Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:02 PM EDT

PDB ID	:	1MLU / pdb_00001mlu
Title	:	NITRIC OXIDE RECOMBINATION TO DOUBLE MUTANTS OF MYOGLOBIN: THE ROLE OF LIGAND DIFFUSION IN A FLUCTUATING HEME POCKET
Authors	:	Quillin, M.L.; Phillips Jr., G.N.
Deposited on	:	1994-06-15
Resolution	:	1.90 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:

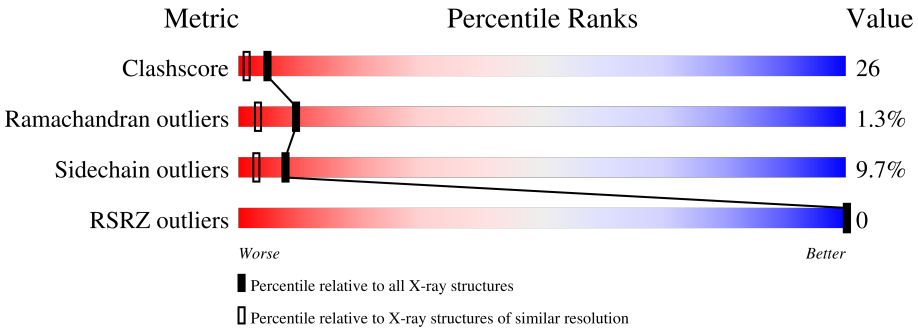
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 <=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	154	60% 21% 16% ·

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	SO4	A	156	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1396 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.

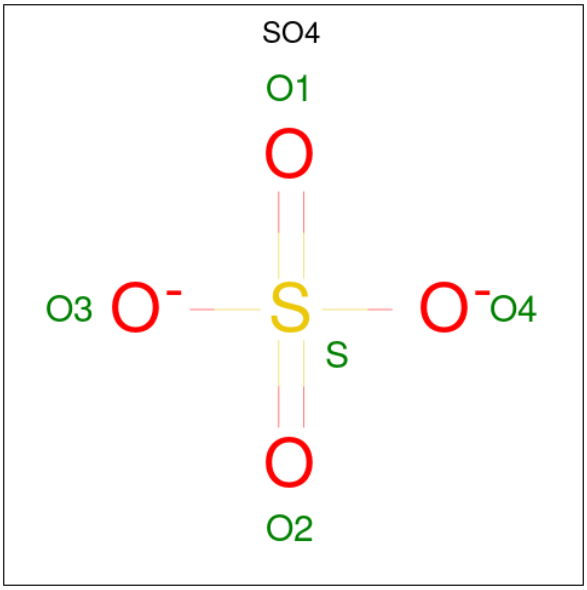
- Molecule 1 is a protein called MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1217	782	216	216	3	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

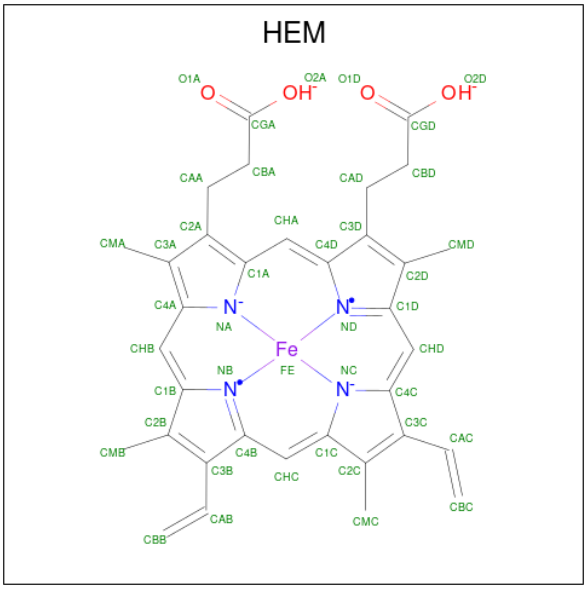
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	GLY	HIS	conflict	UNP P02185
A	68	ALA	VAL	conflict	UNP P02185
A	122	ASN	ASP	conflict	UNP P02185

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



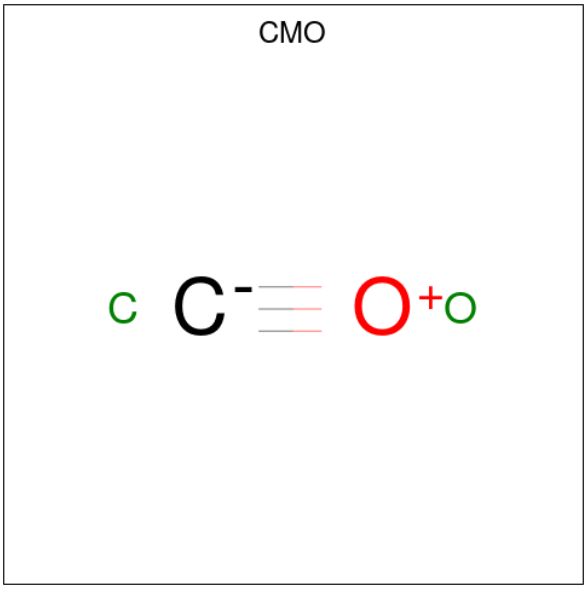
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0

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



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

- Molecule 4 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total	O	0	0
			129	129		

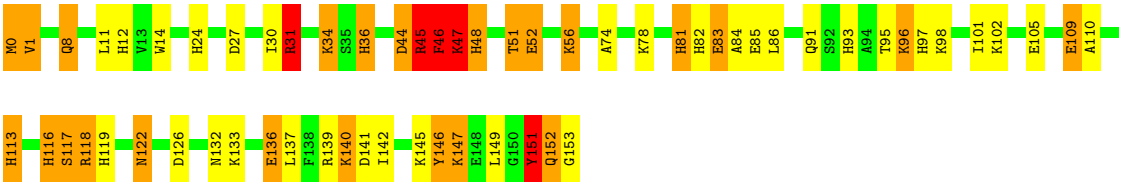
3 Residue-property plots (i)

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 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: MYOGLOBIN

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	91.20Å 91.20Å 45.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 1.90 78.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90) 50.6 (78.98-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.143 , (Not available) 0.135 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	16.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.72 , 132.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	1396	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, CMO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.77	26/1244 (2.1%)	1.83	34/1668 (2.0%)

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	28

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	HIS	ND1-CE1	13.68	1.46	1.32
1	A	81	HIS	CG-ND1	12.28	1.51	1.38
1	A	116	HIS	ND1-CE1	11.68	1.44	1.32
1	A	97	HIS	CD2-NE2	11.62	1.50	1.37
1	A	12	HIS	CG-ND1	10.38	1.49	1.38
1	A	48	HIS	ND1-CE1	9.38	1.42	1.32
1	A	45	ARG	NE-CZ	8.86	1.42	1.33
1	A	97	HIS	ND1-CE1	8.82	1.41	1.32
1	A	93	HIS	CG-CD2	7.82	1.44	1.35
1	A	119	HIS	ND1-CE1	7.73	1.40	1.32
1	A	48	HIS	CB-CG	-7.41	1.39	1.50
1	A	113	HIS	ND1-CE1	7.05	1.39	1.32
1	A	12	HIS	CG-CD2	6.53	1.43	1.35
1	A	36	HIS	CE1-NE2	-6.50	1.26	1.32
1	A	113	HIS	CG-ND1	6.42	1.45	1.38
1	A	24	HIS	CD2-NE2	6.29	1.44	1.37
1	A	118	ARG	CD-NE	-6.12	1.37	1.46
1	A	81	HIS	CD2-NE2	6.10	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	HIS	CB-CG	6.07	1.58	1.50
1	A	12	HIS	ND1-CE1	6.00	1.38	1.32
1	A	119	HIS	CG-CD2	5.54	1.42	1.35
1	A	36	HIS	CG-ND1	-5.51	1.32	1.38
1	A	36	HIS	ND1-CE1	5.49	1.38	1.32
1	A	82	HIS	CB-CG	-5.44	1.42	1.50
1	A	116	HIS	CG-ND1	5.21	1.44	1.38
1	A	81	HIS	ND1-CE1	5.00	1.37	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	HIS	CA-CB-CG	-9.25	104.55	113.80
1	A	48	HIS	CA-CB-CG	8.44	122.24	113.80
1	A	81	HIS	CB-CG-CD2	-7.98	120.83	131.20
1	A	24	HIS	CB-CG-CD2	-7.71	121.18	131.20
1	A	48	HIS	CB-CG-CD2	-7.69	121.21	131.20
1	A	45	ARG	NH1-CZ-NH2	-7.66	109.34	119.30
1	A	93	HIS	CG-CD2-NE2	-7.46	99.74	107.20
1	A	36	HIS	ND1-CG-CD2	-7.13	98.97	106.10
1	A	81	HIS	CA-CB-CG	-7.13	106.67	113.80
1	A	31	ARG	NE-CZ-NH2	-6.88	113.01	119.20
1	A	81	HIS	ND1-CE1-NE2	6.88	115.28	108.40
1	A	116	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	A	118	ARG	NE-CZ-NH2	-6.60	113.26	119.20
1	A	44	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	116	HIS	CE1-NE2-CD2	6.42	115.42	109.00
1	A	46	PHE	CB-CA-C	-6.09	99.51	110.23
1	A	46	PHE	O-C-N	-6.04	115.12	122.25
1	A	116	HIS	ND1-CG-CD2	5.98	112.08	106.10
1	A	117	SER	CB-CA-C	-5.97	100.69	110.85
1	A	151	TYR	O-C-N	-5.90	115.72	123.21
1	A	36	HIS	CG-CD2-NE2	5.86	113.06	107.20
1	A	45	ARG	NE-CZ-NH1	-5.79	115.72	121.50
1	A	12	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	A	48	HIS	ND1-CG-CD2	5.58	111.68	106.10
1	A	93	HIS	CE1-NE2-CD2	5.57	114.56	109.00
1	A	48	HIS	N-CA-C	5.44	119.02	112.38
1	A	8	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	109	GLU	N-CA-CB	-5.42	102.13	110.16
1	A	118	ARG	CB-CG-CD	-5.34	99.02	111.30
1	A	81	HIS	CB-CG-ND1	5.28	130.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	HIS	CG-CD2-NE2	-5.25	101.95	107.20
1	A	136	GLU	N-CA-C	-5.19	105.70	111.36
1	A	122	ASN	N-CA-C	-5.12	106.27	112.88
1	A	14	TRP	CG-CD1-NE1	-5.04	103.65	110.20

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	105	GLU	Sidechain
1	A	109	GLU	Sidechain
1	A	11	LEU	Mainchain
1	A	122	ASN	Mainchain
1	A	126	ASP	Sidechain
1	A	139	ARG	Sidechain
1	A	146	TYR	Sidechain
1	A	151	TYR	Sidechain,Mainchain
1	A	27	ASP	Sidechain
1	A	31	ARG	Sidechain
1	A	34	LYS	Mainchain
1	A	36	HIS	Mainchain
1	A	45	ARG	Sidechain,Mainchain
1	A	46	PHE	Sidechain,Mainchain
1	A	47	LYS	Mainchain
1	A	48	HIS	Sidechain
1	A	51	THR	Mainchain
1	A	52	GLU	Sidechain
1	A	74	ALA	Mainchain
1	A	78	LYS	Mainchain
1	A	83	GLU	Sidechain
1	A	84	ALA	Mainchain
1	A	85	GLU	Sidechain
1	A	96	LYS	Mainchain

5.2 Too-close contacts (i)

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	1217	0	1245	62	0
2	A	5	0	0	3	0
3	A	43	0	30	0	0
4	A	2	0	0	0	0
5	A	129	0	0	20	1
All	All	1396	0	1275	65	1

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 26.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD2	1:A:46:PHE:CE1	1.85	1.10
1:A:45:ARG:HD2	1:A:46:PHE:HE1	1.18	0.99
1:A:145:LYS:N	1:A:145:LYS:HD3	1.84	0.92
1:A:8:GLN:HG2	5:A:315:HOH:O	1.66	0.92
1:A:101:ILE:HG12	1:A:152:GLN:HE22	1.43	0.82
2:A:156:SO4:S	5:A:270:HOH:O	2.39	0.80
1:A:44:ASP:HB2	5:A:313:HOH:O	1.83	0.78
1:A:101:ILE:HG12	1:A:152:GLN:NE2	1.99	0.76
1:A:44:ASP:CG	5:A:313:HOH:O	2.28	0.74
1:A:132:ASN:O	1:A:136:GLU:HG3	1.88	0.74
1:A:0:MET:HG3	1:A:137:LEU:HD13	1.71	0.72
1:A:52:GLU:OE2	1:A:56:LYS:HE3	1.92	0.69
1:A:145:LYS:HD3	1:A:145:LYS:H	1.58	0.68
1:A:147:LYS:HG3	1:A:153:GLY:CA	2.24	0.67
1:A:147:LYS:CB	1:A:153:GLY:HA2	2.25	0.67
1:A:51:THR:HG22	5:A:308:HOH:O	1.94	0.66
1:A:44:ASP:CB	5:A:313:HOH:O	2.40	0.66
1:A:83:GLU:H	1:A:83:GLU:CD	2.02	0.65
1:A:147:LYS:CG	1:A:153:GLY:HA2	2.25	0.65
1:A:145:LYS:N	1:A:145:LYS:CD	2.61	0.63
1:A:146:TYR:HD2	1:A:152:GLN:HE21	1.47	0.62
1:A:133:LYS:HD2	5:A:297:HOH:O	2.00	0.62
1:A:141:ASP:O	1:A:145:LYS:HD3	1.99	0.62
1:A:147:LYS:CA	1:A:153:GLY:HA2	2.36	0.56
1:A:0:MET:C	1:A:1:VAL:HG23	2.31	0.56
2:A:156:SO4:O3	5:A:270:HOH:O	2.17	0.56
1:A:101:ILE:H	1:A:152:GLN:HE22	1.55	0.55
1:A:133:LYS:CD	5:A:297:HOH:O	2.53	0.55
1:A:151:TYR:CD2	1:A:152:GLN:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:O	1:A:145:LYS:HE2	2.09	0.52
1:A:116:HIS:HD2	5:A:252:HOH:O	1.94	0.51
1:A:45:ARG:CD	1:A:46:PHE:CE1	2.78	0.51
1:A:133:LYS:CE	5:A:297:HOH:O	2.59	0.51
1:A:147:LYS:HG3	1:A:153:GLY:HA3	1.92	0.51
2:A:156:SO4:O1	5:A:270:HOH:O	2.19	0.51
1:A:45:ARG:CG	5:A:268:HOH:O	2.59	0.50
1:A:146:TYR:CD2	1:A:151:TYR:HD2	2.30	0.50
1:A:141:ASP:O	1:A:145:LYS:CE	2.60	0.50
1:A:151:TYR:O	1:A:153:GLY:N	2.45	0.49
1:A:95:THR:O	1:A:98:LYS:HE3	2.13	0.48
1:A:141:ASP:O	1:A:145:LYS:CD	2.60	0.48
1:A:45:ARG:HG2	5:A:268:HOH:O	2.12	0.48
1:A:81:HIS:HD2	5:A:269:HOH:O	1.97	0.48
1:A:151:TYR:O	1:A:152:GLN:C	2.54	0.48
1:A:31:ARG:HG2	1:A:110:ALA:HB1	1.97	0.47
1:A:147:LYS:HA	1:A:153:GLY:HA2	1.97	0.47
1:A:30:ILE:HD13	1:A:56:LYS:HD2	1.97	0.46
1:A:147:LYS:HB2	1:A:153:GLY:C	2.40	0.46
1:A:45:ARG:HH11	1:A:46:PHE:HZ	1.64	0.46
1:A:31:ARG:HD2	1:A:113:HIS:CD2	2.51	0.46
1:A:147:LYS:CG	1:A:153:GLY:CA	2.87	0.45
1:A:91:GLN:HA	1:A:149:LEU:HD13	1.98	0.45
1:A:146:TYR:CD2	1:A:151:TYR:CD2	3.05	0.44
1:A:0:MET:C	1:A:1:VAL:CG2	2.91	0.44
1:A:152:GLN:HB2	1:A:153:GLY:H	1.51	0.44
1:A:140:LYS:HD2	5:A:265:HOH:O	2.18	0.43
1:A:118:ARG:HD3	5:A:212:HOH:O	2.18	0.43
1:A:31:ARG:HD3	5:A:255:HOH:O	2.18	0.42
1:A:44:ASP:HA	1:A:47:LYS:HE2	2.00	0.42
1:A:146:TYR:CE2	1:A:151:TYR:HE2	2.38	0.42
1:A:146:TYR:CE2	1:A:151:TYR:CE2	3.07	0.42
1:A:8:GLN:CG	5:A:315:HOH:O	2.44	0.41
1:A:116:HIS:HE1	5:A:214:HOH:O	2.03	0.41
1:A:0:MET:HG3	1:A:137:LEU:CD1	2.45	0.41
1:A:31:ARG:HG2	1:A:110:ALA:CB	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:246:HOH:O	5:A:246:HOH:O[2_655]	2.03	0.17

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	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9 3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	152	GLN

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	124/124 (100%)	112 (90%)	12 (10%)	8 3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	31	ARG
1	A	34	LYS
1	A	45	ARG

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Mol	Chain	Res	Type
1	A	56	LYS
1	A	86	LEU
1	A	96	LYS
1	A	102	LYS
1	A	117	SER
1	A	140	LYS
1	A	142	ILE
1	A	147	LYS

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	81	HIS
1	A	113	HIS
1	A	116	HIS
1	A	152	GLN

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)

3 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	$\#\|Z\|>2$
4	CMO	A	155	3	0,1,1	-	-	-		
2	SO4	A	156	-	4,4,4	0.59	0	6,6,6	0.48	0
3	HEM	A	154	1,4	50,50,50	2.21	19 (38%)	67,82,82	2.11	20 (29%)

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	154	1,4	-	3/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	154	HEM	CHB-C1B	6.94	1.52	1.38
3	A	154	HEM	C4C-NC	4.31	1.47	1.39
3	A	154	HEM	C1D-ND	3.83	1.46	1.38
3	A	154	HEM	CMB-C2B	3.57	1.58	1.50
3	A	154	HEM	C1C-NC	-3.56	1.32	1.39
3	A	154	HEM	CAA-C2A	3.33	1.59	1.51
3	A	154	HEM	C4B-NB	-3.32	1.32	1.38
3	A	154	HEM	C1A-C2A	3.17	1.50	1.44
3	A	154	HEM	CBB-CAB	3.07	1.45	1.30
3	A	154	HEM	CHC-C4B	-3.05	1.32	1.39
3	A	154	HEM	CBC-CAC	2.97	1.44	1.30
3	A	154	HEM	CHB-C4A	-2.60	1.33	1.39
3	A	154	HEM	O2A-CGA	-2.56	1.22	1.30
3	A	154	HEM	FE-NB	2.47	2.02	1.94
3	A	154	HEM	O2D-CGD	-2.33	1.23	1.30
3	A	154	HEM	C1A-NA	-2.25	1.35	1.39
3	A	154	HEM	CHD-C1D	-2.24	1.34	1.39
3	A	154	HEM	CMD-C2D	-2.17	1.46	1.50
3	A	154	HEM	CMA-C3A	2.07	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	154	HEM	C3B-C4B-NB	5.83	113.66	109.47
3	A	154	HEM	C3C-C2C-C1C	4.37	111.18	107.05
3	A	154	HEM	CHD-C1D-ND	4.32	129.07	124.42
3	A	154	HEM	C4C-C3C-C2C	-4.21	103.16	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	154	HEM	C4A-C3A-C2A	-4.20	102.00	106.82
3	A	154	HEM	C3B-C2B-C1B	-4.17	103.28	106.41
3	A	154	HEM	CHD-C4C-NC	4.11	128.93	124.45
3	A	154	HEM	CHB-C4A-C3A	-3.99	115.86	127.43
3	A	154	HEM	CHC-C4B-NB	-3.51	120.64	124.42
3	A	154	HEM	C3A-C4A-NA	3.21	115.29	110.14
3	A	154	HEM	C1A-CHA-C4D	-3.20	118.72	126.25
3	A	154	HEM	C4C-CHD-C1D	-3.09	119.45	126.02
3	A	154	HEM	CHB-C4A-NA	2.71	128.78	123.86
3	A	154	HEM	CMC-C2C-C3C	-2.60	122.15	128.43
3	A	154	HEM	CHA-C4D-ND	2.54	127.50	124.37
3	A	154	HEM	CHD-C4C-C3C	-2.35	121.25	125.21
3	A	154	HEM	C1B-NB-C4B	-2.32	102.46	105.21
3	A	154	HEM	CHA-C1A-NA	2.26	127.97	123.86
3	A	154	HEM	C2B-C1B-NB	2.15	112.31	109.84
3	A	154	HEM	CBD-CAD-C3D	-2.13	106.64	112.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	154	HEM	C2A-CAA-CBA-CGA
3	A	154	HEM	CAA-CBA-CGA-O2A
3	A	154	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

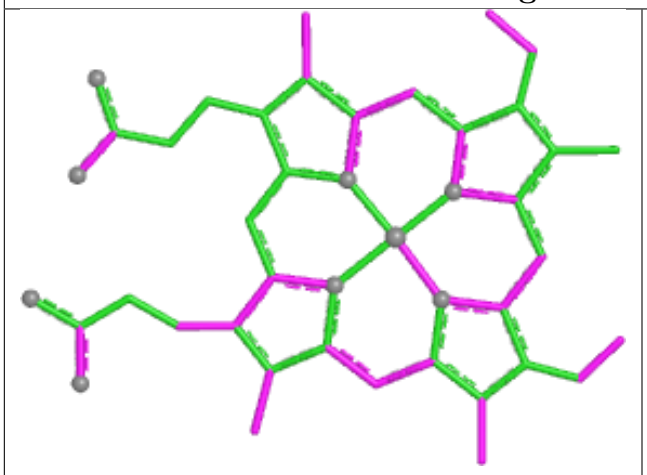
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	156	SO4	3	0

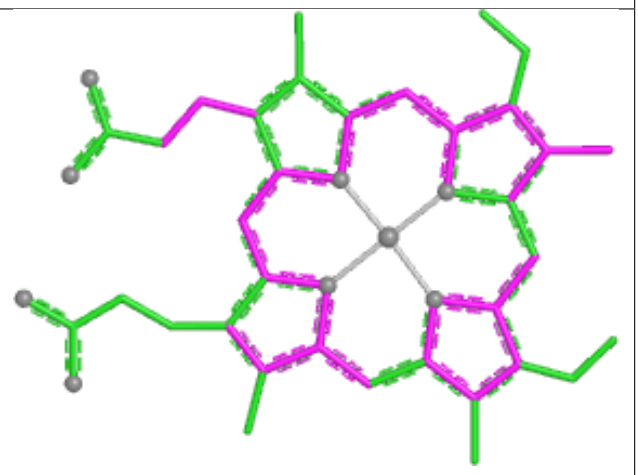
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

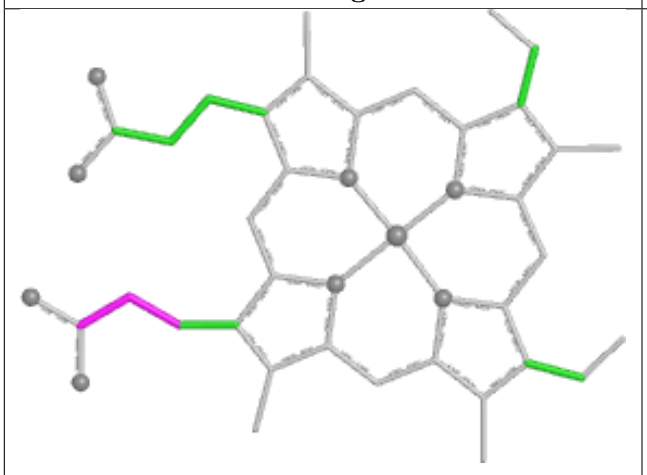
Ligand HEM A 154



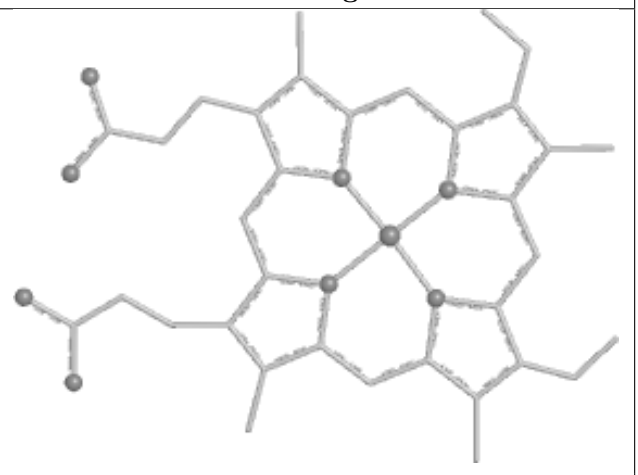
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	154/154 (100%)	-0.97	0 100 100	10, 17, 33, 57	0

There are no RSRZ outliers to report.

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

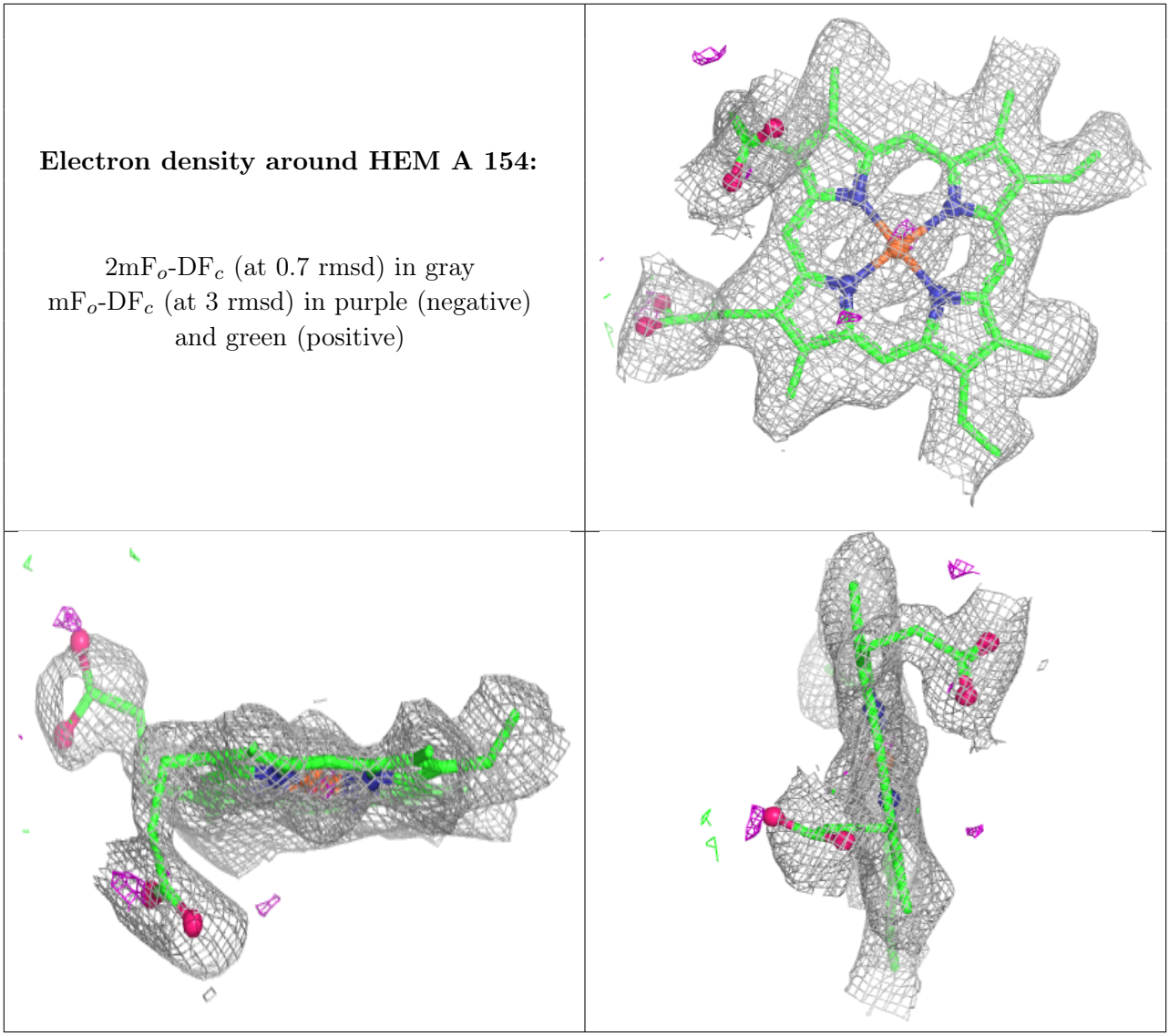
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	SO4	A	156	5/5	0.97	0.06	44,45,46,47	0
3	HEM	A	154	43/43	0.99	0.04	11,13,27,34	0
4	CMO	A	155	2/2	1.00	0.06	13,13,13,15	2

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 154:

$2mF_o$-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.