



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:38 AM UTC

PDB ID : 1Y4V / pdb_00001y4v
Title : T-To-T(High) quaternary transitions in human hemoglobin: betaC93A deoxy low-salt (1 test set)
Authors : Kavanaugh, J.S.; Rogers, P.H.; Arnone, A.
Deposited on : 2004-12-01
Resolution : 1.84 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

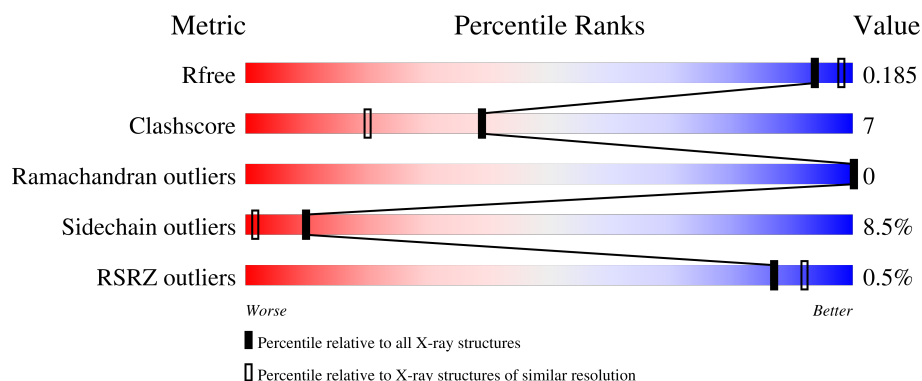
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4750 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 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	18					



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

- Molecule 4 is water.

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.

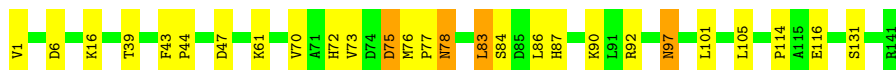
- Molecule 1: Hemoglobin alpha chain

Chain A: 



- Molecule 1: Hemoglobin alpha chain

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.00Å 99.00Å 65.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.84 10.00 – 1.84	Depositor EDS
% Data completeness (in resolution range)	90.8 (10.00-1.84) 89.3 (10.00-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.83Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , 0.230 (Not available) , 0.185	Depositor DCC
R_{free} test set	3145 reflections (6.22%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 76.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.98	1/1097 (0.1%)	1.73	20/1491 (1.3%)
1	C	0.93	0/1097	1.66	11/1491 (0.7%)
2	B	0.99	0/1153	1.71	19/1565 (1.2%)
2	D	0.92	0/1153	1.71	16/1565 (1.0%)
All	All	0.95	1/4500 (0.0%)	1.70	66/6112

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ALA	O-C-N	6.63	129.15	122.12
2	D	11	VAL	CA-C-N	6.57	129.41	120.54
2	D	11	VAL	C-N-CA	6.57	129.41	120.54
2	B	2	HIS	N-CA-CB	6.51	117.64	110.35
1	C	6	ASP	CA-CB-CG	6.43	119.03	112.60
1	C	72	HIS	CA-CB-CG	-6.04	107.76	113.80
2	D	124	PRO	CB-CA-C	5.79	117.98	110.92
2	D	93	ALA	O-C-N	5.78	128.27	122.03
2	D	146	HIS	CA-CB-CG	-5.78	108.02	113.80
1	A	81	SER	CA-C-N	5.74	127.98	120.28
1	A						

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LEU	CA-C-N	5.25	127.32	120.28
1	A	105	LEU	C-N-CA	5.25	127.32	120.28
1	C	97	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	33	PHE	O-C-N	5.23	127.67	122.12
1	A	89	HIS	CA-CB-CG	-5.22	108.58	113.80
1	C	75	ASP	N-CA-CB	-5.21	101.48	111.53
1	C	87	HIS	N-CA-CB	5.17	117.72	110.12
1	A	58	HIS	CA-CB-CG	-5.17	108.63	113.80
1	C	92	ARG	CA-CB-CG	-5.15	103.81	114.10
2	B	72	SER	O-C-N	5.14	127.57	122.12
2	B						

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	48	0	0	0	0
4	D	33	0	0	2	0
All	All	4750	0	4502	62	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 7.

All (62) 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:D:45:PHE:HA	2:D:59:LYS:HD2	1.60	0.83
2:D:66:LYS:HE3	3:D:147:HEM:HAA1	1.66	0.78
2:D:4:THR:HB	2:D:7:GLU:HG3	1.73	0.70
2:B:143:HIS:HB2	4:B:378:HOH:O	1.93	0.68
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.11	0.66
2:B:73:ASP:HB3	4:B:269:HOH:		

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:NZ	1:A:16:LYS:HB3	2.30	0.46
2:B:75:LEU:HA	2:B:78:LEU:HD13	1.97	0.46
2:D:8:LYS:O	2:D:12:THR:HB	2.15	0.46
2:D:48:LEU:HB3	2:D:54:VAL:HG22	1.99	0.45
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.68	0.45
2:B:83:GLY:HA2	4:B:298:HOH:O	2.17	0.45
2:D:51:PRO:O	2:D:55:MET:HG2	2.18	0.43
1:C:86:LEU:CD1	1:C:90:LYS:HD3	2.48	0.43
1:A:133:SER:O	1:A:137:THR:HB	2.19	0.43
1:C:76:MET:N	1:C:77:PRO:HD2	2.34	0.43
2:B:53:ALA:O	2:B:57:ASN:HB2	2.18	0.43
2:D:124:PRO:N	2:D:125:PRO:CD	2.81	0.43
2:B:1:MET:HE2	2:B:81:LEU:HD11	2.0	

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%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
All	All	566/574 (99%)	549 (97%)	17 (3%)	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.

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Mol	Chain	Res	Type
2	B	6	GLU
2	B	8	LYS
2	B	9	SER
2	B	12	THR
2	B	20	VAL
2	B	26	GLU
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	79	ASP
2	B	88	LEU
2	B	104	ARG
2	B	120	LYS
1	C	1	VAL
1	C	61	LYS
1	C	83	LEU
1	C	101	LEU
1	C	105	LEU
2	D	9	SER
2	D	12	THR
2	D	26	GLU
2	D	52	ASP
2	D	61	LYS
2	D	65	LYS
2	D	68	LEU
2	D		

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Mol	Chain	Res	Type
2	D	63	HIS
2	D	102	ASN
2	D	116	HIS
2	D	146	HIS

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](#)

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 $|Z| > 2$

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	147	2	-	7/14/54/54	-
3	HEM	B	147	2	-	3/14/54/54	-
3	HEM	A	142	1	-	4/14/54/54	-
3	HEM	C	142	1	-	6/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	FE-NB	4.48	2.08	1.94
3	A	142	HEM	FE-NB	3.42	2.05	1.94
3	A	142	HEM	FE-NC	3.36	2.06	1.95
3	C	142	HEM	CMD-C2D	3.30	1.57	1.50
3	C	142	HEM	FE-NC	3.24	2.05	1.95
3	B	147	HEM				

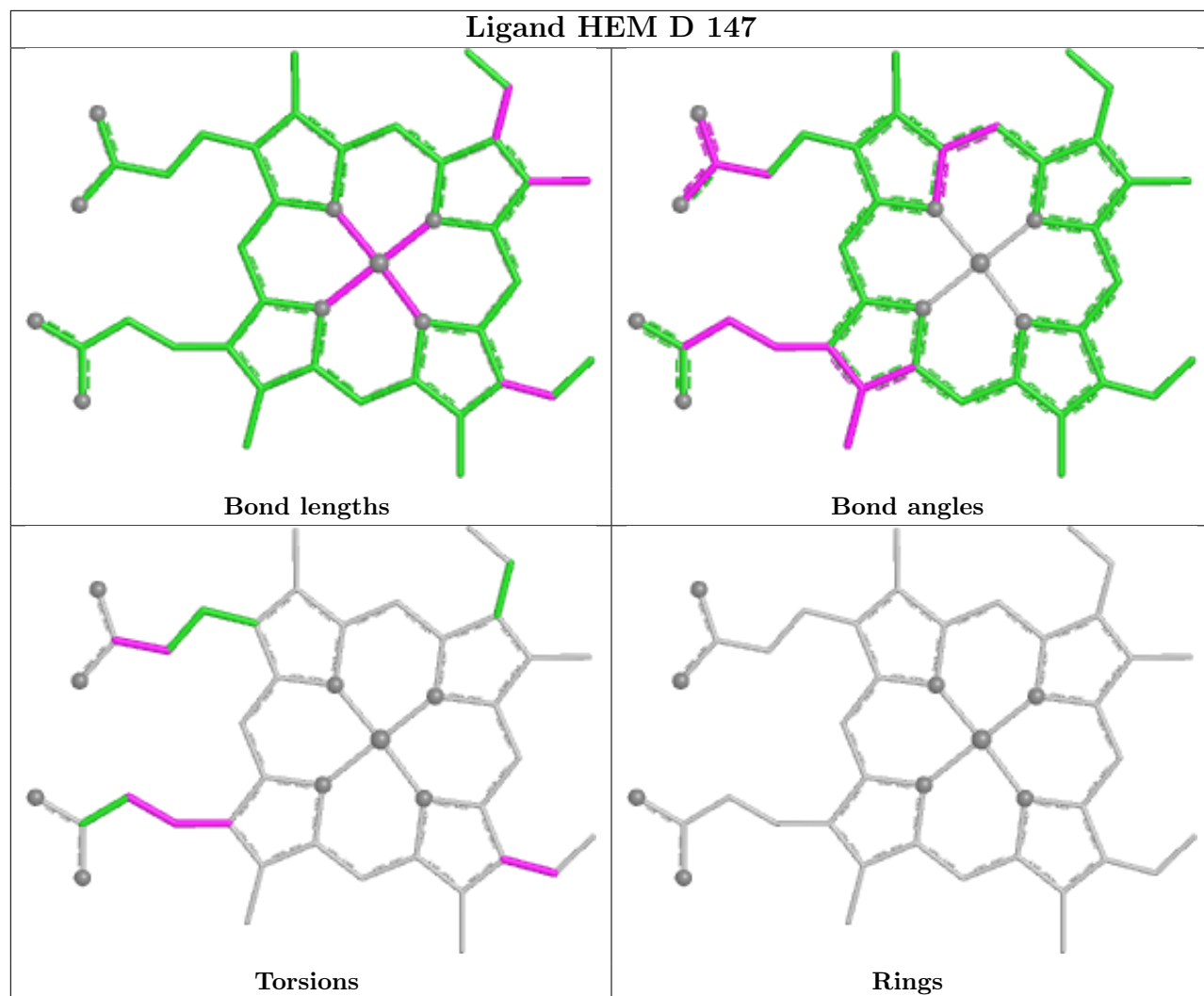
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	O1A-CGA-CBA	-3.01	113.53	123.09
3	D	147	HEM	O1D-CGD-CBD	-3.00	113.57	123.09
3	A	142	HEM	O1A-CGA-CBA	-2.56	114.96	123.09
3	C	142	HEM	O2A-CGA-O1A	2.55	129.90	123.33
3	D	147	HEM	CHD-C1D-ND	2.53	127.15	124.42
3	C	142	HEM	O1D-CGD-CBD	-2.52	115.10	123.09
3	D	147	HEM	CBA-CAA-C2A	2.47	119.37	112.53
3	D	147	HEM	CAA-CBA-CGA	2.47	120.22	113.67
3	D	147	HEM	O2D-CGD-O1D	2.43	129.58	123.33
3	C	142	HEM	CHB-C1B-NB	2.36	127.29	124.37
3	C	1					

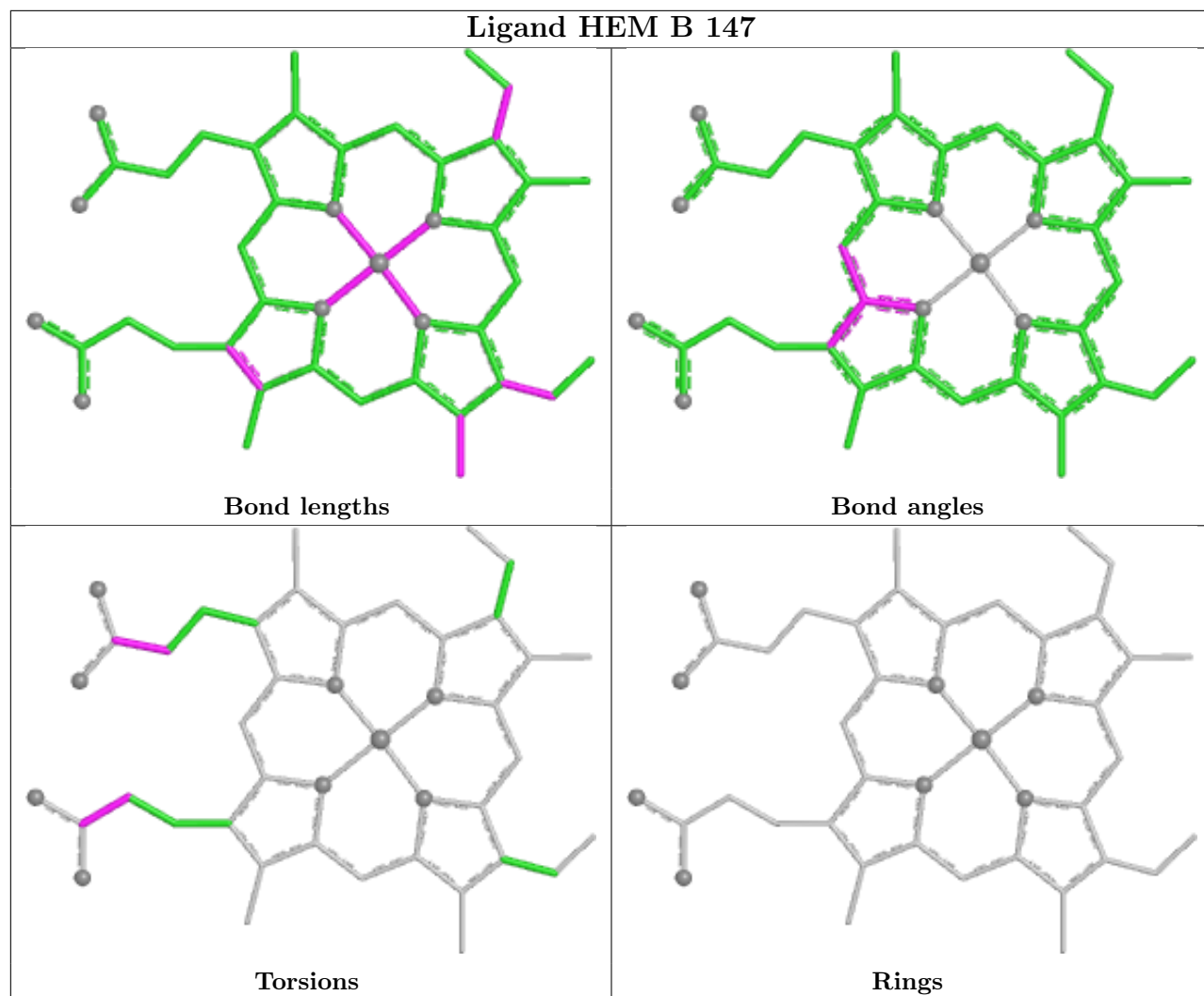
There are no ring outliers.

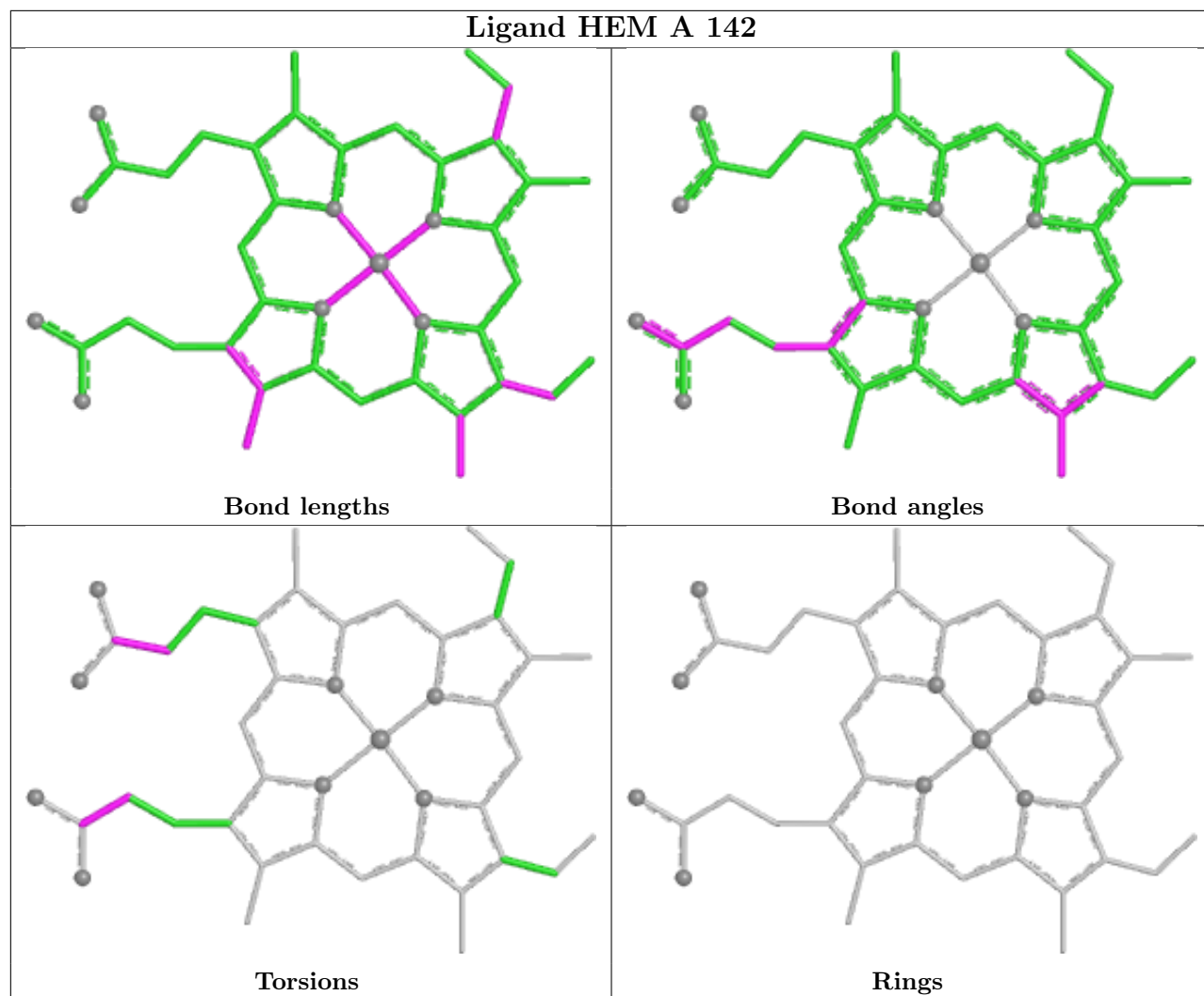
2 monomers are involved in 3 short contacts:

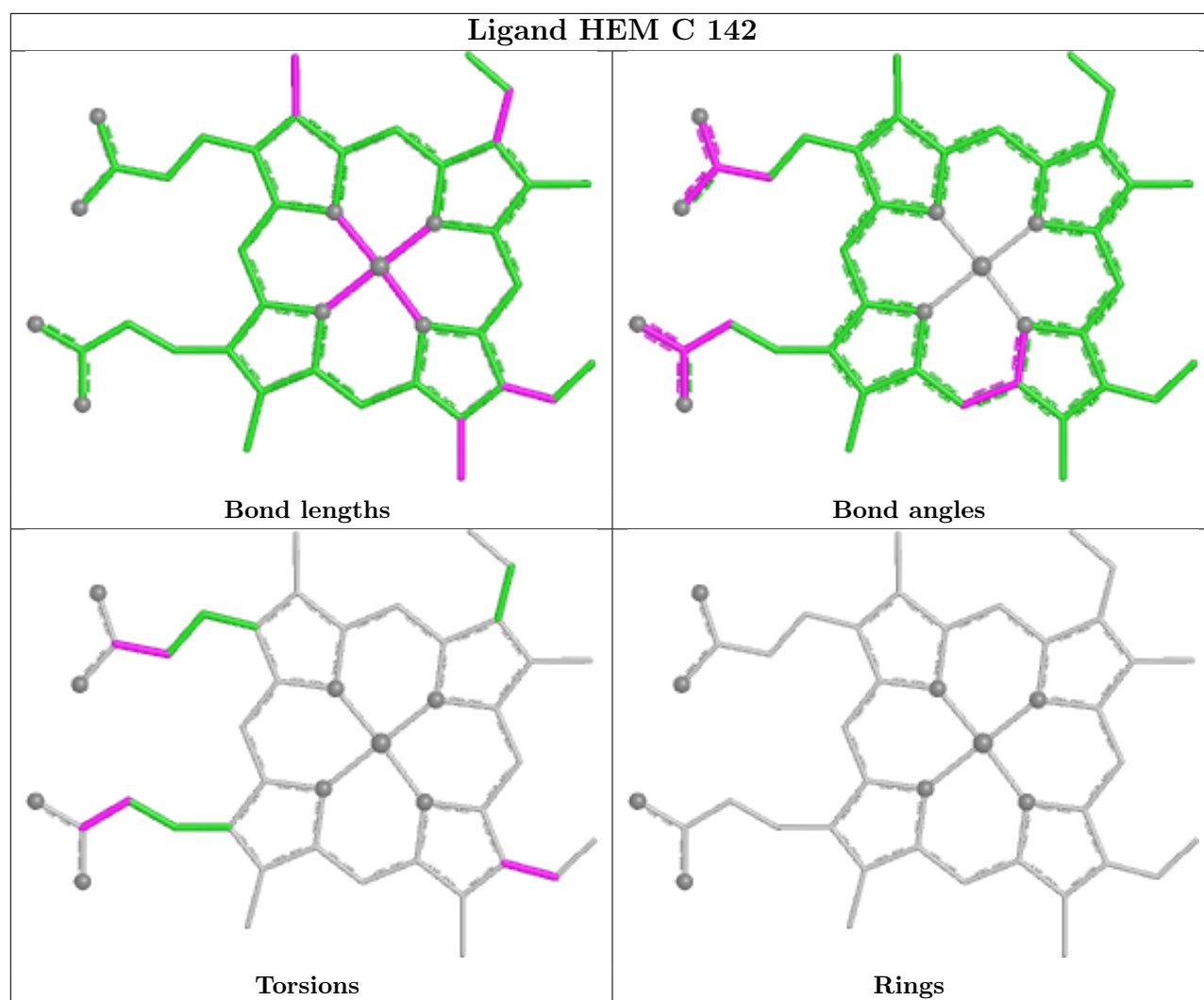
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	147	HEM	2	0
3	B	147	HEM	1	0

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](#)

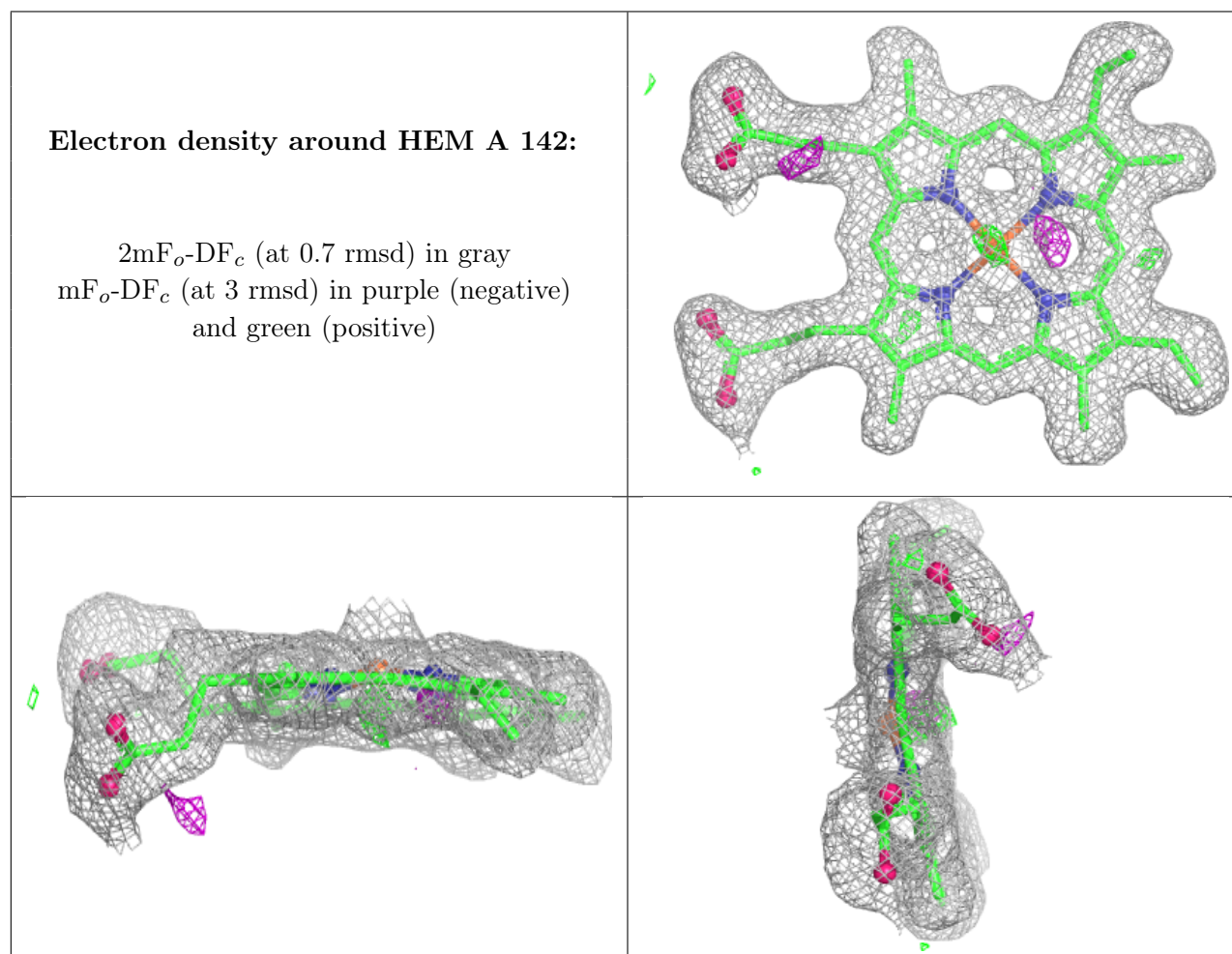
6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.72	0 100 100	10, 17, 34, 46	0
1	C	141/141 (100%)	-0.60	0 100 100	9, 21, 40, 56	0
2	B	146/146 (100%)	-0.61	1 (0%) 84 90	8, 17, 50, 109	0
2	D	146/146 (100%)	-0.35	2 (1%) 73 81	11, 24, 53, 107	0
All	All	574/574 (100%)	-0.57	3 (0%) 87 92	8, 20, 48, 109	0

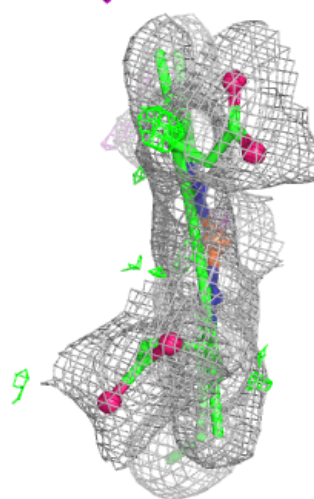
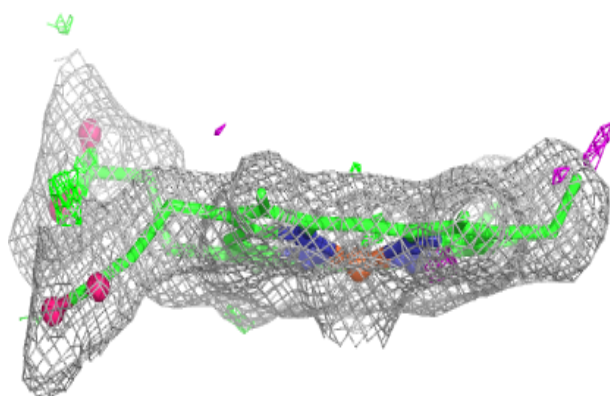
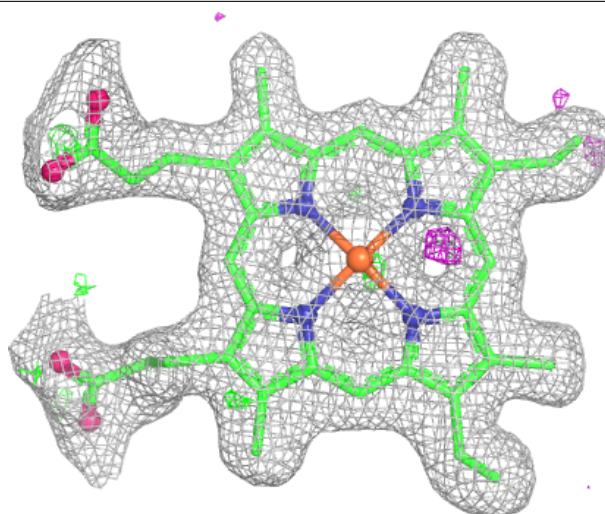
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	A	142	43/43	0.97	0.05	9,15,30,41	0
3	HEM	D	147	43/43	0.97	0.06	12,19,45,56	0
3	HEM	C	142	43/43	0.98	0.05	9,13,35,47	0
3	HEM	B	147	43/43	0.98	0.04	5,10,19,34	0

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.



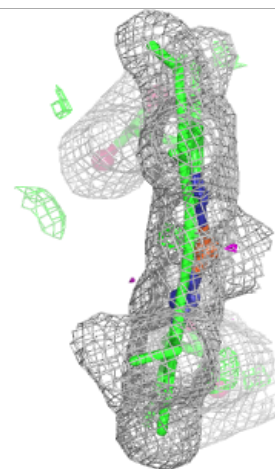
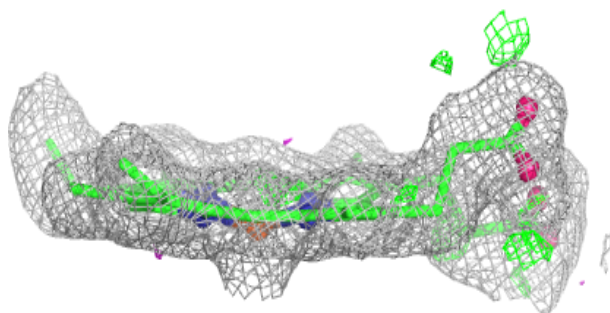
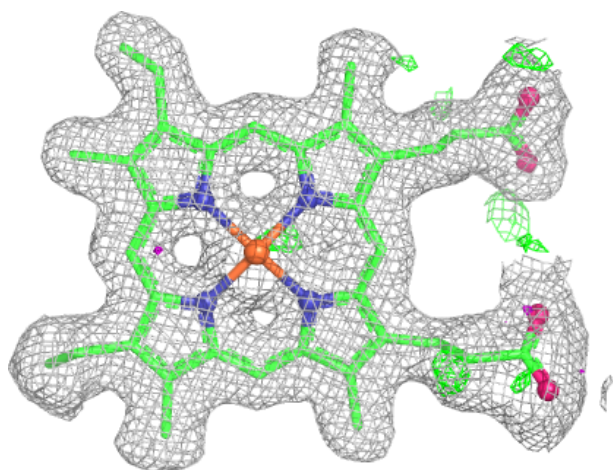
Electron density around HEM D 147:

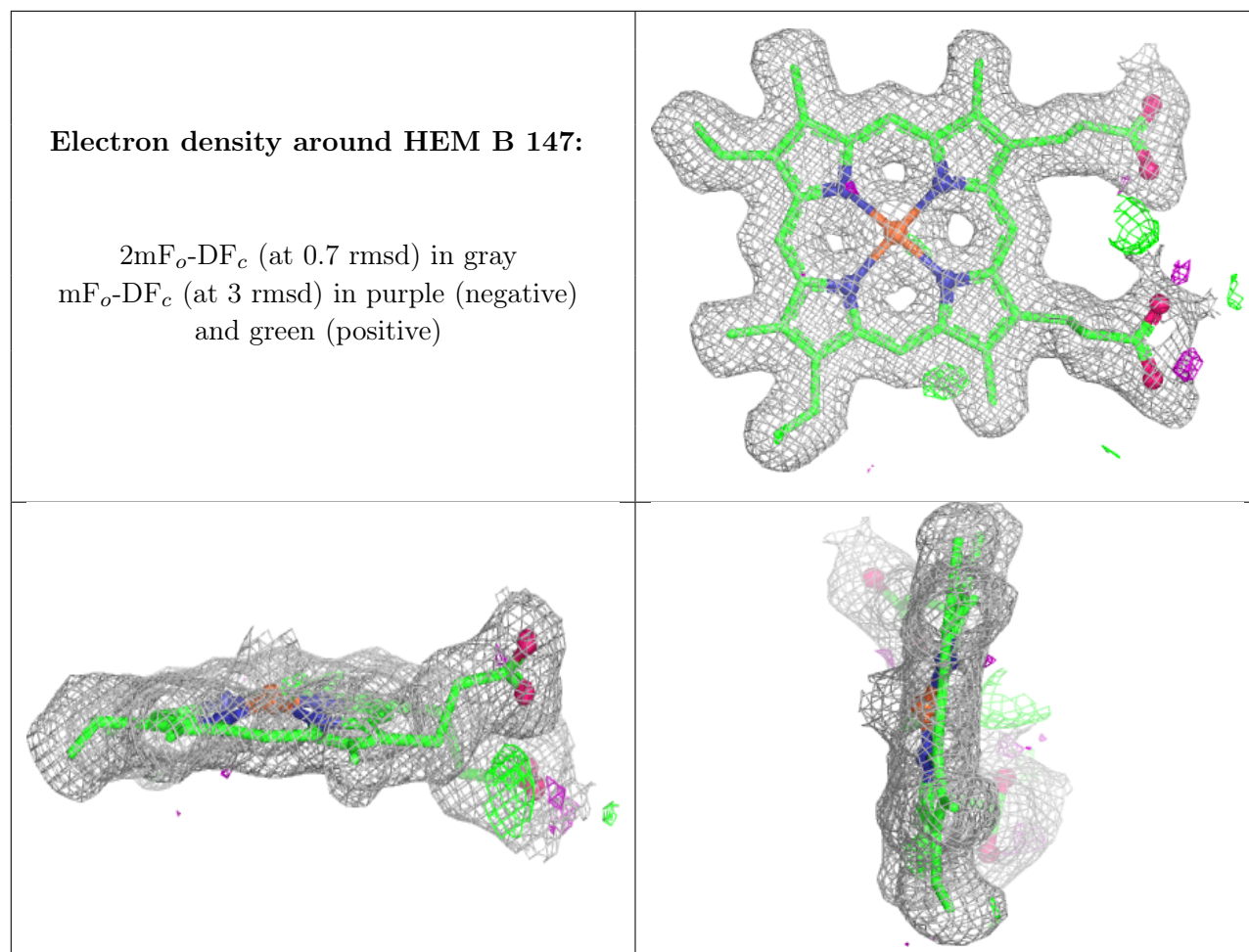
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 142:

$2mF_o-DF_c$ (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.