



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:49 pm BST

PDB ID : 1YCB  
Title : DISTAL POCKET POLARITY IN LIGAND BINDING TO MYOGLOBIN:  
DEOXY AND CARBONMONOXY FORMS OF A THREONINE68 (E11)  
MUTANT INVESTIGATED BY X-RAY CRYSTALLOGRAPHY AND IN-  
FRARED SPECTROSCOPY  
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Deposited on : 1993-08-10  
Resolution : 2.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

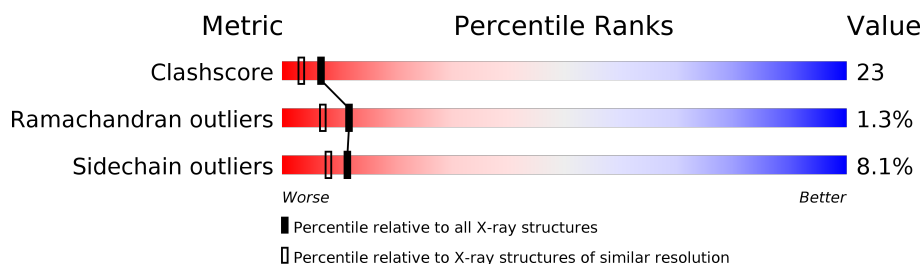
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2589 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
1	A	153	Total	C	N	O	S	53	0	0
			1197	763	208	223	3			
1	B	153	Total	C	N	O	S	51	0	0
			1197	763	208	223	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	THR	VAL	CONFLICT	UNP P02189
B	68	THR	VAL	CONFLICT	UNP P02189

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

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

- Molecule 3 is water.

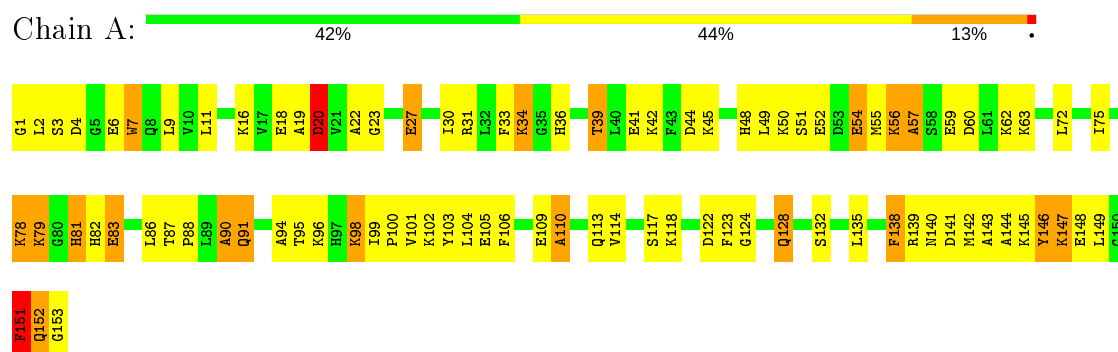
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	66	Total	O	0	0
			66	66		

### 3 Residue-property plots [i](#)

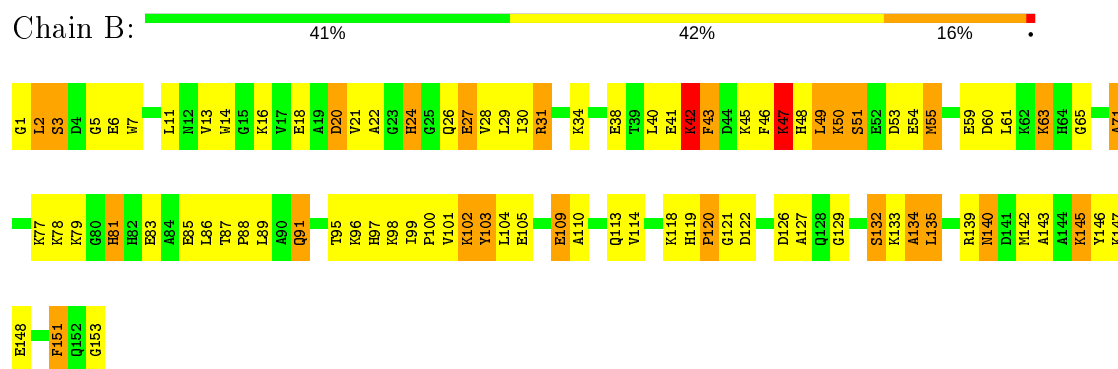
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: MYOGLOBIN



#### • Molecule 1: MYOGLOBIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.60 Å 42.50 Å 92.00 Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 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

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	1.71	7/1222 (0.6%)	2.44	56/1637 (3.4%)
1	B	1.28	6/1222 (0.5%)	2.24	61/1637 (3.7%)
All	All	1.51	13/2444 (0.5%)	2.35	117/3274 (3.6%)

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	2
1	B	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLY	C-OXT	-33.88	0.58	1.23
1	A	62	LYS	CE-NZ	-14.13	1.13	1.49
1	A	56	LYS	CE-NZ	14.03	1.84	1.49
1	B	41	GLU	CG-CD	13.48	1.72	1.51
1	A	102	LYS	CB-CG	9.67	1.78	1.52
1	B	102	LYS	CD-CE	-8.16	1.30	1.51
1	B	34	LYS	CD-CE	-6.86	1.34	1.51
1	A	83	GLU	CB-CG	6.71	1.65	1.52
1	A	44	ASP	CB-CG	6.50	1.65	1.51
1	B	47	LYS	CG-CD	6.47	1.74	1.52
1	B	153	GLY	C-OXT	-5.61	1.12	1.23
1	A	1	GLY	N-CA	5.41	1.54	1.46
1	B	132	SER	CB-OG	5.16	1.49	1.42

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	PHE	O-C-N	-32.97	69.95	122.70
1	A	60	ASP	CB-CG-OD2	-15.89	104.00	118.30
1	A	31	ARG	NE-CZ-NH2	13.37	126.98	120.30
1	B	151	PHE	O-C-N	-12.98	101.93	122.70
1	A	109	GLU	OE1-CD-OE2	12.33	138.10	123.30
1	A	151	PHE	CA-C-N	11.65	142.83	117.20
1	A	139	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	B	60	ASP	CB-CG-OD2	-9.75	109.52	118.30
1	A	45	LYS	CG-CD-CE	9.43	140.18	111.90
1	B	127	ALA	CB-CA-C	9.23	123.95	110.10
1	A	105	GLU	OE1-CD-OE2	9.12	134.24	123.30
1	B	20	ASP	CB-CG-OD1	9.01	126.41	118.30
1	A	146	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	B	102	LYS	CD-CE-NZ	8.70	131.71	111.70
1	B	148	GLU	OE1-CD-OE2	8.69	133.73	123.30
1	A	4	ASP	CB-CG-OD1	-8.59	110.56	118.30
1	A	122	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	A	57	ALA	CB-CA-C	-8.39	97.51	110.10
1	B	60	ASP	OD1-CG-OD2	8.39	139.25	123.30
1	A	49	LEU	CB-CA-C	8.32	126.01	110.20
1	A	31	ARG	CD-NE-CZ	-8.31	111.96	123.60
1	A	44	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	18	GLU	OE1-CD-OE2	8.22	133.16	123.30
1	A	110	ALA	N-CA-CB	-8.12	98.73	110.10
1	A	146	TYR	CB-CG-CD1	8.08	125.85	121.00
1	B	139	ARG	CD-NE-CZ	-7.99	112.41	123.60
1	B	31	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	60	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	B	31	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	B	71	ALA	N-CA-CB	7.56	120.68	110.10
1	B	122	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	B	51	SER	N-CA-CB	-7.51	99.23	110.50
1	B	142	MET	CA-CB-CG	7.50	126.05	113.30
1	A	105	GLU	CG-CD-OE1	-7.39	103.51	118.30
1	A	60	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	20	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	151	PHE	C-N-CA	7.23	139.77	121.70
1	A	113	GLN	O-C-N	-7.21	111.16	122.70
1	A	44	ASP	CA-CB-CG	-6.84	98.34	113.40
1	B	48	HIS	CA-CB-CG	-6.83	102.00	113.60
1	B	132	SER	CA-CB-OG	-6.82	92.78	111.20
1	A	132	SER	CA-CB-OG	-6.76	92.94	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LEU	CB-CG-CD2	-6.75	99.53	111.00
1	B	41	GLU	CG-CD-OE1	6.66	131.62	118.30
1	B	135	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	A	81	HIS	CA-CB-CG	-6.54	102.49	113.60
1	B	103	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	A	98	LYS	CB-CG-CD	6.51	128.53	111.60
1	A	122	ASP	CB-CA-C	-6.36	97.68	110.40
1	A	96	LYS	CG-CD-CE	6.35	130.96	111.90
1	A	44	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	139	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	140	ASN	O-C-N	6.29	132.76	122.70
1	A	2	LEU	N-CA-CB	-6.27	97.86	110.40
1	B	91	GLN	CG-CD-OE1	-6.24	109.13	121.60
1	B	140	ASN	CA-C-O	-6.23	107.01	120.10
1	B	126	ASP	N-CA-CB	-6.21	99.42	110.60
1	B	2	LEU	CB-CG-CD2	-6.17	100.50	111.00
1	B	13	VAL	N-CA-CB	-6.12	98.04	111.50
1	B	22	ALA	CB-CA-C	6.09	119.24	110.10
1	B	89	LEU	CB-CA-C	6.02	121.64	110.20
1	B	18	GLU	OE1-CD-OE2	5.99	130.49	123.30
1	B	40	LEU	CB-CA-C	5.98	121.57	110.20
1	A	7	TRP	O-C-N	-5.95	113.17	122.70
1	A	2	LEU	O-C-N	5.93	132.18	122.70
1	B	42	LYS	CD-CE-NZ	-5.91	98.10	111.70
1	B	134	ALA	CB-CA-C	5.89	118.94	110.10
1	B	104	LEU	O-C-N	-5.78	113.45	122.70
1	B	139	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	B	105	GLU	CA-C-O	5.58	131.82	120.10
1	B	55	MET	CA-C-O	5.58	131.82	120.10
1	A	33	PHE	CG-CD2-CE2	-5.56	114.68	120.80
1	A	22	ALA	CB-CA-C	5.54	118.42	110.10
1	B	16	LYS	CA-CB-CG	-5.53	101.23	113.40
1	B	81	HIS	CA-CB-CG	-5.52	104.21	113.60
1	B	91	GLN	OE1-CD-NE2	5.52	134.60	121.90
1	A	54	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	B	49	LEU	CB-CA-C	5.51	120.67	110.20
1	B	21	VAL	CA-CB-CG1	5.51	119.16	110.90
1	B	151	PHE	CA-C-O	-5.49	108.58	120.10
1	B	24	HIS	O-C-N	-5.47	113.89	123.20
1	B	5	GLY	O-C-N	5.47	131.46	122.70
1	A	16	LYS	CG-CD-CE	5.46	128.28	111.90
1	B	77	LYS	CA-C-N	5.43	129.16	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	GLU	CB-CA-C	-5.42	99.56	110.40
1	A	54	GLU	CG-CD-OE2	5.42	129.13	118.30
1	A	128	GLN	CG-CD-OE1	-5.41	110.79	121.60
1	A	27	GLU	CG-CD-OE1	-5.39	107.52	118.30
1	A	78	LYS	N-CA-CB	5.39	120.30	110.60
1	B	105	GLU	CG-CD-OE2	-5.39	107.53	118.30
1	B	14	TRP	CA-CB-CG	-5.37	103.51	113.70
1	B	55	MET	O-C-N	-5.37	114.11	122.70
1	A	135	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	B	27	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	B	43	PHE	O-C-N	5.33	131.23	122.70
1	B	38	GLU	CG-CD-OE2	5.32	128.93	118.30
1	A	128	GLN	O-C-N	-5.31	114.17	123.20
1	B	89	LEU	CB-CG-CD2	-5.31	101.98	111.00
1	B	120	PRO	CA-C-O	5.28	132.88	120.20
1	B	148	GLU	CG-CD-OE2	-5.26	107.79	118.30
1	A	33	PHE	CD1-CG-CD2	5.24	125.11	118.30
1	A	33	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	B	3	SER	N-CA-CB	-5.20	102.70	110.50
1	B	122	ASP	CB-CA-C	-5.19	100.03	110.40
1	B	51	SER	CB-CA-C	5.18	119.95	110.10
1	B	129	GLY	O-C-N	-5.17	114.43	122.70
1	A	142	MET	CA-CB-CG	5.15	122.06	113.30
1	B	3	SER	O-C-N	-5.15	114.46	122.70
1	A	123	PHE	CB-CG-CD1	-5.15	117.20	120.80
1	A	78	LYS	CB-CA-C	-5.14	100.12	110.40
1	A	90	ALA	CB-CA-C	5.11	117.76	110.10
1	B	105	GLU	CG-CD-OE1	5.10	128.51	118.30
1	A	55	MET	CA-CB-CG	-5.07	104.68	113.30
1	A	109	GLU	CG-CD-OE1	-5.07	108.16	118.30
1	A	51	SER	CB-CA-C	-5.05	100.51	110.10
1	B	122	ASP	N-CA-CB	-5.02	101.56	110.60
1	A	39	THR	CA-CB-CG2	5.02	119.42	112.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PHE	Mainchain,Peptide
1	B	151	PHE	Mainchain

## 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	1197	0	1202	48	0
1	B	1197	0	1203	58	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
3	A	43	0	0	1	0
3	B	66	0	0	6	0
All	All	2589	0	2465	108	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 23.

All (108) 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:154:HEM:HMC1	2:B:154:HEM:HBC2	1.44	0.97
1:B:46:PHE:HB3	1:B:49:LEU:HD12	1.49	0.90
2:B:154:HEM:CMC	2:B:154:HEM:HBC2	2.07	0.84
1:B:50:LYS:O	1:B:51:SER:HB3	1.78	0.83
1:B:110:ALA:O	1:B:114:VAL:HG23	1.84	0.77
1:A:19:ALA:O	1:A:20:ASP:HB2	1.83	0.76
1:A:95:THR:HB	1:B:95:THR:HG21	1.67	0.76
1:B:87:THR:O	1:B:91:GLN:HG3	1.85	0.75
1:A:144:ALA:HA	1:A:147:LYS:HE3	1.68	0.75
1:A:59:GLU:HG3	1:A:63:LYS:HE2	1.70	0.74
1:A:145:LYS:O	1:A:149:LEU:HG	1.88	0.74
1:B:120:PRO:O	1:B:121:GLY:C	2.26	0.73
1:A:30:ILE:O	1:A:34:LYS:HG2	1.89	0.72
1:A:149:LEU:HB2	1:A:151:PHE:HD2	1.54	0.72
1:A:99:ILE:HD12	2:A:154:HEM:CAC	2.20	0.71
1:B:3:SER:OG	1:B:6:GLU:HG3	1.91	0.71
1:A:52:GLU:O	1:A:56:LYS:HG3	1.91	0.69
1:B:98:LYS:O	1:B:100:PRO:HD3	1.93	0.69
1:A:82:HIS:NE2	1:A:141:ASP:OD2	2.20	0.67
1:B:86:LEU:C	1:B:86:LEU:HD23	2.15	0.66
1:A:146:TYR:O	1:A:149:LEU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ASP:OD1	3:B:171:HOH:O	2.14	0.64
1:A:27:GLU:OE2	1:A:118:LYS:NZ	2.31	0.64
1:B:1:GLY:CA	3:B:162:HOH:O	2.46	0.62
1:A:110:ALA:O	1:A:114:VAL:HG23	2.00	0.61
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.36	0.61
1:A:86:LEU:CD2	1:A:141:ASP:HB3	2.32	0.60
1:A:36:HIS:HB2	1:A:39:THR:HG23	1.84	0.60
1:B:87:THR:N	1:B:88:PRO:HD2	2.17	0.59
1:B:1:GLY:HA3	3:B:162:HOH:O	2.01	0.59
1:B:7:TRP:HB3	1:B:79:LYS:HE2	1.84	0.59
1:B:85:GLU:N	1:B:85:GLU:OE1	2.31	0.59
1:A:42:LYS:HE2	1:A:98:LYS:O	2.03	0.58
1:A:149:LEU:HB2	1:A:151:PHE:CD2	2.37	0.58
1:B:42:LYS:HG2	1:B:99:ILE:HD12	1.85	0.58
1:A:87:THR:HB	1:A:88:PRO:HD3	1.87	0.57
1:A:19:ALA:O	1:A:20:ASP:CB	2.47	0.57
1:B:59:GLU:O	1:B:63:LYS:HD2	2.06	0.56
1:A:78:LYS:O	1:A:79:LYS:C	2.43	0.56
1:A:11:LEU:HD11	1:A:79:LYS:HE3	1.86	0.55
1:A:75:ILE:HD13	1:A:86:LEU:HD12	1.88	0.55
1:B:86:LEU:CD2	1:B:145:LYS:HD3	2.37	0.55
1:A:124:GLY:O	1:A:128:GLN:HG3	2.07	0.54
1:B:109:GLU:O	1:B:113:GLN:HG3	2.06	0.54
1:A:147:LYS:CB	1:A:147:LYS:NZ	2.69	0.54
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.90	0.53
2:A:154:HEM:HBC2	2:A:154:HEM:HMC2	1.91	0.52
1:B:24:HIS:O	1:B:28:VAL:HG23	2.09	0.52
1:B:42:LYS:HG2	1:B:99:ILE:CD1	2.38	0.52
1:B:50:LYS:O	1:B:51:SER:CB	2.47	0.51
1:A:90:ALA:O	1:A:94:ALA:HB2	2.09	0.51
1:B:46:PHE:CZ	1:B:61:LEU:HA	2.45	0.51
1:A:140:ASN:O	1:A:143:ALA:HB3	2.11	0.50
1:A:36:HIS:HB2	1:A:39:THR:CG2	2.40	0.50
1:A:57:ALA:HB3	3:A:172:HOH:O	2.11	0.50
1:B:87:THR:OG1	1:B:145:LYS:HE2	2.12	0.50
1:B:29:LEU:HD11	1:B:65:GLY:HA2	1.93	0.50
1:B:11:LEU:CD1	1:B:79:LYS:HE3	2.43	0.49
1:B:87:THR:N	1:B:88:PRO:CD	2.76	0.49
1:A:101:VAL:O	1:A:104:LEU:HB2	2.13	0.48
1:A:50:LYS:N	1:A:54:GLU:OE1	2.40	0.48
1:B:7:TRP:CE2	1:B:79:LYS:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.77	0.48
1:B:119:HIS:N	1:B:120:PRO:HD3	2.28	0.48
1:A:95:THR:HG22	1:A:151:PHE:CE2	2.48	0.48
1:A:23:GLY:O	1:A:27:GLU:HG3	2.13	0.48
1:B:78:LYS:HB3	1:B:78:LYS:HZ3	1.78	0.48
1:B:11:LEU:HD11	1:B:79:LYS:HE3	1.95	0.47
1:B:43:PHE:O	1:B:47:LYS:HG2	2.13	0.47
1:B:96:LYS:HD2	1:B:97:HIS:CE1	2.50	0.47
1:A:99:ILE:HA	1:A:100:PRO:HD2	1.73	0.47
1:B:2:LEU:HD21	1:B:134:ALA:HB2	1.97	0.47
1:A:48:HIS:O	1:A:50:LYS:HG2	2.14	0.46
1:B:97:HIS:O	1:B:98:LYS:HB2	2.15	0.46
1:B:71:ALA:HB2	2:B:154:HEM:CMA	2.45	0.45
1:A:86:LEU:HD11	1:A:138:PHE:CD2	2.52	0.45
1:A:90:ALA:O	1:A:94:ALA:CB	2.64	0.45
1:A:95:THR:HB	1:B:95:THR:CG2	2.41	0.45
1:B:101:VAL:HG22	1:B:146:TYR:CE2	2.52	0.44
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.44	0.44
1:B:31:ARG:CG	3:B:173:HOH:O	2.66	0.44
1:A:103:TYR:O	1:A:106:PHE:N	2.50	0.44
1:B:101:VAL:HG22	1:B:146:TYR:CD2	2.53	0.44
1:A:78:LYS:O	1:A:81:HIS:N	2.50	0.44
1:A:11:LEU:CD1	1:A:79:LYS:HE3	2.47	0.44
1:B:26:GLN:HG2	1:B:30:ILE:HD12	1.99	0.44
1:B:71:ALA:HB2	2:B:154:HEM:HMA1	2.00	0.43
1:B:31:ARG:HG2	3:B:173:HOH:O	2.19	0.43
1:B:46:PHE:CB	1:B:49:LEU:HD12	2.35	0.43
1:B:42:LYS:HE3	1:B:103:TYR:HE2	1.84	0.42
1:B:78:LYS:HB3	1:B:81:HIS:O	2.19	0.42
1:B:140:ASN:HA	1:B:140:ASN:HD22	1.58	0.42
1:B:78:LYS:HD3	3:B:195:HOH:O	2.20	0.42
1:B:143:ALA:O	1:B:146:TYR:HB2	2.19	0.42
1:B:135:LEU:HA	1:B:135:LEU:HD23	1.39	0.41
1:A:147:LYS:HB3	1:A:147:LYS:NZ	2.34	0.41
1:A:36:HIS:CB	1:A:39:THR:HG23	2.49	0.41
1:B:99:ILE:HA	1:B:100:PRO:HD2	1.84	0.41
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.88	0.41
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.66	0.41
1:A:114:VAL:O	1:A:118:LYS:HB2	2.19	0.41
1:A:7:TRP:CE3	1:A:7:TRP:HA	2.56	0.41
2:B:154:HEM:HMC1	2:B:154:HEM:CBC	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:N	1:A:6:GLU:OE1	2.43	0.40
1:B:6:GLU:O	1:B:7:TRP:C	2.60	0.40
1:B:27:GLU:OE2	1:B:118:LYS:HD2	2.21	0.40
1:B:51:SER:O	1:B:54:GLU:N	2.55	0.40
1:B:7:TRP:CD2	1:B:79:LYS:HB3	2.56	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	151/153 (99%)	143 (95%)	4 (3%)	4 (3%)	5	2
1	B	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
All	All	302/306 (99%)	284 (94%)	14 (5%)	4 (1%)	12	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	20	ASP
1	A	79	LYS
1	A	91	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%)	117 (94%)	7 (6%)	21	18
1	B	124/124 (100%)	111 (90%)	13 (10%)	7	4
All	All	248/248 (100%)	228 (92%)	20 (8%)	11	8

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	83	GLU
1	A	117	SER
1	A	138	PHE
1	A	147	LYS
1	A	148	GLU
1	A	152	GLN
1	B	42	LYS
1	B	45	LYS
1	B	47	LYS
1	B	50	LYS
1	B	53	ASP
1	B	63	LYS
1	B	83	GLU
1	B	102	LYS
1	B	109	GLU
1	B	132	SER
1	B	133	LYS
1	B	145	LYS
1	B	147	LYS

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

Mol	Chain	Res	Type
1	A	66	ASN
1	A	91	GLN
1	A	140	ASN
1	B	12	ASN
1	B	26	GLN
1	B	36	HIS
1	B	116	GLN
1	B	128	GLN
1	B	140	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
2	HEM	B	154	1,3	27,50,50	2.29	9 (33%)	17,82,82	2.99	9 (52%)
2	HEM	A	154	1,3	27,50,50	1.96	5 (18%)	17,82,82	2.53	8 (47%)

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
2	HEM	B	154	1,3	-	1/6/54/54	-
2	HEM	A	154	1,3	-	0/6/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	154	HEM	C3C-C2C	-6.13	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C3C-C2C	-4.77	1.33	1.40
2	B	154	HEM	C3C-CAC	4.71	1.57	1.47
2	A	154	HEM	C3B-C2B	-4.34	1.34	1.40
2	A	154	HEM	C3B-CAB	4.13	1.56	1.47
2	B	154	HEM	C3B-C2B	-4.00	1.34	1.40
2	A	154	HEM	C3C-CAC	3.65	1.55	1.47
2	B	154	HEM	C3B-CAB	3.35	1.54	1.47
2	B	154	HEM	CAA-C2A	2.86	1.56	1.52
2	B	154	HEM	CMD-C2D	2.78	1.57	1.51
2	B	154	HEM	C4B-NB	2.68	1.41	1.36
2	B	154	HEM	CAD-C3D	2.65	1.56	1.52
2	B	154	HEM	C4A-NA	2.12	1.40	1.36
2	A	154	HEM	CMB-C2B	2.05	1.56	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CMA-C3A-C4A	-6.53	118.42	128.46
2	B	154	HEM	CAA-CBA-CGA	5.38	121.70	112.67
2	B	154	HEM	CMA-C3A-C2A	5.33	135.00	124.94
2	A	154	HEM	CMA-C3A-C4A	-5.30	120.32	128.46
2	A	154	HEM	CMA-C3A-C2A	4.47	133.37	124.94
2	A	154	HEM	CMD-C2D-C1D	-3.67	122.82	128.46
2	B	154	HEM	CMD-C2D-C1D	-3.58	122.96	128.46
2	A	154	HEM	CMD-C2D-C3D	3.48	131.51	124.94
2	A	154	HEM	CBA-CAA-C2A	-3.33	106.34	112.49
2	A	154	HEM	CBD-CAD-C3D	-3.26	106.48	112.48
2	B	154	HEM	CMD-C2D-C3D	2.91	130.43	124.94
2	B	154	HEM	CBA-CAA-C2A	2.78	117.61	112.49
2	B	154	HEM	CBD-CAD-C3D	-2.31	108.23	112.48
2	B	154	HEM	CMB-C2B-C3B	2.31	128.99	124.68
2	B	154	HEM	CMC-C2C-C3C	2.20	128.78	124.68
2	A	154	HEM	C1D-C2D-C3D	-2.13	105.52	107.00
2	A	154	HEM	CAA-CBA-CGA	2.11	116.20	112.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

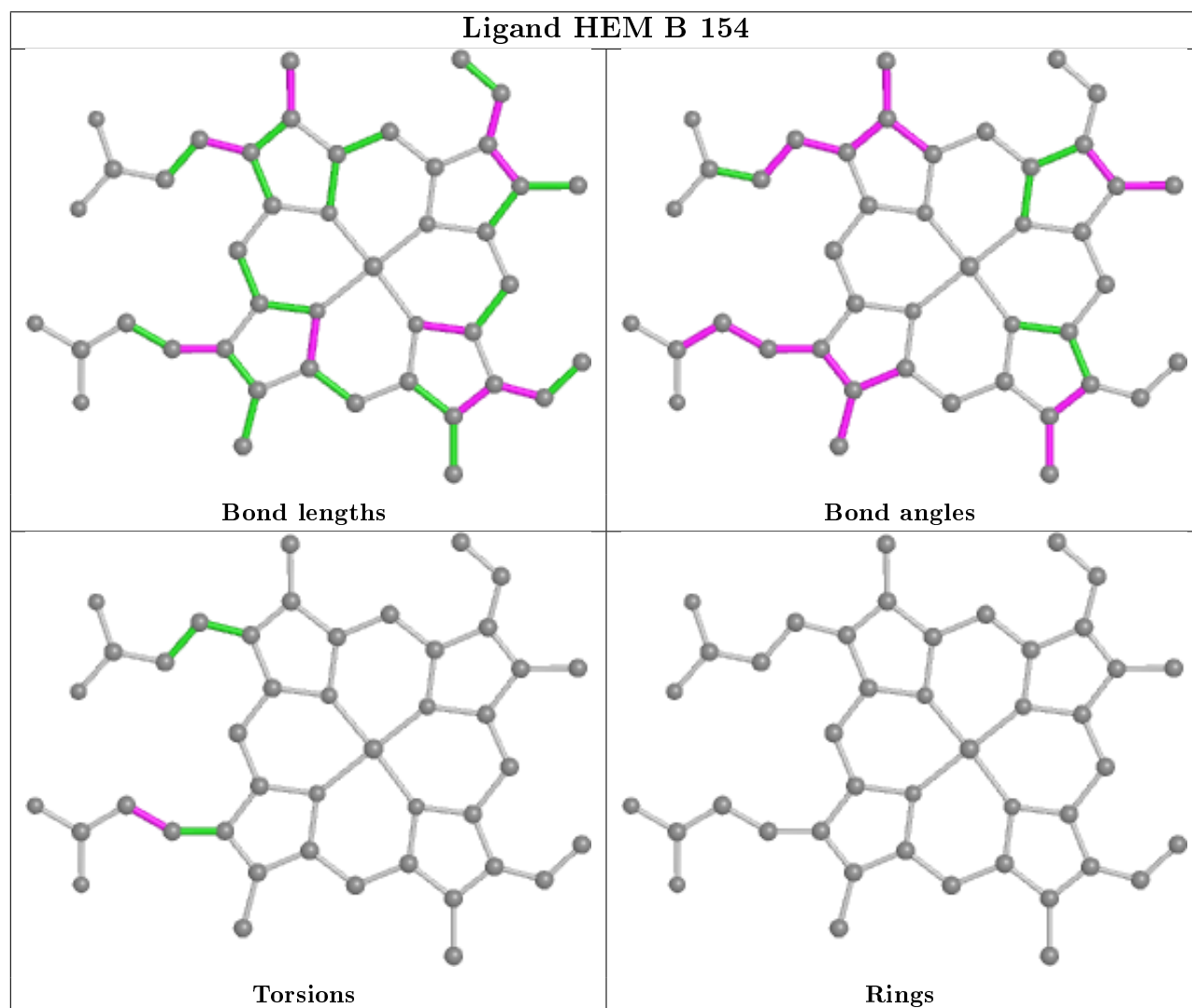
Mol	Chain	Res	Type	Atoms
2	B	154	HEM	C2A-CAA-CBA-CGA

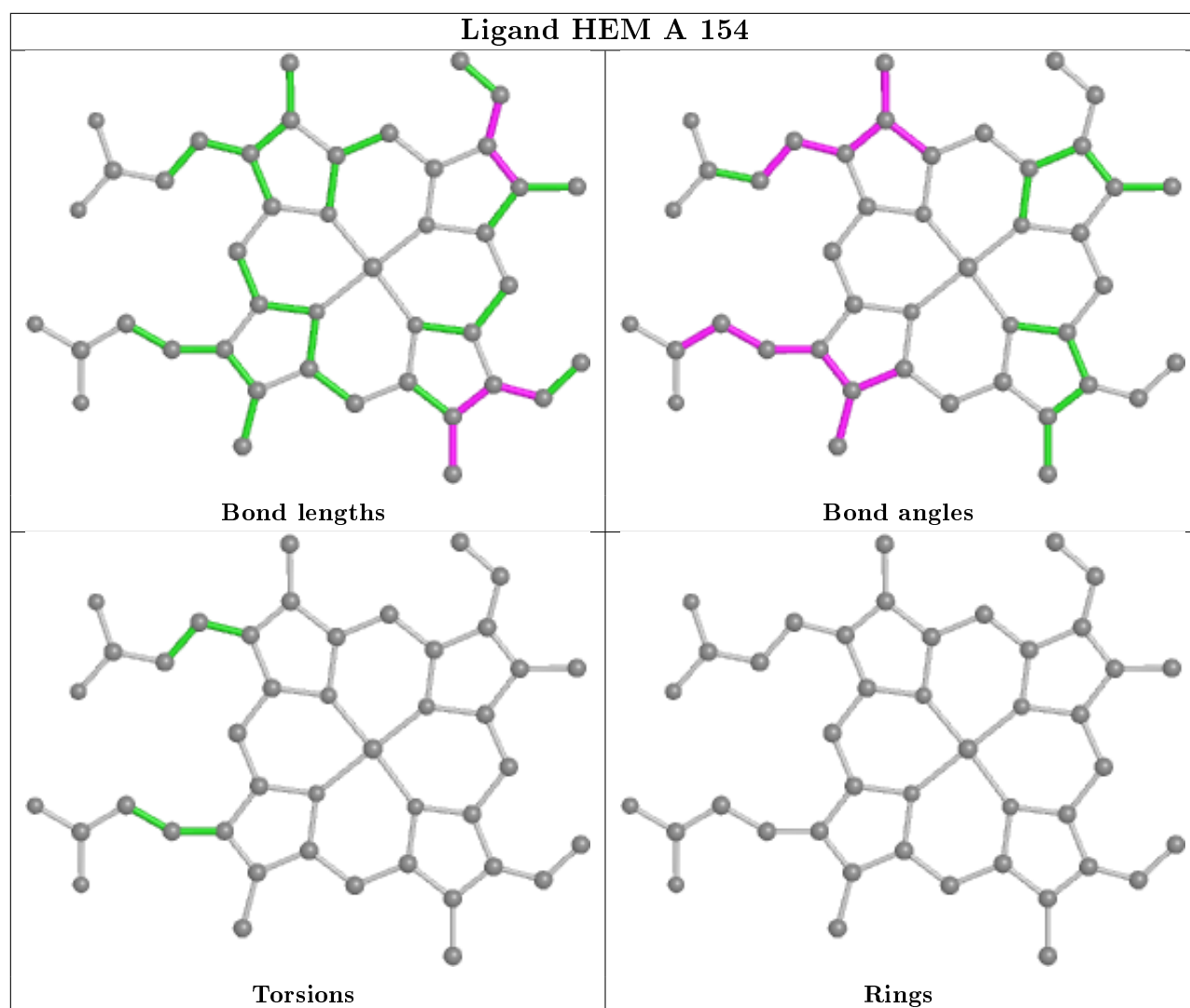
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	HEM	5	0
2	A	154	HEM	2	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.