



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:25 pm BST

PDB ID : 1YCA  
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 : 2.90 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](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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

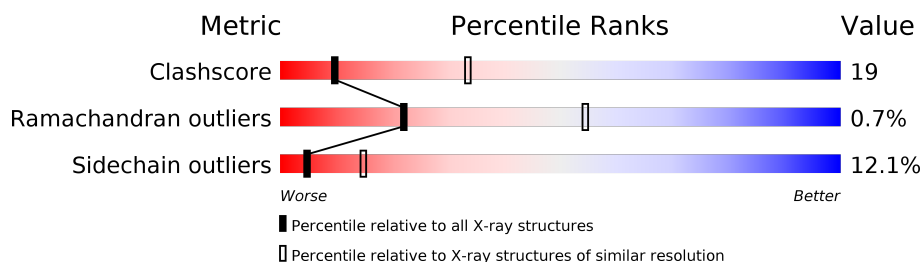
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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 4 unique types of molecules in this entry. The entry contains 2591 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	42	0	0
			1197	763	208	223	3			
1	B	153	Total	C	N	O	S	48	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:  $C_{34}H_{32}FeN_4O_4$ ).



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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 CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 4 is water.

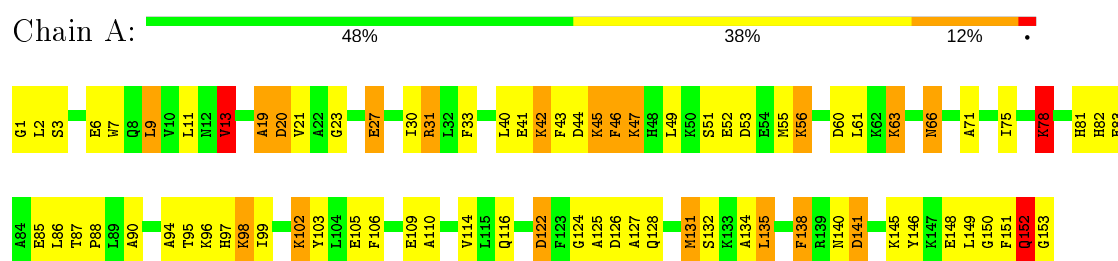
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	58	Total	O	0	0
			58	58		

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

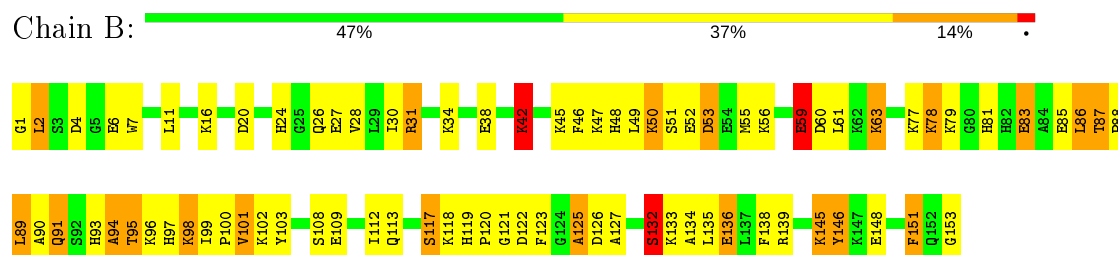
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	124.20 Å   42.50 Å   92.10 Å 90.00°   92.20°   90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2591	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: CMO, 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	1.44	6/1222 (0.5%)	2.21	53/1637 (3.2%)
1	B	1.28	5/1222 (0.4%)	2.34	53/1637 (3.2%)
All	All	1.37	11/2444 (0.5%)	2.27	106/3274 (3.2%)

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	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLY	C-OXT	-22.51	0.80	1.23
1	A	83	GLU	CB-CG	12.19	1.75	1.52
1	B	151	PHE	C-N	-11.93	1.06	1.34
1	A	152	GLN	CA-CB	-8.71	1.34	1.53
1	A	56	LYS	CE-NZ	7.58	1.68	1.49
1	A	63	LYS	CD-CE	7.27	1.69	1.51
1	A	1	GLY	N-CA	6.86	1.56	1.46
1	B	34	LYS	CD-CE	-6.85	1.34	1.51
1	B	136	GLU	CD-OE2	6.26	1.32	1.25
1	B	153	GLY	C-OXT	-5.22	1.13	1.23
1	B	108	SER	CB-OG	5.13	1.49	1.42

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PHE	O-C-N	-28.40	77.26	122.70
1	B	139	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	A	31	ARG	NE-CZ-NH1	-15.23	112.69	120.30
1	A	152	GLN	N-CA-CB	11.10	130.59	110.60
1	A	31	ARG	CD-NE-CZ	-10.97	108.24	123.60
1	A	31	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	B	148	GLU	OE1-CD-OE2	9.14	134.27	123.30
1	B	146	TYR	CB-CG-CD1	9.13	126.48	121.00
1	A	146	TYR	CB-CG-CD2	-8.89	115.66	121.00
1	B	139	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	A	126	ASP	CB-CG-OD1	8.76	126.18	118.30
1	A	49	LEU	CB-CA-C	8.75	126.83	110.20
1	B	60	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	B	27	GLU	OE1-CD-OE2	8.22	133.17	123.30
1	B	53	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	B	146	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	146	TYR	CB-CG-CD1	7.90	125.74	121.00
1	B	136	GLU	CB-CG-CD	7.79	135.22	114.20
1	A	132	SER	CA-CB-OG	-7.54	90.85	111.20
1	B	151	PHE	C-N-CA	7.51	140.47	121.70
1	A	60	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	78	LYS	CA-CB-CG	7.37	129.62	113.40
1	B	59	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	B	123	PHE	CB-CG-CD1	-7.35	115.66	120.80
1	B	20	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	106	PHE	CB-CG-CD1	-7.14	115.80	120.80
1	A	122	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	135	LEU	CB-CG-CD2	-6.99	99.12	111.00
1	A	40	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	B	126	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	127	ALA	CB-CA-C	6.86	120.39	110.10
1	A	21	VAL	CA-CB-CG1	6.76	121.04	110.90
1	B	132	SER	CB-CA-C	-6.71	97.35	110.10
1	B	42	LYS	CD-CE-NZ	-6.66	96.39	111.70
1	A	56	LYS	CD-CE-NZ	6.62	126.92	111.70
1	A	102	LYS	CA-CB-CG	-6.50	99.11	113.40
1	A	131	MET	CG-SD-CE	-6.49	89.81	100.20
1	B	132	SER	CA-CB-OG	-6.44	93.80	111.20
1	B	85	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	A	116	GLN	O-C-N	-6.35	112.54	122.70
1	A	49	LEU	O-C-N	6.35	132.85	122.70
1	A	109	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	A	125	ALA	N-CA-CB	-6.29	101.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PHE	CA-C-O	-6.28	106.92	120.10
1	B	122	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	B	127	ALA	CB-CA-C	6.21	119.41	110.10
1	A	13	VAL	CA-CB-CG2	-6.17	101.65	110.90
1	B	94	ALA	O-C-N	6.11	132.48	122.70
1	B	31	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	A	135	LEU	CB-CG-CD2	-6.06	100.70	111.00
1	A	51	SER	O-C-N	6.04	132.36	122.70
1	B	20	ASP	OD1-CG-OD2	-6.03	111.85	123.30
1	B	86	LEU	CA-CB-CG	6.01	129.12	115.30
1	B	125	ALA	N-CA-CB	-6.00	101.69	110.10
1	A	53	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	112	ILE	CB-CG1-CD1	-5.92	97.34	113.90
1	A	85	GLU	CG-CD-OE1	5.90	130.10	118.30
1	B	4	ASP	CB-CG-OD1	-5.85	113.04	118.30
1	B	136	GLU	CA-CB-CG	5.84	126.26	113.40
1	A	3	SER	O-C-N	-5.82	113.39	122.70
1	A	134	ALA	CB-CA-C	5.78	118.77	110.10
1	A	27	GLU	CG-CD-OE1	-5.76	106.78	118.30
1	B	151	PHE	CA-C-N	5.75	129.86	117.20
1	A	33	PHE	CB-CG-CD2	-5.74	116.79	120.80
1	A	19	ALA	O-C-N	-5.72	113.54	122.70
1	B	94	ALA	N-CA-CB	5.72	118.11	110.10
1	A	66	ASN	CA-C-O	5.65	131.96	120.10
1	B	48	HIS	CB-CA-C	5.64	121.68	110.40
1	B	134	ALA	CB-CA-C	5.63	118.54	110.10
1	B	16	LYS	CB-CA-C	-5.59	99.21	110.40
1	B	122	ASP	OD1-CG-OD2	5.55	133.85	123.30
1	B	77	LYS	CA-C-N	5.50	129.30	117.20
1	A	60	ASP	C-N-CA	5.47	135.38	121.70
1	A	53	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	20	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	71	ALA	N-CA-CB	5.41	117.67	110.10
1	B	122	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	B	103	TYR	O-C-N	5.38	131.30	122.70
1	A	1	GLY	CA-C-O	5.36	130.25	120.60
1	B	27	GLU	CG-CD-OE2	-5.36	107.59	118.30
1	A	9	LEU	N-CA-CB	-5.33	99.73	110.40
1	A	141	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	150	GLY	O-C-N	5.31	131.19	122.70
1	B	26	GLN	O-C-N	-5.30	114.22	122.70
1	A	105	GLU	CA-CB-CG	5.29	125.04	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	1	GLY	N-CA-C	-5.28	99.91	113.10
1	A	27	GLU	CG-CD-OE2	5.26	128.82	118.30
1	A	81	HIS	CA-CB-CG	-5.26	104.66	113.60
1	B	138	PHE	CG-CD2-CE2	-5.22	115.06	120.80
1	A	127	ALA	O-C-N	-5.22	114.35	122.70
1	A	43	PHE	CG-CD1-CE1	-5.19	115.09	120.80
1	A	138	PHE	CB-CA-C	5.18	120.76	110.40
1	B	89	LEU	CB-CA-C	5.18	120.04	110.20
1	B	2	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	B	26	GLN	OE1-CD-NE2	5.17	133.79	121.90
1	B	53	ASP	OD1-CG-OD2	5.17	133.12	123.30
1	A	45	LYS	CD-CE-NZ	-5.13	99.90	111.70
1	A	46	PHE	O-C-N	5.11	130.87	122.70
1	B	148	GLU	N-CA-CB	-5.11	101.41	110.60
1	A	27	GLU	CB-CG-CD	-5.10	100.44	114.20
1	A	103	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	B	103	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	B	91	GLN	N-CA-CB	-5.03	101.54	110.60
1	A	43	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	B	87	THR	CA-CB-CG2	5.03	119.44	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	1203	40	0
1	B	1197	0	1202	49	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	A	49	0	0	4	0
4	B	58	0	0	4	0
All	All	2591	0	2465	91	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 19.

All (91) 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:B:78:LYS:HB3	1:B:78:LYS:HZ3	1.30	0.94
1:B:31:ARG:HD2	4:B:176:HOH:O	1.68	0.93
2:B:154:HEM:HMC2	2:B:154:HEM:HBC2	1.61	0.81
1:B:78:LYS:HB3	1:B:78:LYS:NZ	1.93	0.80
1:A:96:LYS:HE2	4:A:191:HOH:O	1.81	0.79
1:A:42:LYS:NZ	1:A:98:LYS:O	2.18	0.75
2:A:154:HEM:HBC2	2:A:154:HEM:HMC2	1.68	0.74
1:A:42:LYS:HG2	1:A:99:ILE:CD1	2.20	0.72
1:B:46:PHE:HB3	1:B:49:LEU:HD12	1.71	0.71
1:B:42:LYS:HG2	1:B:99:ILE:CD1	2.20	0.71
1:A:87:THR:HB	1:A:88:PRO:HD3	1.72	0.70
1:B:87:THR:HB	1:B:88:PRO:HD3	1.76	0.68
1:B:42:LYS:HG2	1:B:99:ILE:HD12	1.75	0.67
1:A:96:LYS:HD3	1:A:97:HIS:CE1	2.30	0.67
1:B:87:THR:O	1:B:91:GLN:HB2	1.95	0.66
1:B:52:GLU:O	1:B:56:LYS:HG3	1.96	0.65
1:A:86:LEU:CD2	1:A:141:ASP:HB3	2.29	0.62
1:B:118:LYS:NZ	4:B:199:HOH:O	2.31	0.62
1:B:38:GLU:OE1	1:B:38:GLU:N	2.28	0.61
1:A:86:LEU:HD21	1:A:141:ASP:HB3	1.82	0.60
1:A:46:PHE:CZ	1:A:61:LEU:HA	2.37	0.59
1:B:59:GLU:O	1:B:63:LYS:HD2	2.02	0.59
1:B:90:ALA:O	1:B:94:ALA:CB	2.50	0.59
1:B:11:LEU:CD1	1:B:79:LYS:HE3	2.32	0.59
2:B:154:HEM:CMC	2:B:154:HEM:HBC2	2.31	0.59
1:A:31:ARG:NH1	4:A:171:HOH:O	2.35	0.57
1:B:132:SER:O	1:B:136:GLU:HB2	2.06	0.56
1:B:11:LEU:HD11	1:B:79:LYS:HE3	1.89	0.55
1:A:149:LEU:O	1:B:91:GLN:OE1	2.24	0.55
2:A:154:HEM:CMC	2:A:154:HEM:HBC2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:HD23	1:B:145:LYS:HD3	1.89	0.54
1:B:52:GLU:HG2	1:B:56:LYS:HE3	1.89	0.54
1:B:87:THR:N	1:B:88:PRO:CD	2.71	0.54
1:A:110:ALA:O	1:A:114:VAL:HG23	2.08	0.53
1:B:90:ALA:O	1:B:94:ALA:HB2	2.09	0.53
1:B:101:VAL:HG12	1:B:146:TYR:CD2	2.43	0.52
1:A:42:LYS:HG2	1:A:99:ILE:HD13	1.90	0.52
1:A:87:THR:N	1:A:88:PRO:CD	2.74	0.51
1:A:124:GLY:O	1:A:128:GLN:HG3	2.11	0.51
1:A:30:ILE:HG12	1:A:55:MET:HB3	1.93	0.51
1:B:93:HIS:O	1:B:99:ILE:N	2.38	0.50
1:A:7:TRP:O	1:A:11:LEU:HG	2.12	0.49
1:A:19:ALA:O	1:A:20:ASP:HB2	2.12	0.49
1:B:78:LYS:HB3	1:B:81:HIS:O	2.14	0.48
1:B:61:LEU:HD23	1:B:61:LEU:O	2.13	0.48
1:A:140:ASN:ND2	4:A:201:HOH:O	2.46	0.47
1:A:75:ILE:O	1:A:78:LYS:HB2	2.14	0.47
1:A:44:ASP:O	1:A:47:LYS:HG3	2.14	0.47
1:B:61:LEU:HD23	1:B:61:LEU:C	2.35	0.47
1:B:96:LYS:HE3	4:B:213:HOH:O	2.14	0.47
1:B:78:LYS:NZ	1:B:81:HIS:O	2.47	0.46
1:B:96:LYS:HD2	1:B:97:HIS:CE1	2.50	0.46
1:A:135:LEU:HA	1:A:135:LEU:HD23	1.71	0.46
1:A:87:THR:CB	1:A:88:PRO:HD3	2.44	0.46
1:A:99:ILE:HD12	2:A:154:HEM:CAC	2.46	0.46
1:B:2:LEU:HD23	1:B:6:GLU:HB3	1.98	0.46
1:A:31:ARG:HD2	4:A:171:HOH:O	2.16	0.46
1:B:119:HIS:N	1:B:120:PRO:CD	2.78	0.46
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.97	0.46
1:A:23:GLY:O	1:A:27:GLU:HG3	2.15	0.45
1:A:7:TRP:HA	1:A:7:TRP:CE3	2.50	0.45
1:B:89:LEU:HD12	1:B:93:HIS:CE1	2.52	0.45
1:B:11:LEU:HD12	1:B:79:LYS:HE3	1.97	0.45
1:B:78:LYS:CB	1:B:78:LYS:NZ	2.59	0.45
1:A:97:HIS:NE2	2:A:154:HEM:O1A	2.41	0.45
1:B:83:GLU:HG3	1:B:83:GLU:O	2.16	0.44
1:B:24:HIS:O	1:B:28:VAL:HG23	2.17	0.44
1:A:2:LEU:HD23	1:A:6:GLU:HB3	2.00	0.44
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.65	0.44
1:A:87:THR:N	1:A:88:PRO:HD2	2.33	0.44
1:A:95:THR:HB	1:B:95:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.53	0.44
1:A:42:LYS:HG2	1:A:99:ILE:HD11	1.97	0.44
1:A:52:GLU:O	1:A:56:LYS:HG3	2.17	0.44
1:B:120:PRO:O	1:B:121:GLY:C	2.53	0.44
1:A:90:ALA:O	1:A:94:ALA:CB	2.66	0.43
1:B:42:LYS:CG	1:B:99:ILE:CD1	2.95	0.43
1:B:113:GLN:O	1:B:117:SER:HB3	2.18	0.43
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.72	0.43
1:B:101:VAL:HG12	1:B:146:TYR:HD2	1.85	0.42
1:B:50:LYS:O	1:B:51:SER:HB3	2.20	0.42
1:B:98:LYS:O	1:B:100:PRO:HD3	2.20	0.41
1:B:78:LYS:O	1:B:79:LYS:C	2.58	0.41
1:A:13:VAL:CG1	1:A:131:MET:CE	2.98	0.41
1:A:82:HIS:NE2	1:A:141:ASP:OD2	2.39	0.41
1:A:44:ASP:O	1:A:47:LYS:CG	2.68	0.41
1:A:52:GLU:HG2	1:A:56:LYS:CE	2.51	0.41
1:B:125:ALA:N	4:B:203:HOH:O	2.39	0.41
1:B:6:GLU:O	1:B:7:TRP:C	2.59	0.40
1:A:63:LYS:O	1:A:66:ASN:HB3	2.21	0.40
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.90	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%)	146 (97%)	4 (3%)	1 (1%)	22	54
1	B	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	22	54
All	All	302/306 (99%)	289 (96%)	11 (4%)	2 (1%)	22	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	45	LYS

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/124 (100%)	111 (90%)	13 (10%)	7	21
1	B	124/124 (100%)	107 (86%)	17 (14%)	3	11
All	All	248/248 (100%)	218 (88%)	30 (12%)	5	15

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	41	GLU
1	A	42	LYS
1	A	45	LYS
1	A	47	LYS
1	A	78	LYS
1	A	98	LYS
1	A	102	LYS
1	A	122	ASP
1	A	138	PHE
1	A	145	LYS
1	A	148	GLU
1	A	152	GLN
1	B	42	LYS
1	B	47	LYS
1	B	50	LYS
1	B	53	ASP
1	B	59	GLU
1	B	63	LYS
1	B	78	LYS
1	B	83	GLU
1	B	95	THR

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Mol	Chain	Res	Type
1	B	98	LYS
1	B	101	VAL
1	B	102	LYS
1	B	109	GLU
1	B	117	SER
1	B	132	SER
1	B	133	LYS
1	B	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	36	HIS
1	A	91	GLN
1	A	140	ASN
1	B	26	GLN
1	B	36	HIS
1	B	116	GLN
1	B	128	GLN

### 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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  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	CMO	B	155	2	0,1,1	0.00	-	-		
2	HEM	A	154	1,3	27,50,50	2.17	8 (29%)	17,82,82	2.12	8 (47%)
2	HEM	B	154	1,3	27,50,50	2.22	8 (29%)	17,82,82	2.53	8 (47%)
3	CMO	A	155	2	0,1,1	0.00	-	-		

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C3B-C2B	-5.69	1.32	1.40
2	B	154	HEM	C3C-C2C	-5.15	1.33	1.40
2	B	154	HEM	C3B-C2B	-4.78	1.33	1.40
2	B	154	HEM	C3C-CAC	4.59	1.57	1.47
2	A	154	HEM	C3C-C2C	-4.44	1.34	1.40
2	A	154	HEM	C3B-CAB	3.91	1.55	1.47
2	B	154	HEM	C3B-CAB	3.52	1.55	1.47
2	A	154	HEM	C3C-CAC	3.25	1.54	1.47
2	B	154	HEM	CAA-C2A	2.96	1.56	1.52
2	A	154	HEM	CMB-C2B	2.83	1.58	1.51
2	A	154	HEM	C4A-NA	2.29	1.40	1.36
2	B	154	HEM	C4A-NA	2.20	1.40	1.36
2	B	154	HEM	CAD-C3D	2.19	1.56	1.52
2	A	154	HEM	CAA-C2A	2.17	1.55	1.52
2	B	154	HEM	C1A-NA	2.16	1.40	1.36
2	A	154	HEM	CMD-C2D	2.13	1.56	1.51

All (16) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CBD-CAD-C3D	-5.22	102.86	112.48
2	B	154	HEM	CMB-C2B-C3B	4.36	132.83	124.68
2	B	154	HEM	CMD-C2D-C1D	-4.02	122.29	128.46
2	B	154	HEM	CMA-C3A-C4A	-3.74	122.72	128.46
2	A	154	HEM	CMD-C2D-C1D	-3.66	122.85	128.46
2	A	154	HEM	CMD-C2D-C3D	3.27	131.10	124.94
2	A	154	HEM	CMA-C3A-C4A	-3.21	123.54	128.46
2	B	154	HEM	CMD-C2D-C3D	3.17	130.92	124.94
2	A	154	HEM	CAA-CBA-CGA	2.97	117.66	112.67
2	B	154	HEM	CMA-C3A-C2A	2.93	130.47	124.94
2	A	154	HEM	C4C-C3C-C2C	2.57	108.69	106.90
2	A	154	HEM	CMC-C2C-C3C	2.39	129.15	124.68
2	A	154	HEM	CAD-CBD-CGD	2.38	116.66	112.67
2	A	154	HEM	CMB-C2B-C3B	2.37	129.12	124.68
2	B	154	HEM	CAA-CBA-CGA	-2.32	108.77	112.67
2	B	154	HEM	CMC-C2C-C3C	2.02	128.45	124.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

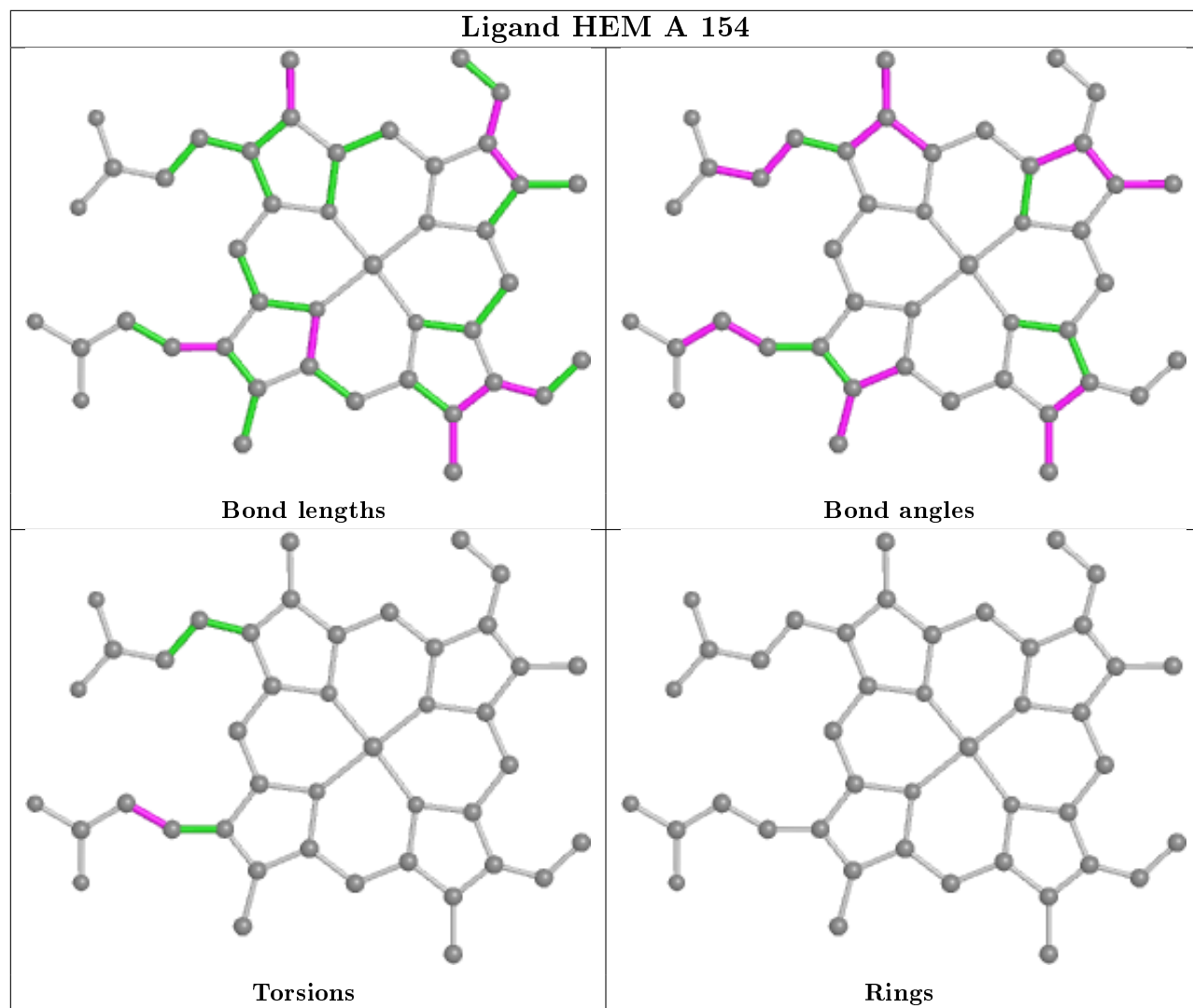
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	C2A-CAA-CBA-CGA
2	B	154	HEM	C2A-CAA-CBA-CGA

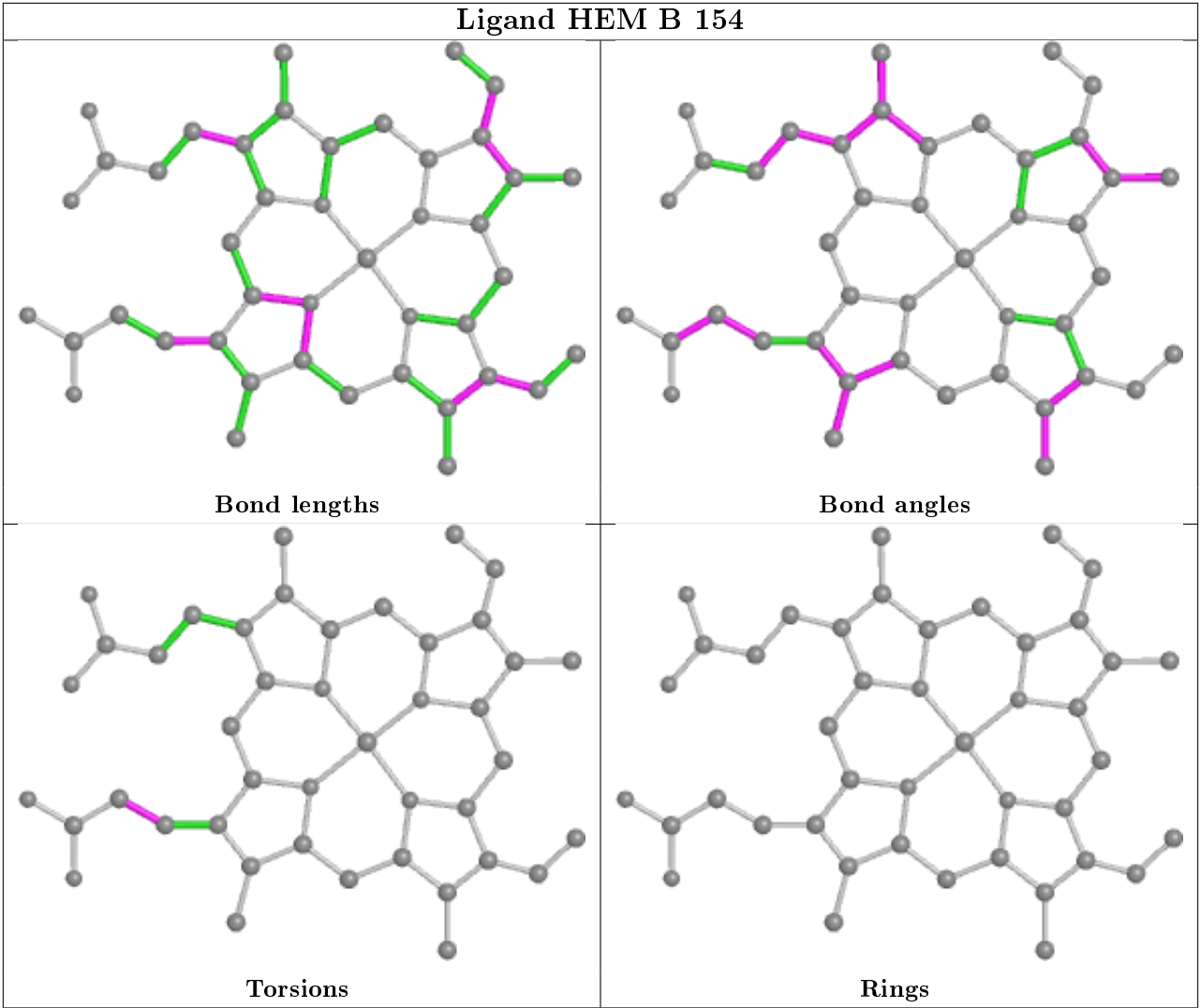
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	4	0
2	B	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	151:PHE	C	152:GLN	N	1.06

## 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.