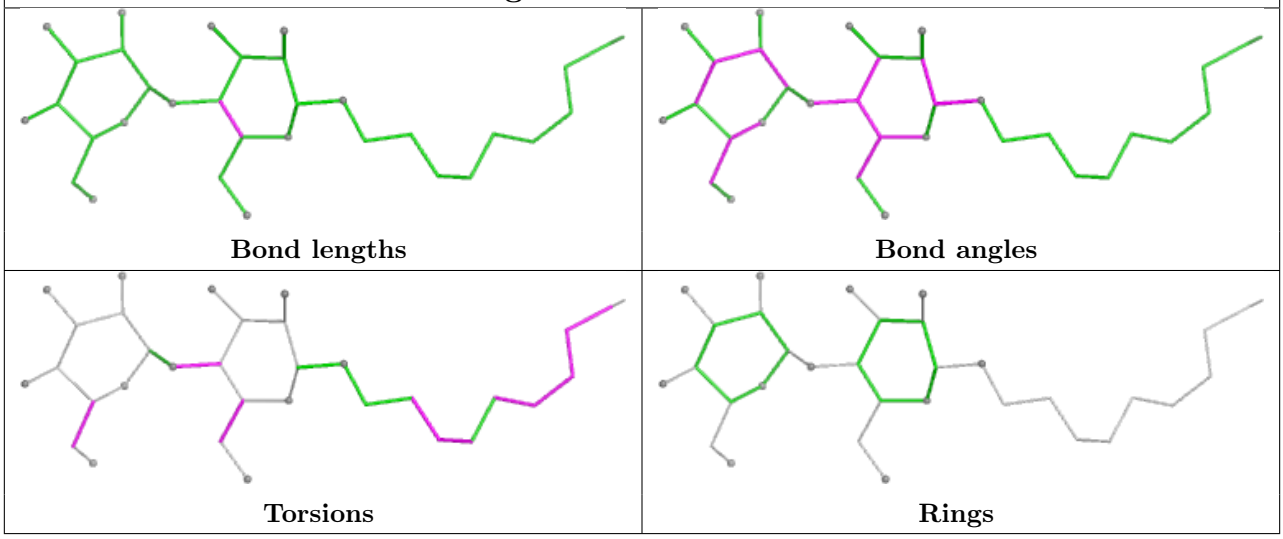
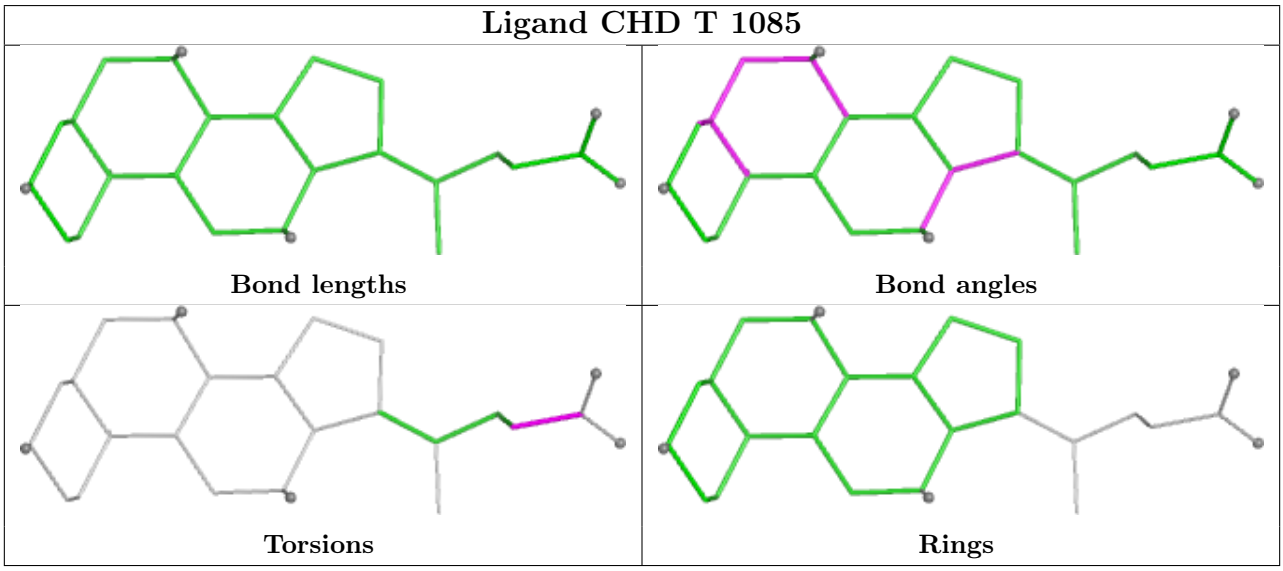


Rings

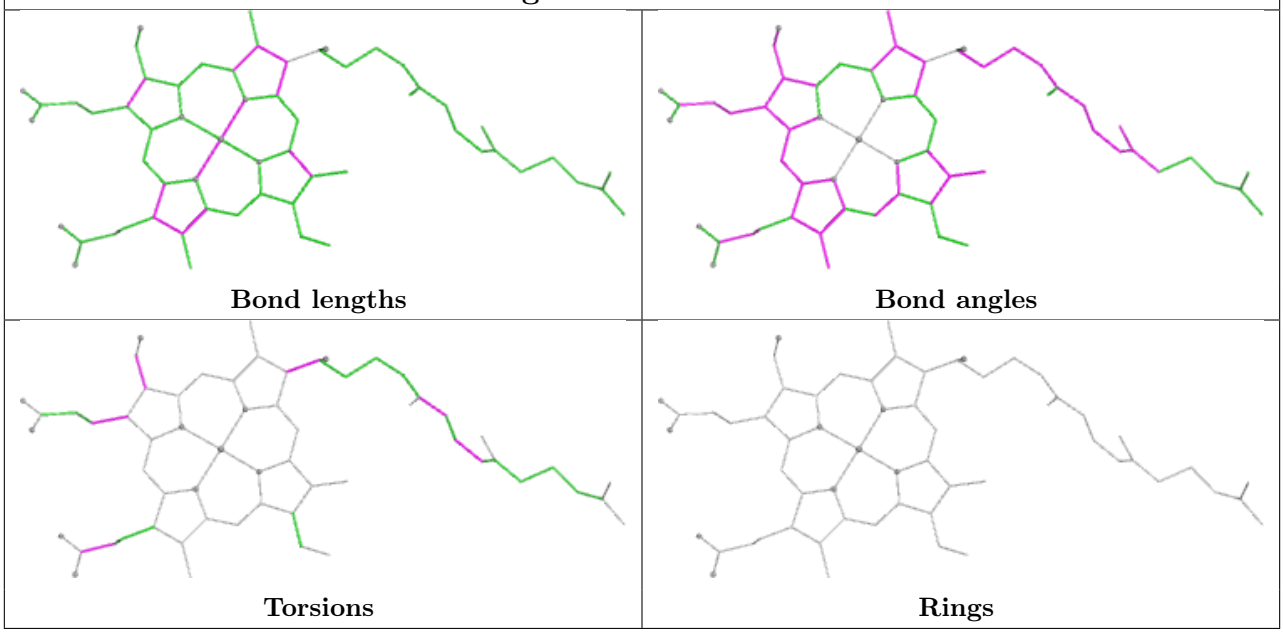
Ligand DMU M 1044



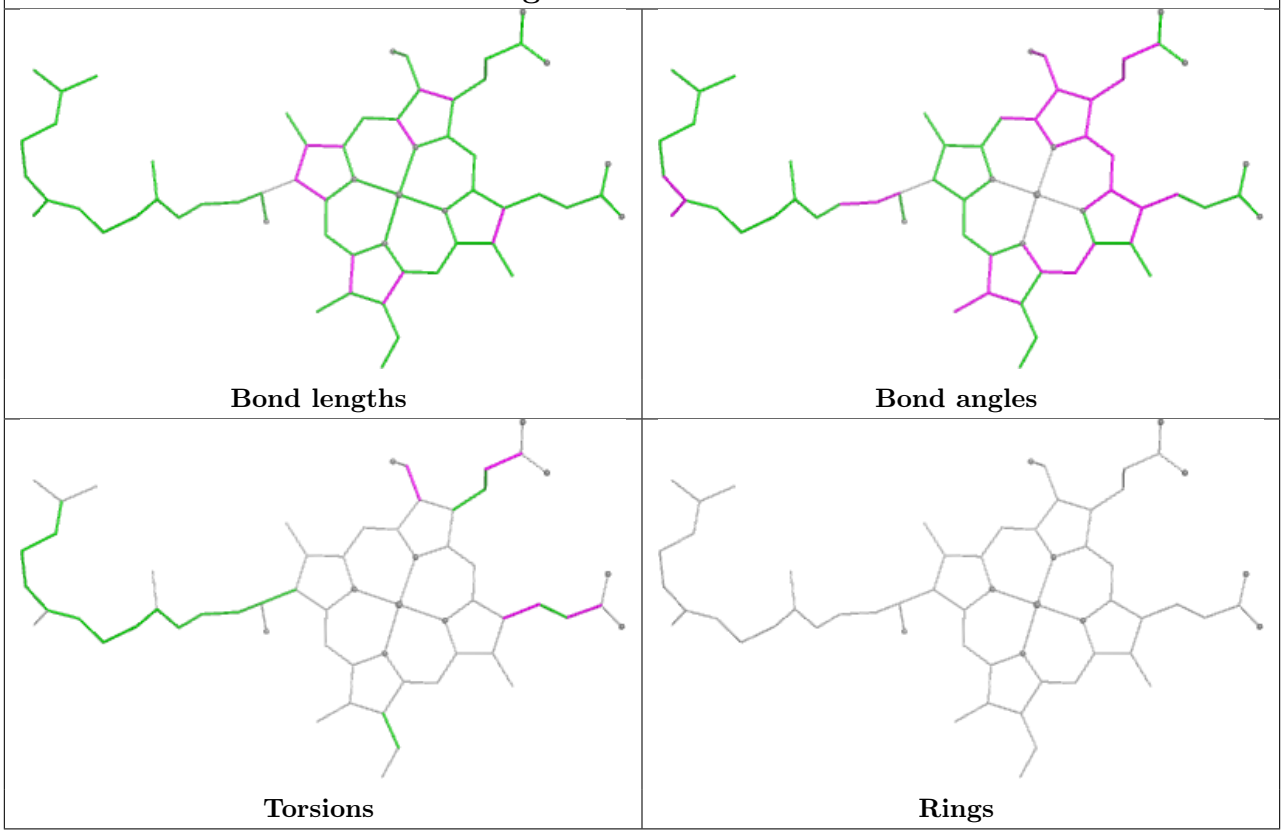
Ligand CHD T 1085



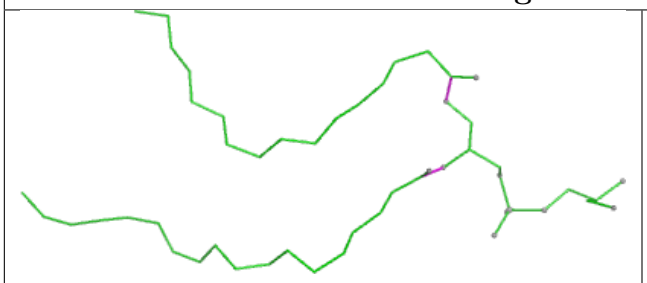
Ligand HEA N 515



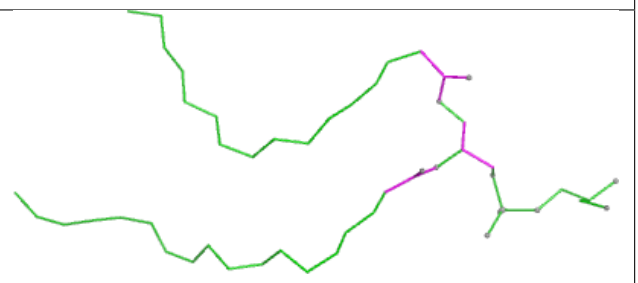
Ligand HEA A 516



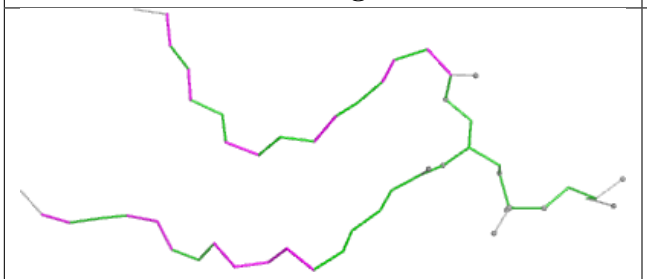
Ligand PGV P 1263



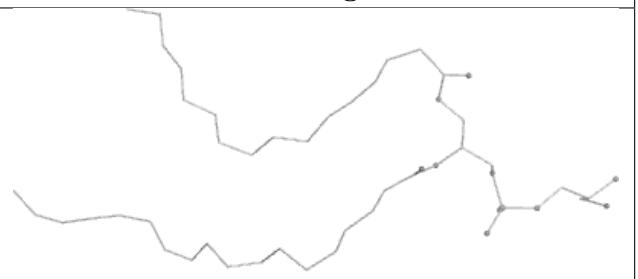
Bond lengths



Bond angles

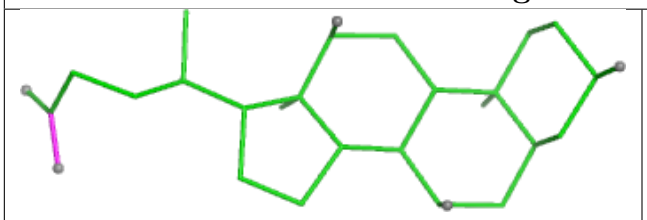


Torsions

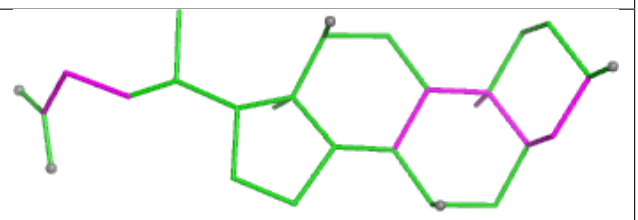


Rings

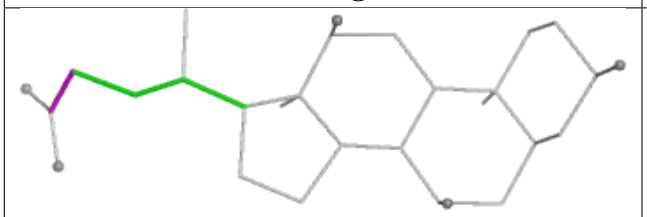
Ligand CHD C 1265



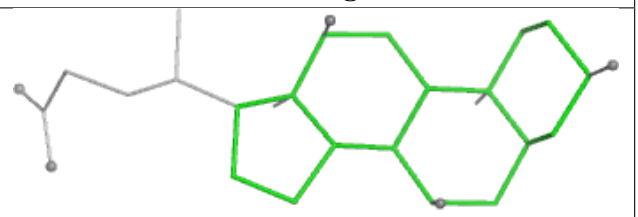
Bond lengths



Bond angles

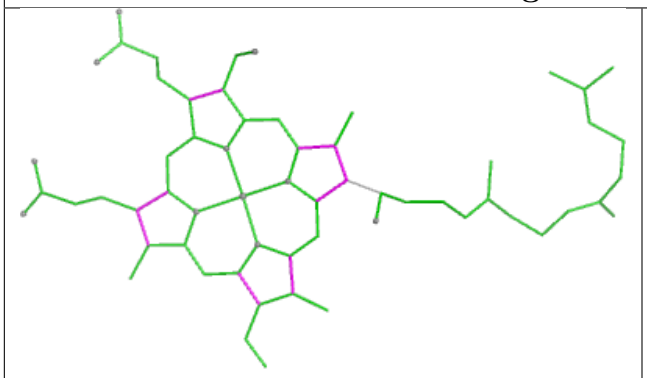


Torsions

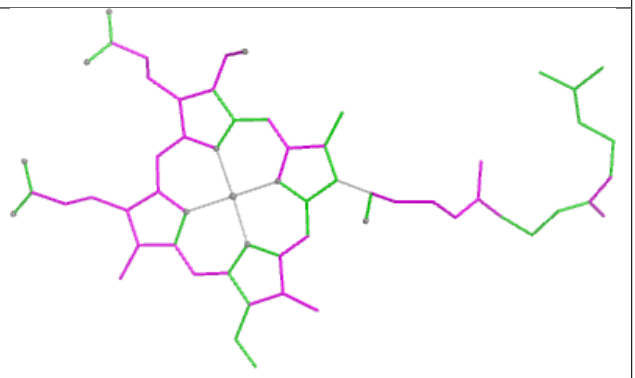


Rings

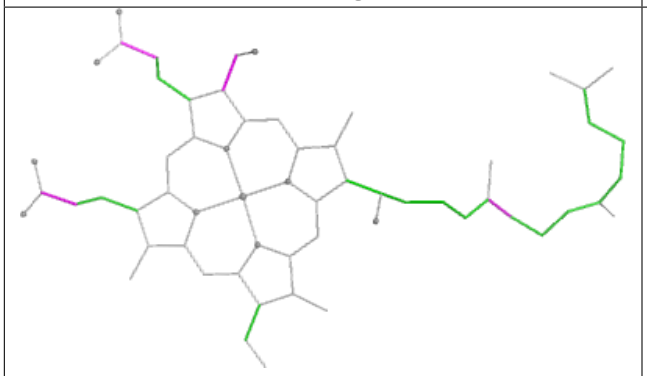
Ligand HEA N 516



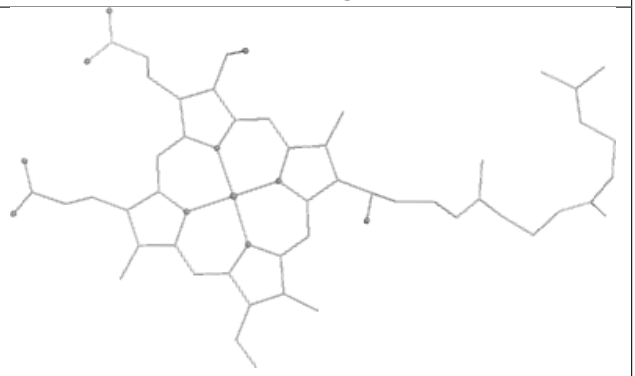
Bond lengths



Bond angles

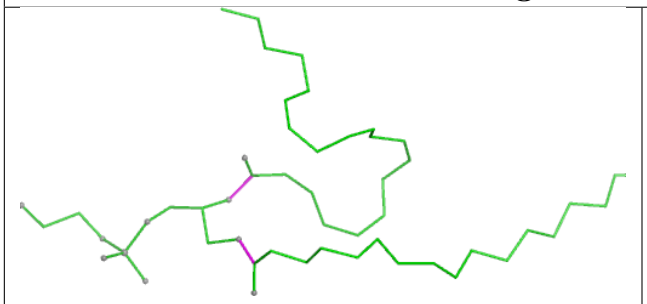


Torsions

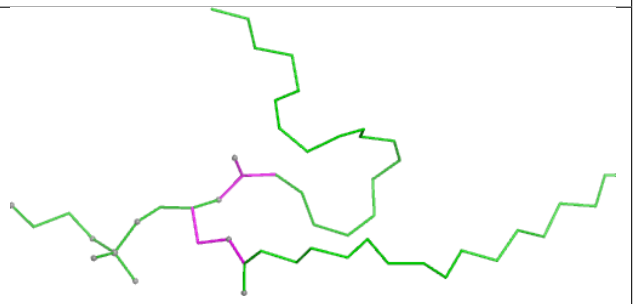


Rings

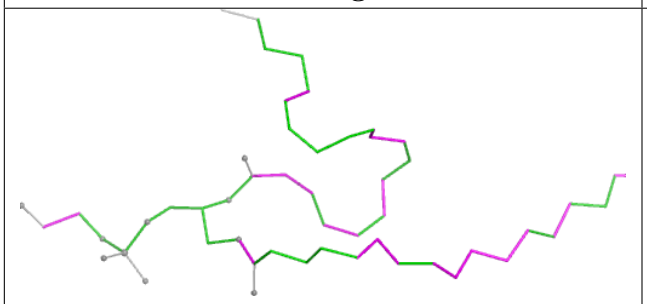
Ligand PEK C 1262



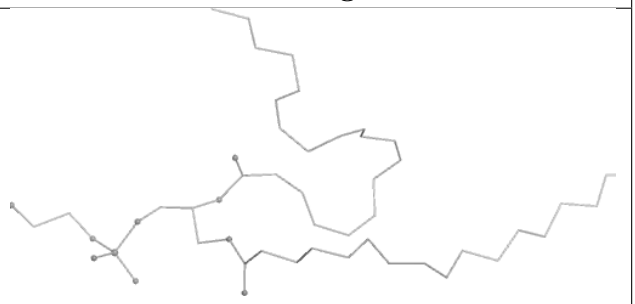
Bond lengths



Bond angles

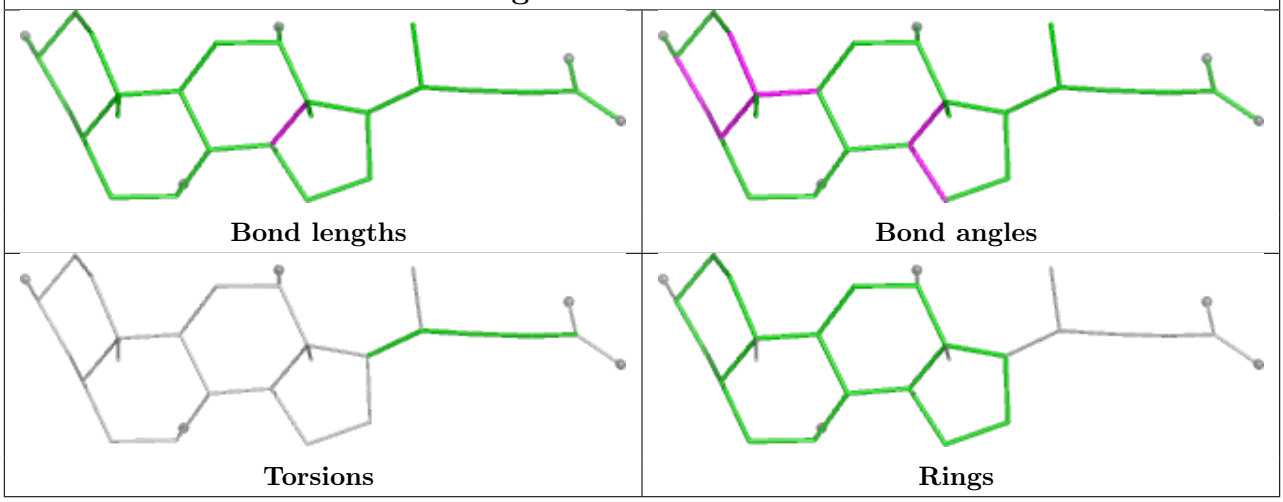


Torsions

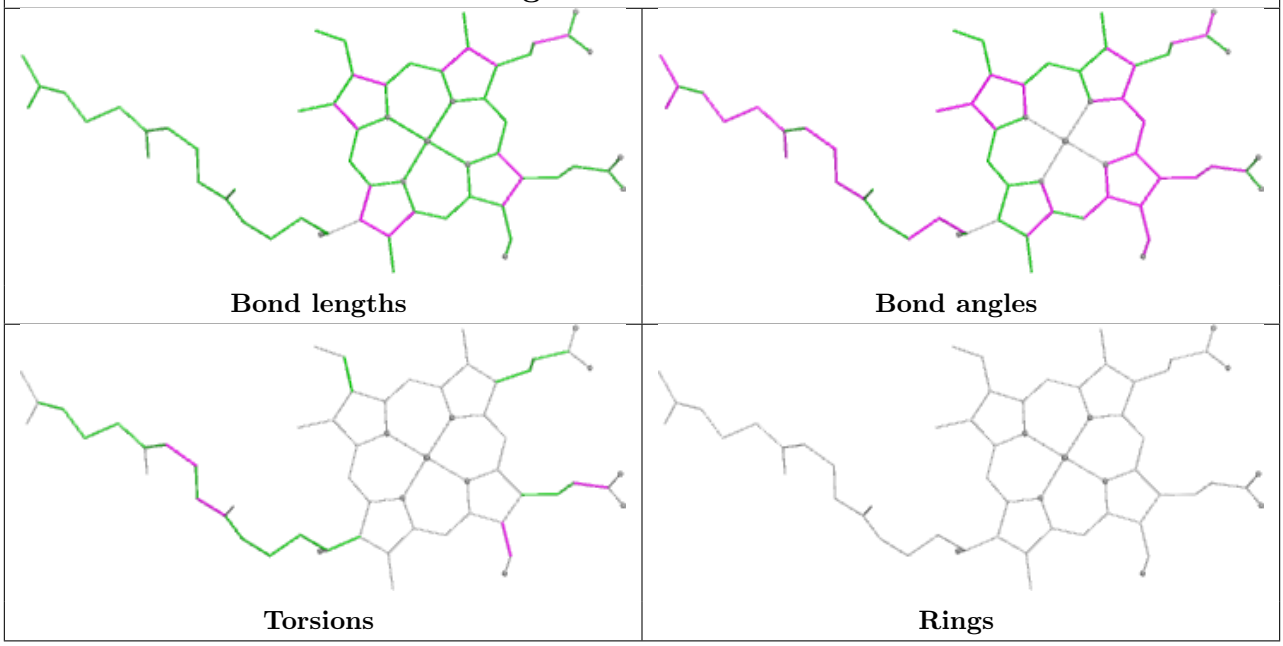


Rings

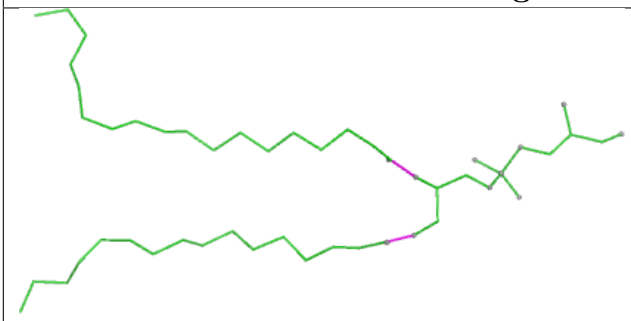
Ligand CHD N 1517



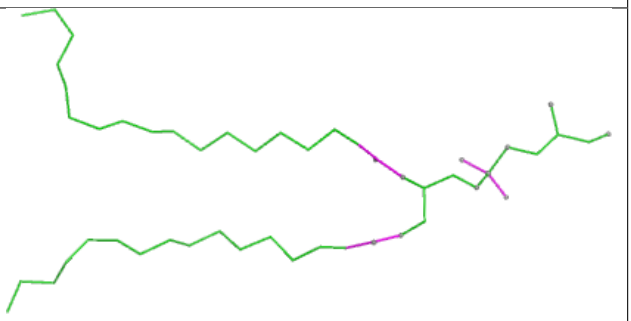
Ligand HEA A 515



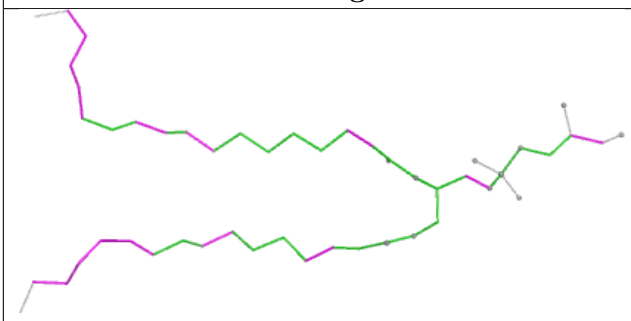
Ligand PGV C 1264



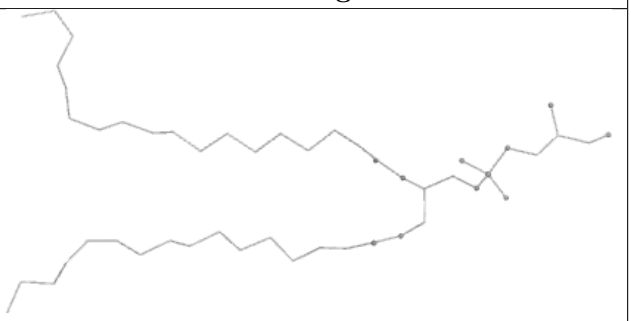
Bond lengths



Bond angles



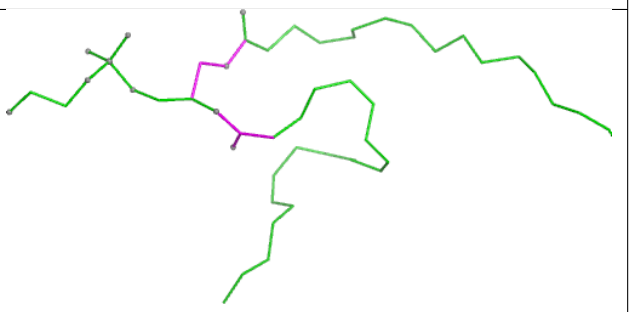
Torsions



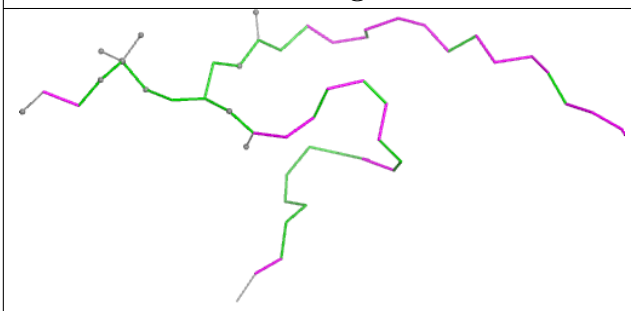
Rings

Ligand PEK P 1262

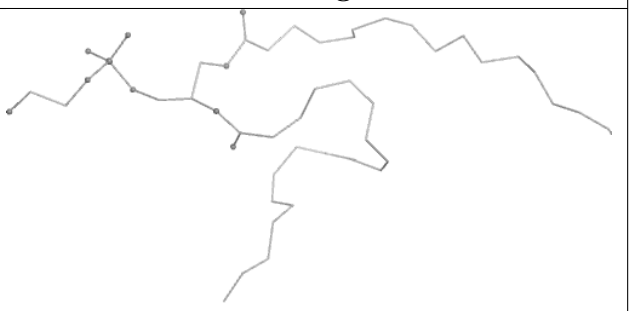
Bond lengths



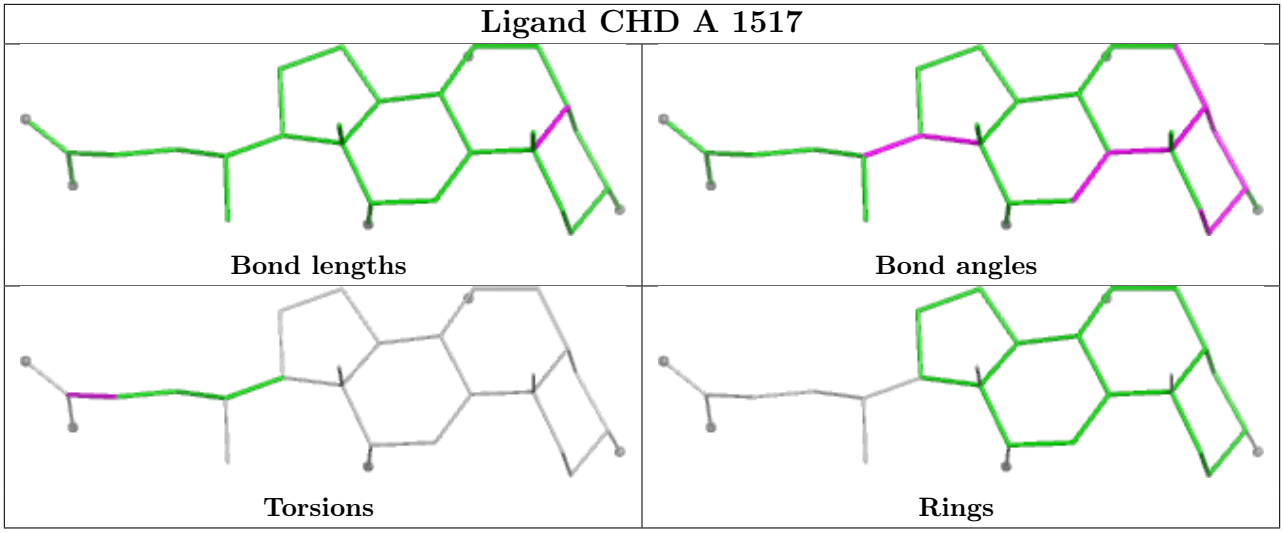
Bond angles



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%)	-0.16	5 (0%)	79	84	24, 29, 36, 56	0
1	N	513/514 (99%)	0.41	19 (3%)	45	52	27, 37, 50, 106	0
2	B	227/227 (100%)	0.46	14 (6%)	26	31	24, 35, 54, 67	0
2	O	226/227 (99%)	1.09	30 (13%)	7	8	32, 46, 82, 136	0
3	C	259/261 (99%)	0.28	5 (1%)	66	74	27, 35, 50, 114	0
3	P	259/261 (99%)	0.53	11 (4%)	40	47	29, 37, 55, 122	0
4	D	144/169 (85%)	0.65	15 (10%)	11	13	30, 38, 64, 99	0
4	Q	144/169 (85%)	1.73	51 (35%)	1	0	40, 59, 91, 210	0
5	E	104/152 (68%)	0.38	5 (4%)	35	41	31, 39, 67, 110	0
5	R	104/152 (68%)	1.01	9 (8%)	16	18	36, 49, 79, 109	0
6	F	93/129 (72%)	0.78	14 (15%)	5	6	29, 40, 83, 243	0
6	S	93/129 (72%)	1.07	16 (17%)	4	4	32, 43, 89, 168	0
7	G	83/97 (85%)	1.41	24 (28%)	1	1	30, 42, 138, 172	0
7	T	83/97 (85%)	1.71	24 (28%)	1	1	30, 47, 146, 256	0
8	H	75/86 (87%)	0.90	10 (13%)	7	8	31, 44, 88, 166	0
8	U	75/86 (87%)	1.41	17 (22%)	2	2	38, 51, 99, 141	0
9	I	71/74 (95%)	1.20	17 (23%)	2	2	31, 47, 90, 126	0
9	V	71/74 (95%)	1.86	29 (40%)	0	0	37, 59, 90, 106	0
10	J	57/80 (71%)	0.93	9 (15%)	5	5	34, 44, 81, 95	0
10	W	57/80 (71%)	1.67	15 (26%)	1	1	38, 50, 100, 127	0
11	K	49/80 (61%)	0.96	5 (10%)	12	13	33, 43, 70, 118	0
11	X	49/80 (61%)	1.86	20 (40%)	0	0	49, 58, 84, 125	0
12	L	46/63 (73%)	0.64	3 (6%)	25	28	27, 37, 58, 137	0
12	Y	46/63 (73%)	1.50	11 (23%)	2	2	37, 50, 89, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/70 (61%)	1.11	8 (18%) 3 3	28, 37, 122, 212	0
13	Z	42/70 (60%)	1.80	12 (28%) 1 1	44, 54, 120, 170	0
All	All	3526/4004 (88%)	0.71	398 (11%) 10 11	24, 39, 81, 256	0

The worst 5 of 398 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	3	ALA	8.6
6	S	96	LEU	8.4
2	O	113	TYR	8.1
10	W	52	TRP	8.0
7	G	36	TRP	7.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	TPO	G	11	11/12	0.75	0.31	73,140,486,493	0
7	TPO	T	11	11/12	0.77	0.28	65,143,410,489	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	DMU	Z	1043	33/33	0.88	0.16	42,72,127,190	0
16	OXY	A	1515	2/2	0.91	0.11	32,32,32,41	0
23	DMU	M	1044	33/33	0.92	0.12	35,51,76,92	0

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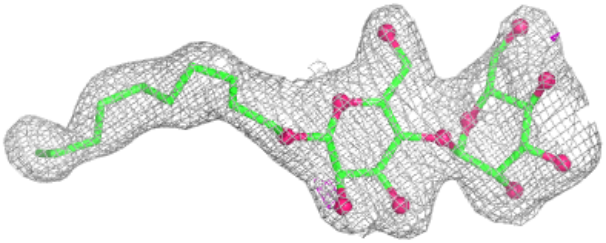
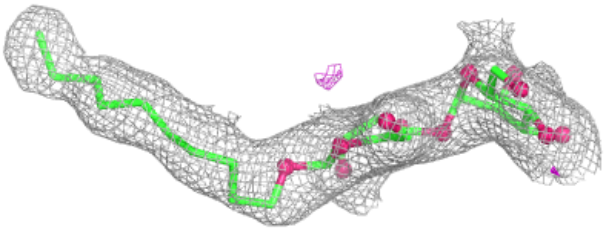
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CHD	P	1265	29/29	0.93	0.11	38,57,66,74	0
18	CHD	A	1517	29/29	0.93	0.09	25,32,44,46	0
18	CHD	C	1265	29/29	0.93	0.10	37,51,65,68	0
16	OXY	N	1515	2/2	0.94	0.12	31,31,31,33	0
20	PEK	C	1262	53/53	0.94	0.14	30,48,94,136	0
20	PEK	P	1262	53/53	0.95	0.17	35,52,149,483	0
21	PGV	P	1263	51/51	0.95	0.12	30,48,80,146	0
21	PGV	P	1264	51/51	0.95	0.13	28,43,86,192	0
18	CHD	T	1085	29/29	0.95	0.08	26,31,46,51	0
18	CHD	N	1517	29/29	0.95	0.08	27,37,42,44	0
21	PGV	C	1263	51/51	0.96	0.12	26,46,86,132	0
21	PGV	C	1264	51/51	0.96	0.12	24,37,97,273	0
18	CHD	G	1085	29/29	0.96	0.07	27,35,48,63	0
14	HEA	N	515	60/60	0.97	0.11	25,38,64,319	0
14	HEA	N	516	60/60	0.97	0.09	21,31,40,48	0
14	HEA	A	516	60/60	0.97	0.08	21,26,34,35	0
14	HEA	A	515	60/60	0.98	0.07	19,26,49,53	0
17	MG	N	1516	1/1	0.98	0.06	35,35,35,35	0
19	CUA	O	228	2/2	0.99	0.04	39,39,39,40	0
22	ZN	S	1097	1/1	0.99	0.03	39,39,39,39	0
15	CU	N	517	1/1	0.99	0.03	32,32,32,32	0
19	CUA	B	228	2/2	0.99	0.02	28,28,28,30	0
17	MG	A	1516	1/1	1.00	0.04	26,26,26,26	0
15	CU	A	517	1/1	1.00	0.01	28,28,28,28	0
22	ZN	F	1097	1/1	1.00	0.01	35,35,35,35	0

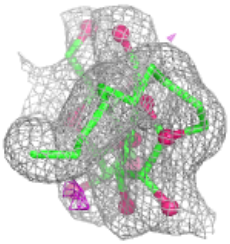
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU Z 1043:

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

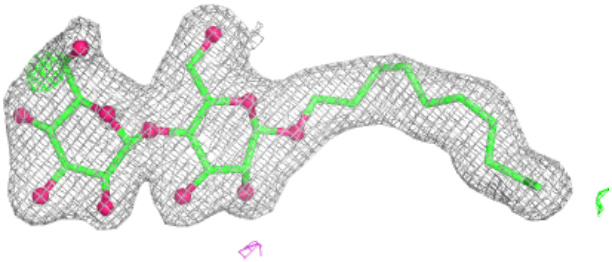


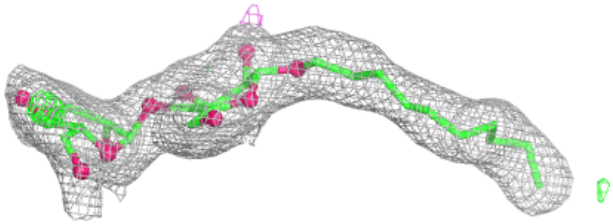


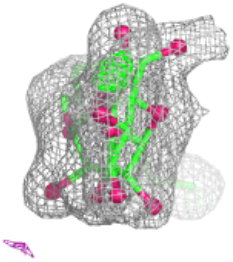


Electron density around DMU M 1044:

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

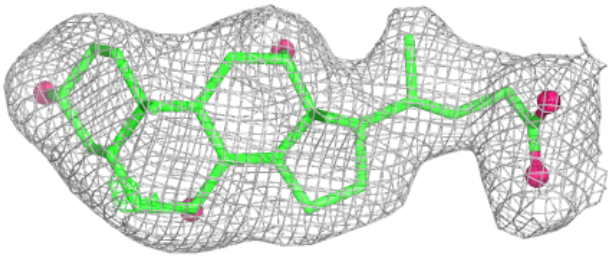


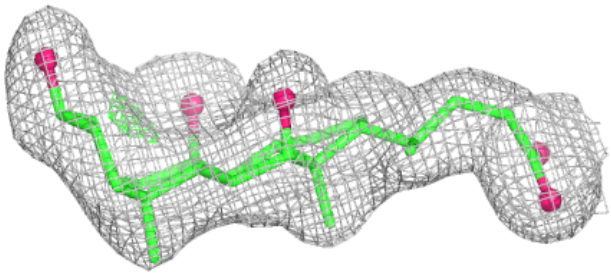


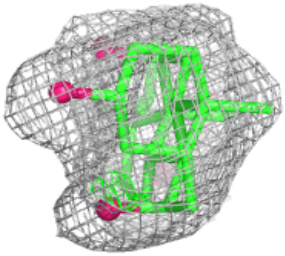


Electron density around CHD P 1265:

$2mF_o$-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 A 1517:

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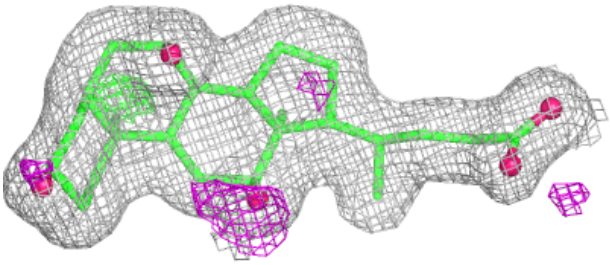
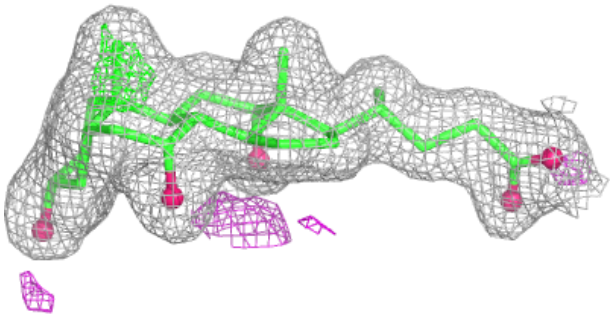
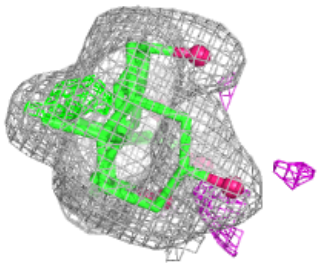
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

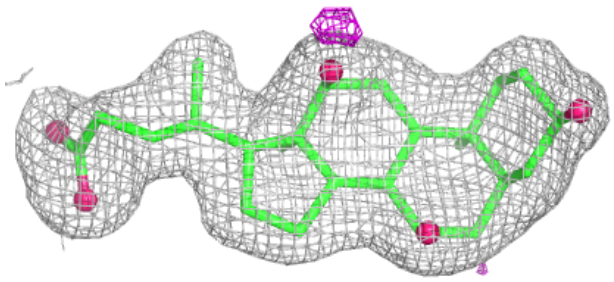


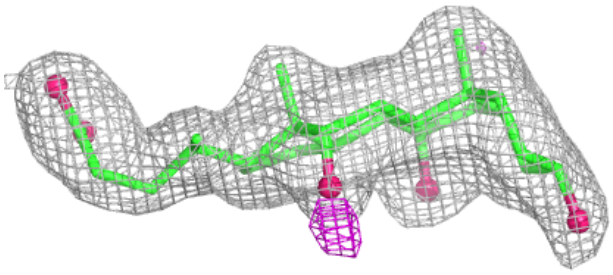


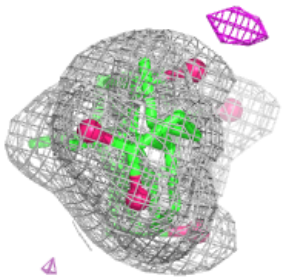


Electron density around CHD C 1265:

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

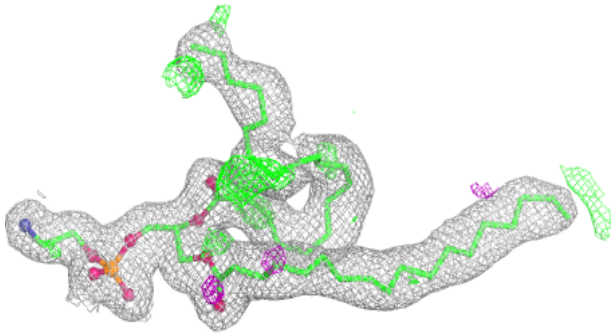


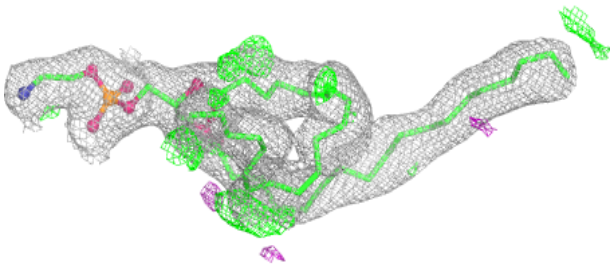


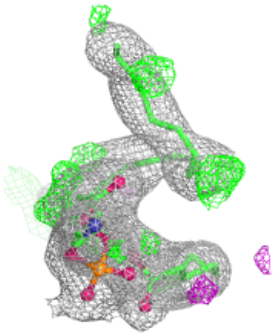


Electron density around PEK C 1262:

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

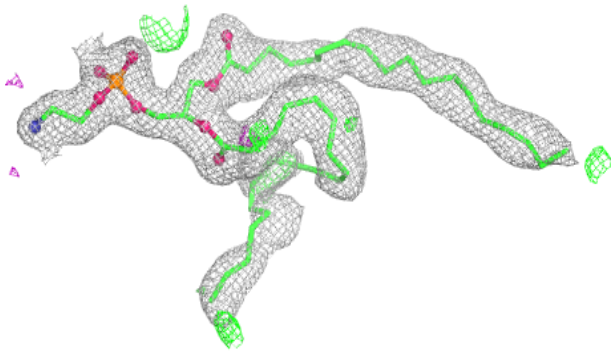


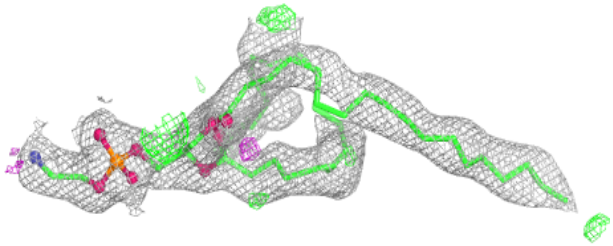


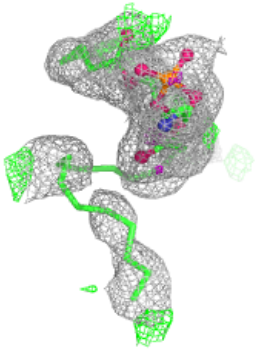


Electron density around PEK P 1262:

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

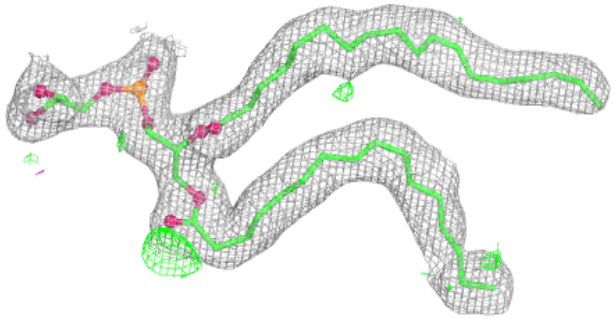


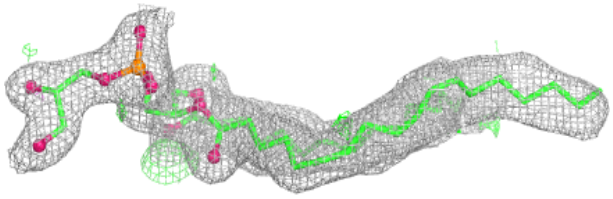


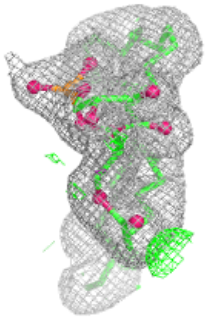


Electron density around PGV P 1263:

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

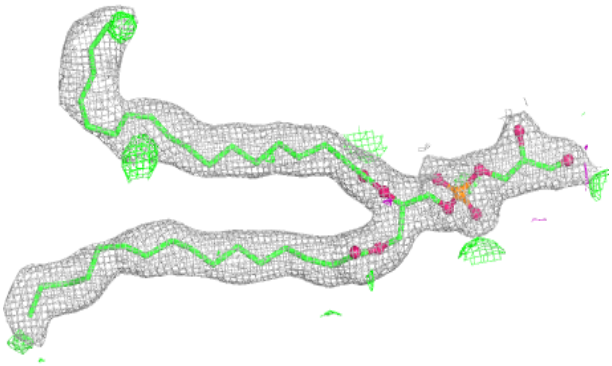


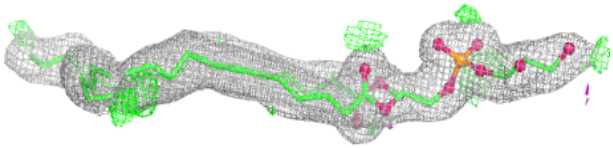


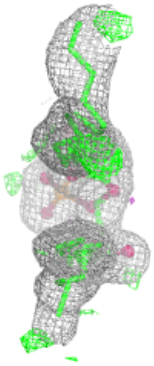


Electron density around PGV P 1264:

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

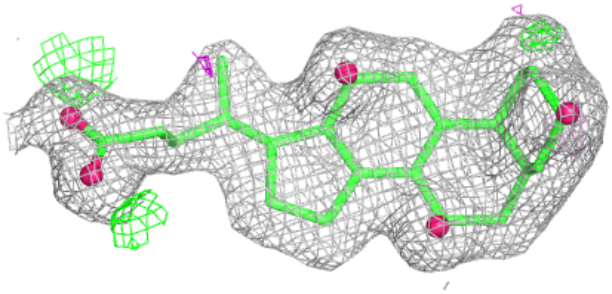


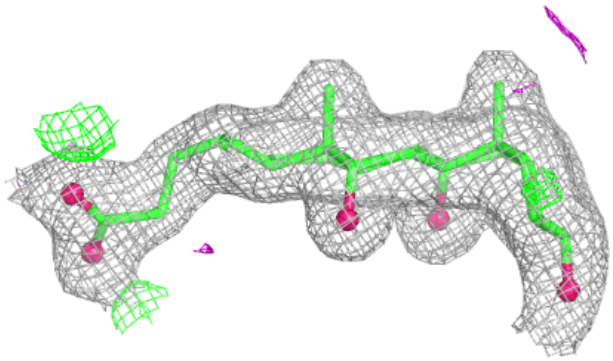


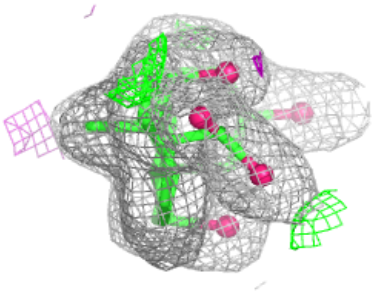


Electron density around CHD T 1085:

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

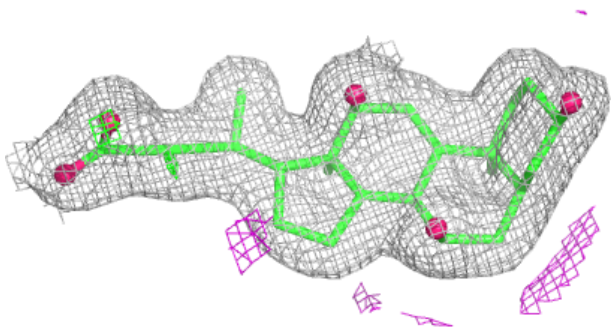


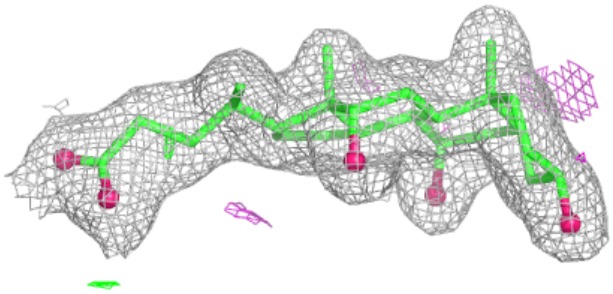


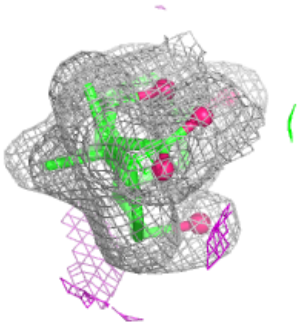


Electron density around CHD N 1517:

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

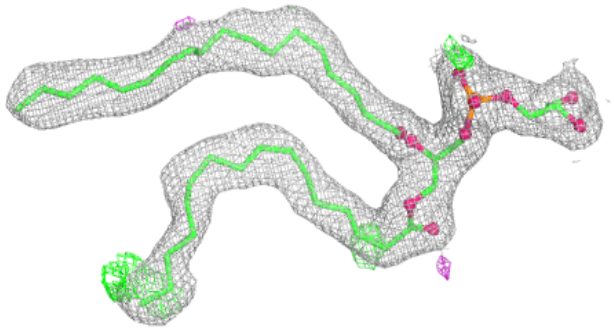


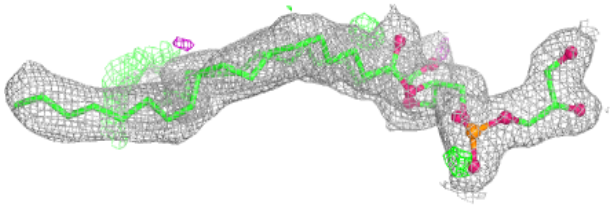


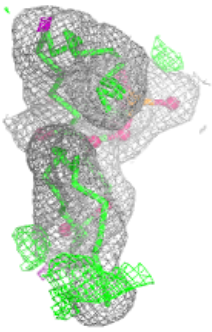


Electron density around PGV C 1263:

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

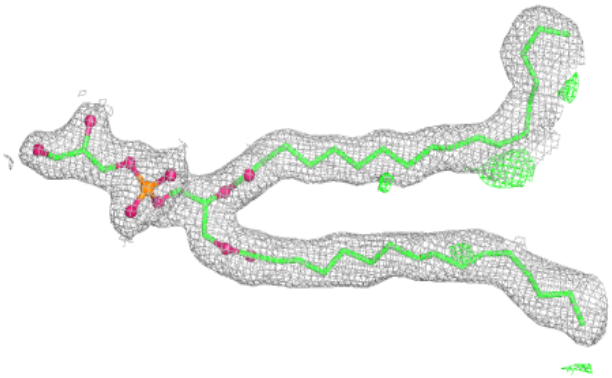


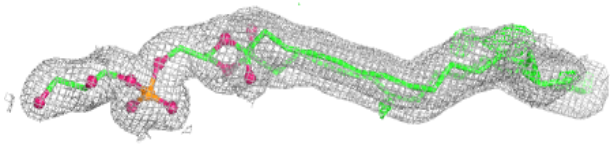


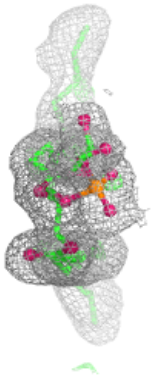


Electron density around PGV C 1264:

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

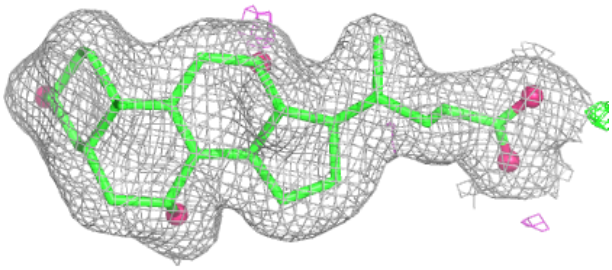


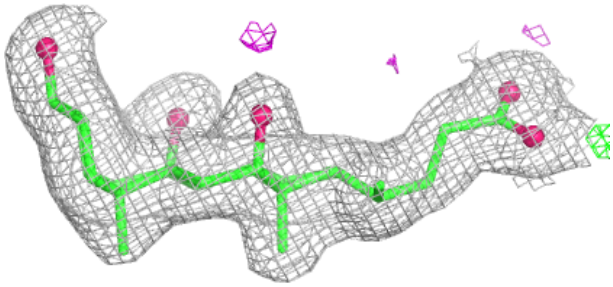


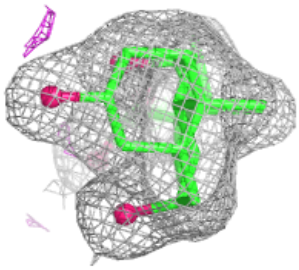


Electron density around CHD G 1085:

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

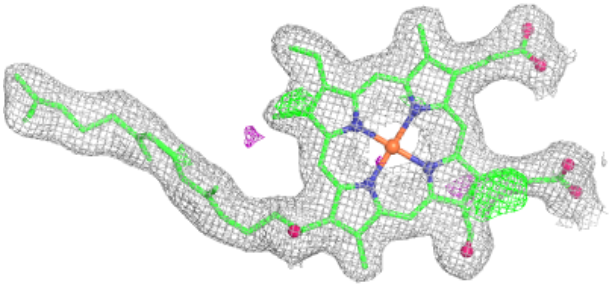


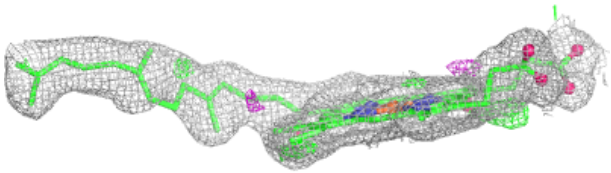


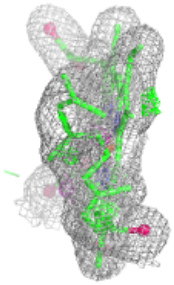


Electron density around HEA N 515:

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

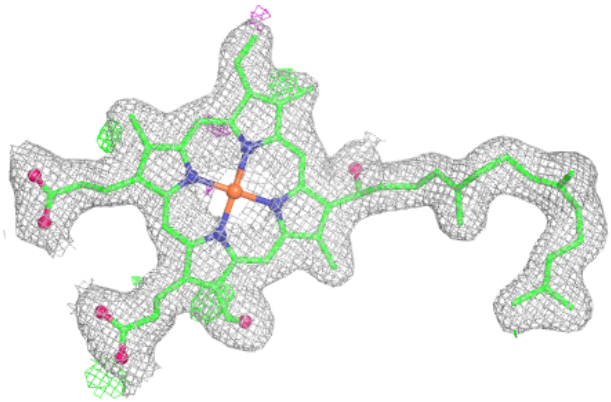


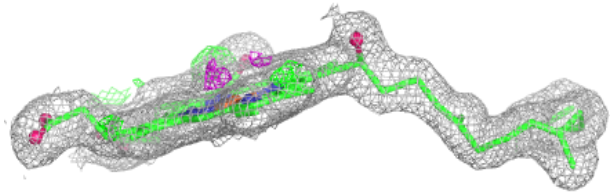


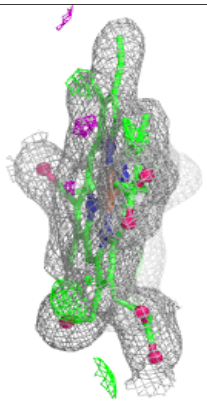


Electron density around HEA N 516:

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

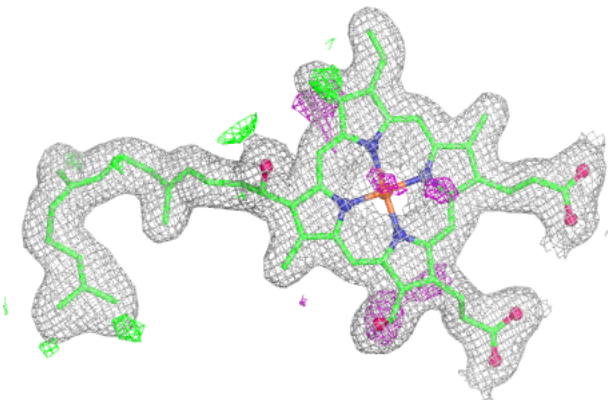


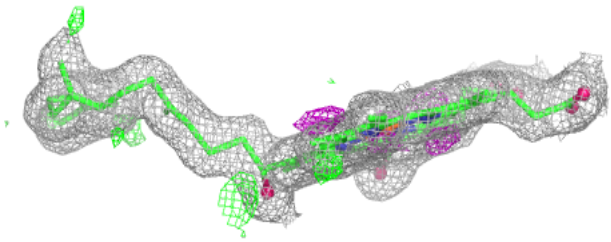


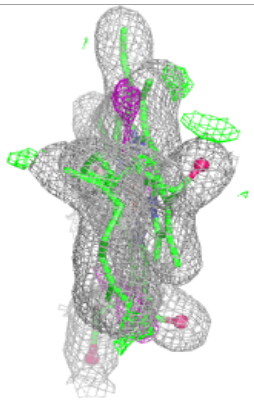


Electron density around HEA A 516:

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

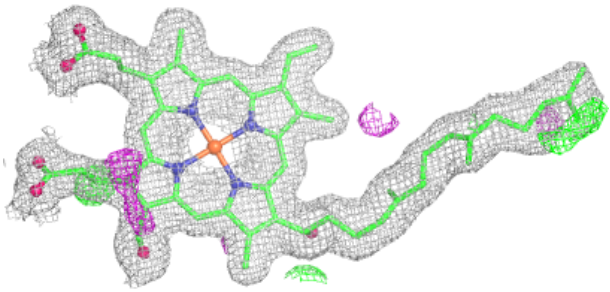


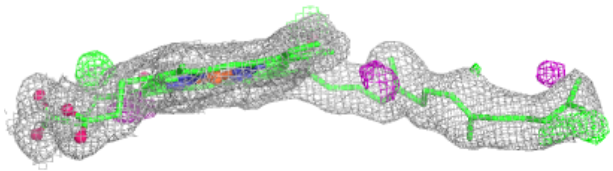




Electron density around HEA A 515:

$2mF_o$-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.