Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:50 am BST

PDB ID	:	2H8F
Title	:	Crystal structure of deoxy hemoglobin from Trematomus bernacchii at pH 6.2
Authors	:	Mazzarella, L.; Vergara, A.; Vitagliano, L.; Merlino, A.; Bonomi, G.; Scala, S.; Verde, C.; di Prisco, G.
Deposited on	:	2006-06-07
Resolution	:	1.30 Å(reported)

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

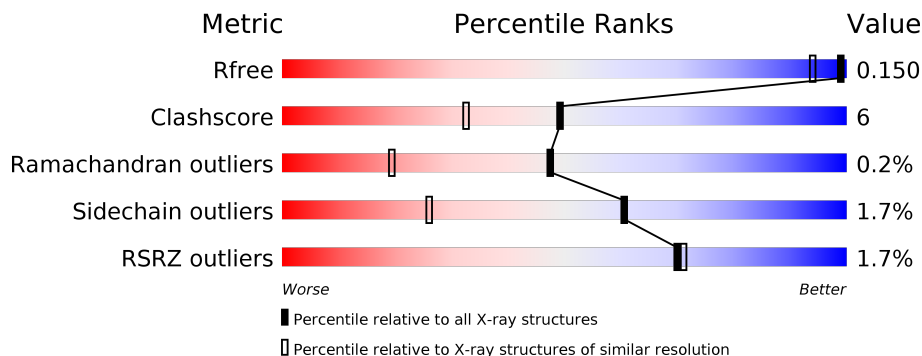|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 >=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 <=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	143	2% / 73% / 23% / •
1	C	143	% / 82% / 17% / •
2	B	146	% / 77% / 21% / •
2	D	146	3% / 74% / 25% / ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5191 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.
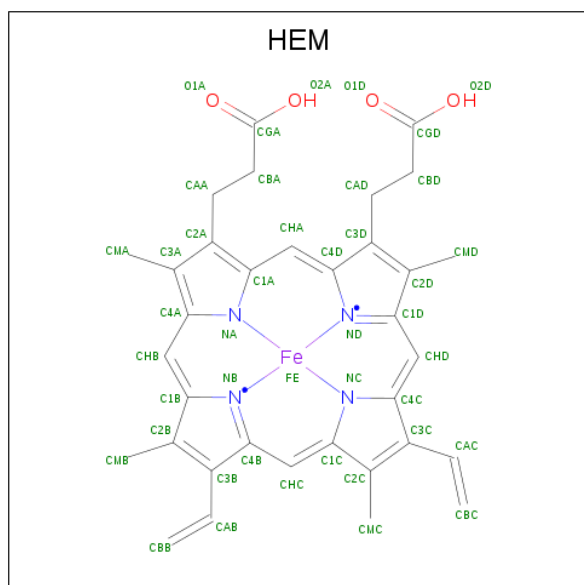
- Molecule 1 is a protein called Hemoglobin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total 1107	C 713	N 190	O 199	S 5	0	2	0
1	C	143	Total 1107	C 713	N 190	O 199	S 5	0	1	0

- Molecule 2 is a protein called Hemoglobin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total 1147	C 733	N 196	O 212	S 6	0	3	0
2	D	146	Total 1147	C 733	N 196	O 212	S 6	0	4	0

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

HEM

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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total 127	O 127	0	0
4	B	118	Total 118	O 118	0	0
4	C	148	Total 148	O 148	0	0
4	D	118	Total 118	O 118	0	0

3 Residue-property plots ⓘ

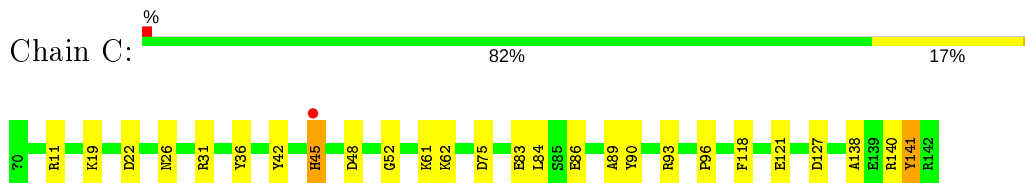These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.
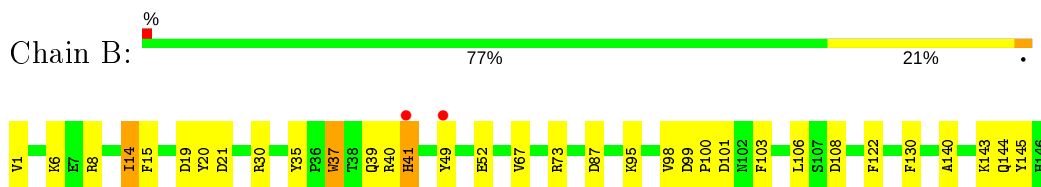
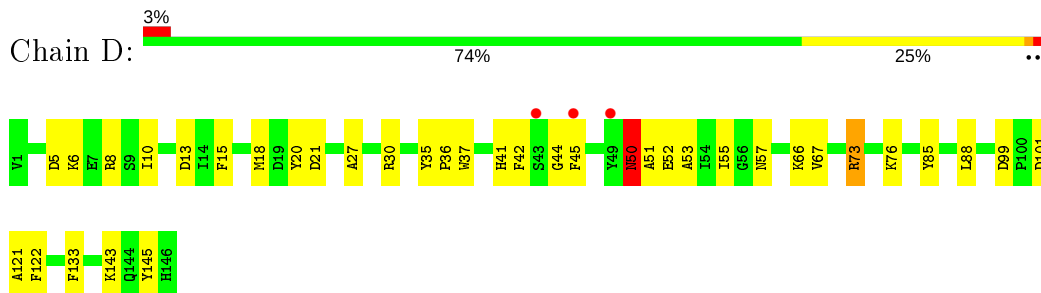- Molecule 1: Hemoglobin alpha subunit

- Molecule 1: Hemoglobin alpha subunit

- Molecule 2: Hemoglobin beta subunit

- Molecule 2: Hemoglobin beta subunit

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.85Å 95.04Å 61.82Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	19.83 – 1.30 19.83 – 1.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.83-1.30) 83.8 (19.83-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 1.29Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.151 , 0.172 0.148 , 0.150	Depositor DCC
R_{free} test set	7541 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 43.0	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.044 for -l,k,h 0.044 for -h,-k,l 0.346 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HEM, ACE

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	0.89	0/1135	1.78	24/1534 (1.6%)
1	C	0.94	0/1135	1.77	27/1534 (1.8%)
2	B	0.94	1/1186 (0.1%)	1.81	29/1605 (1.8%)
2	D	0.89	1/1186 (0.1%)	1.97	30/1605 (1.9%)
All	All	0.91	2/4642 (0.0%)	1.84	110/6278 (1.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	ARG	CZ-NH2	6.30	1.41	1.33
2	B	8	ARG	CZ-NH2	5.42	1.40	1.33

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	8	ARG	NE-CZ-NH1	33.59	137.10	120.30
2	D	8	ARG	NE-CZ-NH2	-19.81	110.39	120.30
2	B	8	ARG	NE-CZ-NH1	19.63	130.11	120.30
1	C	31	ARG	NE-CZ-NH1	17.08	128.84	120.30
2	D	21	ASP	CB-CG-OD1	15.43	132.19	118.30
2	B	40	ARG	NE-CZ-NH2	-15.14	112.73	120.30
1	A	31	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	A	22	ASP	CB-CG-OD1	13.18	130.16	118.30
1	C	90	TYR	CB-CG-CD1	13.11	128.86	121.00
2	D	30	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	A	90[B]	TYR	CB-CG-CD1	12.30	128.38	121.00
2	D	101	ASP	CB-CG-OD2	12.11	129.20	118.30
2	B	30	ARG	NE-CZ-NH1	11.83	126.21	120.30
1	A	31	ARG	NE-CZ-NH2	-11.73	114.44	120.30
1	A	142	ARG	NE-CZ-NH1	11.42	126.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	TYR	CB-CG-CD2	-11.29	114.23	121.00
1	C	140	ARG	NE-CZ-NH1	-10.69	114.96	120.30
1	A	90[B]	TYR	CB-CG-CD2	-9.86	115.08	121.00
1	C	31	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	93	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	B	99	ASP	CB-CG-OD2	-9.25	109.98	118.30
2	D	101	ASP	CB-CG-OD1	-9.24	109.99	118.30
1	C	75	ASP	CB-CG-OD2	9.09	126.48	118.30
1	A	36	TYR	CB-CG-CD1	8.93	126.36	121.00
1	C	42	TYR	CB-CG-CD2	-8.79	115.73	121.00
2	B	30	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	141	TYR	CZ-CE2-CD2	-8.40	112.24	119.80
2	B	35	TYR	CB-CG-CD2	-8.35	115.99	121.00
2	B	101	ASP	CB-CG-OD2	8.28	125.75	118.30
1	C	11	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	121	GLU	CG-CD-OE2	7.97	134.24	118.30
1	A	76	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	11	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	22	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	27	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	142	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	B	130	PHE	CB-CG-CD1	7.09	125.76	120.80
1	C	121	GLU	OE1-CD-OE2	-7.06	114.83	123.30
2	D	35	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	D	18	MET	CG-SD-CE	6.93	111.28	100.20
2	B	40	ARG	NH1-CZ-NH2	6.89	126.98	119.40
2	B	21	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	36	TYR	CG-CD1-CE1	6.67	126.64	121.30
1	C	36	TYR	CB-CG-CD1	6.65	124.99	121.00
1	C	36	TYR	CD1-CE1-CZ	-6.63	113.83	119.80
2	B	8	ARG	NH1-CZ-NH2	-6.63	112.10	119.40
2	D	5	ASP	CB-CG-OD1	6.63	124.27	118.30
2	B	103	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	A	22	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	A	121	GLU	OE1-CD-OE2	-6.53	115.47	123.30
2	D	30	ARG	NH1-CZ-NH2	-6.45	112.31	119.40
2	B	108	ASP	CB-CG-OD1	6.40	124.06	118.30
2	B	73	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	86	GLU	OE1-CD-OE2	-6.38	115.65	123.30
2	D	8	ARG	NH1-CZ-NH2	-6.27	112.51	119.40
2	B	15	PHE	CB-CG-CD1	-6.25	116.43	120.80
2	D	122	PHE	CB-CG-CD2	-6.23	116.44	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	PHE	CB-CG-CD1	-6.13	116.51	120.80
1	A	49	VAL	C-N-CA	6.08	136.90	121.70
1	C	96[A]	PRO	O-C-N	-6.04	113.03	122.70
1	C	96[B]	PRO	O-C-N	-6.04	113.03	122.70
2	B	87	ASP	CB-CG-OD1	6.02	123.72	118.30
2	D	27	ALA	O-C-N	-5.96	113.16	122.70
1	C	118	PHE	CB-CG-CD2	-5.96	116.63	120.80
2	D	36	PRO	O-C-N	-5.95	113.19	122.70
2	D	122	PHE	CZ-CE2-CD2	5.90	127.18	120.10
2	D	99	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	121	GLU	CG-CD-OE2	5.85	130.01	118.30
1	C	75	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	A	99	PHE	CG-CD2-CE2	-5.84	114.38	120.80
2	D	121	ALA	N-CA-CB	5.84	118.27	110.10
2	D	85	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	C	11	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	31	ARG	CD-NE-CZ	-5.79	115.50	123.60
1	A	0	ACE	O-C-N	-5.74	113.52	122.70
2	B	49	TYR	CG-CD2-CE2	-5.73	116.72	121.30
2	B	108	ASP	CB-CG-OD2	-5.69	113.18	118.30
2	B	8	ARG	CD-NE-CZ	-5.64	115.70	123.60
1	C	141	TYR	CG-CD1-CE1	-5.64	116.78	121.30
2	D	15	PHE	CB-CG-CD2	-5.63	116.86	120.80
2	B	14	ILE	O-C-N	-5.59	113.75	122.70
2	D	73	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	117	GLU	OE1-CD-OE2	-5.57	116.62	123.30
2	D	21	ASP	OD1-CG-OD2	-5.56	112.73	123.30
2	D	13	ASP	CA-CB-CG	5.55	125.62	113.40
1	A	117	GLU	CG-CD-OE1	5.55	129.40	118.30
2	B	20	TYR	CD1-CE1-CZ	-5.37	114.96	119.80
2	B	140	ALA	O-C-N	-5.35	114.14	122.70
2	D	108	ASP	CB-CG-OD1	5.35	123.11	118.30
2	B	19	ASP	CB-CG-OD1	5.33	123.10	118.30
2	B	1	VAL	O-C-N	5.32	131.21	122.70
2	D	41	HIS	CA-CB-CG	-5.31	104.57	113.60
2	B	41	HIS	CA-CB-CG	-5.31	104.58	113.60
1	C	11	ARG	CD-NE-CZ	5.29	131.01	123.60
2	D	133	PHE	CG-CD1-CE1	-5.25	115.03	120.80
1	C	141	TYR	CG-CD2-CE2	5.24	125.49	121.30
1	A	11	ARG	CD-NE-CZ	5.23	130.92	123.60
2	B	21	ASP	CB-CG-OD2	-5.16	113.65	118.30
2	D	37	TRP	CD1-NE1-CE2	-5.16	104.36	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	20	TYR	CD1-CE1-CZ	-5.13	115.19	119.80
2	D	50	ASN	CA-CB-CG	-5.11	102.15	113.40
1	A	70	ALA	O-C-N	-5.09	114.56	122.70
1	A	114	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	C	127	ASP	CB-CG-OD1	5.07	122.86	118.30
2	B	37	TRP	CE3-CZ3-CH2	-5.06	115.64	121.20
1	C	19	LYS	CD-CE-NZ	5.04	123.29	111.70
1	C	118	PHE	CD1-CE1-CZ	-5.04	114.06	120.10
2	B	8	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	D	145	TYR	CG-CD1-CE1	-5.04	117.27	121.30
2	D	122	PHE	CB-CG-CD1	5.01	124.31	120.80

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	1107	0	1139	17	0
1	C	1107	0	1141	16	0
2	B	1147	0	1130	9	0
2	D	1147	0	1128	15	0
3	A	43	0	30	2	0
3	B	43	0	30	0	0
3	C	43	0	30	2	0
3	D	43	0	30	3	0
4	A	127	0	0	2	0
4	B	118	0	0	1	0
4	C	148	0	0	5	0
4	D	118	0	0	2	0
All	All	5191	0	4658	55	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.

All (55) 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:143:LYS:HD3	2:B:144:GLN:OE1	1.84	0.78
2:D:66:LYS:HE3	3:D:800:HEM:HAA1	1.72	0.71
2:D:50:ASN:OD1	2:D:52:GLU:HB2	1.92	0.68
1:C:61:LYS:HE3	4:C:1302:HOH:O	1.96	0.65
1:C:83:GLU:HG3	4:C:1184:HOH:O	1.96	0.64
1:C:26:ASN:HD21	1:C:52:GLY:HA2	1.60	0.64
1:C:45:HIS:CD2	1:C:45:HIS:H	2.17	0.62
2:B:41:HIS:CE1	2:B:98:VAL:HA	2.36	0.61
1:C:62:LYS:HE2	4:C:1436:HOH:O	2.02	0.59
1:A:26:ASN:HD22	1:A:56:ILE:HG22	1.70	0.56
2:D:66:LYS:HE3	3:D:800:HEM:CAA	2.35	0.56
2:D:51:ALA:O	2:D:55:ILE:HG13	2.06	0.55
2:B:37:TRP:HA	1:C:93:ARG:HD2	1.86	0.55
1:A:61:LYS:HG3	4:A:1107:HOH:O	2.07	0.54
2:D:44:GLY:HA2	4:D:1476:HOH:O	2.07	0.54
1:A:26:ASN:HD21	1:A:52:GLY:HA2	1.73	0.53
2:D:50:ASN:HB3	2:D:53:ALA:CB	2.39	0.52
1:C:93:ARG:HD3	4:C:1491:HOH:O	2.09	0.52
1:A:97:ALA:HA	1:A:100:LYS:HE2	1.93	0.51
1:A:88:HIS:HA	1:A:92:LEU:HB2	1.92	0.51
2:B:100[B]:PRO:HG3	2:B:145:TYR:CZ	2.46	0.51
1:A:45:HIS:H	1:A:45:HIS:CD2	2.29	0.50
2:D:143:LYS:HD2	4:D:1475:HOH:O	2.12	0.49
1:A:62:LYS:HD2	3:A:200:HEM:HAA1	1.94	0.49
2:D:6:LYS:HE2	2:D:10:ILE:HD11	1.94	0.49
1:A:138:ALA:HA	1:A:141:TYR:CD1	2.48	0.48
1:A:62:LYS:HD2	3:A:200:HEM:CAA	2.43	0.48
1:A:87:GLN:HE21	1:A:87:GLN:HA	1.78	0.48
1:A:49:VAL:O	1:A:49:VAL:HG12	2.13	0.47
1:A:29:LEU:HD12	1:A:60:GLY:HA2	1.97	0.46
2:B:14:ILE:HG13	4:B:1376:HOH:O	2.14	0.46
1:C:138:ALA:HA	1:C:141:TYR:CD1	2.50	0.46
2:D:50:ASN:HB3	2:D:53:ALA:HB2	1.98	0.46
2:D:67:VAL:HG13	3:D:800:HEM:C2B	2.51	0.45
1:A:22:ASP:OD2	1:A:61:LYS:NZ	2.50	0.45
1:A:11:ARG:NH1	4:A:1511:HOH:O	2.46	0.44
1:A:46:TRP:HZ3	1:A:56:ILE:HD13	1.83	0.44
1:A:34:VAL:CG2	1:A:51:PRO:HG3	2.48	0.43
1:C:89:ALA:O	1:C:93:ARG:HD3	2.18	0.43
1:C:62:LYS:HD3	3:C:600:HEM:HBA2	2.01	0.43
2:D:53:ALA:O	2:D:57:ASN:HB2	2.19	0.42
1:C:93:ARG:NH2	4:C:1208:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:HD3	3:C:600:HEM:CGA	2.50	0.42
1:C:83:GLU:HG3	1:C:83:GLU:H	1.49	0.42
2:B:95:LYS:HA	2:B:95:LYS:HD3	1.94	0.42
1:A:29:LEU:HD13	1:A:59:HIS:CD2	2.55	0.41
2:B:67:VAL:HG11	2:B:106:LEU:HD21	2.01	0.41
2:B:100[B]:PRO:HG3	2:B:145:TYR:CE2	2.55	0.41
2:D:73:ARG:CZ	2:D:88:LEU:HD11	2.51	0.41
2:D:76:LYS:HG2	2:D:76:LYS:O	2.21	0.41
1:C:48:ASP:OD1	1:C:48:ASP:N	2.55	0.40
1:C:84:LEU:HD23	1:C:84:LEU:HA	1.91	0.40
2:B:39:GLN:OE1	1:C:93:ARG:NH2	2.55	0.40
2:D:42:PHE:O	2:D:45:PHE:HB2	2.21	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	142/143 (99%)	139 (98%)	3 (2%)	0	100	100
1	C	142/143 (99%)	139 (98%)	3 (2%)	0	100	100
2	B	147/146 (101%)	147 (100%)	0	0	100	100
2	D	147/146 (101%)	143 (97%)	3 (2%)	1 (1%)	22	3
All	All	578/578 (100%)	568 (98%)	9 (2%)	1 (0%)	47	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	50	ASN

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	120/119 (101%)	115 (96%)	5 (4%)	30	2
1	C	120/119 (101%)	119 (99%)	1 (1%)	81	58
2	B	123/120 (102%)	121 (98%)	2 (2%)	62	28
2	D	123/120 (102%)	123 (100%)	0	100	100
All	All	486/478 (102%)	478 (98%)	8 (2%)	60	28

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	45	HIS
1	A	87	GLN
1	A	91	LYS
1	A	116	LYS
2	B	6	LYS
2	B	52	GLU
1	C	45	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	45	HIS
1	A	59	HIS
1	A	87	GLN
2	B	17	HIS
2	B	102	ASN
1	C	26	ASN
2	D	17	HIS
2	D	102	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)

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)

4 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	C	600	1	27,50,50	1.55	5 (18%)	17,82,82	1.87	7 (41%)
3	HEM	B	400	2	27,50,50	2.09	6 (22%)	17,82,82	2.38	6 (35%)
3	HEM	A	200	1	27,50,50	1.67	7 (25%)	17,82,82	1.83	4 (23%)
3	HEM	D	800	2	27,50,50	1.82	6 (22%)	17,82,82	2.17	9 (52%)

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	600	1	-	0/6/54/54	-
3	HEM	B	400	2	-	0/6/54/54	-
3	HEM	A	200	1	-	0/6/54/54	-
3	HEM	D	800	2	-	0/6/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	HEM	C3C-C2C	-6.50	1.31	1.40
3	D	800	HEM	C3C-C2C	-4.79	1.33	1.40
3	B	400	HEM	C3B-C2B	-4.56	1.34	1.40
3	A	200	HEM	C3B-C2B	-3.98	1.34	1.40
3	B	400	HEM	CAA-C2A	3.62	1.57	1.52
3	C	600	HEM	CAD-C3D	3.20	1.57	1.52
3	D	800	HEM	C3B-CAB	3.14	1.54	1.47
3	D	800	HEM	C3B-C2B	-3.13	1.36	1.40
3	A	200	HEM	C3C-C2C	-3.11	1.36	1.40
3	A	200	HEM	CMB-C2B	3.07	1.58	1.51
3	D	800	HEM	C3C-CAC	3.05	1.54	1.47
3	C	600	HEM	C3C-C2C	-2.72	1.36	1.40
3	B	400	HEM	C3C-CAC	2.65	1.53	1.47
3	B	400	HEM	C3B-CAB	2.58	1.53	1.47
3	C	600	HEM	C3B-C2B	-2.56	1.36	1.40
3	C	600	HEM	CAA-C2A	2.38	1.55	1.52
3	D	800	HEM	CAD-C3D	2.31	1.56	1.52
3	A	200	HEM	CAD-C3D	2.26	1.56	1.52
3	A	200	HEM	C4A-NA	2.20	1.40	1.36
3	A	200	HEM	C3C-CAC	2.19	1.52	1.47
3	C	600	HEM	C3C-CAC	2.16	1.52	1.47
3	D	800	HEM	CAA-C2A	2.15	1.55	1.52
3	A	200	HEM	CMD-C2D	2.05	1.55	1.51
3	B	400	HEM	C1A-NA	2.02	1.40	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	HEM	CMA-C3A-C4A	-5.53	119.97	128.46
3	A	200	HEM	CMD-C2D-C1D	-4.13	122.12	128.46
3	B	400	HEM	CMA-C3A-C2A	4.03	132.54	124.94
3	D	800	HEM	CMA-C3A-C4A	-3.96	122.38	128.46
3	A	200	HEM	CBA-CAA-C2A	3.63	119.19	112.49
3	B	400	HEM	CAA-CBA-CGA	3.63	118.77	112.67
3	C	600	HEM	CMA-C3A-C4A	-3.30	123.39	128.46
3	D	800	HEM	CBA-CAA-C2A	3.25	118.48	112.49
3	C	600	HEM	CMD-C2D-C1D	-3.21	123.53	128.46
3	A	200	HEM	CMA-C3A-C4A	-3.13	123.65	128.46
3	B	400	HEM	CMC-C2C-C3C	3.08	130.44	124.68
3	D	800	HEM	CBD-CAD-C3D	2.87	117.76	112.48
3	D	800	HEM	CMC-C2C-C3C	2.76	129.84	124.68
3	D	800	HEM	CAA-CBA-CGA	2.73	117.25	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	600	HEM	CAA-CBA-CGA	2.71	117.22	112.67
3	C	600	HEM	CBA-CAA-C2A	2.68	117.43	112.49
3	B	400	HEM	CBA-CAA-C2A	2.67	117.41	112.49
3	D	800	HEM	CAD-CBD-CGD	2.67	117.15	112.67
3	C	600	HEM	CMD-C2D-C3D	2.60	129.84	124.94
3	D	800	HEM	CMA-C3A-C2A	2.44	129.53	124.94
3	D	800	HEM	CMD-C2D-C1D	-2.42	124.74	128.46
3	A	200	HEM	CMD-C2D-C3D	2.39	129.45	124.94
3	C	600	HEM	CAD-CBD-CGD	2.31	116.54	112.67
3	D	800	HEM	CMB-C2B-C3B	2.23	128.86	124.68
3	C	600	HEM	CMA-C3A-C2A	2.13	128.96	124.94
3	B	400	HEM	CMD-C2D-C1D	-2.13	125.20	128.46

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	C	600	HEM	2	0
3	A	200	HEM	2	0
3	D	800	HEM	3	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 400

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 200

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 800

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	142/143 (99%)	-0.29	3 (2%) 63	63	9, 15, 30, 43	1 (0%)
1	C	142/143 (99%)	-0.41	1 (0%) 87	87	9, 14, 24, 37	0
2	B	146/146 (100%)	-0.35	2 (1%) 75	77	11, 16, 30, 37	0
2	D	146/146 (100%)	-0.10	4 (2%) 54	52	11, 18, 31, 39	1 (0%)
All	All	576/578 (99%)	-0.29	10 (1%) 70	71	9, 16, 30, 43	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	45	PHE	4.5
2	D	49[A]	TYR	4.4
2	D	43	SER	3.1
1	A	45	HIS	2.9
2	B	49	TYR	2.9
1	C	45	HIS	2.5
2	B	41	HIS	2.3
1	A	48	ASP	2.3
1	A	90[B]	TYR	2.1
2	D	120	HIS	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.
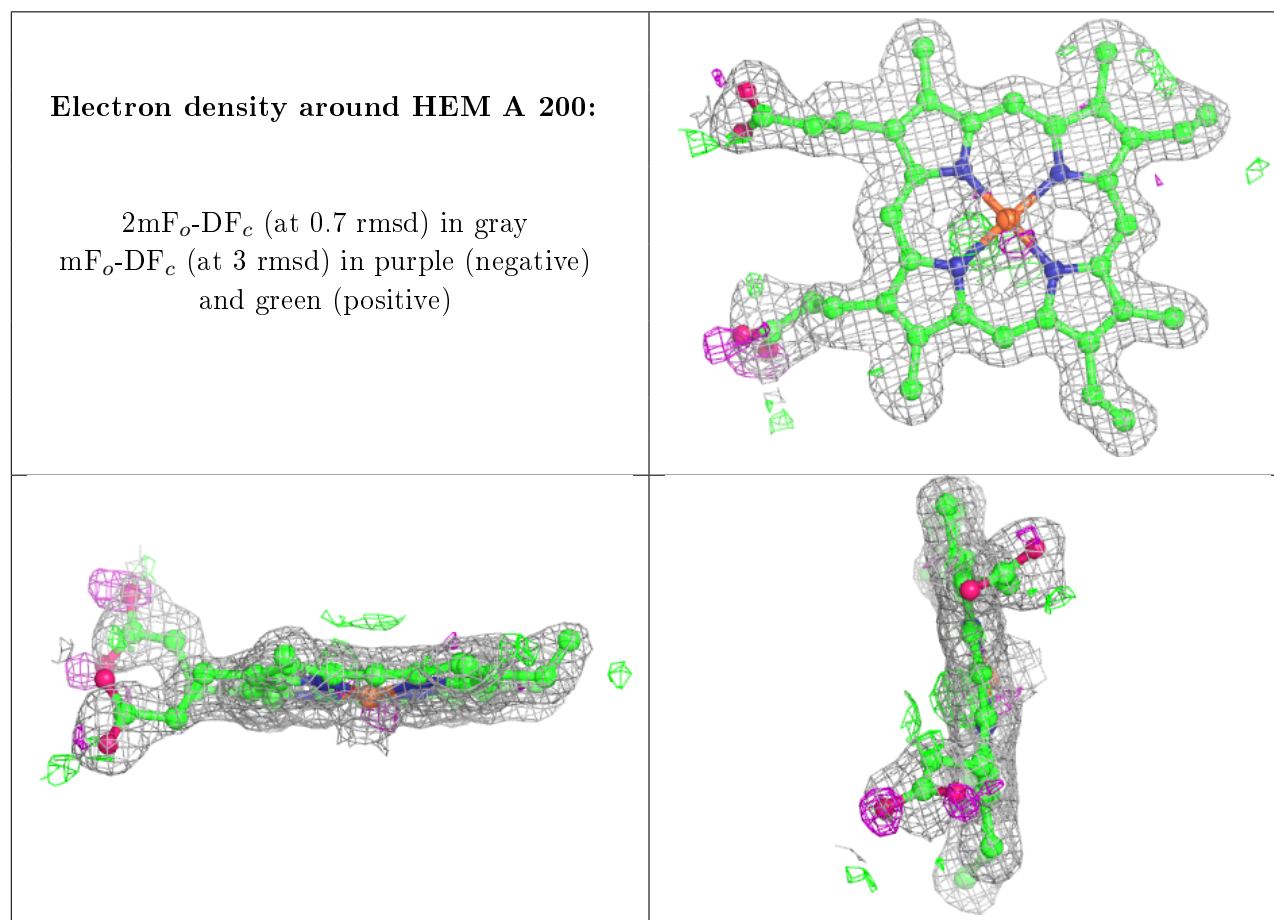
6.3 Carbohydrates (i)

There are no carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
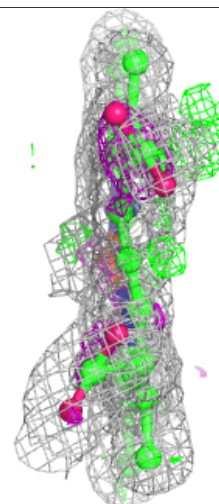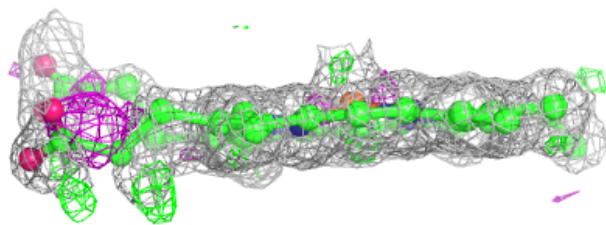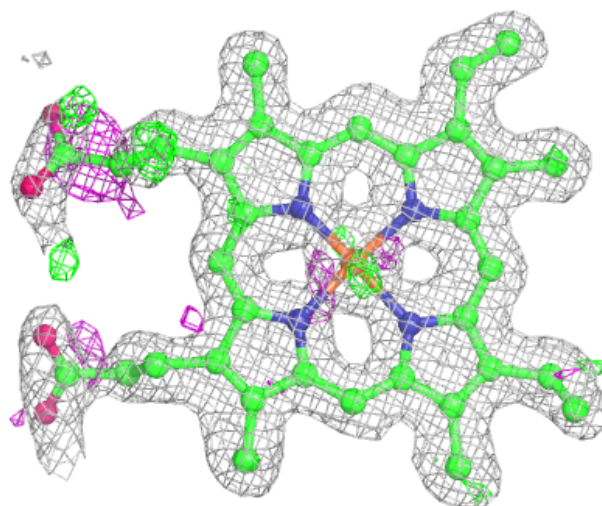
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	A	200	43/43	0.97	0.09	13,19,39,62	0
3	HEM	D	800	43/43	0.97	0.10	14,20,38,53	0
3	HEM	C	600	43/43	0.98	0.08	10,14,35,45	0
3	HEM	B	400	43/43	0.98	0.08	13,18,35,41	0

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.
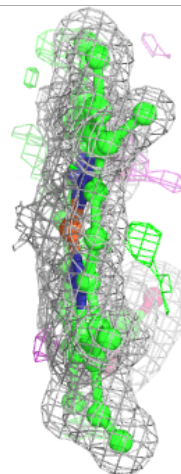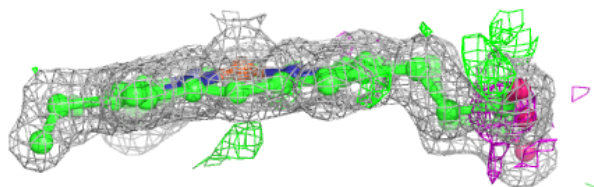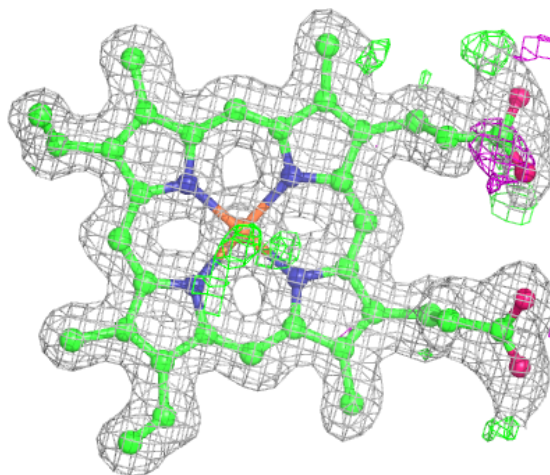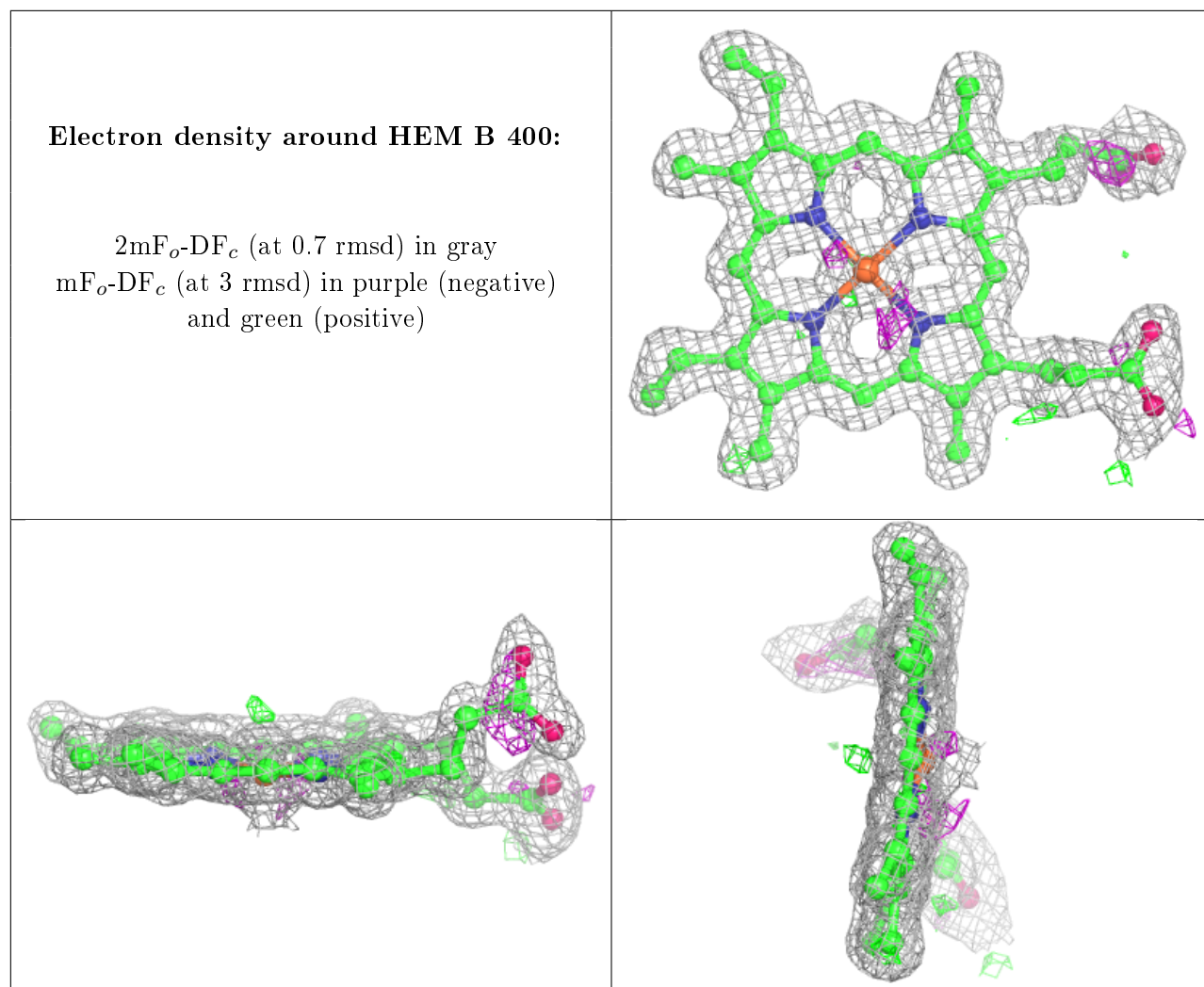
Electron density around HEM A 200:

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

Electron density around HEM D 800:

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

Electron density around HEM C 600:

$2mF_o$-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 B 400:

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.