



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 27, 2021 – 07:59 PM EST

PDB ID : 2GC4  
Title : Structural comparison of the oxidized ternary electron transfer complex of methylamine dehydrogenase, amicyanin and cytochrome c551i from *Paracoccus denitrificans* with the substrate-reduced, copper free complex at 1.9 Å resolution.  
Authors : Chen, Z.; Durley, R.; Davidson, V.L.; Mathews, F.S.  
Deposited on : 2006-03-13  
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](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.

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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	:	2.17.1
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)	:	2.17.1

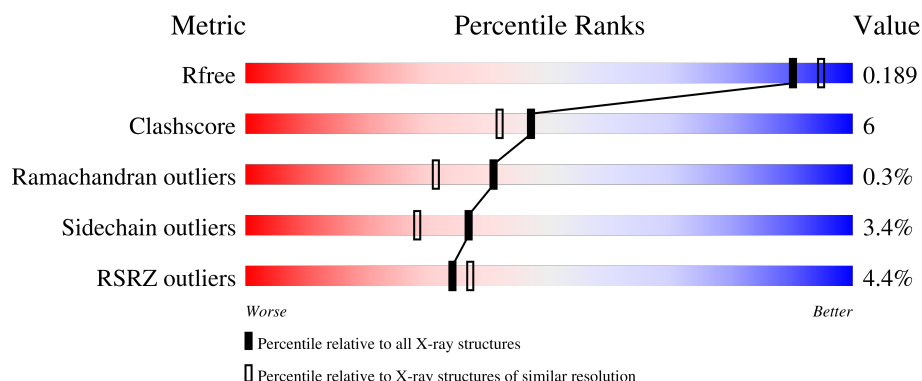
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	386	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
1	E	386	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	I	386	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>
1	M	386	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
2	B	131	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	131	 2% 88% 6% • 5%
2	J	131	 2% 88% 6% • 5%
2	N	131	 4% 87% 7% • 5%
3	C	105	 10% 86% 13% •
3	G	105	 5% 90% 10%
3	K	105	 6% 92% 8%
3	O	105	 16% 75% 21% •
4	D	147	 5% 82% 16% •
4	H	147	 7% 77% 22% •
4	L	147	 5% 80% 18% •
4	P	147	 6% 73% 25% •

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24820 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 Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	E	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	I	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	M	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	F	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	J	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	N	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	TRQ	TRP	modified residue	UNP P22619
F	57	TRQ	TRP	modified residue	UNP P22619
J	57	TRQ	TRP	modified residue	UNP P22619
N	57	TRQ	TRP	modified residue	UNP P22619

- Molecule 3 is a protein called Amicyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	G	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	K	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	O	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			

- Molecule 4 is a protein called Cytochrome c-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	H	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	L	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	P	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cu	0	0
			1	1		
5	G	1	Total	Cu	0	0
			1	1		
5	K	1	Total	Cu	0	0
			1	1		
5	O	1	Total	Cu	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

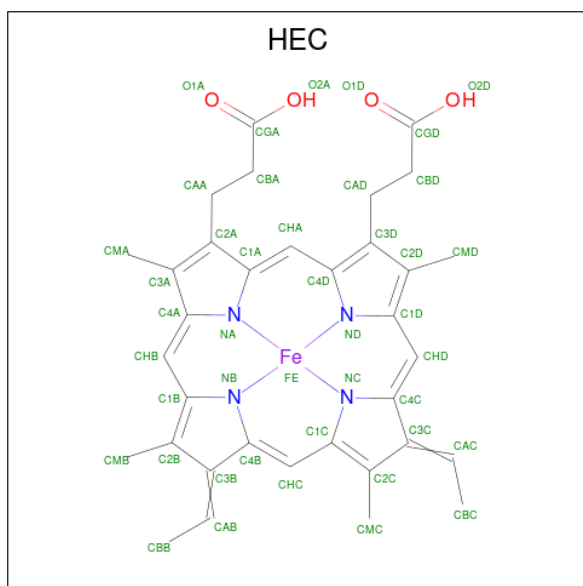
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na	0	0
			1	1		
6	H	1	Total	Na	0	0
			1	1		
6	L	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Na	0	0
			1	1		

- Molecule 7 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is water.

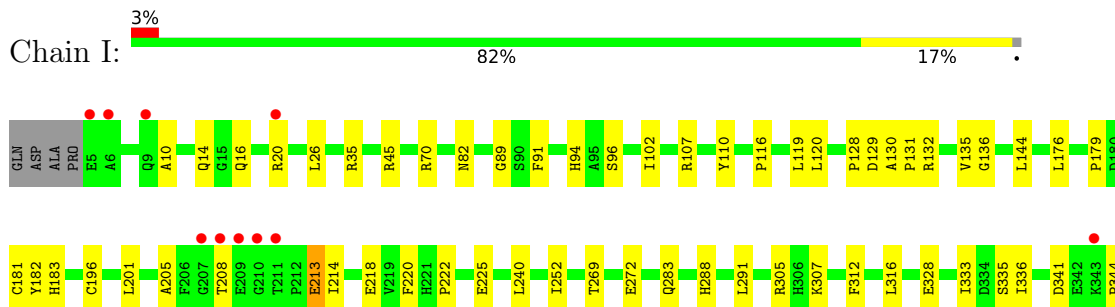
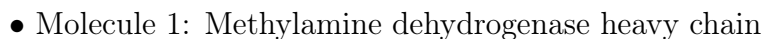
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	170	Total	O	0	0
			170	170		
8	B	54	Total	O	0	0
			54	54		
8	C	19	Total	O	0	0
			19	19		
8	D	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	160	Total 160	O 160	0	0
8	F	60	Total 60	O 60	0	0
8	G	22	Total 22	O 22	0	0
8	H	40	Total 40	O 40	0	0
8	I	155	Total 155	O 155	0	0
8	J	64	Total 64	O 64	0	0
8	K	27	Total 27	O 27	0	0
8	L	48	Total 48	O 48	0	0
8	M	173	Total 173	O 173	0	0
8	N	55	Total 55	O 55	0	0
8	O	14	Total 14	O 14	0	0
8	P	43	Total 43	O 43	0	0

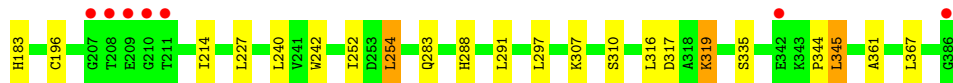
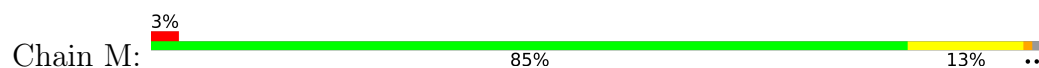
- Molecule 1: Methylamine dehydrogenase heavy chain



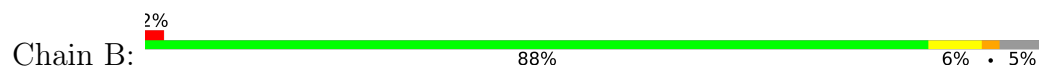




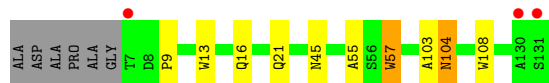
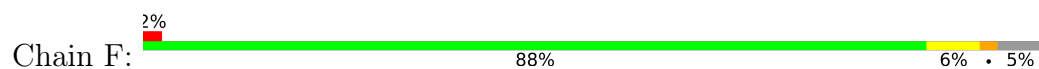
- Molecule 1: Methylamine dehydrogenase heavy chain



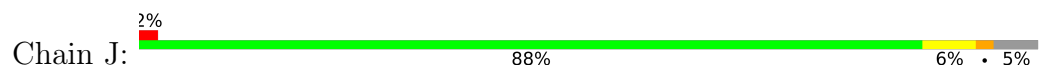
- Molecule 2: Methylamine dehydrogenase light chain



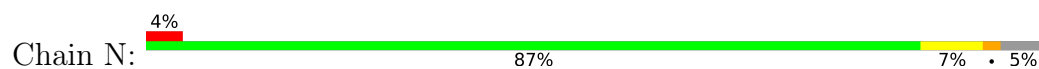
- Molecule 2: Methylamine dehydrogenase light chain



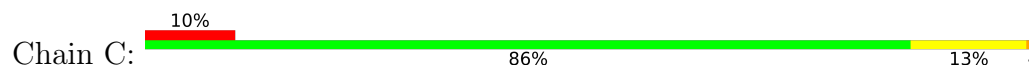
- Molecule 2: Methylamine dehydrogenase light chain



- Molecule 2: Methylamine dehydrogenase light chain

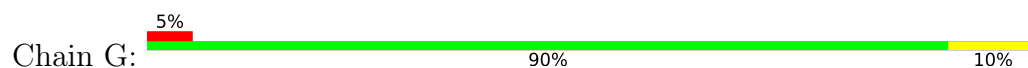


- Molecule 3: Amicyanin

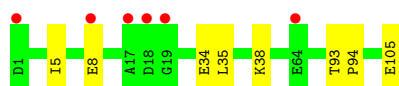




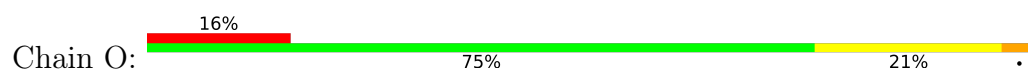
- Molecule 3: Amicyanin



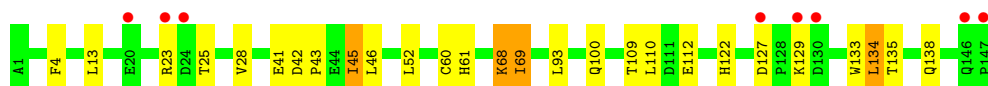
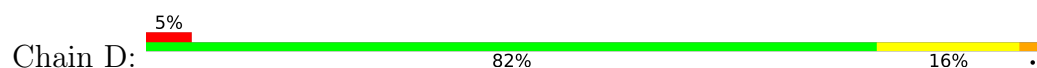
- Molecule 3: Amicyanin



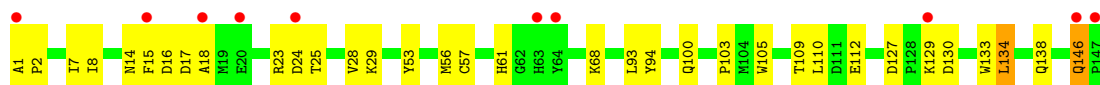
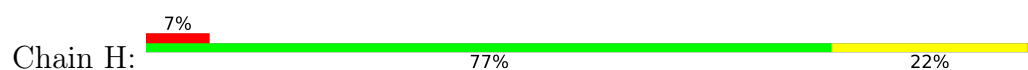
- Molecule 3: Amicyanin



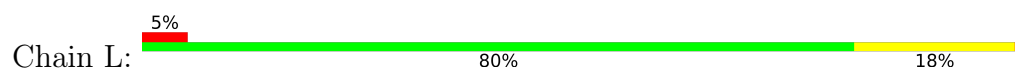
- Molecule 4: Cytochrome c-L



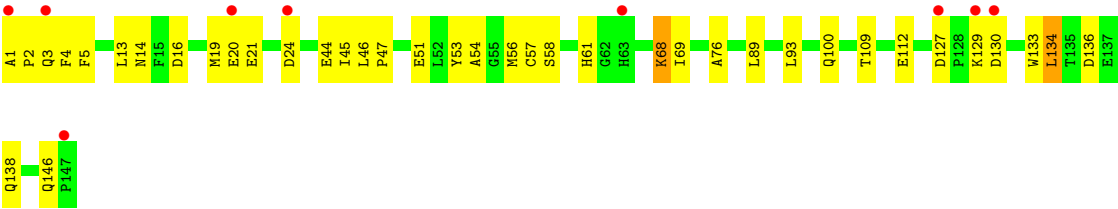
- Molecule 4: Cytochrome c-L



- Molecule 4: Cytochrome c-L



- Molecule 4: Cytochrome c-L



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.37Å 188.98Å 128.84Å 90.00° 99.74° 90.00°	Depositor
Resolution (Å)	29.95 – 1.90 29.95 – 1.84	Depositor EDS
% Data completeness (in resolution range)	84.3 (29.95-1.90) 79.8 (29.95-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.173 , 0.197 0.166 , 0.189	Depositor DCC
$R_{free}$ test set	21026 reflections (7.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	24820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3668e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CU, TRQ, HEC, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/3044	0.64	0/4148
1	E	0.31	0/3044	0.63	0/4148
1	I	0.32	0/3044	0.64	0/4148
1	M	0.32	0/3044	0.64	0/4148
2	B	0.32	0/964	0.61	0/1315
2	F	0.32	0/964	0.61	0/1315
2	J	0.33	0/964	0.61	0/1315
2	N	0.31	0/964	0.61	0/1315
3	C	0.32	0/828	0.55	0/1124
3	G	0.32	0/828	0.58	0/1124
3	K	0.33	0/828	0.60	0/1124
3	O	0.30	0/828	0.57	0/1124
4	D	0.33	0/1180	0.63	1/1605 (0.1%)
4	H	0.37	1/1180 (0.1%)	0.65	1/1605 (0.1%)
4	L	0.35	1/1180 (0.1%)	0.63	1/1605 (0.1%)
4	P	0.34	1/1180 (0.1%)	0.61	1/1605 (0.1%)
All	All	0.32	3/24064 (0.0%)	0.62	4/32768 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	61	HIS	CE1-NE2	5.26	1.44	1.32
4	H	61	HIS	CE1-NE2	5.25	1.44	1.32
4	P	61	HIS	CE1-NE2	5.05	1.44	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	61	HIS	ND1-CG-CD2	8.05	120.07	108.80
4	H	61	HIS	ND1-CG-CD2	8.04	120.06	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	61	HIS	ND1-CG-CD2	7.98	119.97	108.80
4	D	61	HIS	ND1-CG-CD2	7.97	119.95	108.80

There are no chirality outliers.

There are no planarity outliers.

## 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	2967	0	2845	39	0
1	E	2967	0	2845	31	0
1	I	2967	0	2845	39	0
1	M	2967	0	2845	41	0
2	B	956	0	857	11	0
2	F	956	0	857	10	0
2	J	956	0	857	12	0
2	N	956	0	857	12	0
3	C	807	0	794	9	0
3	G	807	0	794	4	0
3	K	807	0	794	6	0
3	O	807	0	794	19	0
4	D	1145	0	1038	19	0
4	H	1145	0	1038	21	0
4	L	1145	0	1038	18	0
4	P	1145	0	1038	23	0
5	C	1	0	0	0	0
5	G	1	0	0	0	0
5	K	1	0	0	0	0
5	O	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	L	1	0	0	0	0
6	P	1	0	0	0	0
7	D	43	0	30	2	0
7	H	43	0	30	2	0
7	L	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	43	0	30	2	0
8	A	170	0	0	4	0
8	B	54	0	0	0	0
8	C	19	0	0	1	0
8	D	36	0	0	0	0
8	E	160	0	0	1	0
8	F	60	0	0	1	0
8	G	22	0	0	0	0
8	H	40	0	0	0	0
8	I	155	0	0	1	0
8	J	64	0	0	1	0
8	K	27	0	0	0	0
8	L	48	0	0	0	0
8	M	173	0	0	2	0
8	N	55	0	0	0	0
8	O	14	0	0	1	0
8	P	43	0	0	0	0
All	All	24820	0	22256	285	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 6.

The worst 5 of 285 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:J:21:GLN:HE22	1:M:11:GLN:HG3	1.28	0.92
2:J:57:TRQ:HB2	2:J:108:TRP:NE1	1.89	0.88
2:B:57:TRQ:HB2	2:B:108:TRP:NE1	1.87	0.88
2:J:21:GLN:NE2	1:M:11:GLN:HG3	1.89	0.88
2:N:57:TRQ:HB2	2:N:108:TRP:NE1	1.88	0.88

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	380/386 (98%)	367 (97%)	12 (3%)	1 (0%)	41	31
1	E	380/386 (98%)	367 (97%)	13 (3%)	0	100	100
1	I	380/386 (98%)	364 (96%)	15 (4%)	1 (0%)	41	31
1	M	380/386 (98%)	366 (96%)	13 (3%)	1 (0%)	41	31
2	B	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	F	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	J	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	N	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
3	C	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	G	103/105 (98%)	98 (95%)	4 (4%)	1 (1%)	15	6
3	K	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	O	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	8	1
4	D	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
4	H	145/147 (99%)	140 (97%)	4 (3%)	1 (1%)	22	12
4	L	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
4	P	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	22	12
All	All	3000/3076 (98%)	2897 (97%)	93 (3%)	10 (0%)	41	31

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	17	ALA
3	O	18	ASP
4	H	68	LYS
3	O	19	GLY
4	P	68	LYS

### 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	308/311 (99%)	296 (96%)	12 (4%)	32	23
1	E	308/311 (99%)	299 (97%)	9 (3%)	42	35
1	I	308/311 (99%)	296 (96%)	12 (4%)	32	23
1	M	308/311 (99%)	298 (97%)	10 (3%)	39	30
2	B	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	F	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	J	104/106 (98%)	102 (98%)	2 (2%)	57	53
2	N	104/106 (98%)	102 (98%)	2 (2%)	57	53
3	C	85/85 (100%)	83 (98%)	2 (2%)	49	43
3	G	85/85 (100%)	81 (95%)	4 (5%)	26	16
3	K	85/85 (100%)	84 (99%)	1 (1%)	71	70
3	O	85/85 (100%)	79 (93%)	6 (7%)	14	6
4	D	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	H	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	L	118/118 (100%)	114 (97%)	4 (3%)	37	28
4	P	118/118 (100%)	110 (93%)	8 (7%)	16	7
All	All	2460/2480 (99%)	2376 (97%)	84 (3%)	37	28

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	134	LEU
3	O	4	THR
1	M	94	HIS
1	M	319	LYS
3	O	48	ARG

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

Mol	Chain	Res	Type
4	H	14	ASN
4	P	30	HIS
1	I	82	ASN
3	O	76	GLN
1	M	288	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	TRQ	J	57	2	13,17,18	4.72	3 (23%)	14,24,26	2.67	5 (35%)
2	TRQ	B	57	2	13,17,18	4.71	3 (23%)	14,24,26	3.04	5 (35%)
2	TRQ	N	57	2	13,17,18	4.71	3 (23%)	14,24,26	2.98	5 (35%)
2	TRQ	F	57	2	13,17,18	4.68	3 (23%)	14,24,26	2.99	5 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	J	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	B	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	N	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	F	57	2	-	0/4/19/21	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	TRQ	CH2-CZ2	-14.80	1.37	1.54
2	J	57	TRQ	CH2-CZ2	-14.76	1.37	1.54
2	N	57	TRQ	CH2-CZ2	-14.59	1.37	1.54
2	F	57	TRQ	CH2-CZ2	-14.57	1.37	1.54
2	N	57	TRQ	CE2-CZ2	-7.59	1.40	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	57	TRQ	O7-CZ2-CH2	6.47	126.61	119.00
2	N	57	TRQ	O7-CZ2-CH2	6.39	126.52	119.00
2	F	57	TRQ	O7-CZ2-CH2	6.32	126.44	119.00
2	B	57	TRQ	O7-CZ2-CE2	-5.93	115.56	121.84
2	N	57	TRQ	O7-CZ2-CE2	-5.83	115.67	121.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	57	TRQ	2	0
2	B	57	TRQ	2	0
2	N	57	TRQ	2	0
2	F	57	TRQ	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	HEC	P	200	4	26,50,50	2.04	11 (42%)	18,82,82	1.95	5 (27%)
7	HEC	D	200	4	26,50,50	2.26	10 (38%)	18,82,82	2.10	7 (38%)
7	HEC	L	200	4	26,50,50	2.00	8 (30%)	18,82,82	2.04	4 (22%)
7	HEC	H	200	4	26,50,50	2.08	9 (34%)	18,82,82	2.06	5 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEC	P	200	4	-	0/6/54/54	-
7	HEC	D	200	4	-	0/6/54/54	-
7	HEC	L	200	4	-	0/6/54/54	-
7	HEC	H	200	4	-	0/6/54/54	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	200	HEC	C3C-C2C	-5.58	1.34	1.40
7	P	200	HEC	C3C-C2C	-4.46	1.36	1.40
7	L	200	HEC	C3C-C2C	-4.25	1.36	1.40
7	P	200	HEC	C3B-C2B	-4.19	1.36	1.40
7	H	200	HEC	C3C-C2C	-4.16	1.36	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	200	HEC	CBD-CAD-C3D	-4.99	103.27	112.49
7	H	200	HEC	CBD-CAD-C3D	-4.52	104.16	112.49
7	D	200	HEC	CBD-CAD-C3D	-4.32	104.52	112.49
7	P	200	HEC	CBD-CAD-C3D	-4.27	104.60	112.49
7	L	200	HEC	CAD-CBD-CGD	4.01	119.40	112.67

There are no chirality outliers.

There are no torsion outliers.

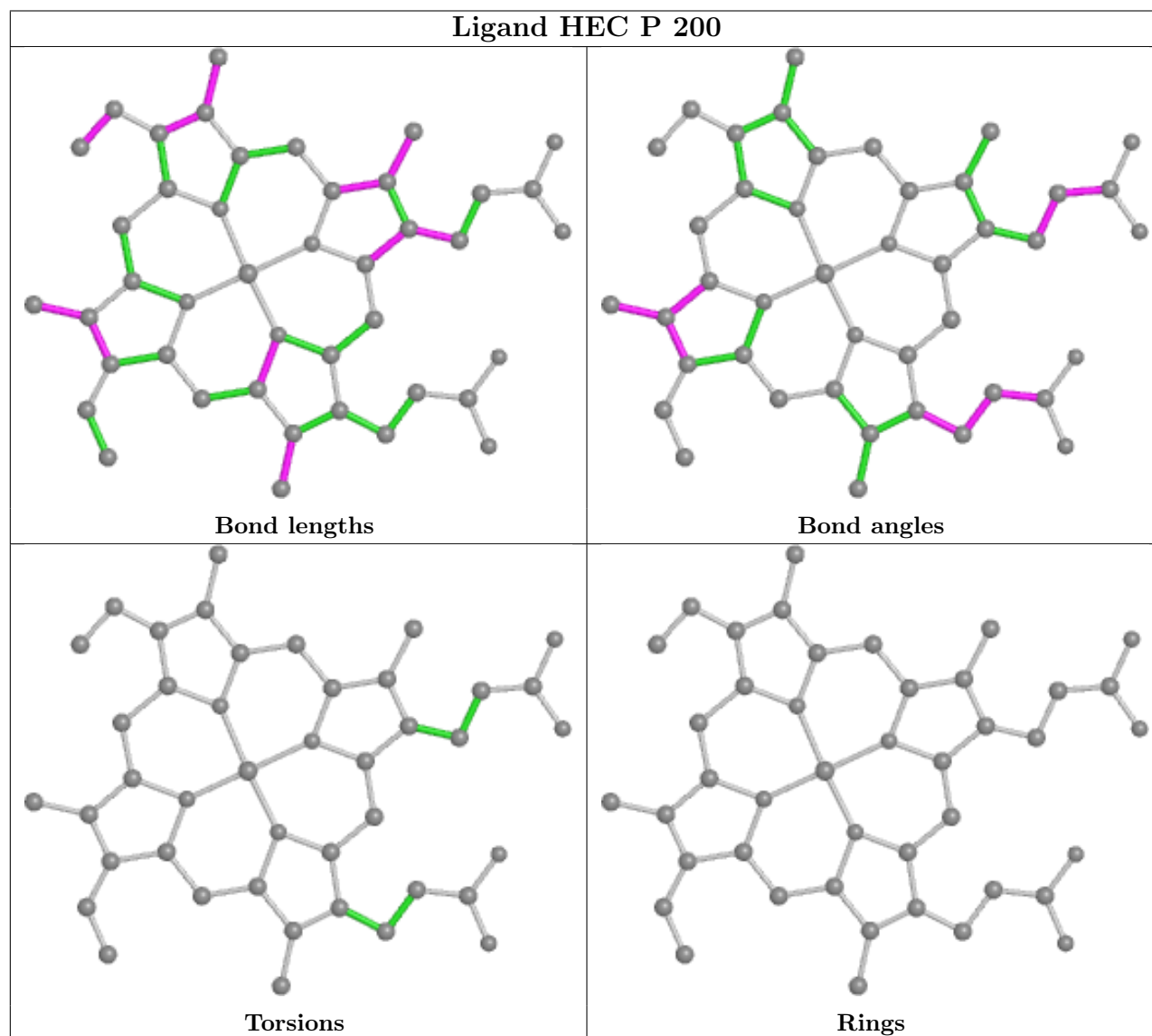
There are no ring outliers.

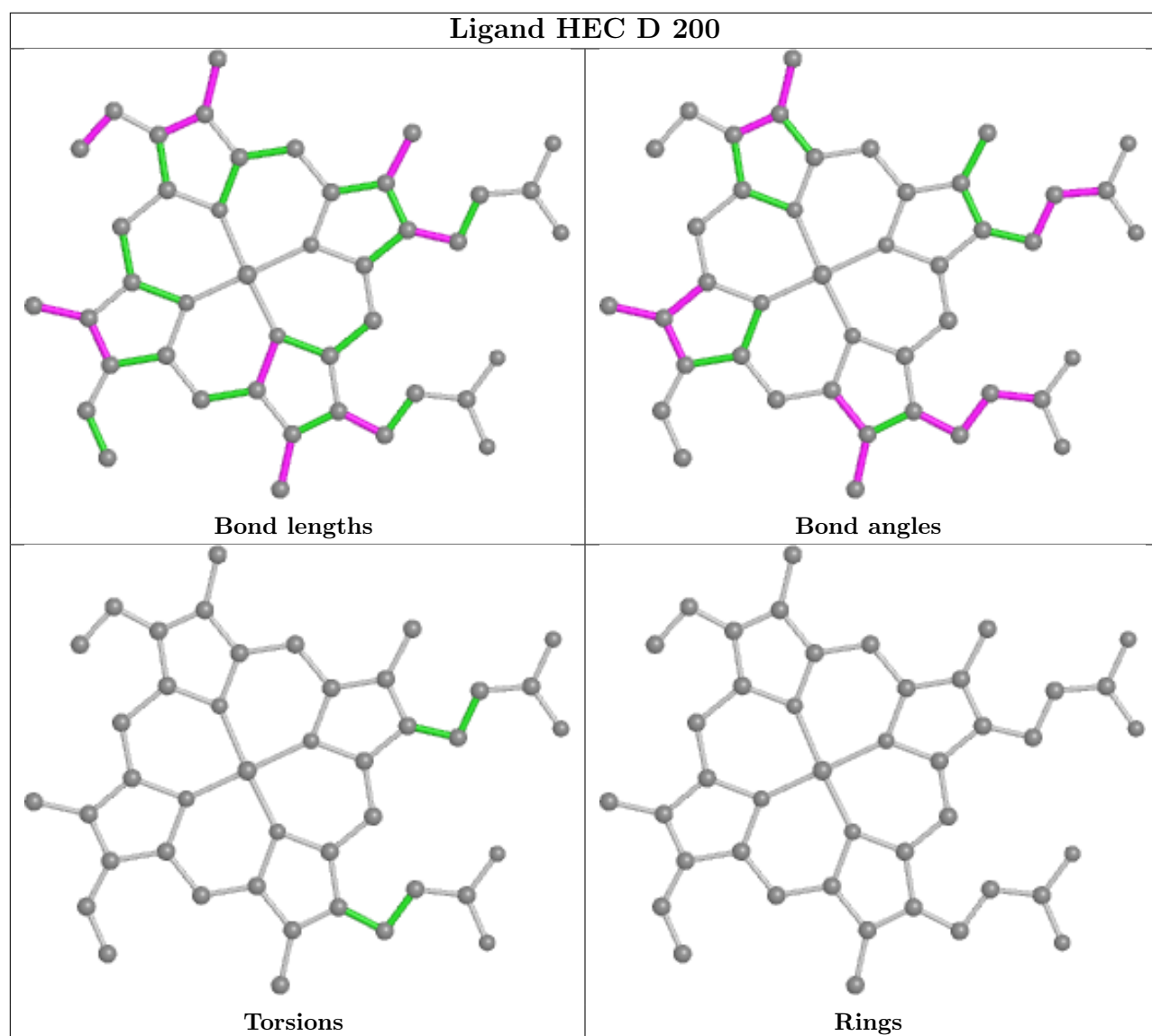
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	200	HEC	2	0
7	D	200	HEC	2	0
7	L	200	HEC	1	0
7	H	200	HEC	2	0

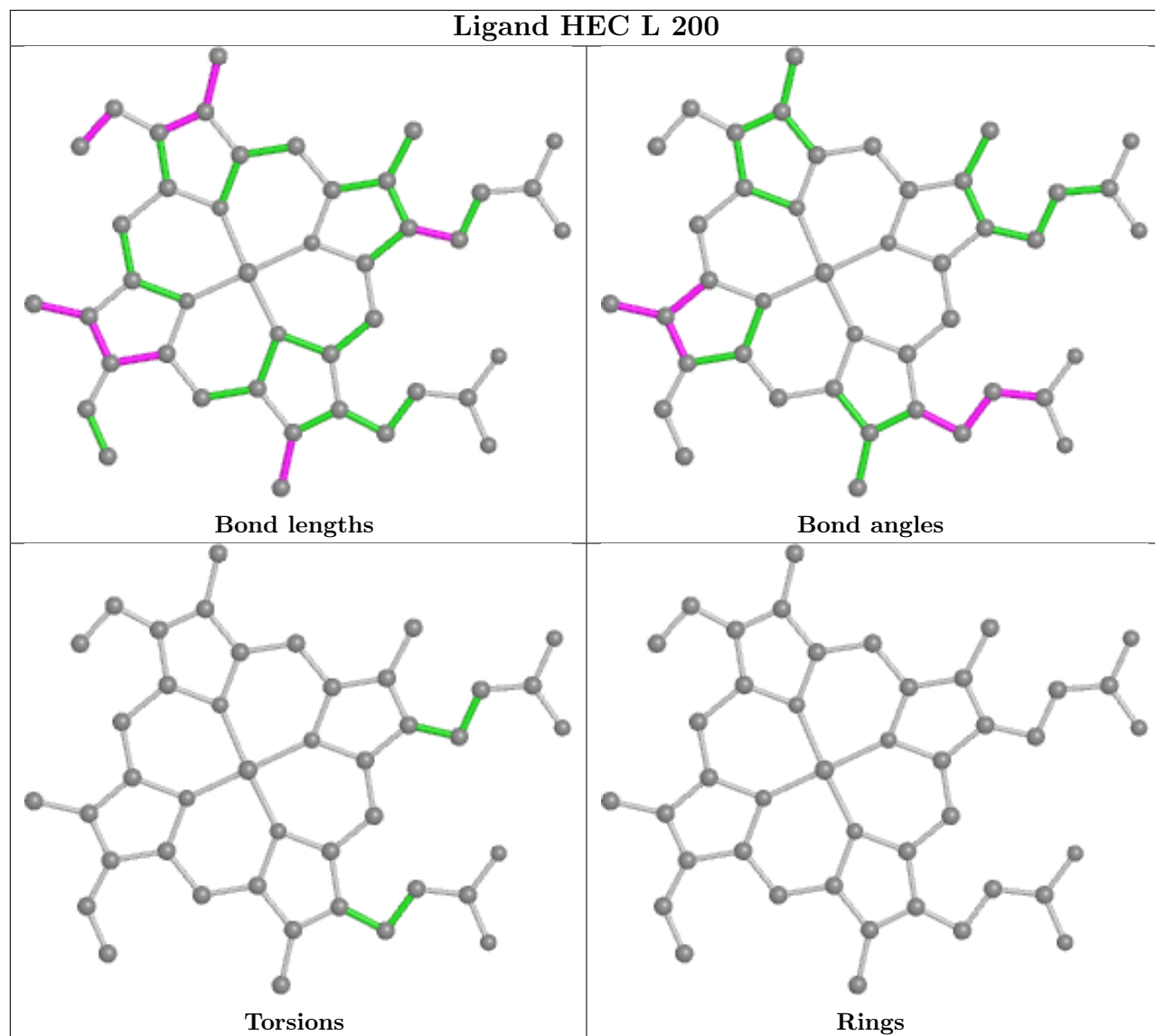
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

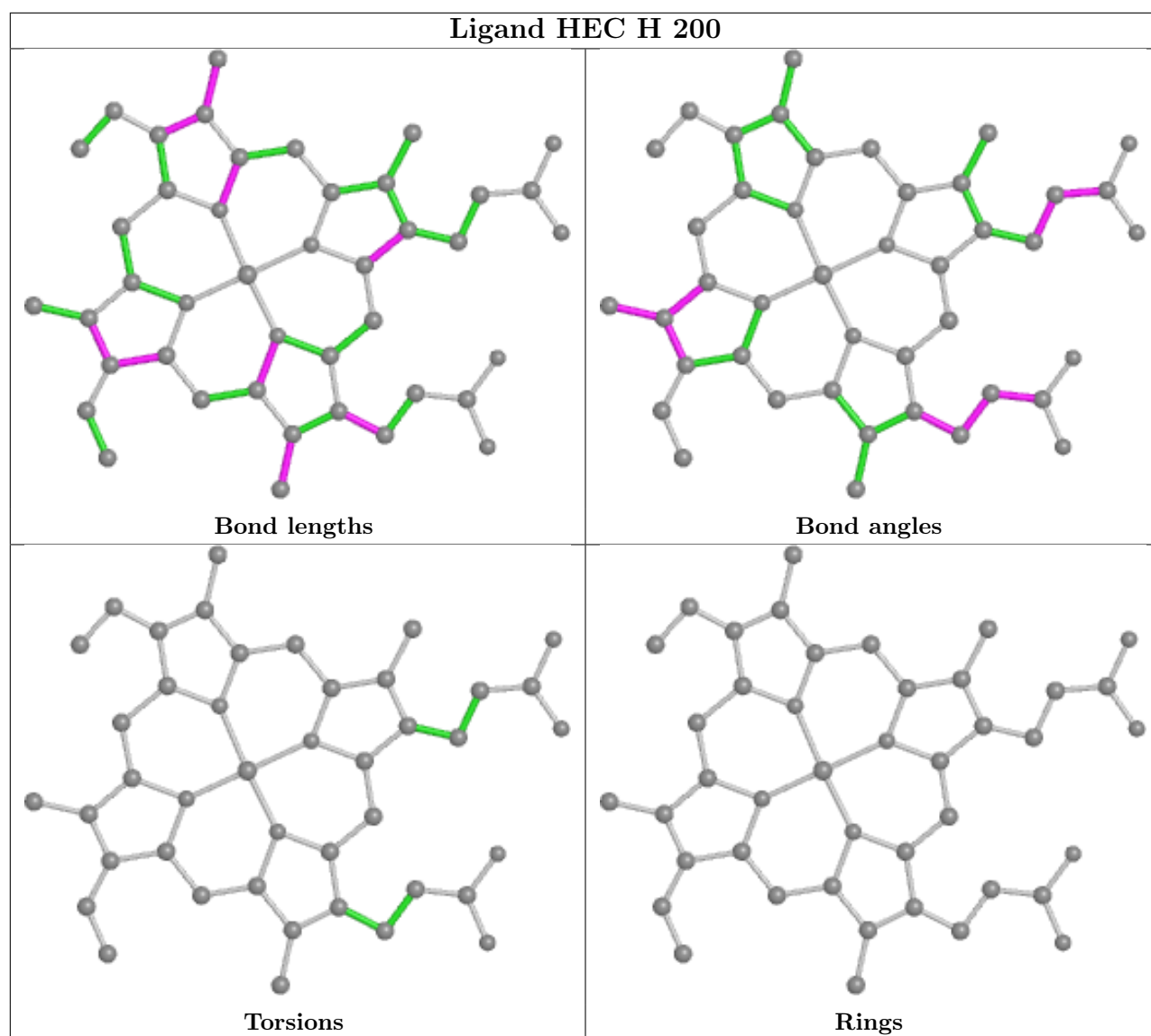
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 HEC L 200





## 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, 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	382/386 (98%)	-0.31	11 (2%) 51 54	21, 29, 49, 87	0
1	E	382/386 (98%)	-0.26	13 (3%) 45 48	21, 30, 51, 89	0
1	I	382/386 (98%)	-0.29	11 (2%) 51 54	21, 29, 53, 88	0
1	M	382/386 (98%)	-0.29	11 (2%) 51 54	20, 29, 50, 89	0
2	B	124/131 (94%)	-0.29	3 (2%) 59 62	22, 28, 48, 86	0
2	F	124/131 (94%)	-0.23	3 (2%) 59 62	20, 26, 46, 86	0
2	J	124/131 (94%)	-0.23	2 (1%) 72 74	19, 24, 45, 86	0
2	N	124/131 (94%)	-0.26	5 (4%) 38 41	22, 29, 49, 85	0
3	C	105/105 (100%)	0.35	10 (9%) 8 9	28, 42, 69, 81	0
3	G	105/105 (100%)	0.00	5 (4%) 30 33	25, 38, 60, 81	0
3	K	105/105 (100%)	-0.17	6 (5%) 23 26	24, 35, 57, 77	0
3	O	105/105 (100%)	0.85	17 (16%) 1 1	32, 51, 76, 88	0
4	D	147/147 (100%)	-0.10	8 (5%) 25 29	24, 35, 62, 76	0
4	H	147/147 (100%)	0.03	10 (6%) 17 19	25, 38, 68, 78	0
4	L	147/147 (100%)	-0.15	8 (5%) 25 29	24, 33, 59, 74	0
4	P	147/147 (100%)	0.11	9 (6%) 21 24	25, 38, 68, 79	0
All	All	3032/3076 (98%)	-0.16	132 (4%) 34 37	19, 31, 61, 89	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	131	SER	14.5
2	F	131	SER	12.7
2	B	131	SER	12.1
1	E	5	GLU	11.0
1	I	208	THR	9.2

## 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, 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( $\text{\AA}^2$ )	Q<0.9
2	TRQ	F	57	16/17	0.96	0.10	20,23,26,27	0
2	TRQ	J	57	16/17	0.96	0.10	20,23,26,27	0
2	TRQ	N	57	16/17	0.96	0.08	21,26,29,29	0
2	TRQ	B	57	16/17	0.97	0.09	23,25,27,29	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

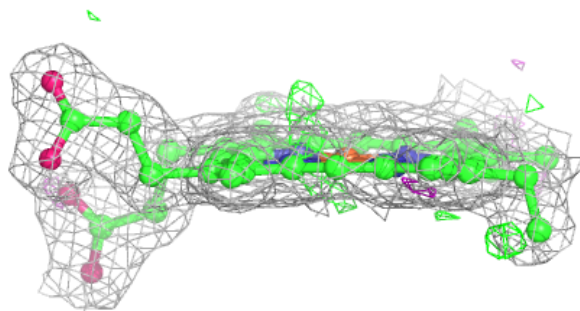
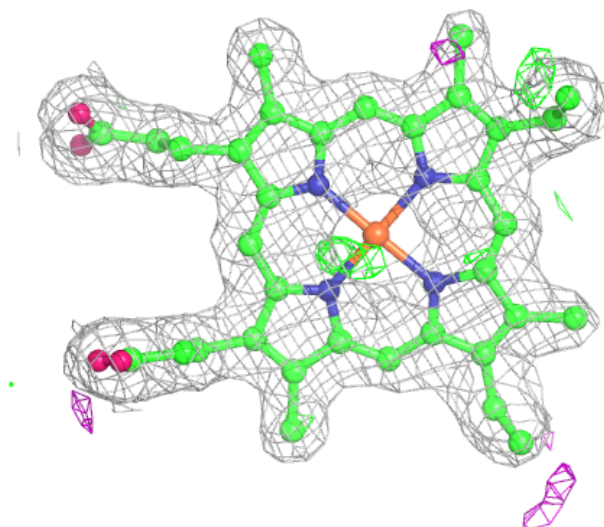
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NA	P	602	1/1	0.98	0.11	28,28,28,28	0
7	HEC	D	200	43/43	0.98	0.11	21,25,29,34	0
7	HEC	H	200	43/43	0.98	0.09	25,29,34,36	0
7	HEC	L	200	43/43	0.98	0.10	20,24,29,33	0
7	HEC	P	200	43/43	0.98	0.11	23,28,31,34	0
5	CU	O	107	1/1	0.99	0.06	39,39,39,39	0
6	NA	D	604	1/1	0.99	0.04	32,32,32,32	0
6	NA	H	603	1/1	0.99	0.12	27,27,27,27	0
5	CU	C	107	1/1	0.99	0.05	33,33,33,33	0
6	NA	L	601	1/1	1.00	0.12	23,23,23,23	0
5	CU	K	107	1/1	1.00	0.09	29,29,29,29	0
5	CU	G	107	1/1	1.00	0.06	32,32,32,32	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.

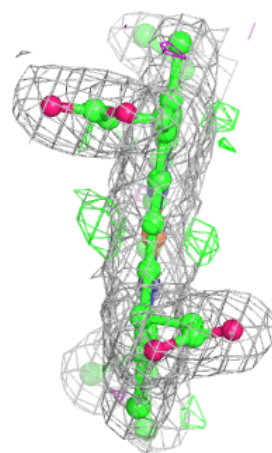
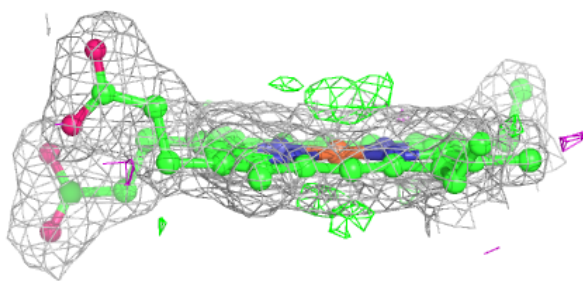
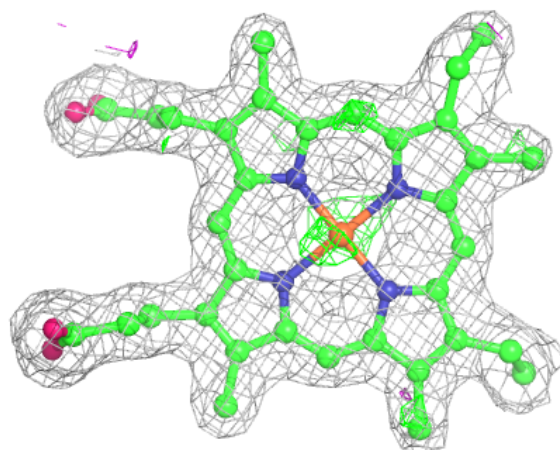
**Electron density around HEC D 200:**

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



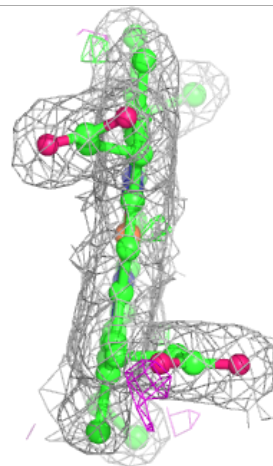
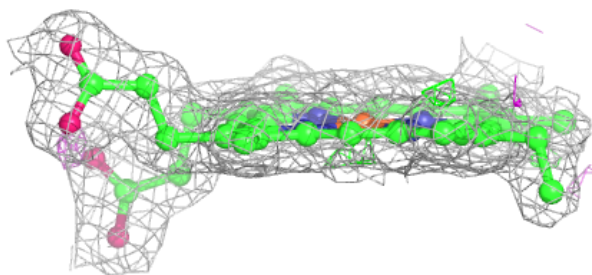
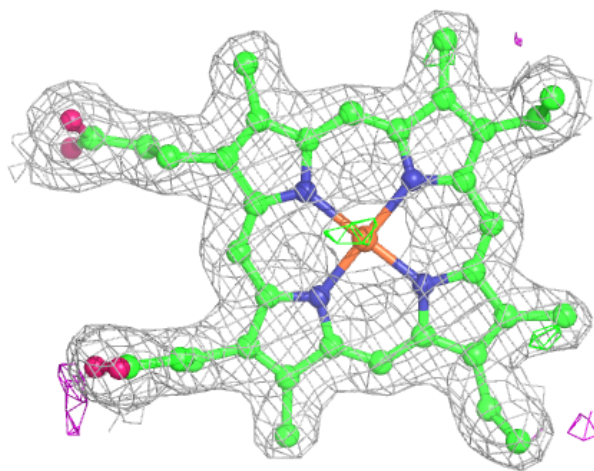
**Electron density around HEC H 200:**

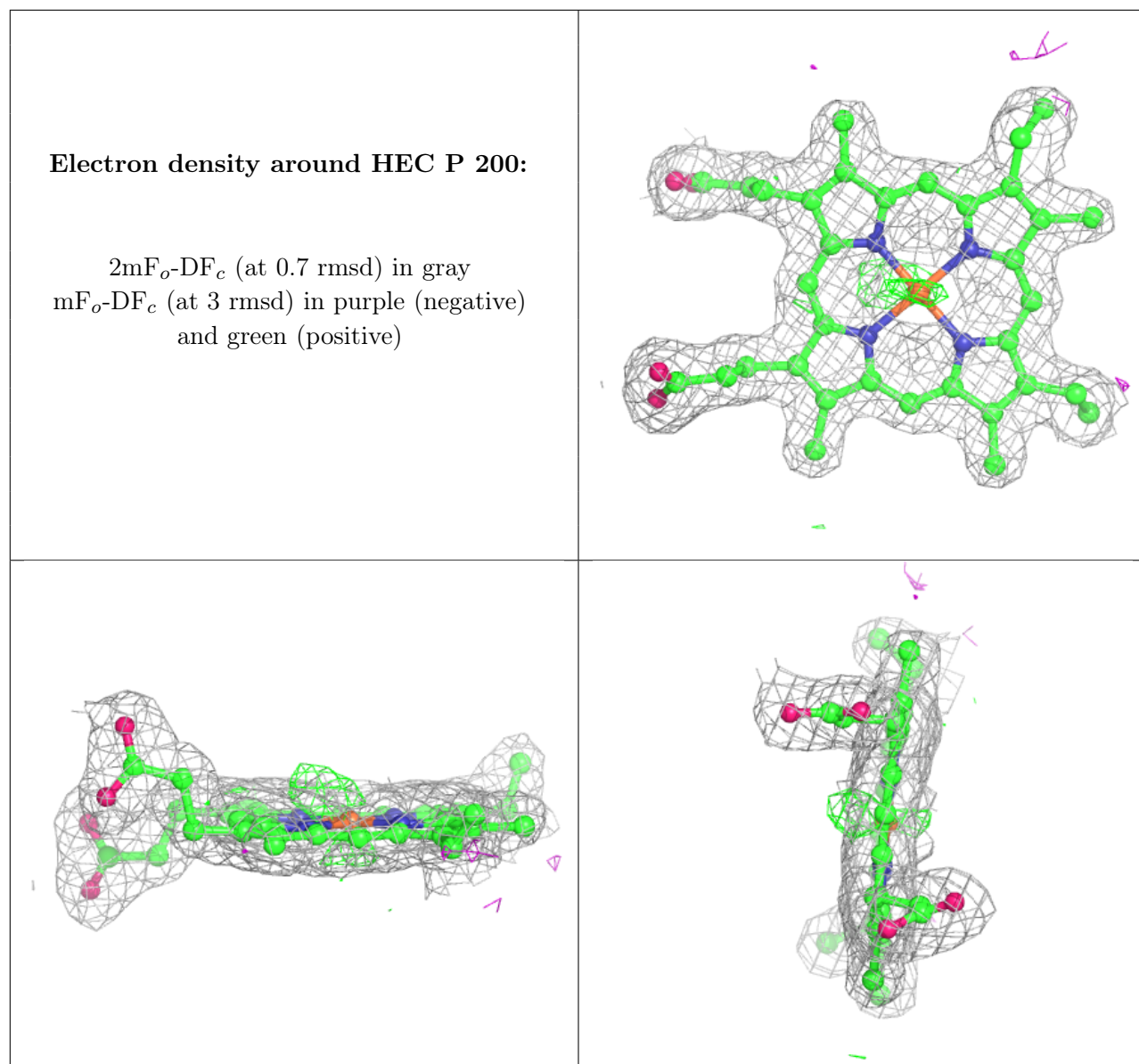
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC L 200:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.