



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 09:40 AM EST

PDB ID : 1LH7
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.

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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

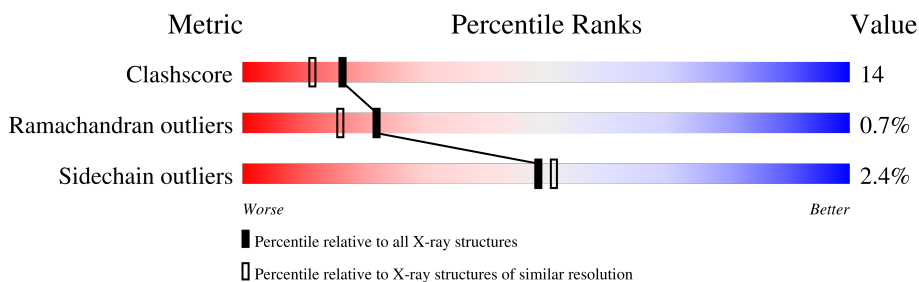
1 Overall quality at a glance

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)

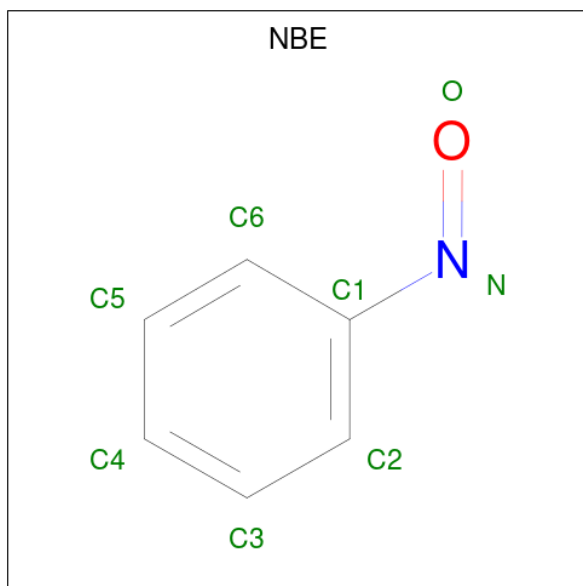
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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
3	NBE	A	155	-	-	X	-

- Molecule 3 is NITROSOBENZENE (three-letter code: NBE) (formula: C₆H₅NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	6	1	1	0	0

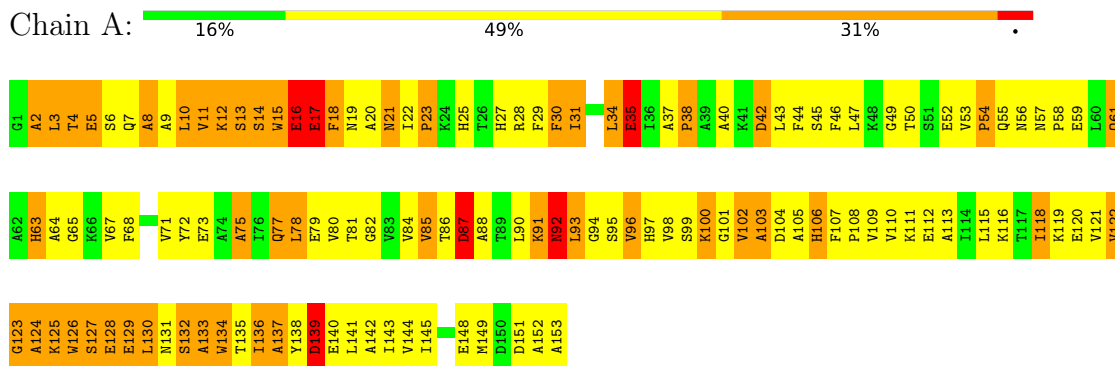
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	64	64	64	0	0

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 (NITROSOBENZENE)



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.23Å 38.25Å 51.88Å 90.00° 90.00° 98.70°	Depositor
Resolution (Å)	(Not available) – 2.00 9.92 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.3 (9.92-1.98)	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) 0.475 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 157.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.52	EDS
Total number of atoms	1295	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.07% 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: HEM, NBE

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	3.32	155/1214 (12.8%)	2.28	56/1648 (3.4%)

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	14

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	TYR	CB-CG	10.85	1.68	1.51
1	A	13	SER	CA-CB	10.21	1.68	1.52
1	A	95	SER	CB-OG	9.87	1.55	1.42
1	A	15	TRP	CD2-CE2	9.79	1.53	1.41
1	A	112	GLU	CG-CD	9.52	1.66	1.51
1	A	35	GLU	CD-OE2	9.52	1.36	1.25
1	A	138	TYR	CZ-OH	9.38	1.53	1.37
1	A	120	GLU	CG-CD	9.15	1.65	1.51
1	A	27	HIS	CG-ND1	8.81	1.58	1.38
1	A	121	VAL	CB-CG2	8.79	1.71	1.52
1	A	132[A]	SER	CA-CB	8.62	1.65	1.52
1	A	132[B]	SER	CA-CB	8.62	1.65	1.52
1	A	132[C]	SER	CA-CB	8.62	1.65	1.52
1	A	72	TYR	CE1-CZ	8.60	1.49	1.38
1	A	14	SER	CB-OG	-8.39	1.31	1.42
1	A	18	PHE	CB-CG	8.29	1.65	1.51
1	A	72	TYR	CG-CD2	8.27	1.50	1.39
1	A	106	HIS	CB-CG	8.24	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	VAL	CB-CG1	8.24	1.70	1.52
1	A	138	TYR	CD2-CE2	8.16	1.51	1.39
1	A	99	SER	N-CA	7.96	1.62	1.46
1	A	45	SER	CB-OG	7.88	1.52	1.42
1	A	5	GLU	CD-OE2	7.85	1.34	1.25
1	A	27	HIS	CE1-NE2	7.79	1.50	1.32
1	A	15	TRP	CG-CD1	7.77	1.47	1.36
1	A	111	LYS	N-CA	7.77	1.61	1.46
1	A	123	GLY	CA-C	7.75	1.64	1.51
1	A	102	VAL	CB-CG1	7.74	1.69	1.52
1	A	13	SER	CB-OG	-7.69	1.32	1.42
1	A	15	TRP	CB-CG	7.66	1.64	1.50
1	A	144	VAL	CB-CG2	7.65	1.69	1.52
1	A	15	TRP	CZ3-CH2	7.57	1.52	1.40
1	A	65	GLY	C-O	7.56	1.35	1.23
1	A	113	ALA	CA-CB	7.49	1.68	1.52
1	A	138	TYR	CD1-CE1	7.47	1.50	1.39
1	A	16	GLU	CD-OE1	7.45	1.33	1.25
1	A	140	GLU	CB-CG	7.45	1.66	1.52
1	A	79	GLU	CB-CG	7.41	1.66	1.52
1	A	122	VAL	N-CA	7.39	1.61	1.46
1	A	73	GLU	CG-CD	7.25	1.62	1.51
1	A	61	GLN	C-O	7.25	1.37	1.23
1	A	97	HIS	CA-CB	7.11	1.69	1.53
1	A	94	GLY	CA-C	7.07	1.63	1.51
1	A	97	HIS	CG-CD2	-7.03	1.23	1.35
1	A	101	GLY	CA-C	6.96	1.62	1.51
1	A	86	THR	N-CA	6.93	1.60	1.46
1	A	68	PHE	C-O	6.91	1.36	1.23
1	A	128	GLU	CD-OE2	-6.89	1.18	1.25
1	A	45	SER	N-CA	6.84	1.60	1.46
1	A	71	VAL	CB-CG1	6.79	1.67	1.52
1	A	134	TRP	CD2-CE2	-6.78	1.33	1.41
1	A	28	ARG	CZ-NH1	6.77	1.41	1.33
1	A	44	PHE	CB-CG	6.76	1.62	1.51
1	A	91	LYS	C-N	-6.74	1.18	1.34
1	A	82	GLY	CA-C	6.73	1.62	1.51
1	A	152	ALA	C-O	6.67	1.36	1.23
1	A	68	PHE	CG-CD2	6.67	1.48	1.38
1	A	75	ALA	N-CA	6.67	1.59	1.46
1	A	11	VAL	N-CA	6.59	1.59	1.46
1	A	152	ALA	N-CA	6.58	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	TYR	C-O	6.56	1.35	1.23
1	A	110	VAL	CB-CG2	6.55	1.66	1.52
1	A	16	GLU	CG-CD	6.52	1.61	1.51
1	A	18	PHE	N-CA	6.51	1.59	1.46
1	A	129	GLU	CD-OE1	6.46	1.32	1.25
1	A	67	VAL	CB-CG2	6.46	1.66	1.52
1	A	85	VAL	CB-CG2	6.44	1.66	1.52
1	A	95	SER	N-CA	6.42	1.59	1.46
1	A	149	MET	C-O	6.42	1.35	1.23
1	A	63	HIS	CE1-NE2	6.41	1.47	1.32
1	A	84	VAL	N-CA	6.27	1.58	1.46
1	A	59	GLU	CD-OE2	6.23	1.32	1.25
1	A	133	ALA	CA-C	6.19	1.69	1.52
1	A	145	ILE	N-CA	6.17	1.58	1.46
1	A	93	LEU	C-N	-6.15	1.22	1.33
1	A	120	GLU	CA-CB	6.14	1.67	1.53
1	A	92	ASN	CB-CG	6.13	1.65	1.51
1	A	92	ASN	C-O	6.07	1.34	1.23
1	A	111	LYS	CB-CG	6.03	1.68	1.52
1	A	35	GLU	CD-OE1	-6.02	1.19	1.25
1	A	116	LYS	N-CA	-6.02	1.34	1.46
1	A	20	ALA	N-CA	-6.02	1.34	1.46
1	A	88	ALA	N-CA	6.01	1.58	1.46
1	A	38	PRO	N-CA	6.00	1.57	1.47
1	A	90	LEU	CA-CB	6.00	1.67	1.53
1	A	15	TRP	C-O	6.00	1.34	1.23
1	A	68	PHE	CE1-CZ	5.97	1.48	1.37
1	A	124	ALA	N-CA	5.96	1.58	1.46
1	A	63	HIS	CG-ND1	5.96	1.51	1.38
1	A	46	PHE	CB-CG	5.96	1.61	1.51
1	A	84	VAL	CB-CG1	5.95	1.65	1.52
1	A	130	LEU	N-CA	5.92	1.58	1.46
1	A	63	HIS	CB-CG	5.92	1.60	1.50
1	A	58	PRO	N-CD	5.91	1.56	1.47
1	A	64	ALA	C-O	5.88	1.34	1.23
1	A	124	ALA	C-O	5.88	1.34	1.23
1	A	134	TRP	N-CA	5.86	1.58	1.46
1	A	107	PHE	N-CA	5.84	1.58	1.46
1	A	52	GLU	N-CA	5.82	1.57	1.46
1	A	115	LEU	N-CA	5.77	1.57	1.46
1	A	68	PHE	N-CA	5.76	1.57	1.46
1	A	52	GLU	CG-CD	-5.71	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	LEU	N-CA	5.71	1.57	1.46
1	A	109	VAL	CA-CB	5.70	1.66	1.54
1	A	44	PHE	CD2-CE2	5.68	1.50	1.39
1	A	104	ASP	N-CA	5.67	1.57	1.46
1	A	64	ALA	N-CA	5.65	1.57	1.46
1	A	98	VAL	CA-CB	-5.59	1.43	1.54
1	A	108	PRO	C-N	5.59	1.47	1.34
1	A	77	GLN	N-CA	-5.57	1.35	1.46
1	A	148	GLU	CG-CD	-5.56	1.43	1.51
1	A	15	TRP	N-CA	5.55	1.57	1.46
1	A	55	GLN	C-O	5.51	1.33	1.23
1	A	30	PHE	N-CA	5.47	1.57	1.46
1	A	87	ASP	CA-C	5.46	1.67	1.52
1	A	53	VAL	CA-CB	5.44	1.66	1.54
1	A	10	LEU	CB-CG	5.41	1.68	1.52
1	A	75	ALA	C-O	5.40	1.33	1.23
1	A	4	THR	C-O	5.39	1.33	1.23
1	A	148	GLU	C-O	5.39	1.33	1.23
1	A	127	SER	CA-CB	5.38	1.61	1.52
1	A	40	ALA	CA-CB	5.37	1.63	1.52
1	A	77	GLN	CG-CD	5.37	1.63	1.51
1	A	15	TRP	NE1-CE2	-5.33	1.30	1.37
1	A	71	VAL	N-CA	5.33	1.57	1.46
1	A	65	GLY	N-CA	5.32	1.54	1.46
1	A	127	SER	C-O	5.30	1.33	1.23
1	A	50	THR	CA-CB	5.30	1.67	1.53
1	A	85	VAL	CA-C	5.30	1.66	1.52
1	A	79	GLU	CA-CB	-5.29	1.42	1.53
1	A	13	SER	N-CA	-5.28	1.35	1.46
1	A	77	GLN	CA-CB	5.27	1.65	1.53
1	A	108	PRO	N-CD	-5.27	1.40	1.47
1	A	100	LYS	C-N	-5.26	1.23	1.33
1	A	125	LYS	CD-CE	5.26	1.64	1.51
1	A	46	PHE	CD2-CE2	5.25	1.49	1.39
1	A	79	GLU	CD-OE1	5.22	1.31	1.25
1	A	30	PHE	CA-CB	5.21	1.65	1.53
1	A	78	LEU	C-N	-5.21	1.22	1.34
1	A	110	VAL	CA-C	5.20	1.66	1.52
1	A	8	ALA	C-O	5.20	1.33	1.23
1	A	91	LYS	CD-CE	5.16	1.64	1.51
1	A	42	ASP	C-N	5.14	1.45	1.34
1	A	103	ALA	CA-C	5.13	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	THR	N-CA	-5.12	1.36	1.46
1	A	148	GLU	CB-CG	5.12	1.61	1.52
1	A	145	ILE	C-O	5.11	1.33	1.23
1	A	43	LEU	CA-CB	5.11	1.65	1.53
1	A	136	ILE	N-CA	-5.11	1.36	1.46
1	A	68	PHE	CA-CB	-5.10	1.42	1.53
1	A	111	LYS	CD-CE	5.09	1.64	1.51
1	A	140	GLU	CG-CD	-5.08	1.44	1.51
1	A	49	GLY	CA-C	-5.08	1.43	1.51
1	A	140	GLU	CD-OE2	5.06	1.31	1.25
1	A	137	ALA	CA-C	5.01	1.66	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	TYR	CB-CG-CD1	-10.50	114.70	121.00
1	A	29	PHE	CB-CG-CD1	-9.03	114.48	120.80
1	A	16	GLU	OE1-CD-OE2	-8.34	113.29	123.30
1	A	87	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	A	15	TRP	CG-CD2-CE3	-8.06	126.65	133.90
1	A	23	PRO	N-CA-CB	7.88	112.75	103.30
1	A	30	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	A	28	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	17	GLU	OE1-CD-OE2	-7.27	114.57	123.30
1	A	68	PHE	CB-CG-CD1	-7.27	115.71	120.80
1	A	124	ALA	CB-CA-C	-7.21	99.29	110.10
1	A	128	GLU	OE1-CD-OE2	-6.98	114.93	123.30
1	A	15	TRP	CD2-CE3-CZ3	-6.82	109.94	118.80
1	A	34	LEU	CB-CG-CD2	6.80	122.57	111.00
1	A	29	PHE	CD1-CG-CD2	6.72	127.03	118.30
1	A	72	TYR	CG-CD1-CE1	-6.70	115.94	121.30
1	A	138	TYR	CB-CG-CD2	6.69	125.02	121.00
1	A	112	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	A	126	TRP	NE1-CE2-CD2	6.52	113.82	107.30
1	A	126	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	A	120	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	73	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	134	TRP	CG-CD1-NE1	-6.42	103.68	110.10
1	A	15	TRP	CH2-CZ2-CE2	-6.34	111.06	117.40
1	A	153	ALA	N-CA-CB	-6.17	101.46	110.10
1	A	80	VAL	CA-CB-CG2	-6.07	101.79	110.90
1	A	46	PHE	CB-CG-CD2	6.05	125.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	TRP	CE2-CD2-CE3	6.01	125.91	118.70
1	A	138	TYR	CD1-CE1-CZ	5.90	125.11	119.80
1	A	15	TRP	CB-CG-CD1	5.86	134.61	127.00
1	A	12	LYS	O-C-N	5.84	132.04	122.70
1	A	15	TRP	NE1-CE2-CZ2	-5.74	124.09	130.40
1	A	138	TYR	CG-CD2-CE2	5.71	125.87	121.30
1	A	149	MET	CA-CB-CG	-5.69	103.63	113.30
1	A	54	PRO	N-CA-CB	5.67	110.10	103.30
1	A	35	GLU	CG-CD-OE1	-5.66	106.99	118.30
1	A	31	ILE	CB-CA-C	-5.63	100.34	111.60
1	A	139	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	110	VAL	O-C-N	-5.43	114.01	122.70
1	A	15	TRP	CD1-NE1-CE2	-5.42	104.12	109.00
1	A	149	MET	O-C-N	5.42	131.37	122.70
1	A	142	ALA	O-C-N	5.40	131.34	122.70
1	A	63	HIS	N-CA-CB	-5.38	100.91	110.60
1	A	72	TYR	CZ-CE2-CD2	-5.33	115.00	119.80
1	A	35	GLU	CB-CA-C	-5.32	99.76	110.40
1	A	126	TRP	CE2-CD2-CE3	5.29	125.05	118.70
1	A	109	VAL	CA-CB-CG1	5.29	118.83	110.90
1	A	139	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	90	LEU	CB-CA-C	5.20	120.09	110.20
1	A	124	ALA	O-C-N	5.13	130.92	122.70
1	A	133	ALA	O-C-N	-5.11	114.52	122.70
1	A	92	ASN	O-C-N	5.07	130.82	122.70
1	A	15	TRP	NE1-CE2-CD2	5.07	112.37	107.30
1	A	68	PHE	O-C-N	5.06	130.80	122.70
1	A	5	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	A	126	TRP	CD1-CG-CD2	5.03	110.33	106.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ALA	Mainchain
1	A	118	ILE	Mainchain
1	A	139	ASP	Sidechain
1	A	151	ASP	Sidechain
1	A	16	GLU	Sidechain
1	A	17	GLU	Sidechain
1	A	19	ASN	Sidechain
1	A	2	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	35	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	61	GLN	Sidechain
1	A	78	LEU	Mainchain
1	A	87	ASP	Sidechain
1	A	92	ASN	Sidechain

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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%)	148 (97%)	4 (3%)	1 (1%)	22 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	NBE	A	155	2	8,8,8	1.29	1 (12%)	9,9,9	1.44	2 (22%)
2	HEM	A	154	1,3	41,50,50	4.16	28 (68%)	45,82,82	2.58	19 (42%)

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	NBE	A	155	2	-	2/2/2/2	0/1/1/1
2	HEM	A	154	1,3	-	1/12/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C1D-C2D	8.92	1.61	1.44
2	A	154	HEM	FE-NB	8.49	2.38	1.96
2	A	154	HEM	CBD-CGD	7.18	1.67	1.50
2	A	154	HEM	CAB-C3B	7.04	1.66	1.47
2	A	154	HEM	CAA-C2A	6.86	1.62	1.52
2	A	154	HEM	C4D-C3D	6.64	1.56	1.45
2	A	154	HEM	C1A-NA	6.44	1.49	1.36
2	A	154	HEM	C3B-C4B	6.36	1.57	1.44
2	A	154	HEM	C3C-CAC	5.42	1.58	1.47
2	A	154	HEM	CMD-C2D	4.96	1.61	1.50
2	A	154	HEM	C4A-NA	4.84	1.46	1.36
2	A	154	HEM	CAD-C3D	4.71	1.63	1.51
2	A	154	HEM	FE-ND	4.39	2.18	1.96
2	A	154	HEM	C1B-C2B	4.33	1.52	1.44
2	A	154	HEM	C4A-CHB	4.01	1.52	1.41
2	A	154	HEM	C3C-C2C	3.93	1.45	1.40
2	A	154	HEM	C2A-C3A	3.62	1.48	1.37
2	A	154	HEM	CMA-C3A	3.60	1.59	1.51
2	A	154	HEM	CBA-CGA	3.46	1.58	1.50
2	A	154	HEM	CMC-C2C	3.29	1.59	1.51
2	A	154	HEM	CMB-C2B	3.10	1.57	1.50
2	A	154	HEM	CHB-C1B	2.90	1.42	1.35
2	A	154	HEM	O1D-CGD	2.75	1.31	1.22
2	A	154	HEM	CBD-CAD	-2.57	1.43	1.52
2	A	154	HEM	O2A-CGA	-2.44	1.22	1.30
2	A	154	HEM	O2D-CGD	-2.20	1.23	1.30
2	A	154	HEM	CBB-CAB	2.12	1.40	1.30
3	A	155	NBE	C4-C3	-2.12	1.32	1.38
2	A	154	HEM	C1A-CHA	2.02	1.46	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	CMA-C3A-C4A	-6.58	118.35	128.46
2	A	154	HEM	C4C-CHD-C1D	6.01	130.49	122.56
2	A	154	HEM	C4B-C3B-C2B	-5.37	102.85	107.11
2	A	154	HEM	CHD-C1D-ND	-4.41	119.64	124.43
2	A	154	HEM	C4A-C3A-C2A	4.33	110.01	107.00
2	A	154	HEM	O2D-CGD-O1D	-3.93	113.50	123.30
2	A	154	HEM	CMA-C3A-C2A	3.55	131.63	124.94
2	A	154	HEM	CHA-C4D-ND	-3.41	120.17	124.38
2	A	154	HEM	C4B-CHC-C1C	3.31	126.93	122.56
2	A	154	HEM	O2A-CGA-O1A	-3.21	115.29	123.30
3	A	155	NBE	C3-C2-C1	2.97	123.73	119.74
2	A	154	HEM	CAA-CBA-CGA	-2.94	105.53	113.76
2	A	154	HEM	C3B-C2B-C1B	2.93	108.66	106.49
2	A	154	HEM	C3C-C4C-NC	-2.81	105.63	110.94
2	A	154	HEM	C3D-C4D-ND	2.79	113.28	110.17
2	A	154	HEM	CAD-CBD-CGD	-2.57	108.06	113.60
2	A	154	HEM	C2C-C3C-C4C	2.43	108.60	106.90
2	A	154	HEM	CAD-C3D-C4D	2.43	128.91	124.66
2	A	154	HEM	CHD-C1D-C2D	2.42	128.76	124.98
2	A	154	HEM	CHC-C4B-NB	-2.19	122.05	124.43
3	A	155	NBE	C4-C5-C6	2.17	123.50	120.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	155	NBE	C2-C1-N-O
3	A	155	NBE	C6-C1-N-O
2	A	154	HEM	CAD-CBD-CGD-O1D

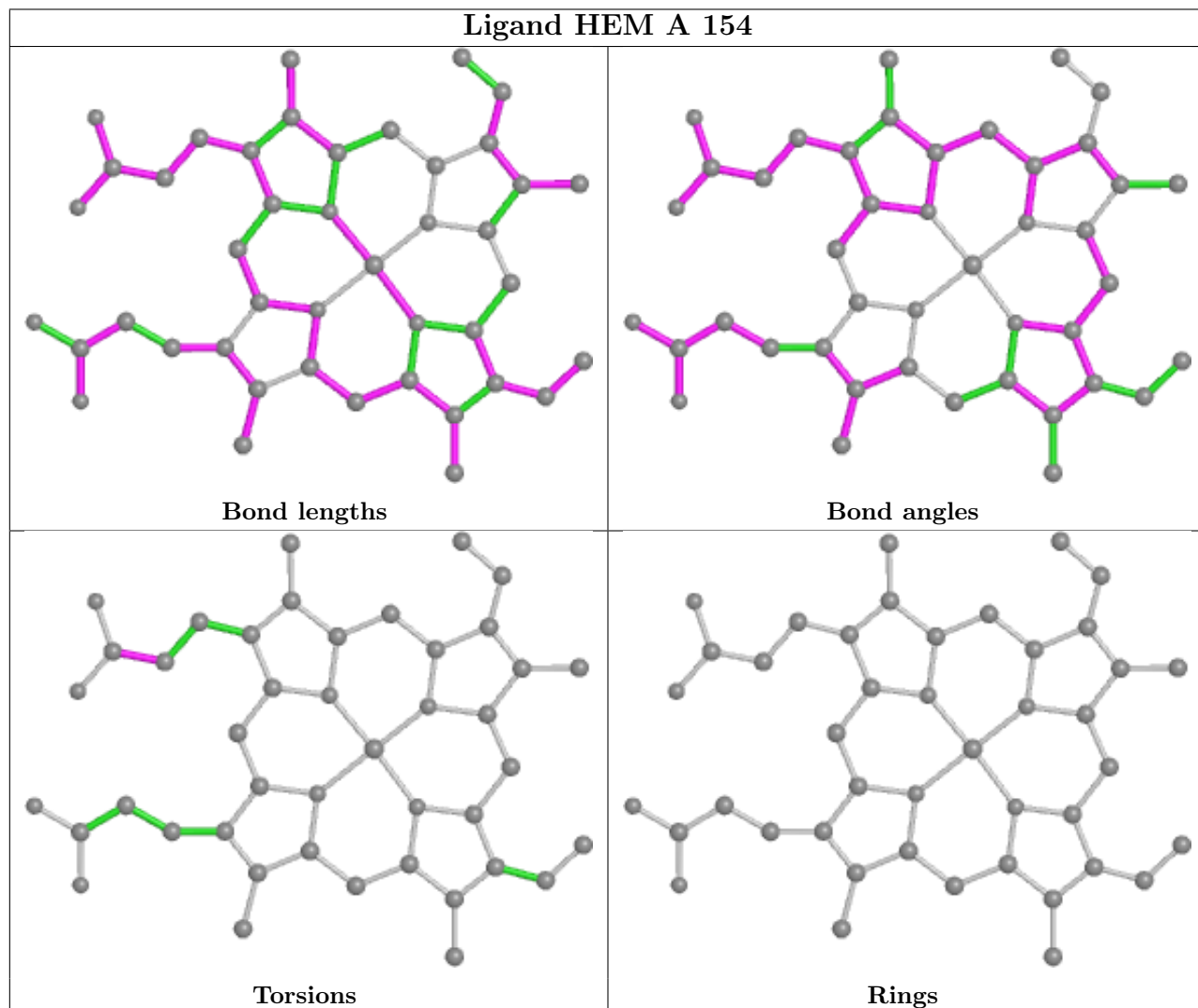
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	NBE	12	0
2	A	154	HEM	7	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	91:LYS	C	92:ASN	N	1.18

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.

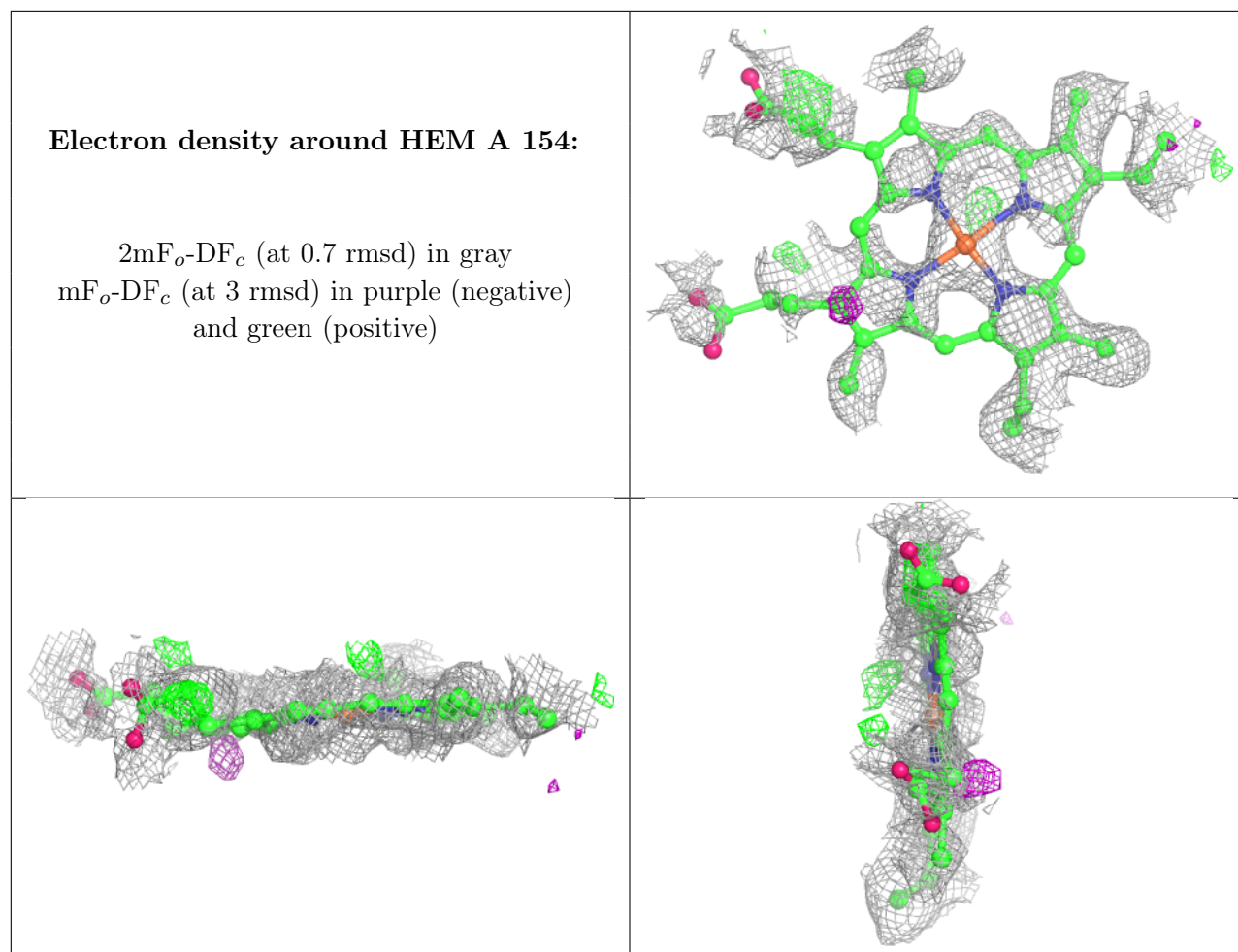
6.3 Carbohydrates

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 depositor's R factor - this section is therefore empty.