



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 03:25 PM EDT

PDB ID : 3CX5 / pdb_00003cx5
Title : Structure of complex III with bound cytochrome c in reduced state and definition of a minimal core interface for electron transfer.
Authors : Solmaz, S.R.N.; Hunte, C.
Deposited on : 2008-04-23
Resolution : 1.90 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (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

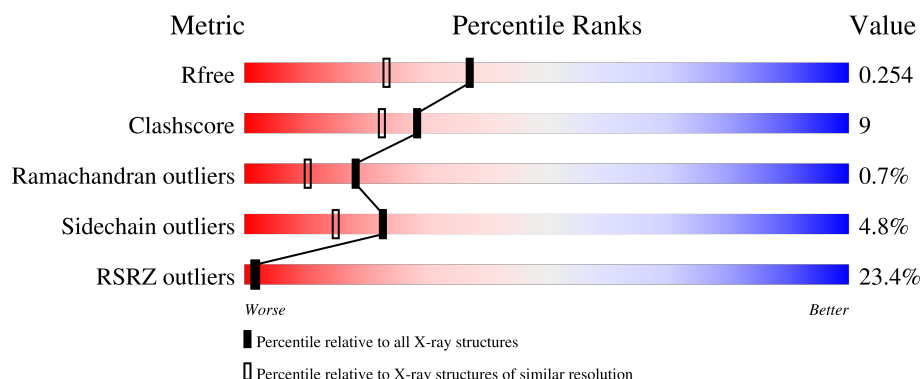
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	25% 78% 20%
1	L	431	21% 76% 21%
2	B	352	26% 76% 22%
2	M	352	26% 70% 25%
3	C	385	2% 81% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	385	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	146	
6	Q	146	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	65	
9	T	65	
10	J	127	
10	U	127	
11	K	107	
11	V	107	
12	W	108	
13	X	2	

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 38020 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			
1	L	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256
L	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			
3	N	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	9			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			
6	Q	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			
7	R	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	0	0	0
			465	310	77	78			
9	T	57	Total	C	N	O	0	0	0
			465	310	77	78			

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			
10	U	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

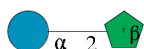
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is a protein called Cytochrome c iso-1.

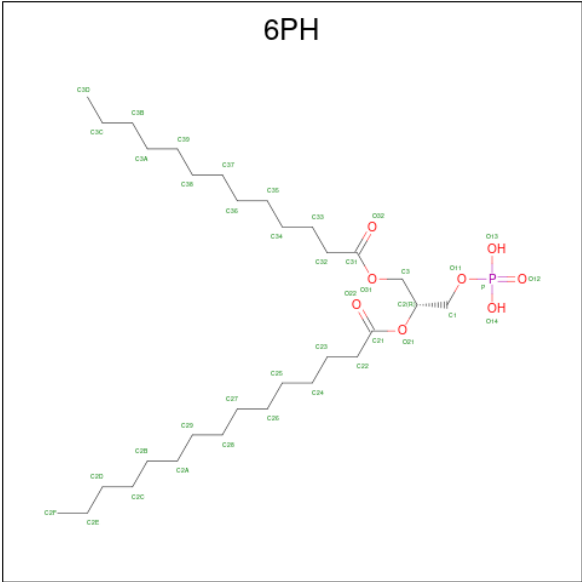
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	1	0
			859	542	153	159	5			

- Molecule 13 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



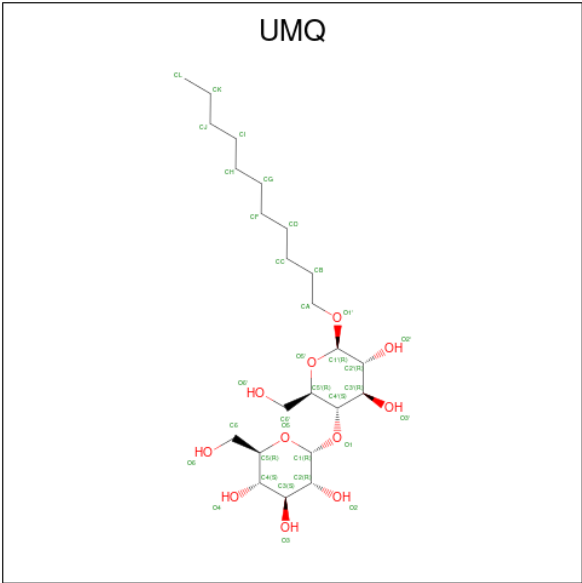
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	X	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 14 is (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (CCD ID: 6PH) (formula: C₃₁H₆₁O₈P).



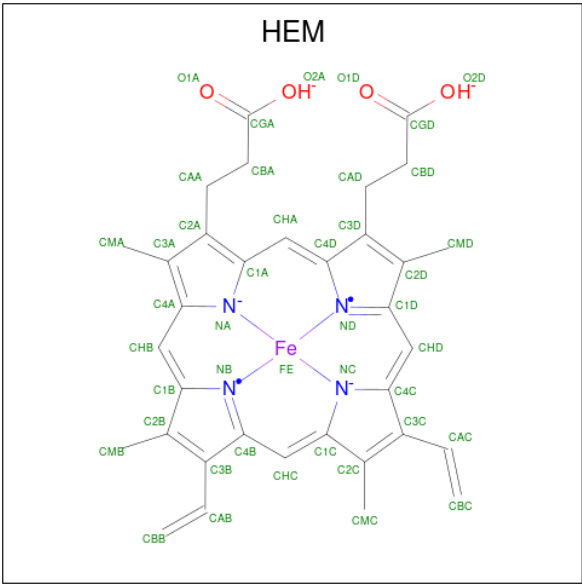
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			40	31	8	1		
14	L	1	Total	C	O	P	0	0
			40	31	8	1		

- Molecule 15 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



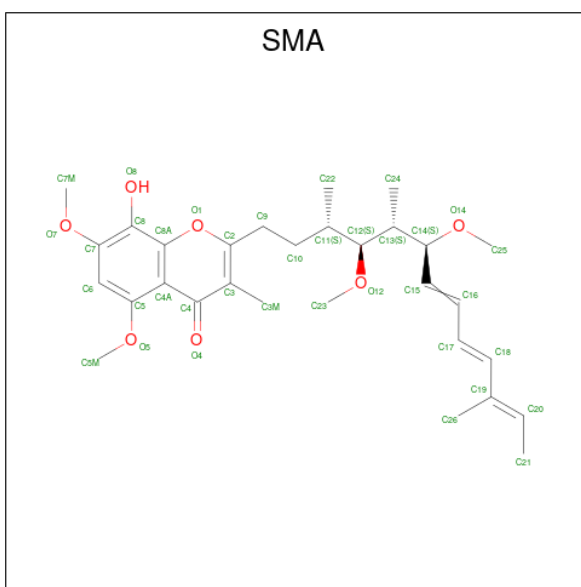
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	C	O	0	0
			34	23	11		
15	L	1	Total	C	O	0	0
			34	23	11		

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



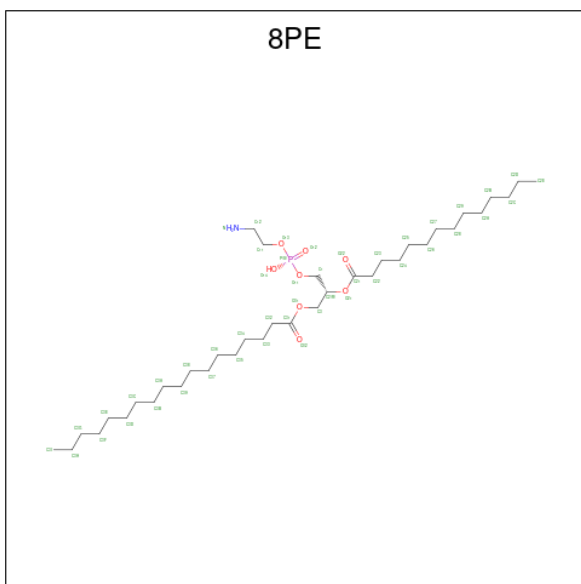
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	W	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 17 is STIGMATELLIN A (CCD ID: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	N	1	Total	C	O	0	0
			37	30	7		

- Molecule 18 is (2R)-3-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(tetradecanoyloxy)propyl octadecanoate (CCD ID: 8PE) (formula: C₃₇H₇₄NO₈P).



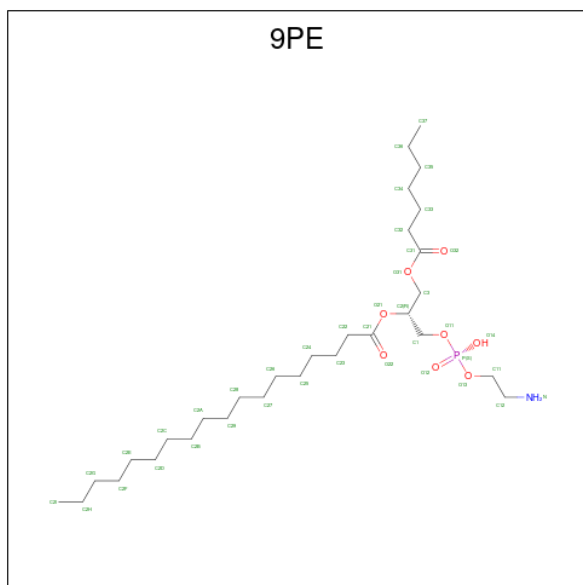
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

Continued on next page...

Continued from previous page...

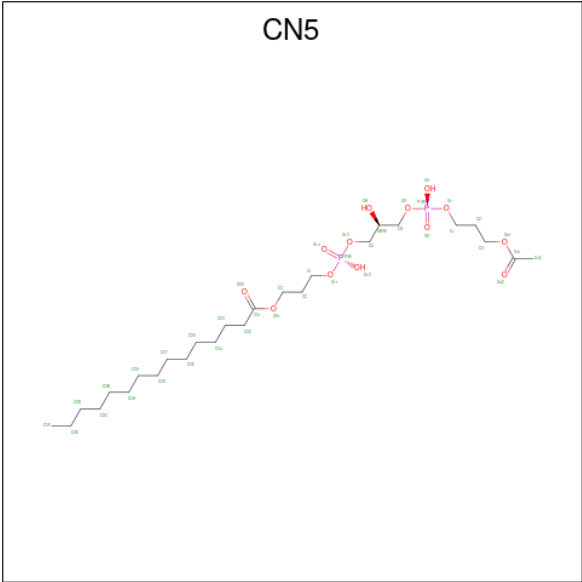
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 19 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P).



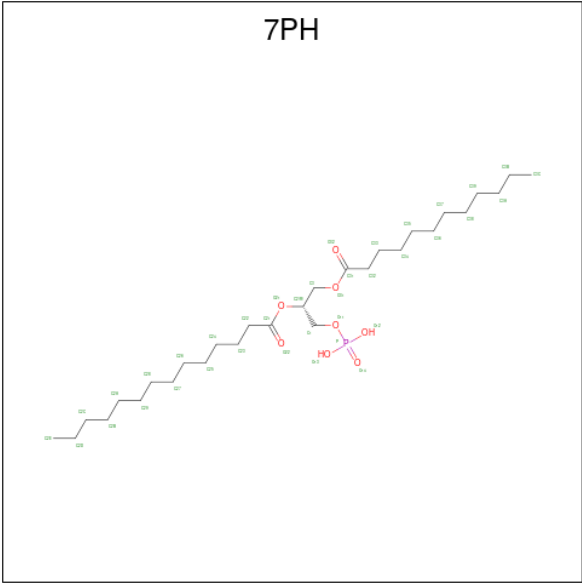
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (5S,11R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-4,6,10,12,16-pentaoxa-5,11-diphosphaoctadec-1-yl pentadecanoate (CCD ID: CN5) (formula: C₂₆H₅₂O₁₃P₂).



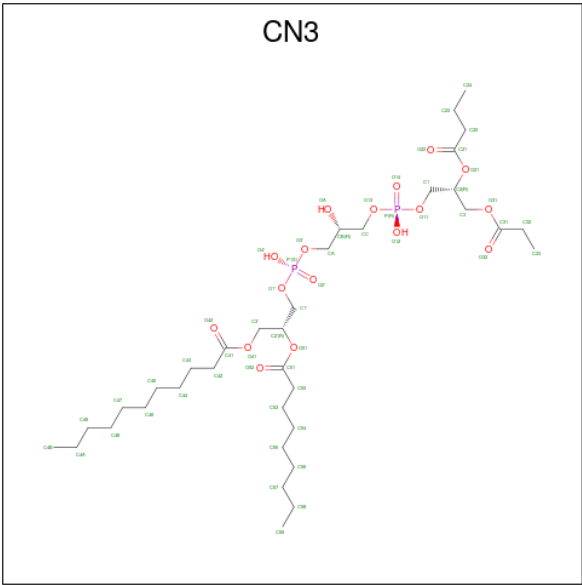
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			41	26	13	2		

- Molecule 21 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



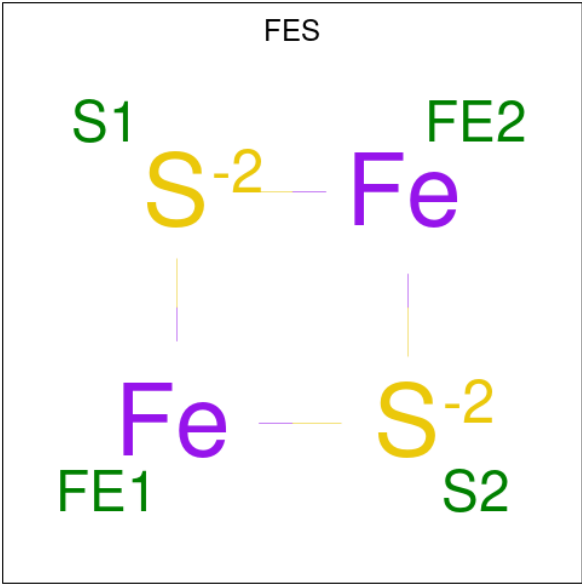
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			38	29	8	1		
21	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 22 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN3) (formula: C₃₆H₆₈O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	D	1	Total	C	O	P	0	0
			55	36	17	2		
22	N	1	Total	C	O	P	0	0
			55	36	17	2		

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	E	1	Total 4	Fe 2	S 2	0	0
23	P	1	Total 4	Fe 2	S 2	0	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	153	Total 153	O 153		0	0
24	B	93	Total 93	O 93		0	0
24	C	161	Total 161	O 161		0	0
24	D	154	Total 154	O 154		0	0
24	E	74	Total 74	O 74		0	0
24	F	16	Total 16	O 16		0	0
24	G	71	Total 71	O 71		0	0
24	H	31	Total 31	O 31		0	0
24	I	11	Total 11	O 11		0	0
24	J	15	Total 15	O 15		0	0
24	K	7	Total 7	O 7		0	0
24	L	170	Total 170	O 170		0	0
24	M	101	Total 101	O 101		0	0
24	N	170	Total 170	O 170		0	0
24	O	173	Total 173	O 173		0	0
24	P	66	Total 66	O 66		0	0
24	Q	27	Total 27	O 27		0	0
24	R	73	Total 73	O 73		0	0

Continued on next page...

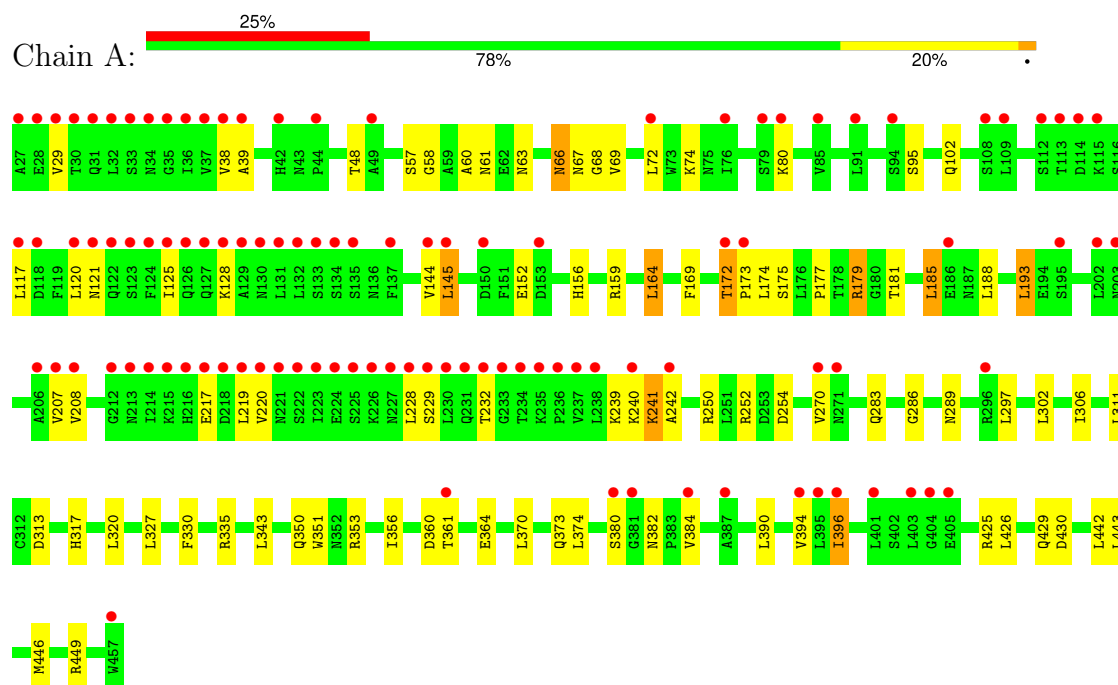
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	S	40	Total 40	O 40	0	0
24	T	12	Total 12	O 12	0	0
24	U	8	Total 8	O 8	0	0
24	V	2	Total 2	O 2	0	0
24	W	20	Total 20	O 20	0	0

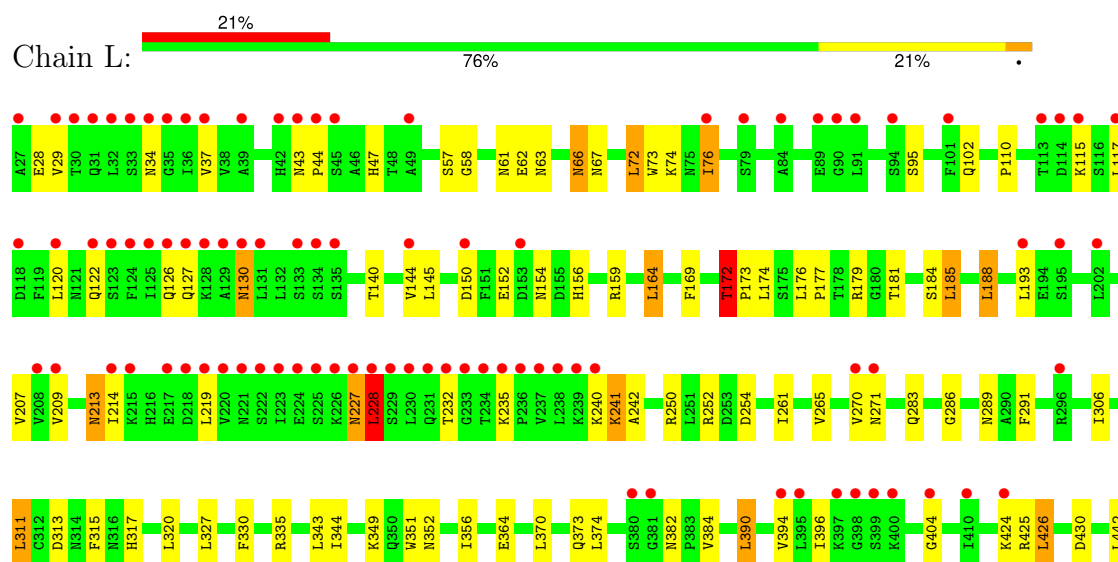
3 Residue-property plots [i](#)

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 b-c1 complex subunit 1, mitochondrial

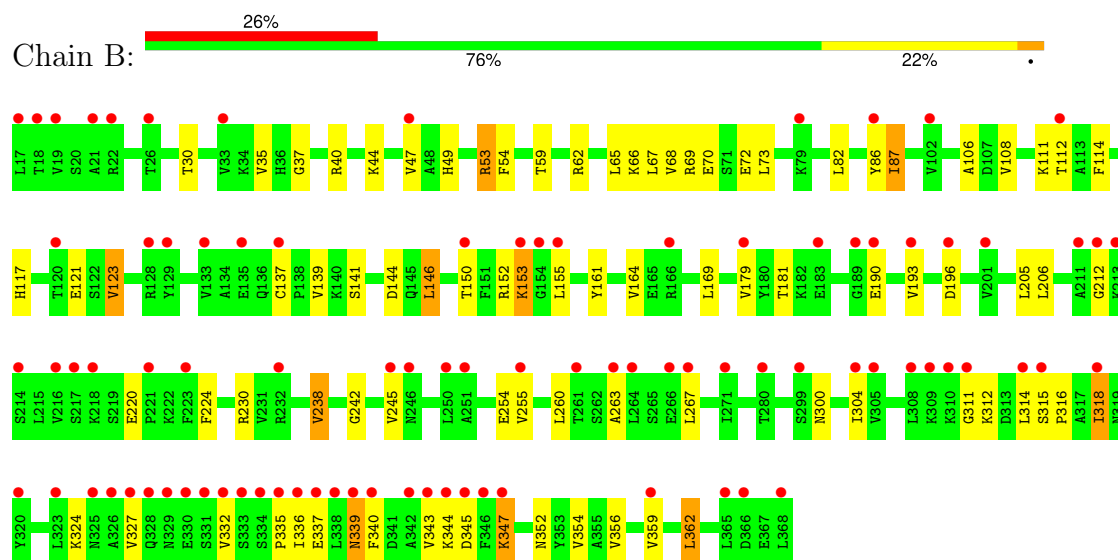


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

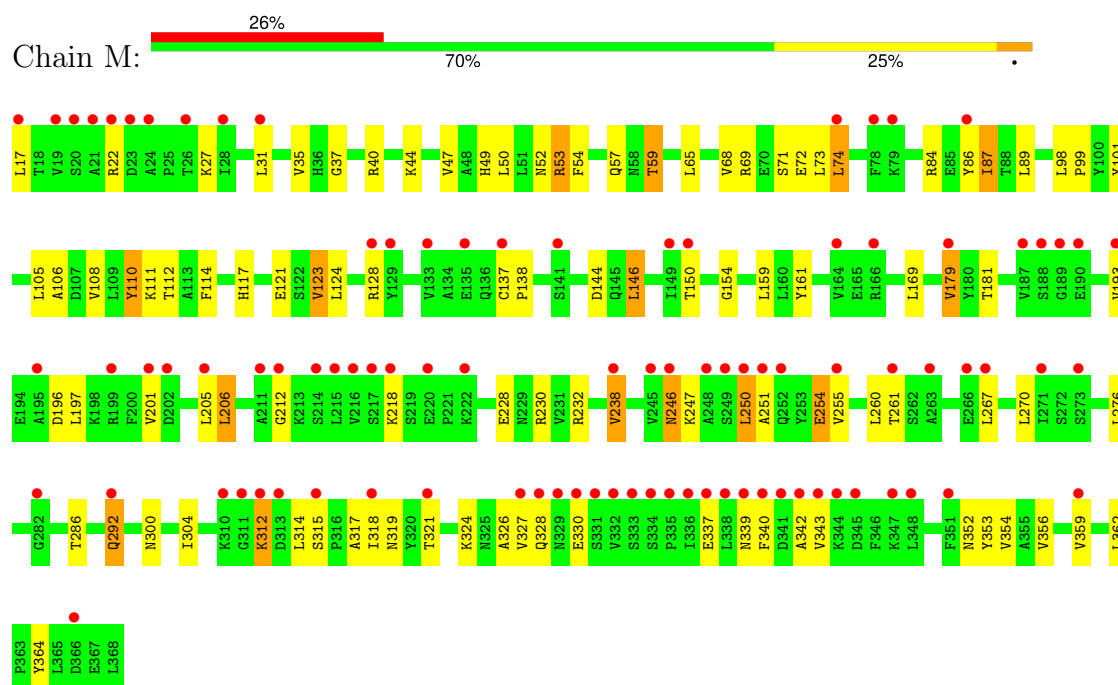




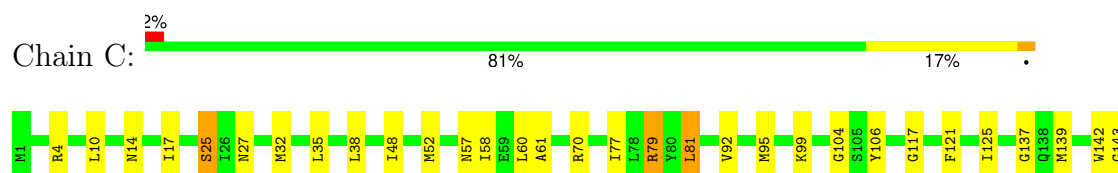
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

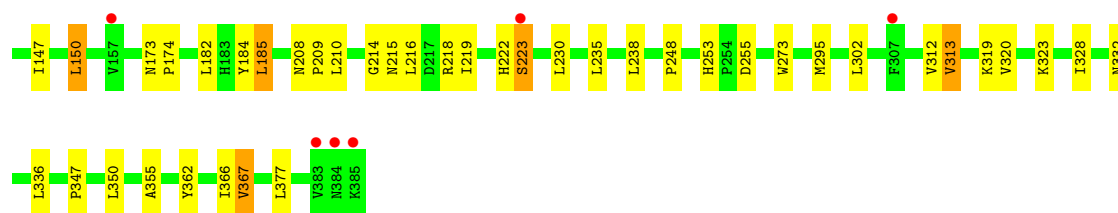


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

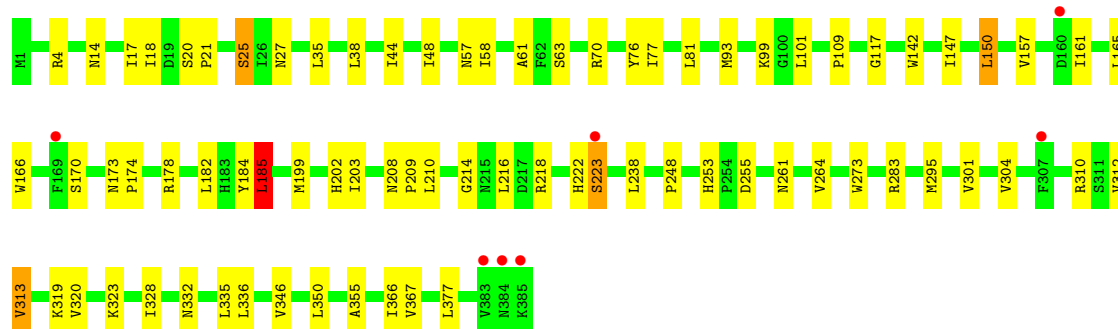
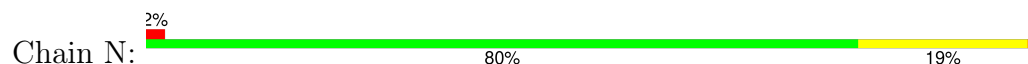


• Molecule 3: CYTOCHROME B

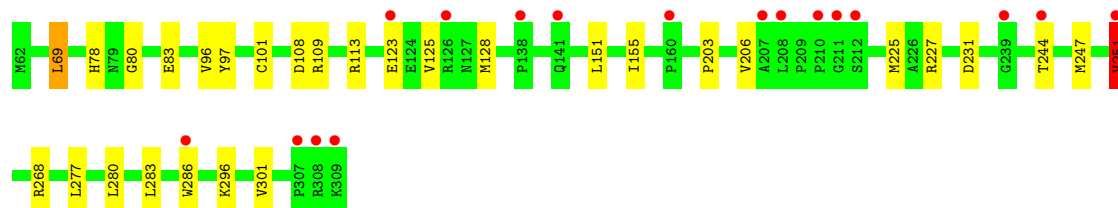
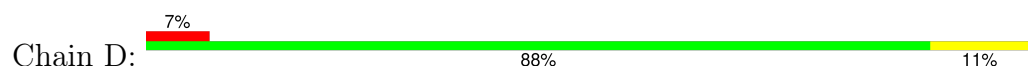




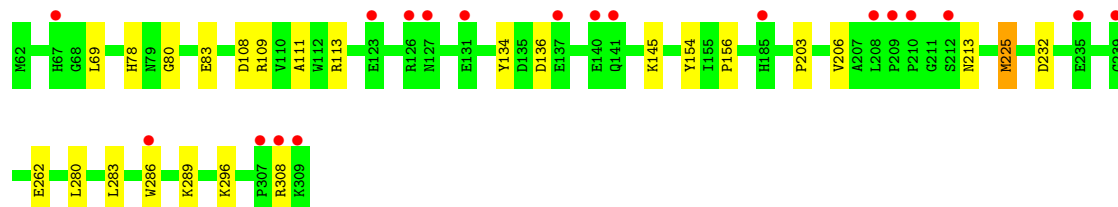
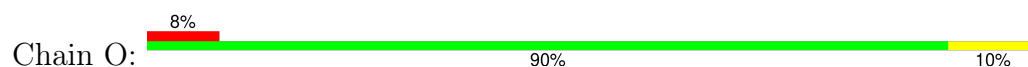
• Molecule 3: CYTOCHROME B



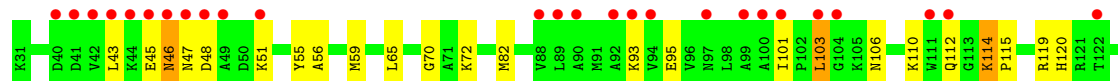
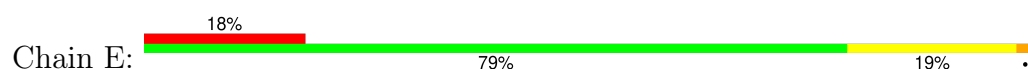
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

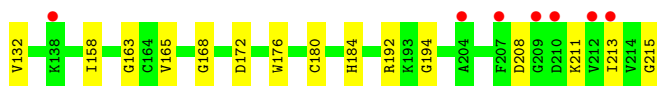


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

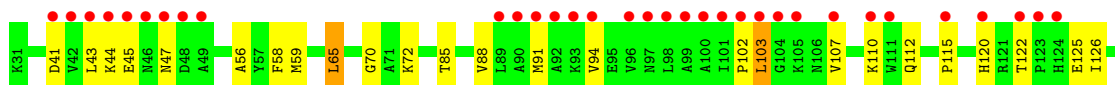
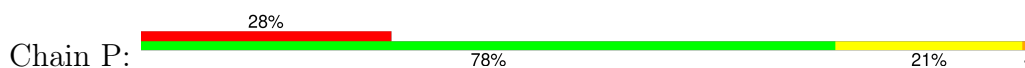


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

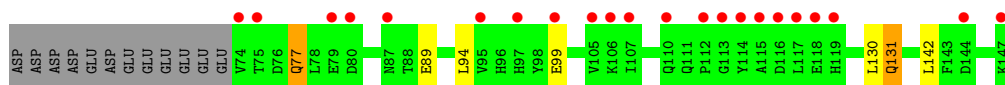
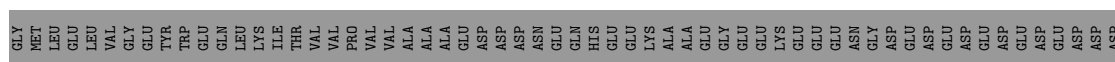




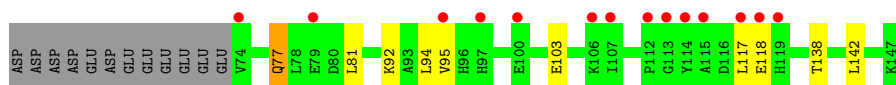
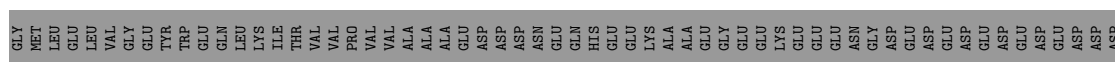
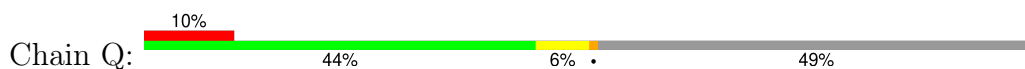
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



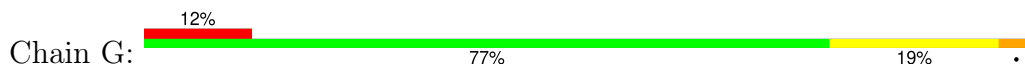
- Molecule 6: Cytochrome b-c1 complex subunit 6



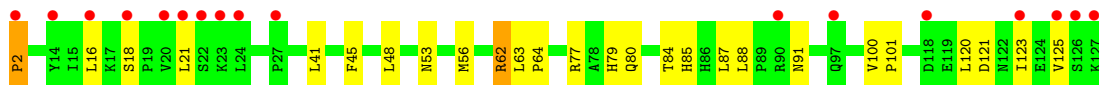
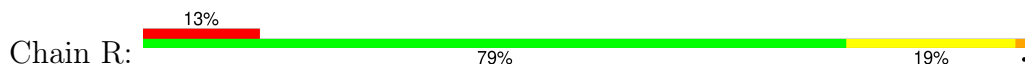
- Molecule 6: Cytochrome b-c1 complex subunit 6



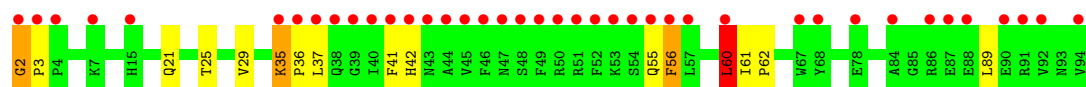
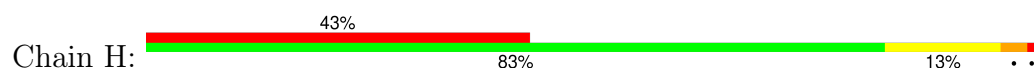
- Molecule 7: Cytochrome b-c1 complex subunit 7



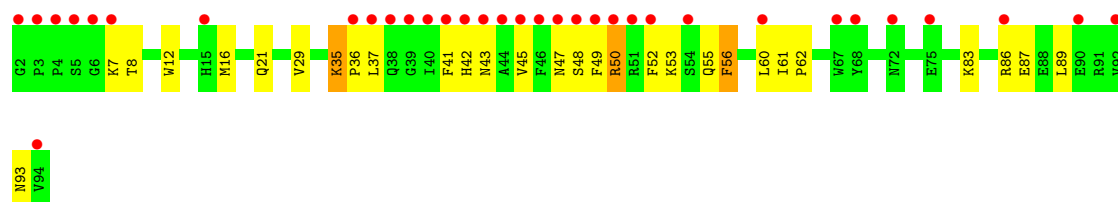
- Molecule 7: Cytochrome b-c1 complex subunit 7



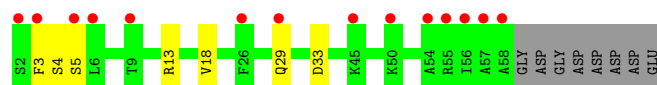
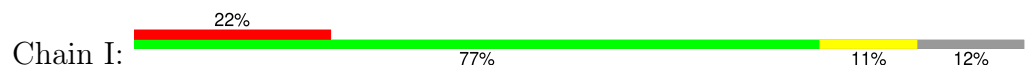
- Molecule 8: Cytochrome b-c1 complex subunit 8



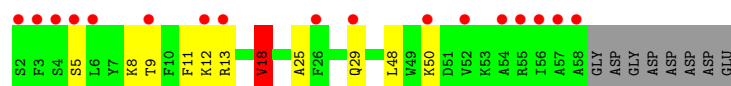
• Molecule 8: Cytochrome b-c1 complex subunit 8



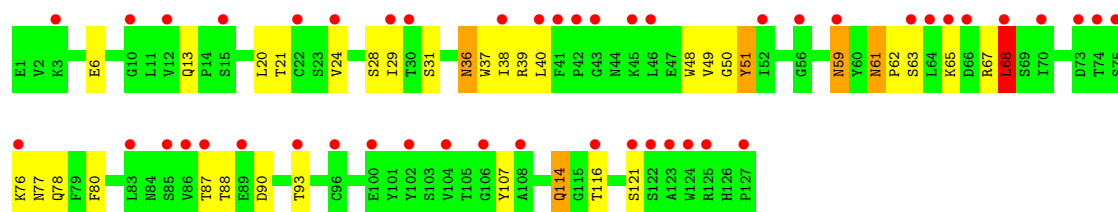
• Molecule 9: Cytochrome b-c1 complex subunit 9



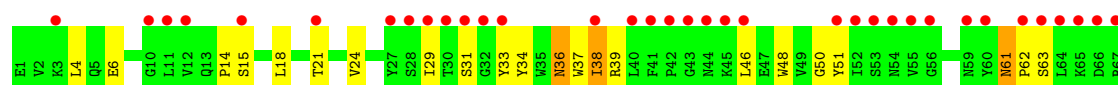
• Molecule 9: Cytochrome b-c1 complex subunit 9



• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

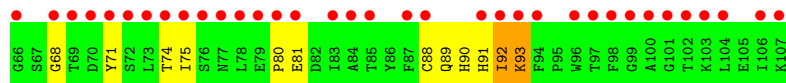
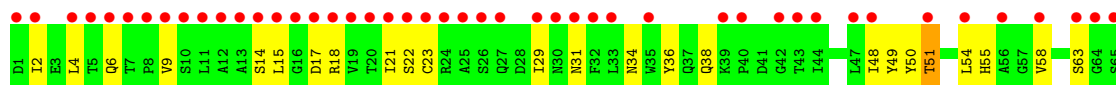
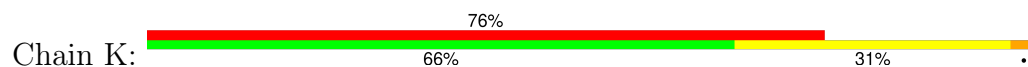


• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

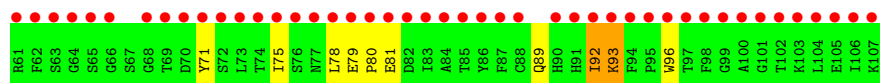




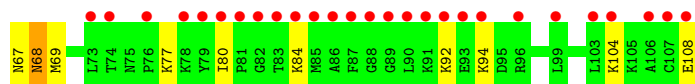
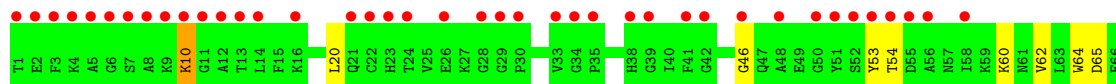
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



• Molecule 12: Cytochrome c iso-1



• Molecule 13: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.12Å 165.09Å 194.37Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	18.99 – 1.90 18.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (18.99-1.90) 95.1 (18.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.263 0.238 , 0.254	Depositor DCC
R_{free} test set	33007 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38020	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 10.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CN3, 8PE, FRU, 6PH, GLC, CN5, 9PE, SMA, M3L, UMQ, HEM, 7PH

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	0.39	0/3405	0.91	6/4614 (0.1%)
1	L	0.39	0/3405	0.90	5/4614 (0.1%)
2	B	0.38	0/2781	0.92	9/3764 (0.2%)
2	M	0.38	0/2781	0.91	8/3764 (0.2%)
3	C	0.53	1/3192 (0.0%)	0.98	12/4354 (0.3%)
3	N	0.54	1/3192 (0.0%)	0.99	14/4354 (0.3%)
4	D	0.43	0/2022	0.95	8/2751 (0.3%)
4	O	0.47	1/2022 (0.0%)	0.96	5/2751 (0.2%)
5	E	0.44	0/1444	0.91	5/1957 (0.3%)
5	P	0.44	0/1444	0.93	5/1957 (0.3%)
6	F	0.36	0/638	0.82	1/858 (0.1%)
6	Q	0.38	0/638	0.82	1/858 (0.1%)
7	G	0.42	0/1040	0.89	2/1408 (0.1%)
7	R	0.46	0/1040	0.89	1/1408 (0.1%)
8	H	0.41	0/804	0.94	6/1088 (0.6%)
8	S	0.41	0/804	0.91	5/1088 (0.5%)
9	I	0.39	0/479	0.84	0/646
9	T	0.41	0/479	0.86	2/646 (0.3%)
10	J	0.36	0/1043	0.84	2/1422 (0.1%)
10	U	0.36	0/1043	0.88	4/1422 (0.3%)
11	K	0.36	0/863	0.72	0/1172
11	V	0.36	0/863	0.73	0/1172
12	W	0.36	0/865	0.89	2/1157 (0.2%)
All	All	0.43	3/36287 (0.0%)	0.91	103/49225 (0.2%)

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
4	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	225	MET	SD-CE	-8.37	1.58	1.79
3	C	367	VAL	CA-CB	5.59	1.57	1.54
3	N	367	VAL	CA-CB	5.18	1.57	1.54

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	33	TYR	N-CA-C	8.39	116.81	108.75
8	H	2	GLY	CA-C-N	8.11	125.50	119.66
8	H	2	GLY	C-N-CA	8.11	125.50	119.66
5	P	163	GLY	N-CA-C	7.93	126.26	115.32
2	M	87	ILE	N-CA-C	-7.83	94.09	107.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	62	0
1	L	3344	0	3321	76	0
2	B	2735	0	2774	70	0
2	M	2735	0	2774	72	0
3	C	3090	0	3129	47	0
3	N	3090	0	3129	46	0
4	D	1961	0	1888	22	0
4	O	1961	0	1888	17	0
5	E	1411	0	1386	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1411	0	1386	29	0
6	F	624	0	581	4	0
6	Q	624	0	581	6	0
7	G	1019	0	1034	22	0
7	R	1019	0	1034	19	0
8	H	773	0	736	10	0
8	S	773	0	736	20	0
9	I	465	0	459	7	0
9	T	465	0	459	9	0
10	J	1015	0	959	31	0
10	U	1015	0	959	27	0
11	K	842	0	820	28	0
11	V	842	0	820	28	0
12	W	859	0	862	14	0
13	X	23	0	21	5	0
14	A	40	0	59	1	0
14	L	40	0	59	3	0
15	A	34	0	44	2	0
15	L	34	0	44	2	0
16	C	86	0	60	2	0
16	D	43	0	30	1	0
16	N	86	0	60	4	0
16	O	43	0	30	0	0
16	W	43	0	30	0	0
17	C	37	0	42	2	0
17	N	37	0	42	1	0
18	C	47	0	73	1	0
18	N	47	0	73	0	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	C	41	0	50	5	0
21	D	38	0	55	2	0
21	O	38	0	55	2	0
22	D	55	0	66	5	0
22	N	55	0	66	5	0
23	E	4	0	0	0	0
23	P	4	0	0	0	0
24	A	153	0	0	2	0
24	B	93	0	0	8	0
24	C	161	0	0	2	0
24	D	154	0	0	5	0
24	E	74	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	16	0	0	0	0
24	G	71	0	0	1	0
24	H	31	0	0	0	0
24	I	11	0	0	0	0
24	J	15	0	0	0	0
24	K	7	0	0	0	0
24	L	170	0	0	0	0
24	M	101	0	0	1	0
24	N	170	0	0	1	0
24	O	173	0	0	7	0
24	P	66	0	0	2	0
24	Q	27	0	0	0	0
24	R	73	0	0	1	0
24	S	40	0	0	0	0
24	T	12	0	0	1	0
24	U	8	0	0	0	0
24	V	2	0	0	0	0
24	W	20	0	0	0	0
All	All	38020	0	36113	641	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 9.

The worst 5 of 641 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)
2:B:150:THR:HG22	2:B:352:ASN:HD22	1.27	1.00
2:M:246:ASN:HD22	2:M:246:ASN:H	1.11	0.99
6:F:77:GLN:H	6:F:77:GLN:HE21	1.12	0.97
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.27	0.97
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.47	0.96

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	429/431 (100%)	408 (95%)	19 (4%)	2 (0%)	24	16
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	14	6
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	9	3
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	36	29
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	36	29
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	36	29
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	30	22
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	11	4
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	5	1
6	F	72/146 (49%)	71 (99%)	1 (1%)	0	100	100
6	Q	72/146 (49%)	70 (97%)	2 (3%)	0	100	100
7	G	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
7	R	124/126 (98%)	123 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	4
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	4
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100	100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	6	1
10	J	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
10	U	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
11	K	105/107 (98%)	91 (87%)	10 (10%)	4 (4%)	2	0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	3	0
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	18	10

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	103	LEU
5	P	103	LEU
2	B	153	LYS
3	C	223	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	228	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	347 (94%)	23 (6%)	16	9
1	L	370/370 (100%)	341 (92%)	29 (8%)	11	5
2	B	301/301 (100%)	288 (96%)	13 (4%)	26	18
2	M	301/301 (100%)	282 (94%)	19 (6%)	16	8
3	C	338/338 (100%)	321 (95%)	17 (5%)	22	14
3	N	338/338 (100%)	322 (95%)	16 (5%)	23	15
4	D	206/206 (100%)	202 (98%)	4 (2%)	50	47
4	O	206/206 (100%)	203 (98%)	3 (2%)	57	56
5	E	151/151 (100%)	148 (98%)	3 (2%)	48	46
5	P	151/151 (100%)	144 (95%)	7 (5%)	24	16
6	F	67/130 (52%)	61 (91%)	6 (9%)	9	3
6	Q	67/130 (52%)	64 (96%)	3 (4%)	24	17
7	G	110/110 (100%)	103 (94%)	7 (6%)	16	8
7	R	110/110 (100%)	106 (96%)	4 (4%)	31	23
8	H	77/77 (100%)	75 (97%)	2 (3%)	40	35
8	S	77/77 (100%)	76 (99%)	1 (1%)	61	61
9	I	47/53 (89%)	47 (100%)	0	100	100
9	T	47/53 (89%)	45 (96%)	2 (4%)	26	18
10	J	112/112 (100%)	104 (93%)	8 (7%)	13	7
10	U	112/112 (100%)	106 (95%)	6 (5%)	20	12
11	K	93/93 (100%)	89 (96%)	4 (4%)	26	18
11	V	93/93 (100%)	89 (96%)	4 (4%)	26	18
12	W	89/88 (101%)	87 (98%)	2 (2%)	45	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3833/3970 (96%)	3650 (95%)	183 (5%)	23	15

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	443	LEU
3	N	238	LEU
2	M	73	LEU
2	M	270	LEU
3	N	377	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
5	P	106	ASN
12	W	44	HIS
6	Q	77	GLN
10	U	54	ASN
6	F	129	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
12	M3L	W	77	12	10,11,12	0.92	0	9,14,16	0.99	1 (11%)

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
12	M3L	W	77	12	-	0/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM2-NZ-CM1	-2.03	103.64	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 monosaccharides 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	$\# Z > 2$
13	GLC	X	1	13	11,11,12	0.62	0	15,15,17	0.79	1 (6%)
13	FRU	X	2	13	11,12,12	0.52	0	10,18,18	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GLC	X	1	13	-	2/2/19/22	0/1/1/1
13	FRU	X	2	13	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	1	GLC	C2-C3-C4	-2.81	105.92	110.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

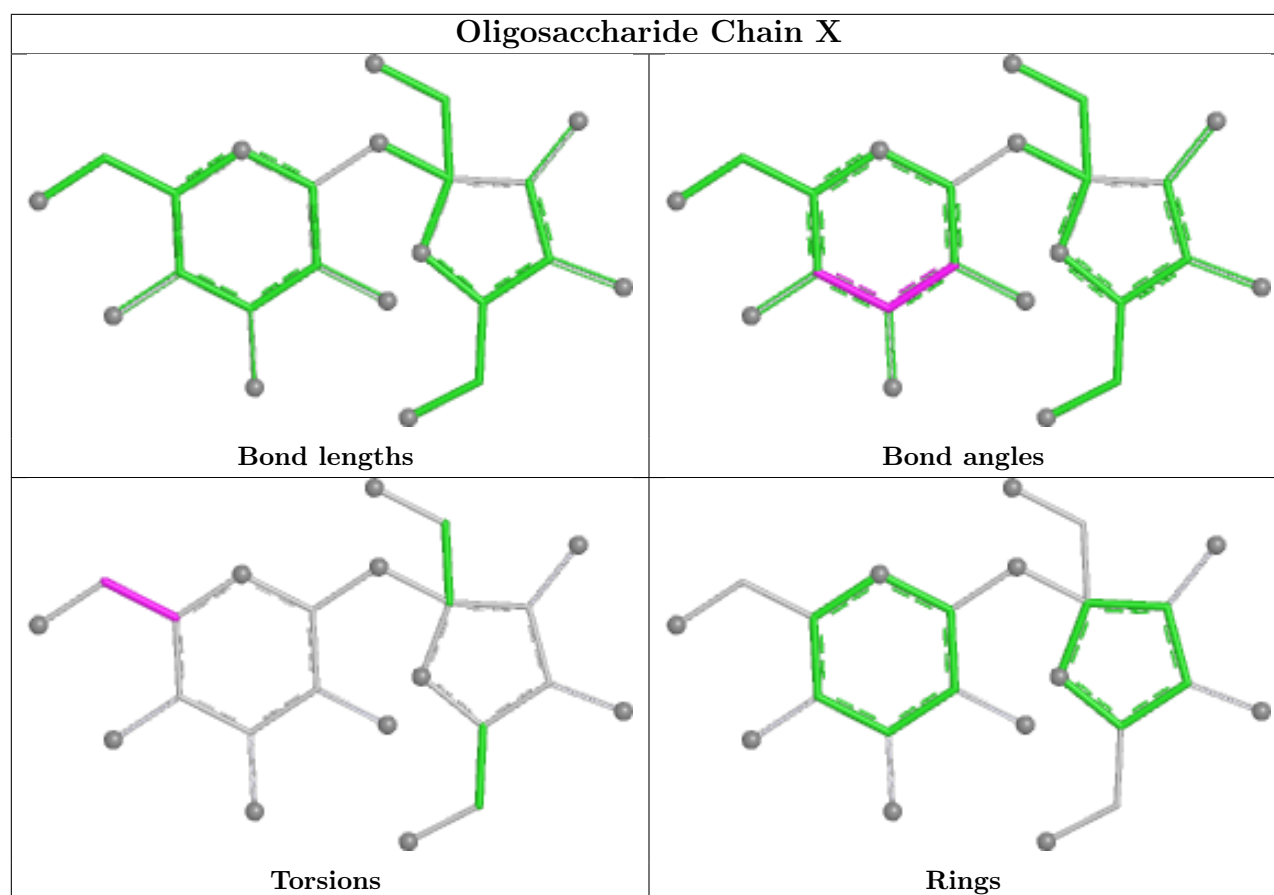
Mol	Chain	Res	Type	Atoms
13	X	1	GLC	C4-C5-C6-O6
13	X	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	1	GLC	1	0
13	X	2	FRU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

24 ligands 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	$\# Z > 2$
19	9PE	C	4011	-	39,39,39	0.71	0	42,44,44	0.97	1 (2%)
22	CN3	D	4031	-	54,54,54	1.54	9 (16%)	60,66,66	1.52	9 (15%)
21	7PH	D	4014	-	37,37,37	1.01	1 (2%)	40,42,42	1.44	8 (20%)
18	8PE	C	4010	-	46,46,46	0.96	2 (4%)	49,51,51	1.19	2 (4%)
14	6PH	L	4113	-	39,39,39	0.99	2 (5%)	42,44,44	1.34	4 (9%)
23	FES	P	4024	5	0,4,4	-	-	-	-	-
14	6PH	A	4013	-	39,39,39	0.99	3 (7%)	42,44,44	1.31	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	9PE	N	4111	-	39,39,39	0.75	0	42,44,44	1.00	1 (2%)
16	HEM	D	4003	4	50,50,50	1.42	5 (10%)	67,82,82	0.84	3 (4%)
16	HEM	C	4001	3	50,50,50	1.36	9 (18%)	67,82,82	0.91	4 (5%)
16	HEM	W	4026	12	50,50,50	1.48	7 (14%)	67,82,82	0.96	5 (7%)
16	HEM	N	4021	3	50,50,50	1.41	11 (22%)	67,82,82	0.92	3 (4%)
22	CN3	N	4131	-	54,54,54	1.52	10 (18%)	60,66,66	1.50	9 (15%)
16	HEM	C	4002	3	50,50,50	1.31	7 (14%)	67,82,82	0.68	0
17	SMA	N	4025	-	38,38,38	0.78	1 (2%)	47,52,52	0.94	3 (6%)
15	UMQ	A	4021	-	35,35,35	0.92	1 (2%)	46,46,46	1.78	7 (15%)
16	HEM	N	4022	3	50,50,50	1.34	7 (14%)	67,82,82	0.76	0
16	HEM	O	4023	4	50,50,50	1.49	7 (14%)	67,82,82	0.83	2 (2%)
21	7PH	O	4114	-	37,37,37	1.01	1 (2%)	40,42,42	1.44	8 (20%)
20	CN5	C	4033	-	40,40,40	1.68	11 (27%)	44,48,48	1.84	9 (20%)
17	SMA	C	4005	-	38,38,38	0.78	0	47,52,52	0.94	4 (8%)
23	FES	E	4004	5	0,4,4	-	-	-	-	-
18	8PE	N	4110	-	46,46,46	0.99	3 (6%)	49,51,51	1.15	2 (4%)
15	UMQ	L	4121	-	35,35,35	0.95	1 (2%)	46,46,46	1.75	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9PE	C	4011	-	-	21/43/43/43	-
22	CN3	D	4031	-	-	28/65/65/65	-
21	7PH	D	4014	-	-	13/39/39/39	-
18	8PE	C	4010	-	-	17/50/50/50	-
14	6PH	L	4113	-	-	19/41/41/41	-
23	FES	P	4024	5	-	-	0/1/1/1
14	6PH	A	4013	-	-	17/41/41/41	-
19	9PE	N	4111	-	-	17/43/43/43	-
16	HEM	D	4003	4	-	8/14/54/54	-
16	HEM	C	4001	3	-	4/14/54/54	-
16	HEM	W	4026	12	-	5/14/54/54	-
16	HEM	N	4021	3	-	6/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CN3	N	4131	-	-	29/65/65/65	-
16	HEM	C	4002	3	-	4/14/54/54	-
17	SMA	N	4025	-	-	1/34/34/34	0/2/2/2
15	UMQ	A	4021	-	-	4/20/60/60	0/2/2/2
16	HEM	N	4022	3	-	4/14/54/54	-
16	HEM	O	4023	4	-	8/14/54/54	-
21	7PH	O	4114	-	-	12/39/39/39	-
20	CN5	C	4033	-	-	18/44/44/44	-
17	SMA	C	4005	-	-	3/34/34/34	0/2/2/2
23	FES	E	4004	5	-	-	0/1/1/1
18	8PE	N	4110	-	-	21/50/50/50	-
15	UMQ	L	4121	-	-	4/20/60/60	0/2/2/2

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	4003	HEM	CBC-CAC	5.00	1.54	1.30
16	O	4023	HEM	CBC-CAC	5.00	1.54	1.30
16	O	4023	HEM	CBB-CAB	4.91	1.54	1.30
16	W	4026	HEM	CBC-CAC	4.83	1.53	1.30
16	D	4003	HEM	CBB-CAB	4.81	1.53	1.30

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	4021	UMQ	CA-O1'-C1'	-8.62	98.95	113.68
15	L	4121	UMQ	CA-O1'-C1'	-8.34	99.44	113.68
20	C	4033	CN5	O1'-C1'-C2'	5.93	130.30	109.28
22	D	4031	CN3	C2'-O51-C51	-5.34	105.03	117.80
22	N	4131	CN3	C2'-O51-C51	-5.09	105.60	117.80

There are no chirality outliers.

5 of 263 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	C	4011	9PE	C1-O11-P-O12
19	C	4011	9PE	C1-O11-P-O13
19	C	4011	9PE	C1-O11-P-O14
19	C	4011	9PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

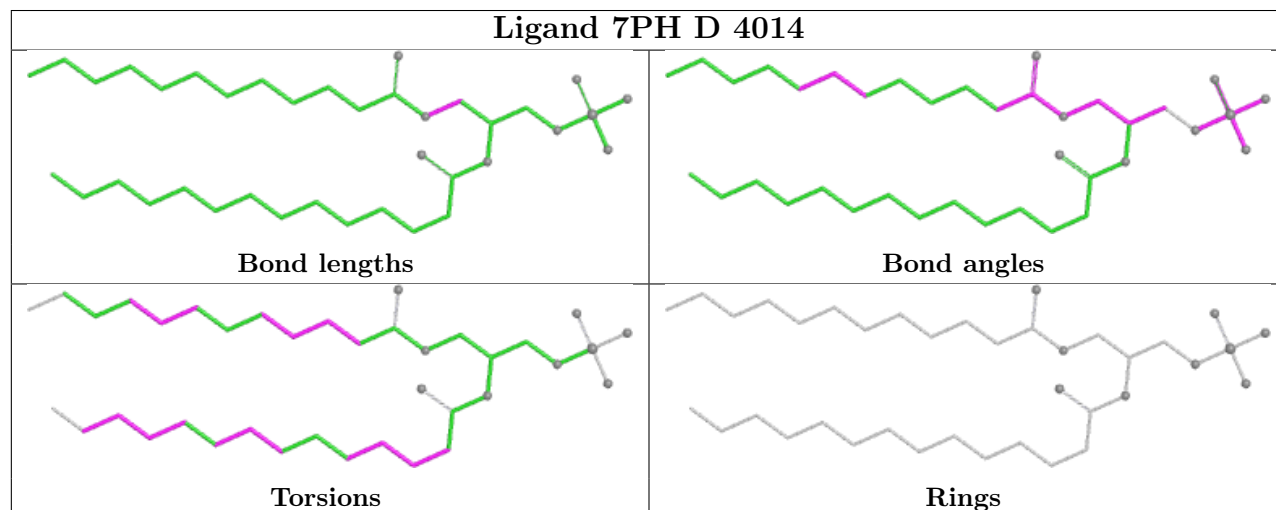
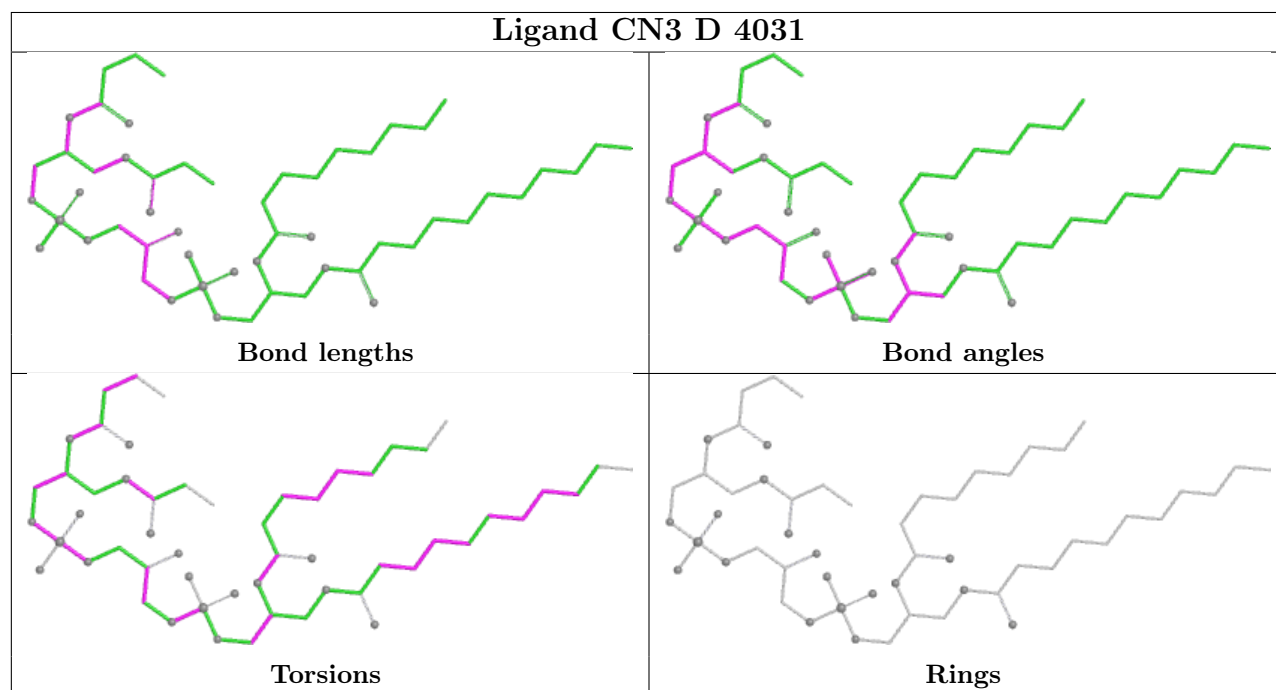
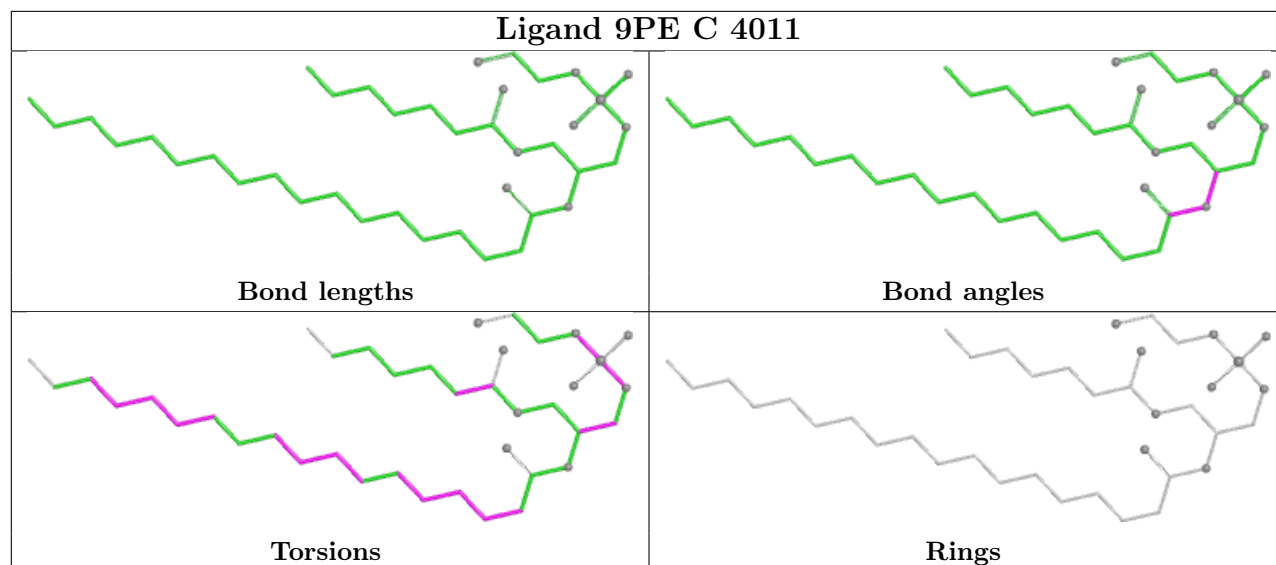
Mol	Chain	Res	Type	Atoms
19	C	4011	9PE	C11-O13-P-O14

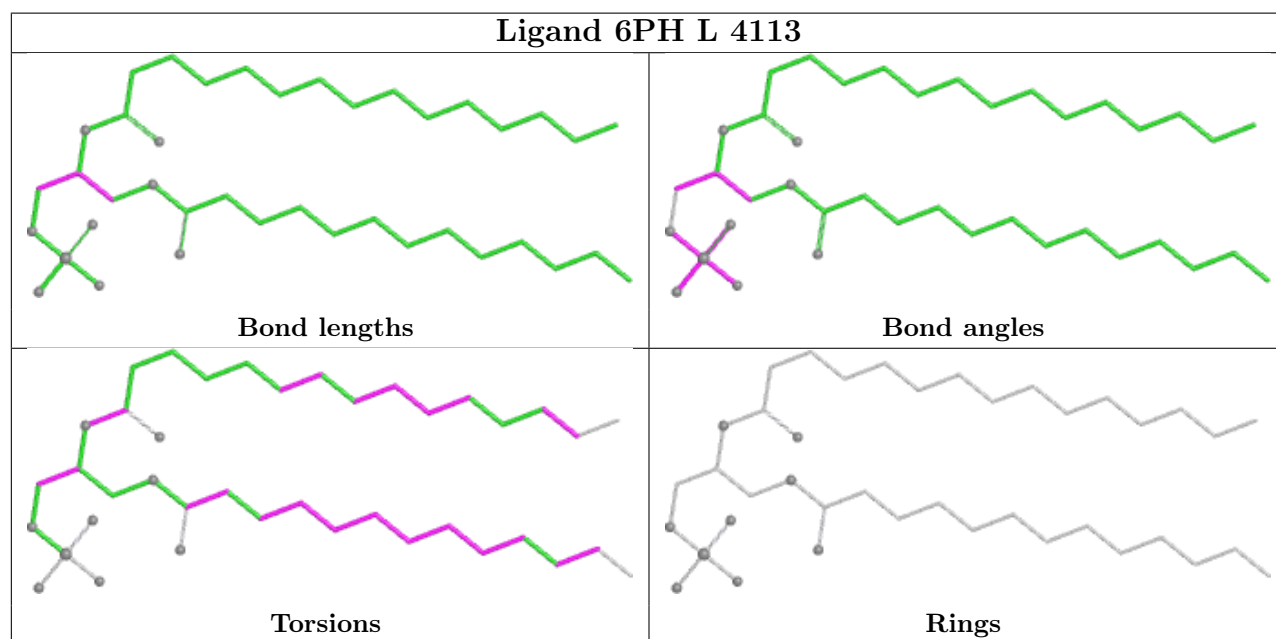
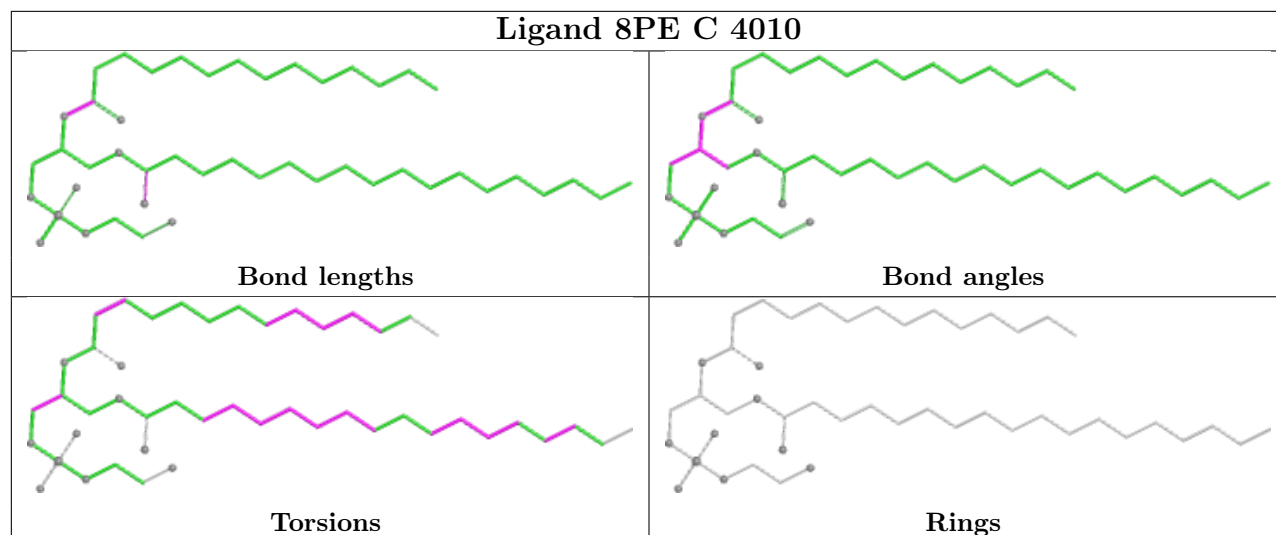
There are no ring outliers.

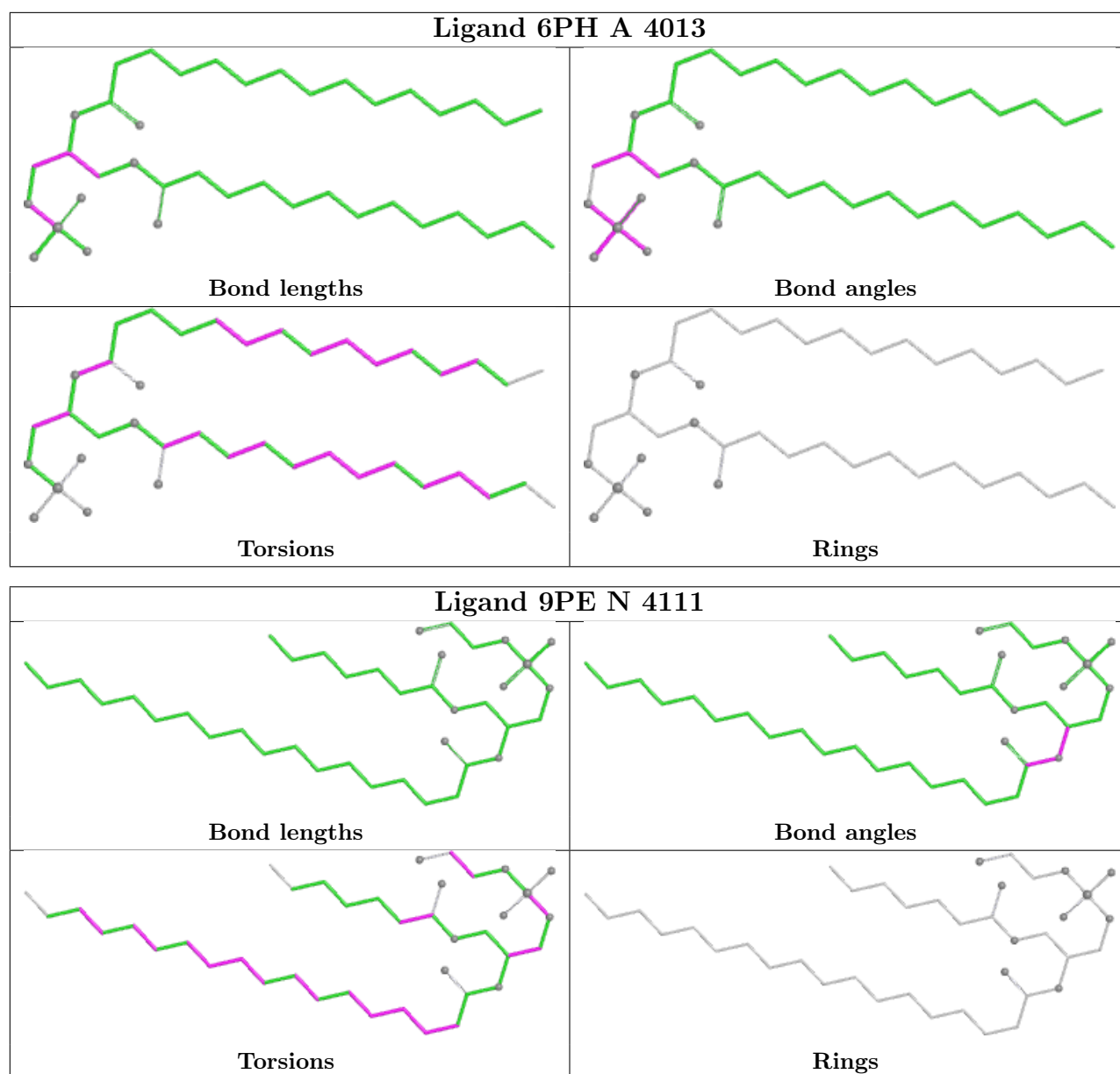
17 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	4031	CN3	5	0
21	D	4014	7PH	2	0
18	C	4010	8PE	1	0
14	L	4113	6PH	3	0
14	A	4013	6PH	1	0
16	D	4003	HEM	1	0
16	C	4001	HEM	1	0
16	N	4021	HEM	2	0
22	N	4131	CN3	5	0
16	C	4002	HEM	1	0
17	N	4025	SMA	1	0
15	A	4021	UMQ	2	0
16	N	4022	HEM	2	0
21	O	4114	7PH	2	0
20	C	4033	CN5	5	0
17	C	4005	SMA	2	0
15	L	4121	UMQ	2	0

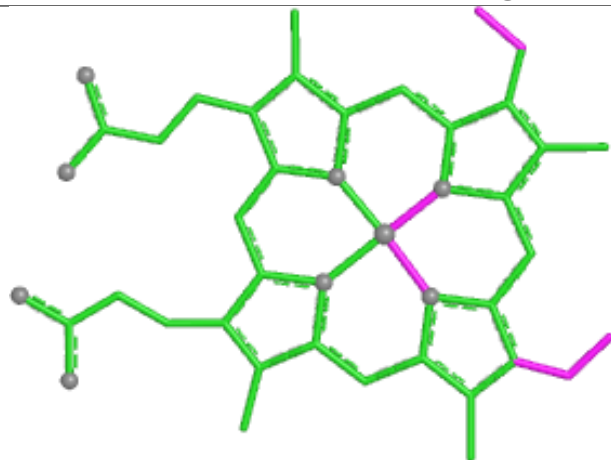
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



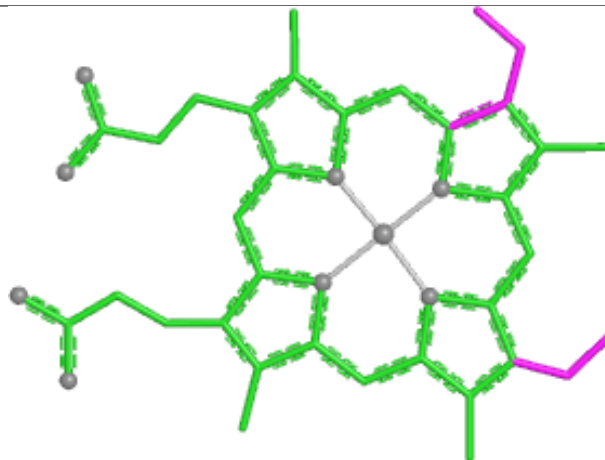




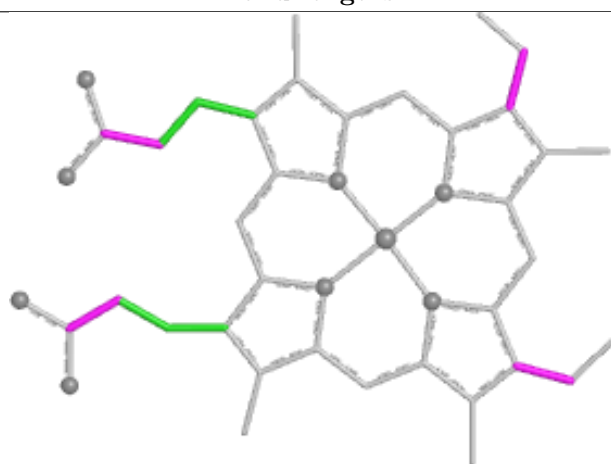
Ligand HEM D 4003



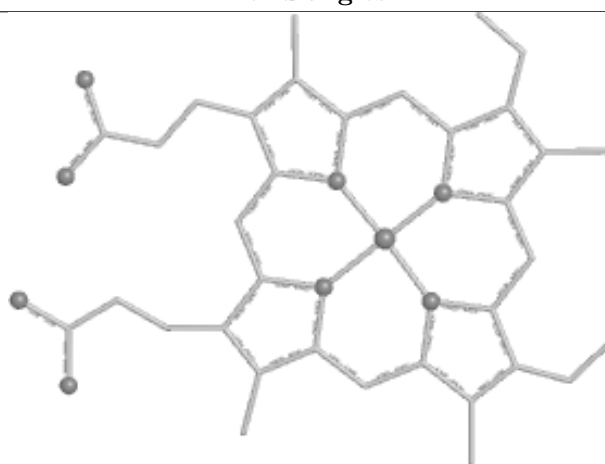
Bond lengths



Bond angles

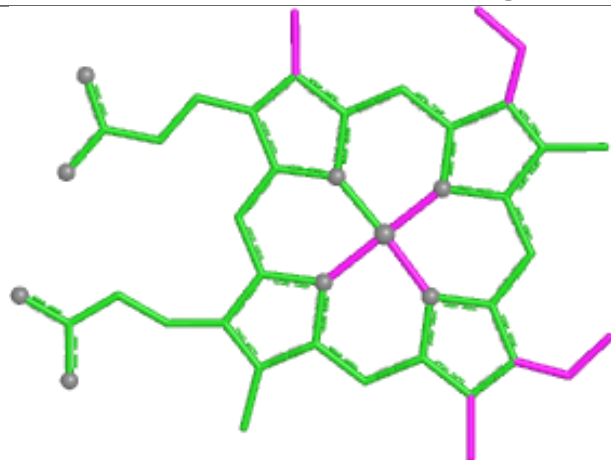


Torsions

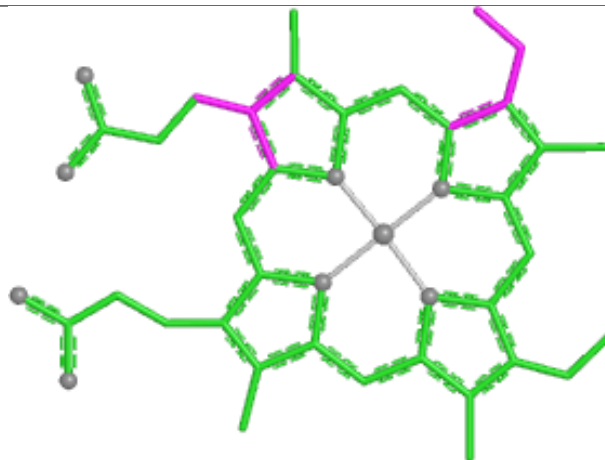


Rings

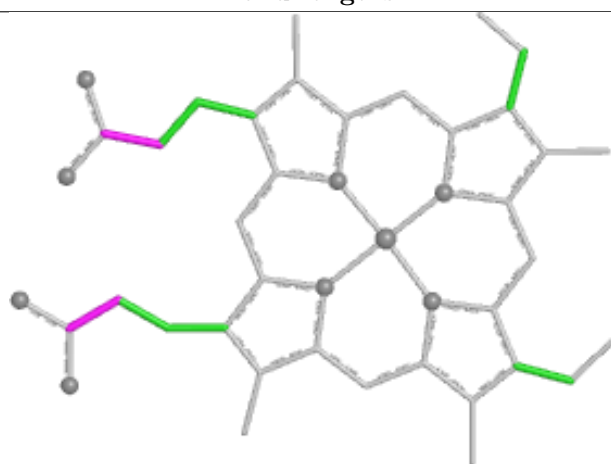
Ligand HEM C 4001



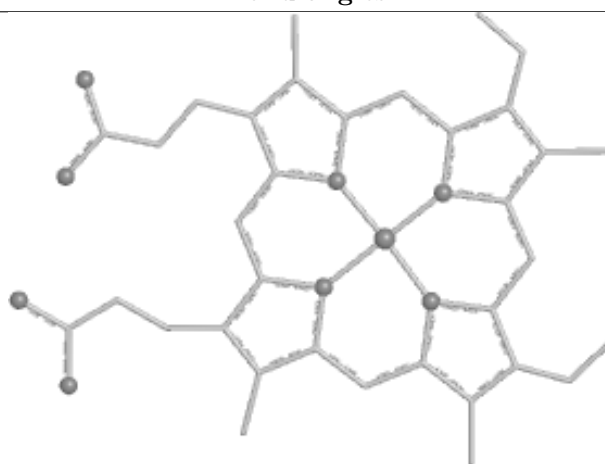
Bond lengths



Bond angles

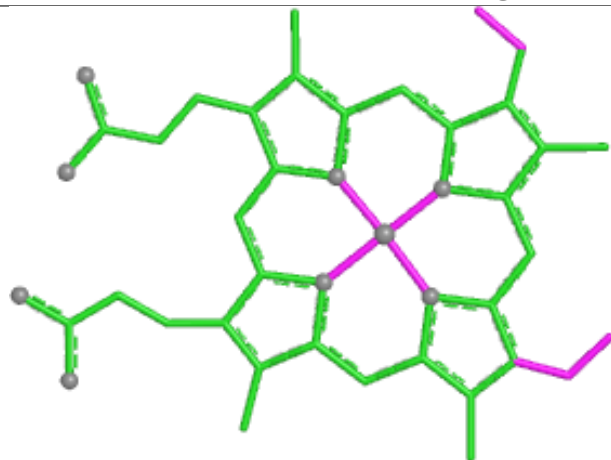


Torsions

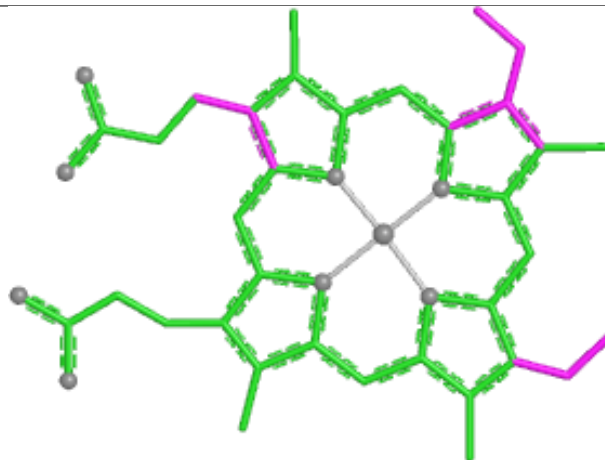


Rings

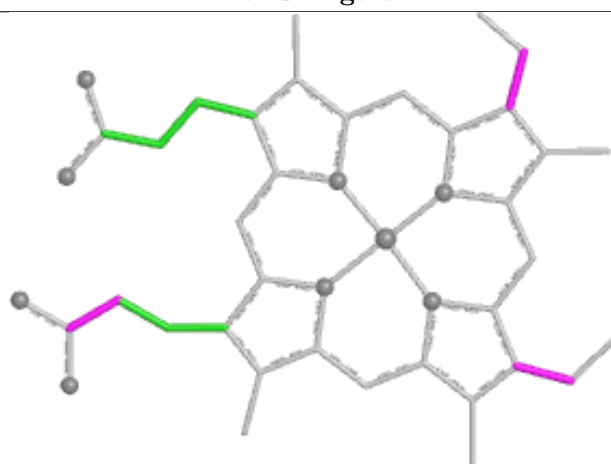
Ligand HEM W 4026



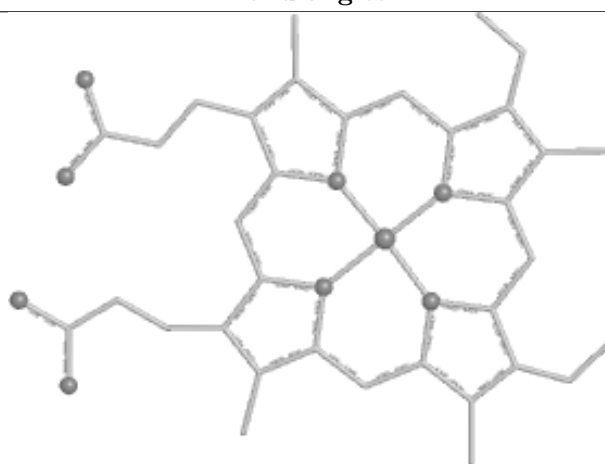
Bond lengths



Bond angles

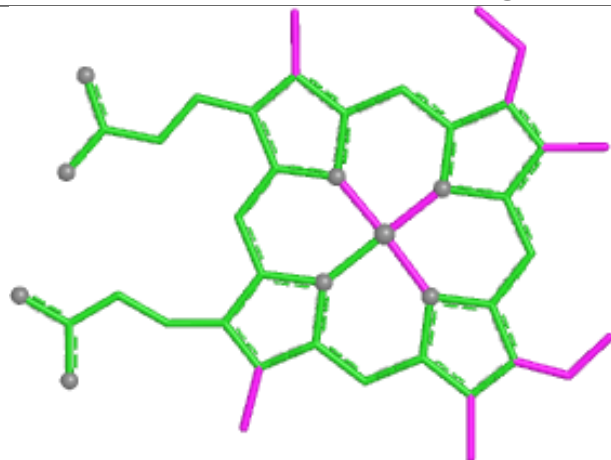


Torsions

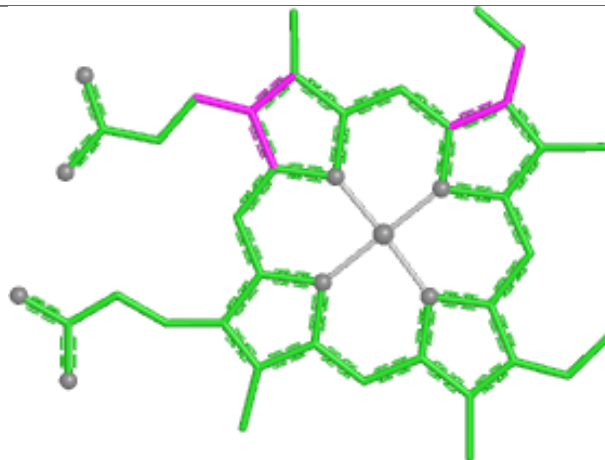


Rings

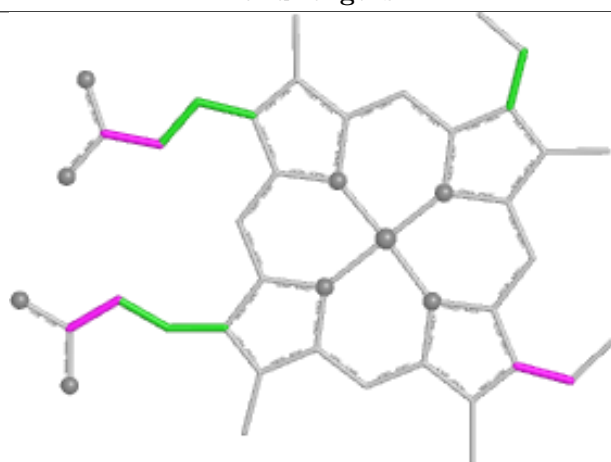
Ligand HEM N 4021



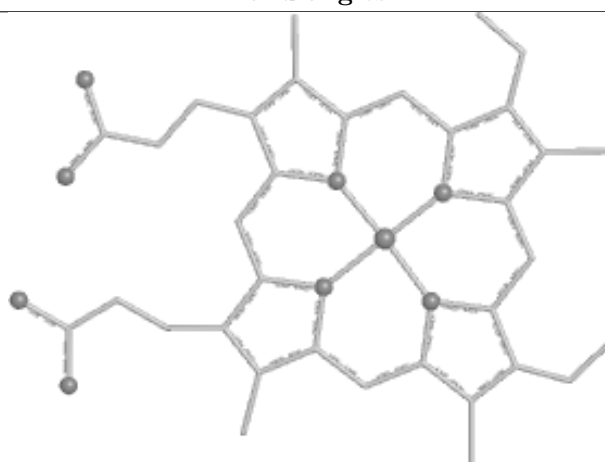
Bond lengths



Bond angles

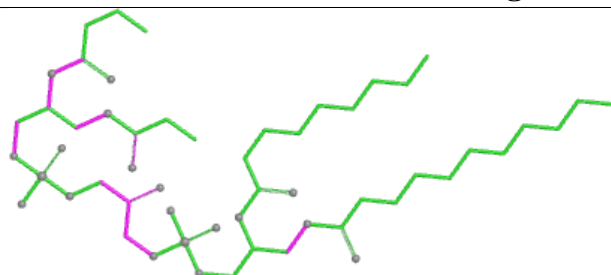


Torsions

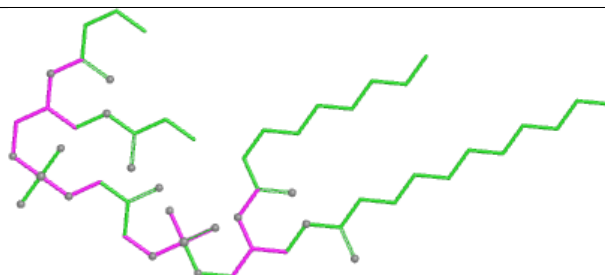


Rings

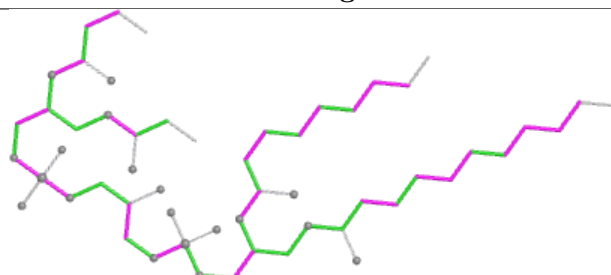
Ligand CN3 N 4131



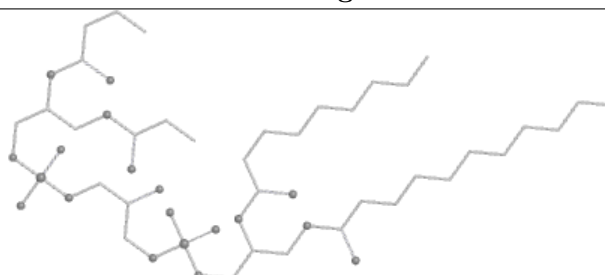
Bond lengths



Bond angles

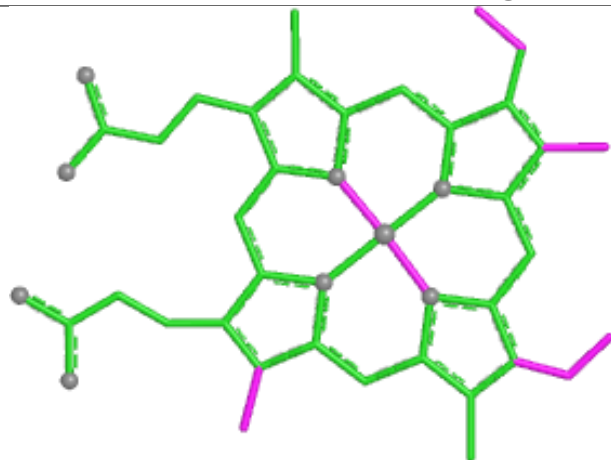


Torsions

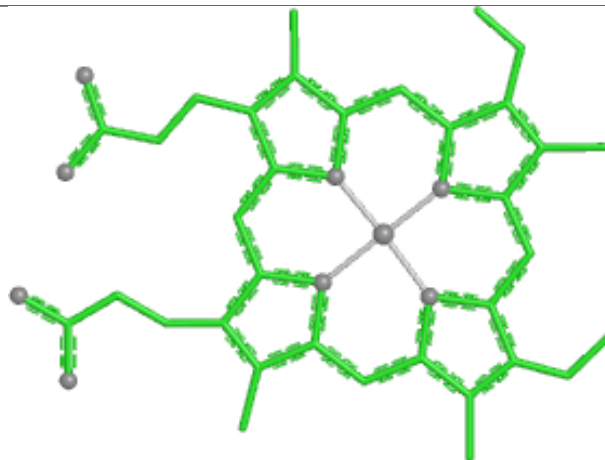


Rings

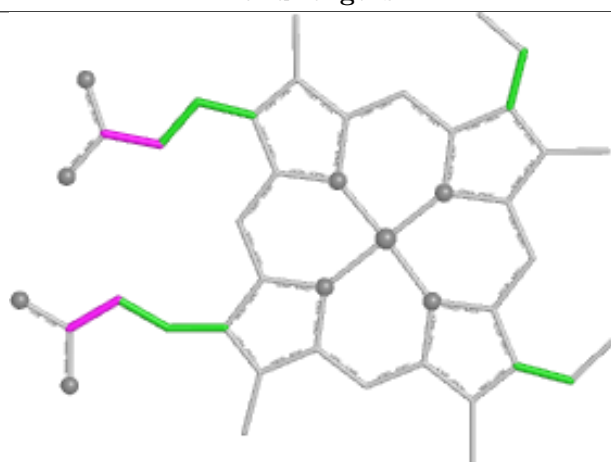
Ligand HEM C 4002



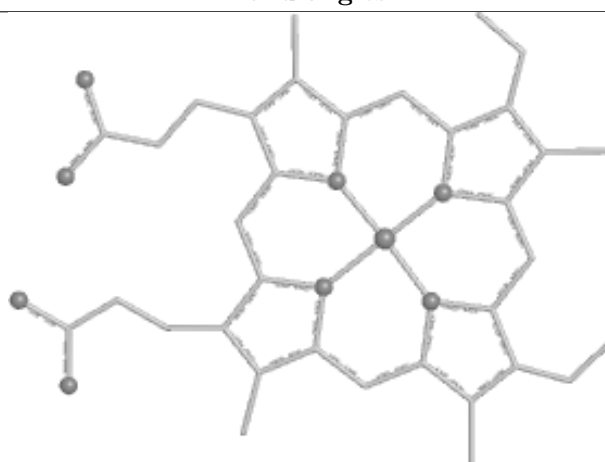
Bond lengths



Bond angles

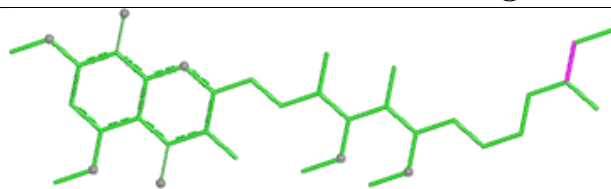


Torsions

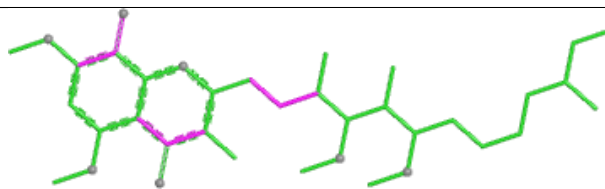


Rings

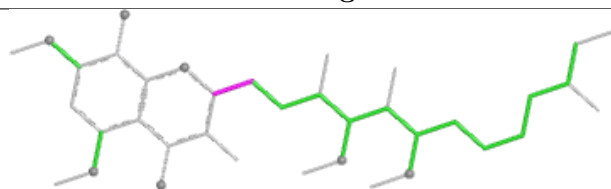
Ligand SMA N 4025



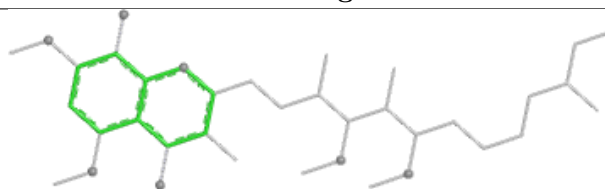
Bond lengths



Bond angles

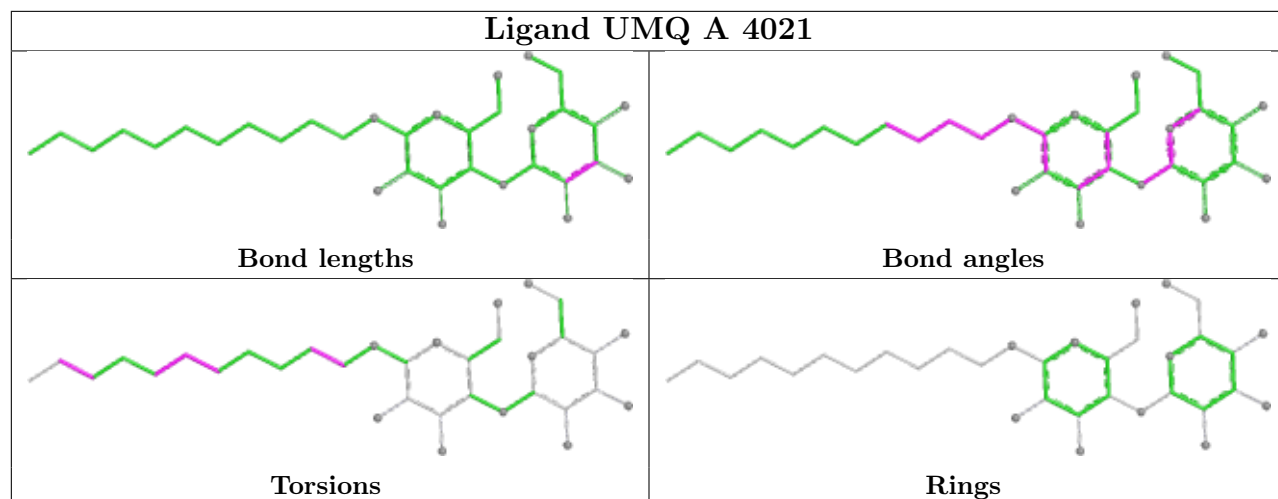


Torsions

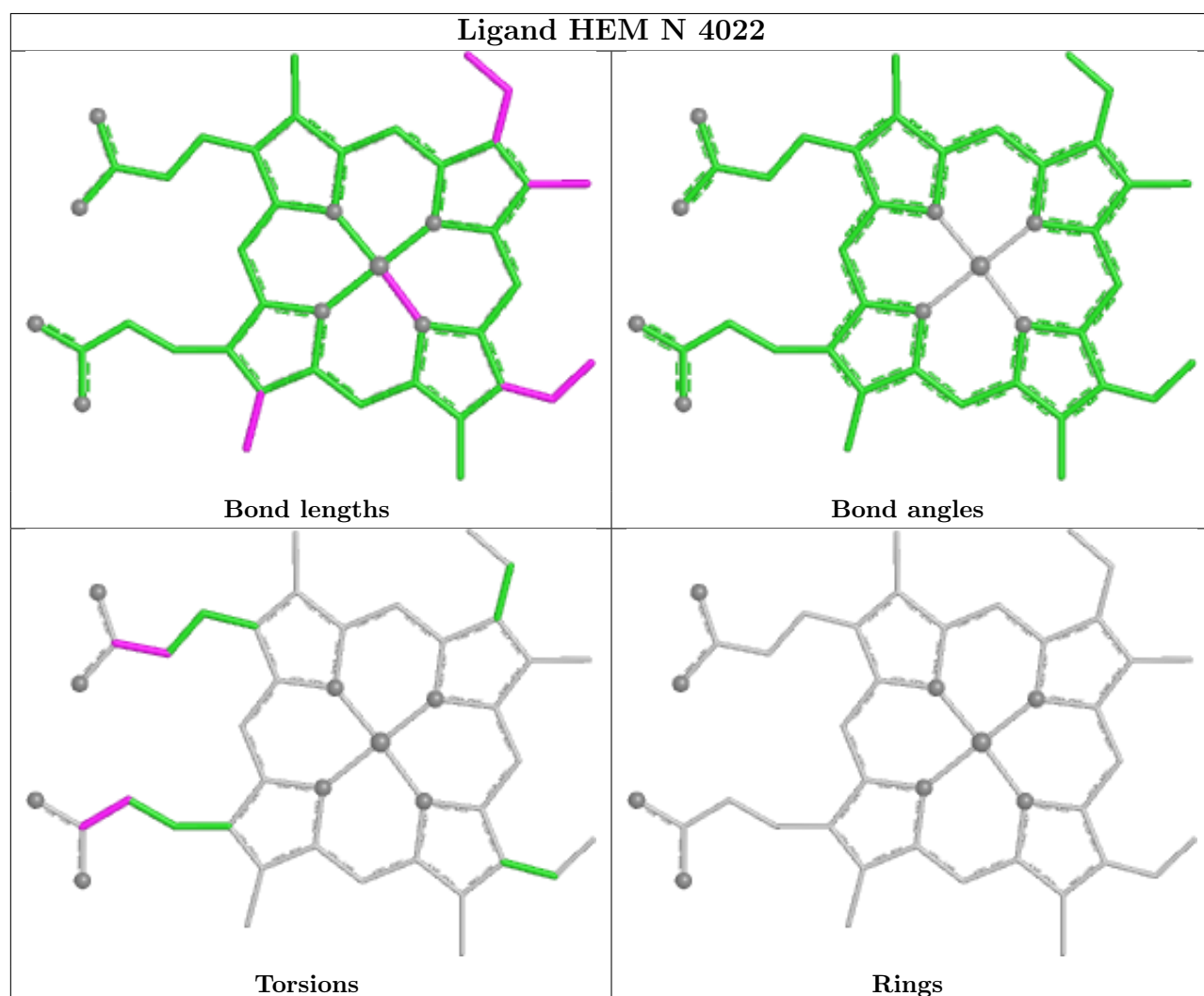


Rings

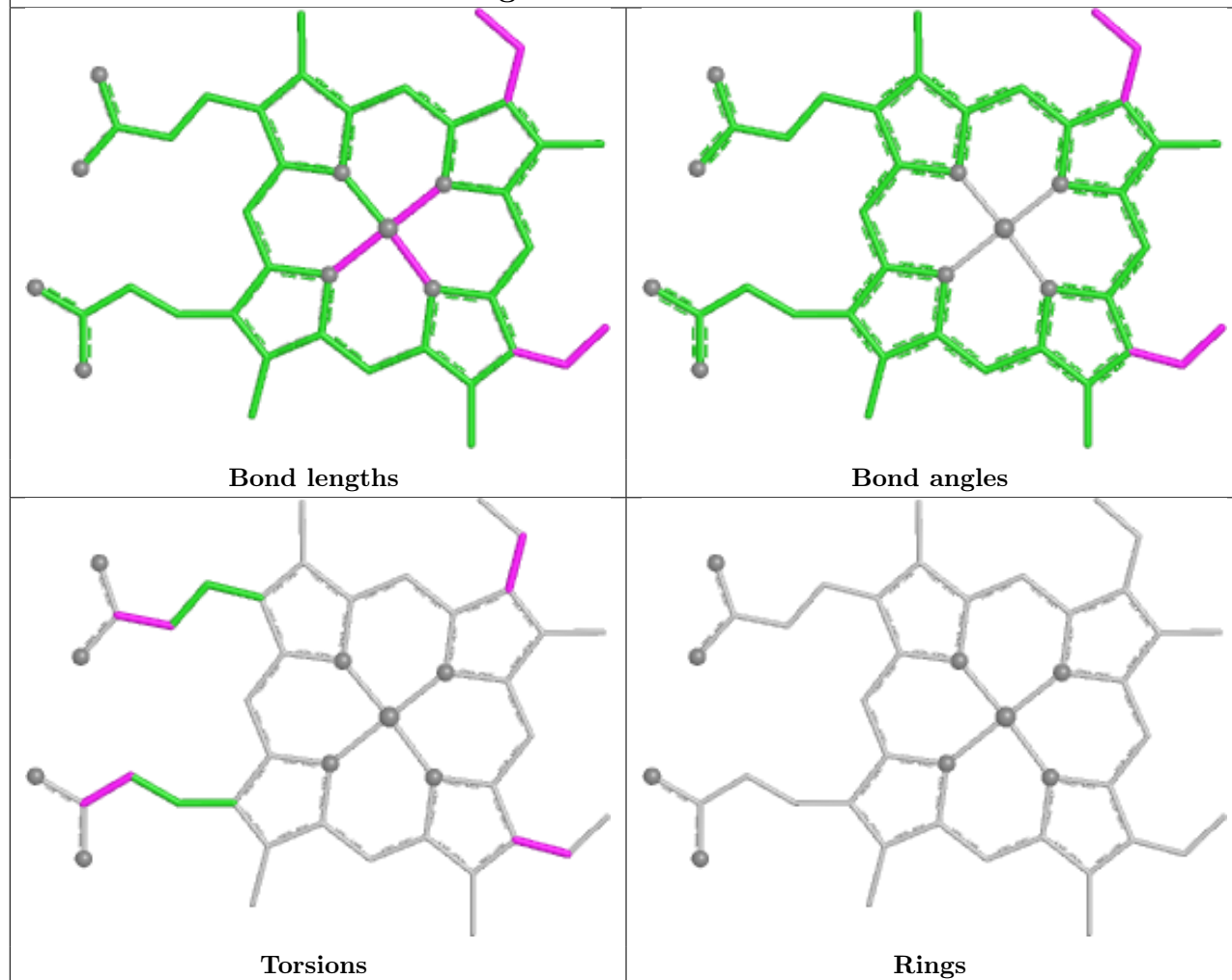
Ligand UMQ A 4021



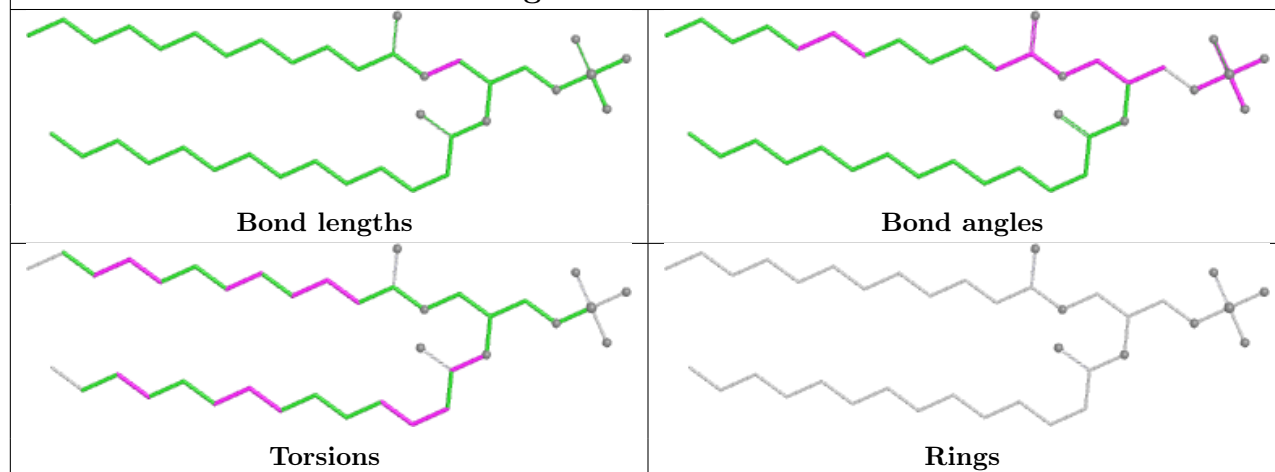
Ligand HEM N 4022

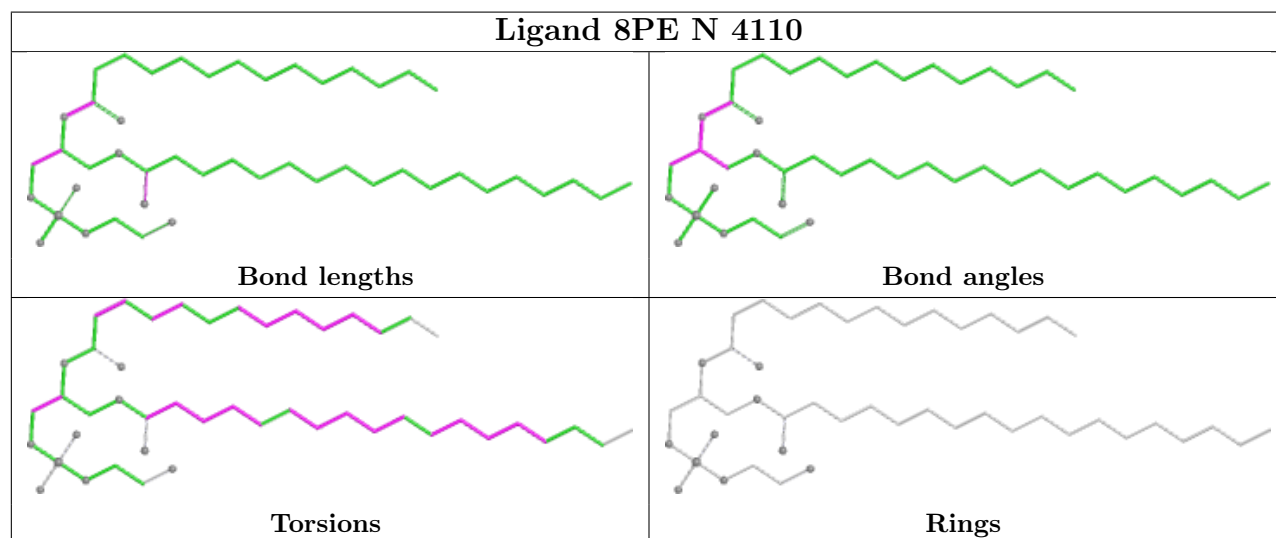
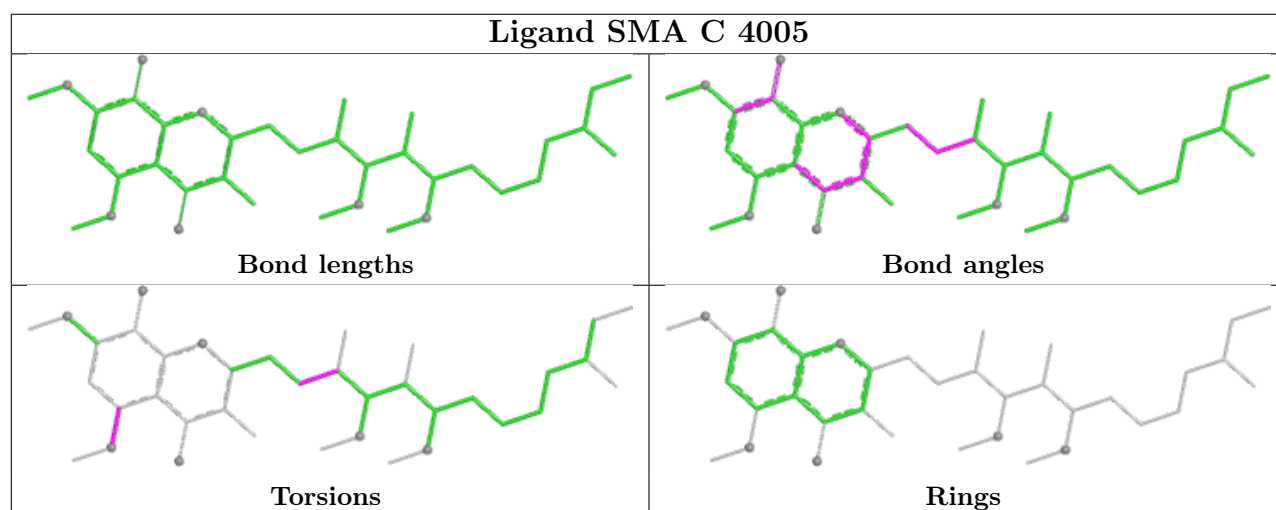
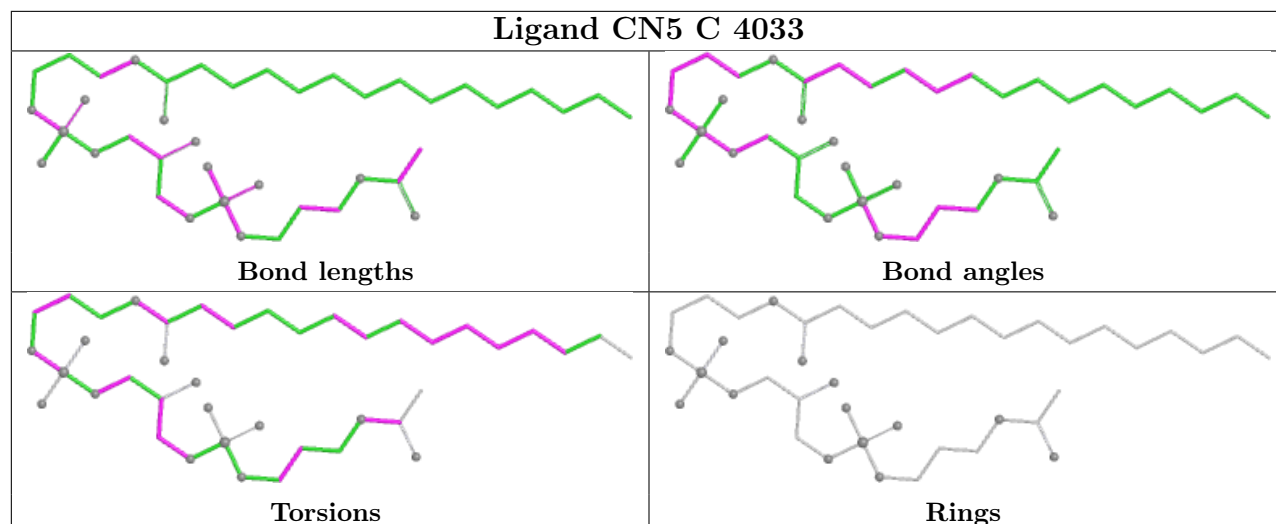


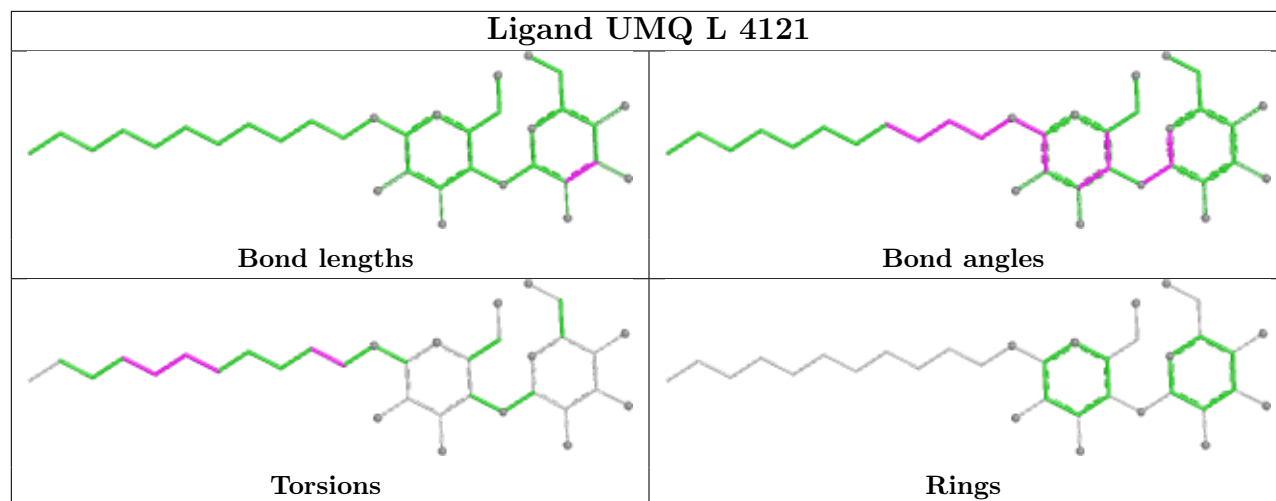
Ligand HEM O 4023



Ligand 7PH O 4114







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	1.28	106 (24%) 2 1	26, 44, 98, 114	0
1	L	431/431 (100%)	1.14	92 (21%) 2 2	25, 42, 90, 113	0
2	B	352/352 (100%)	1.46	90 (25%) 1 1	30, 47, 73, 114	0
2	M	352/352 (100%)	1.46	92 (26%) 1 1	32, 45, 72, 109	0
3	C	385/385 (100%)	0.02	6 (1%) 70 74	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.07	7 (1%) 67 71	19, 26, 37, 88	0
4	D	248/248 (100%)	0.47	17 (6%) 23 24	25, 35, 57, 83	0
4	O	248/248 (100%)	0.38	19 (7%) 19 21	24, 33, 55, 86	0
5	E	185/185 (100%)	0.90	33 (17%) 4 3	24, 40, 69, 94	0
5	P	185/185 (100%)	1.23	51 (27%) 1 1	24, 41, 80, 93	0
6	F	74/146 (50%)	1.45	22 (29%) 1 1	34, 46, 90, 96	0
6	Q	74/146 (50%)	1.27	14 (18%) 3 3	32, 45, 87, 90	0
7	G	126/126 (100%)	0.63	15 (11%) 9 9	26, 37, 60, 78	0
7	R	126/126 (100%)	0.58	17 (13%) 7 7	23, 34, 62, 80	0
8	H	93/93 (100%)	2.24	40 (43%) 0 0	24, 45, 128, 131	0
8	S	93/93 (100%)	1.88	34 (36%) 1 0	22, 43, 113, 119	0
9	I	57/65 (87%)	1.65	14 (24%) 2 1	34, 42, 83, 100	0
9	T	57/65 (87%)	1.65	17 (29%) 1 1	32, 40, 84, 96	0
10	J	127/127 (100%)	1.92	47 (37%) 1 0	40, 57, 71, 80	0
10	U	127/127 (100%)	2.23	66 (51%) 0 0	42, 59, 73, 82	0
11	K	107/107 (100%)	3.41	81 (75%) 0 0	51, 81, 114, 116	0
11	V	107/107 (100%)	3.87	101 (94%) 0 0	60, 92, 120, 122	0
12	W	107/108 (99%)	2.37	67 (62%) 0 0	29, 62, 87, 99	1 (0%)
All	All	4477/4638 (96%)	1.15	1048 (23%) 2 1	18, 41, 90, 131	1 (0%)

The worst 5 of 1048 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	17.5
1	A	230	LEU	15.8
9	I	57	ALA	13.2
1	L	230	LEU	13.1
2	B	336	ILE	12.6

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.

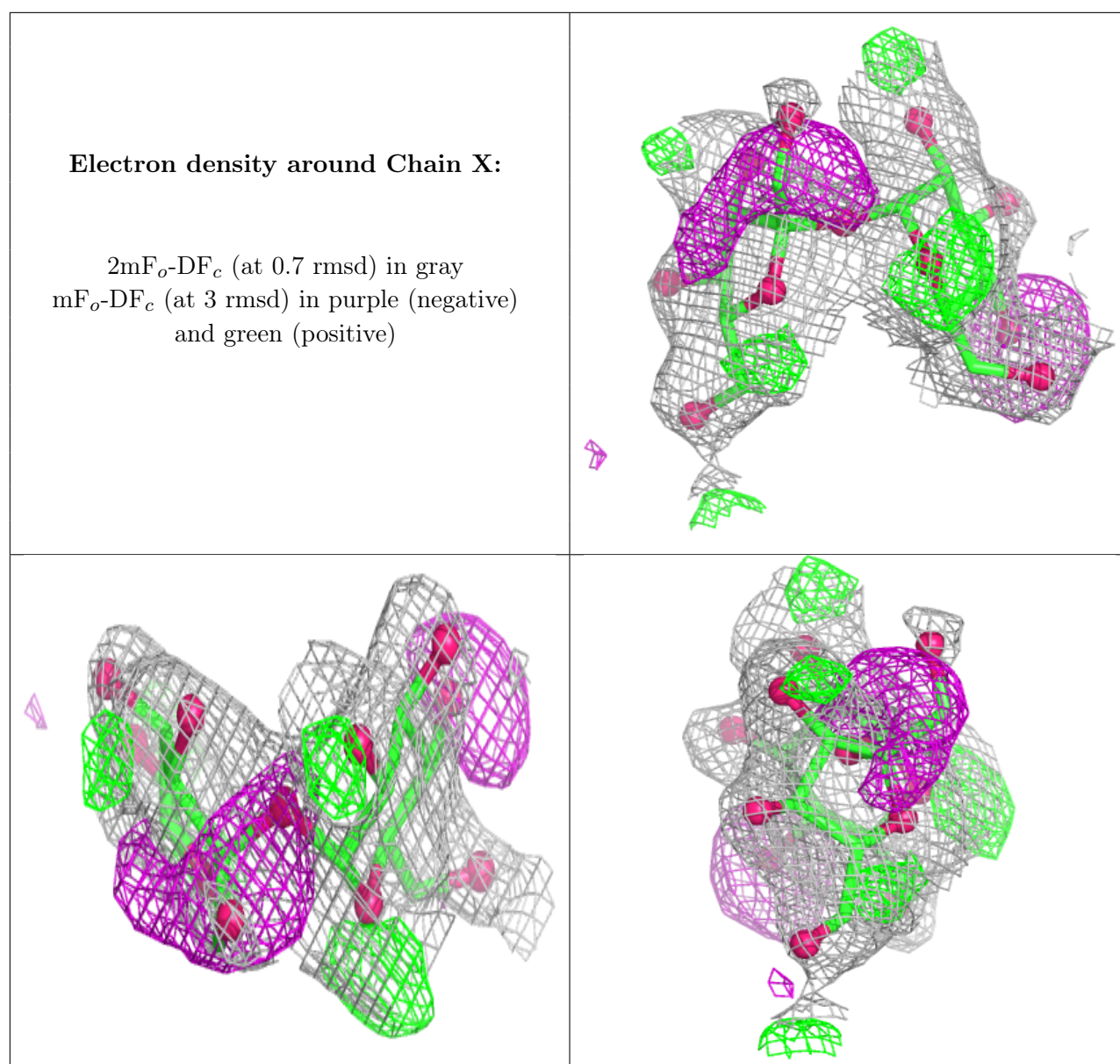
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	M3L	W	77	12/13	0.71	0.22	64,68,72,72	0

6.3 Carbohydrates [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
13	GLC	X	1	11/12	0.70	0.23	70,71,73,76	0
13	FRU	X	2	12/12	0.76	0.19	68,69,72,72	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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
20	CN5	C	4033	41/41	0.70	0.23	76,79,85,86	0
18	8PE	N	4110	47/47	0.83	0.17	43,51,65,67	0
18	8PE	C	4010	47/47	0.83	0.15	39,50,59,60	0
14	6PH	L	4113	40/40	0.84	0.15	51,55,67,68	0
22	CN3	D	4031	55/55	0.84	0.18	48,62,70,71	0

Continued on next page...

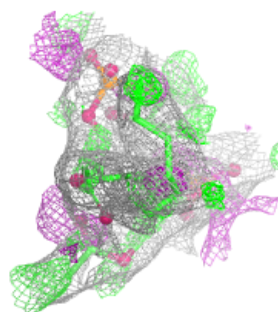
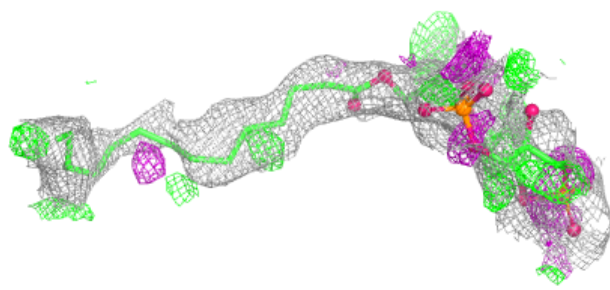
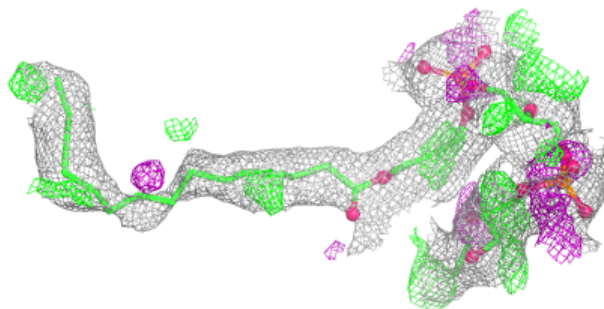
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CN3	N	4131	55/55	0.86	0.17	39,58,66,69	0
19	9PE	N	4111	40/40	0.87	0.14	39,47,62,66	0
14	6PH	A	4013	40/40	0.87	0.14	48,55,61,61	0
19	9PE	C	4011	40/40	0.89	0.13	39,46,70,72	0
21	7PH	O	4114	38/38	0.90	0.11	40,44,52,52	0
16	HEM	W	4026	43/43	0.90	0.15	46,50,54,55	0
21	7PH	D	4014	38/38	0.90	0.12	43,46,62,63	0
15	UMQ	A	4021	34/34	0.92	0.10	32,36,55,56	0
15	UMQ	L	4121	34/34	0.92	0.10	33,35,57,58	0
17	SMA	N	4025	37/37	0.95	0.06	21,24,30,33	0
17	SMA	C	4005	37/37	0.97	0.05	22,24,31,34	0
16	HEM	D	4003	43/43	0.98	0.07	23,29,33,34	0
16	HEM	N	4021	43/43	0.98	0.06	16,20,25,27	0
16	HEM	N	4022	43/43	0.98	0.06	15,18,26,28	0
16	HEM	O	4023	43/43	0.98	0.06	25,28,30,33	0
16	HEM	C	4001	43/43	0.99	0.05	16,21,26,30	0
16	HEM	C	4002	43/43	0.99	0.05	17,20,24,28	0
23	FES	E	4004	4/4	0.99	0.04	27,27,28,31	0
23	FES	P	4024	4/4	0.99	0.04	28,29,31,32	0

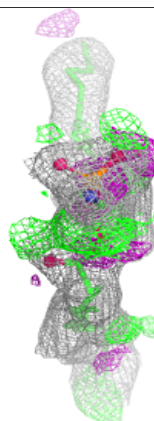
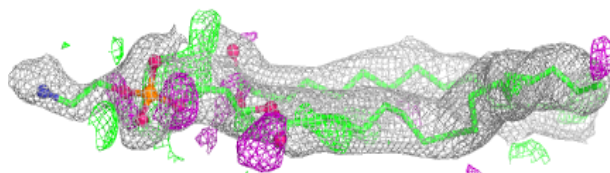
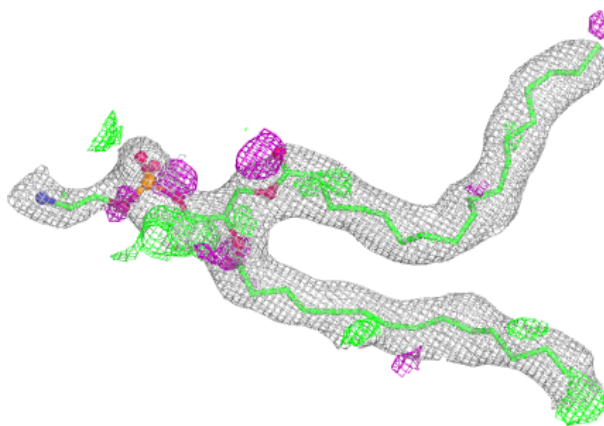
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CN5 C 4033:

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

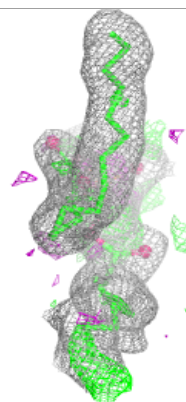
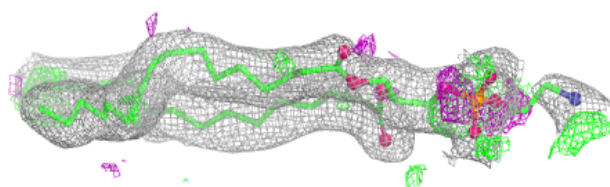
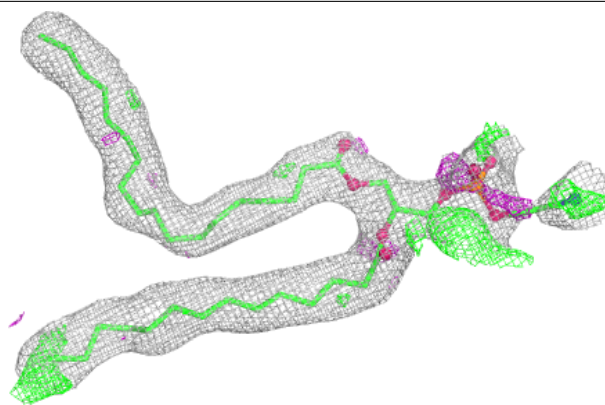
**Electron density around 8PE N 4110:**

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

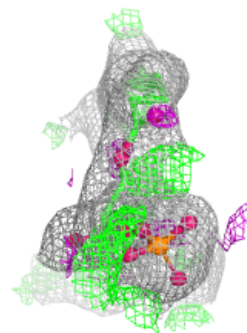
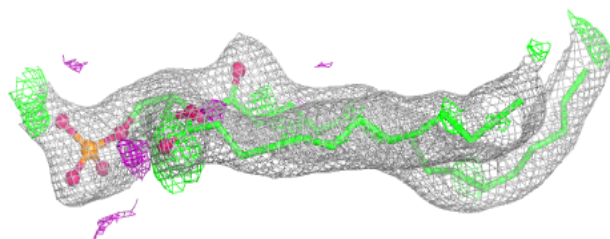
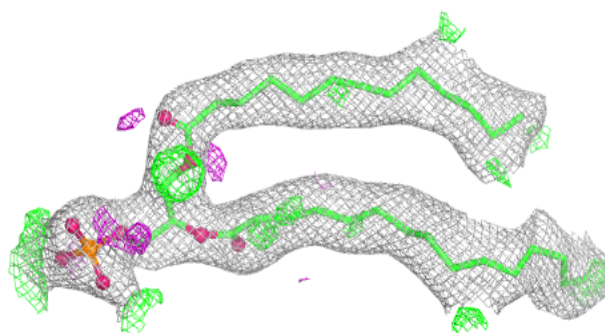


Electron density around 8PE C 4010:

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

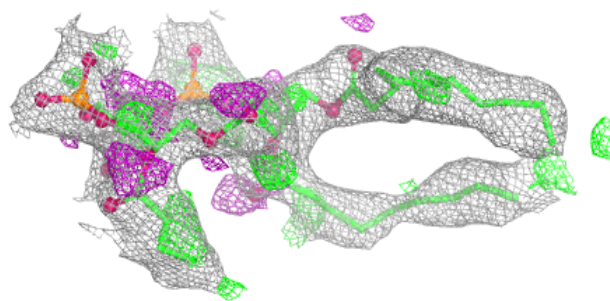
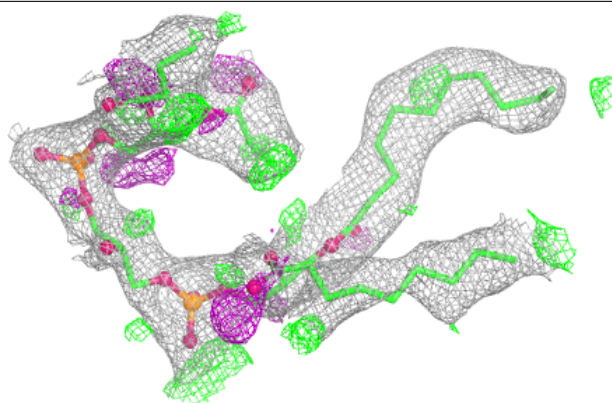
**Electron density around 6PH L 4113:**

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

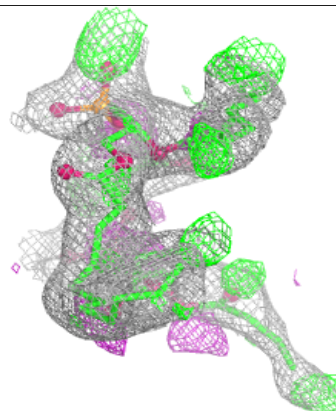
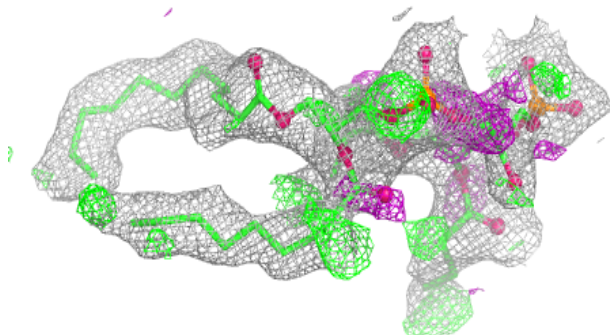
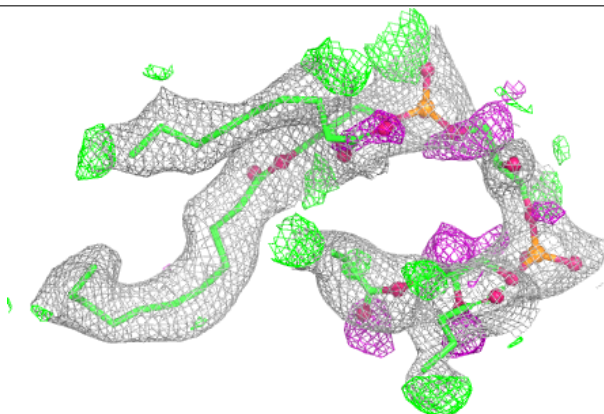


Electron density around CN3 D 4031:

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

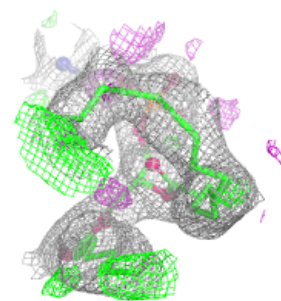
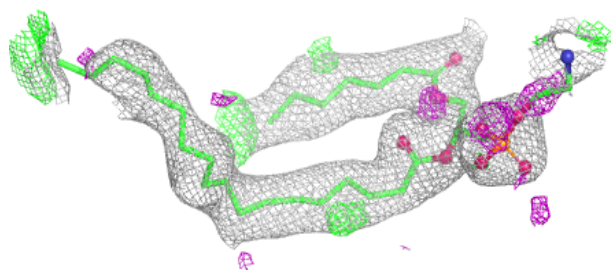
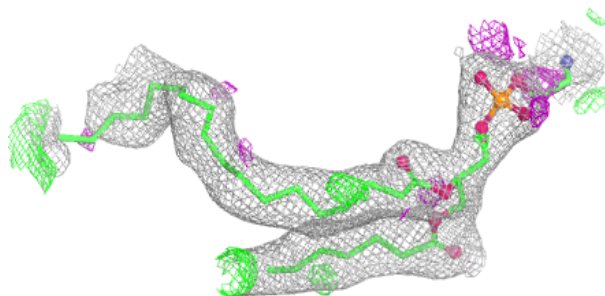
**Electron density around CN3 N 4131:**

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

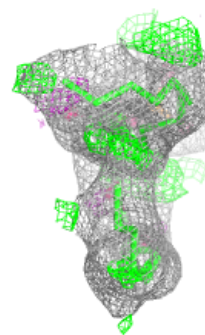
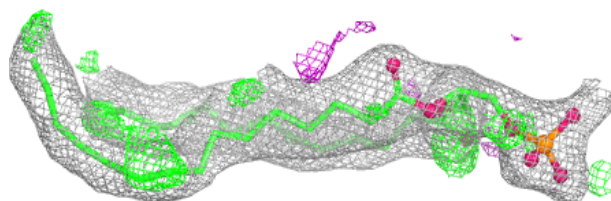
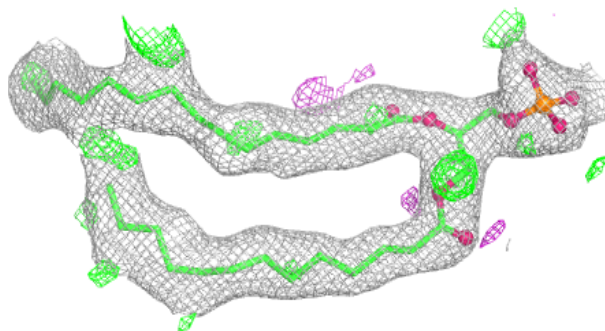


Electron density around 9PE N 4111:

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

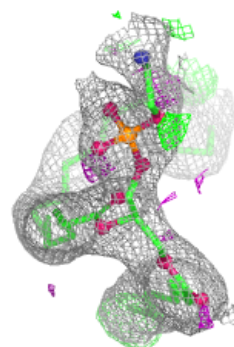
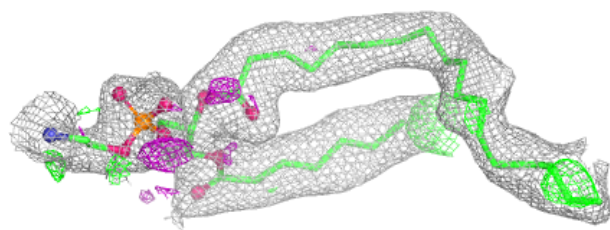
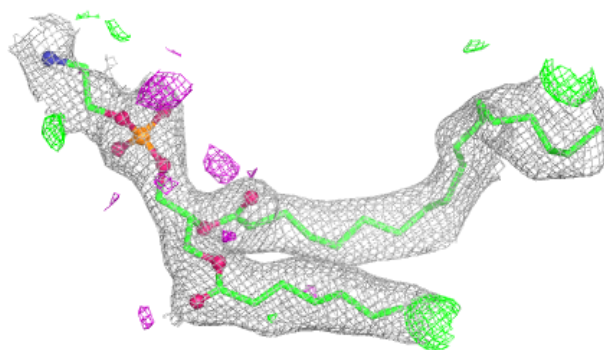
**Electron density around 6PH A 4013:**

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

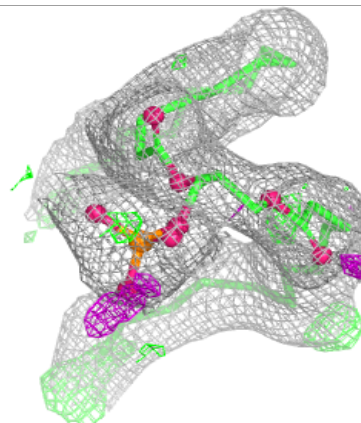
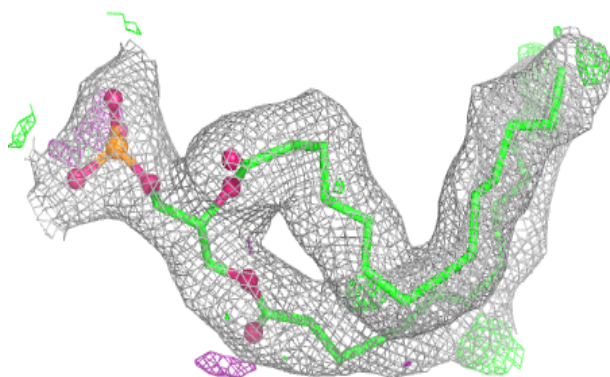
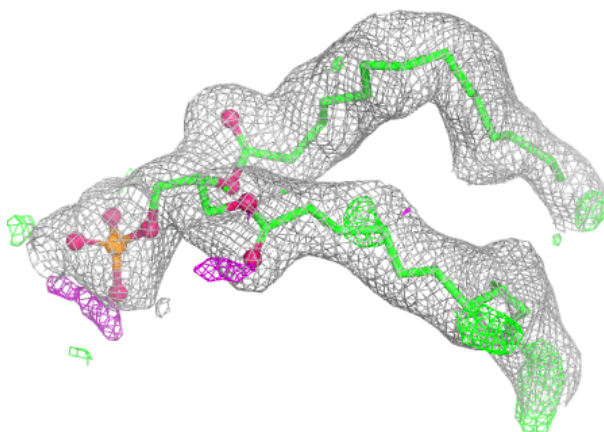


Electron density around 9PE C 4011:

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

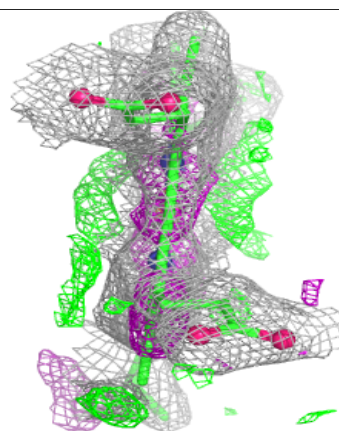
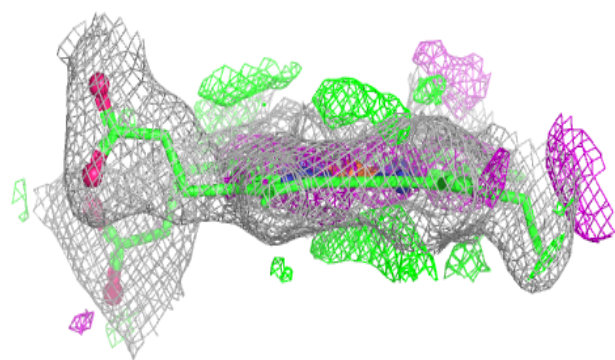
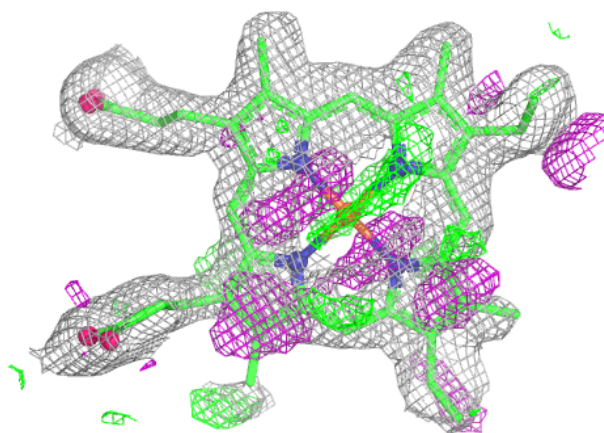
**Electron density around 7PH O 4114:**

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

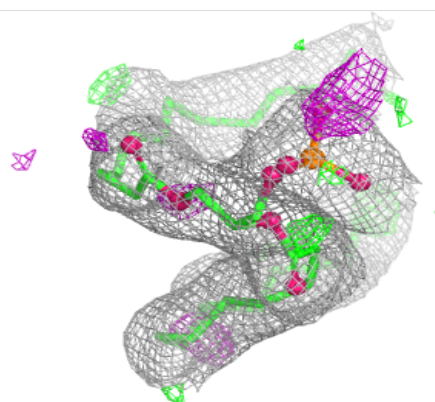
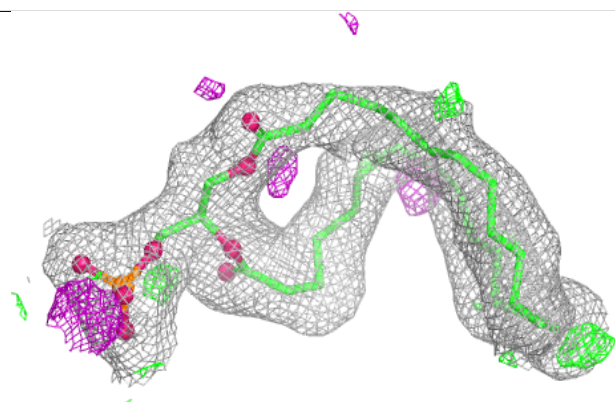
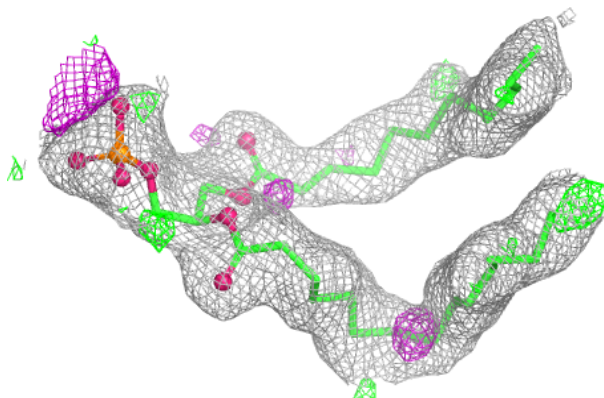


Electron density around HEM W 4026:

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

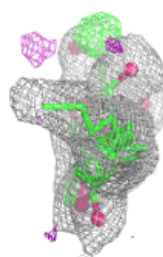
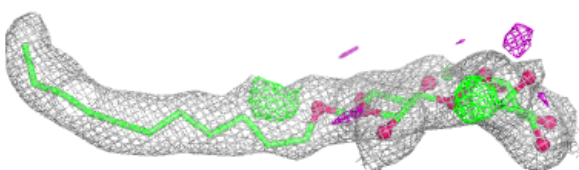
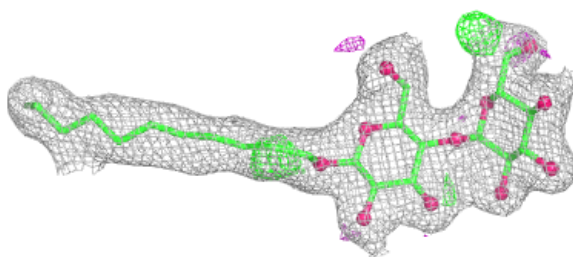
**Electron density around 7PH D 4014:**

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

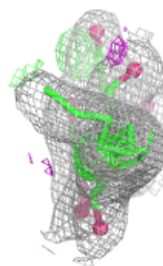
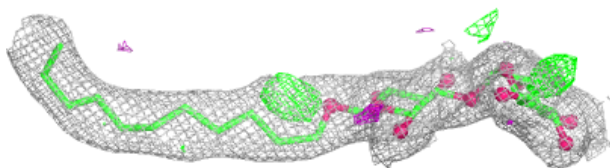
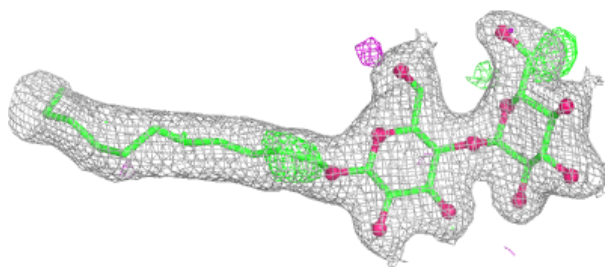


Electron density around UMQ A 4021:

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

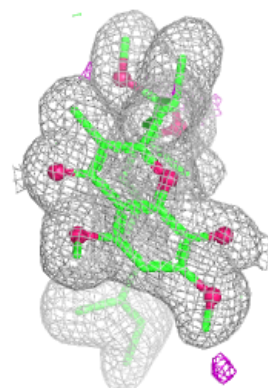
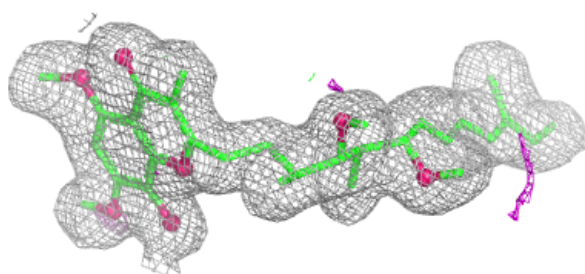
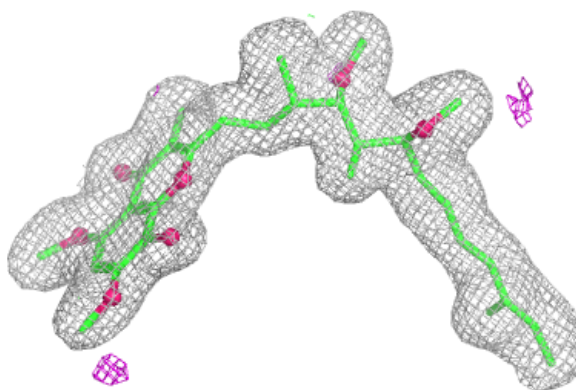
**Electron density around UMQ L 4121:**

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

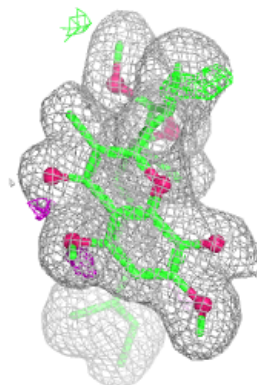
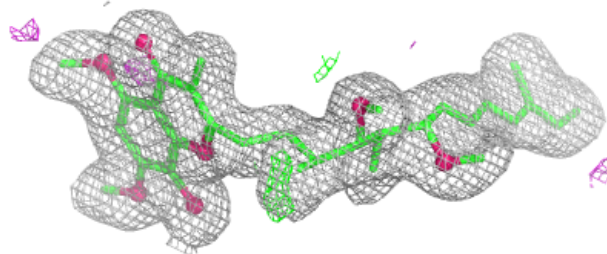
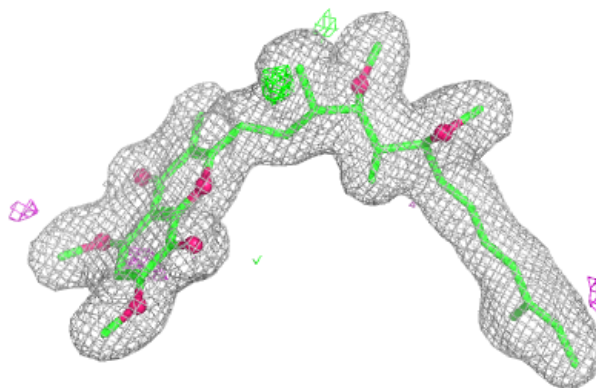


Electron density around SMA N 4025:

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

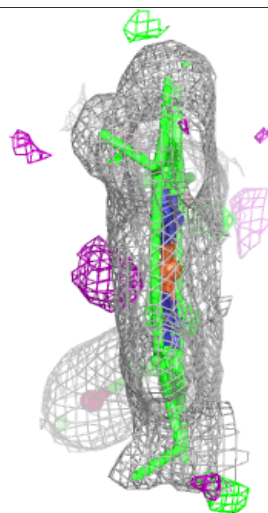
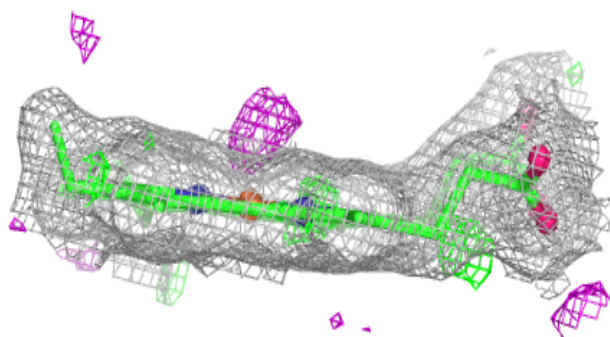
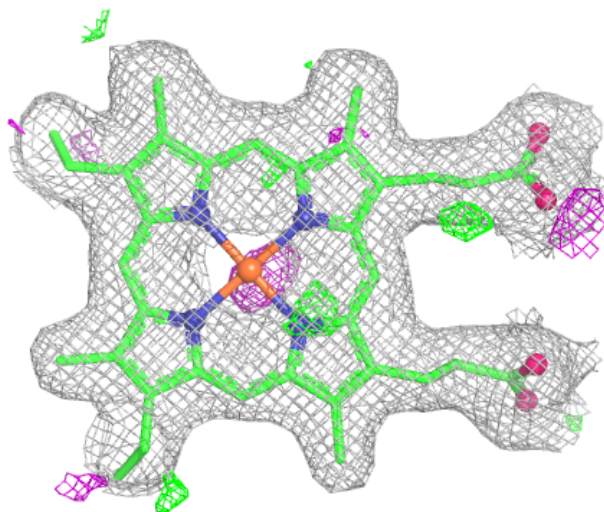
**Electron density around SMA C 4005:**

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



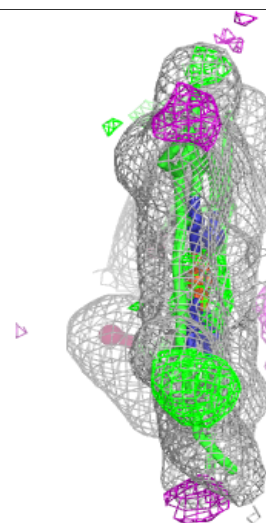
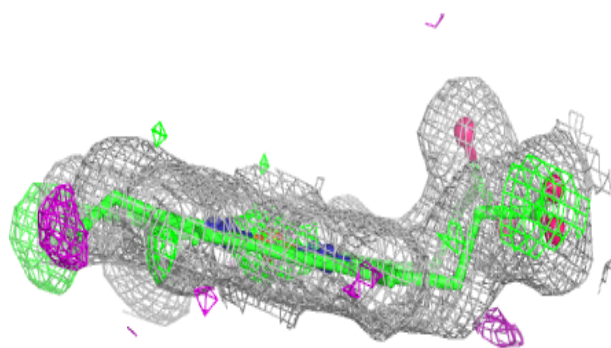
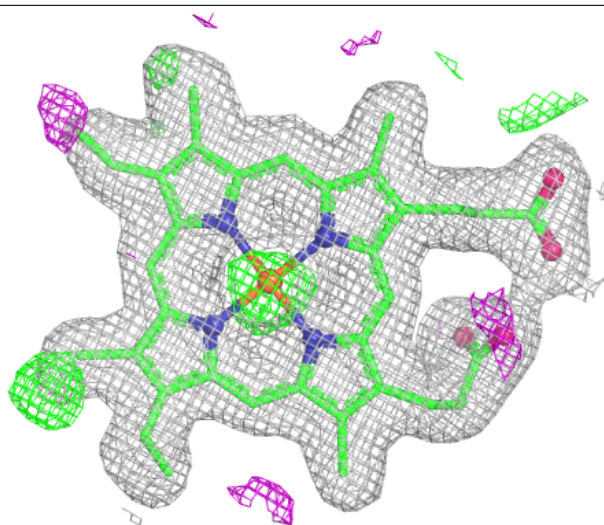
Electron density around HEM D 4003:

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



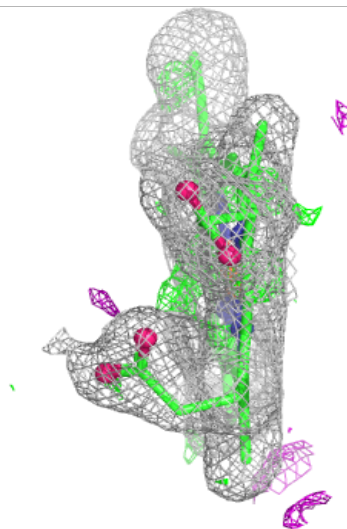
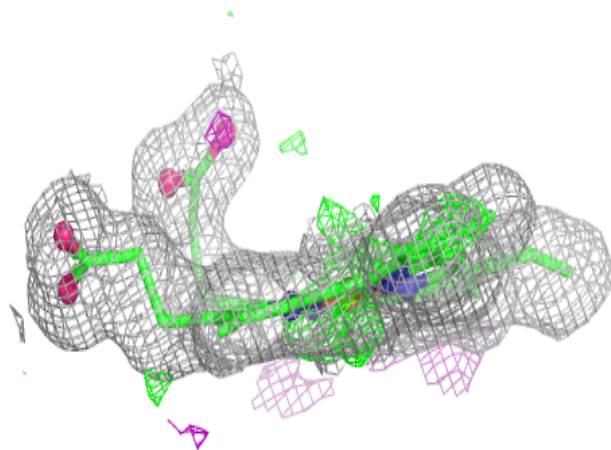
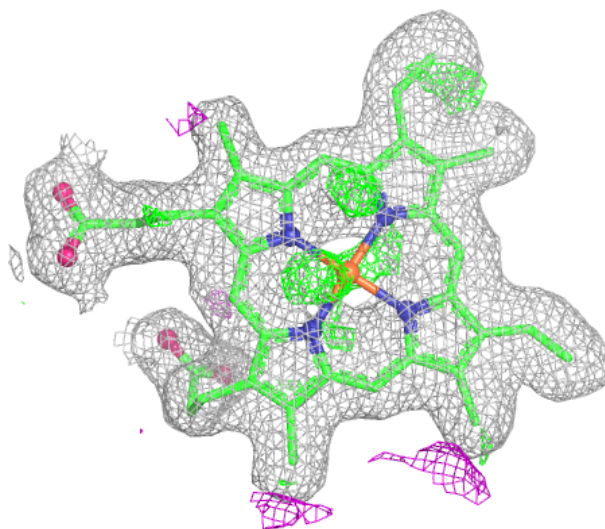
Electron density around HEM N 4021:

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



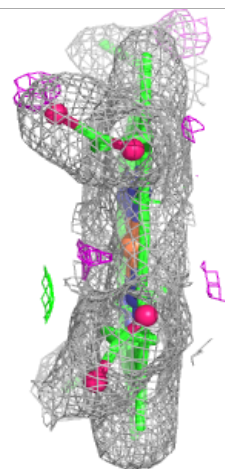
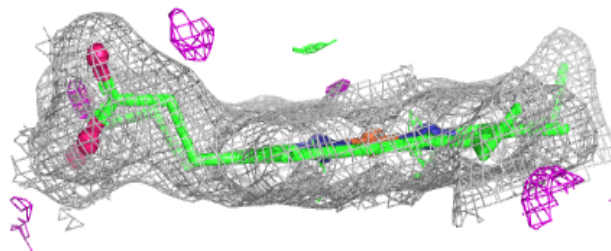
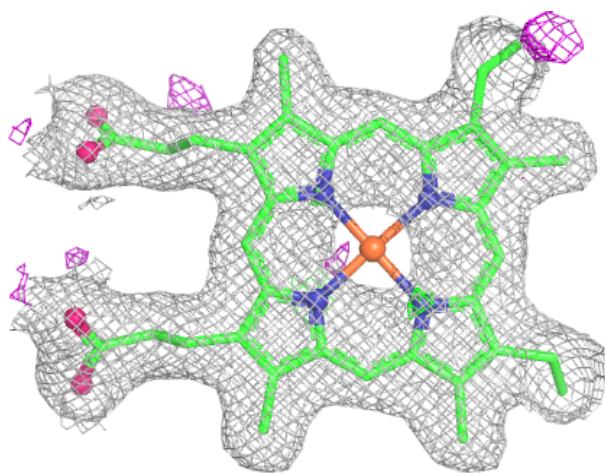
Electron density around HEM N 4022:

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



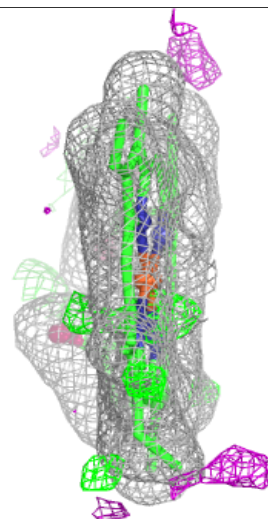
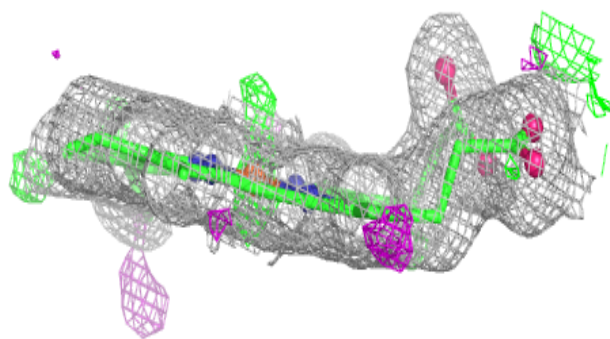
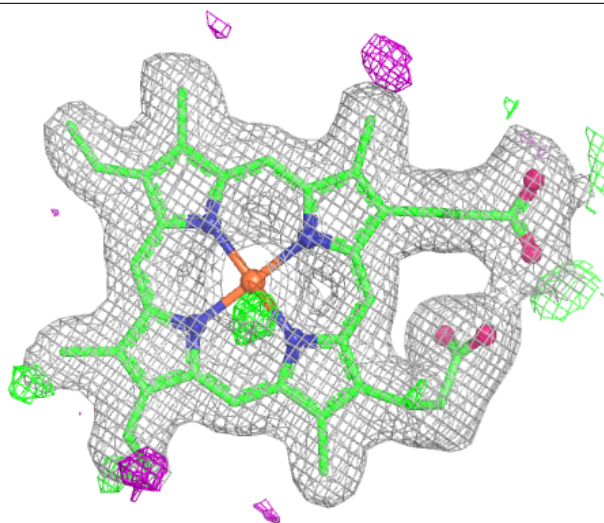
Electron density around HEM O 4023:

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



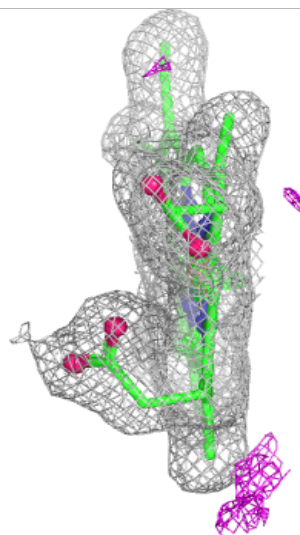
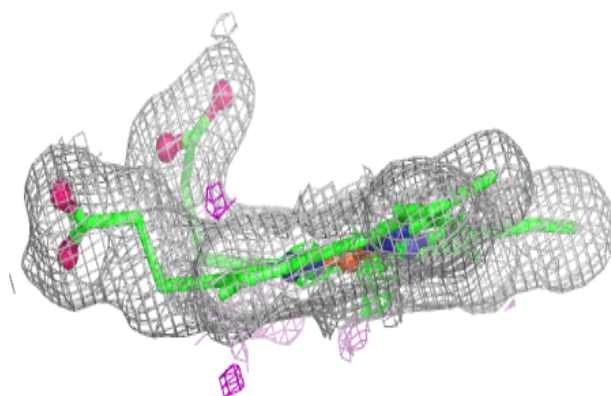
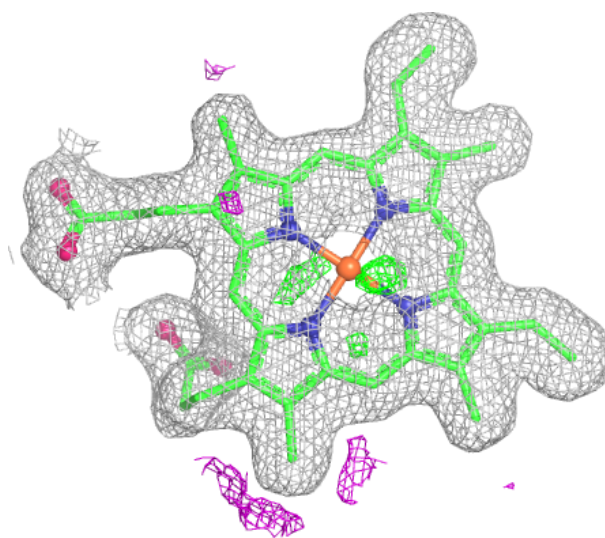
Electron density around HEM C 4001:

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



Electron density around HEM C 4002:

$2mF_o-DF_c$ (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.