



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 01:39 PM EST

PDB ID : 2DHB  
Title : THREE DIMENSIONAL FOURIER SYNTHESIS OF HORSE DEOXY-HAEMOGLOBIN AT 2.8 ANGSTROMS RESOLUTION  
Authors : Perutz, M.F.  
Deposited on : 1973-11-01  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (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) : 2.36

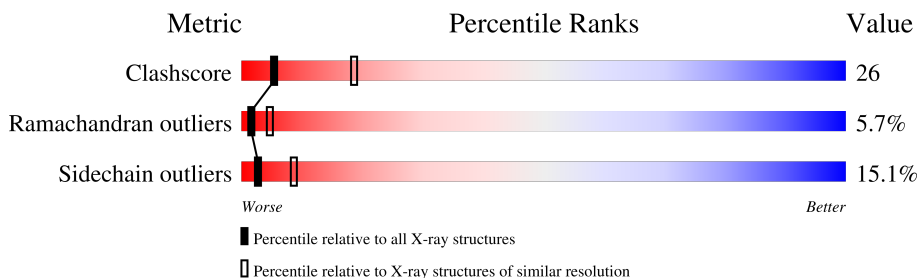
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\geq 3$ , 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	141	 18% 39% 28% 14%
2	B	146	 18% 48% 23% 10%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2289 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 HEMOGLOBIN (DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1069	684	187	196	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ALA	GLY	conflict	UNP P01958
A	65	GLY	ALA	conflict	UNP P01958
A	82	ASP	ASN	conflict	UNP P01958
A	85	ASN	ASP	conflict	UNP P01958

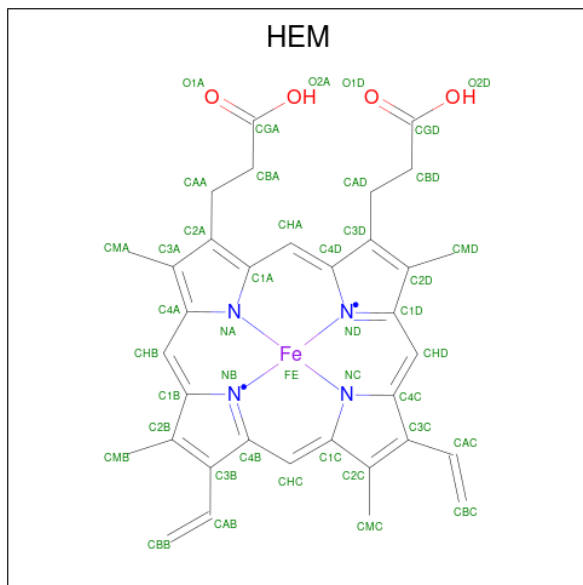
- Molecule 2 is a protein called HEMOGLOBIN (DEOXY) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	146	1132	726	200	204	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	ALA	VAL	conflict	UNP P02062
B	112	LEU	VAL	conflict	UNP P02062
B	114	VAL	LEU	conflict	UNP P02062

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is water.

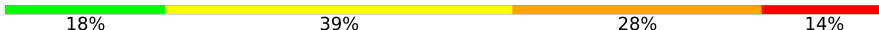
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		

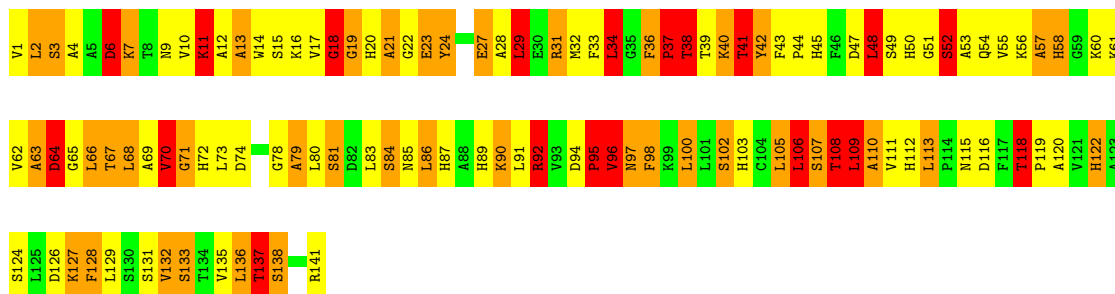
### 3 Residue-property plots

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.

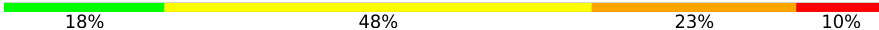
Note EDS was not executed.

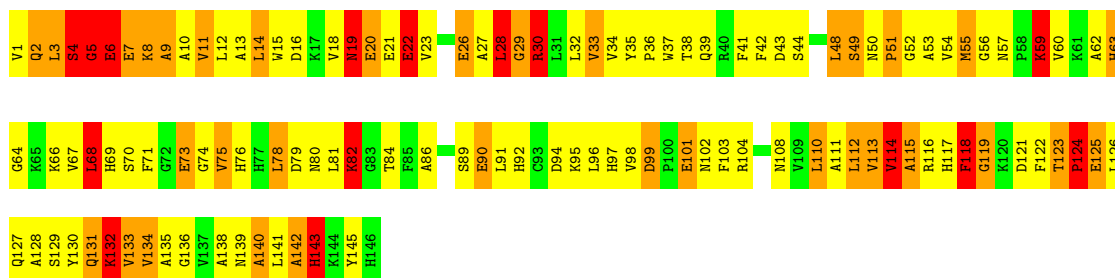
- Molecule 1: HEMOGLOBIN (DEOXY) (ALPHA CHAIN)

Chain A: 



- Molecule 2: HEMOGLOBIN (DEOXY) (BETA CHAIN)

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.96Å 81.70Å 92.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	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	1.26	3/1096 (0.3%)	1.96	26/1487 (1.7%)
2	B	1.25	2/1160 (0.2%)	1.97	23/1569 (1.5%)
All	All	1.25	5/2256 (0.2%)	1.97	49/3056 (1.6%)

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	2	85
2	B	1	90
All	All	3	175

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	TRP	NE1-CE2	-6.85	1.28	1.37
2	B	15	TRP	NE1-CE2	-6.66	1.28	1.37
2	B	37	TRP	NE1-CE2	-6.63	1.28	1.37
1	A	3	SER	CB-OG	5.07	1.48	1.42
1	A	49	SER	CB-OG	5.07	1.48	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LEU	N-CA-CB	9.99	130.38	110.40
2	B	5	GLY	C-N-CA	8.29	142.43	121.70
1	A	108	THR	N-CA-C	7.91	132.36	111.00
1	A	37	PRO	CA-N-CD	-7.32	101.25	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	THR	C-N-CA	7.06	139.35	121.70
1	A	96	VAL	CG1-CB-CG2	-6.95	99.78	110.90
2	B	9	ALA	CA-C-O	-6.83	105.75	120.10
2	B	22	GLU	C-N-CA	6.67	138.38	121.70
2	B	6	GLU	N-CA-C	6.63	128.90	111.00
1	A	92	ARG	NE-CZ-NH1	-6.45	117.08	120.30
2	B	63	HIS	C-N-CA	6.14	135.20	122.30
2	B	19	ASN	CA-C-N	-6.10	103.77	117.20
1	A	133	SER	N-CA-CB	5.99	119.48	110.50
2	B	30	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	A	118	THR	CA-CB-CG2	5.87	120.62	112.40
1	A	62	VAL	CA-CB-CG1	5.86	119.69	110.90
2	B	134	VAL	CA-CB-CG1	5.85	119.68	110.90
1	A	133	SER	CA-C-O	-5.84	107.83	120.10
1	A	6	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	30	ARG	CD-NE-CZ	5.76	131.66	123.60
1	A	38	THR	CA-CB-CG2	5.69	120.37	112.40
2	B	42	PHE	N-CA-C	5.69	126.37	111.00
1	A	137	THR	CA-CB-OG1	5.66	120.88	109.00
1	A	27	GLU	N-CA-CB	-5.63	100.46	110.60
2	B	2	GLN	C-N-CA	5.60	135.71	121.70
1	A	24	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	A	42	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	A	34	LEU	CB-CG-CD1	-5.51	101.64	111.00
2	B	49	SER	C-N-CA	5.50	135.45	121.70
1	A	57	ALA	N-CA-CB	5.49	117.79	110.10
2	B	28	LEU	CB-CA-C	5.46	120.57	110.20
1	A	138	SER	N-CA-CB	5.46	118.68	110.50
1	A	106	LEU	CB-CG-CD2	5.42	120.21	111.00
2	B	114	VAL	CA-CB-CG1	5.37	118.95	110.90
1	A	41	THR	CA-CB-CG2	5.35	119.88	112.40
2	B	124	PRO	CA-N-CD	-5.29	104.09	111.50
2	B	63	HIS	N-CA-CB	5.27	120.08	110.60
2	B	82	LYS	C-N-CA	5.21	133.24	122.30
1	A	48	LEU	CB-CG-CD2	5.19	119.83	111.00
2	B	49	SER	N-CA-C	5.19	125.01	111.00
1	A	11	LYS	N-CA-CB	5.18	119.93	110.60
2	B	26	GLU	OE1-CD-OE2	-5.18	117.09	123.30
2	B	133	VAL	CA-CB-CG1	5.16	118.64	110.90
2	B	118	PHE	CB-CA-C	5.12	120.64	110.40
1	A	115	ASN	N-CA-CB	-5.09	101.43	110.60
2	B	9	ALA	N-CA-CB	5.09	117.22	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	VAL	CA-CB-CG1	5.08	118.52	110.90
1	A	29	LEU	CB-CG-CD1	-5.04	102.43	111.00
2	B	103	PHE	CB-CG-CD2	-5.02	117.28	120.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	108	THR	CA
1	A	109	LEU	CA
2	B	28	LEU	CA

All (175) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	VAL	Mainchain
1	A	100	LEU	Mainchain
1	A	102	SER	Mainchain
1	A	105	LEU	Mainchain
1	A	106	LEU	Mainchain
1	A	107	SER	Mainchain
1	A	108	THR	Peptide
1	A	11	LYS	Mainchain
1	A	110	ALA	Mainchain
1	A	112	HIS	Mainchain
1	A	113	LEU	Mainchain
1	A	118	THR	Mainchain
1	A	12	ALA	Mainchain
1	A	120	ALA	Mainchain
1	A	122	HIS	Mainchain
1	A	124	SER	Mainchain
1	A	126	ASP	Mainchain
1	A	127	LYS	Mainchain
1	A	128	PHE	Mainchain
1	A	13	ALA	Mainchain
1	A	131	SER	Mainchain
1	A	132	VAL	Mainchain
1	A	133	SER	Mainchain
1	A	135	VAL	Mainchain
1	A	136	LEU	Mainchain
1	A	16	LYS	Mainchain
1	A	18	GLY	Mainchain
1	A	19	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	2	LEU	Mainchain
1	A	21	ALA	Mainchain
1	A	23	GLU	Mainchain
1	A	27	GLU	Mainchain
1	A	28	ALA	Mainchain
1	A	29	LEU	Mainchain
1	A	3	SER	Mainchain
1	A	31	ARG	Sidechain
1	A	32	MET	Mainchain
1	A	33	PHE	Mainchain
1	A	34	LEU	Mainchain
1	A	36	PHE	Peptide
1	A	37	PRO	Mainchain
1	A	38	THR	Mainchain
1	A	4	ALA	Mainchain
1	A	41	THR	Mainchain
1	A	42	TYR	Sidechain
1	A	44	PRO	Mainchain
1	A	45	HIS	Mainchain
1	A	48	LEU	Mainchain
1	A	50	HIS	Mainchain
1	A	51	GLY	Mainchain
1	A	52	SER	Mainchain
1	A	53	ALA	Mainchain
1	A	54	GLN	Mainchain
1	A	57	ALA	Mainchain
1	A	58	HIS	Mainchain
1	A	6	ASP	Mainchain
1	A	61	LYS	Mainchain
1	A	63	ALA	Mainchain
1	A	64	ASP	Mainchain
1	A	65	GLY	Mainchain
1	A	67	THR	Mainchain
1	A	68	LEU	Mainchain
1	A	69	ALA	Mainchain
1	A	7	LYS	Mainchain
1	A	70	VAL	Mainchain
1	A	71	GLY	Mainchain
1	A	74	ASP	Mainchain
1	A	78	GLY	Mainchain
1	A	79	ALA	Mainchain
1	A	80	LEU	Mainchain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	A	81	SER	Mainchain
1	A	84	SER	Mainchain
1	A	85	ASN	Mainchain
1	A	86	LEU	Mainchain
1	A	87	HIS	Mainchain
1	A	89	HIS	Mainchain
1	A	9	ASN	Mainchain
1	A	90	LYS	Mainchain
1	A	91	LEU	Mainchain
1	A	92	ARG	Sidechain,Mainchain
1	A	95	PRO	Mainchain
1	A	96	VAL	Mainchain
1	A	97	ASN	Mainchain
1	A	98	PHE	Mainchain
2	B	101	GLU	Sidechain,Mainchain
2	B	104	ARG	Mainchain
2	B	108	ASN	Mainchain
2	B	11	VAL	Mainchain
2	B	110	LEU	Mainchain
2	B	111	ALA	Mainchain
2	B	113	VAL	Mainchain
2	B	114	VAL	Mainchain
2	B	115	ALA	Mainchain
2	B	117	HIS	Mainchain
2	B	118	PHE	Mainchain
2	B	119	GLY	Mainchain
2	B	121	ASP	Mainchain
2	B	123	THR	Peptide,Mainchain
2	B	124	PRO	Mainchain
2	B	125	GLU	Mainchain
2	B	127	GLN	Sidechain,Mainchain
2	B	128	ALA	Mainchain
2	B	130	TYR	Sidechain
2	B	131	GLN	Mainchain
2	B	132	LYS	Mainchain
2	B	135	ALA	Mainchain
2	B	136	GLY	Mainchain
2	B	138	ALA	Mainchain
2	B	14	LEU	Mainchain
2	B	140	ALA	Mainchain
2	B	141	LEU	Mainchain
2	B	142	ALA	Mainchain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	B	145	TYR	Sidechain
2	B	16	ASP	Sidechain,Mainchain
2	B	19	ASN	Sidechain,Mainchain
2	B	20	GLU	Mainchain
2	B	22	GLU	Mainchain
2	B	26	GLU	Mainchain
2	B	27	ALA	Mainchain
2	B	28	LEU	Mainchain
2	B	29	GLY	Mainchain
2	B	30	ARG	Sidechain,Mainchain
2	B	33	VAL	Mainchain
2	B	35	TYR	Sidechain
2	B	38	THR	Mainchain
2	B	39	GLN	Sidechain,Mainchain
2	B	4	SER	Mainchain
2	B	44	SER	Mainchain
2	B	48	LEU	Mainchain
2	B	49	SER	Mainchain
2	B	5	GLY	Mainchain
2	B	50	ASN	Mainchain
2	B	51	PRO	Mainchain
2	B	52	GLY	Mainchain
2	B	55	MET	Mainchain
2	B	56	GLY	Mainchain
2	B	59	LYS	Mainchain
2	B	6	GLU	Mainchain
2	B	60	VAL	Mainchain
2	B	62	ALA	Mainchain
2	B	63	HIS	Mainchain
2	B	64	GLY	Mainchain
2	B	66	LYS	Mainchain
2	B	67	VAL	Mainchain
2	B	68	LEU	Mainchain
2	B	69	HIS	Mainchain
2	B	7	GLU	Mainchain
2	B	70	SER	Mainchain
2	B	71	PHE	Mainchain
2	B	73	GLU	Mainchain
2	B	74	GLY	Mainchain
2	B	75	VAL	Mainchain
2	B	78	LEU	Mainchain
2	B	79	ASP	Sidechain

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Mol	Chain	Res	Type	Group
2	B	8	LYS	Mainchain
2	B	80	ASN	Mainchain
2	B	82	LYS	Mainchain
2	B	84	THR	Mainchain
2	B	86	ALA	Mainchain
2	B	89	SER	Mainchain
2	B	9	ALA	Mainchain
2	B	90	GLU	Mainchain
2	B	94	ASP	Mainchain
2	B	95	LYS	Mainchain
2	B	97	HIS	Mainchain
2	B	99	ASP	Sidechain,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	1069	0	1073	69	52
2	B	1132	0	1120	64	0
3	A	43	0	30	6	0
3	B	43	0	30	2	0
4	A	2	0	0	0	0
All	All	2289	0	2253	119	52

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 (119) 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:83:LEU:HD11	3:A:142:HEM:HMA3	1.50	0.92
2:B:78:LEU:HD21	2:B:133:VAL:HG22	1.49	0.91
1:A:29:LEU:HD11	1:A:58:HIS:HD2	1.39	0.86
2:B:11:VAL:HG11	2:B:133:VAL:HG21	1.61	0.82
1:A:95:PRO:HB3	1:A:137:THR:CG2	2.12	0.80
1:A:84:SER:HB2	1:A:136:LEU:HA	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD13	2:B:124:PRO:C	2.06	0.76
1:A:103:HIS:CE1	2:B:131:GLN:HE22	2.04	0.75
1:A:34:LEU:CD1	2:B:124:PRO:CB	2.65	0.74
2:B:3:LEU:H	2:B:3:LEU:HD12	1.53	0.74
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.53	0.73
2:B:12:LEU:HD11	2:B:76:HIS:HD2	1.52	0.72
2:B:78:LEU:HD21	2:B:133:VAL:CG2	2.18	0.72
1:A:29:LEU:HD11	1:A:58:HIS:CD2	2.25	0.72
1:A:94:ASP:OD2	1:A:96:VAL:HG23	1.89	0.72
1:A:34:LEU:HD11	2:B:124:PRO:CB	2.20	0.71
1:A:34:LEU:HD11	2:B:124:PRO:HB2	1.71	0.70
1:A:70:VAL:O	1:A:73:LEU:HB2	1.93	0.69
2:B:139:ASN:HA	2:B:142:ALA:HB3	1.75	0.69
1:A:111:VAL:HG13	2:B:119:GLY:C	2.15	0.66
1:A:83:LEU:CD1	3:A:142:HEM:HMA3	2.25	0.66
1:A:83:LEU:HD11	3:A:142:HEM:CMA	2.25	0.64
2:B:5:GLY:O	2:B:8:LYS:HB2	1.98	0.64
1:A:31:ARG:HA	1:A:34:LEU:HB2	1.79	0.64
1:A:40:LYS:HE3	1:A:41:THR:HG22	1.81	0.63
2:B:7:GLU:O	2:B:11:VAL:HG23	1.97	0.63
1:A:66:LEU:HD21	3:A:142:HEM:HBB2	1.81	0.62
2:B:22:GLU:HG3	2:B:23:VAL:HG23	1.81	0.62
3:B:147:HEM:HBC2	3:B:147:HEM:HMC1	1.81	0.62
2:B:78:LEU:HD12	2:B:81:LEU:HD11	1.82	0.61
2:B:78:LEU:HA	2:B:81:LEU:HD21	1.81	0.61
2:B:12:LEU:HD11	2:B:76:HIS:CD2	2.34	0.60
1:A:97:ASN:HA	1:A:100:LEU:HD12	1.84	0.60
1:A:34:LEU:CD1	2:B:124:PRO:CA	2.80	0.59
2:B:99:ASP:OD1	2:B:101:GLU:HB3	2.01	0.59
2:B:30:ARG:O	2:B:34:VAL:HG23	2.04	0.57
1:A:40:LYS:NZ	1:A:41:THR:HG22	2.19	0.57
1:A:102:SER:O	1:A:106:LEU:HB2	2.04	0.57
1:A:60:LYS:O	1:A:64:ASP:HB2	2.05	0.57
2:B:11:VAL:HG11	2:B:133:VAL:CG2	2.34	0.57
1:A:122:HIS:CE1	2:B:112:LEU:HD22	2.39	0.56
1:A:103:HIS:HE1	2:B:131:GLN:NE2	2.04	0.56
2:B:41:PHE:HE1	2:B:102:ASN:OD1	1.88	0.56
1:A:29:LEU:CD1	1:A:58:HIS:HD2	2.14	0.55
1:A:103:HIS:CE1	2:B:131:GLN:NE2	2.73	0.55
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	2.36	0.55
2:B:59:LYS:HA	2:B:59:LYS:HE3	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:O	1:A:17:VAL:HG23	2.07	0.54
2:B:19:ASN:C	2:B:21:GLU:H	2.12	0.53
1:A:40:LYS:CE	1:A:41:THR:HG22	2.37	0.53
1:A:111:VAL:HG22	2:B:115:ALA:O	2.08	0.53
1:A:83:LEU:O	1:A:136:LEU:HD22	2.09	0.52
1:A:7:LYS:O	1:A:11:LYS:HG3	2.09	0.52
2:B:48:LEU:HA	2:B:54:VAL:HG22	1.92	0.52
1:A:109:LEU:O	1:A:113:LEU:HB2	2.10	0.51
2:B:22:GLU:CG	2:B:23:VAL:HG23	2.40	0.51
2:B:118:PHE:HB2	2:B:122:PHE:HB2	1.93	0.50
1:A:6:ASP:O	1:A:10:VAL:HG23	2.10	0.50
1:A:84:SER:CB	1:A:136:LEU:HA	2.40	0.50
1:A:106:LEU:HD11	1:A:122:HIS:CD2	2.46	0.50
1:A:83:LEU:HD11	3:A:142:HEM:C3A	2.46	0.49
2:B:68:LEU:HD11	2:B:110:LEU:CD1	2.43	0.49
1:A:2:LEU:HD11	1:A:127:LYS:HB3	1.95	0.49
2:B:32:LEU:HD23	2:B:48:LEU:HD13	1.95	0.48
1:A:37:PRO:O	1:A:40:LYS:HG3	2.13	0.48
1:A:105:LEU:HD23	1:A:129:LEU:HD21	1.95	0.48
1:A:111:VAL:HG13	2:B:119:GLY:CA	2.43	0.48
2:B:4:SER:C	2:B:6:GLU:N	2.67	0.48
2:B:53:ALA:O	2:B:57:ASN:HB2	2.13	0.48
1:A:17:VAL:HG13	1:A:24:TYR:CD1	2.49	0.48
2:B:1:VAL:HG12	2:B:132:LYS:HG2	1.96	0.48
2:B:10:ALA:HA	2:B:13:ALA:HB3	1.96	0.48
2:B:29:GLY:HA3	2:B:55:MET:SD	2.54	0.48
1:A:34:LEU:CD1	2:B:124:PRO:HB3	2.44	0.47
2:B:78:LEU:HA	2:B:81:LEU:CD2	2.42	0.47
2:B:54:VAL:O	2:B:57:ASN:HB3	2.14	0.47
1:A:95:PRO:HB3	1:A:137:THR:HG21	1.94	0.47
1:A:34:LEU:CD1	2:B:124:PRO:C	2.82	0.46
2:B:30:ARG:HD2	2:B:113:VAL:HG22	1.96	0.46
2:B:140:ALA:O	2:B:143:HIS:HB2	2.16	0.45
1:A:47:ASP:O	1:A:52:SER:HB3	2.17	0.45
3:A:142:HEM:HBB2	3:A:142:HEM:CMB	2.47	0.45
1:A:95:PRO:HA	1:A:98:PHE:HD2	1.82	0.45
2:B:75:VAL:O	2:B:78:LEU:HB2	2.17	0.45
1:A:52:SER:HB2	1:A:55:VAL:HB	1.98	0.45
1:A:118:THR:O	2:B:30:ARG:NH2	2.49	0.45
2:B:14:LEU:HD21	2:B:118:PHE:CD1	2.52	0.45
2:B:28:LEU:O	2:B:32:LEU:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:VAL:CG2	2:B:129:SER:HB3	2.47	0.45
2:B:48:LEU:HA	2:B:54:VAL:CG2	2.47	0.45
1:A:17:VAL:HG22	1:A:109:LEU:HD11	1.99	0.44
1:A:128:PHE:O	1:A:132:VAL:HG23	2.17	0.44
1:A:39:THR:HG22	1:A:97:ASN:ND2	2.26	0.44
2:B:34:VAL:O	2:B:36:PRO:HD3	2.17	0.44
1:A:39:THR:C	1:A:41:THR:H	2.22	0.43
1:A:107:SER:O	1:A:110:ALA:N	2.51	0.43
2:B:18:VAL:HG13	2:B:23:VAL:HG11	2.00	0.43
1:A:73:LEU:HD11	1:A:128:PHE:CD1	2.53	0.43
2:B:125:GLU:H	2:B:125:GLU:CD	2.21	0.43
1:A:102:SER:OG	1:A:129:LEU:HB3	2.19	0.43
2:B:4:SER:OG	2:B:7:GLU:HG2	2.18	0.43
1:A:90:LYS:O	1:A:92:ARG:HD2	2.19	0.43
1:A:40:LYS:HD2	1:A:40:LYS:C	2.40	0.42
1:A:84:SER:HB3	1:A:136:LEU:HD23	2.01	0.42
2:B:78:LEU:HD12	2:B:81:LEU:HD21	2.01	0.42
2:B:33:VAL:CG2	2:B:51:PRO:HB3	2.50	0.42
1:A:2:LEU:CD1	1:A:127:LYS:HB3	2.50	0.42
1:A:21:ALA:HB1	1:A:63:ALA:HB1	2.02	0.41
1:A:66:LEU:HD13	1:A:105:LEU:HD21	2.02	0.41
1:A:106:LEU:CD1	1:A:122:HIS:CD2	3.03	0.41
2:B:41:PHE:CZ	2:B:98:VAL:HA	2.55	0.41
1:A:34:LEU:HD13	2:B:124:PRO:CA	2.49	0.41
1:A:111:VAL:HG13	2:B:119:GLY:HA2	2.02	0.41
1:A:38:THR:O	1:A:41:THR:HG23	2.21	0.41
2:B:68:LEU:HD11	2:B:110:LEU:HD11	2.03	0.41
2:B:92:HIS:HA	2:B:96:LEU:HB2	2.04	0.40
1:A:17:VAL:HA	1:A:24:TYR:CE1	2.55	0.40
1:A:70:VAL:HA	1:A:73:LEU:HD13	2.03	0.40
2:B:33:VAL:HG21	2:B:51:PRO:HB3	2.02	0.40

All (52) 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)
1:A:15:SER:OG	1:A:15:SER:OG[3_554]	0.49	1.71
1:A:19:GLY:CA	1:A:70:VAL:O[3_554]	0.55	1.65
1:A:67:THR:CB	1:A:67:THR:CG2[3_554]	1.06	1.14
1:A:19:GLY:CA	1:A:70:VAL:C[3_554]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:CG2	1:A:67:THR:CG2[3_554]	1.17	1.03
1:A:15:SER:CB	1:A:15:SER:CB[3_554]	1.23	0.97
1:A:11:LYS:NZ	1:A:20:HIS:CD2[3_554]	1.31	0.89
1:A:15:SER:CB	1:A:15:SER:OG[3_554]	1.36	0.84
1:A:19:GLY:O	1:A:71:GLY:O[3_554]	1.38	0.82
1:A:11:LYS:NZ	1:A:20:HIS:NE2[3_554]	1.40	0.80
1:A:67:THR:CA	1:A:67:THR:CG2[3_554]	1.50	0.70
1:A:19:GLY:N	1:A:70:VAL:O[3_554]	1.55	0.65
1:A:19:GLY:O	1:A:71:GLY:C[3_554]	1.56	0.64
1:A:19:GLY:N	1:A:70:VAL:C[3_554]	1.60	0.60
1:A:23:GLU:OE1	1:A:71:GLY:O[3_554]	1.67	0.53
1:A:22:GLY:CA	1:A:72:HIS:CE1[3_554]	1.69	0.51
1:A:127:LYS:NZ	1:A:141:ARG:C[4_555]	1.70	0.50
1:A:64:ASP:CB	1:A:68:LEU:CD1[3_554]	1.71	0.49
1:A:19:GLY:C	1:A:71:GLY:O[3_554]	1.77	0.43
1:A:11:LYS:C	1:A:15:SER:O[3_554]	1.79	0.41
1:A:127:LYS:NZ	1:A:141:ARG:OXT[4_555]	1.81	0.39
1:A:127:LYS:CE	1:A:141:ARG:OXT[4_555]	1.82	0.38
1:A:18:GLY:CA	1:A:70:VAL:CG1[3_554]	1.87	0.33
1:A:15:SER:CA	1:A:15:SER:CB[3_554]	1.88	0.32
1:A:19:GLY:CA	1:A:71:GLY:N[3_554]	1.89	0.31
1:A:60:LYS:NZ	1:A:79:ALA:CA[3_554]	1.89	0.31
1:A:18:GLY:C	1:A:70:VAL:CG1[3_554]	1.90	0.30
1:A:19:GLY:C	1:A:71:GLY:C[3_554]	1.91	0.29
1:A:20:HIS:N	1:A:71:GLY:O[3_554]	1.92	0.28
1:A:64:ASP:N	1:A:68:LEU:CD1[3_554]	1.92	0.28
1:A:15:SER:N	1:A:15:SER:CB[3_554]	1.94	0.26
1:A:19:GLY:C	1:A:70:VAL:O[3_554]	1.95	0.25
1:A:64:ASP:CA	1:A:68:LEU:CD1[3_554]	1.96	0.24
1:A:19:GLY:O	1:A:72:HIS:N[3_554]	1.97	0.23
1:A:127:LYS:NZ	1:A:141:ARG:O[4_555]	1.98	0.22
1:A:67:THR:C	1:A:67:THR:CG2[3_554]	1.99	0.21
1:A:11:LYS:O	1:A:15:SER:O[3_554]	2.01	0.19
1:A:60:LYS:O	1:A:68:LEU:CD1[3_554]	2.05	0.15
1:A:20:HIS:N	1:A:71:GLY:CA[3_554]	2.06	0.14
1:A:64:ASP:OD2	1:A:68:LEU:CD2[3_554]	2.08	0.12
1:A:11:LYS:CB	1:A:15:SER:O[3_554]	2.10	0.10
1:A:20:HIS:CA	1:A:71:GLY:O[3_554]	2.10	0.10
1:A:18:GLY:C	1:A:70:VAL:C[3_554]	2.12	0.08
1:A:127:LYS:CE	1:A:141:ARG:C[4_555]	2.13	0.07
1:A:19:GLY:C	1:A:71:GLY:CA[3_554]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:THR:CB	1:A:67:THR:CB[3_554]	2.14	0.06
1:A:64:ASP:OD1	1:A:68:LEU:CB[3_554]	2.15	0.05
1:A:60:LYS:NZ	1:A:79:ALA:N[3_554]	2.16	0.04
1:A:11:LYS:O	1:A:15:SER:CB[3_554]	2.17	0.03
1:A:18:GLY:O	1:A:71:GLY:N[3_554]	2.17	0.03
1:A:15:SER:CA	1:A:15:SER:OG[3_554]	2.19	0.01
1:A:23:GLU:OE1	1:A:71:GLY:C[3_554]	2.19	0.01

## 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	139/141 (99%)	113 (81%)	17 (12%)	9 (6%)	1	3
2	B	144/146 (99%)	108 (75%)	29 (20%)	7 (5%)	2	7
All	All	283/287 (99%)	221 (78%)	46 (16%)	16 (6%)	1	5

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	PRO
1	A	52	SER
1	A	109	LEU
2	B	5	GLY
2	B	19	ASN
2	B	82	LYS
2	B	124	PRO
2	B	143	HIS
2	B	20	GLU
1	A	108	THR
1	A	119	PRO
2	B	22	GLU
1	A	95	PRO

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Mol	Chain	Res	Type
1	A	118	THR
1	A	18	GLY
1	A	43	PHE

### 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	115/115 (100%)	98 (85%)	17 (15%)	<b>3</b> <b>9</b>
2	B	117/117 (100%)	99 (85%)	18 (15%)	<b>2</b> <b>8</b>
All	All	232/232 (100%)	197 (85%)	35 (15%)	<b>3</b> <b>9</b>

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	36	PHE
1	A	38	THR
1	A	40	LYS
1	A	41	THR
1	A	48	LEU
1	A	52	SER
1	A	56	LYS
1	A	64	ASP
1	A	66	LEU
1	A	81	SER
1	A	86	LEU
1	A	92	ARG
1	A	106	LEU
1	A	116	ASP
1	A	137	THR
1	A	138	SER
2	B	2	GLN
2	B	3	LEU
2	B	4	SER

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Mol	Chain	Res	Type
2	B	28	LEU
2	B	43	ASP
2	B	59	LYS
2	B	68	LEU
2	B	73	GLU
2	B	90	GLU
2	B	91	LEU
2	B	112	LEU
2	B	114	VAL
2	B	116	ARG
2	B	123	THR
2	B	126	LEU
2	B	132	LYS
2	B	134	VAL
2	B	143	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	97	ASN
1	A	103	HIS
1	A	122	HIS
2	B	63	HIS
2	B	76	HIS

### 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 monosaccharides 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
3	HEM	A	142	1	41,50,50	2.06	12 (29%)	45,82,82	2.10	9 (20%)
3	HEM	B	147	2	41,50,50	2.09	15 (36%)	45,82,82	2.05	10 (22%)

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	142	1	-	5/12/54/54	-
3	HEM	B	147	2	-	5/12/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	FE-ND	4.59	2.19	1.96
3	A	142	HEM	FE-NB	4.36	2.18	1.96
3	A	142	HEM	FE-ND	4.33	2.18	1.96
3	A	142	HEM	C4D-C3D	-4.03	1.38	1.45
3	B	147	HEM	FE-NB	4.03	2.16	1.96
3	B	147	HEM	C3B-C4B	-3.89	1.37	1.44
3	A	142	HEM	C1D-C2D	-3.71	1.37	1.44
3	B	147	HEM	C4D-C3D	-3.57	1.38	1.45
3	A	142	HEM	C4D-ND	-3.49	1.34	1.40
3	A	142	HEM	C1B-NB	-3.47	1.34	1.40
3	B	147	HEM	C1B-C2B	-3.45	1.37	1.44
3	B	147	HEM	C3C-CAC	-3.39	1.40	1.47
3	A	142	HEM	C3C-CAC	-3.35	1.40	1.47
3	A	142	HEM	C1B-C2B	-3.22	1.38	1.44
3	B	147	HEM	C4D-ND	-3.18	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C1D-C2D	-3.17	1.38	1.44
3	A	142	HEM	C3B-C4B	-3.01	1.38	1.44
3	B	147	HEM	CHB-C1B	2.76	1.42	1.35
3	B	147	HEM	CAB-C3B	-2.62	1.40	1.47
3	A	142	HEM	CHB-C1B	2.57	1.41	1.35
3	A	142	HEM	CHA-C4D	2.45	1.41	1.35
3	B	147	HEM	CHA-C4D	2.45	1.41	1.35
3	B	147	HEM	C1B-NB	-2.44	1.36	1.40
3	B	147	HEM	C3B-C2B	2.40	1.42	1.37
3	A	142	HEM	CAB-C3B	-2.28	1.41	1.47
3	B	147	HEM	C4B-NB	-2.28	1.34	1.38
3	B	147	HEM	C1D-ND	-2.23	1.34	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C4D-ND-C1D	6.44	111.73	105.07
3	A	142	HEM	C1B-NB-C4B	6.44	111.72	105.07
3	B	147	HEM	C4B-CHC-C1C	5.77	130.17	122.56
3	A	142	HEM	C4B-CHC-C1C	5.54	129.87	122.56
3	A	142	HEM	C4C-CHD-C1D	5.25	129.49	122.56
3	A	142	HEM	C4D-ND-C1D	5.19	110.44	105.07
3	B	147	HEM	C1B-NB-C4B	4.87	110.10	105.07
3	B	147	HEM	C4C-CHD-C1D	4.48	128.47	122.56
3	B	147	HEM	C3D-C4D-ND	-3.67	106.08	110.17
3	A	142	HEM	O2D-CGD-CBD	3.09	123.96	114.03
3	A	142	HEM	C3D-C4D-ND	-2.64	107.22	110.17
3	B	147	HEM	C2D-C1D-ND	-2.62	106.75	109.88
3	A	142	HEM	C2B-C1B-NB	-2.48	106.90	109.84
3	B	147	HEM	C3C-C4C-NC	-2.43	106.36	110.94
3	B	147	HEM	C2B-C1B-NB	-2.24	107.19	109.84
3	A	142	HEM	CAD-CBD-CGD	-2.18	108.91	113.60
3	B	147	HEM	CMC-C2C-C3C	2.12	128.64	124.68
3	B	147	HEM	O2D-CGD-CBD	2.03	120.54	114.03
3	A	142	HEM	C2D-C1D-ND	-2.00	107.48	109.88

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C2A-CAA-CBA-CGA
3	A	142	HEM	C3D-CAD-CBD-CGD

*Continued on next page...*

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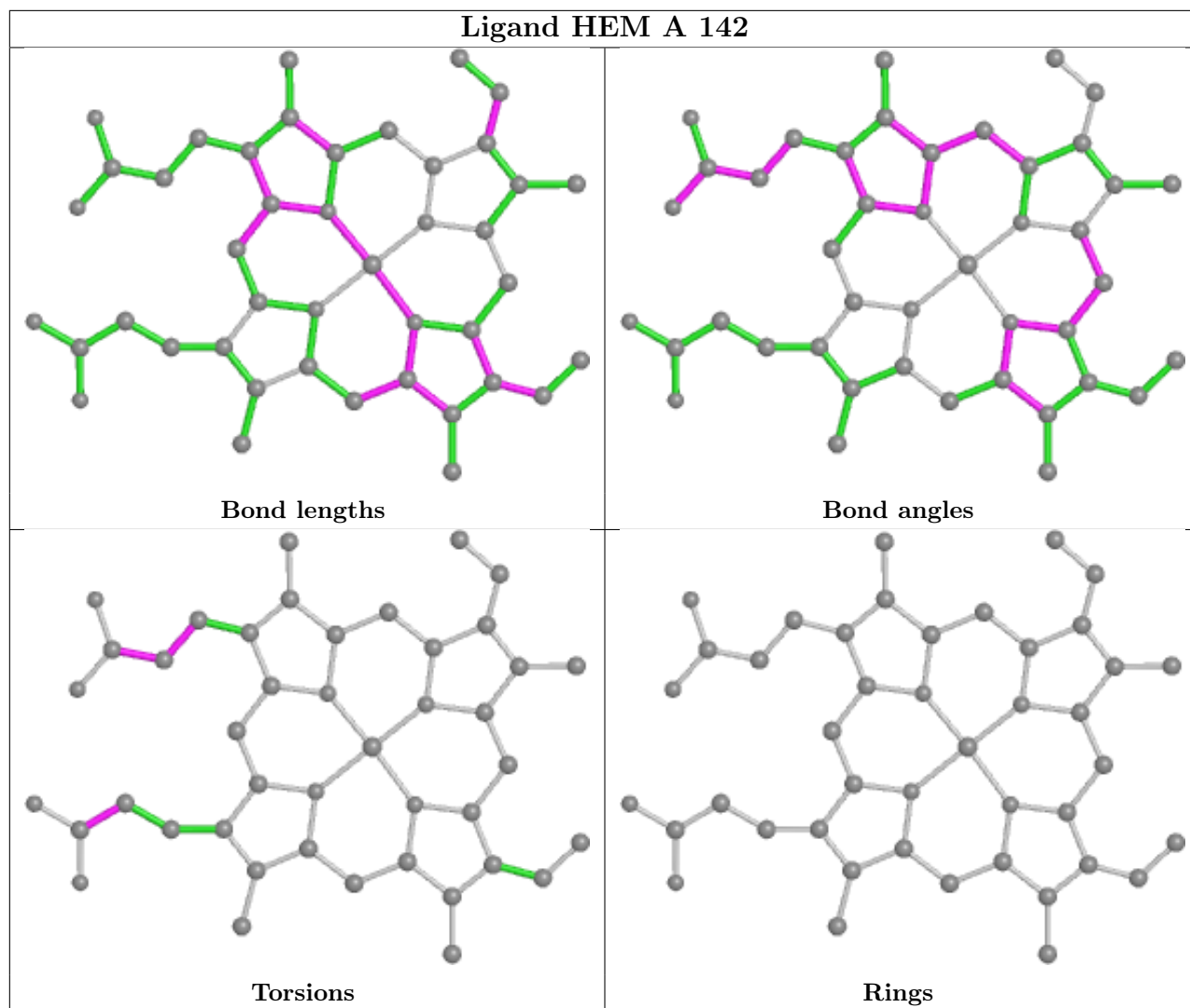
Mol	Chain	Res	Type	Atoms
3	B	147	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

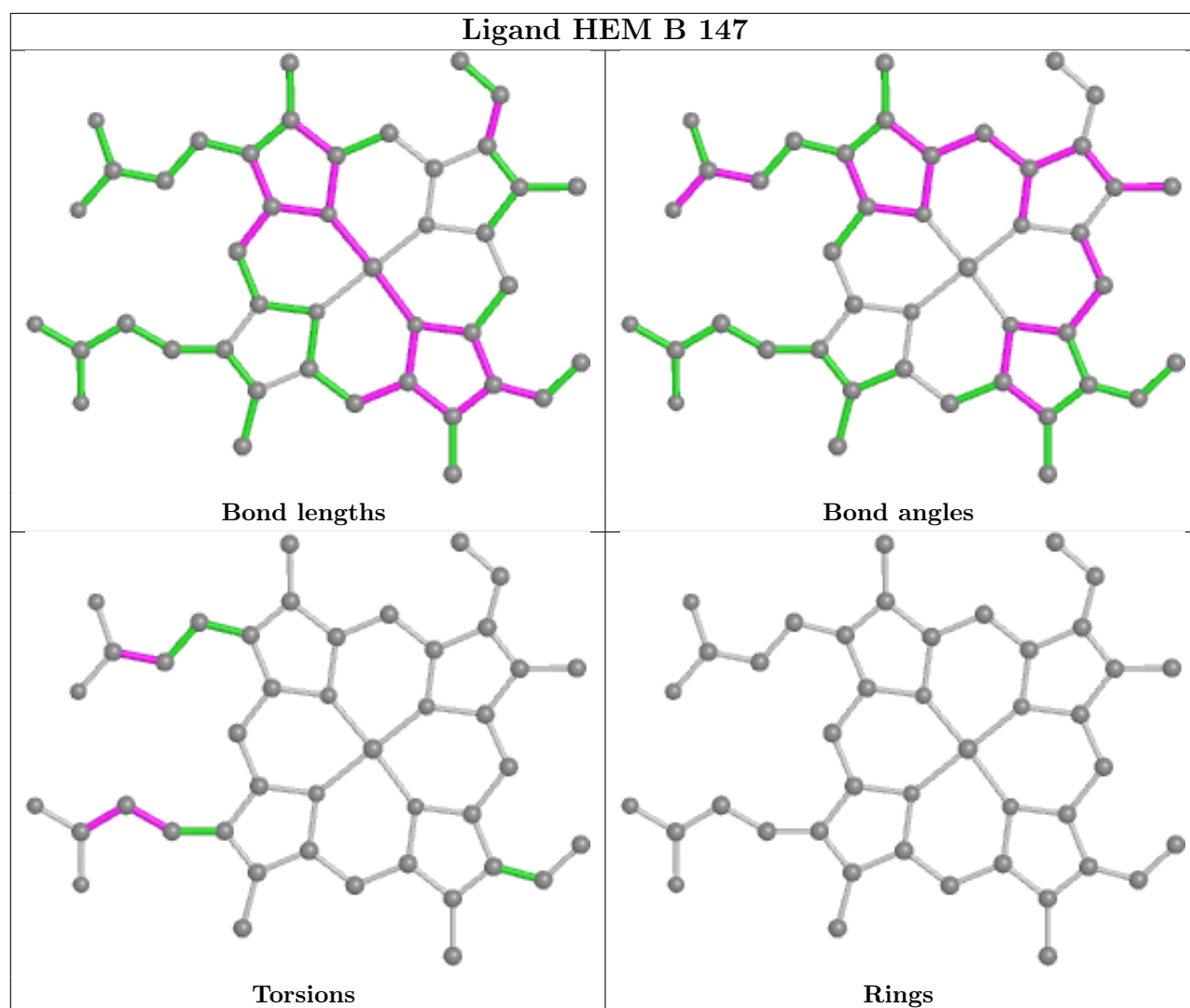
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	142	HEM	6	0
3	B	147	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.