



# wwPDB X-ray Structure Validation Summary Report

Oct 17, 2021 – 05:56 AM EDT

PDB ID : 1MG2  
Title : MUTATION OF ALPHA PHE55 OF METHYLAMINE DEHYDROGENASE ALTERS THE REORGANIZATION ENERGY AND ELECTRONIC COUPLING FOR ITS ELECTRON TRANSFER REACTION WITH AMICYANIN  
Authors : Sun, D.; Chen, Z.W.; Mathews, F.S.; Davidson, V.L.  
Deposited on : 2002-08-14  
Resolution : 2.25 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 : 2.23.2  
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) : 2.23.2

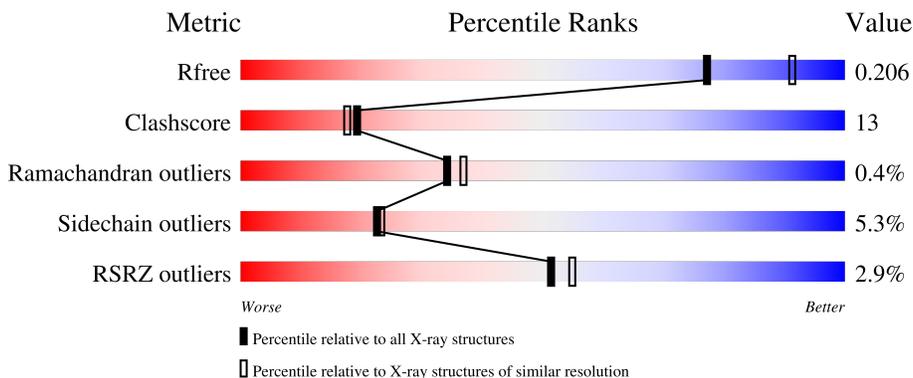
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	390	 2% 73% 23% ..
1	E	390	 2% 73% 23% ..
1	I	390	 2% 75% 21% ..
1	M	390	 2% 74% 22% ..
2	B	131	 % 70% 22% . 5%

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Mol	Chain	Length	Quality of chain
2	F	131	<p>% 71% 21% • 5%</p>
2	J	131	<p>% 73% 19% • 5%</p>
2	N	131	<p>% 72% 21% • 5%</p>
3	C	105	<p>8% 77% 23%</p>
3	G	105	<p>3% 90% 8% •</p>
3	K	105	<p>2% 80% 20%</p>
3	O	105	<p>6% 87% 11% •</p>
4	D	155	<p>% 68% 24% • 5%</p>
4	H	155	<p>7% 73% 19% • 5%</p>
4	L	155	<p>6% 65% 27% • 5%</p>
4	P	155	<p>6% 66% 26% • 5%</p>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25377 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
			Total	C	N	O	S			
1	A	382	2961	1872	509	572	8	0	0	0
1	E	382	2961	1872	509	572	8	0	0	0
1	I	382	2961	1872	509	572	8	0	0	0
1	M	382	2961	1872	509	572	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	PHE	engineered mutation	UNP P29894
A	312	PHE	LEU	SEE REMARK 999	UNP P29894
A	313	VAL	LEU	SEE REMARK 999	UNP P29894
E	55	ALA	PHE	engineered mutation	UNP P29894
E	312	PHE	LEU	SEE REMARK 999	UNP P29894
E	313	VAL	LEU	SEE REMARK 999	UNP P29894
I	55	ALA	PHE	engineered mutation	UNP P29894
I	312	PHE	LEU	SEE REMARK 999	UNP P29894
I	313	VAL	LEU	SEE REMARK 999	UNP P29894
M	55	ALA	PHE	engineered mutation	UNP P29894
M	312	PHE	LEU	SEE REMARK 999	UNP P29894
M	313	VAL	LEU	SEE REMARK 999	UNP P29894

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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

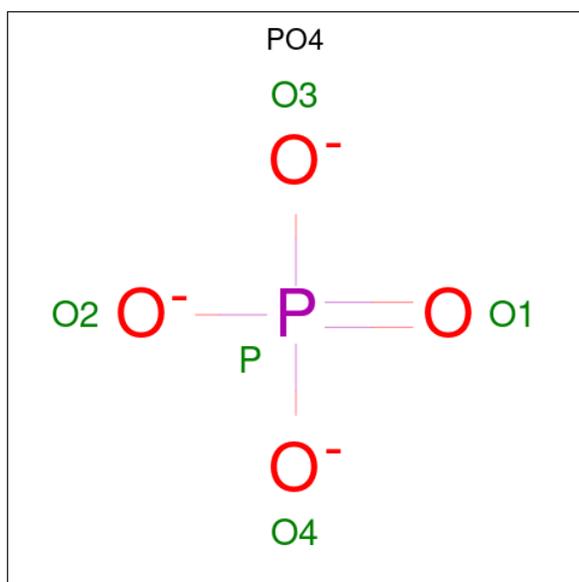
- Molecule 3 is a protein called Amicyanin.

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
			1144	724	182	230	8			
4	H	147	Total	C	N	O	S	0	0	0
			1144	724	182	230	8			
4	L	147	Total	C	N	O	S	0	0	0
			1144	724	182	230	8			
4	P	147	Total	C	N	O	S	0	0	0
			1144	724	182	230	8			

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	I	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0

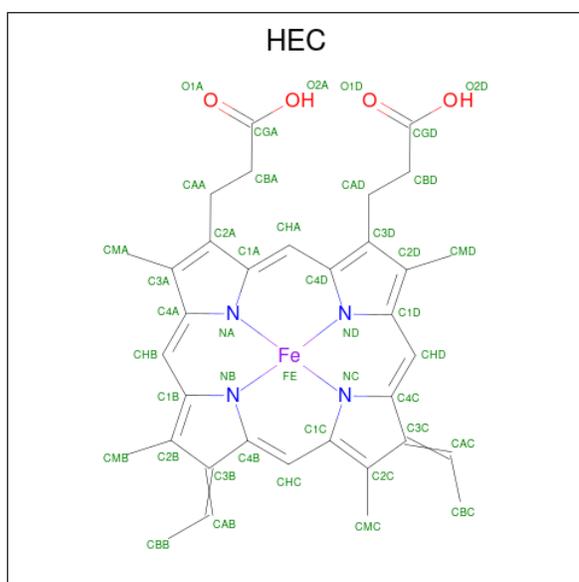
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	218	Total O 218 218	0	0

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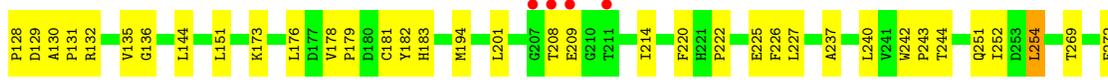
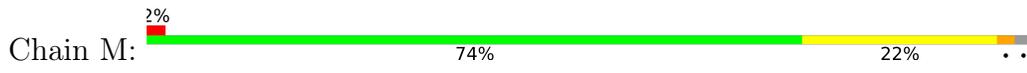
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	74	Total 74	O 74	0	0
9	C	46	Total 46	O 46	0	0
9	D	78	Total 78	O 78	0	0
9	E	223	Total 223	O 223	0	0
9	F	97	Total 97	O 97	0	0
9	G	57	Total 57	O 57	0	0
9	H	55	Total 55	O 55	0	0
9	I	224	Total 224	O 224	0	0
9	J	93	Total 93	O 93	0	0
9	K	56	Total 56	O 56	0	0
9	L	52	Total 52	O 52	0	0
9	M	245	Total 245	O 245	0	0
9	N	78	Total 78	O 78	0	0
9	O	34	Total 34	O 34	0	0
9	P	55	Total 55	O 55	0	0

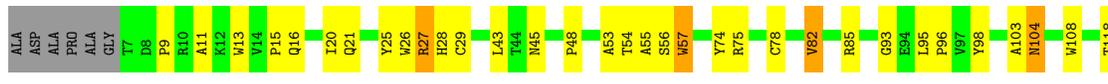




● Molecule 1: Methylamine dehydrogenase, heavy chain



● Molecule 2: Methylamine dehydrogenase, light chain



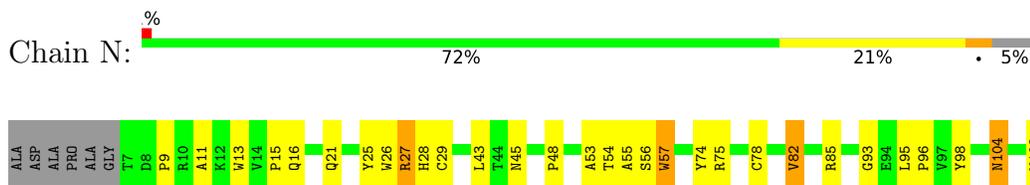
● Molecule 2: Methylamine dehydrogenase, light chain



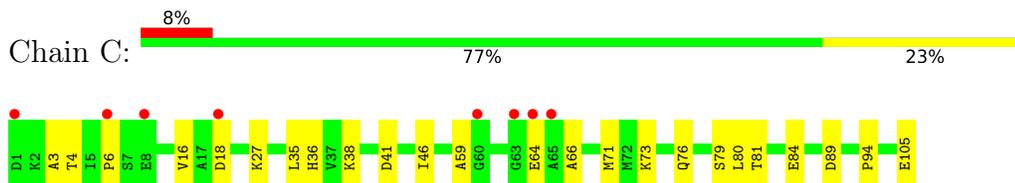
● Molecule 2: Methylamine dehydrogenase, light chain



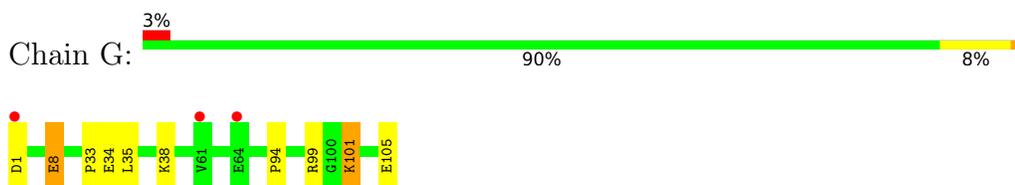
- Molecule 2: Methylamine dehydrogenase, light chain



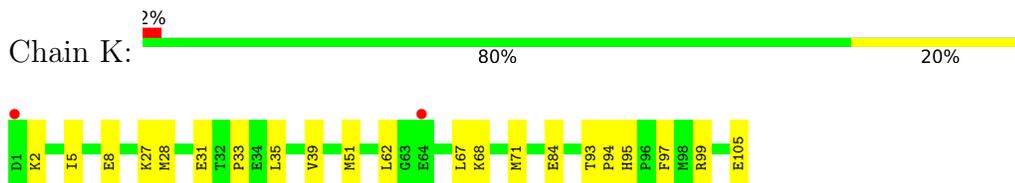
- Molecule 3: Amicyanin



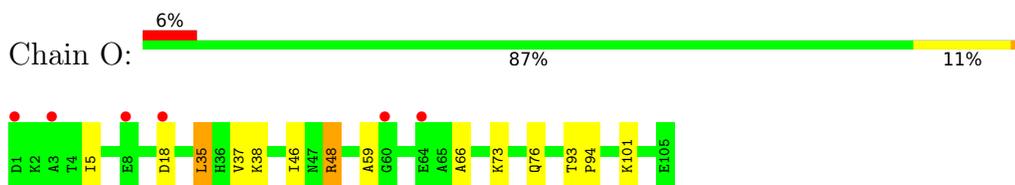
- Molecule 3: Amicyanin



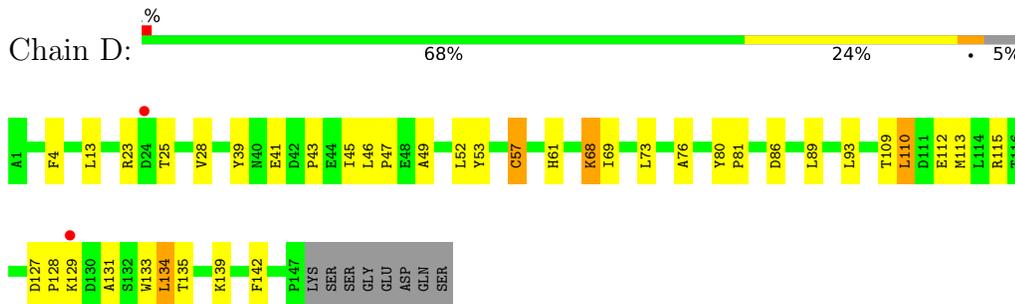
- Molecule 3: Amicyanin



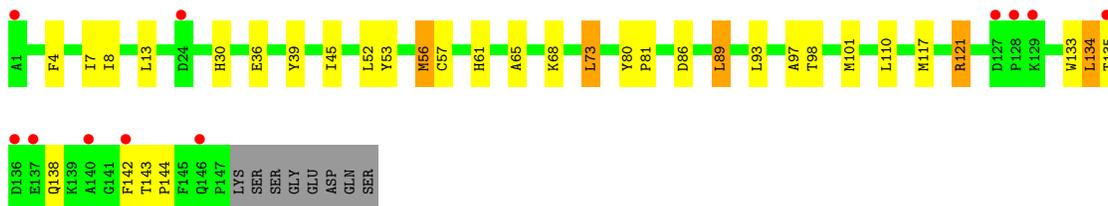
- Molecule 3: Amicyanin



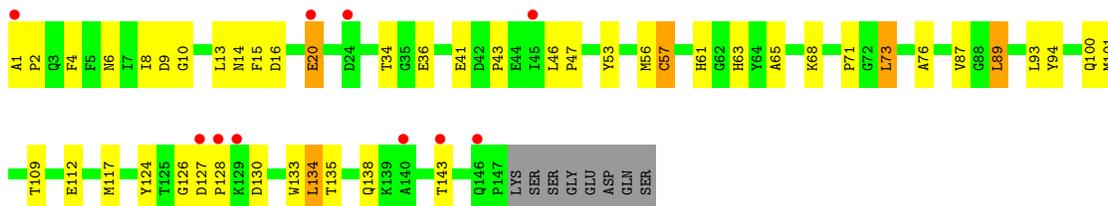
- Molecule 4: CYTOCHROME C-L



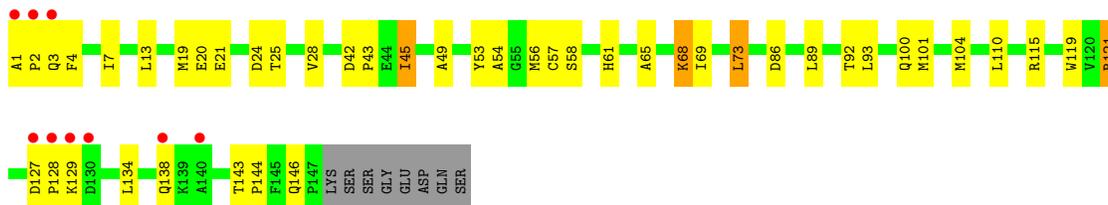
- Molecule 4: CYTOCHROME C-L



• 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, $\alpha$ , $\beta$ , $\gamma$	79.12Å 188.20Å 127.10Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 48.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.25) 83.5 (48.91-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.67 (at 2.20Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.173 , 0.210 0.169 , 0.206	Depositor DCC
$R_{free}$ test set	15487 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.542	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% 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: PO4, NA, HEC, TRQ, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	0/3037	0.64	0/4139
1	E	0.32	0/3037	0.64	0/4139
1	I	0.34	0/3037	0.65	0/4139
1	M	0.33	0/3037	0.65	0/4139
2	B	0.34	0/964	0.61	0/1315
2	F	0.34	0/964	0.61	0/1315
2	J	0.34	0/964	0.61	0/1315
2	N	0.35	0/964	0.61	0/1315
3	C	0.33	0/828	0.56	0/1124
3	G	0.33	0/828	0.59	0/1124
3	K	0.34	0/828	0.61	0/1124
3	O	0.32	0/828	0.59	0/1124
4	D	0.37	0/1179	0.65	1/1605 (0.1%)
4	H	0.36	0/1179	0.67	1/1605 (0.1%)
4	L	0.35	1/1179 (0.1%)	0.63	1/1605 (0.1%)
4	P	0.35	1/1179 (0.1%)	0.63	1/1605 (0.1%)
All	All	0.34	2/24032 (0.0%)	0.63	4/32732 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	61	HIS	CE1-NE2	5.49	1.45	1.32
4	L	61	HIS	CE1-NE2	5.26	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	8.07	120.10	108.80
4	P	61	HIS	ND1-CG-CD2	8.07	120.09	108.80
4	D	61	HIS	ND1-CG-CD2	8.03	120.03	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	61	HIS	ND1-CG-CD2	7.95	119.93	108.80

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	2961	0	2843	90	0
1	E	2961	0	2843	82	0
1	I	2961	0	2843	78	0
1	M	2961	0	2843	89	0
2	B	956	0	869	35	0
2	F	956	0	869	33	0
2	J	956	0	869	32	0
2	N	956	0	869	34	0
3	C	807	0	794	15	0
3	G	807	0	794	7	0
3	K	807	0	794	16	0
3	O	807	0	794	11	0
4	D	1144	0	1038	26	0
4	H	1144	0	1038	23	0
4	L	1144	0	1038	31	0
4	P	1144	0	1038	29	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	I	5	0	0	1	0
5	J	5	0	0	1	0
5	M	5	0	0	0	0
5	N	5	0	0	0	0
6	C	1	0	0	0	0
6	G	1	0	0	0	0
6	K	1	0	0	0	0
6	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	D	43	0	30	1	0
8	H	43	0	30	4	0
8	L	43	0	30	2	0
8	P	43	0	30	4	0
9	A	218	0	0	8	0
9	B	74	0	0	2	0
9	C	46	0	0	0	0
9	D	78	0	0	0	0
9	E	223	0	0	5	0
9	F	97	0	0	2	0
9	G	57	0	0	1	0
9	H	55	0	0	2	0
9	I	224	0	0	6	0
9	J	93	0	0	2	0
9	K	56	0	0	2	0
9	L	52	0	0	2	0
9	M	245	0	0	4	0
9	N	78	0	0	2	0
9	O	34	0	0	0	0
9	P	55	0	0	0	0
All	All	25377	0	22296	564	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 13.

The worst 5 of 564 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:ARG:HB2	1:I:20:ARG:HH21	1.20	1.05
4:H:7:ILE:HG13	4:H:8:ILE:HD12	1.38	1.03
1:A:20:ARG:HB2	1:A:20:ARG:HH21	1.20	1.00
2:J:21:GLN:HE22	1:M:11:GLN:HG3	1.22	1.00
2:N:25:TYR:CE2	2:N:27:ARG:HG3	2.00	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	380/390 (97%)	364 (96%)	15 (4%)	1 (0%)	41	46
1	E	380/390 (97%)	365 (96%)	14 (4%)	1 (0%)	41	46
1	I	380/390 (97%)	365 (96%)	14 (4%)	1 (0%)	41	46
1	M	380/390 (97%)	367 (97%)	12 (3%)	1 (0%)	41	46
2	B	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	F	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	J	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	N	122/131 (93%)	116 (95%)	6 (5%)	0	100	100
3	C	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
3	G	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	K	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	O	103/105 (98%)	97 (94%)	5 (5%)	1 (1%)	15	13
4	D	145/155 (94%)	139 (96%)	5 (3%)	1 (1%)	22	21
4	H	145/155 (94%)	133 (92%)	11 (8%)	1 (1%)	22	21
4	L	145/155 (94%)	136 (94%)	7 (5%)	2 (1%)	11	7
4	P	145/155 (94%)	134 (92%)	9 (6%)	2 (1%)	11	7
All	All	3000/3124 (96%)	2872 (96%)	117 (4%)	11 (0%)	34	37

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	68	LYS
4	H	68	LYS
4	L	10	GLY
4	P	68	LYS
1	A	102	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/311 (99%)	290 (94%)	17 (6%)	21	21
1	E	307/311 (99%)	289 (94%)	18 (6%)	19	19
1	I	307/311 (99%)	292 (95%)	15 (5%)	25	27
1	M	307/311 (99%)	291 (95%)	16 (5%)	23	24
2	B	104/106 (98%)	98 (94%)	6 (6%)	20	20
2	F	104/106 (98%)	98 (94%)	6 (6%)	20	20
2	J	104/106 (98%)	99 (95%)	5 (5%)	25	28
2	N	104/106 (98%)	98 (94%)	6 (6%)	20	20
3	C	85/85 (100%)	81 (95%)	4 (5%)	26	29
3	G	85/85 (100%)	81 (95%)	4 (5%)	26	29
3	K	85/85 (100%)	83 (98%)	2 (2%)	49	58
3	O	85/85 (100%)	82 (96%)	3 (4%)	36	43
4	D	118/125 (94%)	111 (94%)	7 (6%)	19	19
4	H	118/125 (94%)	111 (94%)	7 (6%)	19	19
4	L	118/125 (94%)	110 (93%)	8 (7%)	16	14
4	P	118/125 (94%)	111 (94%)	7 (6%)	19	19
All	All	2456/2508 (98%)	2325 (95%)	131 (5%)	22	23

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	16	GLN
2	N	82	VAL
4	P	121	ARG
1	E	345	LEU
1	E	323	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	82	ASN
4	L	3	GLN
4	P	30	HIS
1	I	284	GLN
2	J	34	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	F	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.26	5 (35%)
2	TRQ	B	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.28	5 (35%)
2	TRQ	J	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.27	5 (35%)
2	TRQ	N	57	2	13,17,18	4.72	3 (23%)	14,24,26	2.25	4 (28%)

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	F	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	J	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	N	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	N	57	TRQ	CH2-CZ2	-14.70	1.37	1.54
2	B	57	TRQ	CH2-CZ2	-14.54	1.37	1.54
2	J	57	TRQ	CH2-CZ2	-14.53	1.37	1.54
2	F	57	TRQ	CH2-CZ2	-14.47	1.37	1.54
2	N	57	TRQ	CE2-CZ2	-7.46	1.40	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	57	TRQ	CZ2-CE2-NE1	5.75	129.13	119.94
2	F	57	TRQ	CZ2-CE2-NE1	5.70	129.05	119.94
2	B	57	TRQ	CZ2-CE2-NE1	5.68	129.01	119.94
2	N	57	TRQ	CZ2-CE2-NE1	5.68	129.00	119.94
2	N	57	TRQ	O7-CZ2-CH2	3.84	123.52	119.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	57	TRQ	2	0
2	B	57	TRQ	3	0
2	J	57	TRQ	3	0
2	N	57	TRQ	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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
5	PO4	J	403	-	4,4,4	1.69	1 (25%)	6,6,6	0.43	0
5	PO4	E	406	-	4,4,4	1.65	0	6,6,6	0.43	0
8	HEC	P	200	4	26,50,50	1.94	2 (7%)	18,82,82	1.76	7 (38%)
5	PO4	N	404	-	4,4,4	1.68	0	6,6,6	0.43	0
5	PO4	I	405	-	4,4,4	1.68	0	6,6,6	0.42	0
5	PO4	B	402	-	4,4,4	1.71	0	6,6,6	0.43	0
5	PO4	F	401	-	4,4,4	1.66	0	6,6,6	0.44	0
8	HEC	D	200	4	26,50,50	1.96	2 (7%)	18,82,82	1.93	7 (38%)
8	HEC	H	200	4	26,50,50	2.00	2 (7%)	18,82,82	1.69	7 (38%)
8	HEC	L	200	4	26,50,50	1.98	3 (11%)	18,82,82	1.88	7 (38%)
5	PO4	M	407	-	4,4,4	1.65	0	6,6,6	0.43	0
5	PO4	A	408	-	4,4,4	1.88	3 (75%)	6,6,6	0.43	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
8	HEC	P	200	4	-	0/6/54/54	-
8	HEC	D	200	4	-	0/6/54/54	-
8	HEC	H	200	4	-	0/6/54/54	-
8	HEC	L	200	4	-	0/6/54/54	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	200	HEC	C3C-C2C	-6.58	1.33	1.40
8	L	200	HEC	C3C-C2C	-6.46	1.34	1.40
8	P	200	HEC	C3C-C2C	-6.31	1.34	1.40
8	D	200	HEC	C3C-C2C	-6.17	1.34	1.40
8	D	200	HEC	C3B-C2B	-4.54	1.36	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	200	HEC	CBD-CAD-C3D	-4.14	104.84	112.49
8	L	200	HEC	CBD-CAD-C3D	-3.52	106.00	112.49
8	H	200	HEC	CMC-C2C-C3C	3.02	129.37	125.82
8	L	200	HEC	CAD-CBD-CGD	2.97	117.66	112.67
8	L	200	HEC	CMC-C2C-C3C	2.92	129.25	125.82

There are no chirality outliers.

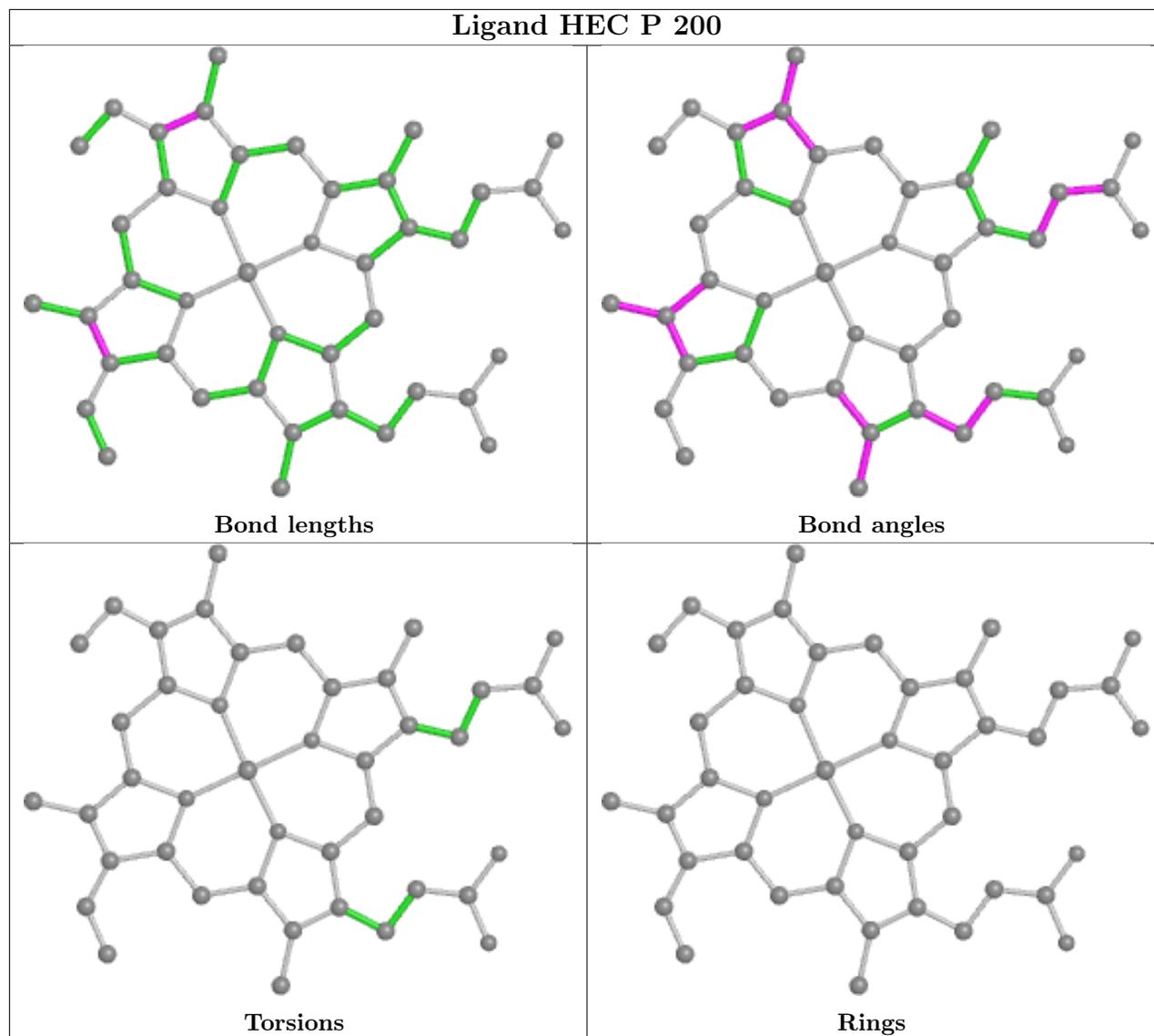
There are no torsion outliers.

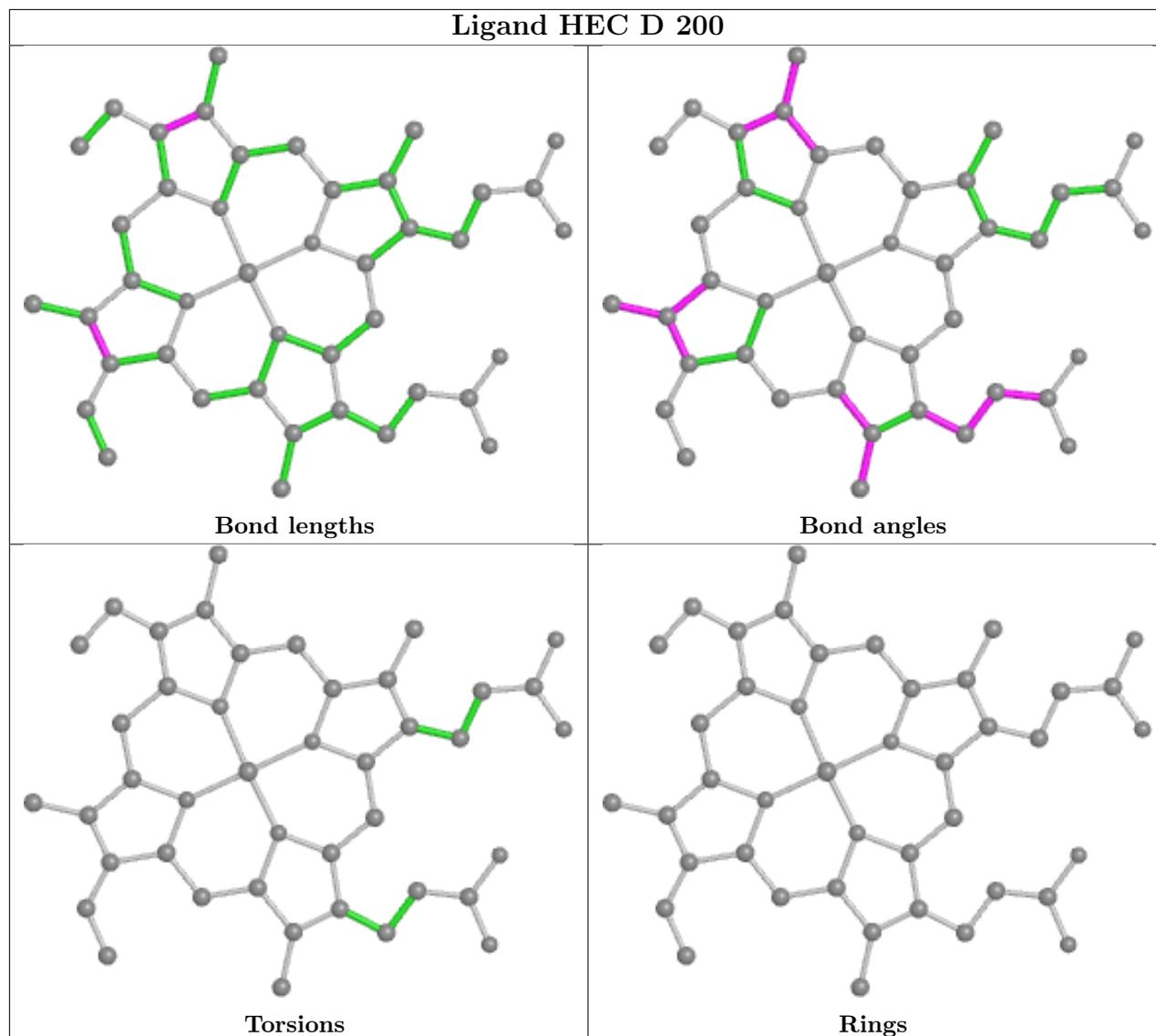
There are no ring outliers.

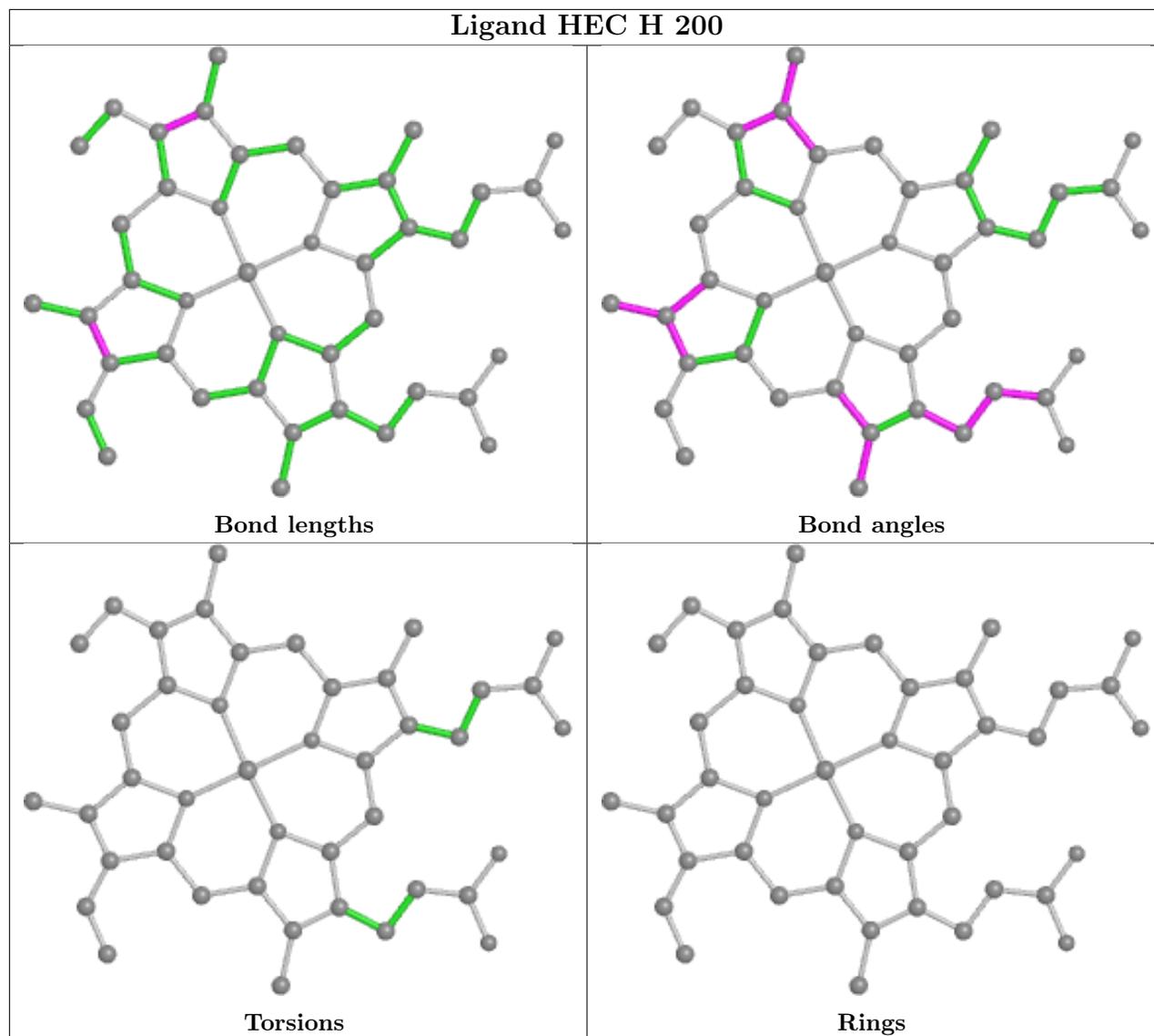
7 monomers are involved in 14 short contacts:

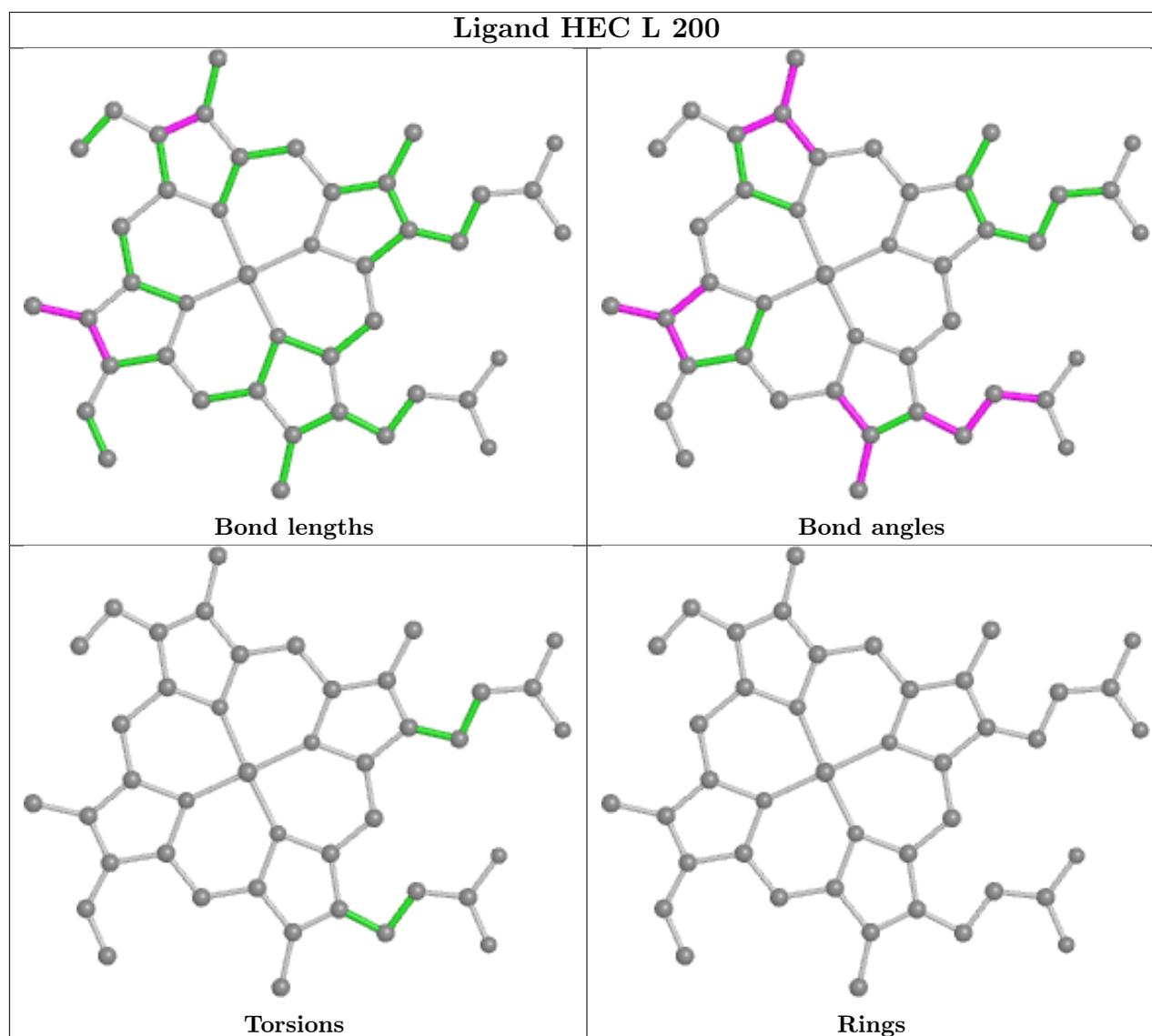
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	403	PO4	1	0
8	P	200	HEC	4	0
5	I	405	PO4	1	0
8	D	200	HEC	1	0
8	H	200	HEC	4	0
8	L	200	HEC	2	0
5	A	408	PO4	1	0

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









## 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	382/390 (97%)	-0.19	9 (2%) 59 62	9, 19, 40, 77	0
1	E	382/390 (97%)	-0.17	8 (2%) 63 66	9, 19, 38, 74	0
1	I	382/390 (97%)	-0.26	9 (2%) 59 62	6, 17, 38, 74	0
1	M	382/390 (97%)	-0.24	7 (1%) 68 71	8, 18, 36, 74	0
2	B	124/131 (94%)	-0.23	1 (0%) 86 87	11, 17, 30, 68	0
2	F	124/131 (94%)	-0.25	1 (0%) 86 87	10, 15, 27, 69	0
2	J	124/131 (94%)	-0.23	1 (0%) 86 87	7, 15, 27, 68	0
2	N	124/131 (94%)	-0.25	1 (0%) 86 87	11, 18, 29, 68	0
3	C	105/105 (100%)	0.24	8 (7%) 13 15	16, 28, 52, 61	0
3	G	105/105 (100%)	-0.27	3 (2%) 51 55	12, 21, 32, 51	0
3	K	105/105 (100%)	-0.28	2 (1%) 66 69	10, 20, 33, 51	0
3	O	105/105 (100%)	0.14	6 (5%) 23 25	16, 28, 53, 66	0
4	D	147/155 (94%)	-0.28	2 (1%) 75 77	13, 22, 47, 59	0
4	H	147/155 (94%)	-0.02	11 (7%) 14 15	15, 26, 57, 70	0
4	L	147/155 (94%)	0.07	10 (6%) 17 18	15, 31, 50, 58	0
4	P	147/155 (94%)	0.07	9 (6%) 21 23	14, 28, 61, 82	0
All	All	3032/3124 (97%)	-0.16	88 (2%) 51 55	6, 20, 45, 82	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	SER	7.8
4	P	129	LYS	7.5
2	F	131	SER	6.2
1	E	386	GLY	6.1
1	E	5	GLU	5.9

## 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(Å <sup>2</sup> )	Q<0.9
2	TRQ	B	57	16/17	0.96	0.11	14,16,19,23	0
2	TRQ	F	57	16/17	0.97	0.11	9,13,16,17	0
2	TRQ	J	57	16/17	0.97	0.10	10,13,15,18	0
2	TRQ	N	57	16/17	0.98	0.09	13,14,18,19	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.

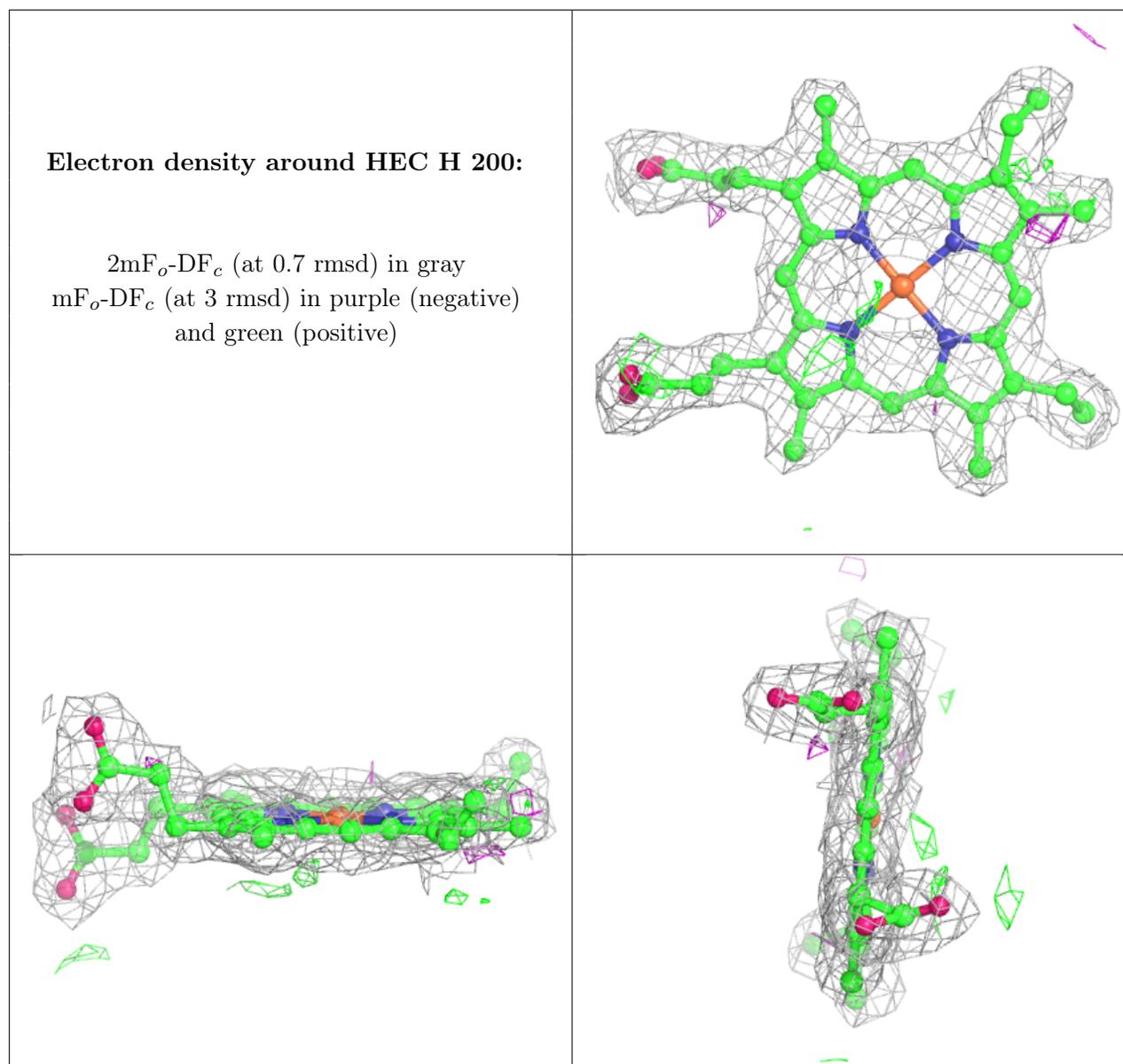
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	M	407	5/5	0.73	0.35	76,76,79,81	0
5	PO4	A	408	5/5	0.76	0.25	51,54,57,58	0
5	PO4	N	404	5/5	0.81	0.28	78,78,81,81	0
5	PO4	J	403	5/5	0.88	0.22	63,64,66,66	0
5	PO4	E	406	5/5	0.88	0.24	69,70,72,73	0
5	PO4	I	405	5/5	0.88	0.23	65,68,69,70	0
5	PO4	F	401	5/5	0.93	0.22	66,67,68,68	0
5	PO4	B	402	5/5	0.97	0.15	51,52,53,54	0
7	NA	H	603	1/1	0.97	0.15	14,14,14,14	0
8	HEC	H	200	43/43	0.97	0.12	12,19,23,29	0
8	HEC	L	200	43/43	0.97	0.12	15,18,22,27	0
8	HEC	P	200	43/43	0.97	0.13	16,25,29,32	0
8	HEC	D	200	43/43	0.98	0.12	6,14,19,25	0
7	NA	L	601	1/1	0.99	0.14	13,13,13,13	0
7	NA	P	602	1/1	0.99	0.10	8,8,8,8	0
7	NA	D	604	1/1	0.99	0.09	22,22,22,22	0
6	CU	C	107	1/1	1.00	0.05	26,26,26,26	0
6	CU	G	107	1/1	1.00	0.07	19,19,19,19	0

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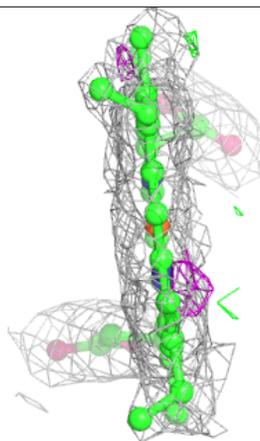
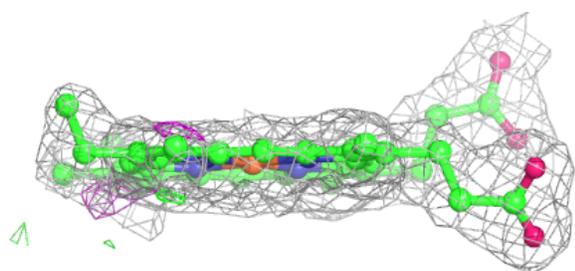
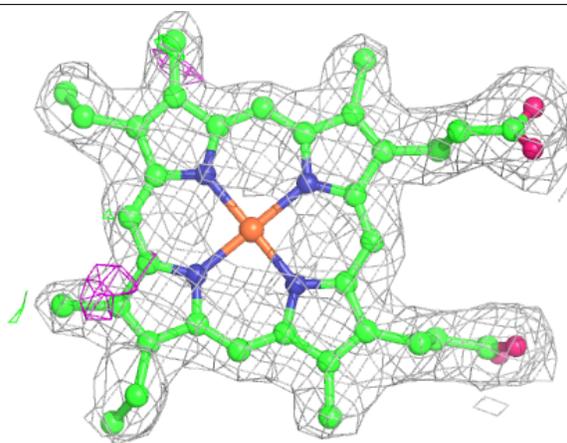
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CU	K	107	1/1	1.00	0.09	18,18,18,18	0
6	CU	O	107	1/1	1.00	0.06	29,29,29,29	0

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.



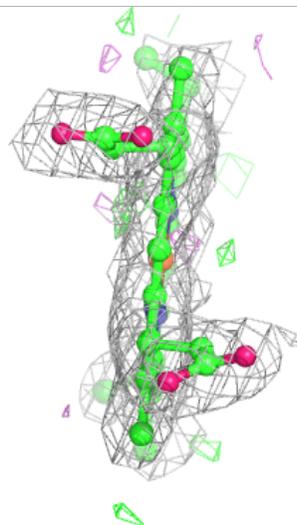
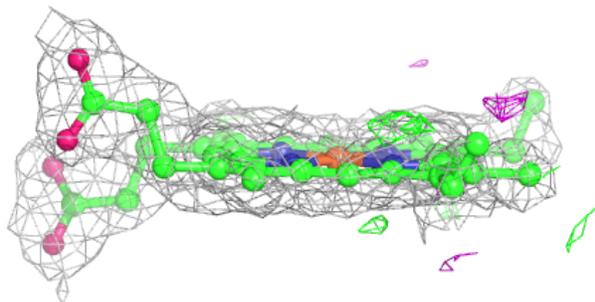
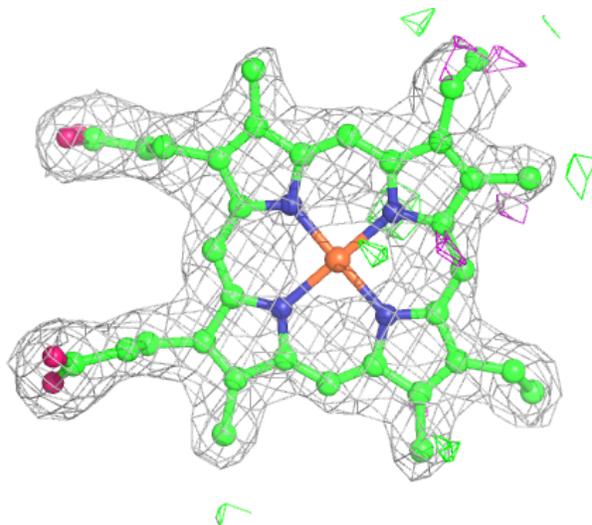
**Electron density around HEC L 200:**

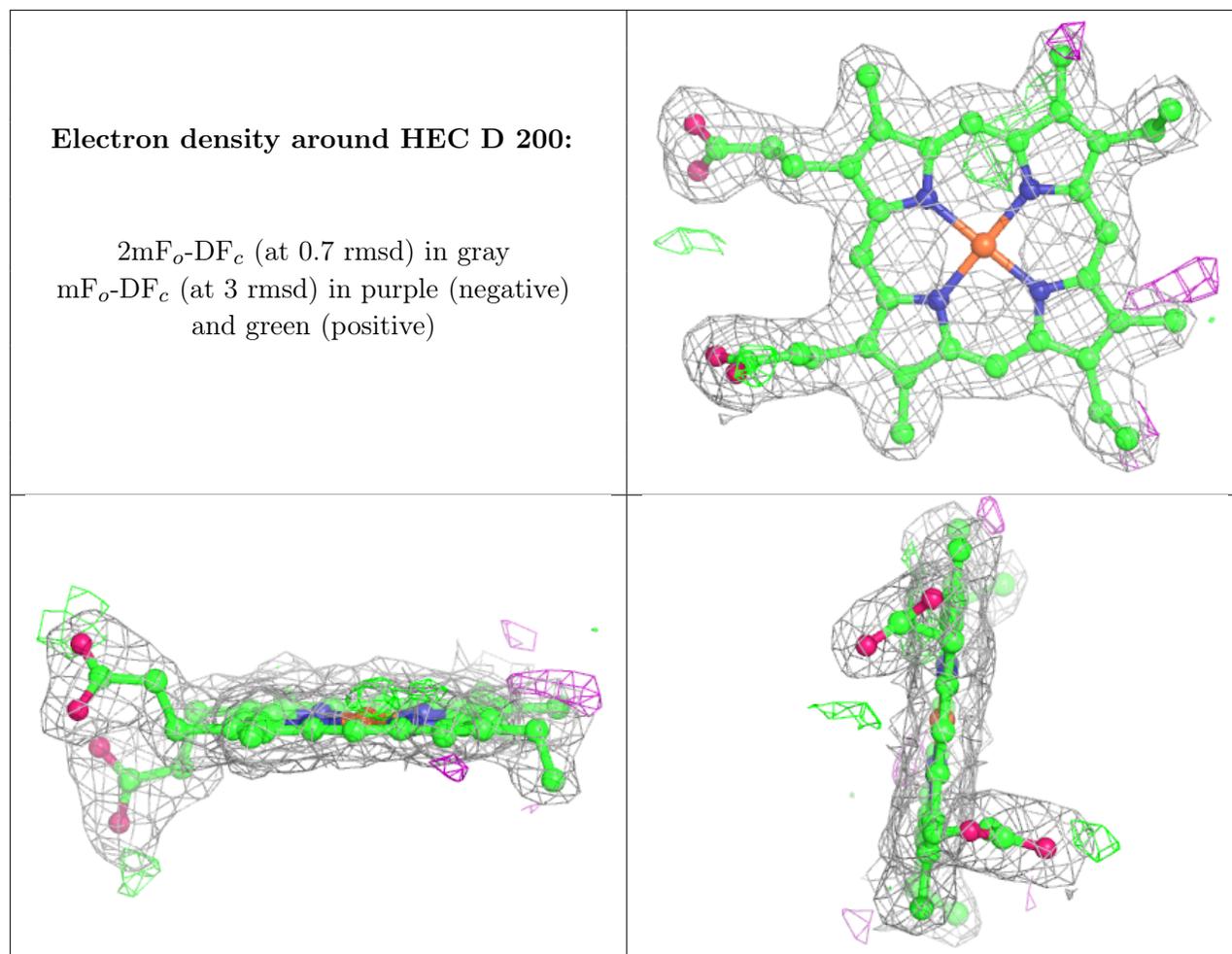
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC P 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 [i](#)

There are no such residues in this entry.