



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 10:36 AM EST

PDB ID : 1LH1
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)
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Deposited on : 1982-04-23
Resolution : 2.00 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

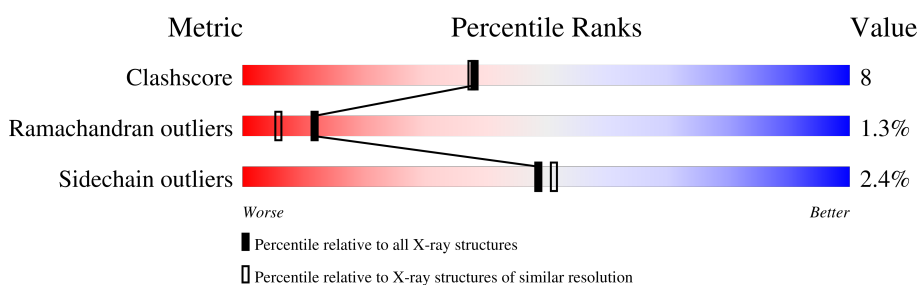
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	154	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1296 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.

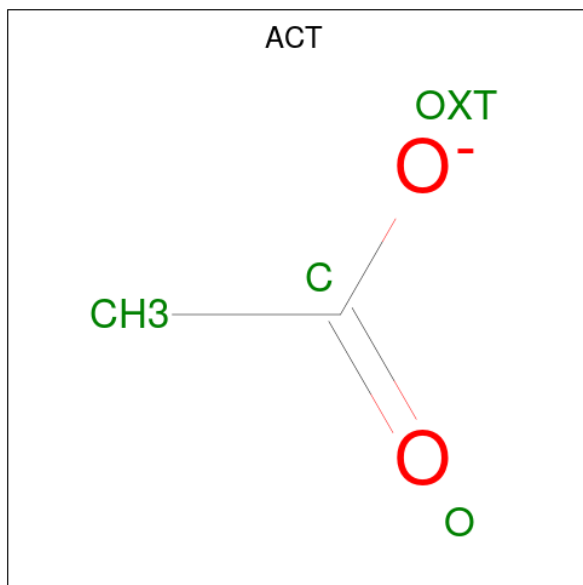
- Molecule 1 is a protein called LEGHEMOGLOBIN (ACETO MET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1180	761	193	225	1	36	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	conflict	UNP P02240
A	150	ASP	ASN	conflict	UNP P02240

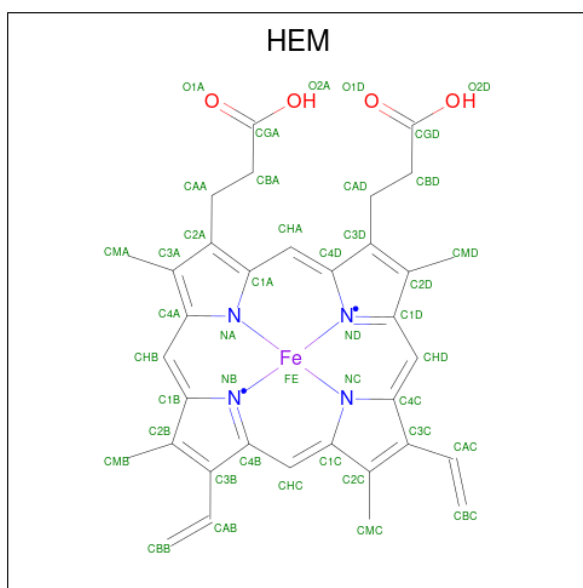
- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



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

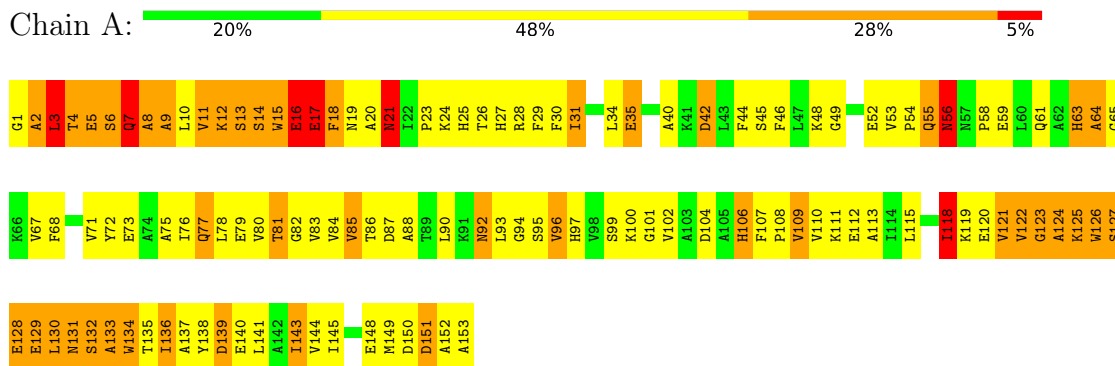
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		

3 Residue-property plots [i](#)

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. 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. 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: LEGHEMOGLOBIN (ACETO MET)



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.33Å 38.40Å 52.40Å 90.00° 90.00° 99.00°	Depositor
Resolution (Å)	(Not available) – 2.00 46.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 99.9 (46.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.520 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 152.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	1296	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, 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	3.35	160/1214 (13.2%)	2.32	64/1648 (3.9%)

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	11

All (160) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	CD2-CE2	11.61	1.55	1.41
1	A	138	TYR	CB-CG	10.52	1.67	1.51
1	A	95	SER	CB-OG	10.43	1.55	1.42
1	A	35	GLU	CD-OE2	9.81	1.36	1.25
1	A	112	GLU	CG-CD	9.61	1.66	1.51
1	A	132[A]	SER	CA-CB	9.36	1.67	1.52
1	A	132[B]	SER	CA-CB	9.36	1.67	1.52
1	A	132[C]	SER	CA-CB	9.36	1.67	1.52
1	A	13	SER	CA-CB	9.27	1.66	1.52
1	A	72	TYR	CE1-CZ	9.12	1.50	1.38
1	A	138	TYR	CZ-OH	9.10	1.53	1.37
1	A	121	VAL	CB-CG2	9.03	1.71	1.52
1	A	106	HIS	CB-CG	8.82	1.66	1.50
1	A	120	GLU	CG-CD	8.63	1.65	1.51
1	A	44	PHE	CB-CG	8.57	1.66	1.51
1	A	15	TRP	CZ3-CH2	8.55	1.53	1.40
1	A	94	GLY	CA-C	8.47	1.65	1.51
1	A	65	GLY	C-O	8.38	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	PHE	CB-CG	8.37	1.65	1.51
1	A	72	TYR	CG-CD2	8.30	1.50	1.39
1	A	40	ALA	CA-CB	8.30	1.69	1.52
1	A	15	TRP	CG-CD1	8.28	1.48	1.36
1	A	123	GLY	CA-C	8.22	1.65	1.51
1	A	138	TYR	CD2-CE2	8.19	1.51	1.39
1	A	15	TRP	CB-CG	8.04	1.64	1.50
1	A	140	GLU	CB-CG	8.00	1.67	1.52
1	A	5	GLU	CD-OE2	8.00	1.34	1.25
1	A	129	GLU	CD-OE1	7.82	1.34	1.25
1	A	15	TRP	CD1-NE1	7.77	1.51	1.38
1	A	68	PHE	CG-CD2	7.65	1.50	1.38
1	A	67	VAL	CB-CG2	7.63	1.68	1.52
1	A	46	PHE	CB-CG	7.61	1.64	1.51
1	A	11	VAL	CB-CG1	7.52	1.68	1.52
1	A	101	GLY	CA-C	7.46	1.63	1.51
1	A	134	TRP	N-CA	7.35	1.61	1.46
1	A	124	ALA	N-CA	7.32	1.60	1.46
1	A	11	VAL	N-CA	7.32	1.60	1.46
1	A	73	GLU	CG-CD	7.31	1.62	1.51
1	A	102	VAL	CB-CG1	7.28	1.68	1.52
1	A	128	GLU	CD-OE2	-7.24	1.17	1.25
1	A	85	VAL	CB-CG2	7.23	1.68	1.52
1	A	110	VAL	CB-CG2	7.22	1.68	1.52
1	A	27	HIS	CE1-NE2	7.21	1.49	1.32
1	A	97	HIS	CA-CB	7.07	1.69	1.53
1	A	79	GLU	CB-CG	7.01	1.65	1.52
1	A	88	ALA	N-CA	6.96	1.60	1.46
1	A	145	ILE	N-CA	6.95	1.60	1.46
1	A	86	THR	N-CA	6.95	1.60	1.46
1	A	6	SER	CA-CB	6.91	1.63	1.52
1	A	71	VAL	CB-CG1	6.78	1.67	1.52
1	A	13	SER	CB-OG	-6.77	1.33	1.42
1	A	68	PHE	N-CA	6.75	1.59	1.46
1	A	106	HIS	ND1-CE1	6.75	1.51	1.34
1	A	148	GLU	CD-OE2	6.70	1.33	1.25
1	A	138	TYR	CD1-CE1	6.68	1.49	1.39
1	A	120	GLU	CA-CB	6.59	1.68	1.53
1	A	152	ALA	C-O	6.58	1.35	1.23
1	A	144	VAL	CB-CG2	6.57	1.66	1.52
1	A	111	LYS	N-CA	6.53	1.59	1.46
1	A	27	HIS	CG-ND1	6.45	1.52	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	SER	N-CA	6.44	1.59	1.46
1	A	16	GLU	CD-OE1	6.43	1.32	1.25
1	A	95	SER	N-CA	6.42	1.59	1.46
1	A	68	PHE	CE1-CZ	6.42	1.49	1.37
1	A	1	GLY	C-O	6.41	1.33	1.23
1	A	61	GLN	C-O	6.41	1.35	1.23
1	A	97	HIS	CG-CD2	-6.41	1.24	1.35
1	A	72	TYR	C-O	6.32	1.35	1.23
1	A	35	GLU	CD-OE1	-6.32	1.18	1.25
1	A	81	THR	CA-CB	6.31	1.69	1.53
1	A	109	VAL	CA-CB	6.26	1.68	1.54
1	A	122	VAL	N-CA	6.25	1.58	1.46
1	A	45	SER	N-CA	6.21	1.58	1.46
1	A	15	TRP	C-O	6.20	1.35	1.23
1	A	45	SER	CB-OG	6.20	1.50	1.42
1	A	134	TRP	CD2-CE2	-6.18	1.33	1.41
1	A	90	LEU	CA-CB	6.15	1.67	1.53
1	A	28	ARG	CZ-NH1	6.13	1.41	1.33
1	A	149	MET	C-O	6.11	1.34	1.23
1	A	130	LEU	N-CA	6.10	1.58	1.46
1	A	143	ILE	CA-CB	6.09	1.68	1.54
1	A	148	GLU	CB-CG	6.08	1.63	1.52
1	A	2	ALA	CA-CB	6.07	1.65	1.52
1	A	64	ALA	N-CA	6.04	1.58	1.46
1	A	18	PHE	N-CA	6.04	1.58	1.46
1	A	79	GLU	CD-OE2	6.03	1.32	1.25
1	A	104	ASP	N-CA	6.01	1.58	1.46
1	A	16	GLU	CG-CD	6.00	1.60	1.51
1	A	75	ALA	C-O	5.97	1.34	1.23
1	A	102	VAL	N-CA	5.94	1.58	1.46
1	A	20	ALA	N-CA	-5.93	1.34	1.46
1	A	76	ILE	C-O	5.90	1.34	1.23
1	A	77	GLN	CG-CD	5.89	1.64	1.51
1	A	124	ALA	C-O	5.87	1.34	1.23
1	A	87	ASP	CA-C	5.86	1.68	1.52
1	A	68	PHE	C-O	5.85	1.34	1.23
1	A	53	VAL	CA-CB	5.83	1.67	1.54
1	A	8	ALA	C-O	5.83	1.34	1.23
1	A	140	GLU	CD-OE2	5.81	1.32	1.25
1	A	77	GLN	CA-CB	5.72	1.66	1.53
1	A	113	ALA	CA-CB	5.69	1.64	1.52
1	A	55	GLN	C-O	5.68	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	9	ALA	CA-CB	5.67	1.64	1.52
1	A	82	GLY	CA-C	5.66	1.60	1.51
1	A	59	GLU	CD-OE2	5.62	1.31	1.25
1	A	84	VAL	N-CA	5.62	1.57	1.46
1	A	81	THR	N-CA	-5.61	1.35	1.46
1	A	106	HIS	CA-CB	5.56	1.66	1.53
1	A	133	ALA	CA-C	5.51	1.67	1.52
1	A	127	SER	CA-CB	5.51	1.61	1.52
1	A	99	SER	C-O	5.50	1.33	1.23
1	A	84	VAL	CB-CG1	5.47	1.64	1.52
1	A	138	TYR	N-CA	5.46	1.57	1.46
1	A	63	HIS	CG-ND1	-5.42	1.26	1.38
1	A	20	ALA	CA-CB	5.41	1.63	1.52
1	A	7	GLN	N-CA	5.41	1.57	1.46
1	A	24	LYS	CD-CE	5.41	1.64	1.51
1	A	127	SER	C-O	5.39	1.33	1.23
1	A	125	LYS	CD-CE	5.39	1.64	1.51
1	A	44	PHE	CD2-CE2	5.38	1.50	1.39
1	A	58	PRO	N-CD	5.38	1.55	1.47
1	A	52	GLU	CG-CD	-5.37	1.43	1.51
1	A	108	PRO	C-N	5.36	1.46	1.34
1	A	110	VAL	CA-C	5.35	1.66	1.52
1	A	49	GLY	CA-C	-5.34	1.43	1.51
1	A	92	ASN	C-O	5.34	1.33	1.23
1	A	14	SER	CB-OG	-5.33	1.35	1.42
1	A	111	LYS	CD-CE	5.31	1.64	1.51
1	A	44	PHE	CD1-CE1	5.30	1.49	1.39
1	A	4	THR	C-O	5.30	1.33	1.23
1	A	21	ASN	N-CA	5.29	1.56	1.46
1	A	71	VAL	N-CA	5.28	1.56	1.46
1	A	141	LEU	CB-CG	5.28	1.67	1.52
1	A	30	PHE	N-CA	5.27	1.56	1.46
1	A	136	ILE	CA-CB	5.27	1.67	1.54
1	A	68	PHE	CE2-CZ	5.26	1.47	1.37
1	A	52	GLU	N-CA	5.23	1.56	1.46
1	A	63	HIS	CA-C	5.22	1.66	1.52
1	A	153	ALA	C-OXT	5.21	1.33	1.23
1	A	85	VAL	CA-C	5.21	1.66	1.52
1	A	141	LEU	N-CA	5.21	1.56	1.46
1	A	68	PHE	CG-CD1	5.20	1.46	1.38
1	A	100	LYS	C-N	-5.20	1.23	1.33
1	A	78	LEU	C-N	-5.20	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	LYS	CB-CG	5.20	1.66	1.52
1	A	79	GLU	C-O	5.20	1.33	1.23
1	A	137	ALA	N-CA	5.19	1.56	1.46
1	A	28	ARG	CZ-NH2	5.14	1.39	1.33
1	A	144	VAL	CA-C	5.12	1.66	1.52
1	A	30	PHE	CA-CB	5.12	1.65	1.53
1	A	104	ASP	C-O	5.11	1.33	1.23
1	A	29	PHE	CG-CD2	5.10	1.46	1.38
1	A	28	ARG	CA-CB	5.09	1.65	1.53
1	A	136	ILE	N-CA	-5.06	1.36	1.46
1	A	148	GLU	C-O	5.04	1.32	1.23
1	A	92	ASN	CB-CG	5.03	1.62	1.51
1	A	115	LEU	N-CA	5.03	1.56	1.46
1	A	152	ALA	N-CA	5.02	1.56	1.46
1	A	2	ALA	C-N	-5.01	1.22	1.34
1	A	11	VAL	CA-CB	-5.00	1.44	1.54

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	TYR	CB-CG-CD1	-11.84	113.90	121.00
1	A	28	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	15	TRP	CG-CD2-CE3	-10.13	124.78	133.90
1	A	112	GLU	OE1-CD-OE2	-9.37	112.06	123.30
1	A	16	GLU	OE1-CD-OE2	-9.13	112.34	123.30
1	A	73	GLU	OE1-CD-OE2	-8.65	112.92	123.30
1	A	138	TYR	CB-CG-CD2	8.23	125.94	121.00
1	A	15	TRP	CD1-NE1-CE2	-8.15	101.67	109.00
1	A	29	PHE	CB-CG-CD1	-7.72	115.39	120.80
1	A	17	GLU	OE1-CD-OE2	-7.50	114.31	123.30
1	A	124	ALA	CB-CA-C	-7.43	98.95	110.10
1	A	15	TRP	CB-CG-CD1	7.31	136.50	127.00
1	A	126	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A	15	TRP	CE2-CD2-CE3	7.04	127.15	118.70
1	A	128	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	A	134	TRP	CG-CD1-NE1	-6.90	103.20	110.10
1	A	15	TRP	CH2-CZ2-CE2	-6.89	110.51	117.40
1	A	87	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	80	VAL	CA-CB-CG2	-6.74	100.80	110.90
1	A	30	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	A	138	TYR	CD1-CE1-CZ	6.69	125.82	119.80
1	A	68	PHE	CB-CG-CD1	-6.58	116.19	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	VAL	CA-CB-CG1	-6.53	101.11	110.90
1	A	72	TYR	CG-CD1-CE1	-6.49	116.11	121.30
1	A	54	PRO	N-CA-CB	6.42	111.01	103.30
1	A	29	PHE	CD1-CG-CD2	6.41	126.64	118.30
1	A	15	TRP	CD2-CE3-CZ3	-6.35	110.54	118.80
1	A	15	TRP	NE1-CE2-CD2	6.27	113.57	107.30
1	A	72	TYR	CZ-CE2-CD2	-6.24	114.19	119.80
1	A	3	LEU	CB-CA-C	6.10	121.79	110.20
1	A	139	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	3	LEU	N-CA-CB	5.89	122.19	110.40
1	A	124	ALA	N-CA-CB	5.85	118.30	110.10
1	A	87	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	15	TRP	NE1-CE2-CZ2	-5.83	123.99	130.40
1	A	126	TRP	NE1-CE2-CD2	5.83	113.13	107.30
1	A	78	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	A	31	ILE	CB-CA-C	-5.74	100.12	111.60
1	A	138	TYR	CG-CD2-CE2	5.57	125.76	121.30
1	A	110	VAL	O-C-N	-5.53	113.85	122.70
1	A	42	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	5	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	A	120	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	A	35	GLU	CB-CA-C	-5.47	99.46	110.40
1	A	151	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	131	ASN	O-C-N	5.44	131.40	122.70
1	A	104	ASP	CB-CA-C	-5.41	99.58	110.40
1	A	3	LEU	CB-CG-CD1	5.35	120.09	111.00
1	A	46	PHE	CB-CG-CD2	5.32	124.52	120.80
1	A	28	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	A	126	TRP	CE2-CD2-CE3	5.27	125.02	118.70
1	A	13	SER	N-CA-CB	-5.21	102.69	110.50
1	A	122	VAL	CB-CA-C	-5.21	101.51	111.40
1	A	126	TRP	CD1-CG-CD2	5.18	110.44	106.30
1	A	107	PHE	N-CA-CB	5.17	119.91	110.60
1	A	23	PRO	N-CA-CB	5.13	109.45	103.30
1	A	15	TRP	CB-CG-CD2	-5.11	119.95	126.60
1	A	56	ASN	CA-CB-CG	-5.10	102.18	113.40
1	A	48	LYS	CB-CA-C	-5.09	100.22	110.40
1	A	21	ASN	CB-CG-OD1	-5.08	111.45	121.60
1	A	118	ILE	CB-CA-C	-5.07	101.46	111.60
1	A	107	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	A	12	LYS	O-C-N	5.06	130.80	122.70
1	A	134	TRP	CD1-CG-CD2	5.06	110.35	106.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ILE	Mainchain
1	A	150	ASP	Sidechain
1	A	151	ASP	Sidechain
1	A	16	GLU	Sidechain
1	A	17	GLU	Sidechain
1	A	21	ASN	Sidechain
1	A	42	ASP	Sidechain
1	A	56	ASN	Sidechain
1	A	7	GLN	Sidechain
1	A	81	THR	Mainchain
1	A	83	VAL	Mainchain

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5.2 Torsion angles [i](#)

5.2.1 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	153/153 (100%)	149 (97%)	2 (1%)	2 (1%)	12 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	3	LEU

5.2.2 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	127/125 (102%)	124 (98%)	3 (2%)	49	51

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	34	LEU
1	A	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	61	GLN
1	A	77	GLN

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.5 Ligand geometry [i](#)

2 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	A	155	1,2	41,50,50	4.07	29 (70%)	45,82,82	2.42	19 (42%)
2	ACT	A	154	3	3,3,3	2.44	2 (66%)	3,3,3	1.55	1 (33%)

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	A	155	1,2	-	2/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C1D-C2D	8.25	1.60	1.44
3	A	155	HEM	CAB-C3B	6.61	1.65	1.47
3	A	155	HEM	C4D-C3D	6.44	1.56	1.45
3	A	155	HEM	FE-NB	6.43	2.28	1.96
3	A	155	HEM	CAA-C2A	6.34	1.61	1.52
3	A	155	HEM	C3B-C4B	6.26	1.57	1.44
3	A	155	HEM	C1B-C2B	6.13	1.56	1.44
3	A	155	HEM	C1A-NA	6.09	1.48	1.36
3	A	155	HEM	CBD-CGD	5.73	1.63	1.50
3	A	155	HEM	FE-ND	5.00	2.21	1.96
3	A	155	HEM	CAD-C3D	4.89	1.64	1.51
3	A	155	HEM	CMD-C2D	4.80	1.61	1.50
3	A	155	HEM	C4A-NA	4.79	1.46	1.36
3	A	155	HEM	C3C-C2C	4.76	1.47	1.40
3	A	155	HEM	C4A-CHB	4.44	1.53	1.41
3	A	155	HEM	CMB-C2B	4.20	1.59	1.50
3	A	155	HEM	CBA-CGA	4.06	1.60	1.50
3	A	155	HEM	CMC-C2C	4.03	1.61	1.51
3	A	155	HEM	C3C-CAC	3.89	1.55	1.47
3	A	155	HEM	O2A-CGA	-3.68	1.18	1.30
2	A	154	ACT	CH3-C	3.52	1.63	1.49
3	A	155	HEM	CMA-C3A	3.28	1.58	1.51
3	A	155	HEM	C2A-C3A	3.27	1.47	1.37
3	A	155	HEM	CBD-CAD	-3.01	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C4D-ND	2.97	1.45	1.40
3	A	155	HEM	O1D-CGD	2.72	1.31	1.22
3	A	155	HEM	CHB-C1B	2.67	1.41	1.35
3	A	155	HEM	CBB-CAB	2.47	1.42	1.30
3	A	155	HEM	C1A-CHA	2.46	1.47	1.41
2	A	154	ACT	OXT-C	-2.34	1.19	1.30
3	A	155	HEM	O2D-CGD	-2.32	1.22	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	CMA-C3A-C4A	-5.91	119.38	128.46
3	A	155	HEM	C2C-C3C-C4C	5.36	110.64	106.90
3	A	155	HEM	C4C-CHD-C1D	4.50	128.50	122.56
3	A	155	HEM	CBA-CAA-C2A	-4.00	105.79	112.62
3	A	155	HEM	C4A-C3A-C2A	3.87	109.69	107.00
3	A	155	HEM	C4B-C3B-C2B	-3.68	104.20	107.11
3	A	155	HEM	O2A-CGA-O1A	-3.59	114.35	123.30
3	A	155	HEM	C3C-C4C-NC	-3.41	104.50	110.94
3	A	155	HEM	CMA-C3A-C2A	3.17	130.92	124.94
3	A	155	HEM	CHD-C1D-ND	-3.14	121.02	124.43
3	A	155	HEM	C4B-CHC-C1C	3.11	126.66	122.56
3	A	155	HEM	CAD-CBD-CGD	-3.06	107.02	113.60
3	A	155	HEM	O2D-CGD-O1D	-2.74	116.47	123.30
3	A	155	HEM	C3D-C4D-ND	2.61	113.07	110.17
2	A	154	ACT	OXT-C-O	-2.61	112.44	122.05
3	A	155	HEM	CMC-C2C-C3C	2.58	129.51	124.68
3	A	155	HEM	CHB-C1B-NB	-2.40	121.42	124.38
3	A	155	HEM	CHC-C4B-NB	-2.39	121.84	124.43
3	A	155	HEM	C4D-ND-C1D	-2.14	102.86	105.07
3	A	155	HEM	CHA-C4D-ND	-2.11	121.77	124.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

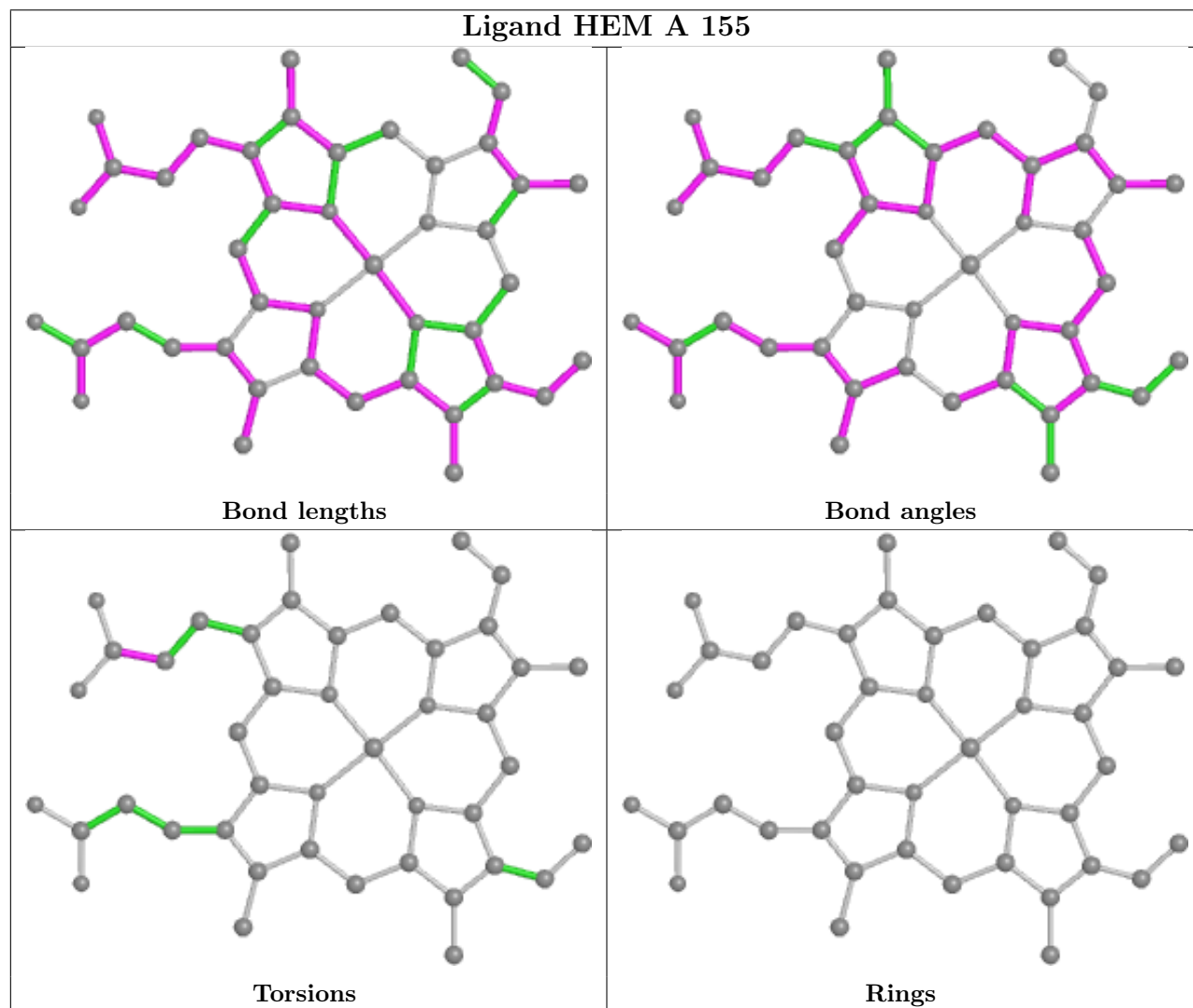
Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAD-CBD-CGD-O1D
3	A	155	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	HEM	3	0
2	A	154	ACT	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.



5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

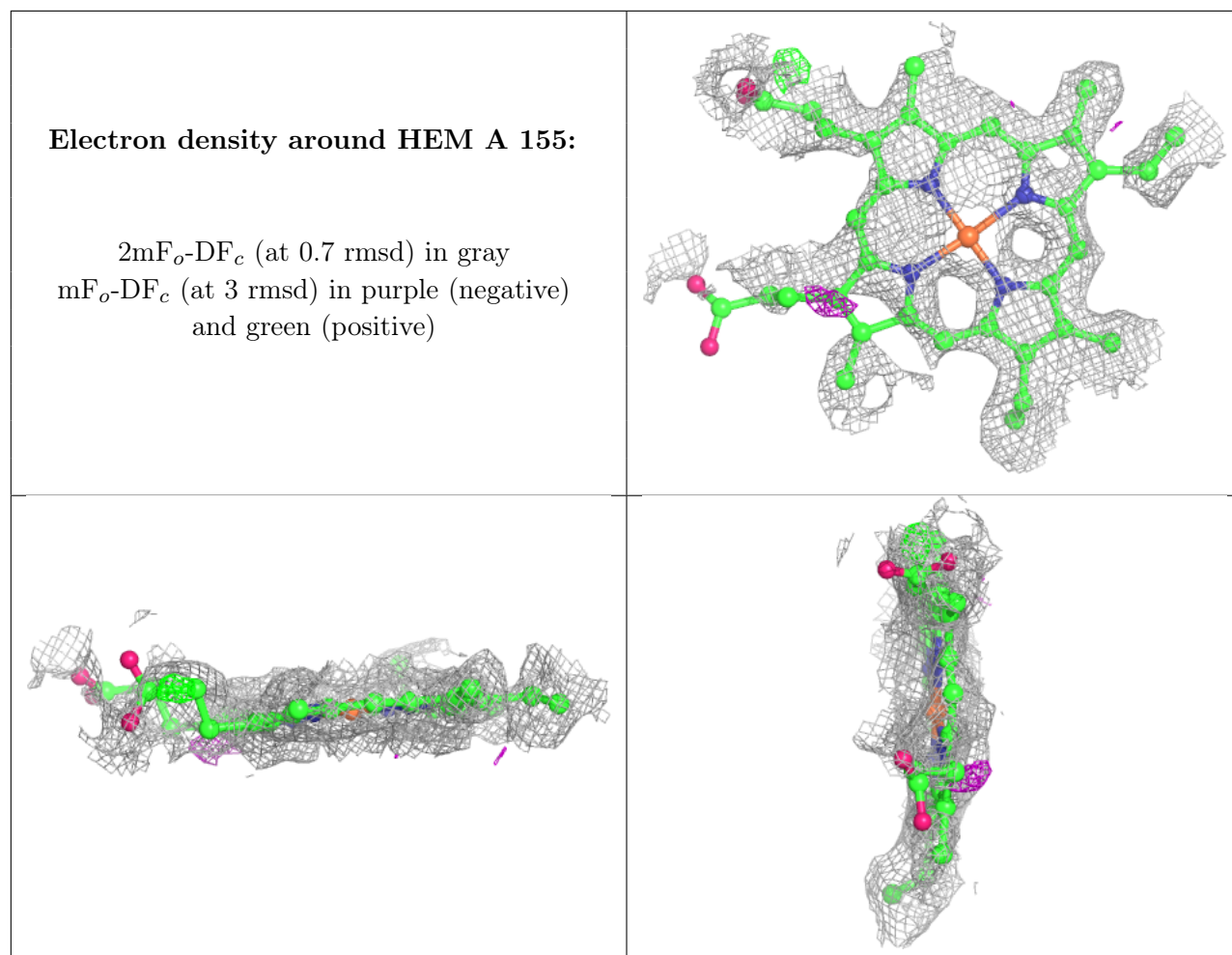
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.