



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:51 PM UTC

PDB ID : 1A4F / pdb_00001a4f
Title : BAR-HEADED GOOSE HEMOGLOBIN (OXY FORM)
Authors : Zhang, J.; Gu, X.
Deposited on : 1998-01-29
Resolution : 2.00 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

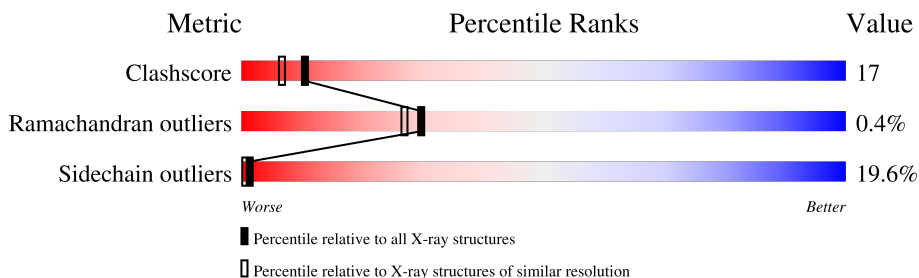
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	26% 46% 22% 6%
2	B	146	34% 45% 16% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2448 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.

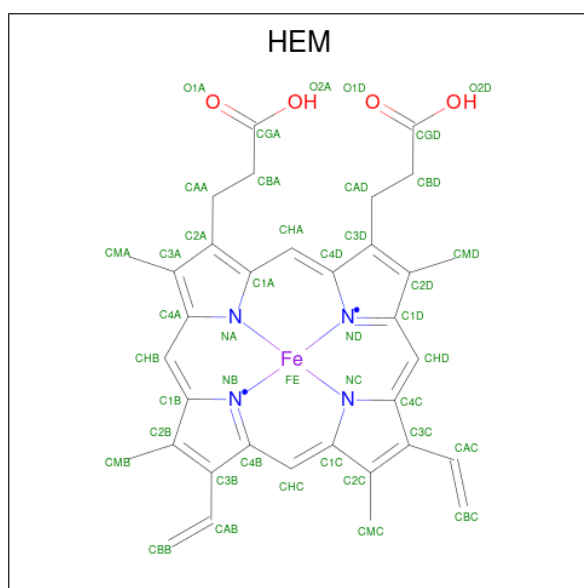
- Molecule 1 is a protein called HEMOGLOBIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1086	698	189	195	4			

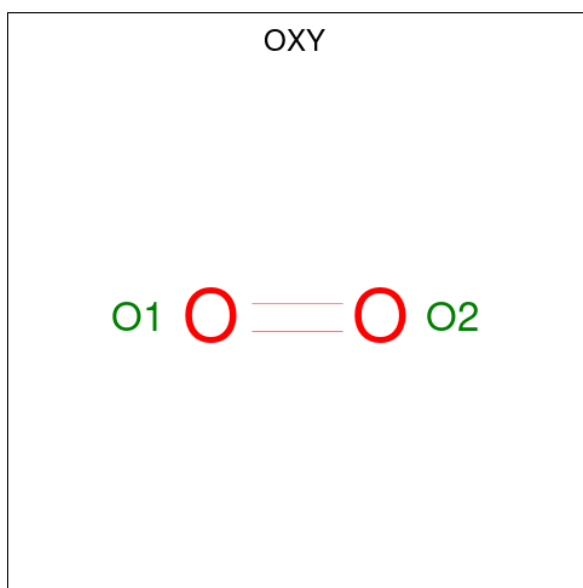
- Molecule 2 is a protein called HEMOGLOBIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	2	0
			1164	751	207	202	4			

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



- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 5 is water.

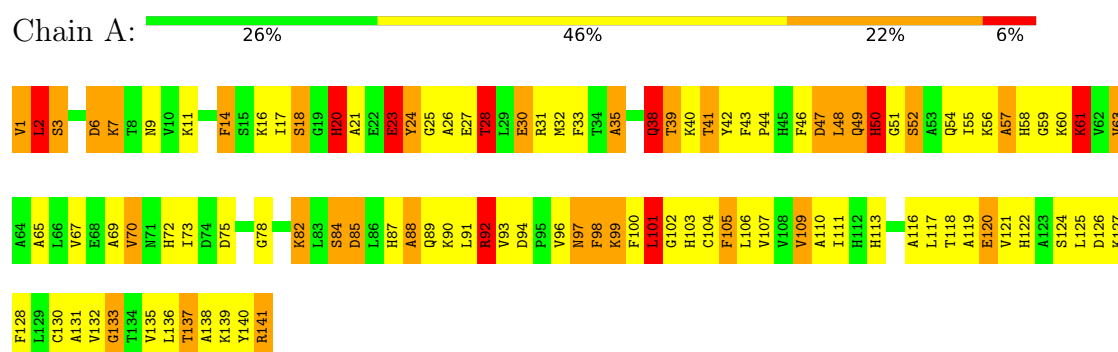
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	57	Total	O	0	0
			57	57		

3 Residue-property plots [i](#)

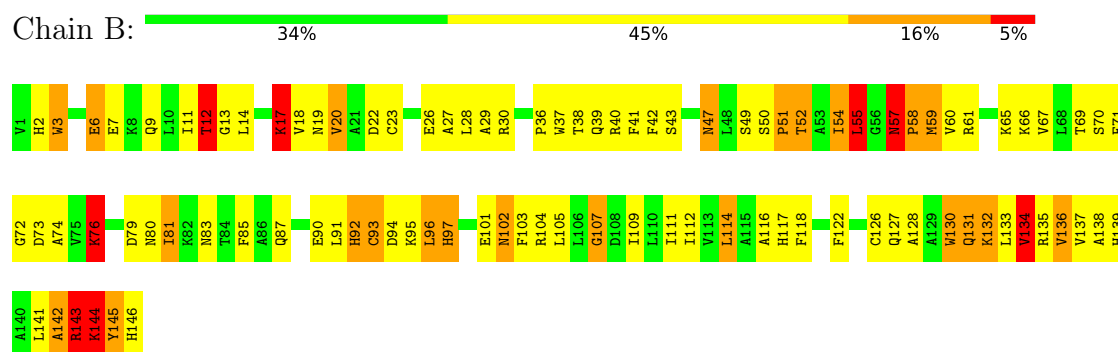
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: HEMOGLOBIN (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 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	81.59Å 81.59Å 107.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	87.1 (10.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2448	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: OXY, 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	1.30	2/1115 (0.2%)	3.06	159/1509 (10.5%)
2	B	1.36	3/1201 (0.2%)	2.84	125/1628 (7.7%)
All	All	1.33	5/2316 (0.2%)	2.95	284/3137 (9.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	VAL	CA-CB	6.80	1.61	1.54
1	A	32	MET	N-CA	5.34	1.52	1.46
2	B	28	LEU	CA-C	-5.17	1.46	1.52
1	A	139	LYS	N-CA	5.08	1.52	1.46
2	B	61	ARG	CA-C	-5.04	1.46	1.52

All (284) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ASP	CA-CB-CG	18.72	131.32	112.60
1	A	31	ARG	NE-CZ-NH1	14.30	135.80	121.50
1	A	82	LYS	CA-CB-CG	13.31	140.72	114.10
2	B	109	ILE	CA-C-O	-12.08	108.39	120.95
2	B	18	VAL	CA-C-O	-12.02	107.34	121.04
2	B	79	ASP	CA-CB-CG	11.78	124.38	112.60
2	B	137	VAL	CA-C-O	-11.45	108.71	120.85
1	A	28	THR	CA-CB-CG2	11.33	129.76	110.50
2	B	87	GLN	CA-CB-CG	10.81	135.72	114.10
1	A	58	HIS	CA-CB-CG	-10.68	103.12	113.80
2	B	83	ASN	CA-C-N	10.67	134.58	120.28
2	B	83	ASN	C-N-CA	10.67	134.58	120.28
1	A	30	GLU	CB-CG-CD	10.46	130.39	112.60
1	A	38	GLN	OE1-CD-NE2	-10.19	112.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	PHE	CA-C-O	-10.09	110.77	122.37
1	A	126	ASP	CA-CB-CG	10.08	122.68	112.60
1	A	31	ARG	NH1-CZ-NH2	-9.94	106.37	119.30
1	A	138	ALA	CA-C-O	-9.87	109.97	120.63
1	A	27	GLU	O-C-N	9.69	132.39	122.12
2	B	142	ALA	CA-C-O	9.51	130.49	119.18
1	A	24	TYR	CA-C-O	-9.41	110.48	120.55
2	B	137	VAL	O-C-N	9.24	131.35	121.83
2	B	7	GLU	N-CA-C	-9.14	101.27	111.14
2	B	80	ASN	CA-CB-CG	9.14	121.74	112.60
2	B	122	PHE	O-C-N	9.10	133.28	122.46
1	A	91	LEU	O-C-N	8.93	134.78	122.46
1	A	49	GLN	CA-CB-CG	8.82	131.74	114.10
1	A	11	LYS	CA-C-N	8.80	129.93	119.99
1	A	11	LYS	C-N-CA	8.80	129.93	119.99
1	A	84	SER	CA-C-O	-8.80	109.85	119.97
2	B	22	ASP	CA-CB-CG	8.80	121.40	112.60
2	B	127	GLN	OE1-CD-NE2	8.78	131.38	122.60
1	A	46	PHE	CA-CB-CG	8.72	122.52	113.80
1	A	102	GLY	CA-C-N	8.68	131.91	120.28
1	A	102	GLY	C-N-CA	8.68	131.91	120.28
2	B	73	ASP	N-CA-C	-8.59	102.00	111.36
2	B	139	HIS	CA-CB-CG	8.49	122.30	113.80
2	B	12	THR	N-CA-C	8.44	120.48	111.28
2	B	102	ASN	OD1-CG-ND2	8.35	130.95	122.60
2	B	28	LEU	CB-CA-C	8.24	123.81	110.88
1	A	40	LYS	CA-C-N	8.21	133.74	120.60
1	A	40	LYS	C-N-CA	8.21	133.74	120.60
1	A	57	ALA	CA-C-O	8.18	129.09	120.42
2	B	30	ARG	CA-C-O	-8.18	111.75	120.42
1	A	100	PHE	O-C-N	8.16	130.90	122.09
1	A	2	LEU	CA-C-O	8.13	132.14	120.51
1	A	82	LYS	CG-CD-CE	8.11	129.95	111.30
1	A	107	VAL	CA-CB-CG2	8.04	124.06	110.40
1	A	94	ASP	CA-C-N	7.83	128.55	119.47
1	A	94	ASP	C-N-CA	7.83	128.55	119.47
1	A	103	HIS	CA-C-N	7.81	132.18	120.31
1	A	103	HIS	C-N-CA	7.81	132.18	120.31
2	B	134	VAL	N-CA-CB	-7.79	96.67	110.77
2	B	41	PHE	CA-CB-CG	-7.74	106.06	113.80
2	B	97	HIS	CA-CB-CG	-7.73	106.07	113.80
1	A	113	HIS	O-C-N	7.67	128.17	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	N-CA-C	-7.61	103.79	113.23
1	A	31	ARG	O-C-N	7.56	130.77	122.15
2	B	143	ARG	CA-C-O	-7.53	111.59	120.10
1	A	9	ASN	O-C-N	7.48	129.77	122.07
2	B	20	VAL	CA-CB-CG2	7.42	123.02	110.40
1	A	92	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	106	LEU	CA-C-N	7.26	130.74	120.42
1	A	106	LEU	C-N-CA	7.26	130.74	120.42
2	B	145	TYR	N-CA-CB	7.19	120.49	110.56
2	B	134	VAL	CB-CA-C	7.18	123.89	112.26
2	B	2	HIS	CA-C-N	-7.15	113.13	123.00
2	B	2	HIS	C-N-CA	-7.15	113.13	123.00
1	A	21	ALA	CA-C-O	7.15	128.35	120.63
2	B	109	ILE	CA-C-N	7.14	130.18	120.54
2	B	109	ILE	C-N-CA	7.14	130.18	120.54
1	A	92	ARG	CD-NE-CZ	-7.13	114.42	124.40
2	B	6	GLU	CA-C-N	7.10	130.09	120.44
2	B	6	GLU	C-N-CA	7.10	130.09	120.44
2	B	111	ILE	CA-C-N	7.10	130.50	120.42
2	B	111	ILE	C-N-CA	7.10	130.50	120.42
1	A	100	PHE	CA-C-O	-7.09	113.39	120.70
2	B	38	THR	CA-CB-OG1	-7.06	99.01	109.60
2	B	57	ASN	N-CA-C	-7.05	99.13	109.50
1	A	48	LEU	N-CA-CB	-7.00	99.85	110.91
1	A	92	ARG	NH1-CZ-NH2	6.97	128.36	119.30
1	A	57	ALA	N-CA-C	6.96	118.94	111.36
2	B	23	CYS	N-CA-C	-6.86	103.04	111.40
1	A	109	VAL	O-C-N	-6.85	114.06	121.80
1	A	35	ALA	CA-C-N	6.85	131.44	123.15
1	A	35	ALA	C-N-CA	6.85	131.44	123.15
1	A	141	ARG	CD-NE-CZ	6.83	133.97	124.40
2	B	61	ARG	NE-CZ-NH1	6.83	128.32	121.50
1	A	113	HIS	CA-CB-CG	-6.79	107.01	113.80
1	A	119	ALA	CA-C-O	6.79	127.77	119.97
1	A	39	THR	CA-CB-OG1	-6.78	99.43	109.60
2	B	58	PRO	CA-C-N	-6.76	109.08	121.52
2	B	58	PRO	C-N-CA	-6.76	109.08	121.52
2	B	114	LEU	N-CA-C	-6.75	103.99	111.82
1	A	82	LYS	CB-CG-CD	6.74	126.79	111.30
1	A	138	ALA	N-CA-CB	6.74	120.16	110.06
2	B	27	ALA	CA-C-O	-6.71	113.44	120.55
1	A	3	SER	O-C-N	6.69	130.60	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	NE-CZ-NH2	-6.69	113.18	119.20
1	A	105	PHE	O-C-N	-6.68	114.53	122.15
2	B	39	GLN	CA-C-N	6.68	129.24	120.28
2	B	39	GLN	C-N-CA	6.68	129.24	120.28
2	B	132	LYS	O-C-N	-6.67	115.05	122.12
2	B	66	LYS	CA-C-O	-6.63	113.39	120.42
1	A	139	LYS	CA-C-N	6.62	134.19	121.54
1	A	139	LYS	C-N-CA	6.62	134.19	121.54
2	B	101	GLU	O-C-N	-6.59	113.60	122.43
1	A	55	ILE	O-C-N	-6.58	115.46	121.91
2	B	57	ASN	O-C-N	6.57	127.85	121.28
2	B	20	VAL	CB-CA-C	6.55	120.99	112.14
1	A	3	SER	N-CA-C	-6.51	100.83	110.46
2	B	134	VAL	CA-CB-CG1	6.49	121.43	110.40
1	A	26	ALA	CA-C-O	6.47	127.28	120.42
2	B	131	GLN	N-CA-CB	6.43	119.57	110.12
2	B	6	GLU	CB-CG-CD	6.37	123.44	112.60
1	A	94	ASP	CA-C-O	-6.37	113.43	119.80
1	A	31	ARG	CG-CD-NE	-6.37	97.99	112.00
1	A	41	THR	CA-CB-CG2	6.37	121.33	110.50
2	B	93	CYS	CA-C-N	6.34	131.43	120.58
2	B	93	CYS	C-N-CA	6.34	131.43	120.58
1	A	133	GLY	CA-C-N	6.34	129.29	120.29
1	A	133	GLY	C-N-CA	6.34	129.29	120.29
2	B	19	ASN	CA-C-O	-6.34	114.33	120.92
2	B	11	ILE	CA-C-N	6.31	128.74	120.28
2	B	11	ILE	C-N-CA	6.31	128.74	120.28
2	B	142	ALA	O-C-N	-6.30	113.46	122.41
1	A	118	THR	CA-C-O	-6.30	114.76	121.88
1	A	107	VAL	N-CA-C	-6.30	104.36	110.72
2	B	13	GLY	O-C-N	6.29	130.88	122.70
2	B	3	TRP	CA-C-O	-6.29	113.53	120.38
1	A	92	ARG	CA-C-N	-6.28	112.28	121.71
1	A	92	ARG	C-N-CA	-6.28	112.28	121.71
2	B	112	ILE	CA-CB-CG2	6.27	121.16	110.50
2	B	76	LYS	CA-C-O	6.25	127.17	119.79
2	B	83	ASN	OD1-CG-ND2	6.25	128.85	122.60
1	A	25	GLY	O-C-N	-6.25	115.47	122.28
2	B	130	TRP	CA-C-O	-6.23	113.82	120.42
2	B	55	LEU	N-CA-CB	-6.22	100.64	110.22
1	A	139	LYS	CB-CG-CD	6.21	125.59	111.30
1	A	99	LYS	CA-C-N	6.19	128.86	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	LYS	C-N-CA	6.19	128.86	120.44
2	B	18	VAL	O-C-N	6.15	129.37	122.67
1	A	9	ASN	N-CA-C	-6.14	104.50	111.07
1	A	127	LYS	O-C-N	6.12	129.79	122.27
2	B	67	VAL	CA-C-O	-6.10	114.70	121.17
1	A	113	HIS	CA-C-N	6.09	125.57	119.24
1	A	113	HIS	C-N-CA	6.09	125.57	119.24
2	B	28	LEU	O-C-N	-6.08	115.80	122.07
2	B	87	GLN	CB-CA-C	6.08	122.34	110.67
2	B	43	SER	CA-C-O	-6.06	113.25	120.10
1	A	38	GLN	CB-CG-CD	6.05	122.88	112.60
1	A	116	ALA	N-CA-C	-6.05	104.61	112.23
1	A	135	VAL	O-C-N	-6.04	115.62	121.90
1	A	59	GLY	CA-C-O	6.03	127.27	121.05
2	B	134	VAL	CA-C-O	6.03	126.98	120.47
1	A	7	LYS	CA-C-O	6.02	126.81	120.42
2	B	61	ARG	CA-C-O	6.02	126.90	120.70
2	B	43	SER	O-C-N	6.01	129.25	122.22
1	A	104	CYS	N-CA-C	-6.01	104.85	111.82
2	B	17	LYS	CA-CB-CG	-6.00	102.09	114.10
1	A	75	ASP	O-C-N	6.00	130.57	122.59
1	A	102	GLY	O-C-N	-5.99	116.20	122.13
1	A	120	GLU	O-C-N	-5.97	114.33	122.33
1	A	26	ALA	O-C-N	-5.97	115.34	122.15
2	B	104	ARG	NE-CZ-NH1	-5.96	115.54	121.50
2	B	69	THR	CA-C-N	5.94	128.73	120.29
2	B	69	THR	C-N-CA	5.94	128.73	120.29
1	A	72	HIS	O-C-N	5.93	130.14	122.19
1	A	23	GLU	N-CA-CB	5.93	119.47	110.28
1	A	49	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	101	LEU	CB-CA-C	5.92	120.25	110.90
2	B	36	PRO	N-CA-CB	5.89	109.44	103.25
2	B	127	GLN	CA-C-N	5.89	128.17	120.28
2	B	127	GLN	C-N-CA	5.89	128.17	120.28
1	A	82	LYS	CB-CA-C	5.88	121.50	109.55
2	B	79	ASP	CA-C-O	-5.87	112.69	118.97
1	A	122	HIS	N-CA-C	-5.85	103.88	111.02
2	B	52	THR	CA-C-O	5.84	126.61	120.42
1	A	50	HIS	N-CA-CB	5.83	118.52	109.48
1	A	98	PHE	O-C-N	5.82	129.43	122.27
1	A	113	HIS	CB-CA-C	-5.80	102.09	111.14
2	B	81	ILE	O-C-N	5.80	127.49	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LYS	CA-C-O	-5.79	113.31	119.97
1	A	67	VAL	CA-C-O	5.77	127.05	121.05
2	B	109	ILE	CB-CG1-CD1	-5.77	101.69	113.80
2	B	144	LYS	N-CA-CB	5.73	119.28	110.46
1	A	58	HIS	N-CA-C	-5.71	105.14	111.36
1	A	98	PHE	CA-CB-CG	-5.70	108.10	113.80
2	B	105	LEU	CA-C-O	-5.70	114.51	120.55
2	B	131	GLN	CB-CG-CD	5.67	122.25	112.60
1	A	99	LYS	CA-C-O	-5.67	113.10	119.79
1	A	49	GLN	N-CA-CB	5.66	118.60	110.06
1	A	56	LYS	CB-CA-C	-5.65	102.01	110.88
2	B	17	LYS	N-CA-CB	-5.63	102.16	110.49
2	B	126	CYS	CA-C-N	5.63	129.26	120.82
2	B	126	CYS	C-N-CA	5.63	129.26	120.82
1	A	47	ASP	CA-C-N	-5.62	114.17	122.83
1	A	47	ASP	C-N-CA	-5.62	114.17	122.83
2	B	51	PRO	N-CA-C	-5.56	105.80	113.53
1	A	14	PHE	CA-CB-CG	-5.56	108.24	113.80
2	B	131	GLN	OE1-CD-NE2	5.53	128.12	122.60
1	A	23	GLU	CA-C-O	-5.52	113.62	119.97
1	A	31	ARG	CA-C-O	-5.52	114.57	120.42
1	A	131	ALA	N-CA-C	-5.51	104.91	111.69
1	A	61	LYS	CG-CD-CE	5.51	123.97	111.30
1	A	20	HIS	CB-CA-C	-5.50	101.99	111.45
1	A	6	ASP	O-C-N	5.48	128.40	122.15
2	B	103	PHE	N-CA-C	-5.47	105.40	111.36
1	A	30	GLU	CG-CD-OE2	5.46	130.97	118.40
2	B	47	ASN	N-CA-C	5.46	117.14	108.67
2	B	143	ARG	CB-CG-CD	-5.46	98.74	111.30
1	A	30	GLU	CA-C-O	-5.46	114.77	120.55
1	A	70	VAL	N-CA-C	-5.45	105.19	110.42
1	A	42	TYR	CA-C-O	-5.45	112.70	119.18
2	B	112	ILE	N-CA-CB	5.45	118.75	110.58
2	B	107	GLY	N-CA-C	-5.44	106.08	113.37
1	A	124	SER	O-C-N	5.39	129.24	122.23
1	A	78	GLY	CA-C-O	-5.39	115.18	121.00
2	B	92	HIS	CA-CB-CG	-5.39	108.41	113.80
1	A	38	GLN	CG-CD-NE2	5.38	124.48	116.40
2	B	22	ASP	CB-CG-OD1	5.38	130.78	118.40
2	B	60	VAL	O-C-N	-5.38	116.65	121.87
1	A	50	HIS	CA-CB-CG	5.38	119.18	113.80
1	A	9	ASN	CA-C-O	-5.37	115.18	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CA-C-N	-5.37	113.93	121.72
1	A	46	PHE	C-N-CA	-5.37	113.93	121.72
1	A	50	HIS	N-CA-C	-5.36	102.36	110.24
1	A	98	PHE	CA-C-O	-5.36	113.81	119.97
2	B	109	ILE	O-C-N	5.36	127.07	121.87
1	A	100	PHE	N-CA-C	-5.36	105.36	111.14
1	A	65	ALA	O-C-N	5.35	128.85	122.27
2	B	7	GLU	O-C-N	5.35	127.86	122.09
1	A	128	PHE	CA-C-N	5.32	127.40	120.28
1	A	128	PHE	C-N-CA	5.32	127.40	120.28
1	A	84	SER	N-CA-CB	5.31	118.51	110.28
2	B	11	ILE	CA-C-O	-5.31	115.02	121.18
1	A	97	ASN	CA-C-N	-5.31	112.24	120.31
1	A	97	ASN	C-N-CA	-5.31	112.24	120.31
2	B	3	TRP	N-CA-CB	-5.30	102.25	110.57
1	A	93	VAL	CA-C-O	-5.30	114.81	121.11
2	B	41	PHE	N-CA-CB	-5.29	101.77	110.40
2	B	42	PHE	CA-C-N	5.27	127.87	120.28
2	B	42	PHE	C-N-CA	5.27	127.87	120.28
1	A	63	VAL	O-C-N	-5.27	115.15	122.05
2	B	138	ALA	N-CA-C	-5.26	105.54	111.28
1	A	46	PHE	N-CA-C	-5.26	101.99	110.14
2	B	102	ASN	CB-CG-ND2	-5.25	108.53	116.40
2	B	122	PHE	N-CA-C	-5.24	99.44	108.56
1	A	33	PHE	O-C-N	-5.24	115.58	122.39
2	B	134	VAL	CA-C-N	5.24	127.57	120.44
2	B	134	VAL	C-N-CA	5.24	127.57	120.44
1	A	48	LEU	CA-C-O	-5.23	113.41	120.15
1	A	16	LYS	O-C-N	-5.22	115.85	122.27
1	A	91	LEU	N-CA-C	5.22	119.36	112.89
1	A	126	ASP	N-CA-CB	5.16	117.70	110.12
2	B	59	MET	N-CA-C	-5.15	106.15	112.90
2	B	103	PHE	CA-C-N	5.14	127.59	120.29
2	B	103	PHE	C-N-CA	5.14	127.59	120.29
2	B	103	PHE	N-CA-CB	5.13	117.76	110.16
1	A	132	VAL	CA-C-N	5.13	125.67	119.98
1	A	132	VAL	C-N-CA	5.13	125.67	119.98
1	A	87	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
1	A	117	LEU	O-C-N	-5.11	115.86	122.56
1	A	47	ASP	N-CA-C	-5.11	101.43	109.25
2	B	128	ALA	N-CA-C	5.11	116.85	111.28
1	A	121	VAL	CG1-CB-CG2	-5.09	99.60	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ALA	CA-C-O	5.09	126.67	120.31
1	A	137	THR	CA-CB-CG2	5.08	119.14	110.50
2	B	55	LEU	CA-C-O	5.08	125.84	120.10
1	A	118	THR	N-CA-CB	-5.08	103.38	110.38
2	B	66	LYS	CB-CA-C	-5.07	102.23	110.85
1	A	135	VAL	CB-CA-C	5.07	118.66	112.02
1	A	130[A]	CYS	CA-C-O	-5.06	114.15	119.97
1	A	130[B]	CYS	CA-C-O	-5.06	114.15	119.97
2	B	144	LYS	N-CA-C	-5.06	107.13	113.15
1	A	96	VAL	CA-C-O	-5.05	115.16	120.57
1	A	31	ARG	CD-NE-CZ	5.05	131.47	124.40
2	B	58	PRO	N-CD-CG	-5.04	95.63	103.20
1	A	119	ALA	O-C-N	-5.03	116.08	122.27
1	A	101	LEU	CA-C-N	5.03	125.67	119.99
1	A	101	LEU	C-N-CA	5.03	125.67	119.99
1	A	52	SER	N-CA-C	-5.02	103.71	110.24
1	A	85	ASP	N-CA-CB	5.01	117.57	110.16
2	B	85	PHE	CA-C-O	-5.00	113.50	119.35

There are no chirality outliers.

There are no planarity outliers.

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	1086	0	1096	33	0
2	B	1164	0	1174	45	0
3	A	43	0	30	1	0
3	B	43	0	30	6	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	51	0	0	0	0
5	B	57	0	0	4	0
All	All	2448	0	2330	79	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 17.

All (79) 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:141:LEU:CD1	3:B:150:HEM:HBB2	1.93	0.99
1:A:92:ARG:HA	1:A:140:TYR:OH	1.62	0.98
2:B:141:LEU:HD12	3:B:150:HEM:HBB2	1.49	0.92
2:B:3:TRP:CZ3	2:B:132:LYS:HD2	2.04	0.92
2:B:91:LEU:O	2:B:96:LEU:HD22	1.74	0.88
2:B:143:ARG:HD3	5:B:180:HOH:O	1.84	0.76
1:A:92:ARG:HA	1:A:140:TYR:HH	1.50	0.74
2:B:91:LEU:HG	2:B:96:LEU:CD2	2.20	0.70
2:B:92:HIS:HA	2:B:96:LEU:HD23	1.74	0.70
2:B:57:ASN:HD22	2:B:59:MET:H	1.39	0.69
2:B:40[A]:ARG:NH2	5:B:167:HOH:O	2.20	0.69
1:A:92:ARG:CA	1:A:140:TYR:OH	2.39	0.68
3:B:150:HEM:HMC2	3:B:150:HEM:HBC2	1.75	0.67
2:B:96:LEU:O	2:B:97:HIS:HB2	1.95	0.66
1:A:14:PHE:O	1:A:18:SER:HB2	1.96	0.65
1:A:70:VAL:O	1:A:73:ILE:HB	1.96	0.65
2:B:37:TRP:HE1	2:B:102:ASN:HD21	1.43	0.65
2:B:132:LYS:O	2:B:136:VAL:HG13	1.97	0.65
2:B:91:LEU:HG	2:B:96:LEU:HD21	1.78	0.63
2:B:141:LEU:HD11	3:B:150:HEM:HBB2	1.79	0.62
2:B:93:CYS:SG	2:B:145:TYR:CE2	2.93	0.62
2:B:26[A]:GLU:OE1	2:B:117:HIS:NE2	2.31	0.59
2:B:51:PRO:O	2:B:55:LEU:HB2	2.03	0.58
3:B:150:HEM:HBC2	3:B:150:HEM:CMC	2.34	0.58
1:A:57:ALA:O	1:A:61:LYS:HG2	2.03	0.57
2:B:57:ASN:ND2	2:B:59:MET:H	2.03	0.56
2:B:71:PHE:O	2:B:74:ALA:HB3	2.05	0.56
2:B:107:GLY:HA3	2:B:134:VAL:HG13	1.86	0.56
2:B:72:GLY:O	2:B:76:LYS:HG2	2.06	0.56
2:B:142:ALA:O	2:B:145:TYR:HB2	2.05	0.56
1:A:49:GLN:O	1:A:50:HIS:C	2.49	0.55
2:B:47:ASN:OD1	2:B:49:SER:HB3	2.06	0.55
2:B:130:TRP:CE3	2:B:133:LEU:HD23	2.42	0.55
1:A:101:LEU:HD12	1:A:101:LEU:O	2.07	0.54
2:B:12:THR:HG22	5:B:202:HOH:O	2.07	0.54
2:B:130:TRP:CZ3	2:B:133:LEU:HD23	2.43	0.54
1:A:28:THR:HG21	1:A:105:PHE:HD1	1.74	0.53
1:A:47:ASP:N	1:A:54:GLN:OE1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD12	1:A:101:LEU:C	2.35	0.52
1:A:51:GLY:O	1:A:52:SER:C	2.50	0.51
2:B:3:TRP:CH2	2:B:132:LYS:HD2	2.45	0.51
2:B:93:CYS:SG	2:B:145:TYR:CD2	3.03	0.51
1:A:110:ALA:HB1	2:B:116:ALA:HB2	1.95	0.49
1:A:17:ILE:CD1	1:A:105:PHE:HZ	2.26	0.49
1:A:3:SER:O	1:A:6:ASP:HB2	2.13	0.49
2:B:90:GLU:O	2:B:94:ASP:HB2	2.13	0.48
1:A:61:LYS:HE3	3:A:150:HEM:O2A	2.12	0.48
1:A:88:ALA:O	1:A:140:TYR:CE1	2.67	0.48
2:B:17:LYS:HB3	2:B:118:PHE:CE1	2.49	0.48
2:B:29:ALA:HB1	2:B:55:LEU:HD13	1.95	0.48
2:B:76:LYS:N	2:B:76:LYS:HD2	2.20	0.47
1:A:92:ARG:C	1:A:140:TYR:OH	2.57	0.47
2:B:17:LYS:HB3	2:B:118:PHE:HE1	1.80	0.46
2:B:50:SER:O	2:B:54:ILE:N	2.44	0.46
1:A:14:PHE:CE2	1:A:17:ILE:HD11	2.50	0.46
2:B:57:ASN:HA	2:B:58:PRO:HD3	1.75	0.46
2:B:144:LYS:C	2:B:146:HIS:H	2.25	0.45
1:A:20:HIS:HB3	1:A:23:GLU:HG2	1.99	0.45
2:B:81:ILE:HD12	2:B:136:VAL:CG2	2.47	0.45
2:B:12:THR:CG2	5:B:202:HOH:O	2.63	0.44
2:B:51:PRO:O	2:B:55:LEU:HD22	2.18	0.43
1:A:2:LEU:HD12	1:A:2:LEU:N	2.33	0.43
1:A:43:PHE:N	1:A:44:PRO:CD	2.81	0.43
3:B:150:HEM:HMC2	3:B:150:HEM:CBC	2.47	0.43
2:B:143:ARG:C	2:B:145:TYR:H	2.26	0.43
2:B:91:LEU:C	2:B:96:LEU:HD22	2.43	0.43
1:A:98:PHE:CE1	1:A:137:THR:HG22	2.54	0.42
1:A:133:GLY:O	1:A:137:THR:HG23	2.19	0.42
2:B:92:HIS:HA	2:B:96:LEU:CD2	2.46	0.42
2:B:114:LEU:HD22	2:B:118:PHE:HE2	1.83	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.87	0.42
1:A:17:ILE:HB	1:A:24:TYR:HD2	1.85	0.41
1:A:51:GLY:C	1:A:52:SER:O	2.62	0.41
1:A:38:GLN:H	1:A:38:GLN:HE21	1.68	0.41
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.67	0.41
1:A:1:VAL:O	1:A:2:LEU:C	2.64	0.41
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.86	0.41
1:A:24:TYR:O	1:A:28:THR:HG23	2.20	0.40
1:A:35:ALA:HB1	2:B:131:GLN:HG3	2.03	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	140/141 (99%)	134 (96%)	5 (4%)	1 (1%)	18	14
2	B	146/146 (100%)	141 (97%)	5 (3%)	0	100	100
All	All	286/287 (100%)	275 (96%)	10 (4%)	1 (0%)	30	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU

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	115/114 (101%)	89 (77%)	26 (23%)	1	0
2	B	123/121 (102%)	103 (84%)	20 (16%)	2	1
All	All	238/235 (101%)	192 (81%)	46 (19%)	1	1

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	7	LYS

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Mol	Chain	Res	Type
1	A	18	SER
1	A	20	HIS
1	A	23	GLU
1	A	28	THR
1	A	30	GLU
1	A	38	GLN
1	A	41	THR
1	A	48	LEU
1	A	50	HIS
1	A	60	LYS
1	A	61	LYS
1	A	63	VAL
1	A	82	LYS
1	A	84	SER
1	A	85	ASP
1	A	89	GLN
1	A	90	LYS
1	A	92	ARG
1	A	99	LYS
1	A	101	LEU
1	A	109	VAL
1	A	111	ILE
1	A	120	GLU
1	A	141	ARG
2	B	6	GLU
2	B	9	GLN
2	B	12	THR
2	B	14	LEU
2	B	17	LYS
2	B	20	VAL
2	B	52	THR
2	B	54	ILE
2	B	55	LEU
2	B	57	ASN
2	B	65	LYS
2	B	70	SER
2	B	76	LYS
2	B	95	LYS
2	B	96	LEU
2	B	134	VAL
2	B	135	ARG
2	B	136	VAL

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Mol	Chain	Res	Type
2	B	143	ARG
2	B	144	LYS

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

Mol	Chain	Res	Type
1	A	9	ASN
1	A	20	HIS
1	A	38	GLN
1	A	97	ASN
2	B	39	GLN
2	B	57	ASN
2	B	83	ASN
2	B	102	ASN
2	B	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	A	150	1,4	50,50,50	1.43	8 (16%)	67,82,82	1.75	18 (26%)
3	HEM	B	150	2,4	50,50,50	1.48	9 (18%)	67,82,82	1.50	9 (13%)
4	OXY	B	151	3	1,1,1	0.03	0	-		
4	OXY	A	151	3	1,1,1	0.10	0	-		

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	150	1,4	-	0/14/54/54	-
3	HEM	B	150	2,4	-	2/14/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	150	HEM	FE-NB	3.63	2.06	1.94
3	B	150	HEM	CAB-C3B	3.27	1.56	1.47
3	A	150	HEM	FE-NC	3.12	2.05	1.95
3	A	150	HEM	CAC-C3C	2.94	1.55	1.47
3	A	150	HEM	CAB-C3B	2.89	1.55	1.47
3	A	150	HEM	FE-ND	2.88	2.03	1.94
3	B	150	HEM	C2A-C3A	-2.74	1.31	1.38
3	B	150	HEM	C3D-C2D	-2.67	1.31	1.36
3	B	150	HEM	CMA-C3A	2.49	1.55	1.50
3	B	150	HEM	FE-NB	2.37	2.02	1.94
3	B	150	HEM	CAC-C3C	2.28	1.53	1.47
3	A	150	HEM	C2A-C3A	-2.28	1.33	1.38
3	A	150	HEM	CMB-C2B	2.26	1.55	1.50
3	B	150	HEM	O1D-CGD	2.18	1.29	1.22
3	A	150	HEM	CAD-C3D	2.16	1.56	1.51
3	B	150	HEM	CHD-C4C	2.14	1.42	1.38
3	B	150	HEM	CMC-C2C	2.01	1.54	1.50

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	150	HEM	CMB-C2B-C1B	-4.66	117.75	125.03
3	B	150	HEM	O2A-CGA-O1A	4.50	134.90	123.33
3	B	150	HEM	C3B-C2B-C1B	3.79	109.26	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	150	HEM	CHA-C4D-ND	-3.78	119.69	124.37
3	A	150	HEM	CHD-C4C-NC	3.66	128.44	124.45
3	A	150	HEM	CHA-C4D-C3D	3.60	131.87	125.23
3	B	150	HEM	O1A-CGA-CBA	-3.59	111.72	123.09
3	A	150	HEM	O1D-CGD-CBD	-3.55	111.82	123.09
3	B	150	HEM	CBA-CAA-C2A	2.91	120.59	112.53
3	A	150	HEM	C3B-C2B-C1B	2.87	108.56	106.41
3	B	150	HEM	CHB-C1B-NB	2.75	127.76	124.37
3	B	150	HEM	CMB-C2B-C1B	-2.75	120.74	125.03
3	A	150	HEM	O2A-CGA-O1A	2.73	130.36	123.33
3	A	150	HEM	CHA-C1A-C2A	2.58	130.95	125.30
3	B	150	HEM	O1D-CGD-CBD	-2.50	115.15	123.09
3	A	150	HEM	CMA-C3A-C4A	-2.50	121.61	125.42
3	A	150	HEM	C1A-CHA-C4D	2.37	131.82	126.25
3	A	150	HEM	C4A-CHB-C1B	-2.34	120.74	126.25
3	A	150	HEM	CMA-C3A-C2A	2.23	130.35	125.62
3	A	150	HEM	O1A-CGA-CBA	-2.23	116.03	123.09
3	A	150	HEM	C4C-C3C-C2C	2.18	108.71	106.81
3	A	150	HEM	CMB-C2B-C3B	2.15	133.62	128.43
3	A	150	HEM	CAC-C3C-C4C	-2.14	119.72	124.82
3	B	150	HEM	CAD-CBD-CGD	-2.10	108.10	113.67
3	A	150	HEM	C4D-C3D-C2D	2.09	109.94	106.89
3	A	150	HEM	O2D-CGD-CBD	2.06	120.52	114.00
3	B	150	HEM	CMC-C2C-C1C	2.06	128.36	124.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	150	HEM	C2B-C3B-CAB-CBB
3	B	150	HEM	C4B-C3B-CAB-CBB

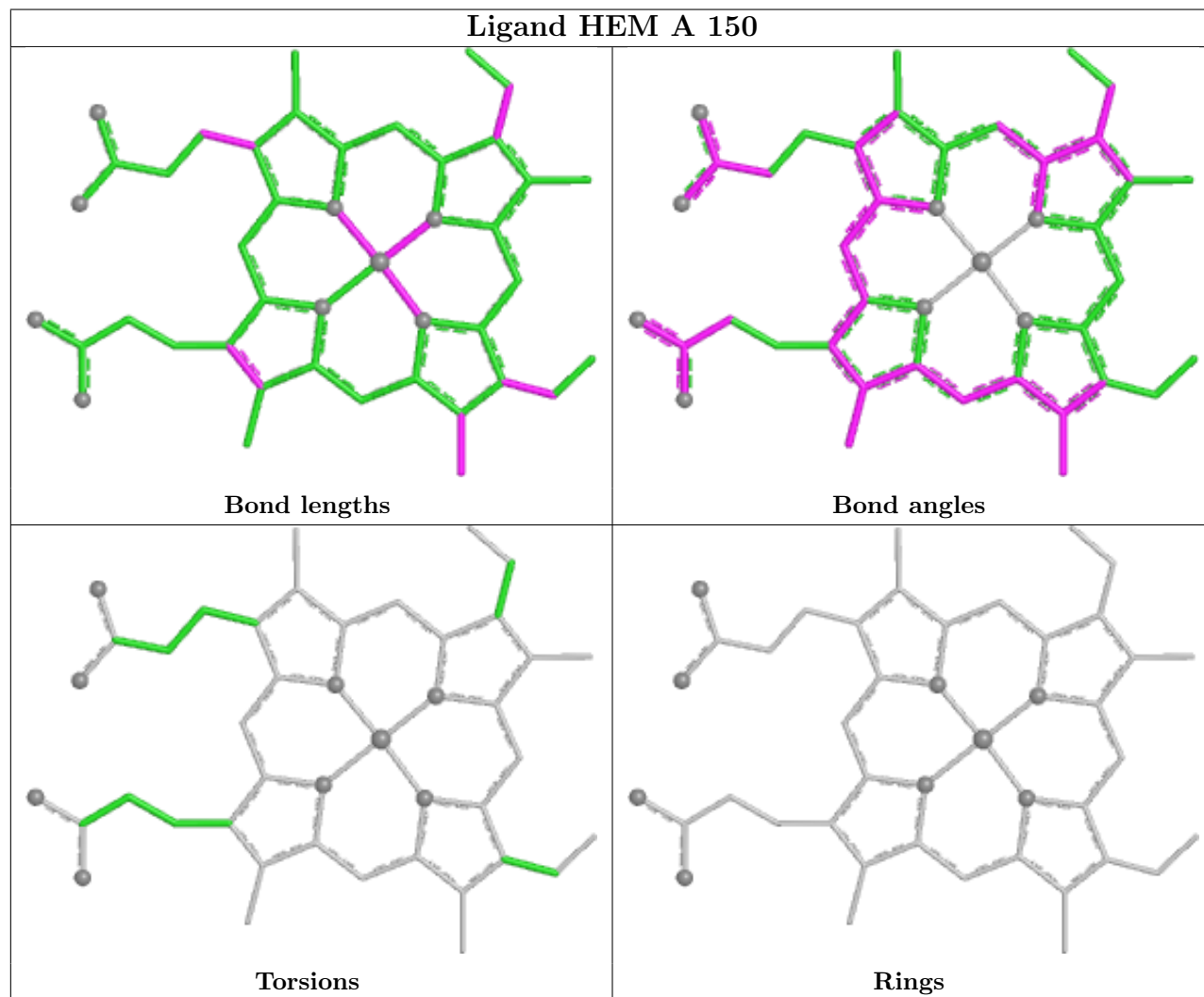
There are no ring outliers.

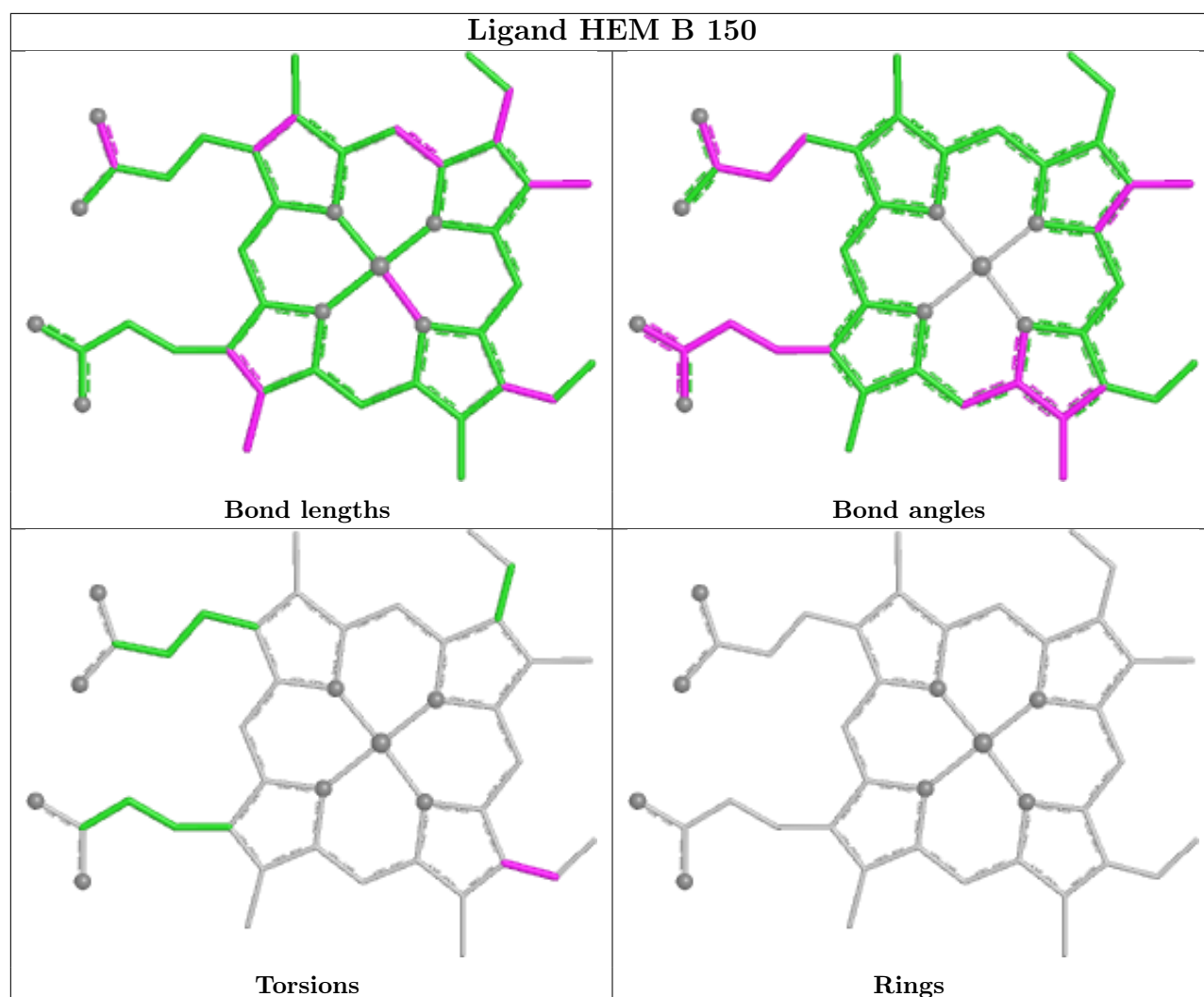
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	150	HEM	1	0
3	B	150	HEM	6	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.