



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 2HHB / pdb_00002hhb
Title : THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT
1.74 ANGSTROMS RESOLUTION
Authors : Fermi, G.; Perutz, M.F.
Deposited on : 1984-03-07
Resolution : 1.74 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

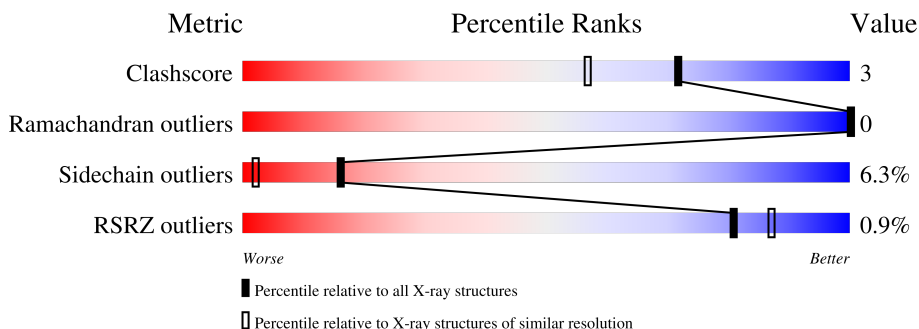
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 ≥ 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	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4779 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.

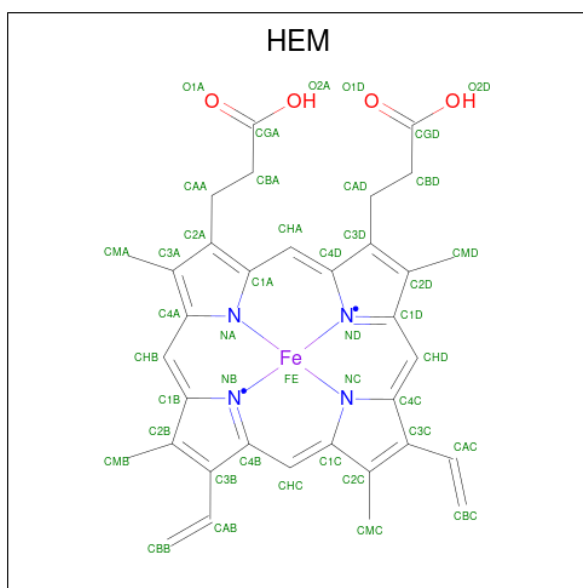
- Molecule 1 is a protein called HEMOGLOBIN (DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN (DEOXY) (BETA CHAIN).

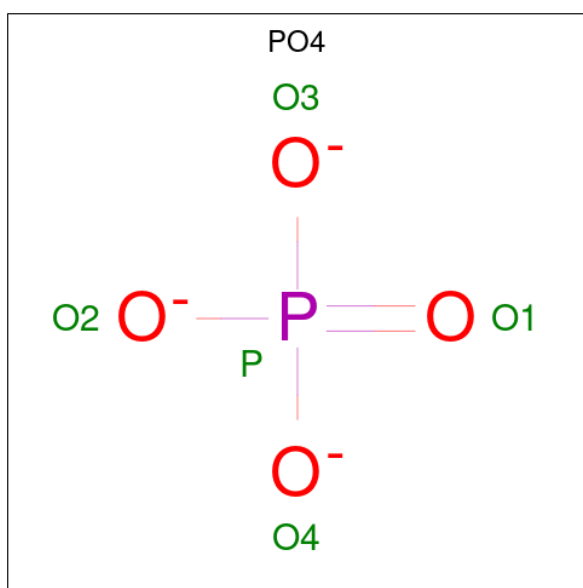
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

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



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	P		
			1	1	0	0
4	D	1	Total	P		
			1	1	0	0

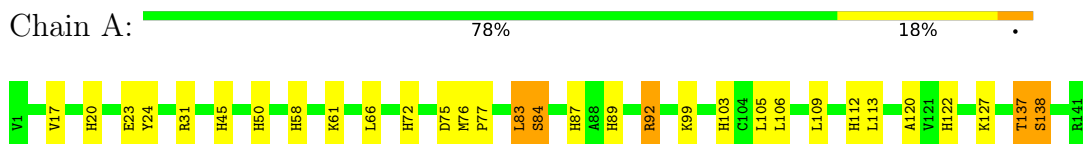
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O		
			58	58	0	0
5	B	58	Total	O		
			58	58	0	0
5	C	58	Total	O		
			58	58	0	0
5	D	47	Total	O		
			47	47	0	0

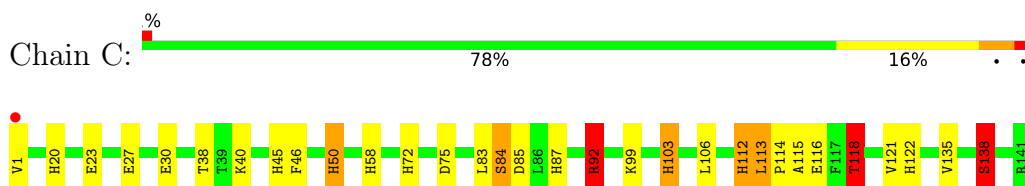
3 Residue-property plots

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

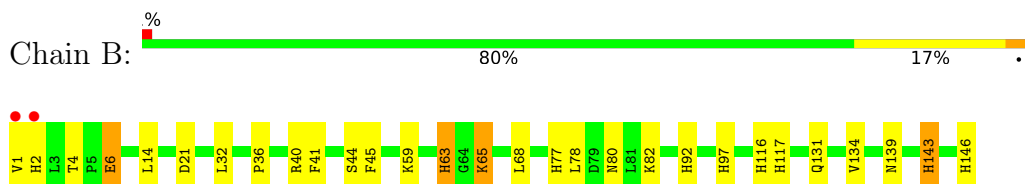
- Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)



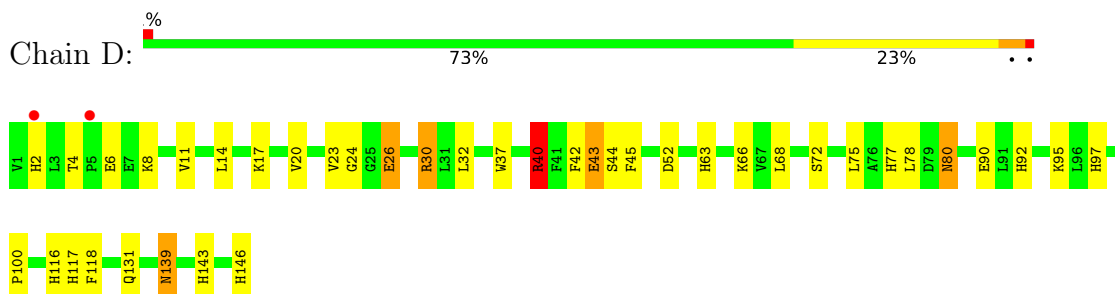
- Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)



- Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)



- Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.15Å 83.59Å 53.80Å 90.00° 99.34° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.74 62.31 – 1.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.74) 99.5 (62.31-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.74Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.160 , (Not available) 0.168 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4779	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, HEM

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	1.62	20/1097 (1.8%)	1.74	22/1491 (1.5%)
1	C	1.60	16/1097 (1.5%)	1.79	20/1491 (1.3%)
2	B	1.71	20/1153 (1.7%)	1.73	15/1566 (1.0%)
2	D	1.65	20/1153 (1.7%)	1.91	24/1566 (1.5%)
All	All	1.65	76/4500 (1.7%)	1.80	81/6114 (1.3%)

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
1	A	0	1
1	C	0	1
2	D	0	2
All	All	0	4

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	HIS	CE1-NE2	12.55	1.45	1.32
1	A	112	HIS	ND1-CE1	12.48	1.45	1.32
2	B	117	HIS	CE1-NE2	12.43	1.45	1.32
2	B	2	HIS	CE1-NE2	12.24	1.44	1.32
2	B	143	HIS	ND1-CE1	11.76	1.44	1.32
2	B	2	HIS	ND1-CE1	11.48	1.44	1.32
2	B	143	HIS	CE1-NE2	11.41	1.44	1.32
2	D	143	HIS	ND1-CE1	11.15	1.43	1.32
1	C	20	HIS	ND1-CE1	10.84	1.43	1.32
2	D	77	HIS	ND1-CE1	10.84	1.43	1.32
2	D	143	HIS	CE1-NE2	10.72	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	HIS	ND1-CE1	10.58	1.43	1.32
1	A	45	HIS	CE1-NE2	10.39	1.43	1.32
2	B	146	HIS	ND1-CE1	10.38	1.43	1.32
1	C	20	HIS	CE1-NE2	10.37	1.43	1.32
2	B	117	HIS	ND1-CE1	10.09	1.42	1.32
1	A	122	HIS	CE1-NE2	9.84	1.42	1.32
1	A	112	HIS	CE1-NE2	9.55	1.42	1.32
1	C	72	HIS	CE1-NE2	9.51	1.42	1.32
2	B	63	HIS	ND1-CE1	9.45	1.42	1.32
1	A	122	HIS	ND1-CE1	9.35	1.42	1.32
2	B	116	HIS	ND1-CE1	8.99	1.41	1.32
2	D	92	HIS	ND1-CE1	8.74	1.41	1.32
2	D	63	HIS	ND1-CE1	8.59	1.41	1.32
1	C	58	HIS	ND1-CE1	8.24	1.40	1.32
1	C	87	HIS	ND1-CE1	8.19	1.40	1.32
1	A	89	HIS	ND1-CE1	8.02	1.40	1.32
2	D	117	HIS	ND1-CE1	7.93	1.40	1.32
2	D	77	HIS	CE1-NE2	7.84	1.40	1.32
2	D	2	HIS	CG-ND1	7.82	1.46	1.38
2	B	116	HIS	CE1-NE2	7.82	1.40	1.32
1	A	20	HIS	ND1-CE1	7.68	1.40	1.32
2	D	97	HIS	ND1-CE1	7.49	1.40	1.32
2	D	146	HIS	CE1-NE2	7.43	1.40	1.32
1	C	58	HIS	CE1-NE2	7.43	1.40	1.32
1	C	50	HIS	CE1-NE2	7.42	1.40	1.32
1	A	45	HIS	ND1-CE1	7.41	1.40	1.32
1	A	72	HIS	ND1-CE1	7.39	1.40	1.32
1	C	45	HIS	CE1-NE2	7.30	1.39	1.32
2	D	45	PHE	C-N	-7.06	1.23	1.33
2	B	77	HIS	CE1-NE2	7.04	1.39	1.32
2	B	97	HIS	ND1-CE1	6.95	1.39	1.32
1	A	20	HIS	CE1-NE2	6.95	1.39	1.32
2	B	63	HIS	CG-ND1	6.90	1.45	1.38
1	C	72	HIS	ND1-CE1	6.85	1.39	1.32
1	A	89	HIS	CE1-NE2	6.77	1.39	1.32
2	D	116	HIS	CE1-NE2	6.68	1.39	1.32
1	A	50	HIS	CE1-NE2	6.66	1.39	1.32
2	B	92	HIS	ND1-CE1	6.63	1.39	1.32
2	B	97	HIS	CE1-NE2	6.44	1.39	1.32
2	D	2	HIS	CD2-NE2	6.38	1.44	1.37
1	A	92	ARG	CD-NE	-6.37	1.37	1.46
2	B	77	HIS	ND1-CE1	6.21	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	HIS	CE1-NE2	6.17	1.38	1.32
1	A	87	HIS	CE1-NE2	6.15	1.38	1.32
1	C	50	HIS	ND1-CE1	6.15	1.38	1.32
1	A	58	HIS	ND1-CE1	6.11	1.38	1.32
1	C	122	HIS	CE1-NE2	6.03	1.38	1.32
2	D	116	HIS	ND1-CE1	6.01	1.38	1.32
2	D	2	HIS	CG-CD2	5.71	1.42	1.35
2	D	97	HIS	CE1-NE2	5.70	1.38	1.32
2	D	146	HIS	ND1-CE1	5.68	1.38	1.32
2	B	117	HIS	CD2-NE2	5.61	1.44	1.37
1	C	122	HIS	ND1-CE1	5.58	1.38	1.32
2	B	2	HIS	CG-ND1	5.57	1.44	1.38
1	A	50	HIS	ND1-CE1	5.53	1.38	1.32
1	C	92	ARG	CZ-NH1	5.44	1.40	1.32
2	B	117	HIS	CG-ND1	5.41	1.44	1.38
1	A	120	ALA	C-N	-5.35	1.27	1.33
2	D	30	ARG	CD-NE	-5.30	1.38	1.46
2	B	146	HIS	CE1-NE2	5.23	1.37	1.32
1	C	103	HIS	ND1-CE1	5.21	1.37	1.32
1	A	138	SER	CB-OG	-5.12	1.31	1.42
1	C	112	HIS	CE1-NE2	5.10	1.37	1.32
1	C	112	HIS	C-N	-5.03	1.27	1.33
1	A	122	HIS	CD2-NE2	5.00	1.43	1.37

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	ARG	CD-NE-CZ	14.27	144.38	124.40
2	D	139	ASN	CA-CB-CG	-13.97	98.63	112.60
2	D	30	ARG	NE-CZ-NH2	-13.74	106.83	119.20
2	D	30	ARG	NE-CZ-NH1	11.57	133.07	121.50
2	D	43	GLU	CB-CG-CD	-11.18	93.59	112.60
2	D	139	ASN	OD1-CG-ND2	10.88	133.48	122.60
1	C	92	ARG	CD-NE-CZ	-10.32	109.94	124.40
2	B	2	HIS	CA-CB-CG	-9.80	104.00	113.80
1	A	137	THR	CA-CB-CG2	9.78	127.12	110.50
1	C	118	THR	N-CA-CB	-8.48	97.83	110.05
2	D	40	ARG	N-CA-CB	-8.46	96.19	110.49
1	C	114	PRO	O-C-N	-7.92	113.62	122.18
1	A	17	VAL	N-CA-C	-7.83	102.82	110.72
2	B	139	ASN	CA-CB-CG	-7.47	105.13	112.60
1	A	75	ASP	N-CA-CB	-7.34	102.99	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	HIS	CA-CB-CG	-7.28	106.52	113.80
1	C	138	SER	CA-CB-OG	-7.23	96.63	111.10
2	B	45	PHE	CA-CB-CG	7.11	120.91	113.80
1	C	38	THR	OG1-CB-CG2	-7.07	95.17	109.30
1	C	92	ARG	NE-CZ-NH2	-7.06	112.84	119.20
1	C	118	THR	CA-CB-CG2	7.03	122.45	110.50
2	D	26	GLU	CB-CG-CD	-7.01	100.69	112.60
1	A	127	LYS	N-CA-CB	-7.00	99.80	110.16
2	D	80	ASN	OD1-CG-ND2	6.81	129.41	122.60
2	D	17	LYS	CB-CG-CD	-6.69	95.91	111.30
1	C	23	GLU	CB-CG-CD	-6.67	101.26	112.60
2	B	44	SER	N-CA-CB	-6.58	99.14	110.32
1	C	84	SER	CB-CA-C	-6.46	100.06	110.79
2	D	40	ARG	CG-CD-NE	-6.44	97.84	112.00
1	A	138	SER	CA-CB-OG	-6.43	98.23	111.10
2	D	52	ASP	CA-CB-CG	-6.42	106.17	112.60
1	A	92	ARG	CD-NE-CZ	-6.38	115.47	124.40
1	C	84	SER	N-CA-CB	6.28	119.36	110.12
1	C	115	ALA	N-CA-C	6.27	120.66	112.89
2	D	42	PHE	CA-C-N	-6.15	109.58	121.58
2	D	42	PHE	C-N-CA	-6.15	109.58	121.58
1	A	84	SER	CA-C-O	-6.15	114.03	120.55
1	A	72	HIS	CA-CB-CG	-6.08	107.72	113.80
2	B	97	HIS	CA-CB-CG	-6.02	107.78	113.80
1	C	113	LEU	CA-C-N	6.00	125.48	119.24
1	C	113	LEU	C-N-CA	6.00	125.48	119.24
2	B	143	HIS	ND1-CG-CD2	5.92	112.02	106.10
2	B	80	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	113	LEU	CA-C-N	5.73	125.20	119.24
1	A	113	LEU	C-N-CA	5.73	125.20	119.24
2	B	139	ASN	CB-CA-C	-5.72	101.29	110.79
2	B	65	LYS	N-CA-CB	-5.71	101.71	110.16
1	A	17	VAL	O-C-N	5.70	127.70	121.83
2	B	134	VAL	N-CA-CB	5.65	119.06	110.58
1	A	127	LYS	CB-CA-C	5.60	120.38	110.85
2	D	80	ASN	CB-CA-C	5.60	121.21	111.86
1	C	58	HIS	CA-CB-CG	-5.58	108.22	113.80
2	D	90	GLU	CB-CG-CD	-5.58	103.12	112.60
1	A	23	GLU	N-CA-CB	-5.57	101.92	110.16
1	C	72	HIS	CA-CB-CG	-5.54	108.26	113.80
1	C	46	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	99	LYS	CA-CB-CG	-5.53	103.04	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	143	HIS	ND1-CG-CD2	5.47	111.58	106.10
2	D	8	LYS	CA-CB-CG	-5.47	103.15	114.10
1	A	106	LEU	N-CA-CB	-5.46	102.09	110.12
2	D	11	VAL	O-C-N	5.46	127.58	121.90
2	B	41	PHE	CA-CB-CG	-5.43	108.37	113.80
2	B	36	PRO	N-CA-CB	5.37	108.85	103.48
1	C	40	LYS	CB-CG-CD	-5.29	99.13	111.30
1	A	92	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	C	75	ASP	N-CA-CB	-5.28	103.43	111.19
1	A	31	ARG	O-C-N	5.28	127.71	122.12
1	A	61	LYS	O-C-N	5.25	128.14	122.15
1	C	114	PRO	N-CA-C	-5.24	105.30	113.78
1	A	137	THR	N-CA-CB	-5.19	102.81	110.49
2	D	72	SER	O-C-N	5.18	127.61	122.12
1	A	112	HIS	ND1-CG-CD2	5.16	111.26	106.10
2	B	117	HIS	ND1-CG-CD2	5.15	111.25	106.10
2	B	14	LEU	CD1-CG-CD2	5.14	122.10	110.80
2	D	43	GLU	O-C-N	5.13	129.92	122.43
2	B	14	LEU	N-CA-CB	-5.12	102.60	110.12
2	D	118	PHE	CA-CB-CG	-5.05	108.75	113.80
2	D	100	PRO	N-CA-CB	5.03	108.30	103.52
1	A	127	LYS	CG-CD-CE	-5.02	99.75	111.30
2	D	43	GLU	N-CA-C	5.01	119.25	113.18
1	A	122	HIS	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	TYR	Sidechain
1	C	92	ARG	Sidechain
2	D	30	ARG	Sidechain
2	D	40	ARG	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	1069	0	1073	5	0
1	C	1069	0	1073	11	1
2	B	1123	0	1118	7	0
2	D	1123	0	1118	8	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	58	0	0	0	0
5	B	58	0	0	0	2
5	C	58	0	0	0	1
5	D	47	0	0	0	0
All	All	4779	0	4502	30	2

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 3.

All (30) 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:C:118:THR:HG22	1:C:121:VAL:H	1.50	0.75
2:D:23:VAL:HG12	2:D:68:LEU:HD11	1.81	0.62
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.86	0.59
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.87	0.57
2:D:66:LYS:HE2	3:D:148:HEM:HAA2	1.86	0.57
1:C:27:GLU:OE2	1:C:112:HIS:HE1	1.88	0.56
2:B:82:LYS:HE3	2:B:143:HIS:CE1	2.41	0.56
1:A:66:LEU:CD1	1:A:105:LEU:HD21	2.37	0.54
2:B:6:GLU:H	2:B:6:GLU:CD	2.17	0.53
2:B:4:THR:HB	2:B:6:GLU:OE2	2.08	0.53
2:D:37:TRP:O	2:D:40:ARG:HB2	2.10	0.52
3:D:148:HEM:HBC2	3:D:148:HEM:HMC2	1.92	0.52
1:C:83:LEU:HD11	3:C:142:HEM:HMA1	1.92	0.52
1:C:113:LEU:HB3	1:C:116:GLU:HG2	1.92	0.50
1:A:66:LEU:HD11	1:A:105:LEU:HD21	1.94	0.49
2:D:24:GLY:N	2:D:68:LEU:HD12	2.29	0.47
1:C:113:LEU:HB3	1:C:116:GLU:CG	2.46	0.46
2:D:24:GLY:CA	2:D:68:LEU:HD12	2.44	0.46
1:A:76:MET:N	1:A:77:PRO:HD2	2.30	0.46
2:D:4:THR:HB	2:D:6:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.76	0.45
2:B:63:HIS:HE1	3:B:148:HEM:C4D	2.35	0.45
1:C:113:LEU:HD22	1:C:116:GLU:HG3	1.97	0.44
2:B:4:THR:OG1	2:B:6:GLU:HG2	2.18	0.44
1:C:92:ARG:HH11	1:C:92:ARG:HD2	1.66	0.44
1:C:30:GLU:OE2	1:C:50:HIS:HD2	2.01	0.43
1:C:135:VAL:O	1:C:138:SER:HB2	2.18	0.43
2:D:95:LYS:HD3	2:D:95:LYS:HA	1.73	0.41
2:B:21:ASP:OD1	2:B:65:LYS:HG3	2.20	0.41
1:C:30:GLU:OE2	1:C:50:HIS:CD2	2.74	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASP:OD2	5:B:205:HOH:O[2_657]	1.42	0.78
5:B:205:HOH:O	5:C:160:HOH:O[2_647]	2.02	0.18

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%)	136 (98%)	3 (2%)	0	100	100
1	C	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	566/574 (99%)	557 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	107 (95%)	6 (5%)	20	4
1	C	113/113 (100%)	107 (95%)	6 (5%)	20	4
2	B	118/118 (100%)	111 (94%)	7 (6%)	18	3
2	D	118/118 (100%)	108 (92%)	10 (8%)	10	1
All	All	462/462 (100%)	433 (94%)	29 (6%)	16	2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LEU
1	A	84	SER
1	A	92	ARG
1	A	109	LEU
1	A	137	THR
1	A	138	SER
2	B	1	VAL
2	B	6	GLU
2	B	32	LEU
2	B	40	ARG
2	B	59	LYS
2	B	68	LEU
2	B	78	LEU
1	C	1	VAL
1	C	84	SER
1	C	99	LYS
1	C	106	LEU
1	C	118	THR
1	C	138	SER
2	D	14	LEU
2	D	20	VAL
2	D	26	GLU
2	D	32	LEU
2	D	43	GLU

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Mol	Chain	Res	Type
2	D	44	SER
2	D	75	LEU
2	D	78	LEU
2	D	80	ASN
2	D	139	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	72	HIS
1	A	103	HIS
2	B	80	ASN
1	C	50	HIS
1	C	68	ASN
1	C	72	HIS
1	C	103	HIS
1	C	112	HIS
2	D	63	HIS
2	D	77	HIS
2	D	80	ASN
2	D	139	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are modelled with single atom - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	C	142	1	50,50,50	1.48	10 (20%)	67,82,82	0.90	1 (1%)
3	HEM	A	142	1	50,50,50	1.79	6 (12%)	67,82,82	1.01	3 (4%)
3	HEM	D	148	2	50,50,50	1.64	9 (18%)	67,82,82	1.11	3 (4%)
3	HEM	B	148	2	50,50,50	1.26	4 (8%)	67,82,82	1.03	3 (4%)

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	142	1	-	4/14/54/54	-
3	HEM	A	142	1	-	2/14/54/54	-
3	HEM	D	148	2	-	4/14/54/54	-
3	HEM	B	148	2	-	3/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NB	6.95	2.16	1.94
3	A	142	HEM	FE-NC	6.10	2.15	1.95
3	D	148	HEM	FE-NA	5.46	2.13	1.95
3	C	142	HEM	FE-NB	4.78	2.09	1.94
3	D	148	HEM	FE-NC	4.20	2.09	1.95
3	C	142	HEM	FE-NA	4.04	2.08	1.95
3	A	142	HEM	FE-ND	3.79	2.06	1.94
3	B	148	HEM	FE-ND	3.72	2.06	1.94
3	D	148	HEM	FE-ND	3.61	2.06	1.94
3	B	148	HEM	FE-NA	3.22	2.05	1.95
3	D	148	HEM	C4A-NA	-2.96	1.34	1.39
3	D	148	HEM	FE-NB	2.92	2.03	1.94
3	C	142	HEM	O2A-CGA	-2.81	1.21	1.30
3	C	142	HEM	O2D-CGD	-2.74	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CHD-C1D	2.71	1.45	1.39
3	C	142	HEM	FE-ND	2.70	2.03	1.94
3	D	148	HEM	CBA-CGA	2.67	1.56	1.50
3	C	142	HEM	C4B-NB	-2.50	1.33	1.38
3	C	142	HEM	FE-NC	2.45	2.03	1.95
3	A	142	HEM	FE-NA	2.45	2.03	1.95
3	A	142	HEM	O2A-CGA	-2.39	1.22	1.30
3	B	148	HEM	O2A-CGA	-2.26	1.23	1.30
3	C	142	HEM	CBC-CAC	2.26	1.41	1.30
3	A	142	HEM	CHC-C1C	2.25	1.42	1.38
3	D	148	HEM	C1C-NC	-2.15	1.35	1.39
3	D	148	HEM	C4A-C3A	2.10	1.48	1.43
3	B	148	HEM	CBB-CAB	2.08	1.40	1.30
3	C	142	HEM	C2A-C3A	-2.05	1.33	1.38
3	C	142	HEM	CBD-CGD	2.05	1.55	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	HEM	C3B-C4B-NB	4.05	112.38	109.47
3	B	148	HEM	C3B-C4B-NB	3.41	111.92	109.47
3	A	142	HEM	O1D-CGD-CBD	-2.96	113.70	123.09
3	A	142	HEM	O2D-CGD-CBD	2.88	123.09	114.00
3	D	148	HEM	CAA-CBA-CGA	2.49	120.27	113.67
3	C	142	HEM	CHD-C1D-ND	2.27	126.86	124.42
3	B	148	HEM	CAD-C3D-C2D	-2.23	123.70	127.87
3	B	148	HEM	O1D-CGD-CBD	-2.08	116.50	123.09
3	A	142	HEM	CHC-C4B-NB	2.07	126.65	124.42
3	D	148	HEM	O2A-CGA-CBA	2.04	120.46	114.00

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	148	HEM	C2B-C3B-CAB-CBB
3	A	142	HEM	C2B-C3B-CAB-CBB
3	D	148	HEM	C4B-C3B-CAB-CBB
3	D	148	HEM	CAD-CBD-CGD-O1D
3	D	148	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAA-CBA-CGA-O2A

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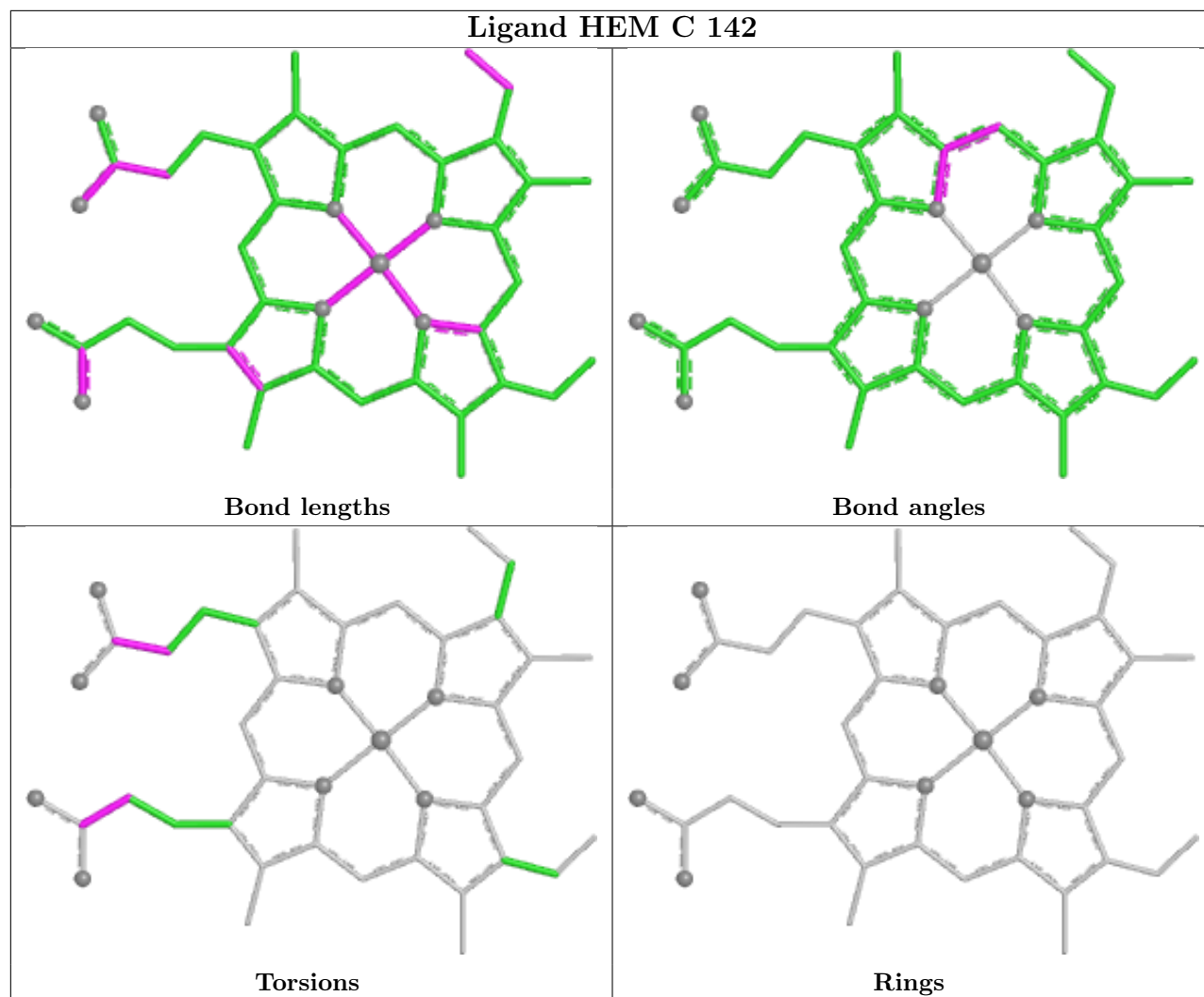
Mol	Chain	Res	Type	Atoms
3	B	148	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAA-CBA-CGA-O1A
3	B	148	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O1A
3	B	148	HEM	CAD-CBD-CGD-O1D

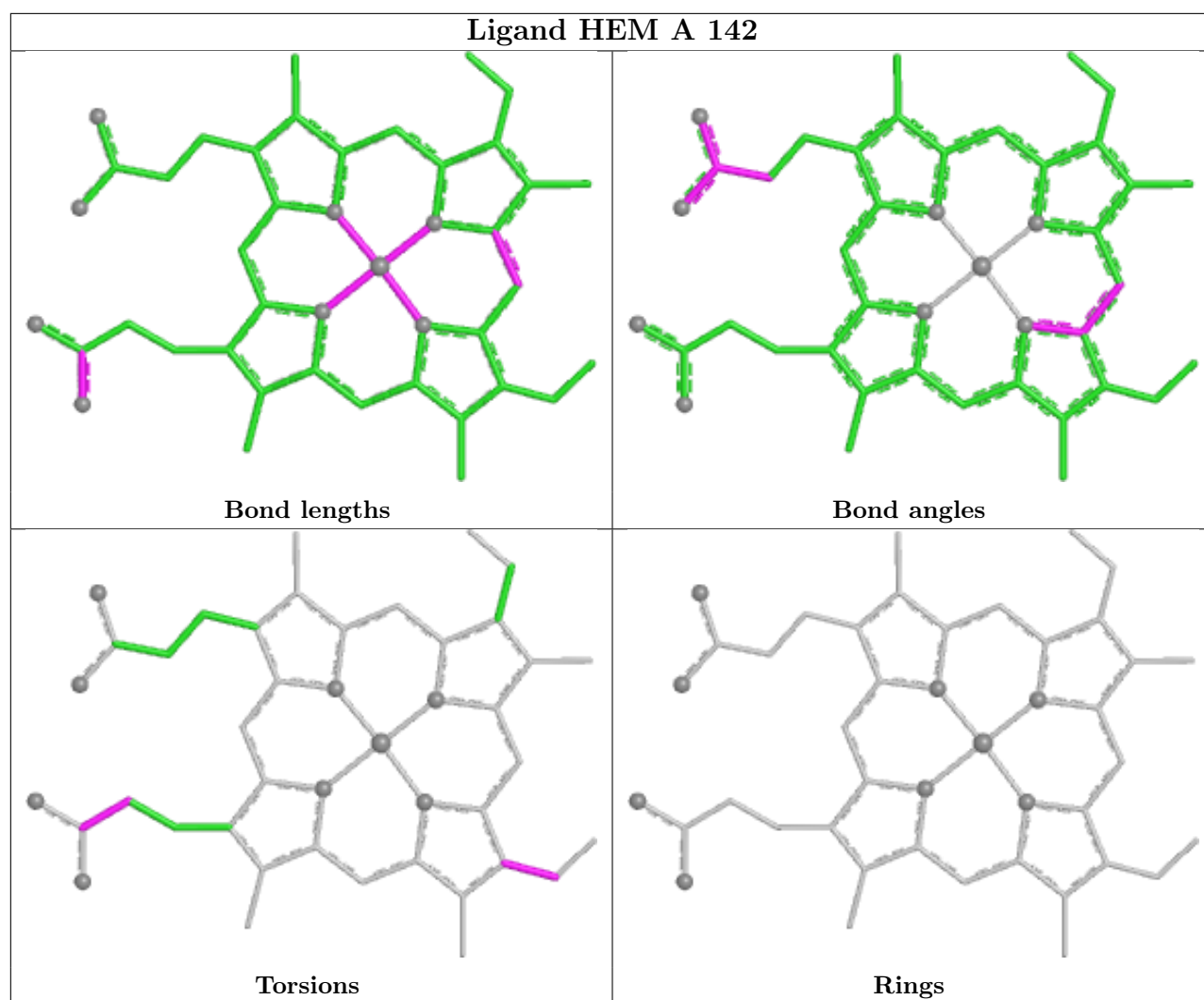
There are no ring outliers.

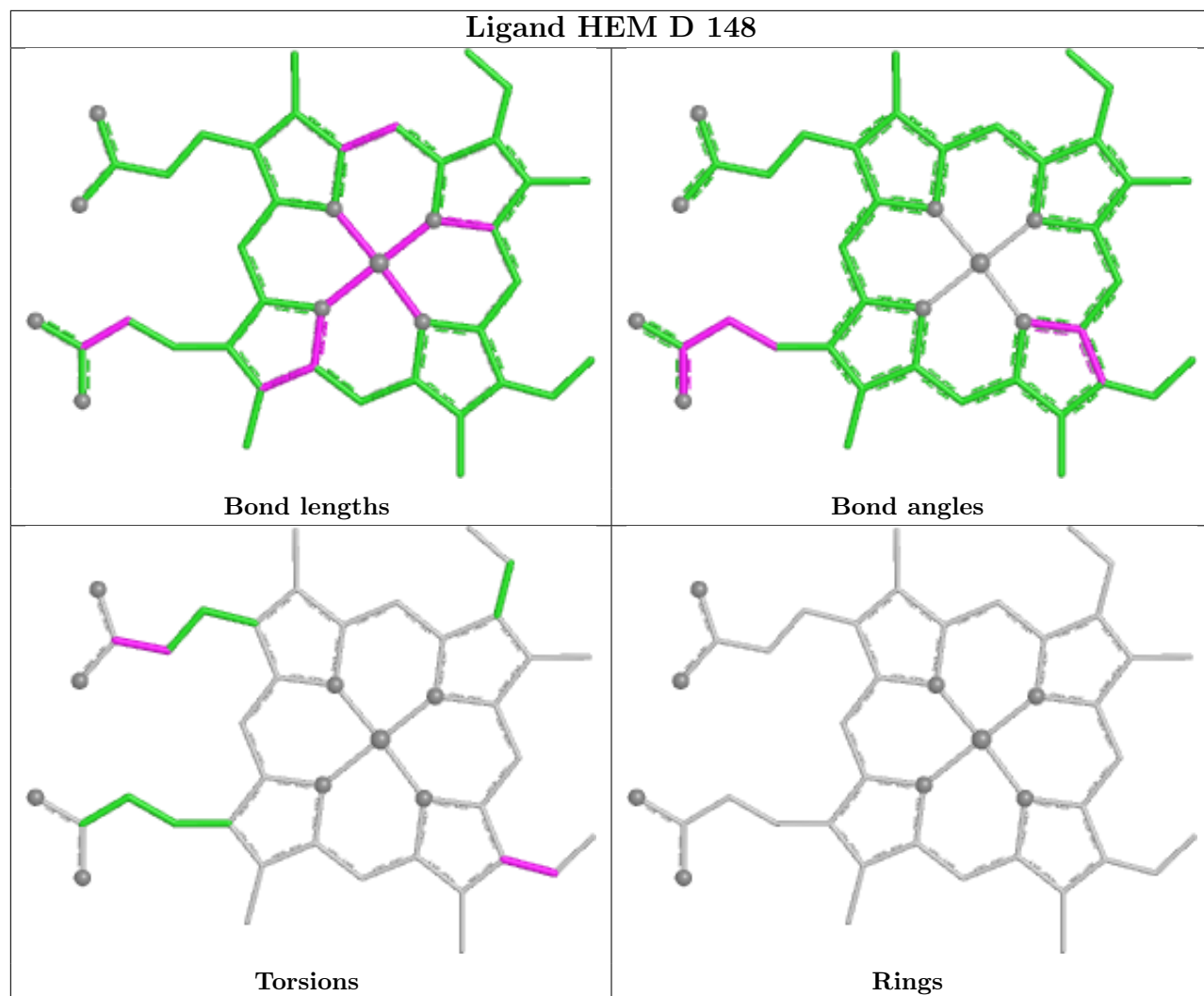
3 monomers are involved in 4 short contacts:

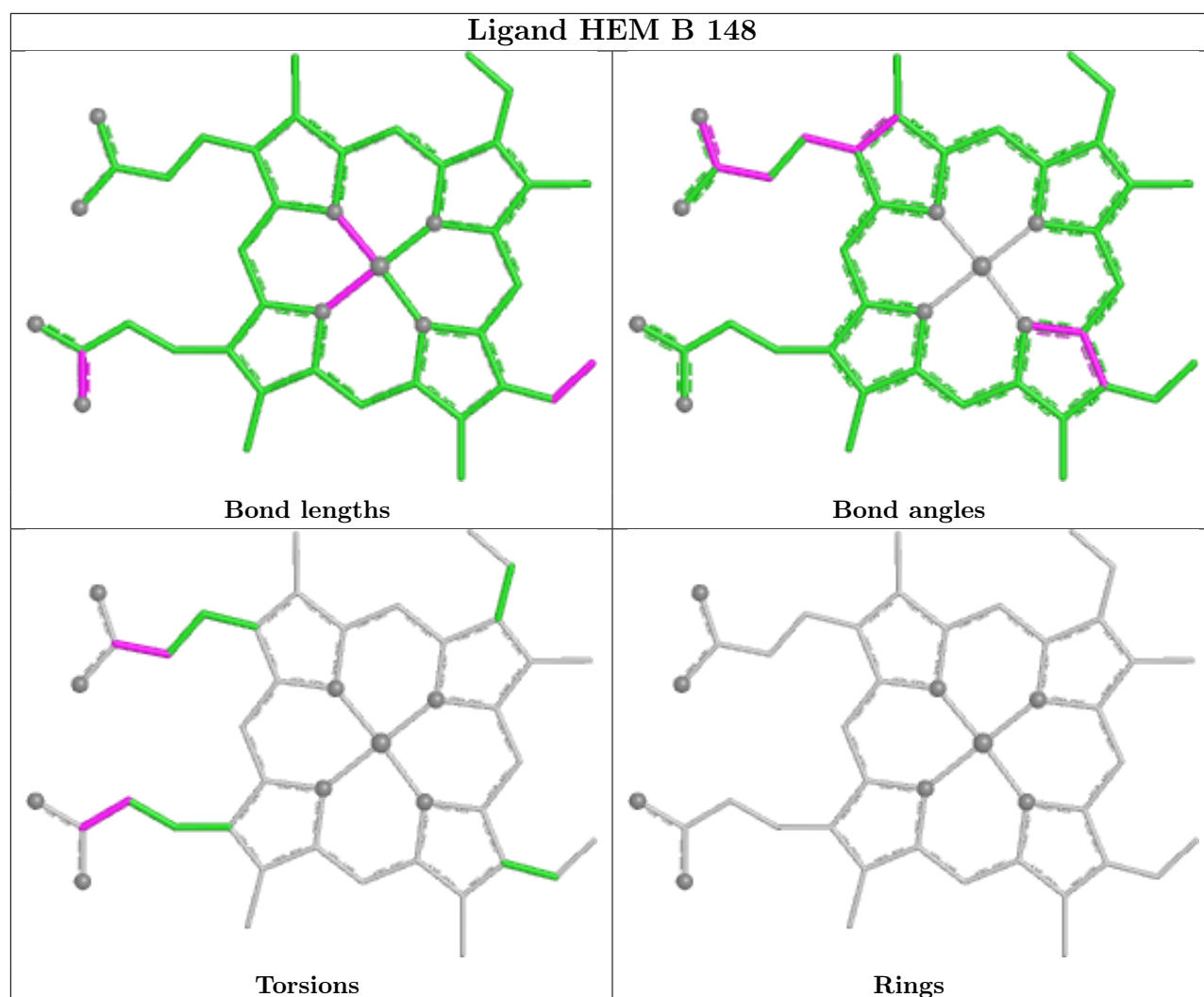
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	142	HEM	1	0
3	D	148	HEM	2	0
3	B	148	HEM	1	0

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, 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	141/141 (100%)	-0.15	0 100 100	12, 22, 38, 45	0
1	C	141/141 (100%)	-0.19	1 (0%) 84 89	12, 21, 37, 45	0
2	B	146/146 (100%)	-0.12	2 (1%) 73 80	12, 22, 40, 56	0
2	D	146/146 (100%)	-0.03	2 (1%) 73 80	13, 24, 44, 53	0
All	All	574/574 (100%)	-0.12	5 (0%) 81 87	12, 22, 40, 56	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	VAL	3.9
1	C	1	VAL	2.9
2	B	2	HIS	2.8
2	D	2	HIS	2.7
2	D	5	PRO	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 oligosaccharides in this entry.

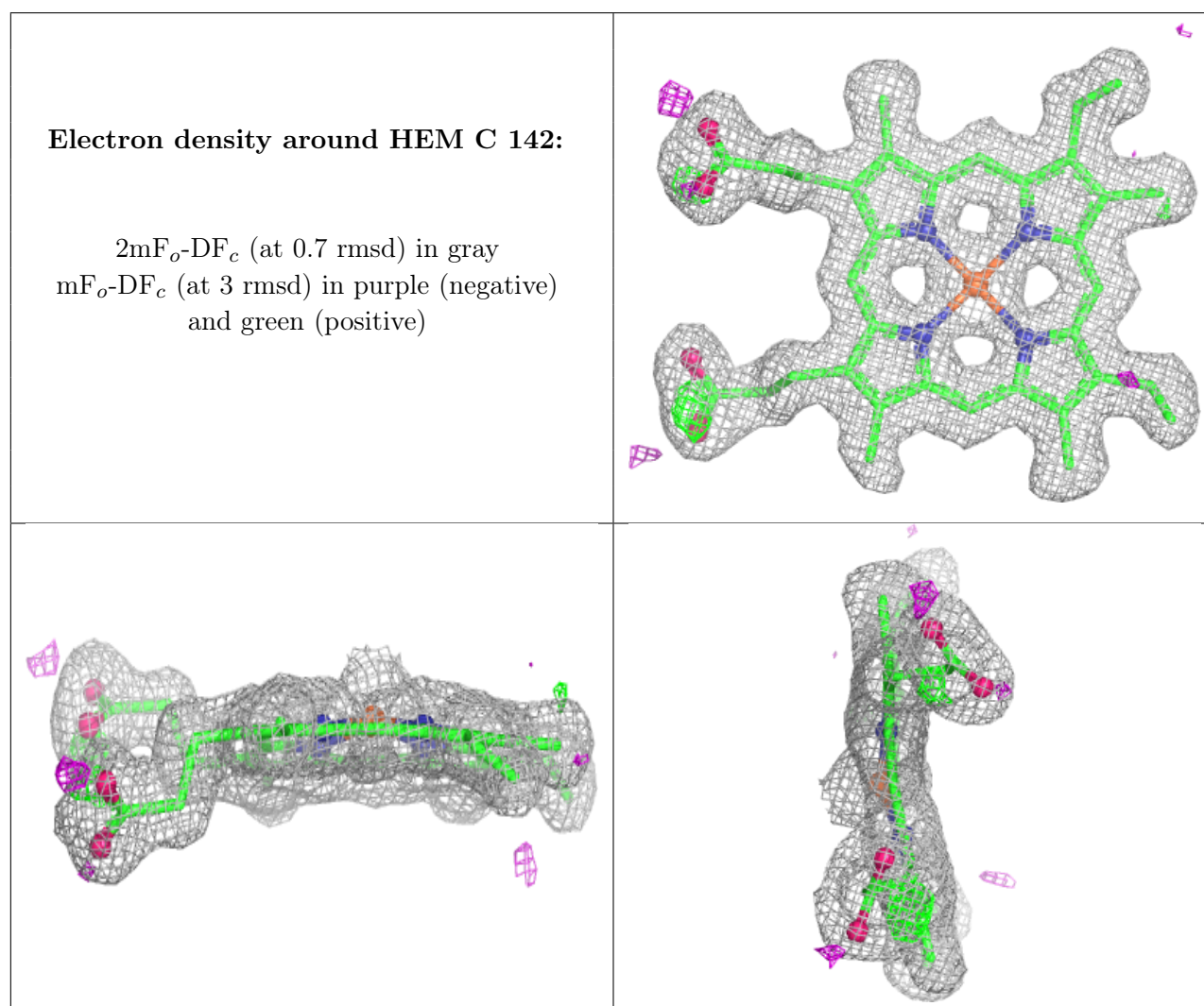
6.4 Ligands [i](#)

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.

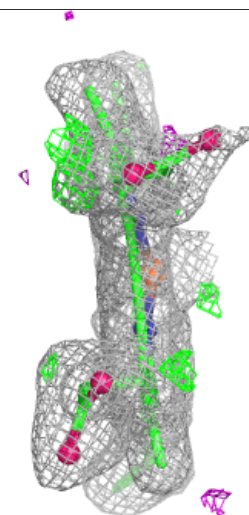
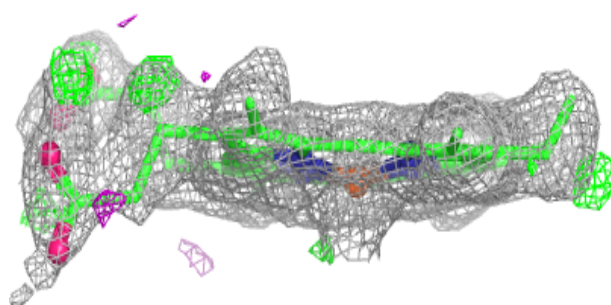
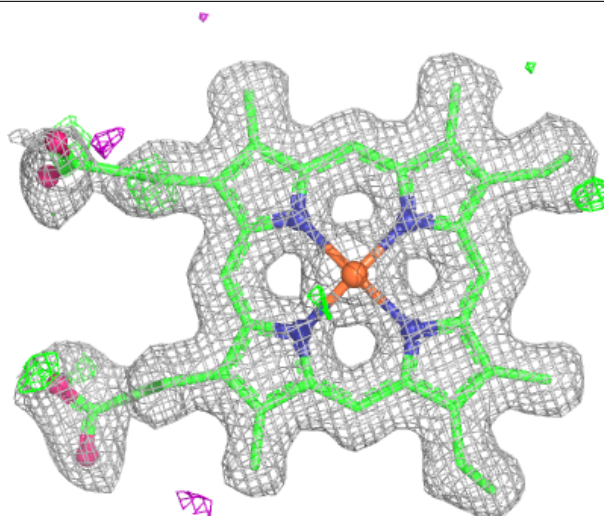
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	B	147	1/5	0.74	0.20	32,32,32,32	0
4	PO4	D	147	1/5	0.83	0.14	31,31,31,31	0
3	HEM	C	142	43/43	0.98	0.05	7,15,32,41	0
3	HEM	D	148	43/43	0.98	0.06	11,18,46,60	0
3	HEM	A	142	43/43	0.98	0.06	10,18,41,46	0
3	HEM	B	148	43/43	0.98	0.06	7,17,35,48	0

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.



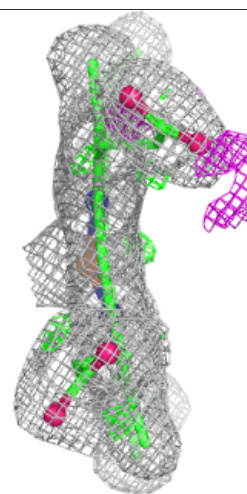
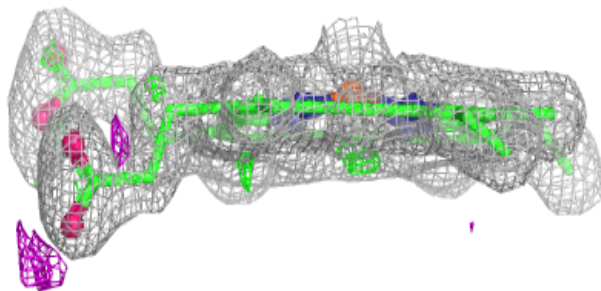
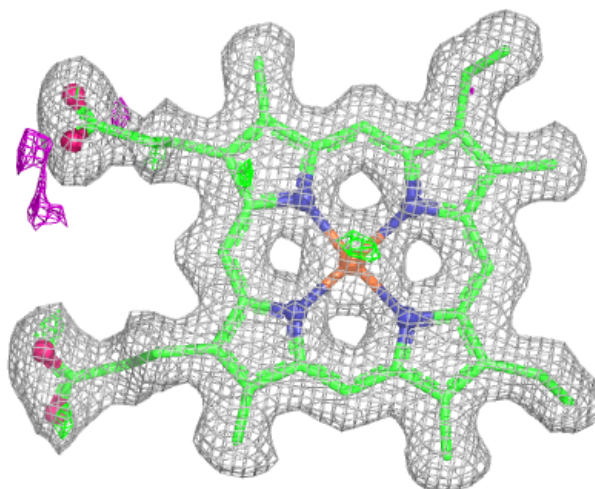
Electron density around HEM D 148:

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



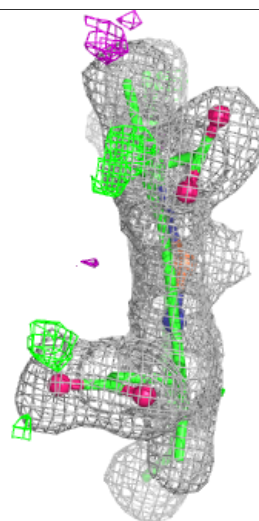
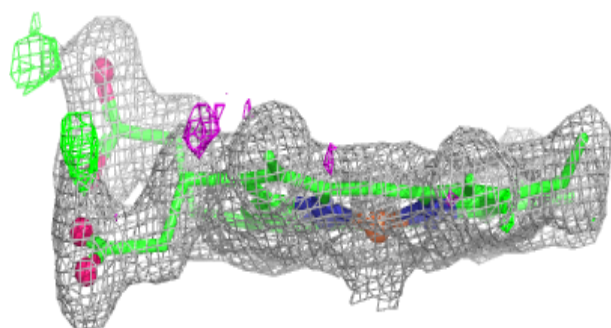
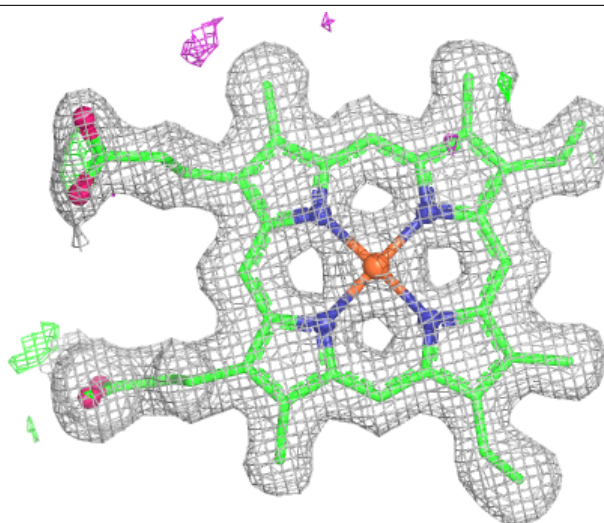
Electron density around HEM A 142:

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



Electron density around HEM B 148:

$2mF_o-DF_c$ (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.