



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:13 pm BST

PDB ID : 1QPW  
Title : CRYSTAL STRUCTURE DETERMINATION OF PORCINE  
HEMOGLOBIN AT 1.8Å RESOLUTION  
Authors : Lu, T.-H.; Panneerselvam, K.; Liaw, Y.-C.; Kan, P.; Lee, C.-J.  
Deposited on : 1999-05-30  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.11  
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) : 2.11

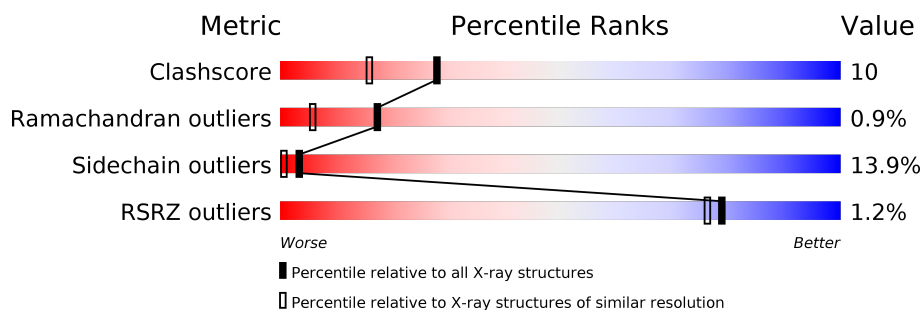
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on 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	141	<div> <div></div> <div>64% 28% 8% .</div> </div>
1	C	141	<div> <div></div> <div>70% 23% 6% .</div> </div>
2	B	146	<div> <div></div> <div>60% 29% 9% .</div> </div>
2	D	146	<div> <div></div> <div>68% 23% 8% .</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5148 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 PORCINE HEMOGLOBIN (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	C	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			

- Molecule 2 is a protein called PORCINE HEMOGLOBIN (BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			
2	D	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			

There are 2 discrepancies between the modelled and reference sequences:

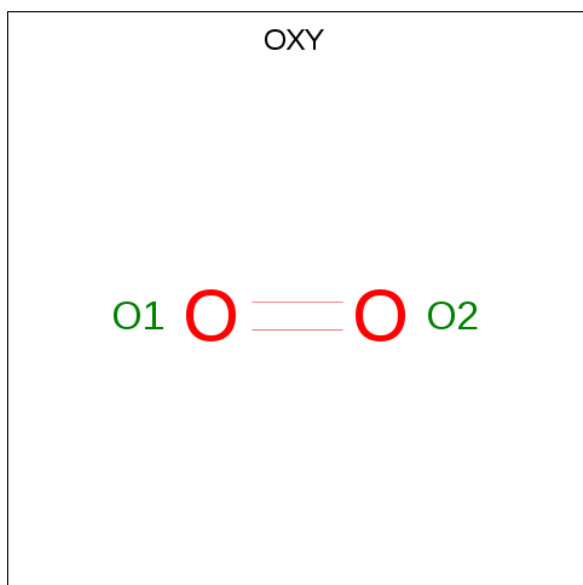
Chain	Residue	Modelled	Actual	Comment	Reference
B	125	ASP	ASN	CONFLICT	UNP P01965
D	125	ASP	ASN	CONFLICT	UNP P02067

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula:  $O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			2	2		

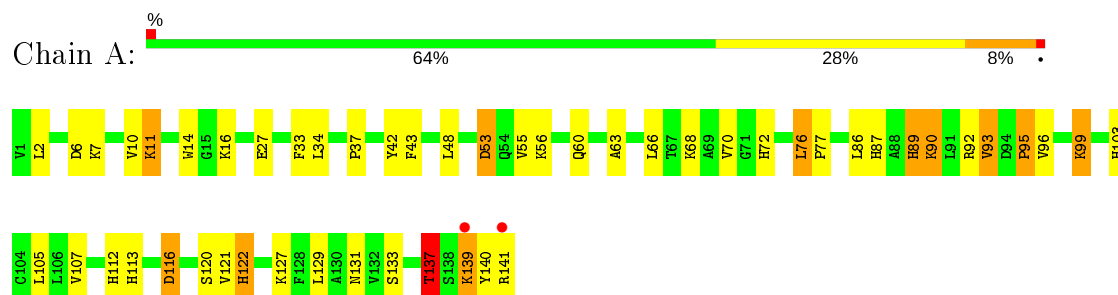
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	143	Total	O	0	0
			143	143		
5	C	135	Total	O	0	0
			135	135		
5	D	192	Total	O	0	0
			192	192		

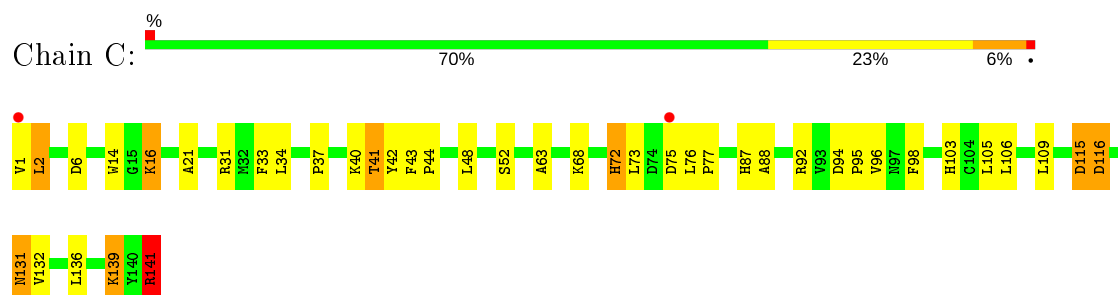
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

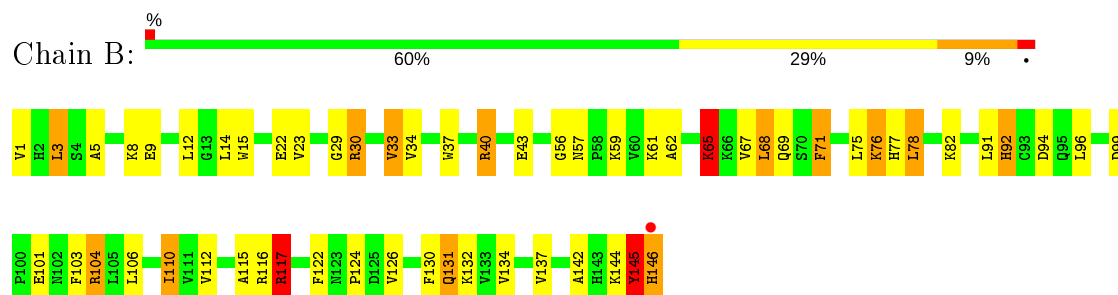
#### • Molecule 1: PORCINE HEMOGLOBIN (ALPHA SUBUNIT)



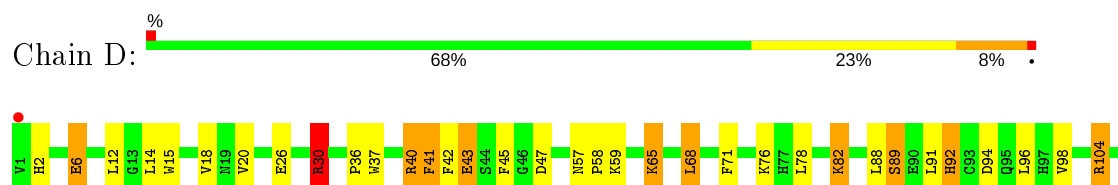
#### • Molecule 1: PORCINE HEMOGLOBIN (ALPHA SUBUNIT)



#### • Molecule 2: PORCINE HEMOGLOBIN (BETA SUBUNIT)



#### • Molecule 2: PORCINE HEMOGLOBIN (BETA SUBUNIT)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.10Å 72.27Å 114.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 58.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (8.00-1.80) 70.4 (58.58-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.207 , 0.251 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 100.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OXY

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	1.00	1/1091 (0.1%)	1.68	17/1480 (1.1%)
1	C	1.11	1/1091 (0.1%)	1.66	13/1480 (0.9%)
2	B	1.06	1/1160 (0.1%)	1.81	23/1568 (1.5%)
2	D	1.07	1/1160 (0.1%)	1.80	30/1568 (1.9%)
All	All	1.06	4/4502 (0.1%)	1.74	83/6096 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	CD2-NE2	-6.30	1.24	1.38
2	D	92	HIS	CD2-NE2	-6.09	1.24	1.38
2	B	92	HIS	CD2-NE2	-5.40	1.26	1.38
1	A	93	VAL	CA-CB	5.20	1.65	1.54

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	141	ARG	NE-CZ-NH2	-12.35	114.12	120.30
2	B	117	ARG	NE-CZ-NH1	11.80	126.20	120.30
2	B	116	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	D	37	TRP	CD1-CG-CD2	9.77	114.11	106.30
2	D	116	ARG	NE-CZ-NH1	9.14	124.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	117	ARG	NE-CZ-NH1	8.96	124.78	120.30
2	D	117	ARG	NE-CZ-NH2	-8.63	115.99	120.30
2	D	30	ARG	NE-CZ-NH2	8.46	124.53	120.30
2	D	37	TRP	CE2-CD2-CG	-8.35	100.62	107.30
2	B	15	TRP	CD1-CG-CD2	8.33	112.96	106.30
2	D	40	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	B	30	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	B	76	LYS	CA-C-N	-7.86	99.91	117.20
1	A	14	TRP	CD1-CG-CD2	7.80	112.54	106.30
2	B	71	PHE	CB-CG-CD1	-7.77	115.36	120.80
2	D	116	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	D	43	GLU	CA-CB-CG	7.68	130.30	113.40
1	C	31	ARG	NE-CZ-NH1	7.67	124.13	120.30
2	D	15	TRP	CD1-CG-CD2	7.54	112.33	106.30
2	B	116	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	42	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	C	14	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	D	104	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	C	87	HIS	CE1-NE2-CD2	7.21	124.61	106.60
2	D	37	TRP	CG-CD2-CE3	7.20	140.38	133.90
2	D	15	TRP	CE2-CD2-CG	-7.07	101.64	107.30
2	B	15	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	C	116	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	14	TRP	CD1-CG-CD2	6.74	111.69	106.30
2	D	92	HIS	CE1-NE2-CD2	6.58	123.04	106.60
1	A	14	TRP	CE2-CD2-CG	-6.57	102.05	107.30
2	B	40	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	137	THR	N-CA-CB	-6.47	98.01	110.30
2	B	30	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	141	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	B	146	HIS	CG-ND1-CE1	6.34	117.08	108.20
2	D	104	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	B	99	ASP	CB-CG-OD1	6.18	123.87	118.30
2	B	94	ASP	CB-CG-OD2	6.15	123.84	118.30
2	D	30	ARG	NE-CZ-NH1	-6.14	117.23	120.30
2	D	18	VAL	CA-CB-CG2	-6.12	101.71	110.90
2	B	145	TYR	CA-C-N	6.12	130.66	117.20
2	B	37	TRP	CE2-CD2-CG	-6.09	102.43	107.30
2	B	37	TRP	CD1-CG-CD2	6.07	111.16	106.30
2	D	94	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	14	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	C	42	TYR	CB-CG-CD1	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	ASP	CB-CG-OD2	5.93	123.64	118.30
2	B	110	ILE	CA-CB-CG1	-5.91	99.76	111.00
1	C	141	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	121	VAL	CG1-CB-CG2	-5.87	101.50	110.90
2	B	65	LYS	CA-CB-CG	5.85	126.27	113.40
2	D	15	TRP	CG-CD2-CE3	5.85	139.16	133.90
2	D	47	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	87	HIS	CG-CD2-NE2	-5.79	98.19	109.20
2	B	146	HIS	N-CA-CB	-5.69	100.35	110.60
1	A	53	ASP	CB-CG-OD2	5.65	123.39	118.30
2	D	41	PHE	CB-CG-CD1	-5.65	116.85	120.80
2	B	131	GLN	CG-CD-NE2	5.64	130.23	116.70
1	C	41	THR	CA-CB-CG2	-5.59	104.58	112.40
1	A	112	HIS	CA-C-N	5.52	129.34	117.20
1	A	116	ASP	N-CA-CB	-5.50	100.70	110.60
2	D	37	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	27	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	A	14	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	76	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	90	LYS	CA-CB-CG	5.38	125.25	113.40
2	B	1	VAL	CA-C-N	5.38	129.03	117.20
2	B	78	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	55	VAL	CG1-CB-CG2	-5.31	102.40	110.90
2	D	15	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	A	89	HIS	CA-CB-CG	5.29	122.59	113.60
1	A	53	ASP	CA-CB-CG	5.26	124.98	113.40
2	D	6	GLU	CA-CB-CG	5.22	124.89	113.40
2	B	103	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	C	16	LYS	CA-CB-CG	5.14	124.71	113.40
2	D	82	LYS	CB-CG-CD	5.14	124.96	111.60
2	D	104	ARG	CA-CB-CG	5.11	124.65	113.40
2	D	65	LYS	CA-CB-CG	5.11	124.64	113.40
2	D	92	HIS	CG-CD2-NE2	-5.10	99.51	109.20
2	D	88	LEU	CA-C-N	5.06	128.32	117.20
1	C	96	VAL	CG1-CB-CG2	-5.04	102.83	110.90
2	D	145	TYR	CA-C-N	-5.04	106.12	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	145	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1064	0	1060	26	0
1	C	1064	0	1060	23	0
2	B	1135	0	1134	28	0
2	D	1135	0	1134	24	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	4	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	104	0	0	4	0
5	B	143	0	0	0	0
5	C	135	0	0	2	0
5	D	192	0	0	3	0
All	All	5148	0	4508	90	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 10.

All (90) 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:22:GLU:HB2	2:B:117:ARG:HH21	1.42	0.83
2:D:89:SER:HB2	2:D:144:LYS:HB2	1.58	0.82
1:A:6:ASP:O	1:A:10:VAL:HG23	1.83	0.79
2:B:146:HIS:HB3	2:D:132:LYS:HG2	1.68	0.74
1:C:72:HIS:HB3	1:C:75:ASP:HB3	1.72	0.71
1:C:76:LEU:HB3	1:C:77:PRO:HD3	1.73	0.70
1:C:98:PHE:HD1	3:C:850:HEM:HBB2	1.62	0.63
2:B:22:GLU:HB2	2:B:117:ARG:NH2	2.11	0.63
2:D:91:LEU:HD23	2:D:92:HIS:CE1	2.39	0.58
2:D:98:VAL:HG13	3:D:950:HEM:HBC2	1.84	0.58
1:A:107:VAL:HG13	2:B:115:ALA:HB2	1.86	0.56
1:C:1:VAL:HG12	1:C:2:LEU:H	1.70	0.56
2:B:5:ALA:O	2:B:9:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:O	1:A:137:THR:HB	2.05	0.56
2:B:62:ALA:O	2:B:65:LYS:HG3	2.06	0.55
1:A:34:LEU:HD12	2:B:124:PRO:CB	2.36	0.55
1:A:122:HIS:HD2	2:B:30:ARG:HD3	1.71	0.55
1:C:21:ALA:HB1	1:C:63:ALA:HB1	1.89	0.55
1:C:103:HIS:HD2	5:C:862:HOH:O	1.88	0.55
2:D:89:SER:HB3	2:D:141:LEU:O	2.07	0.54
1:A:140:TYR:HB2	5:A:692:HOH:O	2.08	0.54
2:B:106:LEU:HD23	3:B:750:HEM:HAB	1.90	0.54
2:B:59:LYS:HD2	2:B:59:LYS:N	2.24	0.53
1:A:96:VAL:O	1:A:99:LYS:HG2	2.09	0.53
2:D:14:LEU:HD23	2:D:126:VAL:HG11	1.91	0.52
2:B:145:TYR:O	2:B:146:HIS:HD2	1.93	0.51
1:A:7:LYS:O	1:A:11:LYS:HG2	2.11	0.51
2:D:91:LEU:O	2:D:96:LEU:HG	2.11	0.50
1:A:127:LYS:HD3	1:C:141:ARG:HA	1.93	0.50
2:B:104:ARG:N	2:B:104:ARG:HD3	2.26	0.50
1:A:139:LYS:N	1:A:139:LYS:HD2	2.26	0.50
1:A:87:HIS:HB3	1:A:93:VAL:HG13	1.92	0.50
1:A:140:TYR:HB3	2:D:36:PRO:HG2	1.92	0.50
2:B:57:ASN:O	2:B:61:LYS:HG2	2.11	0.50
1:C:1:VAL:HG11	1:C:73:LEU:O	2.12	0.49
1:A:16:LYS:HG2	1:A:116:ASP:OD2	2.13	0.49
1:A:95:PRO:HD3	1:A:140:TYR:OH	2.12	0.49
1:A:68:LYS:O	1:A:72:HIS:HD2	1.97	0.48
2:D:123:ASN:OD1	2:D:126:VAL:HG23	2.14	0.48
1:C:132:VAL:O	1:C:136:LEU:HD12	2.15	0.47
2:D:141:LEU:CD1	3:D:950:HEM:HAB	2.44	0.47
1:C:68:LYS:HD2	5:C:910:HOH:O	2.15	0.47
1:C:40:LYS:HZ2	1:C:48:LEU:HD13	1.80	0.47
1:C:68:LYS:O	1:C:72:HIS:HD2	1.99	0.46
2:B:122:PHE:HA	2:B:126:VAL:HG21	1.98	0.46
1:C:98:PHE:CD1	3:C:850:HEM:HBB2	2.48	0.46
1:A:34:LEU:HD12	2:B:124:PRO:HB2	1.97	0.46
1:C:88:ALA:CB	1:C:139:LYS:HB2	2.45	0.46
2:D:20:VAL:HG22	2:D:68:LEU:HD23	1.98	0.46
2:D:91:LEU:HD22	3:D:950:HEM:HBA2	1.97	0.45
2:D:12:LEU:HD23	5:D:1137:HOH:O	2.15	0.45
2:D:26:GLU:O	2:D:30:ARG:HG3	2.15	0.45
2:B:71:PHE:CE1	2:B:137:VAL:HG21	2.52	0.45
2:B:3:LEU:HD12	2:B:8:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:O	1:C:109:LEU:HG	2.16	0.45
2:B:146:HIS:CE1	1:C:37:PRO:HG2	2.52	0.45
1:A:113:HIS:HB3	1:A:116:ASP:HB3	1.98	0.45
2:D:43:GLU:HG2	5:D:1051:HOH:O	2.17	0.44
2:D:2:HIS:HB2	5:D:1036:HOH:O	2.16	0.44
2:B:142:ALA:O	2:B:145:TYR:HB2	2.18	0.44
2:B:30:ARG:O	2:B:34:VAL:HG23	2.17	0.44
1:A:63:ALA:HA	1:A:66:LEU:HD12	2.00	0.43
2:B:145:TYR:O	2:B:146:HIS:CD2	2.71	0.43
2:D:57:ASN:HA	2:D:58:PRO:HD3	1.85	0.43
2:B:29:GLY:O	2:B:33:VAL:HG12	2.18	0.43
1:C:33:PHE:CE2	1:C:48:LEU:HD22	2.53	0.43
1:A:66:LEU:O	1:A:70:VAL:HG23	2.18	0.43
1:A:76:LEU:N	1:A:77:PRO:CD	2.82	0.42
1:C:2:LEU:HD21	1:C:131:ASN:ND2	2.33	0.42
1:C:72:HIS:N	1:C:72:HIS:CD2	2.88	0.42
2:D:14:LEU:CD2	2:D:126:VAL:HG11	2.49	0.42
1:C:103:HIS:HE1	2:D:131:GLN:OE1	2.02	0.42
1:C:94:ASP:HA	1:C:95:PRO:HD3	1.89	0.42
2:D:91:LEU:CD2	3:D:950:HEM:HBA2	2.50	0.42
2:B:92:HIS:CD2	2:B:96:LEU:HD12	2.55	0.41
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.03	0.41
1:C:41:THR:O	1:C:44:PRO:HD3	2.20	0.41
2:D:107:GLY:HA3	2:D:134:VAL:HG13	2.03	0.41
5:A:654:HOH:O	2:D:41:PHE:HZ	2.03	0.41
2:B:14:LEU:HD22	2:B:130:PHE:CE2	2.55	0.41
1:A:34:LEU:HD12	2:B:124:PRO:HB3	2.03	0.41
1:A:60:GLN:HG2	5:A:749:HOH:O	2.21	0.40
2:D:65:LYS:HE3	2:D:65:LYS:HB2	1.59	0.40
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.57	0.40
1:C:2:LEU:HB3	1:C:6:ASP:HB2	2.01	0.40
2:D:42:PHE:O	2:D:45:PHE:HB2	2.21	0.40
1:A:139:LYS:HA	5:A:718:HOH:O	2.21	0.40
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.97	0.40
2:B:56:GLY:H	2:B:61:LYS:HD3	1.86	0.40
2:B:68:LEU:HD22	2:B:68:LEU:HA	1.84	0.40

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	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	11	3
1	C	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	22	10
2	B	144/146 (99%)	136 (94%)	6 (4%)	2 (1%)	11	3
2	D	144/146 (99%)	132 (92%)	12 (8%)	0	100	100
All	All	566/574 (99%)	533 (94%)	28 (5%)	5 (1%)	17	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77	HIS
2	B	145	TYR
1	A	43	PHE
1	A	37	PRO
1	C	43	PHE

### 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	111/111 (100%)	95 (86%)	16 (14%)	3	0
1	C	111/111 (100%)	99 (89%)	12 (11%)	6	1
2	B	119/119 (100%)	96 (81%)	23 (19%)	1	0
2	D	119/119 (100%)	106 (89%)	13 (11%)	6	1
All	All	460/460 (100%)	396 (86%)	64 (14%)	3	1

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	53	ASP
1	A	56	LYS
1	A	86	LEU
1	A	89	HIS
1	A	90	LYS
1	A	92	ARG
1	A	95	PRO
1	A	99	LYS
1	A	105	LEU
1	A	120	SER
1	A	122	HIS
1	A	129	LEU
1	A	131	ASN
1	A	137	THR
1	A	139	LYS
2	B	3	LEU
2	B	12	LEU
2	B	23	VAL
2	B	33	VAL
2	B	40	ARG
2	B	43	GLU
2	B	65	LYS
2	B	67	VAL
2	B	68	LEU
2	B	69	GLN
2	B	75	LEU
2	B	76	LYS
2	B	78	LEU
2	B	82	LYS
2	B	91	LEU
2	B	101	GLU
2	B	104	ARG
2	B	110	ILE
2	B	112	VAL
2	B	117	ARG
2	B	132	LYS
2	B	134	VAL
2	B	144	LYS
1	C	2	LEU
1	C	16	LYS
1	C	34	LEU

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Mol	Chain	Res	Type
1	C	52	SER
1	C	72	HIS
1	C	92	ARG
1	C	106	LEU
1	C	115	ASP
1	C	116	ASP
1	C	131	ASN
1	C	139	LYS
1	C	141	ARG
2	D	6	GLU
2	D	30	ARG
2	D	40	ARG
2	D	59	LYS
2	D	68	LEU
2	D	71	PHE
2	D	76	LYS
2	D	78	LEU
2	D	82	LYS
2	D	89	SER
2	D	104	ARG
2	D	144	LYS
2	D	146	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	89	HIS
1	A	103	HIS
1	A	122	HIS
2	B	146	HIS
1	C	72	HIS
1	C	103	HIS
1	C	131	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
3	HEM	D	950	2,5	27,50,50	2.14	12 (44%)	17,82,82	1.18	2 (11%)
4	OXY	C	851	3	1,1,1	0.11	0	-		
4	OXY	B	751	3	1,1,1	0.09	0	-		
3	HEM	B	750	2,4	27,50,50	1.61	8 (29%)	17,82,82	1.73	7 (41%)
3	HEM	A	650	1,5	27,50,50	2.03	8 (29%)	17,82,82	1.63	2 (11%)
3	HEM	C	850	1,4	27,50,50	1.97	8 (29%)	17,82,82	1.70	4 (23%)

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
3	HEM	C	850	1,4	-	0/6/54/54	-
3	HEM	A	650	1,5	-	0/6/54/54	-
3	HEM	B	750	2,4	-	0/6/54/54	-
3	HEM	D	950	2,5	-	0/6/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	950	HEM	C3C-C2C	-5.37	1.32	1.40
3	A	650	HEM	C3C-C2C	-5.01	1.33	1.40
3	C	850	HEM	C3C-C2C	-4.31	1.34	1.40
3	A	650	HEM	C1D-ND	3.70	1.43	1.36
3	A	650	HEM	C3C-CAC	-3.62	1.40	1.47
3	C	850	HEM	C3C-CAC	-3.52	1.40	1.47
3	C	850	HEM	C3B-C2B	-3.45	1.35	1.40
3	A	650	HEM	C3B-CAB	-3.34	1.41	1.47
3	D	950	HEM	C3B-CAB	-3.23	1.41	1.47
3	C	850	HEM	CBB-CAB	3.22	1.50	1.29
3	B	750	HEM	C3B-CAB	-3.21	1.41	1.47
3	C	850	HEM	CBC-CAC	3.15	1.50	1.29
3	D	950	HEM	C3B-C2B	-3.09	1.36	1.40
3	D	950	HEM	C1A-NA	3.08	1.42	1.36
3	D	950	HEM	C3C-CAC	-3.06	1.41	1.47
3	B	750	HEM	C1C-C2C	3.05	1.49	1.42
3	A	650	HEM	CBC-CAC	2.94	1.48	1.29
3	D	950	HEM	CBC-CAC	2.93	1.48	1.29
3	C	850	HEM	C3B-CAB	-2.79	1.42	1.47
3	D	950	HEM	C4D-C3D	2.75	1.48	1.42
3	D	950	HEM	CBB-CAB	2.70	1.47	1.29
3	B	750	HEM	C3C-CAC	-2.66	1.42	1.47
3	B	750	HEM	C1D-ND	2.65	1.41	1.36
3	C	850	HEM	C1C-C2C	2.63	1.48	1.42
3	A	650	HEM	C3B-C2B	-2.50	1.36	1.40
3	A	650	HEM	CBB-CAB	2.46	1.45	1.29
3	D	950	HEM	C1B-C2B	2.41	1.48	1.42
3	C	850	HEM	C4A-NA	2.40	1.41	1.36
3	A	650	HEM	C4D-C3D	2.39	1.48	1.42
3	D	950	HEM	CAD-C3D	2.31	1.56	1.52
3	B	750	HEM	CBB-CAB	2.28	1.44	1.29
3	B	750	HEM	C1A-NA	2.22	1.40	1.36
3	D	950	HEM	C4B-NB	2.07	1.40	1.36
3	B	750	HEM	C3C-C2C	-2.04	1.37	1.40
3	D	950	HEM	C4A-NA	2.03	1.40	1.36
3	B	750	HEM	CBC-CAC	2.01	1.42	1.29

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	850	HEM	CAA-CBA-CGA	-3.72	106.42	112.67
3	A	650	HEM	C1D-C2D-C3D	-3.57	104.51	107.00
3	C	850	HEM	C1D-C2D-C3D	-3.38	104.64	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	950	HEM	CAD-CBD-CGD	2.82	117.40	112.67
3	B	750	HEM	C4C-C3C-C2C	-2.74	104.99	106.90
3	B	750	HEM	CAD-CBD-CGD	-2.70	108.14	112.67
3	A	650	HEM	CAD-CBD-CGD	-2.42	108.61	112.67
3	B	750	HEM	C1D-C2D-C3D	-2.40	105.33	107.00
3	C	850	HEM	C4A-C3A-C2A	-2.38	105.34	107.00
3	B	750	HEM	CMB-C2B-C3B	2.26	128.91	124.68
3	B	750	HEM	C4A-C3A-C2A	2.24	108.56	107.00
3	B	750	HEM	CAA-CBA-CGA	2.11	116.22	112.67
3	D	950	HEM	C3B-C4B-NB	2.09	111.91	109.21
3	C	850	HEM	CBD-CAD-C3D	-2.02	108.75	112.48
3	B	750	HEM	C3B-C4B-NB	2.02	111.82	109.21

There are no chirality outliers.

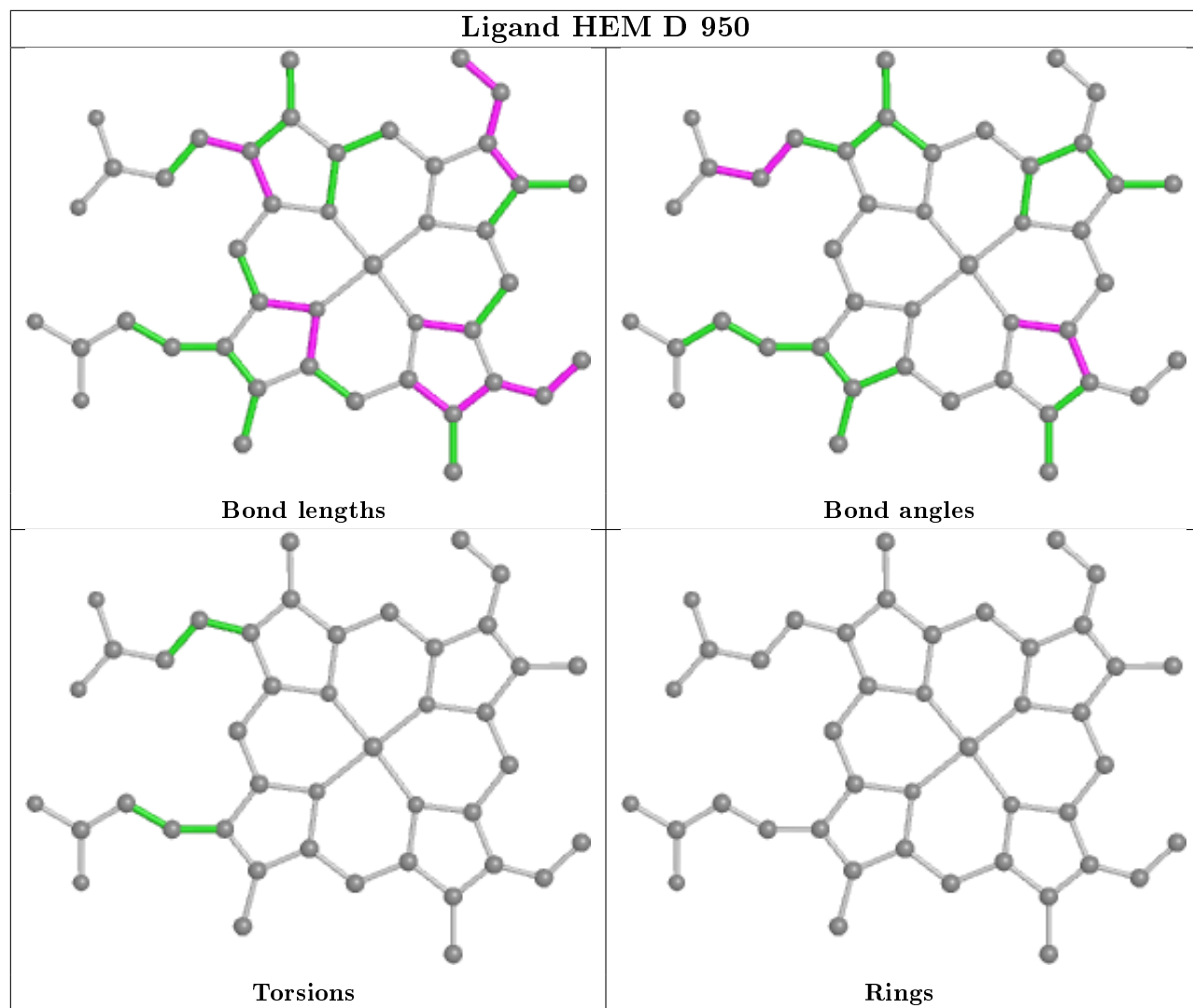
There are no torsion outliers.

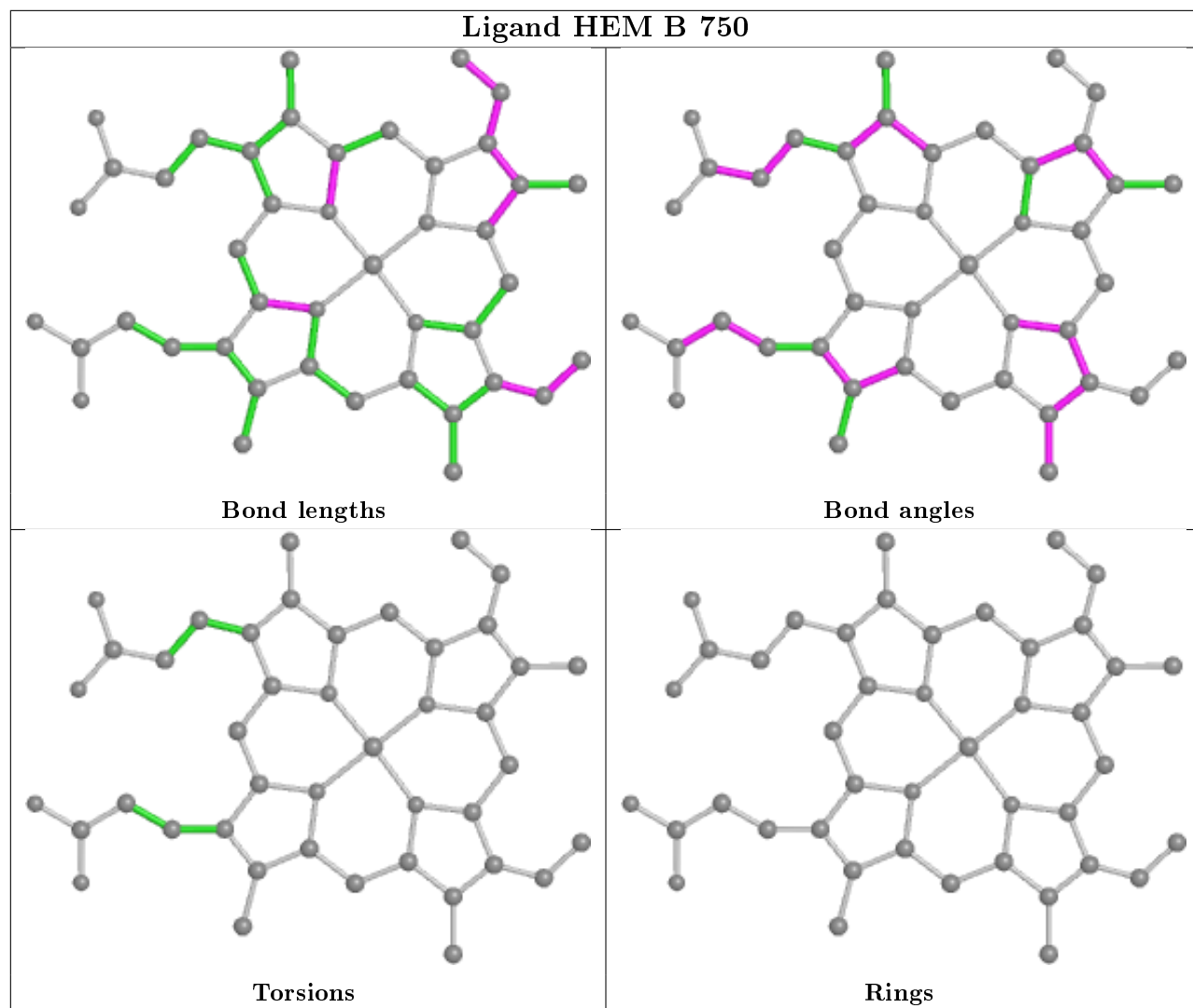
There are no ring outliers.

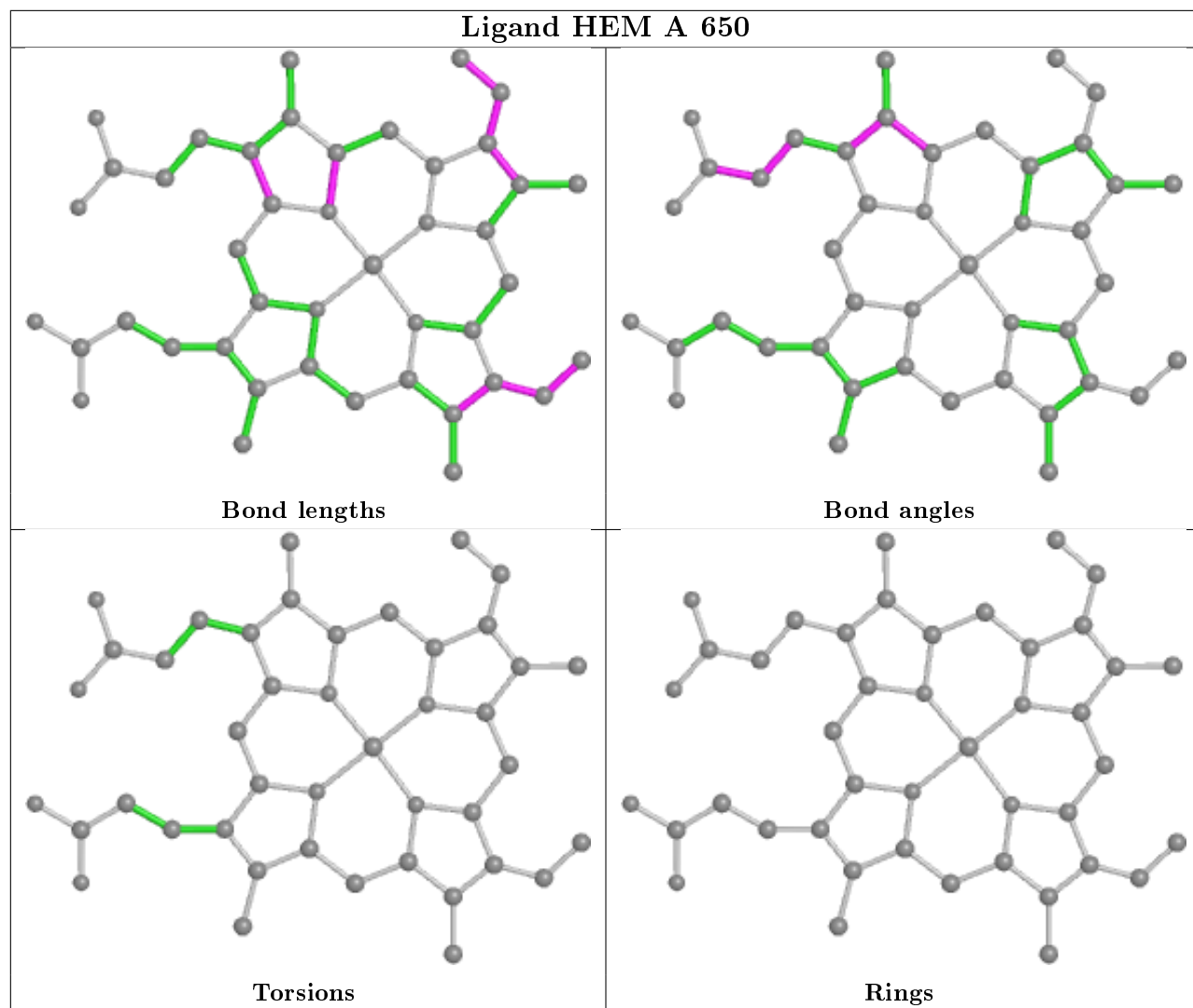
3 monomers are involved in 7 short contacts:

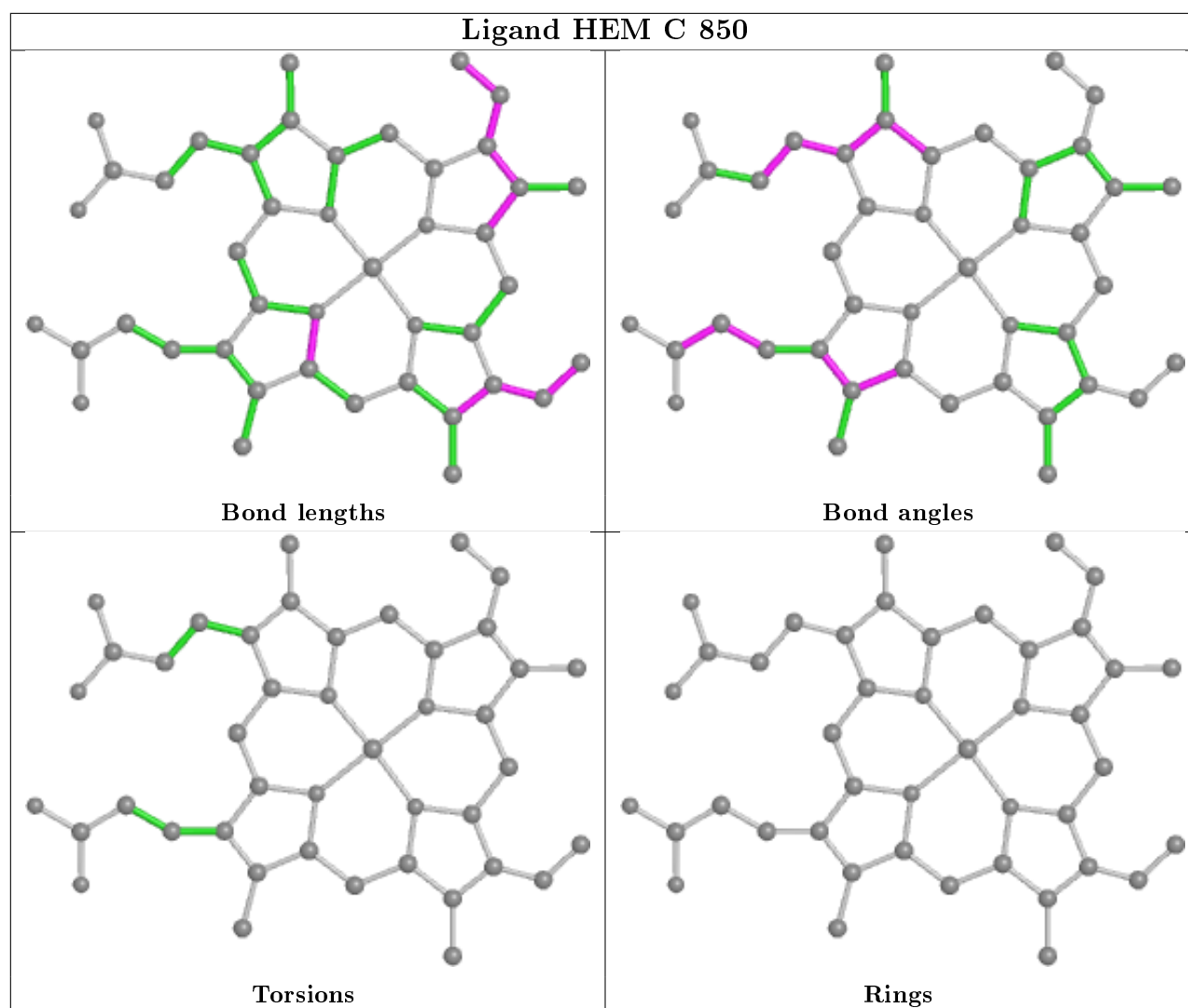
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	950	HEM	4	0
3	B	750	HEM	1	0
3	C	850	HEM	2	0

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.









## 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	141/141 (100%)	-0.38	2 (1%) 75 72	17, 30, 49, 61	0
1	C	141/141 (100%)	-0.39	2 (1%) 75 72	16, 27, 44, 62	0
2	B	146/146 (100%)	-0.20	1 (0%) 87 86	18, 35, 53, 61	0
2	D	146/146 (100%)	-0.32	2 (1%) 75 72	11, 32, 49, 66	0
All	All	574/574 (100%)	-0.32	7 (1%) 79 76	11, 32, 50, 66	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	146	HIS	4.1
1	C	1	VAL	3.6
1	A	141	ARG	2.7
2	D	1	VAL	2.5
1	C	75	ASP	2.4
2	B	146	HIS	2.3
1	A	139	LYS	2.1

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

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

### 6.3 Carbohydrates ⓘ

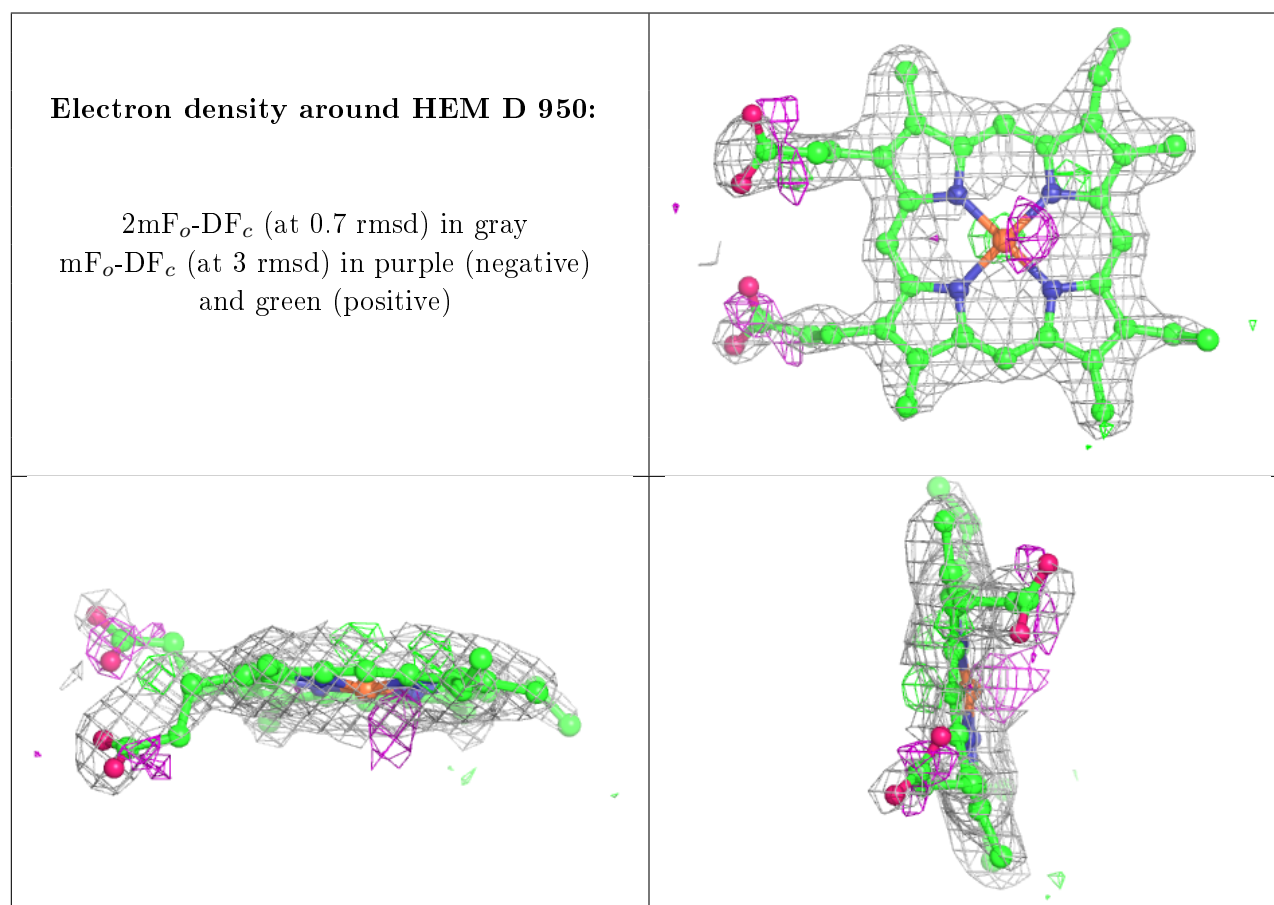
There are no carbohydrates in this entry.

## 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.

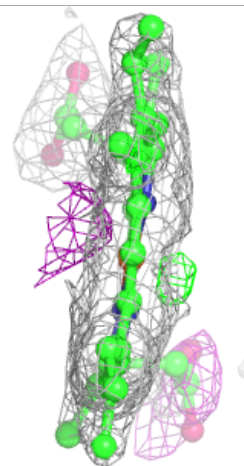
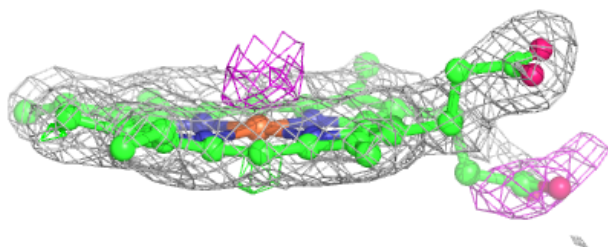
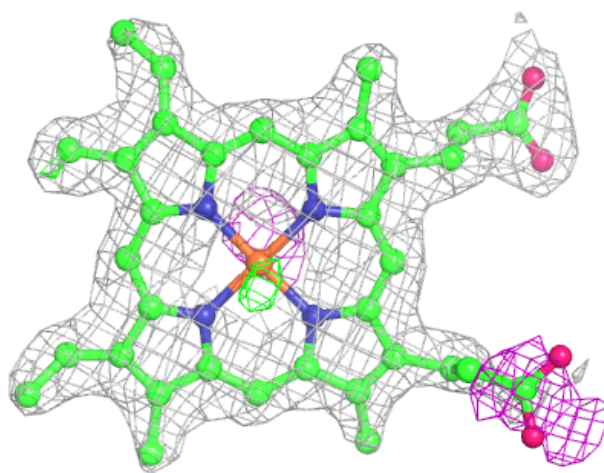
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	OXY	B	751	2/2	0.93	0.26	40,40,40,41	0
3	HEM	D	950	43/43	0.94	0.15	36,45,60,65	0
3	HEM	B	750	43/43	0.96	0.12	29,36,54,65	0
3	HEM	C	850	43/43	0.97	0.08	11,26,44,52	0
3	HEM	A	650	43/43	0.97	0.10	19,28,39,42	0
4	OXY	C	851	2/2	0.98	0.15	36,36,36,37	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.



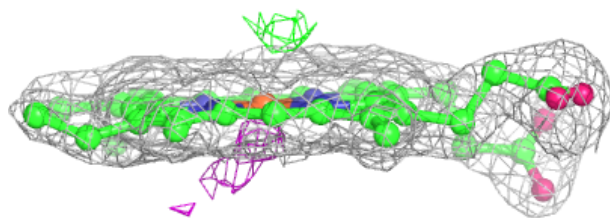
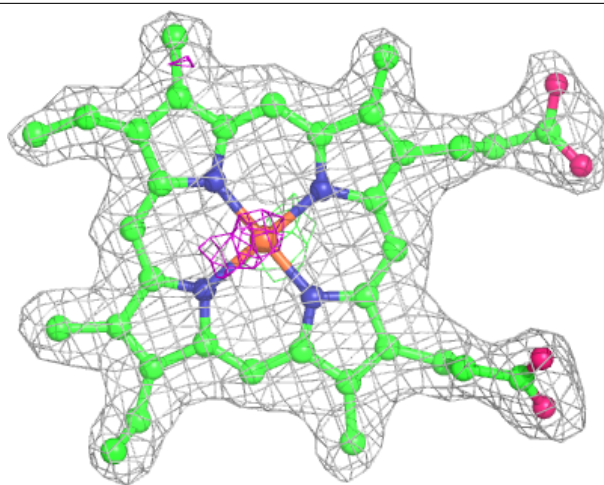
**Electron density around HEM B 750:**

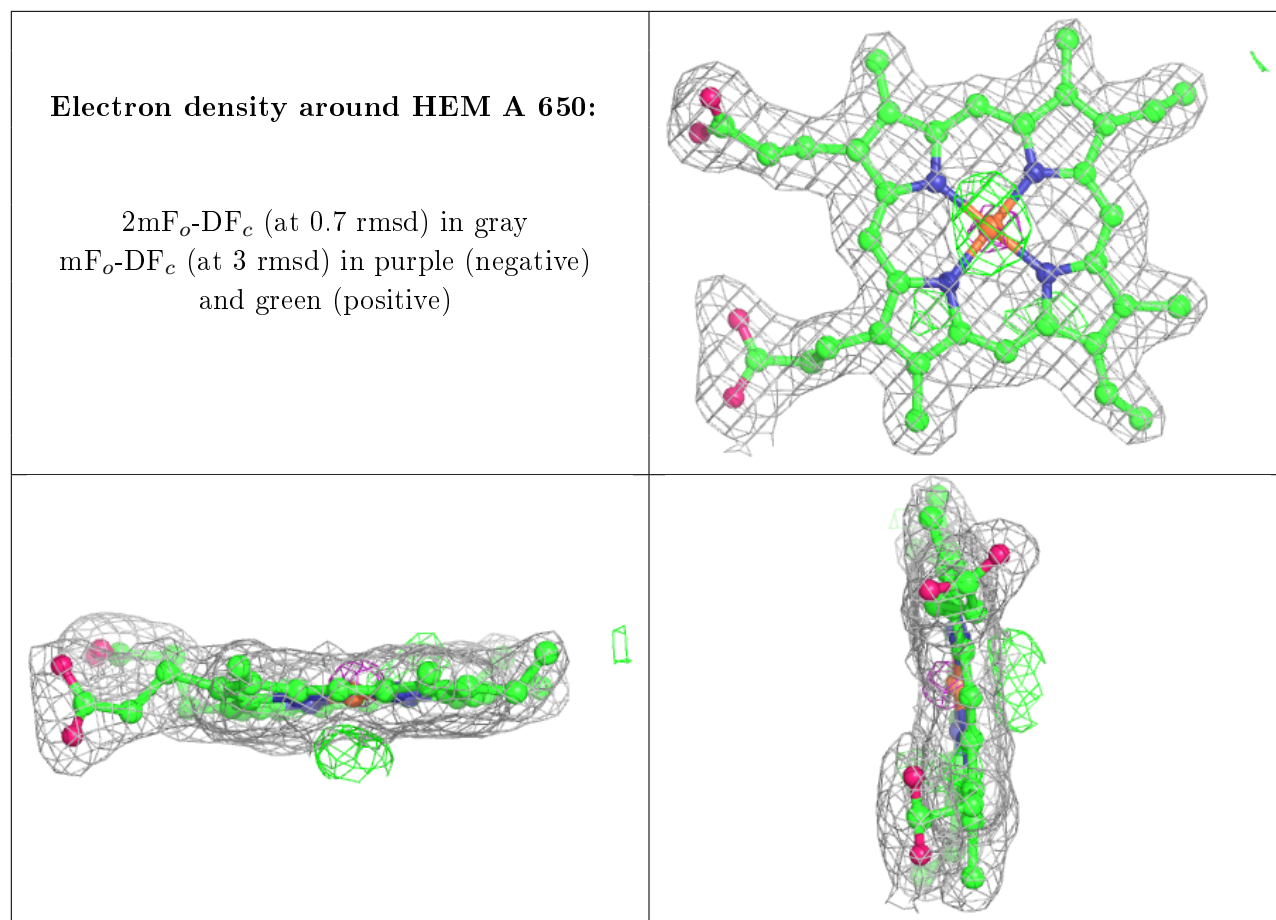
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 850:**

$2mF_o-DF_c$  (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.