



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 02:28 PM UTC

PDB ID : 3IC0 / pdb_00003ic0
Title : Crystal Structure of liganded hemoglobin in complex with a potent antisickling agent, INN-298
Authors : Safo, M.K.; Musayev, F.N.; Gandhi, A.K.; Jorge, P.
Deposited on : 2009-07-17
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

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

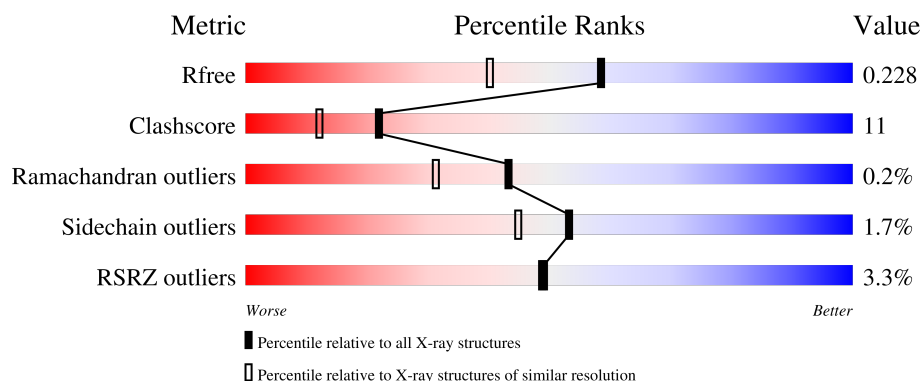
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	79% 19% .
1	C	141	90% 9% .
2	B	146	7% 79% 18% .
2	D	146	6% 75% 24% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5057 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.

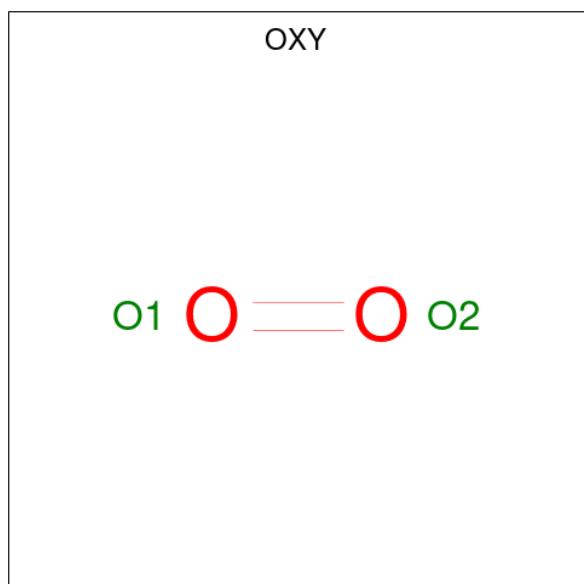
- Molecule 1 is a protein called Hemoglobin subunit alpha.

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 subunit beta.

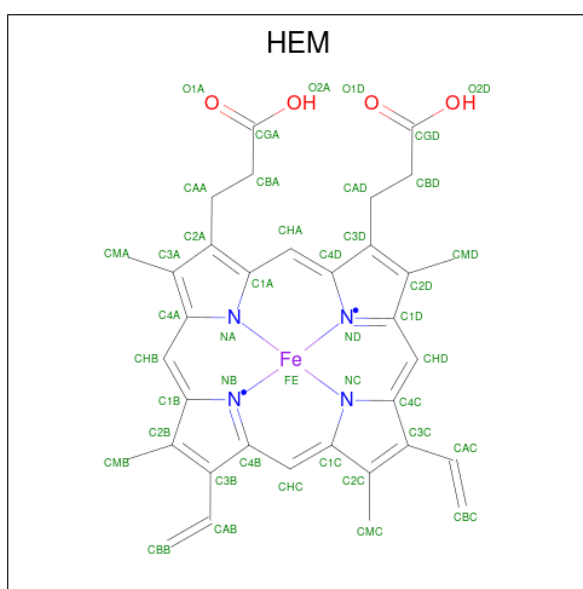
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



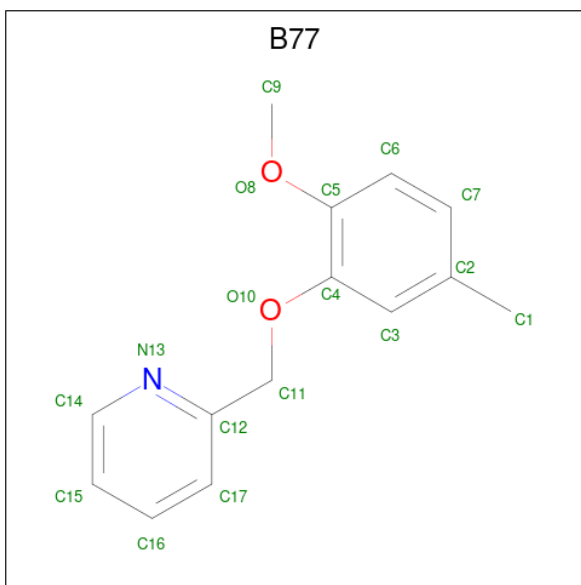
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 2 2	0	0
3	B	1	Total O 2 2	0	0
3	C	1	Total O 2 2	0	0
3	D	1	Total O 2 2	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 2-[(2-methoxy-5-methylphenoxy)methyl]pyridine (CCD ID: B77) (formula: $C_{14}H_{15}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	14	1	2		
5	A	1	Total	C	N	O	0	0
			17	14	1	2		
5	C	1	Total	C	N	O	0	0
			17	14	1	2		
5	C	1	Total	C	N	O	0	0
			17	14	1	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	113	Total	O	0	0
			113	113		
7	B	75	Total	O	0	0
			75	75		
7	C	138	Total	O	0	0
			138	138		
7	D	89	Total	O	0	0
			89	89		

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 subunit alpha

Chain A: 



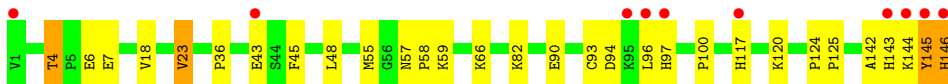
- Molecule 1: Hemoglobin subunit alpha

Chain C: 



- Molecule 2: Hemoglobin subunit beta

Chain B: 



- Molecule 2: Hemoglobin subunit beta

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.98Å 91.98Å 143.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.78 – 1.80 27.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.78-1.80) 99.9 (27.78-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.230 0.196 , 0.228	Depositor DCC
R_{free} test set	3337 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5057	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: B77, HEM, OXY, SO4

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	0.87	0/1097	1.07	5/1491 (0.3%)
1	C	1.01	0/1097	1.04	2/1491 (0.1%)
2	B	0.80	0/1153	1.10	11/1566 (0.7%)
2	D	0.91	0/1153	1.08	4/1566 (0.3%)
All	All	0.90	0/4500	1.07	22/6114 (0.4%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	TYR	CA-C-N	8.41	136.84	121.70
2	B	145	TYR	C-N-CA	8.41	136.84	121.70
1	A	87	HIS	N-CA-C	7.15	120.11	111.82
1	C	47	ASP	N-CA-C	-6.40	98.75	108.67
2	D	22	GLU	N-CA-C	6.21	121.25	113.43
2	B	145	TYR	O-C-N	6.09	130.69	122.59
2	B	145	TYR	CB-CA-C	-6.02	98.43	110.42
2	B	146	HIS	N-CA-CB	5.99	120.68	110.50
2	B	145	TYR	N-CA-C	-5.98	98.06	110.80
2	B	23	VAL	N-CA-C	5.91	116.65	110.62
2	D	49	SER	N-CA-C	5.83	119.49	112.38
2	B	48	LEU	N-CA-C	-5.82	103.91	111.71
2	D	118	PHE	N-CA-C	5.70	120.23	113.28
1	C	17	VAL	N-CA-C	-5.48	105.03	110.62
2	B	96	LEU	N-CA-C	5.43	119.07	112.23
2	D	36	PRO	N-CA-C	5.40	121.63	113.81
1	A	47	ASP	N-CA-C	-5.37	99.76	108.41
1	A	65	ALA	N-CA-C	-5.30	105.58	111.36
2	B	36	PRO	N-CA-C	5.06	121.15	113.81
2	B	145	TYR	CA-C-O	5.05	127.74	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CA-C-N	5.03	125.30	119.47
1	A	94	ASP	C-N-CA	5.03	125.30	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1071	31	0
1	C	1069	0	1071	10	0
2	B	1123	0	1118	35	0
2	D	1123	0	1118	29	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	0	0
5	A	34	0	29	5	0
5	C	34	0	29	3	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
7	A	113	0	0	7	0
7	B	75	0	0	4	0
7	C	138	0	0	2	0
7	D	89	0	0	3	0
All	All	5057	0	4556	98	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 11.

All (98) 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:HIS:HA	2:B:146:HIS:HB3	1.20	1.11
2:B:142:ALA:O	2:B:146:HIS:HA	1.76	0.86
2:B:146:HIS:HD2	2:D:146:HIS:CD2	1.95	0.85
2:D:143:HIS:HA	2:D:146:HIS:CD2	2.17	0.79
2:B:4:THR:HG22	2:B:7:GLU:H	1.49	0.77
1:A:45:HIS:H	1:A:45:HIS:CD2	2.02	0.75
2:B:90:GLU:HB2	2:B:144:LYS:HE3	1.68	0.75
2:B:4:THR:HG23	7:B:235:HOH:O	1.87	0.74
1:C:89:HIS:HB3	6:C:146:SO4:O2	1.87	0.73
2:B:143:HIS:HA	2:B:146:HIS:CB	2.11	0.73
4:B:148:HEM:HMC2	4:B:148:HEM:HBC2	1.73	0.71
2:B:100:PRO:HG3	2:B:145:TYR:CE2	2.26	0.70
1:A:118:THR:HG21	7:A:231:HOH:O	1.90	0.69
2:B:146:HIS:CD2	2:D:146:HIS:CD2	2.80	0.69
2:B:146:HIS:C	2:D:139:ASN:OD1	2.36	0.69
2:D:144:LYS:HD3	7:D:161:HOH:O	1.93	0.67
2:B:100:PRO:HG3	2:B:145:TYR:HE2	1.59	0.66
2:D:59:LYS:HE2	7:D:263:HOH:O	1.96	0.66
1:A:118:THR:HG23	1:A:121:VAL:H	1.60	0.66
2:D:89:SER:OG	2:D:144:LYS:HG2	1.96	0.66
2:D:97:HIS:HD2	7:D:203:HOH:O	1.78	0.65
1:A:99:LYS:NZ	7:A:433:HOH:O	2.30	0.64
2:D:142:ALA:O	2:D:145:TYR:HB2	1.98	0.64
5:A:145:B77:H3	7:A:412:HOH:O	1.98	0.64
1:C:85:ASP:HA	1:C:89:HIS:CD2	2.33	0.63
1:A:99:LYS:HE2	5:A:145:B77:H17	1.83	0.60
1:C:133:SER:HB3	5:C:145:B77:H9B	1.83	0.60
1:C:102:SER:OG	5:C:145:B77:H7	2.02	0.60
2:B:146:HIS:OXT	2:D:139:ASN:OD1	2.20	0.59
2:B:90:GLU:CB	2:B:144:LYS:HE3	2.32	0.59
7:A:209:HOH:O	2:B:120:LYS:HG2	2.01	0.59
1:C:16:LYS:NZ	7:C:422:HOH:O	2.29	0.59
1:A:116:GLU:HG2	7:A:328:HOH:O	2.03	0.58
2:B:18:VAL:HG13	2:B:23:VAL:HG21	1.88	0.56
2:B:43:GLU:OE2	1:C:92:ARG:NH1	2.38	0.56
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.88	0.56
1:A:102:SER:OG	5:A:145:B77:H7	2.05	0.56
2:B:82:LYS:HE3	2:B:143:HIS:CE1	2.42	0.55
2:D:2:HIS:O	2:D:3:LEU:HB2	2.07	0.55
1:A:45:HIS:H	1:A:45:HIS:HD2	1.51	0.54
2:D:93:CYS:SG	2:D:145:TYR:CE2	3.00	0.54
1:A:7:LYS:NZ	1:A:74:ASP:OD1	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LYS:HE3	2:B:143:HIS:NE2	2.23	0.53
1:A:16:LYS:HG3	1:A:116:GLU:HG3	1.91	0.53
2:B:142:ALA:O	2:B:146:HIS:CA	2.52	0.53
2:B:4:THR:HG21	7:B:236:HOH:O	2.09	0.53
2:B:146:HIS:HD2	2:D:146:HIS:NE2	2.07	0.52
1:A:66:LEU:O	1:A:70:VAL:HG23	2.10	0.52
2:B:90:GLU:CA	2:B:144:LYS:HE3	2.41	0.51
2:B:93:CYS:SG	2:B:144:LYS:HB2	2.51	0.50
1:A:99:LYS:CE	5:A:145:B77:H17	2.41	0.50
1:A:119:PRO:HG2	2:B:55:MET:HG3	1.93	0.50
1:A:118:THR:HG22	1:A:121:VAL:HG23	1.93	0.49
2:B:143:HIS:CA	2:B:146:HIS:HB3	2.14	0.49
2:D:75:LEU:HA	2:D:78:LEU:HD21	1.93	0.49
1:A:118:THR:HG22	1:A:121:VAL:CG2	2.42	0.49
1:A:118:THR:CG2	1:A:121:VAL:HG23	2.42	0.49
2:D:91:LEU:HD12	2:D:95:LYS:HD3	1.93	0.49
2:B:117:HIS:NE2	7:B:294:HOH:O	2.28	0.48
2:D:19:ASN:ND2	2:D:22:GLU:OE1	2.46	0.48
1:A:118:THR:OG1	1:A:119:PRO:HD2	2.14	0.48
1:C:90:LYS:HD2	7:C:218:HOH:O	2.14	0.48
2:B:94:ASP:O	2:B:97:HIS:CE1	2.67	0.48
1:A:85:ASP:O	1:A:89:HIS:HB2	2.14	0.47
2:D:90:GLU:HA	2:D:144:LYS:HG3	1.96	0.47
2:D:74:GLY:O	2:D:78:LEU:HD23	2.15	0.47
2:D:65:LYS:HE3	2:D:65:LYS:HB2	1.70	0.46
1:A:140:TYR:HA	1:C:3:SER:HB3	1.97	0.46
2:B:66:LYS:NZ	7:B:299:HOH:O	2.49	0.46
1:A:40:LYS:NZ	7:A:220:HOH:O	2.49	0.45
1:A:47:ASP:N	1:A:54:GLN:OE1	2.38	0.45
2:B:90:GLU:HA	2:B:144:LYS:HG3	1.97	0.45
1:A:85:ASP:HA	1:A:89:HIS:CD2	2.52	0.45
2:D:94:ASP:OD2	2:D:144:LYS:HE2	2.16	0.45
1:A:41:THR:HG21	7:A:219:HOH:O	2.17	0.45
2:D:1:VAL:HG11	2:D:81:LEU:HD12	2.00	0.45
2:D:4:THR:OG1	2:D:7:GLU:HG3	2.17	0.44
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.87	0.44
2:D:82:LYS:HD2	2:D:143:HIS:CD2	2.53	0.44
2:B:90:GLU:HB2	2:B:144:LYS:CE	2.43	0.44
1:A:133:SER:HB3	5:A:145:B77:H9B	2.00	0.43
1:C:34:LEU:HD12	2:D:124:PRO:HB2	2.00	0.43
1:A:45:HIS:CD2	1:A:45:HIS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:ARG:HE	2:D:104:ARG:HB2	1.47	0.42
2:D:1:VAL:HG23	2:D:1:VAL:O	2.20	0.42
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.90	0.42
1:A:118:THR:CG2	1:A:121:VAL:H	2.32	0.42
2:B:124:PRO:HB2	2:B:125:PRO:HD3	2.01	0.42
2:B:4:THR:HG22	2:B:6:GLU:N	2.34	0.41
2:D:18:VAL:HG13	2:D:23:VAL:HG21	2.01	0.41
1:A:118:THR:OG1	1:A:119:PRO:CD	2.69	0.41
2:B:45:PHE:HA	2:B:59:LYS:HD2	2.01	0.41
2:B:143:HIS:C	2:B:145:TYR:H	2.28	0.40
1:C:95:PRO:O	5:C:145:B77:H9A	2.21	0.40
2:D:100:PRO:HD3	2:D:145:TYR:CE2	2.57	0.40
1:A:58:HIS:HE1	4:A:143:HEM:CHA	2.35	0.40
2:B:57:ASN:HA	2:B:58:PRO:HD3	1.90	0.40
2:D:2:HIS:HB2	2:D:132:LYS:NZ	2.37	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%)	134 (96%)	5 (4%)	0	100	100
1	C	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	140 (97%)	3 (2%)	1 (1%)	18	8
All	All	566/574 (99%)	554 (98%)	11 (2%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	HIS

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	113/113 (100%)	111 (98%)	2 (2%)	51	43
1	C	113/113 (100%)	110 (97%)	3 (3%)	39	27
2	B	118/118 (100%)	117 (99%)	1 (1%)	73	70
2	D	118/118 (100%)	116 (98%)	2 (2%)	53	45
All	All	462/462 (100%)	454 (98%)	8 (2%)	53	45

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

Mol	Chain	Res	Type
1	A	52	SER
1	A	141	ARG
2	B	4	THR
1	C	52	SER
1	C	92	ARG
1	C	109	LEU
2	D	2	HIS
2	D	73	ASP

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

Mol	Chain	Res	Type
1	A	45	HIS
2	B	63	HIS
2	B	80	ASN
2	B	97	HIS
2	B	146	HIS
1	C	45	HIS
1	C	68	ASN
2	D	77	HIS

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Mol	Chain	Res	Type
2	D	146	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	$\# Z > 2$
5	B77	C	145	-	18,18,18	2.04	7 (38%)	23,23,23	1.24	1 (4%)
5	B77	C	144	1	18,18,18	2.25	8 (44%)	23,23,23	1.24	3 (13%)
3	OXY	A	142	4	1,1,1	0.24	0	-		
3	OXY	B	147	4	1,1,1	0.04	0	-		
4	HEM	A	143	1,3	50,50,50	1.91	17 (34%)	67,82,82	1.35	6 (8%)
4	HEM	B	148	3,2	50,50,50	1.66	12 (24%)	67,82,82	1.50	13 (19%)
6	SO4	D	149	-	4,4,4	0.45	0	6,6,6	0.17	0
4	HEM	D	148	3,2	50,50,50	1.59	10 (20%)	67,82,82	1.53	9 (13%)
5	B77	A	145	-	18,18,18	2.17	8 (44%)	23,23,23	1.10	1 (4%)
6	SO4	C	146	-	4,4,4	0.46	0	6,6,6	0.09	0
3	OXY	C	142	4	1,1,1	0.14	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	B77	A	144	1	18,18,18	2.12	6 (33%)	23,23,23	1.13	1 (4%)
4	HEM	C	143	1,3	50,50,50	1.61	10 (20%)	67,82,82	1.50	12 (17%)
3	OXY	D	147	4	1,1,1	0.27	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
5	B77	C	145	-	-	0/7/7/7	0/2/2/2
5	B77	C	144	1	-	0/7/7/7	0/2/2/2
4	HEM	B	148	3,2	-	2/14/54/54	-
4	HEM	A	143	1,3	-	4/14/54/54	-
4	HEM	D	148	3,2	-	4/14/54/54	-
5	B77	A	145	-	-	1/7/7/7	0/2/2/2
5	B77	A	144	1	-	0/7/7/7	0/2/2/2
4	HEM	C	143	1,3	-	5/14/54/54	-

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	148	HEM	C4C-NC	-4.79	1.30	1.39
4	C	143	HEM	CMA-C3A	4.20	1.59	1.50
5	A	145	B77	O8-C5	4.10	1.43	1.37
4	A	143	HEM	CHC-C1C	4.00	1.46	1.38
5	C	144	B77	O8-C5	3.99	1.43	1.37
4	A	143	HEM	C3C-C4C	-3.97	1.39	1.46
5	C	145	B77	O8-C5	3.90	1.43	1.37
5	A	144	B77	O10-C4	3.88	1.45	1.37
5	C	144	B77	C7-C6	3.68	1.44	1.38
4	B	148	HEM	CBC-CAC	3.61	1.47	1.30
5	C	144	B77	C3-C4	3.61	1.45	1.38
5	A	145	B77	C3-C4	3.52	1.44	1.38
4	B	148	HEM	C1C-NC	-3.50	1.33	1.39
4	C	143	HEM	C1A-C2A	-3.46	1.37	1.44
5	A	145	B77	C7-C6	3.44	1.44	1.38
4	B	148	HEM	CMA-C3A	3.41	1.57	1.50
4	A	143	HEM	CMC-C2C	3.39	1.57	1.50
4	A	143	HEM	CMB-C2B	3.34	1.57	1.50
5	A	144	B77	C3-C4	3.29	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	143	HEM	FE-ND	3.29	2.05	1.94
4	D	148	HEM	C1D-ND	-3.28	1.32	1.38
4	A	143	HEM	CHD-C1D	3.27	1.46	1.39
4	B	148	HEM	C3D-C2D	3.25	1.43	1.36
5	A	144	B77	C16-C15	3.12	1.45	1.38
5	C	144	B77	C6-C5	3.11	1.46	1.39
4	B	148	HEM	FE-NC	3.11	2.05	1.95
4	C	143	HEM	CBB-CAB	3.09	1.45	1.30
4	D	148	HEM	C1A-C2A	3.07	1.50	1.44
4	C	143	HEM	CBC-CAC	3.03	1.45	1.30
4	C	143	HEM	CHD-C4C	3.02	1.44	1.38
5	C	145	B77	O10-C4	2.94	1.43	1.37
4	C	143	HEM	FE-ND	2.92	2.03	1.94
5	A	144	B77	O8-C5	2.90	1.41	1.37
5	A	144	B77	C17-C12	2.88	1.45	1.38
5	C	145	B77	C16-C17	2.88	1.43	1.38
4	D	148	HEM	CAB-C3B	-2.84	1.39	1.47
4	B	148	HEM	CAB-C3B	-2.82	1.39	1.47
5	C	144	B77	O10-C4	2.79	1.42	1.37
5	C	145	B77	C17-C12	2.78	1.44	1.38
4	A	143	HEM	C3C-C2C	-2.78	1.31	1.37
5	C	145	B77	C3-C4	2.76	1.43	1.38
5	A	144	B77	C6-C5	2.75	1.45	1.39
5	C	144	B77	C16-C15	2.73	1.44	1.38
4	A	143	HEM	C4D-ND	2.66	1.44	1.40
4	A	143	HEM	FE-NB	2.61	2.02	1.94
4	A	143	HEM	CHA-C1A	2.57	1.45	1.39
5	A	145	B77	C3-C2	2.53	1.42	1.39
4	D	148	HEM	CBC-CAC	2.51	1.42	1.30
4	B	148	HEM	FE-ND	2.50	2.02	1.94
5	C	145	B77	C16-C15	2.49	1.43	1.38
4	D	148	HEM	C2A-C3A	-2.49	1.32	1.38
4	B	148	HEM	CMD-C2D	2.48	1.55	1.50
4	D	148	HEM	CHA-C1A	-2.45	1.33	1.39
4	A	143	HEM	CBC-CAC	2.45	1.42	1.30
5	A	145	B77	C6-C5	2.40	1.44	1.39
4	B	148	HEM	C4D-C3D	-2.38	1.41	1.45
5	C	144	B77	C3-C2	2.37	1.42	1.39
4	D	148	HEM	C1B-C2B	-2.35	1.39	1.44
5	A	145	B77	C16-C17	2.34	1.42	1.38
4	C	143	HEM	CAC-C3C	-2.28	1.41	1.47
4	A	143	HEM	C4D-C3D	-2.24	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	143	HEM	CBB-CAB	2.22	1.41	1.30
4	C	143	HEM	CMC-C2C	2.21	1.55	1.50
4	B	148	HEM	CBB-CAB	2.20	1.41	1.30
4	D	148	HEM	CBD-CGD	2.20	1.55	1.50
4	A	143	HEM	CHD-C4C	2.19	1.42	1.38
4	A	143	HEM	C1C-C2C	-2.17	1.41	1.45
5	A	145	B77	O10-C4	2.15	1.41	1.37
5	C	144	B77	C17-C12	2.14	1.43	1.38
5	A	145	B77	C17-C12	2.13	1.43	1.38
5	C	145	B77	C6-C5	2.13	1.44	1.39
4	A	143	HEM	CHB-C1B	2.12	1.42	1.38
4	B	148	HEM	C1D-ND	2.11	1.43	1.38
4	B	148	HEM	O2D-CGD	-2.09	1.23	1.30
4	C	143	HEM	C1B-C2B	2.04	1.48	1.44
4	D	148	HEM	CHD-C4C	2.04	1.42	1.38
4	C	143	HEM	CHD-C1D	2.02	1.43	1.39
4	A	143	HEM	FE-NA	2.01	2.01	1.95

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	143	HEM	C3B-C4B-NB	5.64	113.52	109.47
4	D	148	HEM	C3C-C2C-C1C	-5.17	102.15	107.05
4	C	143	HEM	CMD-C2D-C1D	-5.02	117.20	125.03
4	B	148	HEM	C4C-C3C-C2C	-3.92	103.41	106.81
5	C	144	B77	C14-N13-C12	3.86	122.83	117.41
4	B	148	HEM	C1D-C2D-C3D	-3.73	103.05	106.98
5	C	145	B77	C14-N13-C12	3.66	122.54	117.41
5	A	144	B77	C14-N13-C12	3.50	122.33	117.41
4	B	148	HEM	CAB-C3B-C2B	-3.36	117.50	128.43
4	D	148	HEM	CAB-C3B-C2B	-3.21	117.99	128.43
5	A	145	B77	C14-N13-C12	3.20	121.90	117.41
4	C	143	HEM	C1A-C2A-C3A	2.99	111.49	106.87
4	B	148	HEM	C3B-C4B-NB	2.95	111.59	109.47
4	D	148	HEM	C2D-C1D-ND	2.92	113.28	109.90
4	C	143	HEM	CMD-C2D-C3D	2.70	133.45	126.15
4	A	143	HEM	CAD-C3D-C2D	-2.68	122.84	127.87
4	B	148	HEM	CHC-C4B-NB	-2.59	121.64	124.42
4	C	143	HEM	CMA-C3A-C4A	2.58	129.34	125.42
4	C	143	HEM	C3C-C2C-C1C	-2.49	104.69	107.05
4	D	148	HEM	C2A-C1A-NA	-2.48	107.40	110.15
4	C	143	HEM	C4A-C3A-C2A	-2.40	104.07	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	148	HEM	CAC-C3C-C4C	-2.38	119.13	124.82
4	D	148	HEM	C2B-C1B-NB	2.38	112.58	109.84
4	D	148	HEM	CMB-C2B-C1B	2.34	128.68	125.03
4	B	148	HEM	CMB-C2B-C1B	2.31	128.64	125.03
4	B	148	HEM	CHA-C1A-NA	2.29	128.01	123.86
4	B	148	HEM	CBD-CAD-C3D	-2.28	106.23	112.53
4	B	148	HEM	C2A-C1A-NA	-2.27	107.63	110.15
4	B	148	HEM	CAB-C3B-C4B	2.26	134.38	124.39
4	C	143	HEM	CMB-C2B-C1B	-2.24	121.53	125.03
4	B	148	HEM	CMA-C3A-C4A	2.24	128.83	125.42
4	B	148	HEM	CAD-C3D-C2D	-2.21	123.72	127.87
5	C	144	B77	C15-C14-N13	-2.16	119.99	123.42
4	D	148	HEM	C4C-C3C-C2C	2.16	108.68	106.81
4	A	143	HEM	CBD-CAD-C3D	-2.12	106.67	112.53
4	C	143	HEM	CAA-C2A-C3A	-2.12	122.33	127.07
4	A	143	HEM	C2B-C1B-NB	2.11	112.26	109.84
4	C	143	HEM	CHD-C1D-ND	2.10	126.68	124.42
4	A	143	HEM	CHC-C4B-NB	-2.09	122.18	124.42
4	C	143	HEM	C4C-C3C-C2C	2.07	108.61	106.81
4	D	148	HEM	C1B-NB-C4B	-2.07	102.76	105.21
5	C	144	B77	O8-C5-C4	2.05	118.18	115.40
4	C	143	HEM	CHD-C4C-NC	-2.03	122.24	124.45
4	B	148	HEM	CAA-C2A-C3A	-2.02	122.53	127.07
4	A	143	HEM	C4D-C3D-C2D	2.02	109.83	106.89
4	C	143	HEM	C1D-C2D-C3D	2.02	109.10	106.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	148	HEM	C2B-C3B-CAB-CBB
4	D	148	HEM	C4B-C3B-CAB-CBB
5	A	145	B77	C12-C11-O10-C4
4	A	143	HEM	CAD-CBD-CGD-O2D
4	D	148	HEM	CAD-CBD-CGD-O2D
4	D	148	HEM	CAD-CBD-CGD-O1D
4	A	143	HEM	CAA-CBA-CGA-O1A
4	A	143	HEM	CAD-CBD-CGD-O1D
4	C	143	HEM	CAD-CBD-CGD-O1D
4	A	143	HEM	CAA-CBA-CGA-O2A
4	C	143	HEM	CAD-CBD-CGD-O2D
4	B	148	HEM	CAD-CBD-CGD-O1D

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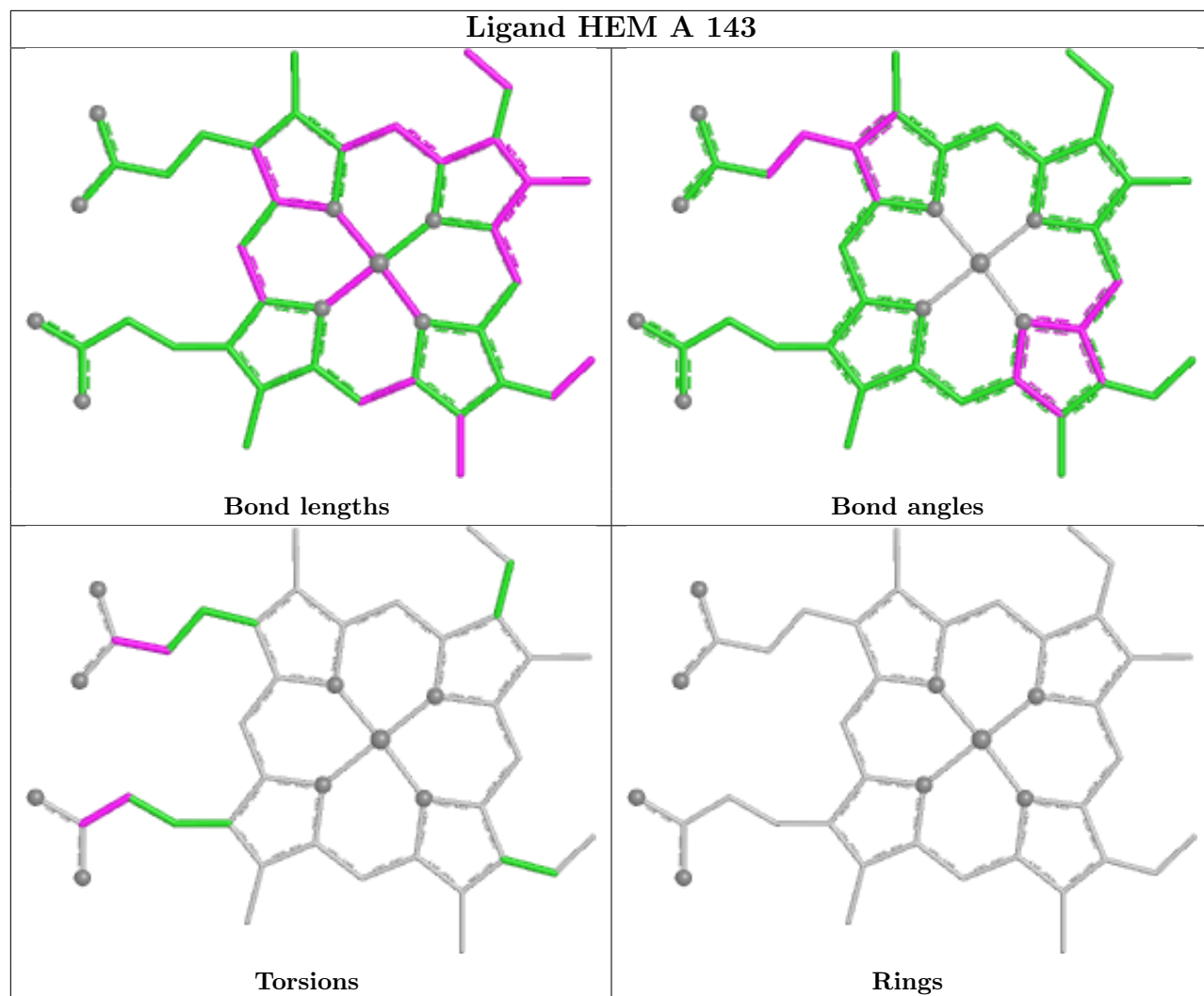
Mol	Chain	Res	Type	Atoms
4	B	148	HEM	CAD-CBD-CGD-O2D
4	C	143	HEM	CAA-CBA-CGA-O2A
4	C	143	HEM	CAA-CBA-CGA-O1A
4	C	143	HEM	C4C-C3C-CAC-CBC

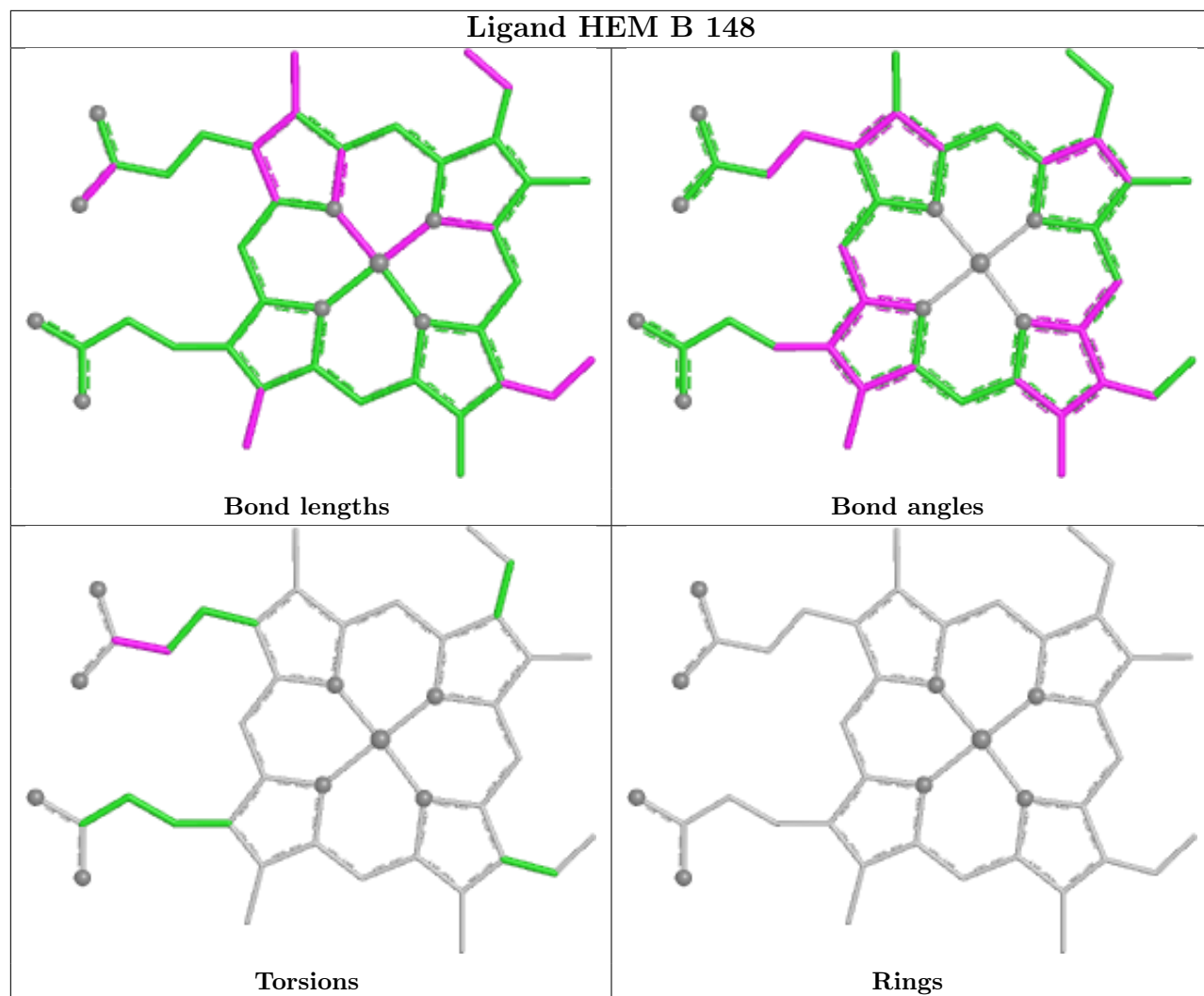
There are no ring outliers.

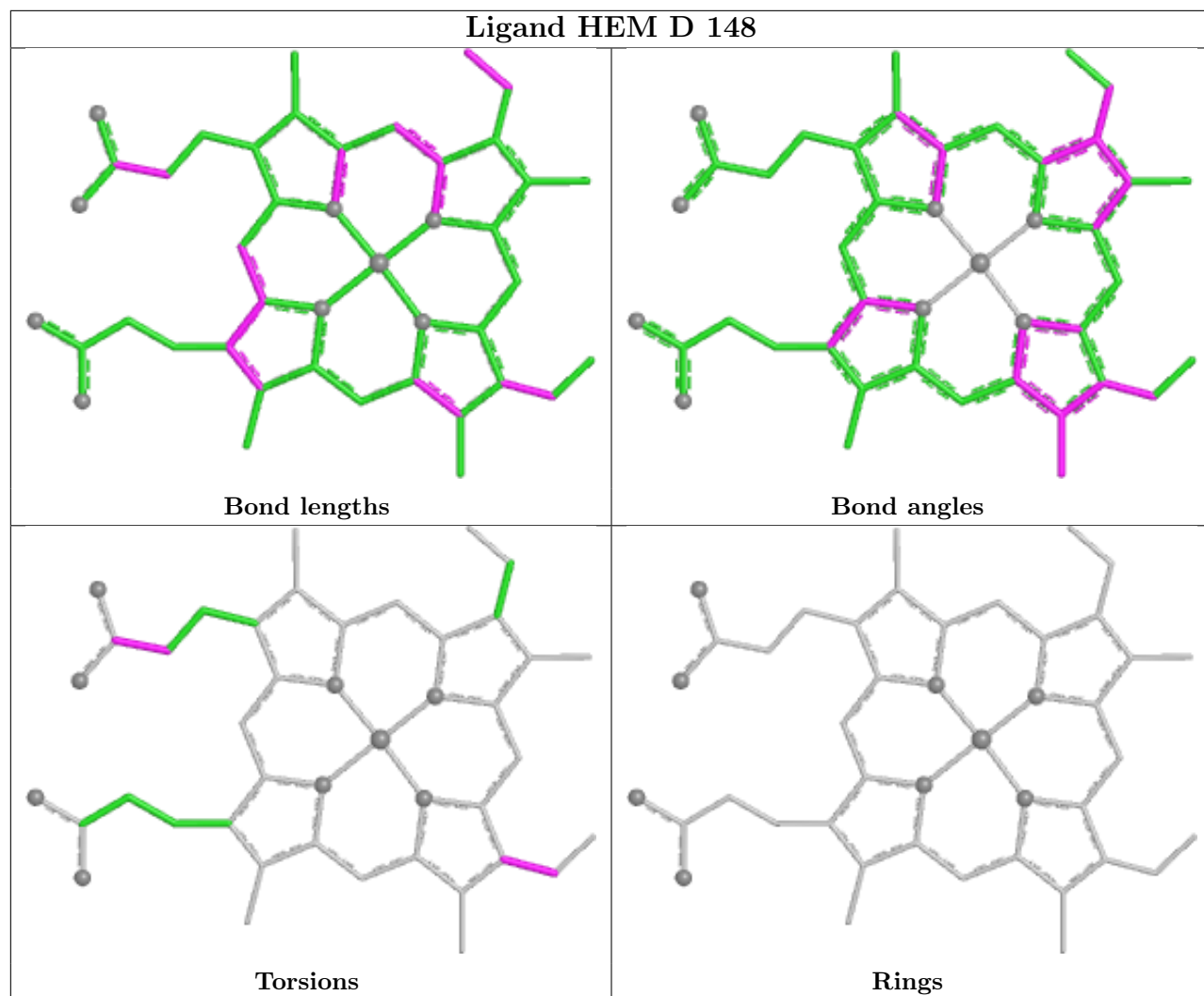
5 monomers are involved in 11 short contacts:

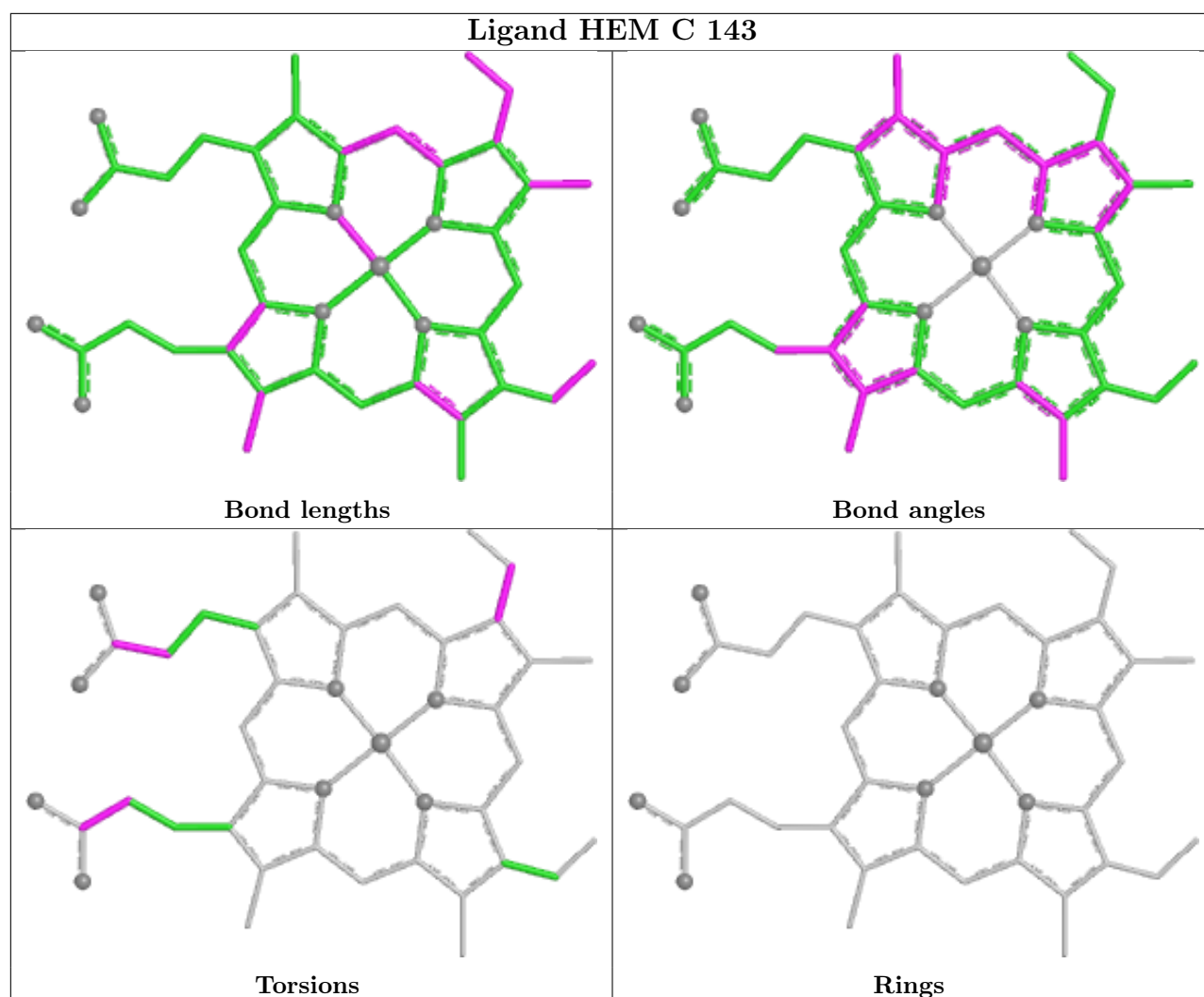
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	145	B77	3	0
4	A	143	HEM	1	0
4	B	148	HEM	1	0
5	A	145	B77	5	0
6	C	146	SO4	1	0

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%)	-0.28	0 100 100	18, 29, 40, 57	0
1	C	141/141 (100%)	-0.53	0 100 100	15, 23, 36, 52	0
2	B	146/146 (100%)	0.17	10 (6%) 23 22	19, 32, 62, 98	0
2	D	146/146 (100%)	-0.08	9 (6%) 26 25	17, 28, 68, 90	0
All	All	574/574 (100%)	-0.17	19 (3%) 49 49	15, 28, 52, 98	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	145	TYR	7.0
2	B	146	HIS	5.4
2	D	1	VAL	5.0
2	D	145	TYR	4.4
2	D	2	HIS	3.7
2	B	143	HIS	3.5
2	D	3	LEU	3.4
2	D	144	LYS	3.2
2	D	146	HIS	3.2
2	D	4	THR	2.6
2	B	1	VAL	2.6
2	B	97	HIS	2.5
2	D	143	HIS	2.4
2	B	95	LYS	2.4
2	B	43	GLU	2.2
2	D	5	PRO	2.2
2	B	117	HIS	2.2
2	B	144	LYS	2.1
2	B	96	LEU	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

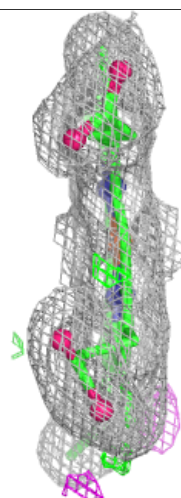
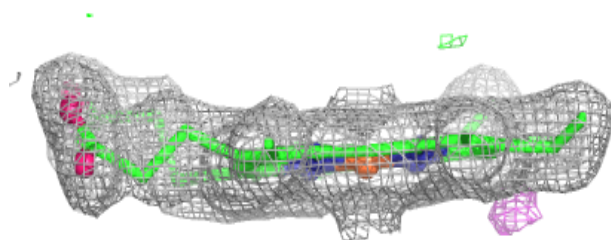
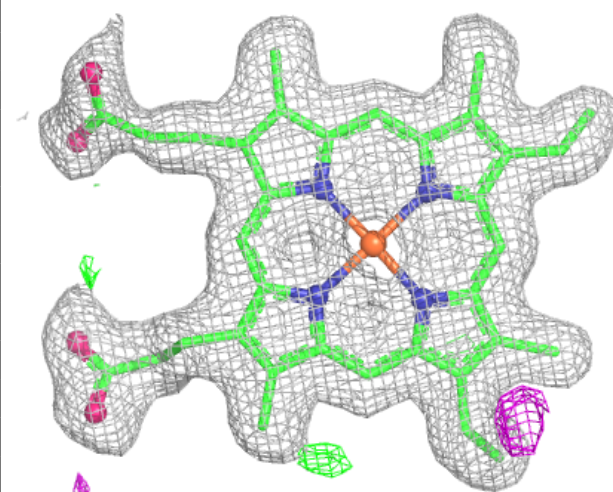
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	C	146	5/5	0.74	0.15	97,97,98,98	0
6	SO4	D	149	5/5	0.75	0.15	90,91,91,92	0
5	B77	A	145	17/17	0.79	0.27	35,44,54,55	16
5	B77	C	145	17/17	0.80	0.32	45,51,58,59	17
5	B77	C	144	17/17	0.97	0.05	19,22,25,25	0
3	OXY	D	147	2/2	0.97	0.12	31,31,31,32	0
5	B77	A	144	17/17	0.97	0.05	20,24,29,30	0
3	OXY	B	147	2/2	0.97	0.10	34,34,34,38	0
3	OXY	C	142	2/2	0.98	0.09	23,23,23,27	0
3	OXY	A	142	2/2	0.98	0.12	30,30,30,36	0
4	HEM	A	143	43/43	0.98	0.05	17,22,42,48	0
4	HEM	B	148	43/43	0.98	0.06	17,28,42,51	0
4	HEM	C	143	43/43	0.98	0.05	17,21,39,49	0
4	HEM	D	148	43/43	0.98	0.06	19,24,40,49	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.

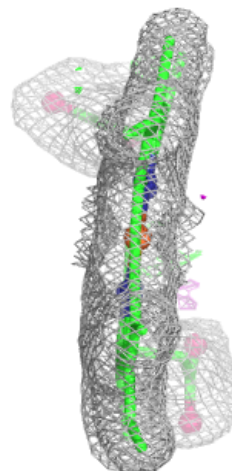
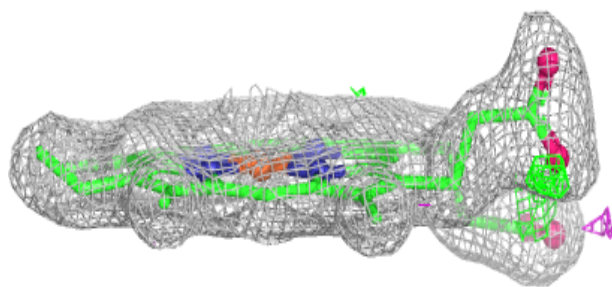
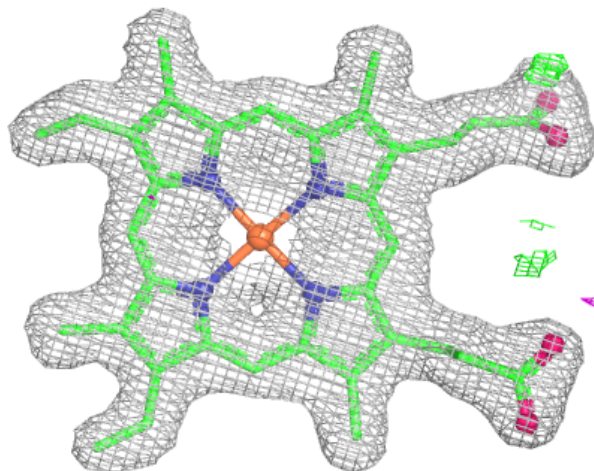
Electron density around HEM A 143:

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



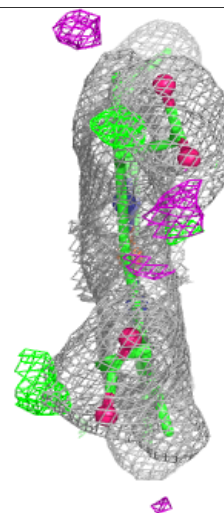
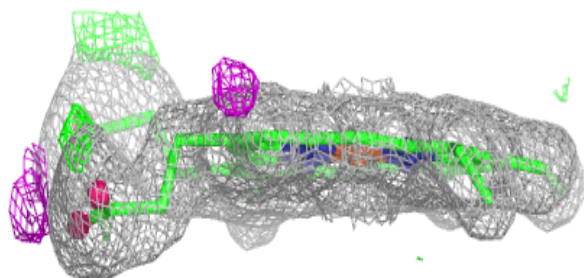
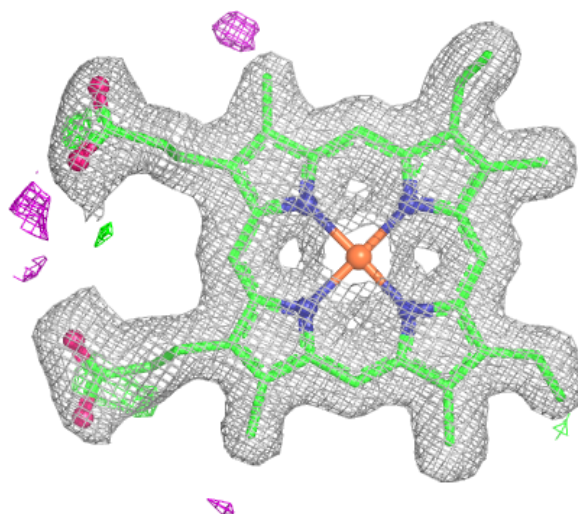
Electron density around HEM B 148:

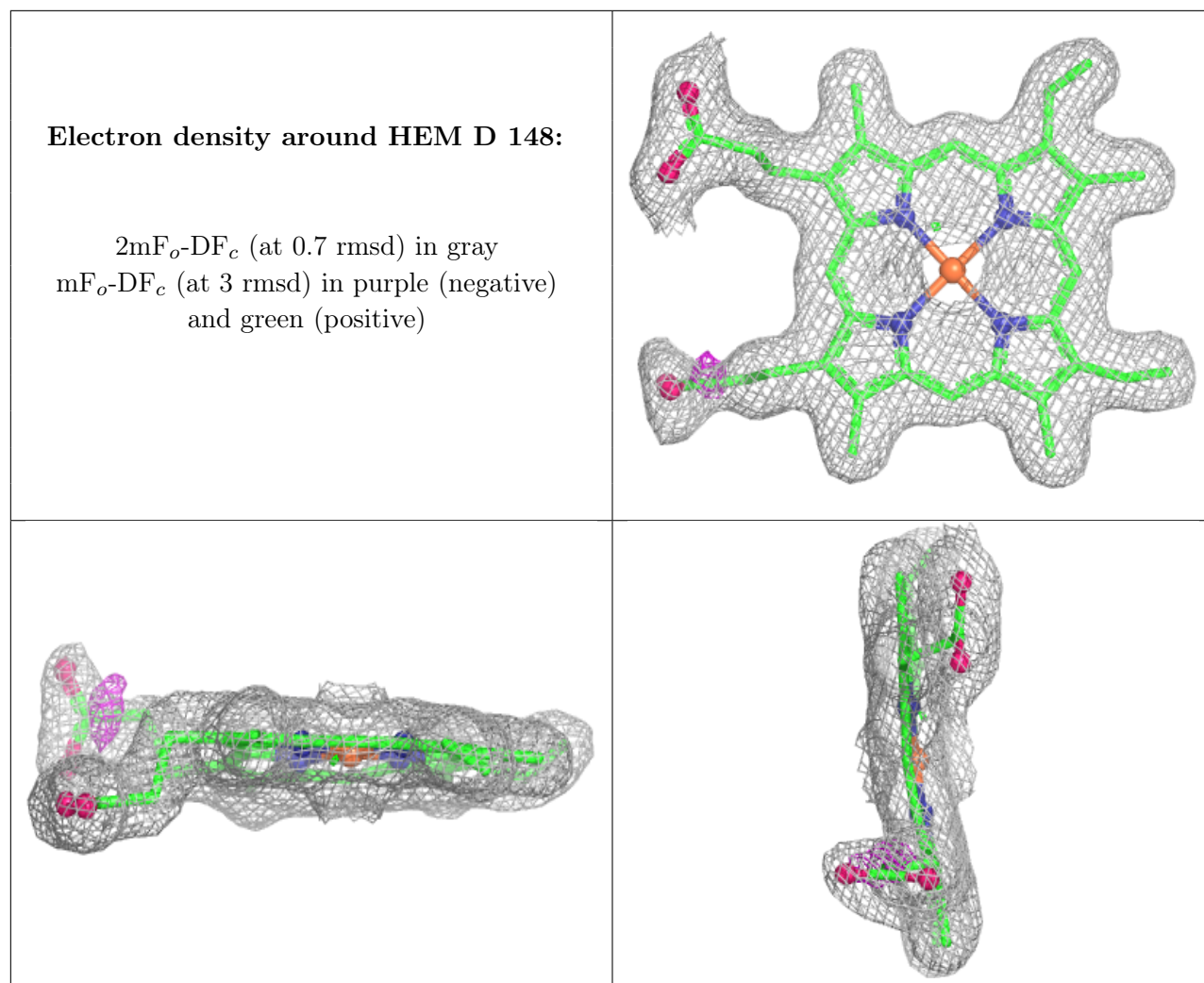
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 143:

$2mF_o-DF_c$ (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.