



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:25 PM UTC

PDB ID : 2PGH / pdb_00002pgh
Title : STRUCTURE DETERMINATION OF AQUOMET PORCINE
HEMOGLOBIN AT 2.8 ANGSTROM RESOLUTION
Authors : Katz, D.S.; White, S.P.; Huang, W.; Kumar, R.; Christianson, D.W.
Deposited on : 1994-09-16
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

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

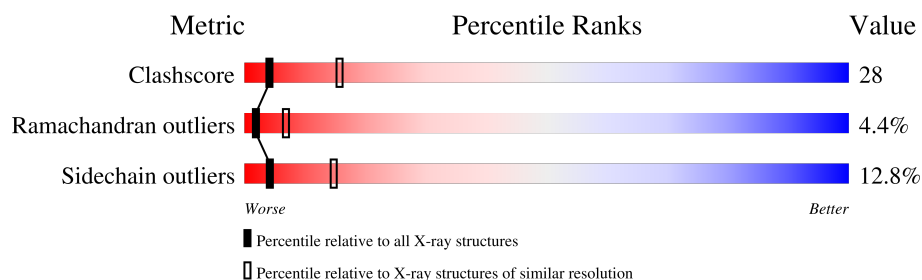
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 ≥ 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	48% 38% 11% .
1	C	141	46% 39% 12% .
2	B	146	41% 43% 14% .
2	D	146	47% 40% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4700 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 (AQUO MET) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	C	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			

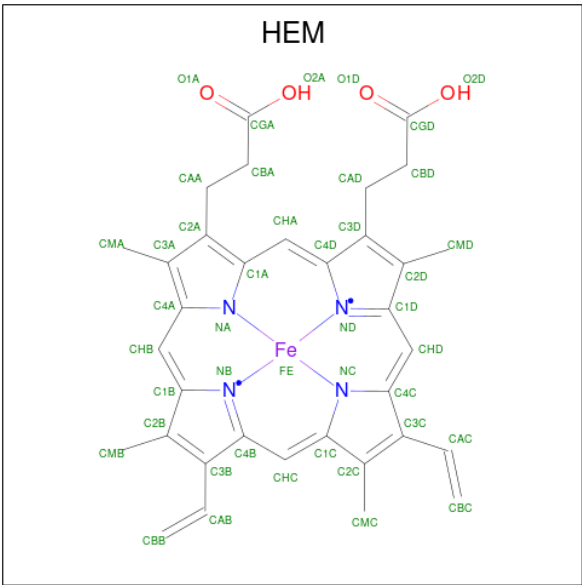
- Molecule 2 is a protein called HEMOGLOBIN (AQUO MET) (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			
2	D	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	125	ASP	ASN	conflict	UNP P02067
D	125	ASP	ASN	conflict	UNP P02067

- 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		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is water.

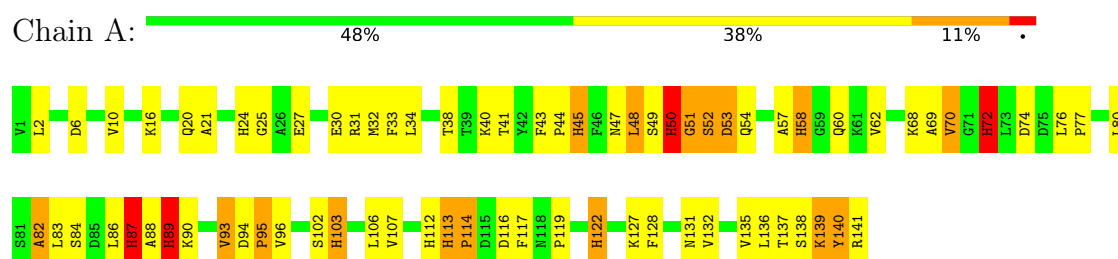
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	34	Total	O	0	0
			34	34		
4	C	45	Total	O	0	0
			45	45		
4	D	31	Total	O	0	0
			31	31		

3 Residue-property plots

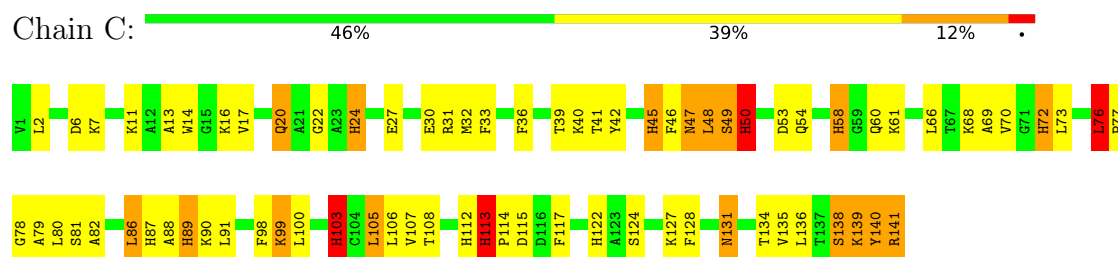
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

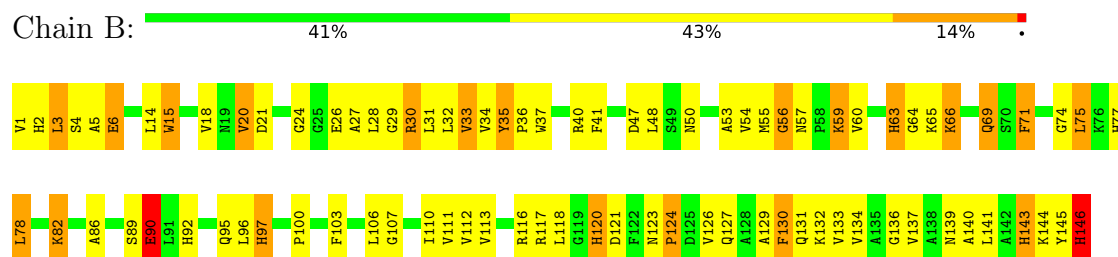
• Molecule 1: HEMOGLOBIN (AQUO MET) (ALPHA CHAIN)



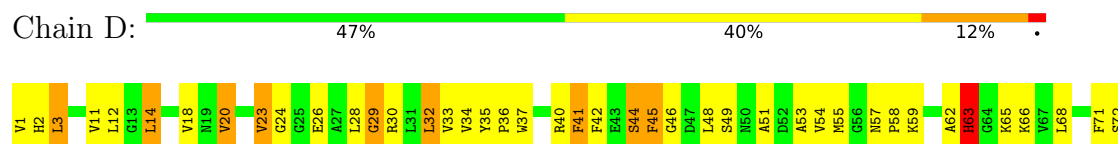
• Molecule 1: HEMOGLOBIN (AQUO MET) (ALPHA CHAIN)



• Molecule 2: HEMOGLOBIN (AQUO MET) (BETA CHAIN)



• Molecule 2: HEMOGLOBIN (AQUO MET) (BETA CHAIN)





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.60 Å 72.80 Å 115.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.50 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.50-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4700	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.02	3/1091 (0.3%)	1.73	31/1480 (2.1%)
1	C	1.10	10/1091 (0.9%)	1.95	37/1480 (2.5%)
2	B	0.93	5/1160 (0.4%)	1.53	31/1568 (2.0%)
2	D	0.94	4/1160 (0.3%)	1.49	30/1568 (1.9%)
All	All	1.00	22/4502 (0.5%)	1.68	129/6096 (2.1%)

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	4
1	C	0	4
2	B	0	2
2	D	0	2
All	All	0	12

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	HIS	CG-CD2	7.47	1.44	1.35
1	C	113	HIS	CG-CD2	7.25	1.43	1.35
2	B	120	HIS	CG-CD2	7.22	1.43	1.35
1	C	72	HIS	CG-CD2	7.22	1.43	1.35
1	C	113	HIS	CB-CG	6.48	1.59	1.50
1	C	72	HIS	CB-CG	6.15	1.58	1.50
1	C	72	HIS	ND1-CE1	6.13	1.38	1.32
1	C	58	HIS	CG-CD2	5.90	1.42	1.35
1	C	72	HIS	CD2-NE2	5.87	1.44	1.37
2	B	120	HIS	CG-ND1	5.86	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	HIS	CG-CD2	5.81	1.42	1.35
2	D	2	HIS	CD2-NE2	5.62	1.44	1.37
2	D	2	HIS	CG-CD2	5.58	1.42	1.35
1	C	113	HIS	CD2-NE2	5.45	1.43	1.37
1	C	50	HIS	CG-CD2	5.33	1.41	1.35
2	B	120	HIS	ND1-CE1	5.28	1.37	1.32
1	A	50	HIS	CB-CG	5.25	1.57	1.50
1	A	50	HIS	ND1-CE1	5.20	1.37	1.32
2	D	120	HIS	CG-CD2	5.16	1.41	1.35
2	D	97	HIS	CG-CD2	5.15	1.41	1.35
2	B	63	HIS	CB-CG	-5.06	1.43	1.50
1	C	45	HIS	CD2-NE2	5.02	1.43	1.37

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	HIS	CA-CB-CG	44.56	158.36	113.80
1	A	113	HIS	CA-CB-CG	20.68	134.48	113.80
1	A	58	HIS	CA-CB-CG	-15.85	97.95	113.80
2	D	77	HIS	CA-CB-CG	14.45	128.25	113.80
2	D	146	HIS	CA-CB-CG	13.30	127.10	113.80
1	A	24	HIS	CA-CB-CG	12.71	126.51	113.80
2	B	77	HIS	CA-CB-CG	12.06	125.86	113.80
1	C	89	HIS	CA-CB-CG	11.92	125.72	113.80
1	A	89	HIS	CB-CG-CD2	-11.51	116.23	131.20
1	C	122	HIS	CA-CB-CG	11.03	124.83	113.80
1	C	112	HIS	ND1-CG-CD2	10.05	116.15	106.10
1	C	112	HIS	CB-CG-CD2	-9.61	118.71	131.20
1	C	112	HIS	CG-CD2-NE2	-9.31	97.89	107.20
2	B	63	HIS	ND1-CG-CD2	9.13	115.23	106.10
1	A	89	HIS	CA-CB-CG	8.94	122.74	113.80
1	C	87	HIS	CA-CB-CG	-8.89	104.91	113.80
1	C	87	HIS	CB-CG-CD2	-8.71	119.87	131.20
2	B	63	HIS	CG-CD2-NE2	-8.46	98.74	107.20
1	C	103	HIS	CG-CD2-NE2	-8.31	98.89	107.20
1	C	58	HIS	ND1-CG-CD2	8.10	114.20	106.10
2	B	92	HIS	ND1-CG-CD2	8.10	114.20	106.10
2	B	120	HIS	CB-CG-CD2	-8.02	120.77	131.20
2	D	96	LEU	N-CA-C	7.93	121.44	111.69
2	B	146	HIS	CB-CG-CD2	-7.82	121.03	131.20
2	D	97	HIS	ND1-CG-CD2	7.81	113.91	106.10
1	A	103	HIS	ND1-CG-CD2	7.79	113.89	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	HIS	CB-CG-CD2	-7.79	121.08	131.20
1	A	103	HIS	CG-CD2-NE2	-7.77	99.43	107.20
2	B	2	HIS	CG-CD2-NE2	-7.75	99.45	107.20
2	D	2	HIS	CG-CD2-NE2	-7.72	99.47	107.20
2	D	2	HIS	ND1-CG-CD2	7.65	113.75	106.10
1	A	122	HIS	CB-CG-CD2	-7.64	121.26	131.20
1	A	89	HIS	ND1-CG-CD2	7.64	113.74	106.10
1	A	87	HIS	CG-CD2-NE2	-7.63	99.57	107.20
1	A	122	HIS	ND1-CG-CD2	7.62	113.72	106.10
1	C	103	HIS	ND1-CG-CD2	7.58	113.68	106.10
2	B	15	TRP	N-CA-C	-7.55	103.53	112.89
1	A	52	SER	N-CA-C	-7.51	96.30	109.06
1	C	50	HIS	CA-CB-CG	7.32	121.12	113.80
1	A	94	ASP	CA-C-N	7.29	128.96	119.84
1	A	94	ASP	C-N-CA	7.29	128.96	119.84
2	D	143	HIS	ND1-CG-CD2	7.29	113.39	106.10
2	B	2	HIS	ND1-CG-CD2	7.27	113.37	106.10
1	A	112	HIS	CB-CG-CD2	-7.23	121.80	131.20
1	A	132	VAL	N-CA-C	-7.14	103.22	111.00
1	A	89	HIS	CG-CD2-NE2	-7.11	100.09	107.20
1	C	58	HIS	CG-CD2-NE2	-7.11	100.09	107.20
1	A	122	HIS	CG-CD2-NE2	-7.11	100.09	107.20
1	C	45	HIS	CB-CG-CD2	-7.07	122.01	131.20
1	C	87	HIS	CG-CD2-NE2	-6.98	100.22	107.20
2	D	66	LYS	N-CA-C	-6.97	103.61	111.07
1	A	87	HIS	ND1-CG-CD2	6.93	113.03	106.10
2	D	97	HIS	CB-CG-CD2	-6.92	122.20	131.20
2	D	77	HIS	CG-CD2-NE2	-6.89	100.31	107.20
2	B	75	LEU	N-CA-C	-6.87	101.44	110.43
2	D	2	HIS	CB-CG-CD2	-6.80	122.36	131.20
2	B	78	LEU	N-CA-C	6.78	119.30	111.02
2	B	3	LEU	N-CA-C	-6.77	100.77	110.59
2	B	97	HIS	ND1-CG-CD2	6.73	112.83	106.10
2	B	137	VAL	N-CA-C	-6.72	104.10	110.42
1	C	58	HIS	ND1-CE1-NE2	6.72	115.12	108.40
2	B	140	ALA	N-CA-C	-6.67	103.93	111.14
1	A	24	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	A	112	HIS	ND1-CG-CD2	6.62	112.72	106.10
2	D	143	HIS	CG-CD2-NE2	-6.59	100.61	107.20
2	B	143	HIS	CB-CG-CD2	-6.56	122.67	131.20
2	D	77	HIS	ND1-CG-CD2	6.46	112.56	106.10
1	C	24	HIS	CB-CG-CD2	-6.46	122.80	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	HIS	ND1-CG-CD2	6.44	112.54	106.10
1	A	122	HIS	CA-CB-CG	6.43	120.23	113.80
2	B	92	HIS	CA-CB-CG	-6.39	107.41	113.80
2	B	143	HIS	CG-CD2-NE2	-6.39	100.81	107.20
2	D	97	HIS	ND1-CE1-NE2	6.35	114.75	108.40
1	C	103	HIS	CB-CG-ND1	-6.34	113.19	122.70
2	D	120	HIS	ND1-CE1-NE2	6.34	114.74	108.40
2	B	77	HIS	CG-CD2-NE2	-6.28	100.92	107.20
1	C	58	HIS	CG-ND1-CE1	-6.24	98.69	109.30
1	C	58	HIS	CB-CG-CD2	-6.19	123.15	131.20
2	B	120	HIS	CA-CB-CG	6.19	119.99	113.80
2	B	71	PHE	N-CA-C	-6.15	104.49	111.07
1	C	48	LEU	N-CA-C	6.13	117.79	110.44
1	A	87	HIS	CB-CG-CD2	-6.09	123.29	131.20
1	C	14	TRP	N-CA-C	-6.06	104.59	111.14
1	A	103	HIS	CB-CG-CD2	-6.06	123.32	131.20
1	C	24	HIS	ND1-CE1-NE2	6.05	114.45	108.40
1	A	112	HIS	CG-CD2-NE2	-5.92	101.28	107.20
1	C	105	LEU	N-CA-C	-5.91	104.23	112.45
2	B	143	HIS	CA-CB-CG	-5.89	107.91	113.80
2	D	63	HIS	CG-CD2-NE2	-5.83	101.37	107.20
2	B	92	HIS	CG-CD2-NE2	-5.79	101.41	107.20
2	B	97	HIS	CB-CG-CD2	-5.74	123.74	131.20
2	D	92	HIS	CB-CG-CD2	-5.74	123.74	131.20
2	B	77	HIS	ND1-CG-CD2	5.72	111.82	106.10
2	D	63	HIS	ND1-CG-CD2	5.68	111.78	106.10
2	B	95	GLN	N-CA-C	5.67	117.26	111.14
2	D	35	TYR	CA-C-N	5.57	126.80	119.84
2	D	35	TYR	C-N-CA	5.57	126.80	119.84
2	D	97	HIS	CG-CD2-NE2	-5.56	101.64	107.20
2	D	146	HIS	ND1-CG-CD2	5.54	111.64	106.10
1	C	89	HIS	ND1-CG-CD2	5.53	111.63	106.10
1	C	87	HIS	ND1-CG-CD2	5.52	111.62	106.10
2	D	146	HIS	CG-CD2-NE2	-5.52	101.68	107.20
1	C	76	LEU	CA-C-N	5.51	124.97	119.24
1	C	76	LEU	C-N-CA	5.51	124.97	119.24
1	A	72	HIS	CG-CD2-NE2	-5.48	101.72	107.20
1	C	20	GLN	N-CA-C	5.45	119.02	112.38
1	C	42	TYR	N-CA-C	-5.41	106.68	113.28
1	A	45	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	C	91	LEU	N-CA-C	-5.38	105.97	112.54
2	B	97	HIS	ND1-CE1-NE2	5.35	113.75	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	23	VAL	N-CA-C	5.32	115.77	110.23
1	C	50	HIS	CB-CG-CD2	-5.31	124.29	131.20
2	D	97	HIS	CG-ND1-CE1	-5.27	100.33	109.30
2	D	92	HIS	CG-CD2-NE2	-5.27	101.93	107.20
2	D	63	HIS	ND1-CE1-NE2	5.26	113.66	108.40
2	D	29	GLY	N-CA-C	-5.25	106.14	112.49
2	B	77	HIS	N-CA-C	-5.24	107.42	112.97
1	C	117	PHE	N-CA-C	-5.24	101.72	109.83
1	A	25	GLY	N-CA-C	-5.21	106.09	112.77
1	C	50	HIS	CG-CD2-NE2	-5.16	102.04	107.20
2	B	5	ALA	N-CA-C	-5.16	107.01	113.72
1	C	89	HIS	CG-CD2-NE2	-5.14	102.06	107.20
1	A	72	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	57	ALA	N-CA-C	-5.09	105.73	111.28
1	A	89	HIS	ND1-CE1-NE2	5.07	113.47	108.40
2	B	90	GLU	N-CA-C	-5.04	105.68	111.07
2	D	135	ALA	N-CA-C	-5.03	105.69	111.07
1	C	112	HIS	CG-ND1-CE1	-5.03	100.75	109.30
1	C	122	HIS	CG-CD2-NE2	-5.01	102.19	107.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	HIS	Sidechain
1	A	72	HIS	Sidechain
1	A	87	HIS	Sidechain
1	A	89	HIS	Sidechain
2	B	146	HIS	Sidechain
2	B	35	TYR	Sidechain
1	C	103	HIS	Sidechain
1	C	113	HIS	Sidechain
1	C	58	HIS	Sidechain
1	C	89	HIS	Sidechain
2	D	63	HIS	Sidechain
2	D	97	HIS	Sidechain

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	1064	0	1060	58	0
1	C	1064	0	1060	61	0
2	B	1135	0	1134	72	0
2	D	1135	0	1134	76	0
3	A	43	0	30	2	0
3	B	43	0	30	6	0
3	C	43	0	30	2	0
3	D	43	0	30	12	0
4	A	20	0	0	3	0
4	B	34	0	0	1	0
4	C	45	0	0	11	0
4	D	31	0	0	2	0
All	All	4700	0	4508	250	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 28.

All (250) 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:14:LEU:HD21	2:B:126:VAL:HG11	1.45	0.98
2:B:106:LEU:HD23	3:B:147:HEM:HBB2	1.50	0.92
2:B:146:HIS:OXT	2:D:132:LYS:HD2	1.69	0.90
2:B:34:VAL:O	2:B:36:PRO:HD3	1.75	0.85
2:D:116:ARG:HG3	2:D:116:ARG:HH11	1.41	0.83
1:A:127:LYS:HE3	1:C:141:ARG:HG3	1.61	0.83
1:A:2:LEU:HG	1:A:131:ASN:HD21	1.44	0.81
1:A:2:LEU:HG	1:A:131:ASN:ND2	1.97	0.79
1:A:127:LYS:NZ	1:C:141:ARG:HB2	1.96	0.79
2:B:121:ASP:HB2	4:B:156:HOH:O	1.82	0.78
1:C:103:HIS:O	1:C:107:VAL:HG23	1.84	0.78
2:D:91:LEU:O	2:D:95:GLN:HB3	1.83	0.78
3:C:142:HEM:HBB1	4:C:152:HOH:O	1.85	0.76
2:D:18:VAL:HG13	2:D:23:VAL:HG21	1.67	0.75
2:B:28:LEU:HD23	2:B:60:VAL:HG13	1.67	0.74
2:B:3:LEU:HD11	2:B:133:VAL:HG22	1.69	0.74
1:C:32:MET:SD	4:C:155:HOH:O	2.45	0.74
2:B:31:LEU:HD12	2:B:35:TYR:HD2	1.53	0.74
2:D:111:VAL:HG13	2:D:122:PHE:HZ	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:VAL:HG23	2:D:3:LEU:HG	1.72	0.71
2:B:107:GLY:O	2:B:111:VAL:HG23	1.91	0.71
1:C:76:LEU:HD23	1:C:131:ASN:ND2	2.04	0.70
2:B:59:LYS:HE3	2:B:59:LYS:HA	1.73	0.69
1:C:46:PHE:HD1	1:C:54:GLN:NE2	1.92	0.67
2:D:51:ALA:O	2:D:55:MET:HG2	1.94	0.67
3:C:142:HEM:CBB	4:C:152:HOH:O	2.42	0.67
2:D:91:LEU:HD21	3:D:147:HEM:CBA	2.24	0.67
2:B:141:LEU:CD1	3:B:147:HEM:HAB	2.23	0.67
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.30	0.66
2:B:141:LEU:HD12	3:B:147:HEM:HAB	1.77	0.66
1:A:30:GLU:O	1:A:34:LEU:HD12	1.96	0.66
2:D:91:LEU:HD21	3:D:147:HEM:HBA1	1.79	0.65
2:D:91:LEU:O	2:D:96:LEU:HG	1.98	0.64
2:D:116:ARG:HG3	2:D:116:ARG:NH1	2.13	0.64
1:A:70:VAL:HG23	1:A:128:PHE:CZ	2.34	0.63
1:C:61:LYS:CD	4:C:153:HOH:O	2.47	0.63
2:D:62:ALA:O	2:D:65:LYS:HG2	1.99	0.63
2:D:92:HIS:CD2	2:D:96:LEU:HD12	2.34	0.63
2:B:15:TRP:HH2	2:B:71:PHE:HD2	1.46	0.62
2:D:48:LEU:HD23	2:D:54:VAL:HG22	1.80	0.62
1:A:127:LYS:HZ2	1:C:141:ARG:HB2	1.62	0.62
1:C:22:GLY:HA3	1:C:60:GLN:NE2	2.15	0.62
2:D:141:LEU:HD11	3:D:147:HEM:CAB	2.31	0.61
1:A:30:GLU:OE2	1:A:50:HIS:HA	2.01	0.61
1:A:41:THR:O	1:A:44:PRO:HD3	2.01	0.60
2:B:82:LYS:HD3	2:B:82:LYS:H	1.66	0.60
1:A:127:LYS:HD2	1:C:141:ARG:HD2	1.84	0.60
2:D:48:LEU:HD21	4:D:166:HOH:O	2.02	0.60
1:C:113:HIS:HB3	4:C:167:HOH:O	2.01	0.59
2:B:26:GLU:O	2:B:30:ARG:HB2	2.03	0.59
2:B:90:GLU:OE2	2:B:144:LYS:HG3	2.02	0.59
2:D:132:LYS:NZ	2:D:132:LYS:HB3	2.18	0.59
1:A:119:PRO:HB3	2:B:33:VAL:HG21	1.85	0.59
2:B:28:LEU:O	2:B:32:LEU:HD13	2.02	0.59
2:B:50:ASN:OD1	2:B:53:ALA:HB2	2.03	0.59
2:D:3:LEU:HD12	2:D:78:LEU:HD13	1.84	0.59
1:A:84:SER:OG	1:A:136:LEU:HA	2.02	0.58
2:D:95:GLN:HG2	2:D:96:LEU:HD23	1.85	0.58
1:C:13:ALA:O	1:C:17:VAL:HG23	2.04	0.58
1:A:137:THR:HG22	1:A:137:THR:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:LEU:HD22	1:C:6:ASP:CB	2.34	0.58
1:A:119:PRO:HG2	2:B:55:MET:HE2	1.86	0.57
1:C:61:LYS:HD2	4:C:153:HOH:O	2.02	0.57
1:C:7:LYS:HG2	1:C:73:LEU:HD13	1.85	0.57
1:C:68:LYS:HG3	1:C:72:HIS:CD2	2.40	0.57
2:D:26:GLU:HG2	2:D:30:ARG:HD2	1.87	0.57
3:D:147:HEM:HAA2	4:D:173:HOH:O	2.04	0.57
2:B:31:LEU:HD12	2:B:35:TYR:CD2	2.37	0.57
1:A:52:SER:O	1:A:54:GLN:N	2.38	0.56
2:B:15:TRP:CH2	2:B:71:PHE:HD2	2.23	0.56
1:C:69:ALA:HB1	1:C:76:LEU:HD11	1.85	0.56
2:D:63:HIS:CE1	3:D:147:HEM:C1A	2.93	0.56
2:B:71:PHE:HZ	2:B:134:VAL:HG12	1.69	0.56
1:C:22:GLY:HA3	1:C:60:GLN:HE22	1.70	0.56
2:D:141:LEU:HD11	3:D:147:HEM:HAB	1.86	0.56
1:A:2:LEU:CG	1:A:131:ASN:HD21	2.17	0.56
1:C:27:GLU:OE1	1:C:108:THR:HG23	2.04	0.56
1:A:88:ALA:O	1:A:89:HIS:ND1	2.39	0.55
2:B:40:ARG:HG2	2:B:40:ARG:O	2.06	0.55
2:D:111:VAL:HG13	2:D:122:PHE:CZ	2.38	0.55
2:B:4:SER:OG	2:B:6:GLU:HG2	2.07	0.55
1:A:127:LYS:HZ1	1:C:141:ARG:HB2	1.70	0.54
1:C:80:LEU:HD12	1:C:135:VAL:HG11	1.89	0.54
1:C:68:LYS:NZ	1:C:72:HIS:NE2	2.56	0.54
2:D:40:ARG:HG3	2:D:41:PHE:N	2.24	0.53
2:B:129:ALA:O	2:B:133:VAL:HG23	2.08	0.53
1:C:105:LEU:HD22	4:C:158:HOH:O	2.08	0.53
1:A:119:PRO:CG	2:B:55:MET:HE2	2.39	0.53
1:A:88:ALA:HB3	1:A:139:LYS:HB2	1.90	0.52
1:C:11:LYS:HE3	1:C:73:LEU:HD12	1.92	0.52
2:D:40:ARG:HG3	2:D:41:PHE:H	1.74	0.52
2:B:35:TYR:HD1	2:B:37:TRP:CH2	2.28	0.52
2:D:48:LEU:CD2	2:D:54:VAL:HG22	2.39	0.52
2:D:141:LEU:CD1	3:D:147:HEM:HAB	2.40	0.52
1:C:2:LEU:HD22	1:C:6:ASP:HB2	1.92	0.52
2:D:63:HIS:HE1	3:D:147:HEM:C1A	2.27	0.52
1:C:33:PHE:HB3	1:C:40:LYS:HG2	1.91	0.51
2:B:71:PHE:CZ	2:B:134:VAL:HG12	2.46	0.51
2:D:23:VAL:HG22	2:D:117:ARG:HD3	1.91	0.51
2:D:45:PHE:O	2:D:57:ASN:ND2	2.42	0.51
2:B:24:GLY:O	2:B:64:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:O	2:B:97:HIS:HB2	2.10	0.51
1:C:131:ASN:HB2	4:C:165:HOH:O	2.10	0.51
2:D:41:PHE:HB3	3:D:147:HEM:HMD2	1.92	0.51
1:A:140:TYR:HB2	4:A:148:HOH:O	2.10	0.50
1:C:66:LEU:HD22	1:C:128:PHE:CZ	2.46	0.50
2:D:32:LEU:HD11	2:D:42:PHE:CE2	2.46	0.50
2:D:123:ASN:OD1	2:D:126:VAL:HG23	2.12	0.50
2:D:28:LEU:O	2:D:28:LEU:HG	2.12	0.50
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.95	0.49
2:D:85:PHE:CE1	2:D:88:LEU:HD22	2.47	0.49
2:D:20:VAL:CG2	2:D:68:LEU:HB3	2.42	0.49
1:A:127:LYS:CE	1:C:141:ARG:HG3	2.37	0.49
2:D:20:VAL:HG22	2:D:68:LEU:HB3	1.95	0.49
1:A:47:ASN:HB2	1:A:52:SER:OG	2.13	0.48
1:A:114:PRO:HB3	2:B:116:ARG:HG2	1.94	0.48
1:C:49:SER:O	1:C:50:HIS:HB2	2.14	0.48
1:A:49:SER:OG	1:A:50:HIS:N	2.46	0.48
1:A:96:VAL:HG12	1:A:96:VAL:O	2.13	0.48
2:D:44:SER:C	2:D:46:GLY:H	2.21	0.48
2:D:53:ALA:O	2:D:57:ASN:HB2	2.13	0.48
2:B:34:VAL:C	2:B:36:PRO:HD3	2.38	0.48
1:C:86:LEU:HD23	1:C:86:LEU:O	2.12	0.48
2:D:41:PHE:HB3	3:D:147:HEM:CMD	2.44	0.48
2:D:92:HIS:HB3	2:D:98:VAL:CG2	2.44	0.48
1:A:40:LYS:HG3	1:A:48:LEU:CD1	2.43	0.48
1:C:138:SER:HA	4:C:151:HOH:O	2.14	0.47
1:C:99:LYS:HD2	1:C:99:LYS:C	2.39	0.47
1:C:99:LYS:HD2	1:C:99:LYS:O	2.14	0.47
1:A:16:LYS:HG3	4:A:154:HOH:O	2.14	0.47
2:D:40:ARG:O	2:D:42:PHE:N	2.48	0.47
1:A:84:SER:HB3	1:A:139:LYS:HG2	1.96	0.47
1:A:114:PRO:CB	2:B:116:ARG:HG2	2.45	0.47
1:C:138:SER:C	1:C:140:TYR:H	2.21	0.47
2:D:58:PRO:HG2	2:D:59:LYS:H	1.80	0.47
1:A:47:ASN:OD1	1:A:54:GLN:NE2	2.48	0.47
1:A:52:SER:O	1:A:53:ASP:C	2.57	0.47
2:D:29:GLY:O	2:D:33:VAL:HG23	2.15	0.47
2:B:4:SER:HG	2:B:6:GLU:HG2	1.81	0.46
2:B:50:ASN:O	2:B:54:VAL:HG23	2.15	0.46
2:D:98:VAL:HG23	2:D:98:VAL:O	2.14	0.46
2:B:27:ALA:HB1	2:B:110:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:HIS:CD2	1:C:41:THR:HG21	2.50	0.46
1:C:115:ASP:HB3	4:C:178:HOH:O	2.14	0.46
1:A:113:HIS:HB3	4:A:153:HOH:O	2.15	0.46
2:B:127:GLN:O	2:B:131:GLN:HG2	2.15	0.46
1:C:99:LYS:HE2	1:C:100:LEU:CD2	2.46	0.46
2:B:14:LEU:HB2	2:B:118:LEU:HD11	1.97	0.46
2:B:82:LYS:H	2:B:82:LYS:CD	2.27	0.46
2:B:100:PRO:HA	2:B:103:PHE:CD2	2.51	0.46
1:C:99:LYS:HE2	1:C:100:LEU:HD21	1.97	0.46
1:C:131:ASN:C	1:C:131:ASN:HD22	2.24	0.46
2:D:144:LYS:NZ	2:D:144:LYS:HA	2.30	0.46
2:B:82:LYS:CD	2:B:82:LYS:N	2.79	0.45
1:C:36:PHE:CD1	1:C:100:LEU:HD13	2.50	0.45
2:B:14:LEU:HD22	2:B:118:LEU:CD1	2.46	0.45
2:D:1:VAL:CG2	2:D:3:LEU:HG	2.42	0.45
2:D:90:GLU:HA	2:D:93:CYS:HB3	1.97	0.45
2:B:1:VAL:HG21	2:B:132:LYS:HG2	1.99	0.45
2:B:32:LEU:HD12	2:B:32:LEU:N	2.32	0.45
2:B:29:GLY:O	2:B:33:VAL:HG22	2.15	0.45
2:D:3:LEU:HD12	2:D:78:LEU:CD1	2.46	0.45
2:B:18:VAL:HA	2:B:117:ARG:HD3	1.99	0.45
2:B:27:ALA:CB	2:B:110:ILE:HG12	2.47	0.45
2:B:50:ASN:OD1	2:B:53:ALA:CB	2.65	0.45
2:D:132:LYS:HB3	2:D:132:LYS:HZ2	1.81	0.45
2:B:30:ARG:NH2	2:B:116:ARG:HD3	2.32	0.45
2:B:3:LEU:HD11	2:B:133:VAL:CG2	2.43	0.45
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.17	0.45
1:C:103:HIS:CE1	2:D:108:ASN:HD22	2.35	0.45
1:A:102:SER:O	1:A:103:HIS:C	2.60	0.44
1:C:66:LEU:O	1:C:70:VAL:HG23	2.16	0.44
1:C:82:ALA:O	1:C:86:LEU:HB2	2.16	0.44
2:D:30:ARG:O	2:D:34:VAL:HG23	2.16	0.44
2:D:93:CYS:HB2	2:D:145:TYR:CD1	2.52	0.44
1:A:6:ASP:O	1:A:10:VAL:HG23	2.16	0.44
2:B:47:ASP:C	2:B:48:LEU:HG	2.41	0.44
1:A:27:GLU:OE2	1:A:31:ARG:NH1	2.50	0.44
1:C:36:PHE:O	1:C:39:THR:HG23	2.18	0.44
1:A:68:LYS:O	1:A:72:HIS:HD2	1.99	0.44
2:D:14:LEU:HD13	2:D:14:LEU:O	2.18	0.44
2:B:31:LEU:HD22	2:B:106:LEU:HD13	2.00	0.44
1:C:47:ASN:C	1:C:47:ASN:ND2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:HD3	4:C:153:HOH:O	2.14	0.44
1:A:58:HIS:O	1:A:62:VAL:HG23	2.17	0.43
1:A:107:VAL:O	1:A:107:VAL:HG12	2.17	0.43
2:B:63:HIS:O	2:B:66:LYS:HB2	2.18	0.43
2:D:91:LEU:HD21	3:D:147:HEM:HBA2	1.99	0.43
2:D:116:ARG:NH1	2:D:116:ARG:CG	2.81	0.43
2:B:18:VAL:HG12	2:B:117:ARG:HD3	2.00	0.43
2:B:123:ASN:HD22	2:B:124:PRO:HD2	1.83	0.43
1:A:138:SER:O	1:A:140:TYR:N	2.51	0.43
1:C:114:PRO:HB3	2:D:116:ARG:O	2.18	0.43
1:A:93:VAL:CG1	3:A:142:HEM:HAC	2.49	0.43
1:C:80:LEU:O	1:C:82:ALA:N	2.51	0.43
2:D:71:PHE:O	2:D:75:LEU:HD13	2.17	0.43
1:A:41:THR:C	1:A:43:PHE:H	2.25	0.43
2:B:145:TYR:HB3	2:B:146:HIS:H	1.54	0.43
2:D:44:SER:O	2:D:46:GLY:N	2.51	0.43
2:D:118:LEU:O	2:D:119:GLY:C	2.61	0.43
1:A:45:HIS:ND1	1:A:45:HIS:N	2.65	0.43
2:B:56:GLY:O	2:B:57:ASN:C	2.62	0.43
2:B:130:PHE:O	2:B:134:VAL:HG22	2.19	0.43
1:A:88:ALA:HB1	1:A:140:TYR:N	2.34	0.43
1:C:30:GLU:OE1	1:C:50:HIS:HD2	2.02	0.43
2:D:107:GLY:HA3	2:D:134:VAL:HG13	2.01	0.43
2:B:41:PHE:CD2	3:B:147:HEM:HBC1	2.54	0.42
1:C:20:GLN:HB3	1:C:24:HIS:CE1	2.54	0.42
2:D:11:VAL:HG23	2:D:12:LEU:N	2.34	0.42
2:B:15:TRP:HH2	2:B:71:PHE:CD2	2.32	0.42
2:B:65:LYS:O	2:B:69:GLN:HB2	2.20	0.42
1:C:76:LEU:HD12	1:C:76:LEU:HA	1.89	0.42
1:A:32:MET:HE1	3:A:142:HEM:HBC2	2.00	0.42
2:B:41:PHE:HD2	3:B:147:HEM:HBC1	1.85	0.42
2:D:118:LEU:HD23	2:D:118:LEU:HA	1.74	0.42
1:A:49:SER:O	1:A:51:GLY:N	2.52	0.42
2:B:66:LYS:HZ2	2:B:66:LYS:HB3	1.84	0.42
2:B:66:LYS:HB3	2:B:66:LYS:NZ	2.35	0.42
1:A:87:HIS:HA	1:A:93:VAL:HG23	2.00	0.42
2:D:32:LEU:HD11	2:D:42:PHE:CD2	2.54	0.42
2:D:143:HIS:O	2:D:145:TYR:N	2.49	0.42
1:C:16:LYS:HD2	1:C:16:LYS:O	2.19	0.42
1:C:127:LYS:O	1:C:128:PHE:C	2.61	0.42
2:D:24:GLY:HA2	2:D:68:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:O	1:A:21:ALA:C	2.64	0.41
1:A:119:PRO:HA	2:B:30:ARG:HH11	1.85	0.41
1:C:36:PHE:CG	1:C:100:LEU:HD13	2.55	0.41
1:C:76:LEU:N	1:C:77:PRO:CD	2.83	0.41
2:D:91:LEU:CD2	3:D:147:HEM:HBA1	2.48	0.41
2:D:40:ARG:C	2:D:42:PHE:N	2.78	0.41
1:A:69:ALA:HB1	1:A:76:LEU:HD21	2.03	0.41
1:C:98:PHE:HE1	1:C:136:LEU:HD12	1.86	0.41
1:A:41:THR:HG21	2:D:97:HIS:CG	2.55	0.41
1:A:76:LEU:N	1:A:77:PRO:CD	2.84	0.41
2:B:96:LEU:HD13	3:B:147:HEM:C2D	2.55	0.41
1:A:95:PRO:HG2	2:D:37:TRP:CE3	2.56	0.41
2:B:26:GLU:CD	2:B:113:VAL:HG13	2.45	0.41
2:B:133:VAL:O	2:B:136:GLY:N	2.53	0.41
1:C:45:HIS:ND1	1:C:45:HIS:N	2.66	0.41
2:D:23:VAL:CG2	2:D:117:ARG:HD3	2.50	0.41
2:D:92:HIS:HA	2:D:96:LEU:HB2	2.02	0.41
2:D:132:LYS:H	2:D:132:LYS:HG2	1.73	0.41
1:A:139:LYS:O	1:A:141:ARG:N	2.53	0.40
1:A:135:VAL:C	1:A:137:THR:H	2.29	0.40
2:B:14:LEU:HD21	2:B:126:VAL:CG1	2.31	0.40
1:C:16:LYS:HE2	1:C:113:HIS:ND1	2.37	0.40
1:C:78:GLY:O	1:C:79:ALA:C	2.63	0.40
1:A:82:ALA:O	1:A:83:LEU:C	2.64	0.40
2:D:115:ALA:HB2	2:D:122:PHE:CD2	2.56	0.40
2:D:57:ASN:HA	2:D:58:PRO:HD2	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	139/141 (99%)	110 (79%)	20 (14%)	9 (6%)	1	3
1	C	139/141 (99%)	126 (91%)	7 (5%)	6 (4%)	2	7
2	B	144/146 (99%)	120 (83%)	18 (12%)	6 (4%)	2	7
2	D	144/146 (99%)	118 (82%)	22 (15%)	4 (3%)	4	14
All	All	566/574 (99%)	474 (84%)	67 (12%)	25 (4%)	2	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	53	ASP
1	A	140	TYR
1	C	81	SER
2	D	45	PHE
1	A	51	GLY
1	A	89	HIS
1	A	117	PHE
1	A	139	LYS
1	C	90	LYS
2	D	49	SER
1	A	82	ALA
2	B	74	GLY
2	B	86	ALA
2	B	120	HIS
1	C	53	ASP
1	C	88	ALA
2	D	144	LYS
1	A	114	PRO
2	B	56	GLY
2	B	143	HIS
1	C	50	HIS
1	C	139	LYS
2	D	41	PHE
2	B	20	VAL

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	111/111 (100%)	98 (88%)	13 (12%)	5	18
1	C	111/111 (100%)	97 (87%)	14 (13%)	4	15
2	B	119/119 (100%)	102 (86%)	17 (14%)	3	11
2	D	119/119 (100%)	104 (87%)	15 (13%)	4	15
All	All	460/460 (100%)	401 (87%)	59 (13%)	4	15

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	60	GLN
1	A	70	VAL
1	A	74	ASP
1	A	80	LEU
1	A	86	LEU
1	A	89	HIS
1	A	90	LYS
1	A	93	VAL
1	A	95	PRO
1	A	106	LEU
1	A	116	ASP
1	A	122	HIS
2	B	6	GLU
2	B	20	VAL
2	B	21	ASP
2	B	30	ARG
2	B	33	VAL
2	B	59	LYS
2	B	66	LYS
2	B	69	GLN
2	B	75	LEU
2	B	78	LEU
2	B	82	LYS
2	B	89	SER
2	B	90	GLU
2	B	112	VAL
2	B	124	PRO
2	B	130	PHE
2	B	139	ASN
1	C	47	ASN

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Mol	Chain	Res	Type
1	C	48	LEU
1	C	49	SER
1	C	76	LEU
1	C	86	LEU
1	C	99	LYS
1	C	106	LEU
1	C	124	SER
1	C	131	ASN
1	C	134	THR
1	C	138	SER
1	C	139	LYS
1	C	140	TYR
1	C	141	ARG
2	D	3	LEU
2	D	14	LEU
2	D	20	VAL
2	D	32	LEU
2	D	36	PRO
2	D	44	SER
2	D	72	SER
2	D	82	LYS
2	D	90	GLU
2	D	101	GLU
2	D	116	ARG
2	D	127	GLN
2	D	132	LYS
2	D	144	LYS
2	D	145	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	72	HIS
1	A	103	HIS
2	B	63	HIS
2	B	69	GLN
2	B	97	HIS
2	B	123	ASN
2	B	127	GLN
2	B	131	GLN
1	C	47	ASN

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Mol	Chain	Res	Type
1	C	50	HIS
1	C	60	GLN
1	C	89	HIS
1	C	103	HIS
1	C	112	HIS
1	C	131	ASN
2	D	63	HIS
2	D	97	HIS
2	D	108	ASN
2	D	139	ASN
2	D	146	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	HEM	C	142	4,1	50,50,50	1.70	14 (28%)	67,82,82	2.01	15 (22%)
3	HEM	B	147	2	50,50,50	1.78	14 (28%)	67,82,82	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	D	147	4,2	50,50,50	1.42	6 (12%)	67,82,82	1.38	13 (19%)
3	HEM	A	142	4,1	50,50,50	1.53	11 (22%)	67,82,82	1.64	12 (17%)

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	C	142	4,1	-	10/14/54/54	-
3	HEM	B	147	2	-	9/14/54/54	-
3	HEM	D	147	4,2	-	6/14/54/54	-
3	HEM	A	142	4,1	-	7/14/54/54	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CAC-C3C	-4.40	1.35	1.47
3	C	142	HEM	CAB-C3B	-4.26	1.36	1.47
3	C	142	HEM	CAC-C3C	-4.18	1.36	1.47
3	B	147	HEM	C3B-C4B	4.12	1.52	1.44
3	B	147	HEM	C1A-C2A	3.89	1.52	1.44
3	D	147	HEM	CAB-C3B	-3.81	1.37	1.47
3	D	147	HEM	C4A-C3A	3.47	1.51	1.43
3	A	142	HEM	C4D-C3D	3.45	1.50	1.45
3	C	142	HEM	C3B-C2B	-3.31	1.30	1.37
3	B	147	HEM	C1B-C2B	3.20	1.51	1.44
3	A	142	HEM	CAB-C3B	-3.20	1.38	1.47
3	B	147	HEM	C1D-C2D	3.15	1.50	1.44
3	B	147	HEM	C4B-NB	3.11	1.44	1.38
3	C	142	HEM	CHC-C1C	2.96	1.44	1.38
3	B	147	HEM	C4D-C3D	2.96	1.50	1.45
3	C	142	HEM	FE-ND	2.94	2.04	1.94
3	A	142	HEM	C3B-C4B	2.84	1.50	1.44
3	C	142	HEM	CHC-C4B	2.64	1.45	1.39
3	C	142	HEM	CHB-C1B	-2.63	1.33	1.38
3	D	147	HEM	CAC-C3C	-2.59	1.40	1.47
3	B	147	HEM	FE-NB	2.55	2.02	1.94
3	D	147	HEM	FE-ND	2.53	2.02	1.94
3	C	142	HEM	C2A-C3A	-2.52	1.32	1.38
3	A	142	HEM	C3B-C2B	-2.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NB	2.47	2.02	1.94
3	B	147	HEM	C3C-C4C	2.43	1.50	1.46
3	A	142	HEM	CHA-C4D	2.42	1.43	1.38
3	D	147	HEM	C3D-C2D	-2.40	1.31	1.36
3	A	142	HEM	FE-NC	-2.39	1.87	1.95
3	D	147	HEM	FE-NA	2.29	2.02	1.95
3	A	142	HEM	CHD-C4C	2.26	1.42	1.38
3	B	147	HEM	CMB-C2B	2.23	1.55	1.50
3	B	147	HEM	CBB-CAB	2.22	1.41	1.30
3	A	142	HEM	C1C-NC	-2.21	1.35	1.39
3	C	142	HEM	C3D-C2D	-2.17	1.32	1.36
3	B	147	HEM	C3B-C2B	2.17	1.41	1.37
3	C	142	HEM	C3C-C2C	-2.15	1.32	1.37
3	B	147	HEM	CBC-CAC	2.10	1.40	1.30
3	B	147	HEM	FE-NA	2.09	2.02	1.95
3	C	142	HEM	C3B-C4B	2.09	1.49	1.44
3	C	142	HEM	CBB-CAB	2.08	1.40	1.30
3	B	147	HEM	CAC-C3C	-2.07	1.41	1.47
3	C	142	HEM	C4A-NA	-2.05	1.35	1.39
3	A	142	HEM	FE-NA	2.05	2.01	1.95
3	C	142	HEM	CHD-C4C	2.00	1.42	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CBD-CAD-C3D	5.77	128.50	112.53
3	C	142	HEM	CMB-C2B-C1B	5.70	133.94	125.03
3	C	142	HEM	C3B-C2B-C1B	-5.06	102.61	106.41
3	B	147	HEM	CAA-C2A-C1A	4.82	134.35	124.94
3	A	142	HEM	CAD-C3D-C4D	4.46	132.47	124.70
3	C	142	HEM	CBA-CAA-C2A	-4.13	101.12	112.53
3	C	142	HEM	C4B-C3B-C2B	4.06	111.01	107.28
3	C	142	HEM	C2B-C1B-NB	4.05	114.50	109.84
3	C	142	HEM	CAA-C2A-C1A	3.94	132.64	124.94
3	A	142	HEM	CAD-C3D-C2D	-3.89	120.59	127.87
3	A	142	HEM	CHD-C1D-ND	-3.87	120.25	124.42
3	D	147	HEM	CMD-C2D-C1D	3.64	130.72	125.03
3	C	142	HEM	CHB-C1B-NB	-3.43	120.12	124.37
3	D	147	HEM	CMA-C3A-C4A	3.43	130.63	125.42
3	A	142	HEM	CHC-C4B-NB	-3.18	121.00	124.42
3	B	147	HEM	C2B-C1B-NB	3.13	113.44	109.84
3	C	142	HEM	CAA-C2A-C3A	-2.82	120.74	127.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	C2D-C1D-ND	2.70	113.03	109.90
3	D	147	HEM	CBD-CAD-C3D	2.70	120.00	112.53
3	C	142	HEM	CMD-C2D-C1D	2.69	129.24	125.03
3	A	142	HEM	CAA-C2A-C1A	2.68	130.17	124.94
3	B	147	HEM	CAA-C2A-C3A	-2.65	121.12	127.07
3	C	142	HEM	CMA-C3A-C4A	2.64	129.44	125.42
3	D	147	HEM	C3B-C4B-NB	2.60	111.34	109.47
3	A	142	HEM	C1B-NB-C4B	-2.52	102.22	105.21
3	D	147	HEM	CAD-C3D-C4D	2.51	129.06	124.70
3	D	147	HEM	C3D-C4D-ND	2.49	112.90	110.17
3	B	147	HEM	CAD-C3D-C4D	2.47	128.99	124.70
3	D	147	HEM	CHD-C1D-ND	-2.46	121.77	124.42
3	B	147	HEM	C1A-C2A-C3A	-2.44	103.10	106.87
3	A	142	HEM	C2B-C1B-NB	2.42	112.62	109.84
3	A	142	HEM	C4C-C3C-C2C	-2.42	104.72	106.81
3	B	147	HEM	C3B-C4B-NB	2.41	111.20	109.47
3	D	147	HEM	C4D-ND-C1D	-2.38	102.39	105.21
3	A	142	HEM	CMD-C2D-C1D	2.37	128.74	125.03
3	C	142	HEM	CHC-C4B-C3B	2.36	129.79	125.07
3	A	142	HEM	C3B-C4B-NB	2.36	111.17	109.47
3	D	147	HEM	C4C-C3C-C2C	-2.31	104.81	106.81
3	C	142	HEM	CHD-C1D-ND	-2.26	121.99	124.42
3	D	147	HEM	CMD-C2D-C3D	-2.24	120.10	126.15
3	C	142	HEM	CHC-C4B-NB	-2.23	122.03	124.42
3	B	147	HEM	C4A-NA-C1A	-2.13	102.35	105.82
3	C	142	HEM	CMB-C2B-C3B	-2.11	123.31	128.43
3	D	147	HEM	CHB-C4A-NA	-2.08	120.09	123.86
3	D	147	HEM	C4A-NA-C1A	-2.08	102.43	105.82
3	A	142	HEM	C4A-NA-C1A	-2.07	102.45	105.82
3	D	147	HEM	C2A-C1A-NA	2.02	112.40	110.15

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C2B-C3B-CAB-CBB
3	A	142	HEM	C2C-C3C-CAC-CBC
3	A	142	HEM	C4C-C3C-CAC-CBC
3	A	142	HEM	C4D-C3D-CAD-CBD
3	B	147	HEM	C1A-C2A-CAA-CBA
3	B	147	HEM	C2B-C3B-CAB-CBB
3	B	147	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	C	142	HEM	C2C-C3C-CAC-CBC
3	C	142	HEM	C2D-C3D-CAD-CBD
3	D	147	HEM	C3D-CAD-CBD-CGD
3	B	147	HEM	C3A-C2A-CAA-CBA
3	C	142	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2D-C3D-CAD-CBD
3	C	142	HEM	C2B-C3B-CAB-CBB
3	A	142	HEM	C4B-C3B-CAB-CBB
3	C	142	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	C3D-CAD-CBD-CGD
3	D	147	HEM	C2B-C3B-CAB-CBB
3	B	147	HEM	C2A-CAA-CBA-CGA
3	C	142	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	C2C-C3C-CAC-CBC
3	C	142	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAD-CBD-CGD-O1D

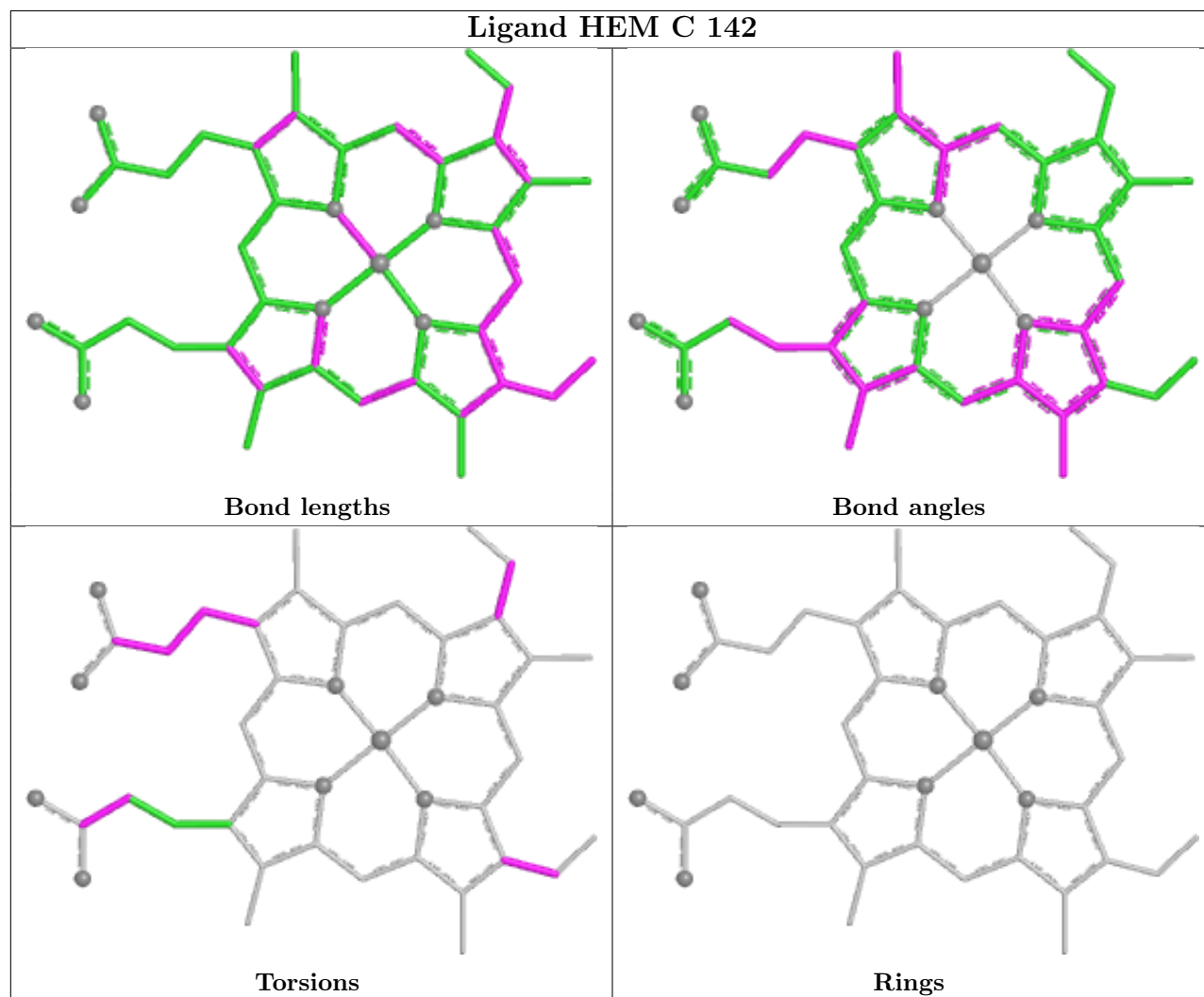
There are no ring outliers.

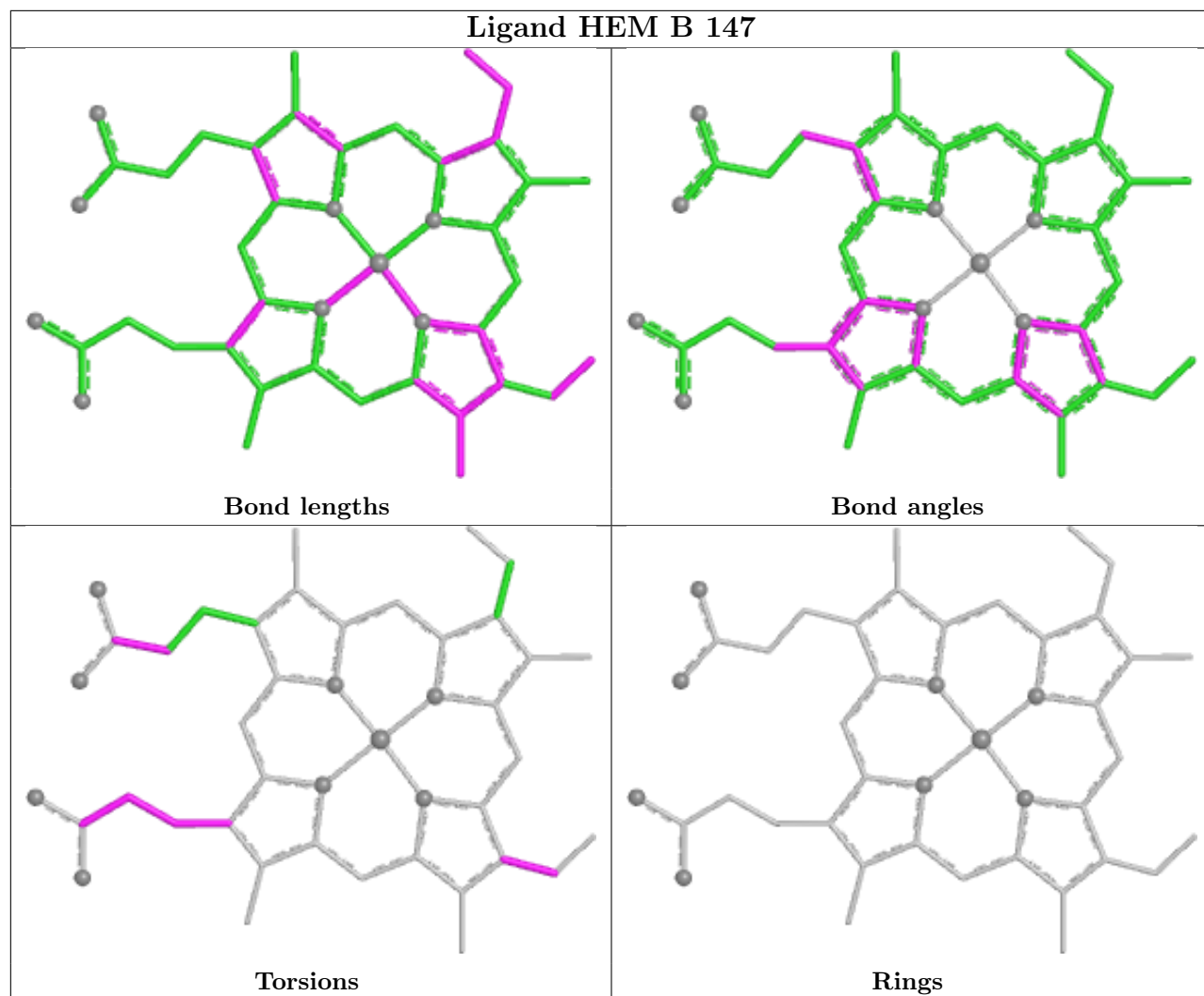
4 monomers are involved in 22 short contacts:

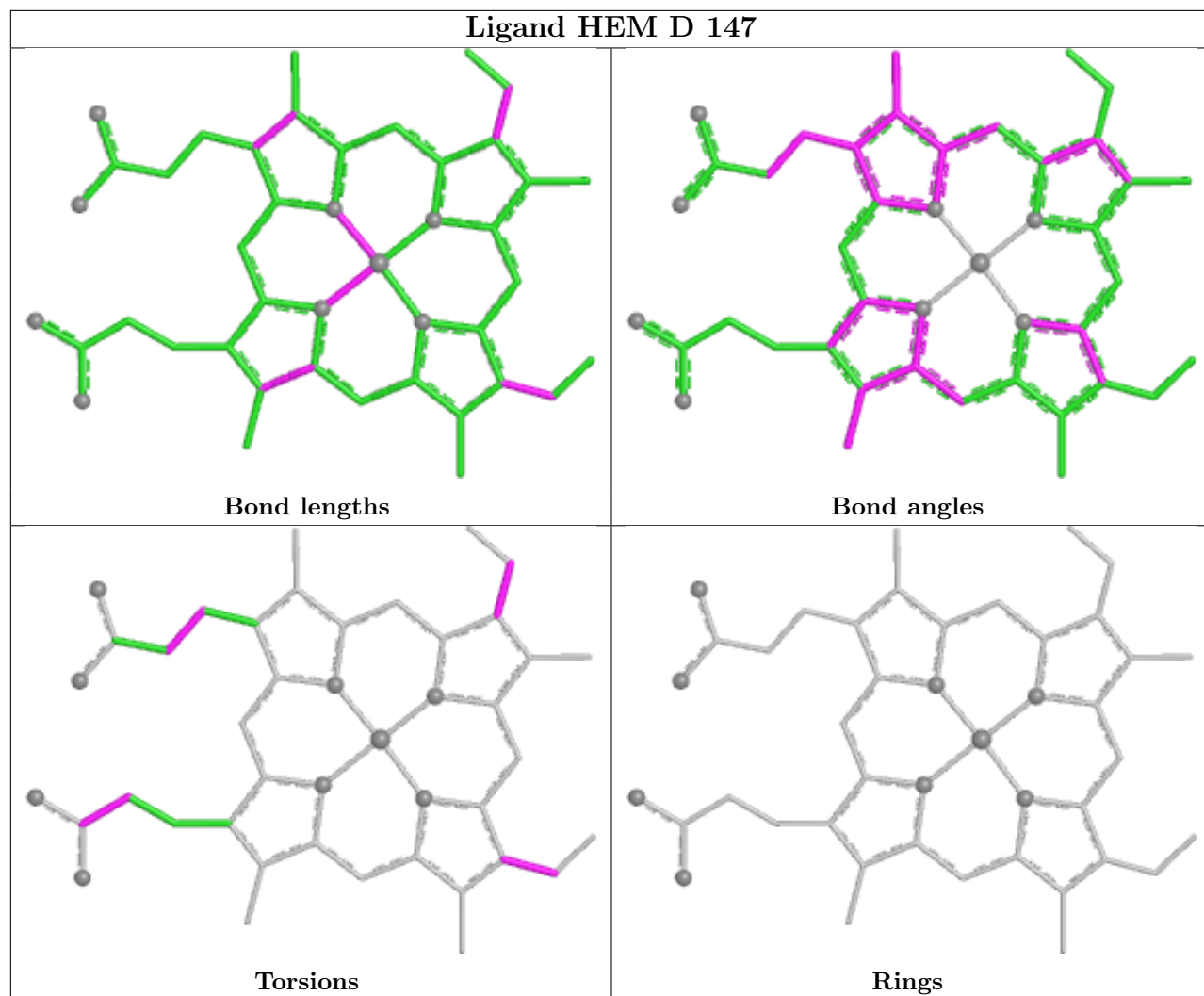
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	142	HEM	2	0
3	B	147	HEM	6	0
3	D	147	HEM	12	0
3	A	142	HEM	2	0

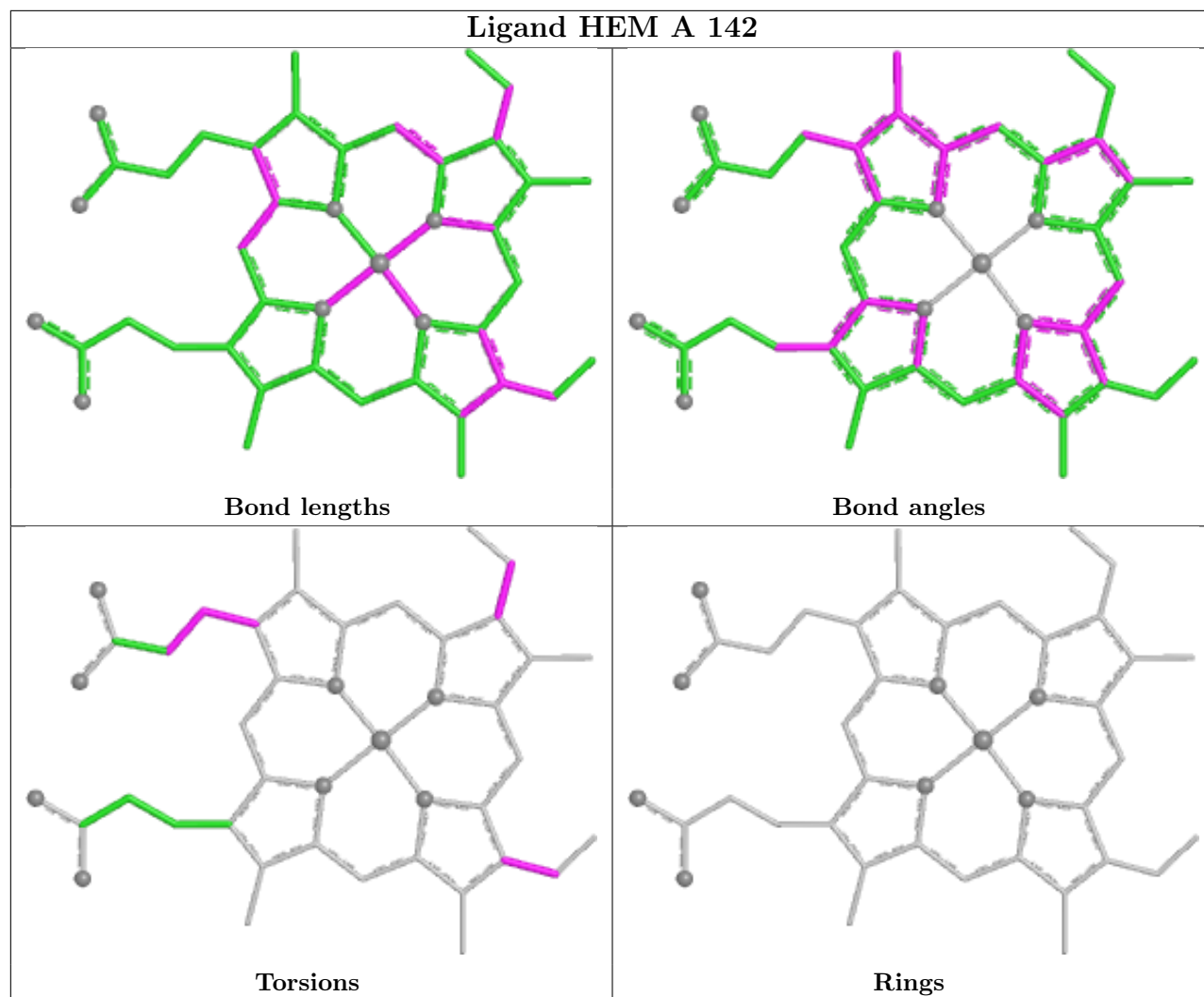
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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