



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 01:32 PM EDT

PDB ID : 1Q90  
Title : Structure of the cytochrome b6f (plastohydroquinone : plastocyanin oxidoreductase) from Chlamydomonas reinhardtii  
Authors : Stroebel, D.; Choquet, Y.; Popot, J.-L.; Picot, D.  
Deposited on : 2003-08-22  
Resolution : 3.10 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

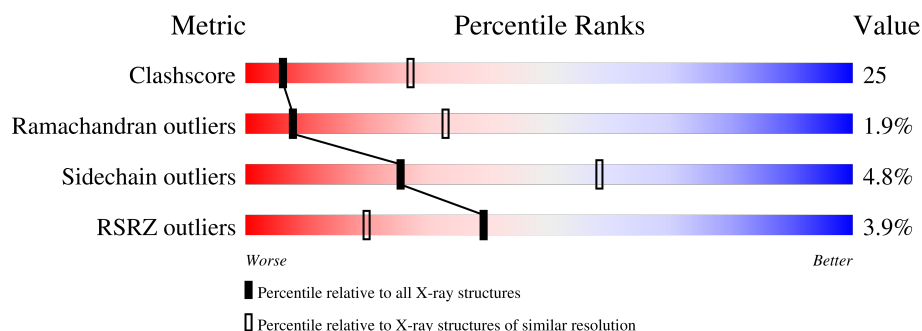
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	292	<div> <div>6%</div> <div>59%</div> <div>37%</div> <div>.</div> </div>
2	B	215	<div> <div>57%</div> <div>40%</div> <div>..</div> </div>
3	C	127	<div> <div>24%</div> <div>42%</div> <div>53%</div> <div>5%</div> <div>.</div> </div>
4	D	159	<div> <div>47%</div> <div>45%</div> <div>6%</div> <div>.</div> </div>
5	R	49	<div> <div>6%</div> <div>57%</div> <div>16%</div> <div>6%</div> <div>20%</div> </div>
6	G	37	<div> <div>65%</div> <div>16%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
7	L	32	
8	M	39	
9	N	31	

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
14	CLA	D	910	X	-	-	-
16	LMG	D	953	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 7778 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 Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2266	1457	387	417	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	HIS	-	expression tag	UNP P23577
A	288	HIS	-	expression tag	UNP P23577
A	289	HIS	-	expression tag	UNP P23577
A	290	HIS	-	expression tag	UNP P23577
A	291	HIS	-	expression tag	UNP P23577
A	292	HIS	-	expression tag	UNP P23577

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1681	1117	270	281	13			

- Molecule 3 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	126	Total	C	N	O	S	0	0	0
			955	606	163	181	5			

- Molecule 4 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	156	Total	C	N	O	S	0	0	0
			1201	807	185	204	5			

- Molecule 5 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	39	Total	C	N	O	S	0	0	0
			283	184	46	51	2			

- Molecule 6 is a protein called Cytochrome b6f complex subunit petG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	30	Total	C	N	O	S	0	0	0
			224	154	31	37	2			

- Molecule 7 is a protein called Cytochrome b6f complex subunit petL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	32	Total	C	N	O	S	0	0	0
			242	168	34	39	1			

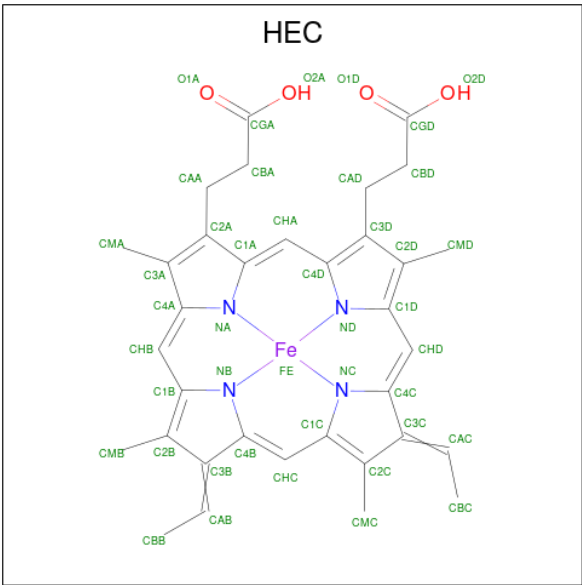
- Molecule 8 is a protein called Cytochrome b6f complex subunit PETM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	M	34	Total	C	N	O	S	0	0	0
			247	162	37	46	2			

- Molecule 9 is a protein called Cytochrome b6f complex subunit PETN.

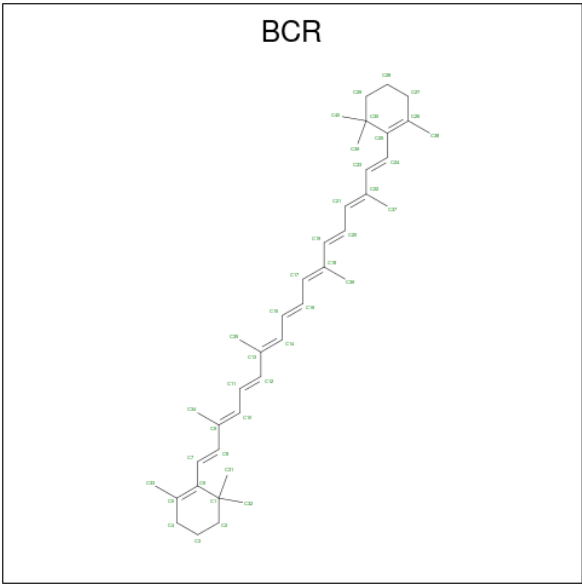
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	31	Total	C	N	O	S	0	0	0
			231	152	37	40	2			

- Molecule 10 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



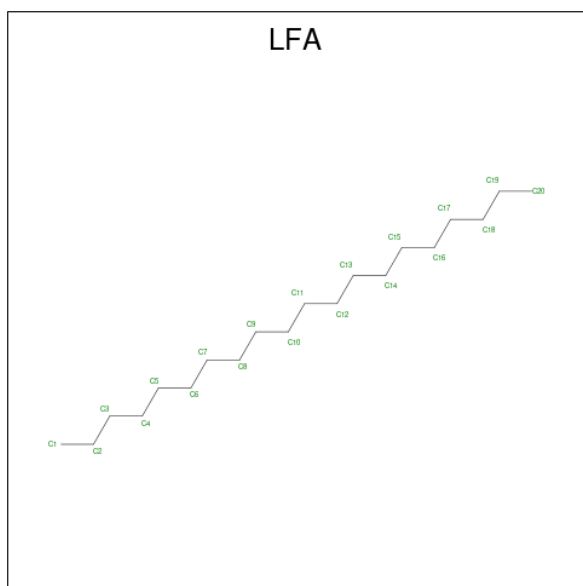
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



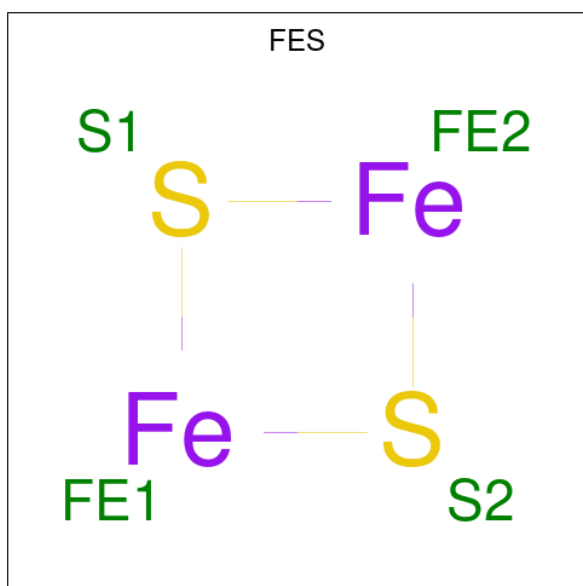
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 27 27	0	0

- Molecule 12 is EICOSANE (three-letter code: LFA) (formula:  $C_{20}H_{42}$ ).



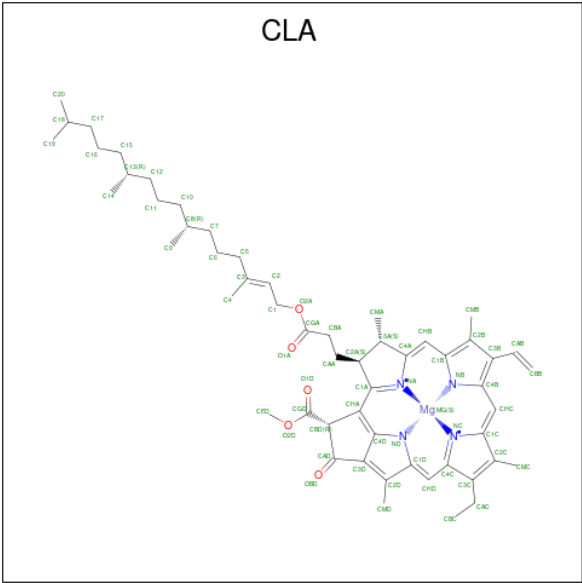
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C 20 20	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



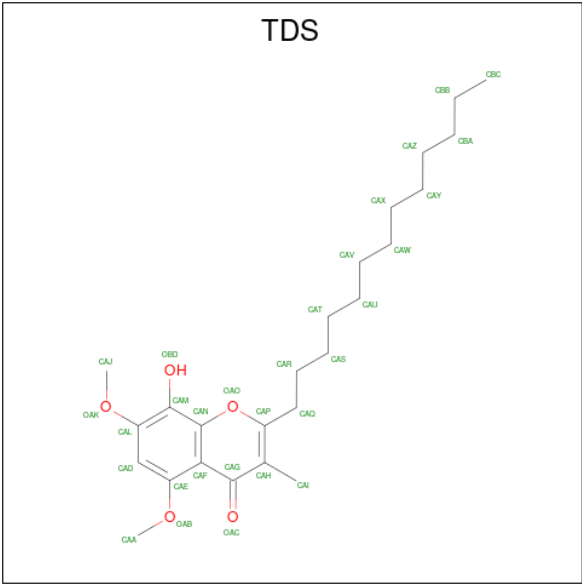
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

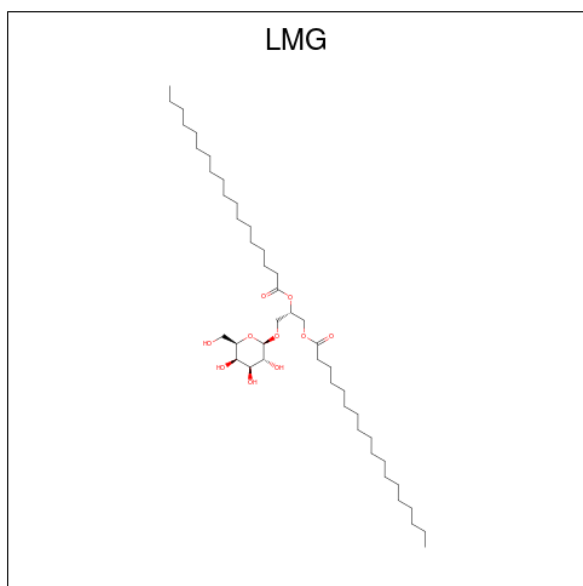
- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula:  $C_{25}H_{38}O_5$ ).





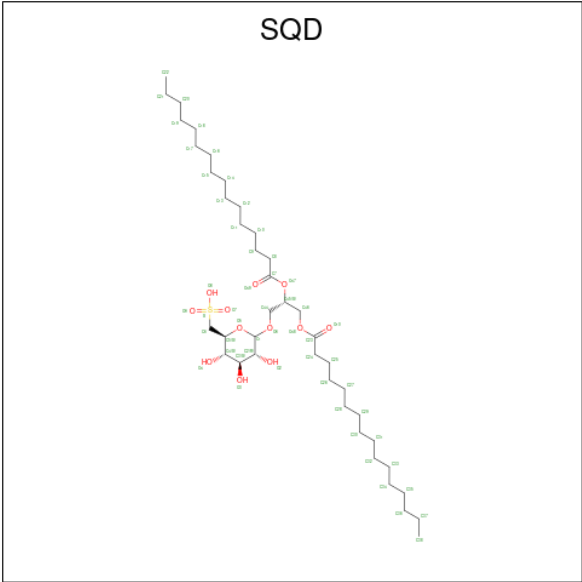
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	C	O	0	0
			30	25	5		

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	C	O	0	0
			53	43	10		
16	L	1	Total	C	O	0	0
			42	32	10		

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	R	1	Total	C	O	S	0	0
			33	20	12	1		

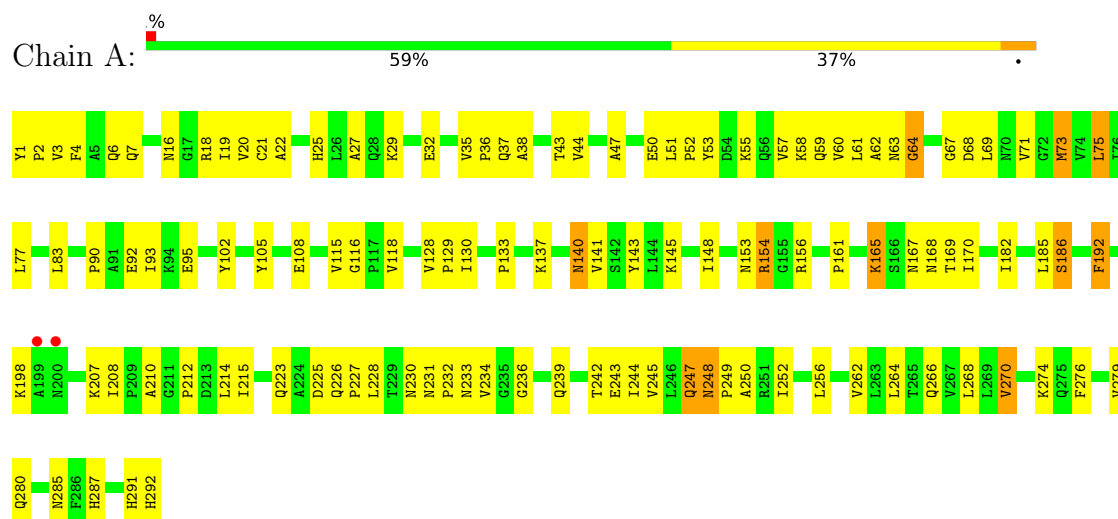
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	B	2	Total	O	0	0
			2	2		

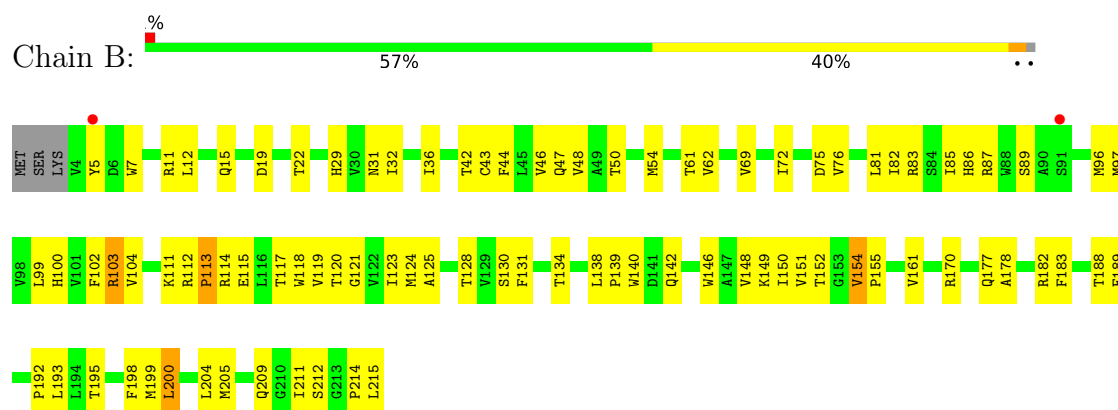
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

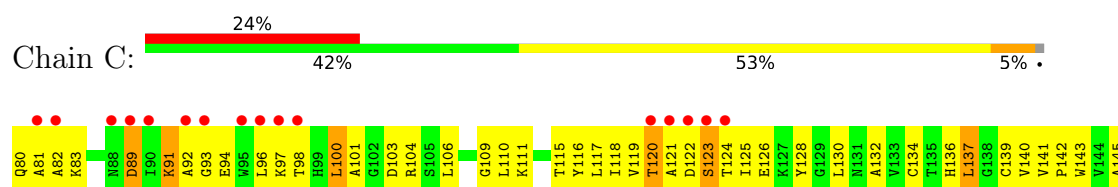
#### • Molecule 1: Apocytochrome f



#### • Molecule 2: Cytochrome b6

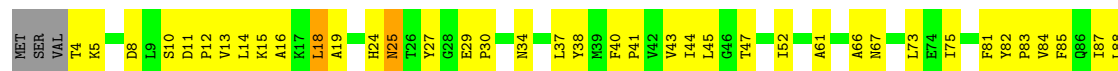


#### • Molecule 3: Cytochrome B6-F complex iron-sulfur subunit

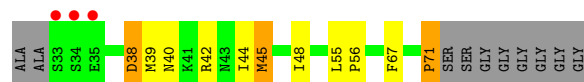




• Molecule 4: Cytochrome b6-f complex subunit 4



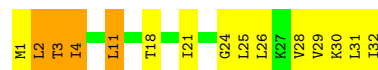
• Molecule 5: Cytochrome B6-F complex iron-sulfur subunit



• Molecule 6: Cytochrome b6f complex subunit petG



• Molecule 7: Cytochrome b6f complex subunit petL



• Molecule 8: Cytochrome b6f complex subunit PETM



• Molecule 9: Cytochrome b6f complex subunit PETN



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.45Å 171.21Å 351.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.42 – 3.10 35.14 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-3.10) 92.7 (35.14-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.261 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 77.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, SQD, CLA, TDS, FES, LMG, LFA, BCR

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	0.36	0/2318	0.64	0/3148
2	B	0.48	0/1732	0.64	0/2360
3	C	0.29	0/979	0.55	0/1333
4	D	0.38	0/1238	0.62	0/1698
5	R	0.46	0/289	0.94	1/393 (0.3%)
6	G	0.42	0/228	0.60	0/313
7	L	0.39	0/244	0.61	0/329
8	M	0.42	0/248	0.64	0/335
9	N	0.56	0/237	0.57	0/321
All	All	0.40	0/7513	0.63	1/10230 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	R	71	PRO	CA-N-CD	-13.91	92.03	111.50

There are no chirality outliers.

There are no planarity outliers.

### 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	2266	0	2301	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1681	0	1692	105	0
3	C	955	0	922	67	0
4	D	1201	0	1256	88	0
5	R	283	0	291	13	0
6	G	224	0	248	9	0
7	L	242	0	286	12	0
8	M	247	0	263	19	0
9	N	231	0	230	19	0
10	A	43	0	30	4	0
10	B	129	0	95	8	0
11	B	27	0	35	3	0
12	B	20	0	42	2	0
13	C	4	0	0	1	0
14	D	65	0	72	5	0
15	D	30	0	38	2	0
16	D	53	0	79	3	0
16	L	42	0	54	4	0
17	R	33	0	29	1	0
18	B	2	0	0	0	0
All	All	7778	0	7963	386	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 25.

The worst 5 of 386 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:31:ASN:HA	9:N:98:LEU:HD22	1.24	1.18
3:C:178:HIS:HB2	3:C:190:SER:HB2	1.34	1.10
2:B:50:THR:HG23	2:B:86:HIS:HD1	1.07	1.07
1:A:59:GLN:HE22	1:A:156:ARG:HG3	1.27	1.00
2:B:142:GLN:NE2	4:D:67:ASN:H	1.63	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/292 (99%)	263 (91%)	21 (7%)	6 (2%)	7	30
2	B	210/215 (98%)	179 (85%)	29 (14%)	2 (1%)	15	49
3	C	122/127 (96%)	96 (79%)	22 (18%)	4 (3%)	4	21
4	D	154/159 (97%)	134 (87%)	15 (10%)	5 (3%)	4	22
5	R	37/49 (76%)	32 (86%)	5 (14%)	0	100	100
6	G	28/37 (76%)	24 (86%)	4 (14%)	0	100	100
7	L	30/32 (94%)	25 (83%)	5 (17%)	0	100	100
8	M	32/39 (82%)	31 (97%)	0	1 (3%)	4	23
9	N	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	932/981 (95%)	811 (87%)	103 (11%)	18 (2%)	8	33

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	89	ASP
1	A	140	ASN
1	A	165	LYS
1	A	198	LYS
3	C	100	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	246/246 (100%)	233 (95%)	13 (5%)	22	54
2	B	179/182 (98%)	171 (96%)	8 (4%)	27	60
3	C	99/100 (99%)	96 (97%)	3 (3%)	41	71
4	D	131/134 (98%)	126 (96%)	5 (4%)	33	66
5	R	30/32 (94%)	27 (90%)	3 (10%)	7	28
6	G	25/30 (83%)	25 (100%)	0	100	100
7	L	27/27 (100%)	23 (85%)	4 (15%)	3	13
8	M	26/29 (90%)	24 (92%)	2 (8%)	13	41
9	N	24/24 (100%)	24 (100%)	0	100	100
All	All	787/804 (98%)	749 (95%)	38 (5%)	25	58

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	118	ASN
7	L	11	LEU
5	R	38	ASP
7	L	2	LEU
8	M	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	34	ASN
5	R	43	ASN
9	N	74	GLN
4	D	121	GLN
2	B	47	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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
16	LMG	D	953	-	53,53,55	1.39	8 (15%)	61,61,63	1.46	6 (9%)
17	SQD	R	950	-	32,33,54	2.07	9 (28%)	41,44,65	3.06	11 (26%)
11	BCR	B	904	-	27,27,41	1.56	5 (18%)	34,35,56	1.93	11 (32%)
10	HEC	B	903	18,2	32,50,50	1.98	7 (21%)	24,82,82	2.25	9 (37%)
13	FES	C	210	3	0,4,4	-	-	-	-	-
16	LMG	L	951	-	42,42,55	1.35	7 (16%)	50,50,63	1.50	5 (10%)
15	TDS	D	920	-	28,31,31	2.46	11 (39%)	35,40,40	2.62	14 (40%)
14	CLA	D	910	-	65,73,73	1.55	12 (18%)	76,113,113	1.93	11 (14%)
12	LFA	B	960	-	19,19,19	0.43	0	18,18,18	0.62	0
10	HEC	B	902	2	32,50,50	1.59	6 (18%)	24,82,82	1.58	5 (20%)
10	HEC	B	901	2	32,50,50	1.76	5 (15%)	24,82,82	1.50	4 (16%)
10	HEC	A	900	1	32,50,50	2.02	10 (31%)	24,82,82	2.08	8 (33%)

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
16	LMG	D	953	-	-	9/48/68/70	0/1/1/1
17	SQD	R	950	-	-	10/28/48/69	0/1/1/1
10	HEC	B	903	18,2	-	3/10/54/54	-
11	BCR	B	904	-	-	2/21/38/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMG	L	951	-	-	8/37/57/70	0/1/1/1
13	FES	C	210	3	-	-	0/1/1/1
15	TDS	D	920	-	-	6/16/17/17	0/2/2/2
14	CLA	D	910	-	2/2/15/20	9/37/115/115	-
12	LFA	B	960	-	-	11/17/17/17	-
10	HEC	B	902	2	-	4/10/54/54	-
10	HEC	B	901	2	-	3/10/54/54	-
10	HEC	A	900	1	-	3/10/54/54	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	950	SQD	C4-C3	6.81	1.69	1.52
10	A	900	HEC	C2B-C3B	-5.63	1.34	1.40
10	B	903	HEC	C2B-C3B	-5.55	1.35	1.40
10	A	900	HEC	C3C-C2C	-5.50	1.35	1.40
15	D	920	TDS	OAQ-CAP	4.97	1.42	1.35

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	910	CLA	C4A-NA-C1A	12.42	112.29	106.71
15	D	920	TDS	CAQ-CAP-CAH	9.29	133.55	120.39
17	R	950	SQD	O7-S-C6	8.91	117.53	106.94
17	R	950	SQD	O5-C1-O6	8.66	130.49	109.97
17	R	950	SQD	O6-C1-C2	7.27	119.65	108.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	910	CLA	C8
14	D	910	CLA	ND

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	901	HEC	C2A-CAA-CBA-CGA
15	D	920	TDS	CAH-CAP-CAQ-CAR
17	R	950	SQD	O5-C1-O6-C44
17	R	950	SQD	C5-C6-S-O7

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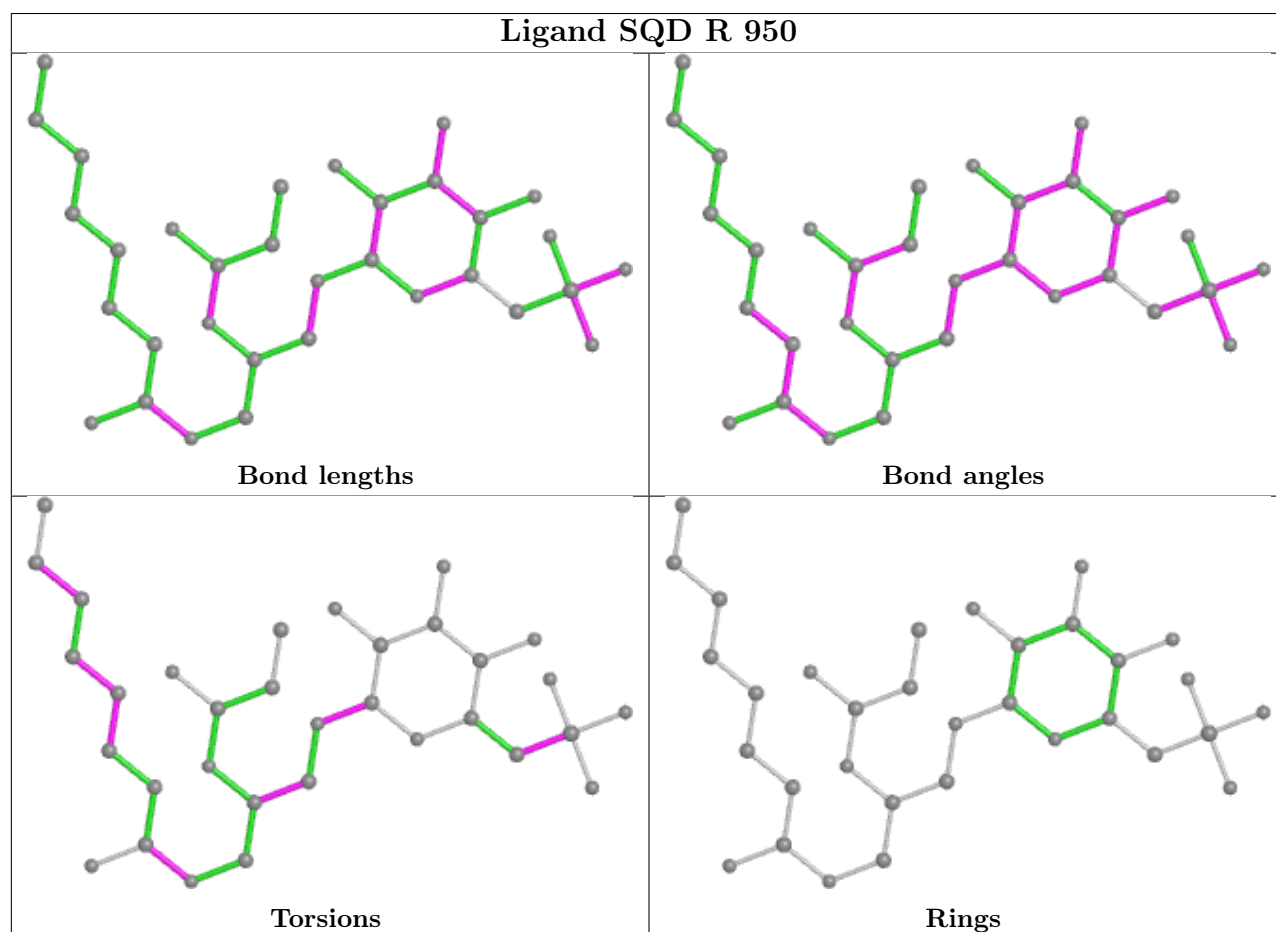
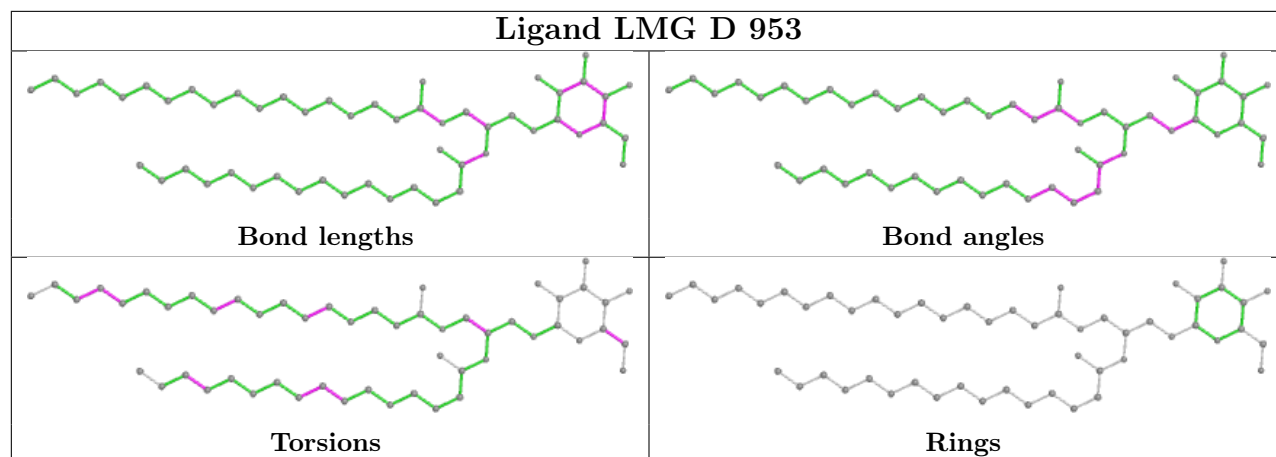
Mol	Chain	Res	Type	Atoms
17	R	950	SQD	C5-C6-S-O8

There are no ring outliers.

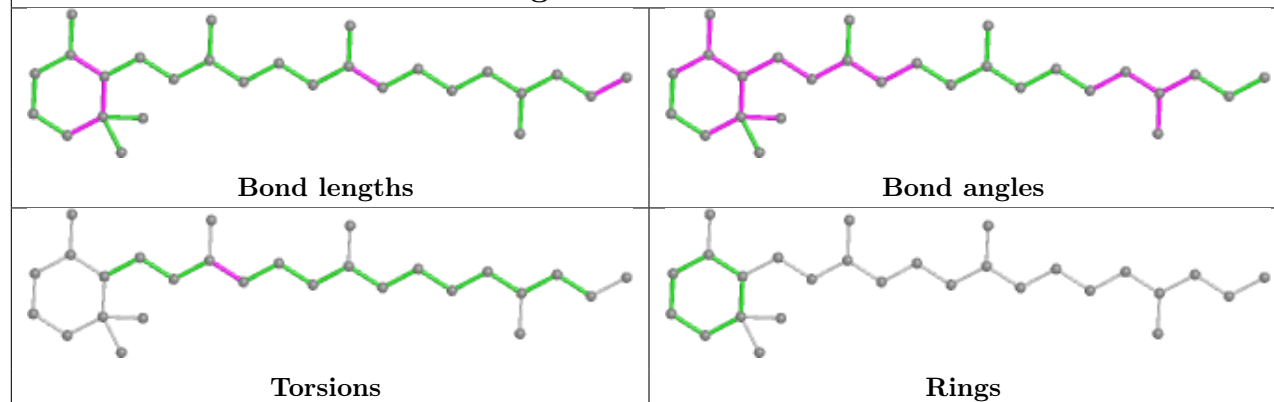
12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	953	LMG	3	0
17	R	950	SQD	1	0
11	B	904	BCR	3	0
10	B	903	HEC	1	0
13	C	210	FES	1	0
16	L	951	LMG	4	0
15	D	920	TDS	2	0
14	D	910	CLA	5	0
12	B	960	LFA	2	0
10	B	902	HEC	1	0
10	B	901	HEC	6	0
10	A	900	HEC	4	0

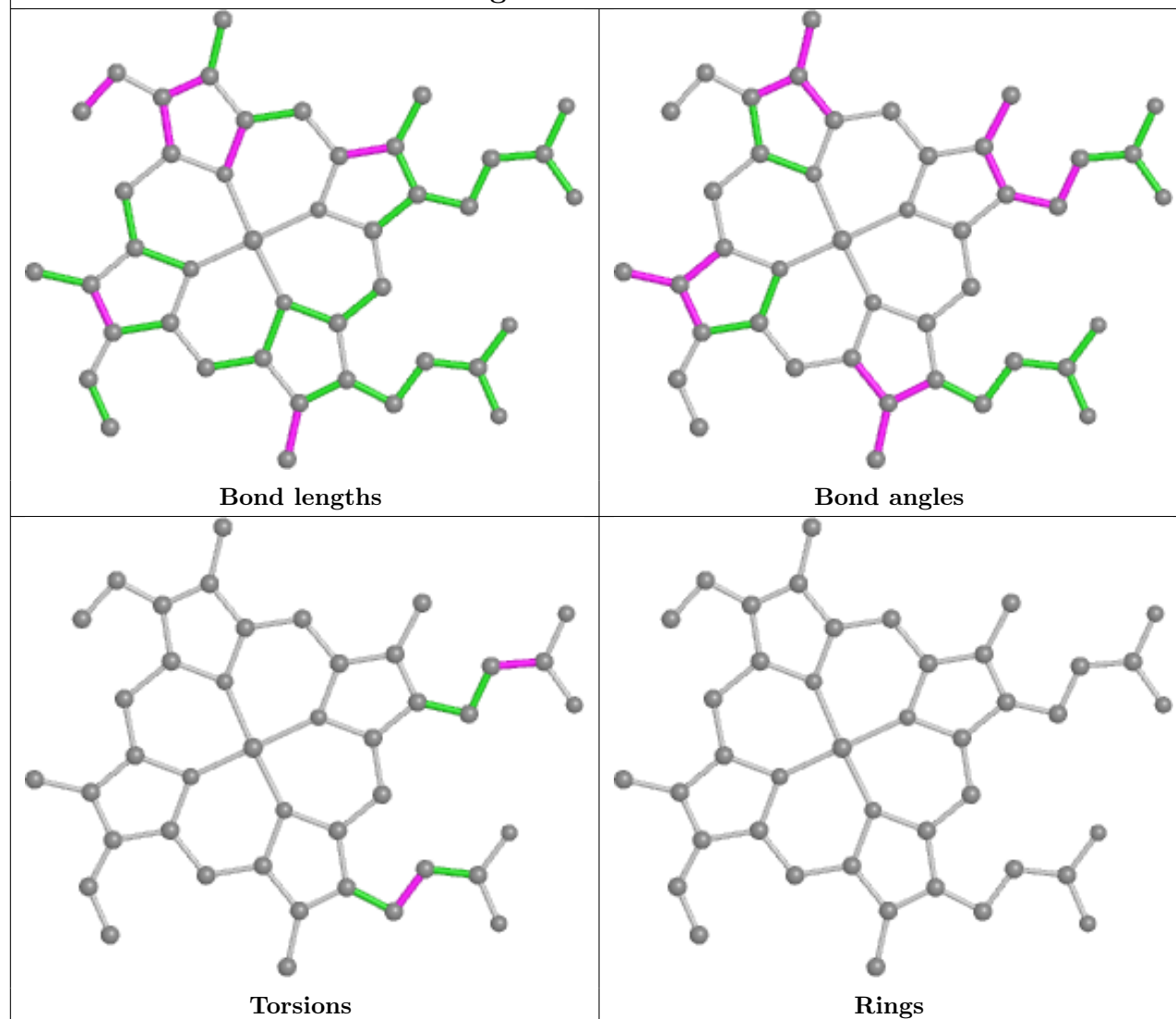
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

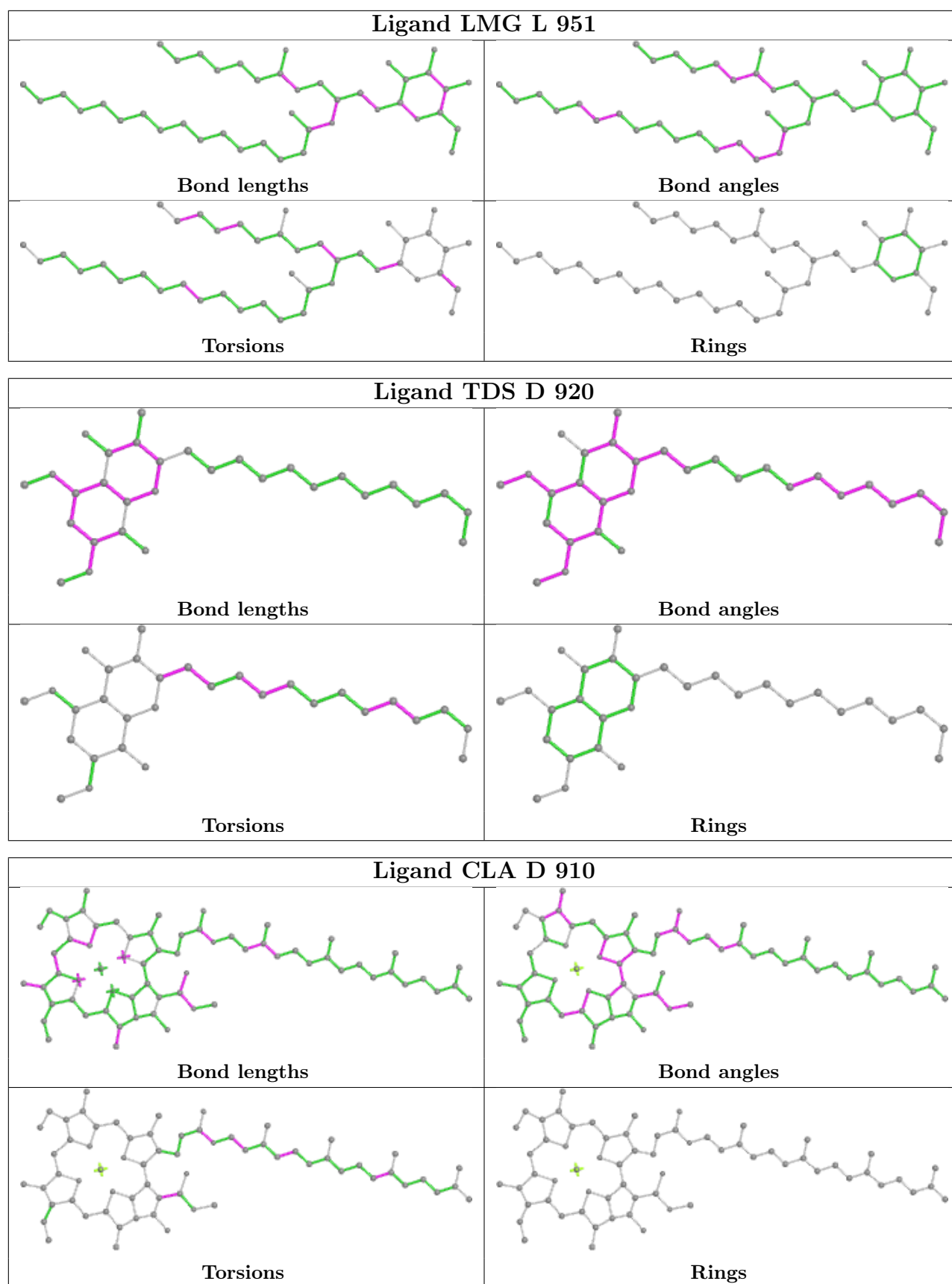


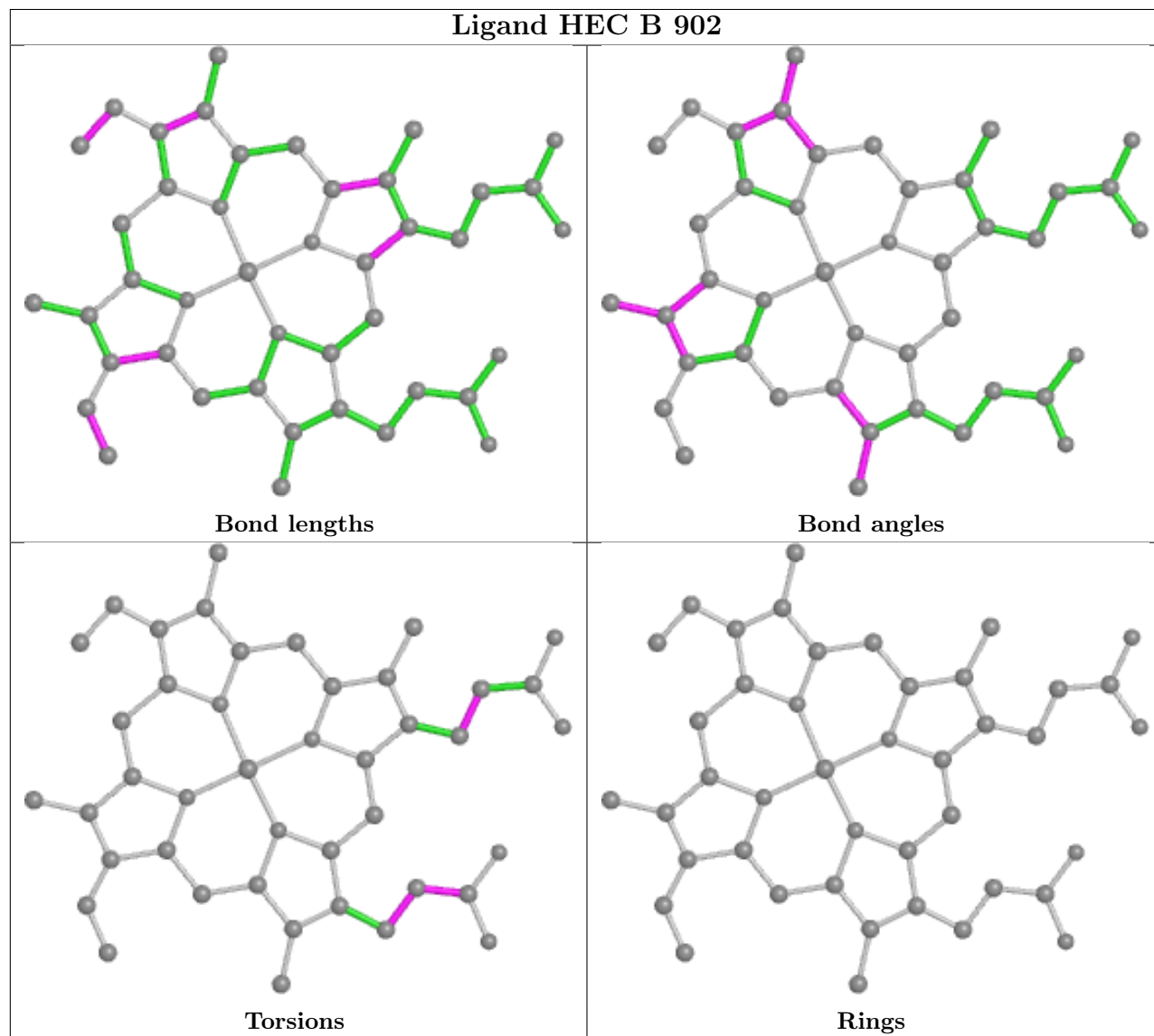
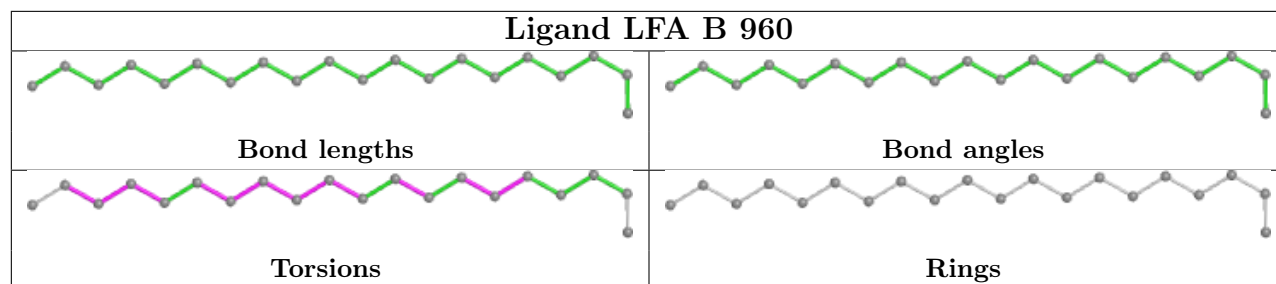
## Ligand BCR B 904



## Ligand HEC B 903

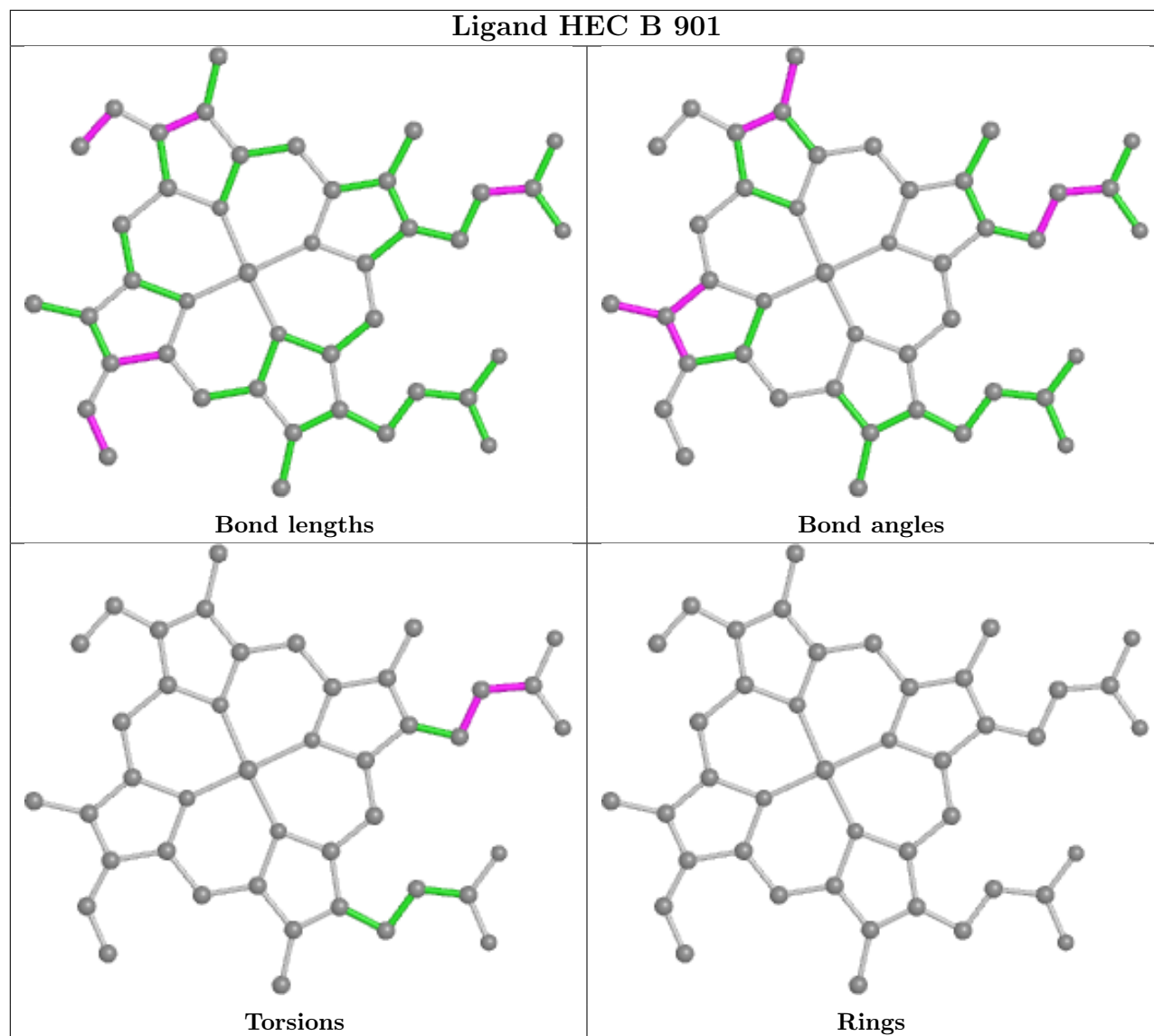


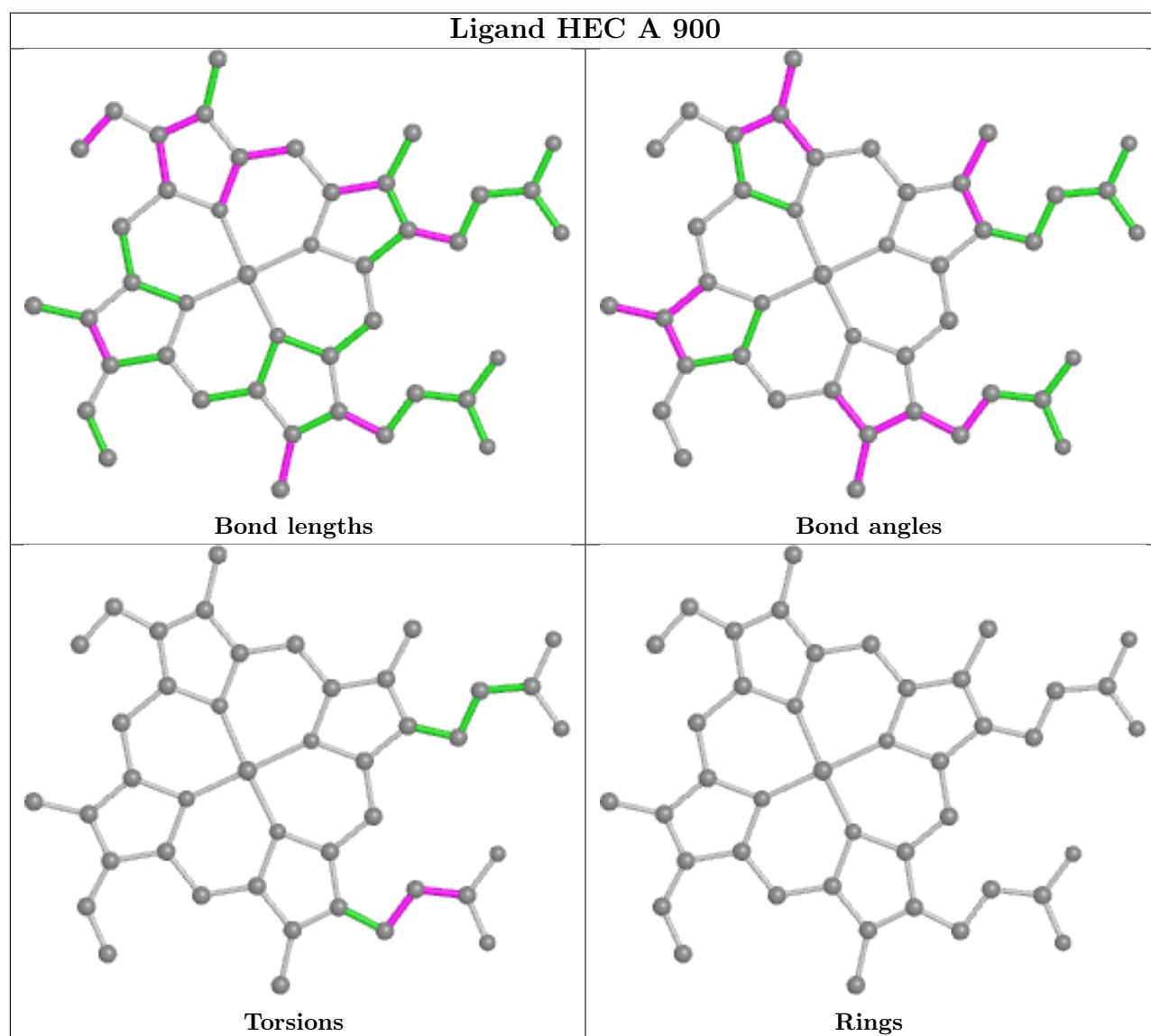






## Ligand HEC B 901





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	292/292 (100%)	-0.16	2 (0%) 87 75	42, 66, 102, 131	3 (1%)
2	B	212/215 (98%)	-0.10	2 (0%) 84 69	29, 47, 76, 114	0
3	C	126/127 (99%)	1.00	30 (23%) 0 0	70, 121, 159, 180	0
4	D	156/159 (98%)	-0.19	0 100 100	37, 62, 96, 131	0
5	R	39/49 (79%)	-0.10	3 (7%) 13 5	37, 51, 135, 159	0
6	G	30/37 (81%)	-0.21	0 100 100	41, 54, 77, 97	0
7	L	32/32 (100%)	-0.31	0 100 100	46, 65, 86, 126	0
8	M	34/39 (87%)	-0.40	0 100 100	41, 57, 83, 130	0
9	N	31/31 (100%)	-0.35	0 100 100	36, 50, 68, 91	0
All	All	952/981 (97%)	-0.02	37 (3%) 39 20	29, 62, 135, 180	3 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	33	SER	4.1
3	C	186	LEU	3.7
3	C	196	ASP	3.6
3	C	93	GLY	3.6
3	C	81	ALA	3.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

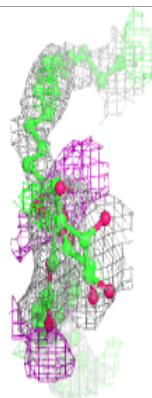
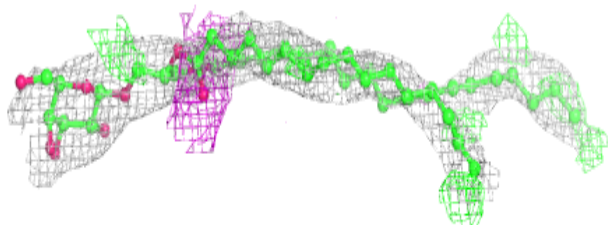
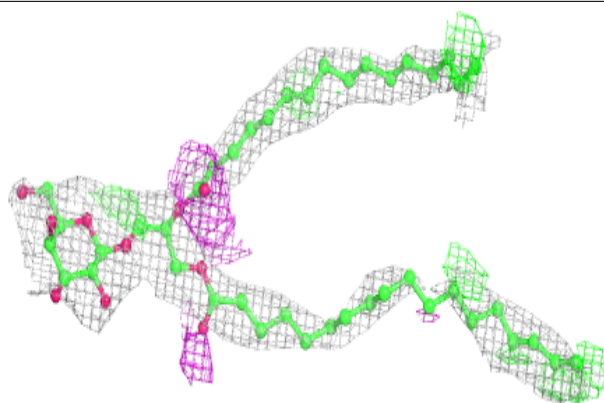
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	LMG	D	953	53/55	0.63	0.43	88,88,107,107	0
16	LMG	L	951	42/55	0.77	0.33	78,85,85,85	0
11	BCR	B	904	27/40	0.85	0.40	49,49,64,64	0
15	TDS	D	920	30/30	0.87	0.30	87,89,89,89	0
14	CLA	D	910	65/65	0.88	0.28	63,70,92,94	0
12	LFA	B	960	20/20	0.91	0.29	59,59,59,59	0
17	SQD	R	950	33/54	0.93	0.19	62,62,111,111	0
10	HEC	B	903	43/43	0.95	0.21	53,53,53,53	0
10	HEC	A	900	43/43	0.95	0.22	63,67,77,80	0
10	HEC	B	902	43/43	0.97	0.19	35,43,48,50	0
10	HEC	B	901	43/43	0.97	0.21	30,37,45,50	0
13	FES	C	210	4/4	0.99	0.09	62,62,63,65	0

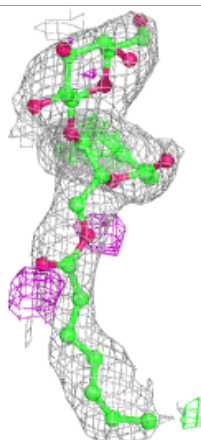
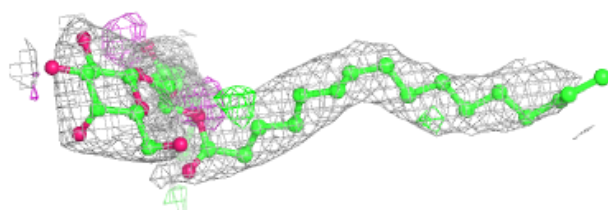
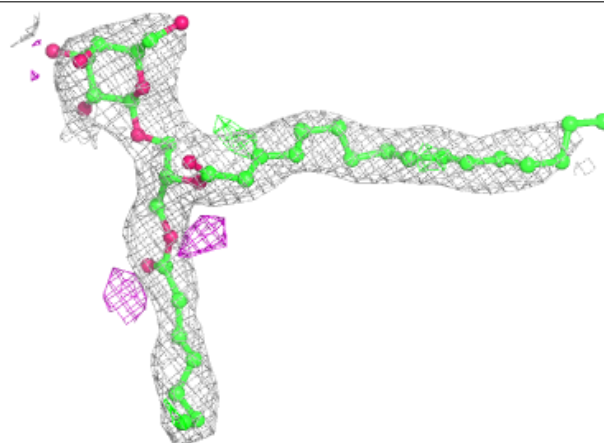
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMG D 953:**

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

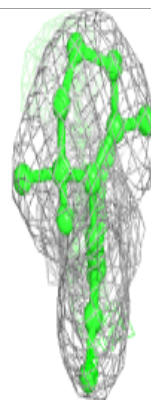
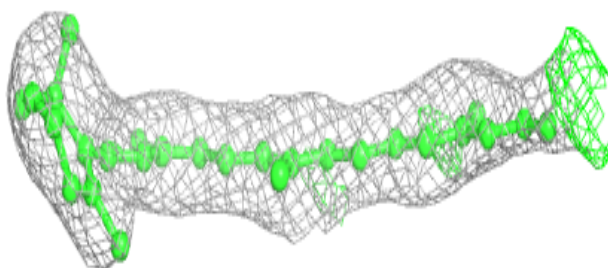
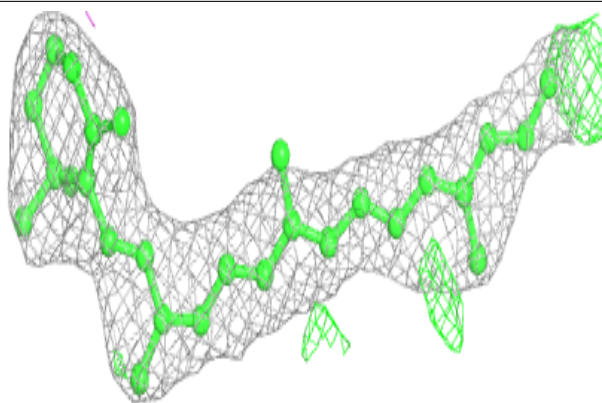
**Electron density around LMG L 951:**

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

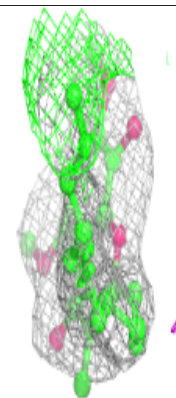
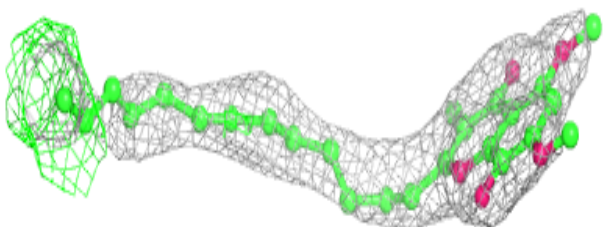
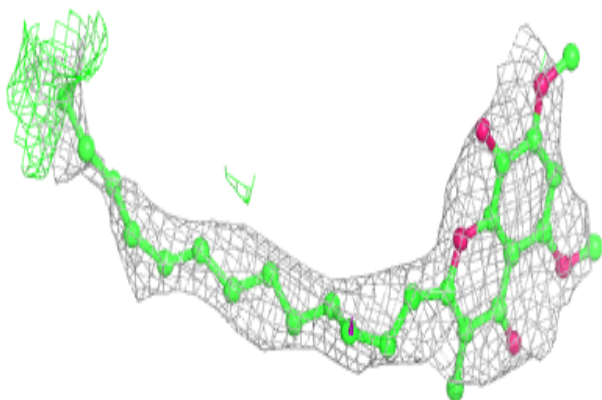


**Electron density around BCR B 904:**

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

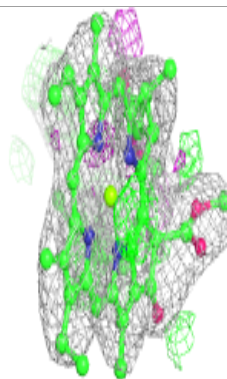
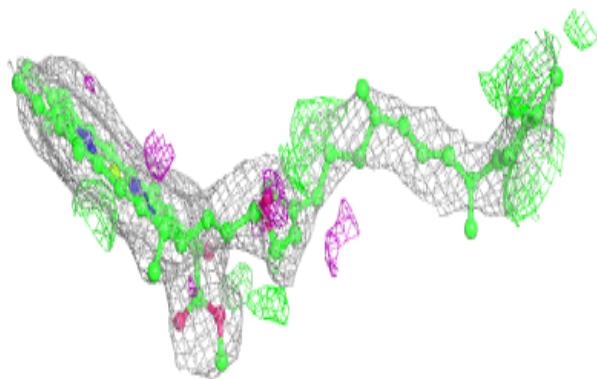
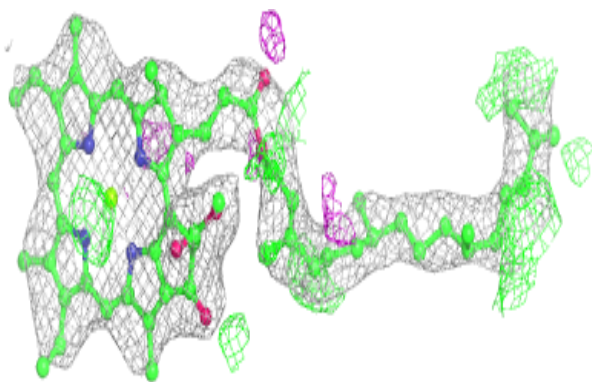
**Electron density around TDS D 920:**

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

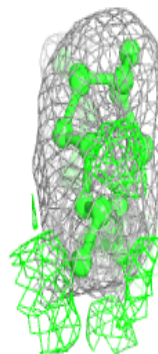
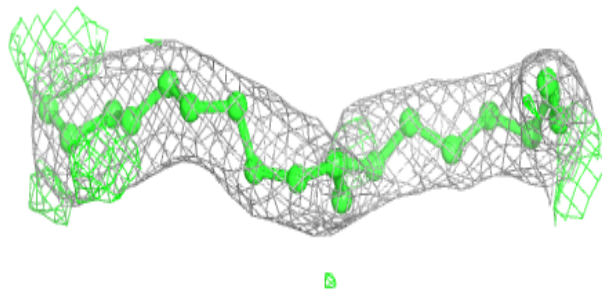
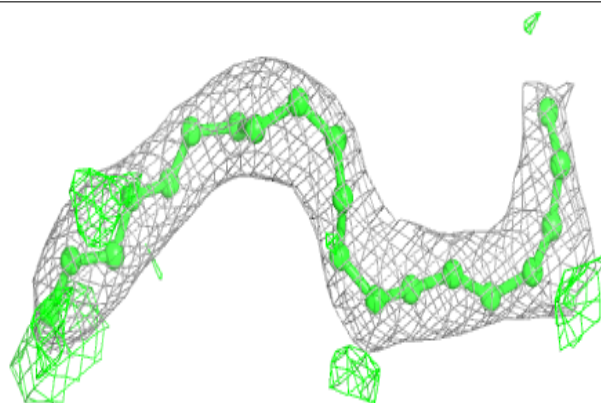


**Electron density around CLA D 910:**

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

**Electron density around LFA B 960:**

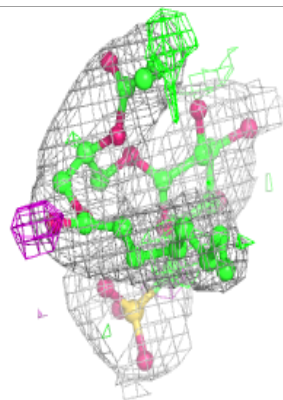
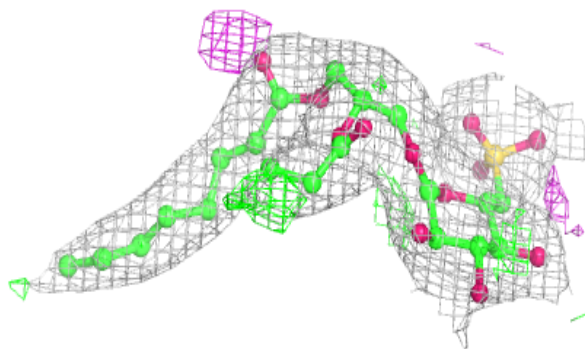
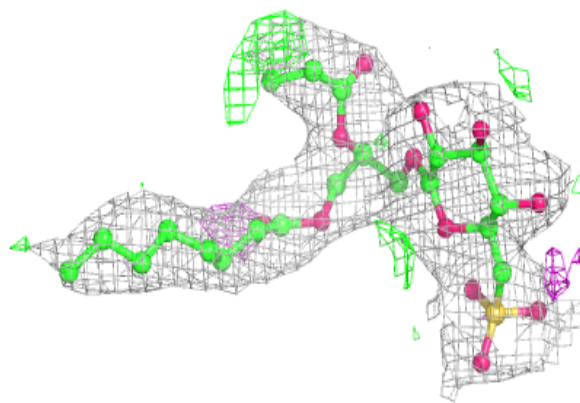
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SQD R 950:**

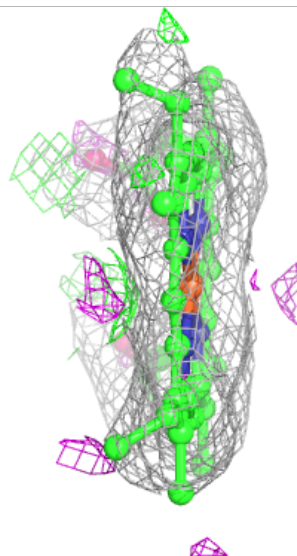
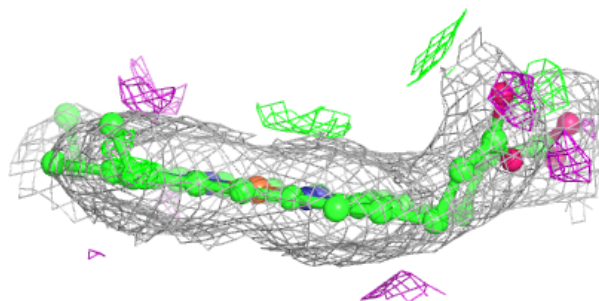
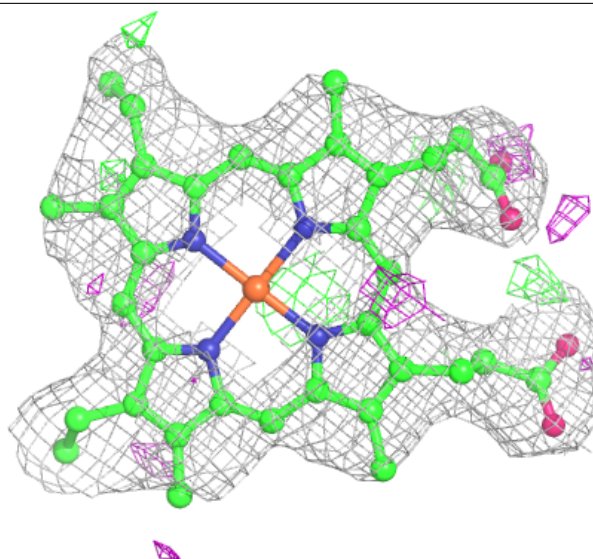
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





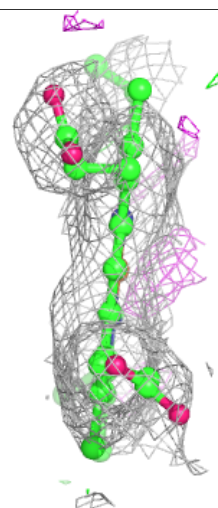
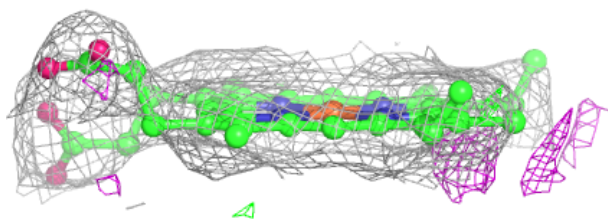
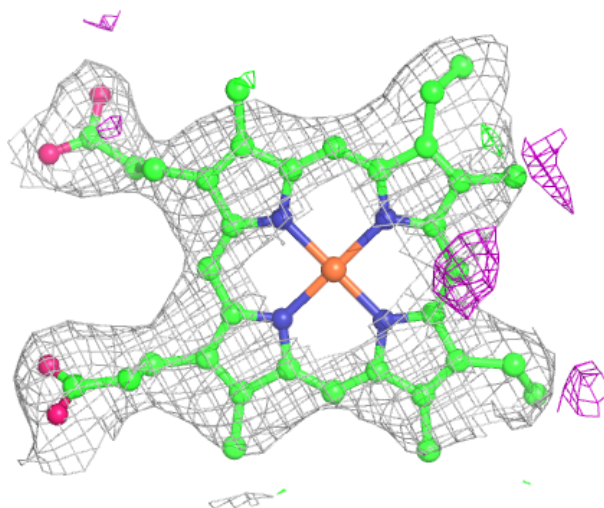
**Electron density around HEC B 903:**

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



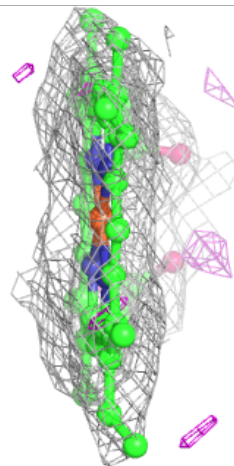
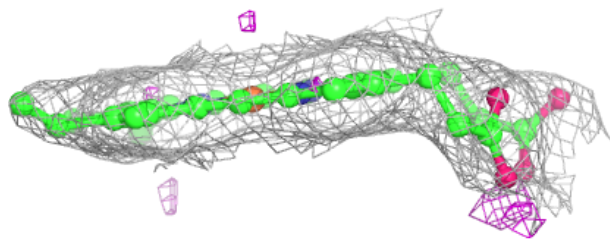
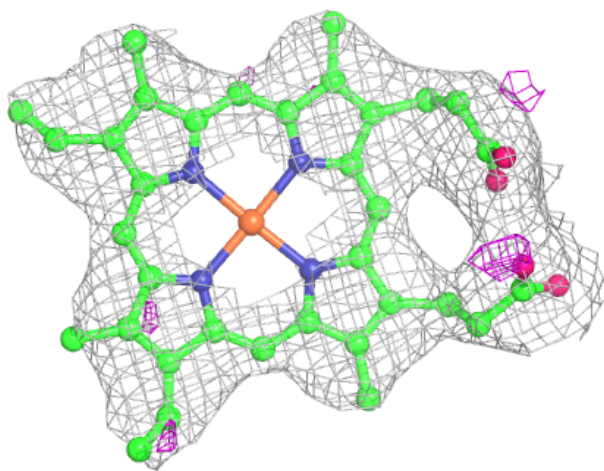
**Electron density around HEC A 900:**

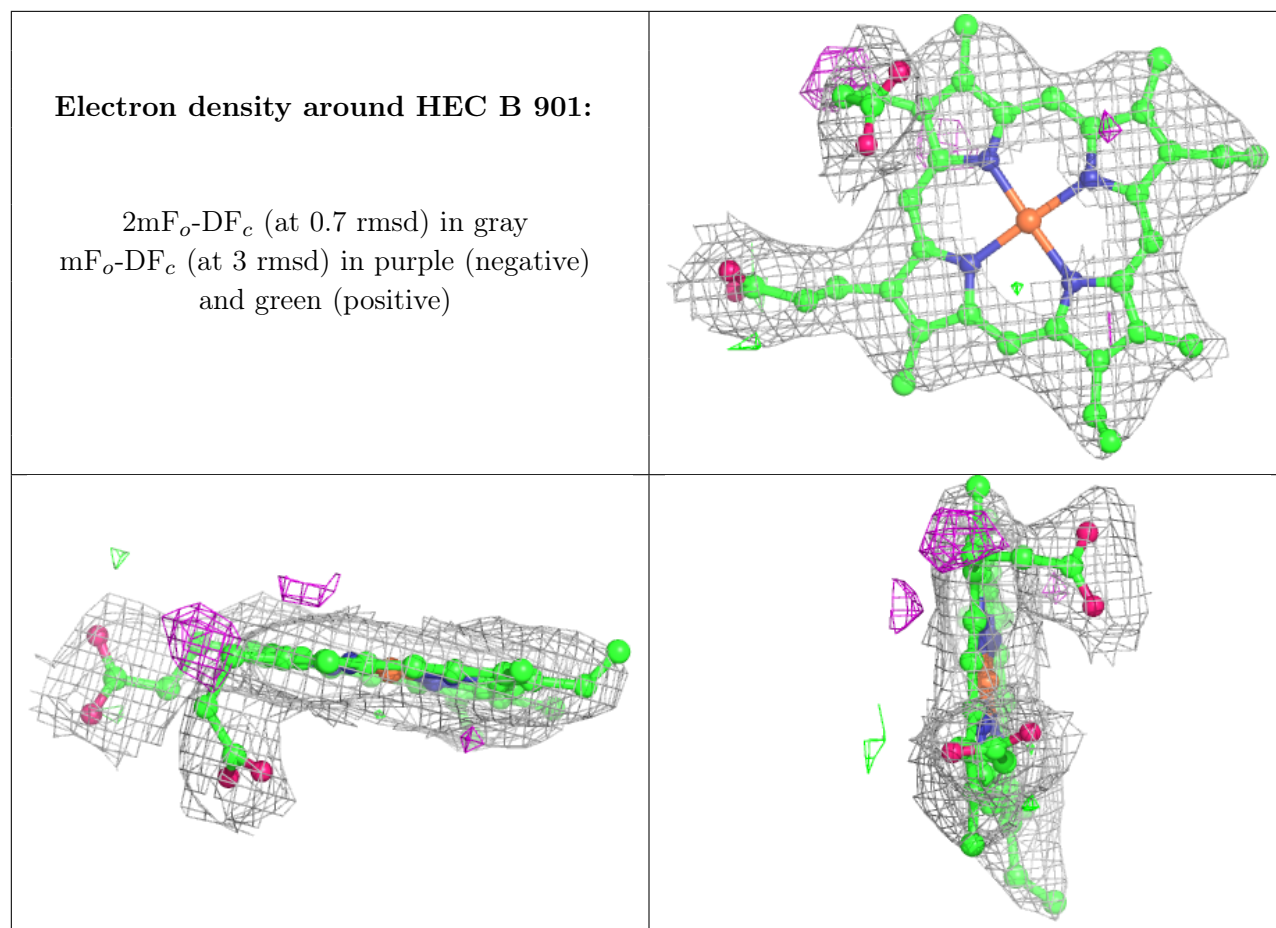
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC B 902:**

$2mF_o-DF_c$  (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.