



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:31 AM UTC

PDB ID : 1HDB / pdb_00001hdb
Title : ANALYSIS OF THE CRYSTAL STRUCTURE, MOLECULAR MODELING AND INFRARED SPECTROSCOPY OF THE DISTAL BETA-HEME POCKET VALINE67(E11)-THREONINE MUTATION OF HEMOGLOBIN
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Deposited on : 1995-04-14
Resolution : 2.20 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

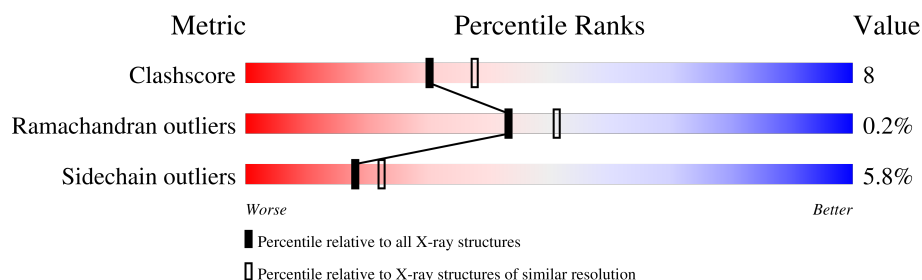
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	 66% 29% . .
1	C	141	 65% 26% 7% .
2	B	146	 60% 34% 7%
2	D	146	 63% 32% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5000 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) BETA-V67T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN (DEOXY) BETA-V67T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	723	195	202	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	723	195	202	3			

There are 2 discrepancies between the modelled and reference sequences:

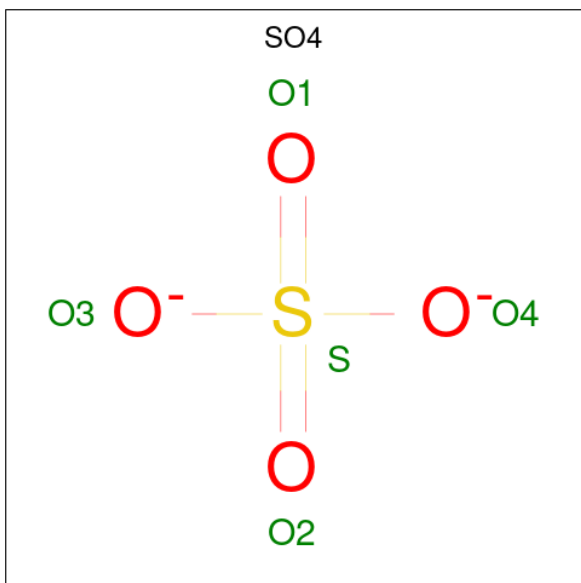
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	THR	VAL	engineered mutation	UNP P02023
D	67	THR	VAL	engineered mutation	UNP P02023

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

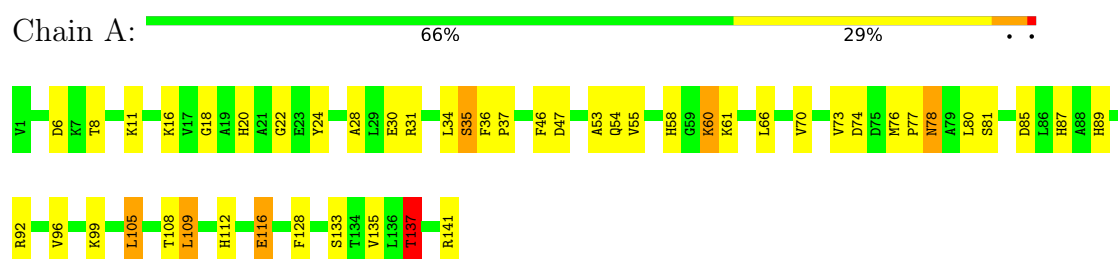
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	112	Total	O	0	0
			112	112		
5	C	120	Total	O	0	0
			120	120		
5	D	92	Total	O	0	0
			92	92		

3 Residue-property plots [i](#)

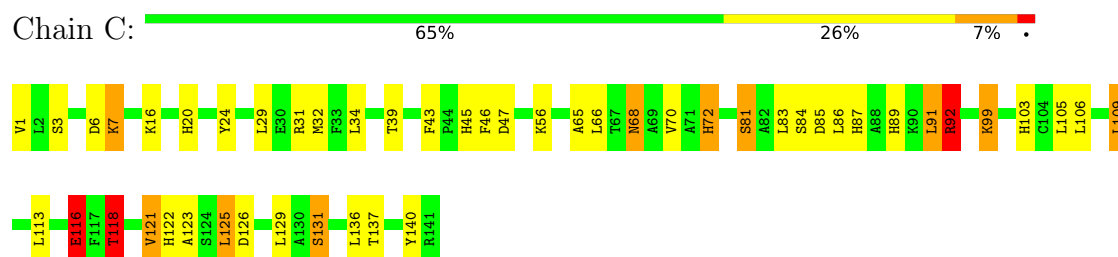
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

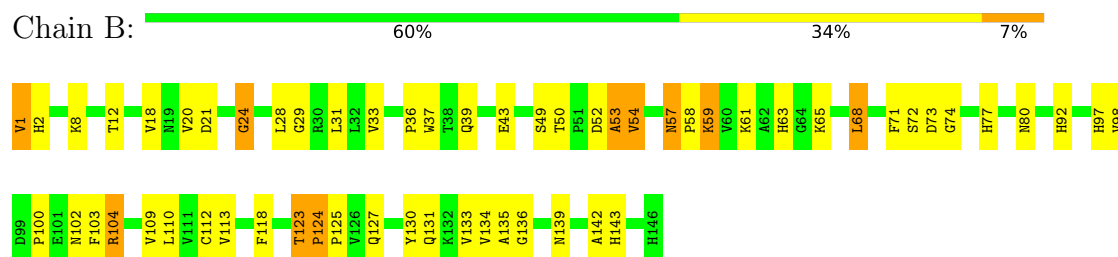
• Molecule 1: HEMOGLOBIN (DEOXY) BETA-V67T



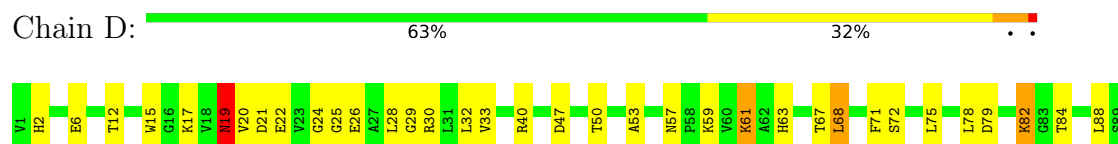
• Molecule 1: HEMOGLOBIN (DEOXY) BETA-V67T



• Molecule 2: HEMOGLOBIN (DEOXY) BETA-V67T



• Molecule 2: HEMOGLOBIN (DEOXY) BETA-V67T





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.54Å 83.19Å 54.02Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5000	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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, SO4

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	1.29	0/1097	2.18	40/1491 (2.7%)
1	C	1.35	2/1097 (0.2%)	2.10	39/1491 (2.6%)
2	B	1.31	2/1153 (0.2%)	2.18	55/1566 (3.5%)
2	D	1.28	2/1153 (0.2%)	2.20	51/1566 (3.3%)
All	All	1.31	6/4500 (0.1%)	2.17	185/6114 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	SER	N-CA	6.07	1.53	1.46
2	B	123	THR	CA-CB	5.62	1.60	1.53
1	C	103	HIS	ND1-CE1	5.57	1.38	1.32
2	D	123	THR	CA-CB	5.15	1.60	1.53
2	D	67	THR	CA-CB	5.11	1.61	1.53
2	B	98	VAL	N-CA	5.07	1.52	1.46

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CA-CB-CG	21.14	134.94	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	HIS	CA-CB-CG	-11.29	102.51	113.80
2	D	2	HIS	CA-CB-CG	-10.39	103.41	113.80
1	C	46	PHE	CA-CB-CG	9.89	123.69	113.80
1	A	31	ARG	CD-NE-CZ	9.21	137.29	124.40
2	B	102	ASN	CA-C-N	8.71	131.95	120.28
2	B	102	ASN	C-N-CA	8.71	131.95	120.28
2	D	24	GLY	CA-C-N	8.47	129.38	119.98
2	D	24	GLY	C-N-CA	8.47	129.38	119.98
2	B	135	ALA	O-C-N	8.34	130.96	122.12
1	C	72	HIS	CA-CB-CG	-8.29	105.51	113.80
1	C	118	THR	N-CA-CB	-8.26	98.15	110.05
1	C	89	HIS	CA-CB-CG	-8.13	105.67	113.80
1	A	47	ASP	N-CA-C	-8.13	95.33	108.41
2	D	72	SER	O-C-N	7.88	130.47	122.12
2	D	103	PHE	O-C-N	7.86	130.46	122.12
1	A	6	ASP	O-C-N	7.83	130.13	122.07
1	A	78	ASN	CA-CB-CG	-7.80	104.80	112.60
2	D	15	TRP	CA-C-N	7.79	128.75	120.03
2	D	15	TRP	C-N-CA	7.79	128.75	120.03
2	B	24	GLY	CA-C-N	7.72	128.55	119.98
2	B	24	GLY	C-N-CA	7.72	128.55	119.98
1	A	6	ASP	CA-C-O	-7.57	112.87	120.82
1	C	24	TYR	CA-C-N	7.41	128.16	119.94
1	C	24	TYR	C-N-CA	7.41	128.16	119.94
2	B	127	GLN	CA-C-N	7.38	130.50	120.54
2	B	127	GLN	C-N-CA	7.38	130.50	120.54
2	B	124	PRO	CB-CA-C	7.26	119.78	110.92
1	A	22	GLY	CA-C-O	-7.10	113.33	121.00
2	D	88	LEU	CA-C-O	-7.07	113.05	120.55
1	C	29	LEU	O-C-N	6.96	129.49	122.12
2	D	28	LEU	CA-C-O	-6.89	113.58	120.82
1	C	68	ASN	CA-C-O	-6.87	113.27	120.55
2	D	96	LEU	CA-C-O	-6.80	111.72	119.41
1	C	84	SER	CA-C-O	-6.76	113.25	120.42
1	C	68	ASN	O-C-N	6.72	129.24	122.12
1	C	65	ALA	CA-C-N	6.63	129.71	120.29
1	C	65	ALA	C-N-CA	6.63	129.71	120.29
1	A	87	HIS	CA-CB-CG	6.62	120.42	113.80
1	C	56	LYS	CA-C-N	6.59	127.26	119.94
1	C	56	LYS	C-N-CA	6.59	127.26	119.94
1	C	68	ASN	OD1-CG-ND2	-6.50	116.10	122.60
2	D	12	THR	CA-CB-OG1	-6.46	99.91	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	VAL	N-CA-C	6.44	117.39	108.89
2	B	31	LEU	O-C-N	6.42	128.69	122.07
1	C	85	ASP	N-CA-CB	6.42	119.56	110.12
2	D	30	ARG	NE-CZ-NH2	-6.42	113.42	119.20
2	B	73	ASP	CA-CB-CG	6.39	119.00	112.60
2	D	26	GLU	CB-CA-C	-6.32	100.92	110.90
1	A	54	GLN	CA-C-O	-6.29	114.17	120.90
1	C	7	LYS	CA-C-N	6.27	128.96	120.44
1	C	7	LYS	C-N-CA	6.27	128.96	120.44
2	B	77	HIS	CA-CB-CG	-6.26	107.54	113.80
1	C	81	SER	N-CA-C	6.26	121.69	111.37
1	C	92	ARG	NE-CZ-NH2	-6.21	113.61	119.20
2	B	97	HIS	CA-C-N	-6.20	114.96	122.90
2	B	97	HIS	C-N-CA	-6.20	114.96	122.90
2	B	103	PHE	N-CA-CB	6.20	119.24	110.12
2	B	57	ASN	OD1-CG-ND2	6.15	128.75	122.60
2	B	52	ASP	CA-CB-CG	6.14	118.75	112.60
1	C	91	LEU	O-C-N	6.13	128.71	122.09
2	B	52	ASP	CA-C-O	-6.12	113.94	120.42
1	C	125	LEU	CA-C-O	6.11	127.02	120.55
1	C	31	ARG	CD-NE-CZ	6.09	132.93	124.40
2	D	82	LYS	CA-C-N	6.09	126.74	119.98
2	D	82	LYS	C-N-CA	6.09	126.74	119.98
1	A	35	SER	CA-C-N	6.04	131.26	122.98
1	A	35	SER	C-N-CA	6.04	131.26	122.98
2	D	15	TRP	CB-CA-C	6.03	120.81	110.79
2	D	139	ASN	OD1-CG-ND2	-6.02	116.58	122.60
2	B	63	HIS	CA-C-N	6.00	126.60	119.94
2	B	63	HIS	C-N-CA	6.00	126.60	119.94
1	C	123	ALA	CA-C-O	-6.00	114.53	120.70
1	A	58	HIS	CA-CB-CG	-5.99	107.81	113.80
2	B	133	VAL	N-CA-CB	5.96	116.88	110.62
1	C	126	ASP	CB-CA-C	5.95	120.96	110.85
2	B	74	GLY	CA-C-O	5.94	126.46	119.45
2	B	133	VAL	CA-C-O	-5.93	115.24	121.41
2	D	57	ASN	CA-C-N	5.92	125.46	119.19
2	D	57	ASN	C-N-CA	5.92	125.46	119.19
2	D	72	SER	N-CA-CB	5.90	118.80	110.12
2	B	104	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	24	TYR	CA-C-N	5.87	127.48	120.14
1	A	24	TYR	C-N-CA	5.87	127.48	120.14
2	D	124	PRO	CB-CA-C	5.85	118.06	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	VAL	N-CA-C	-5.83	104.83	110.72
2	D	131	GLN	CB-CG-CD	5.83	122.51	112.60
1	A	96	VAL	CA-C-N	5.82	129.16	120.31
1	A	96	VAL	C-N-CA	5.82	129.16	120.31
1	C	116	GLU	CA-C-O	-5.80	112.11	119.31
2	B	112	CYS	CA-C-O	-5.80	114.41	120.55
2	D	61	LYS	CA-C-O	-5.80	114.92	121.00
1	A	135	VAL	CA-C-O	-5.79	115.09	121.29
2	D	127	GLN	OE1-CD-NE2	-5.77	116.83	122.60
2	B	54	VAL	O-C-N	5.74	128.16	121.96
1	C	136	LEU	N-CA-C	5.74	119.38	112.38
2	D	94	ASP	N-CA-CB	5.74	118.65	110.16
2	D	106	LEU	CA-C-N	5.73	126.30	119.94
2	D	106	LEU	C-N-CA	5.73	126.30	119.94
1	A	47	ASP	CA-C-O	-5.73	114.45	120.58
2	B	63	HIS	N-CA-CB	5.72	118.63	110.16
1	A	11	LYS	CA-C-N	5.71	128.20	120.44
1	A	11	LYS	C-N-CA	5.71	128.20	120.44
2	B	104	ARG	CD-NE-CZ	-5.70	116.42	124.40
1	A	116	GLU	CG-CD-OE1	5.68	131.45	118.40
1	C	99	LYS	O-C-N	5.66	128.60	122.15
2	D	143	HIS	CA-C-O	-5.66	114.84	120.90
2	D	127	GLN	O-C-N	5.65	127.90	122.03
2	B	134	VAL	CA-C-O	-5.64	115.08	120.95
1	A	37	PRO	N-CA-C	5.64	120.91	113.86
2	B	110	LEU	CA-C-O	-5.64	114.90	120.82
1	C	81	SER	CA-CB-OG	-5.63	99.83	111.10
2	D	111	VAL	O-C-N	5.63	127.43	121.91
1	C	3	SER	CA-C-N	5.62	125.29	119.05
1	C	3	SER	C-N-CA	5.62	125.29	119.05
1	A	112	HIS	CA-CB-CG	-5.62	108.18	113.80
1	A	112	HIS	CA-C-O	-5.61	112.97	118.97
1	C	34	LEU	CA-C-O	-5.56	114.07	120.24
2	D	67	THR	CA-CB-OG1	-5.55	101.27	109.60
2	B	92	HIS	O-C-N	5.54	128.47	122.15
2	D	115	ALA	CA-C-N	5.54	127.70	120.28
2	D	115	ALA	C-N-CA	5.54	127.70	120.28
2	D	102	ASN	CA-C-N	5.52	127.68	120.28
2	D	102	ASN	C-N-CA	5.52	127.68	120.28
1	A	108	THR	CA-C-O	5.51	126.78	121.00
1	A	135	VAL	CB-CA-C	5.50	118.68	111.81
2	D	132	LYS	N-CA-CB	5.49	118.29	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ALA	CA-C-N	5.48	127.93	120.54
1	A	53	ALA	C-N-CA	5.48	127.93	120.54
2	B	118	PHE	CA-CB-CG	-5.47	108.33	113.80
2	B	110	LEU	O-C-N	5.47	127.70	122.07
2	B	28	LEU	CA-C-N	5.47	126.05	119.98
2	B	28	LEU	C-N-CA	5.47	126.05	119.98
1	C	47	ASP	N-CA-C	-5.46	100.27	108.96
1	A	74	ASP	N-CA-C	-5.46	106.39	113.16
2	D	97	HIS	CA-CB-CG	-5.44	108.36	113.80
2	B	136	GLY	CA-C-N	5.42	127.89	120.46
2	B	136	GLY	C-N-CA	5.42	127.89	120.46
1	C	125	LEU	O-C-N	-5.41	116.38	122.12
1	C	109	LEU	N-CA-CB	5.40	117.90	110.07
2	D	103	PHE	N-CA-CB	5.40	118.05	110.12
2	D	40	ARG	CD-NE-CZ	5.38	131.93	124.40
2	B	130	TYR	N-CA-CB	5.38	118.50	110.22
2	B	97	HIS	CA-CB-CG	-5.37	108.43	113.80
2	D	63	HIS	CA-CB-CG	-5.37	108.43	113.80
2	D	47	ASP	O-C-N	5.37	129.80	122.82
1	A	137	THR	CA-CB-CG2	5.34	119.58	110.50
1	A	20	HIS	CA-CB-CG	-5.34	108.46	113.80
2	B	53	ALA	CA-C-N	5.33	127.75	120.77
2	B	53	ALA	C-N-CA	5.33	127.75	120.77
2	D	90	GLU	CA-C-O	-5.33	114.90	120.55
2	B	72	SER	CB-CA-C	5.33	119.33	110.81
2	B	112	CYS	N-CA-CB	5.32	117.95	110.12
1	A	141	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	B	71	PHE	CA-C-N	5.32	127.72	120.54
2	B	71	PHE	C-N-CA	5.32	127.72	120.54
1	A	55	VAL	N-CA-C	5.30	115.51	110.42
2	D	22	GLU	N-CA-C	5.30	119.84	112.90
2	D	84	THR	N-CA-C	5.29	117.12	111.36
2	B	49	SER	N-CA-C	5.28	117.03	111.28
1	C	6	ASP	O-C-N	5.28	127.79	122.09
1	A	128	PHE	CB-CA-C	5.26	119.21	110.90
2	B	130	TYR	CA-C-N	5.22	127.80	120.28
2	B	130	TYR	C-N-CA	5.22	127.80	120.28
2	D	61	LYS	CB-CA-C	-5.22	102.92	110.96
2	B	49	SER	CA-C-O	-5.22	115.02	120.55
1	A	108	THR	CA-C-N	5.21	127.52	120.38
1	A	108	THR	C-N-CA	5.21	127.52	120.38
2	D	19	ASN	OD1-CG-ND2	-5.21	117.39	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	HIS	N-CA-CB	5.20	118.34	110.28
1	C	20	HIS	CA-CB-CG	-5.19	108.61	113.80
2	B	134	VAL	N-CA-CB	5.18	117.58	110.54
2	D	99	ASP	O-C-N	5.17	125.62	121.38
2	D	25	GLY	CA-C-N	5.14	127.43	120.44
2	D	25	GLY	C-N-CA	5.14	127.43	120.44
2	D	143	HIS	CA-CB-CG	-5.12	108.68	113.80
1	A	30	GLU	CA-CB-CG	5.11	124.33	114.10
1	C	122	HIS	CA-CB-CG	5.09	118.89	113.80
2	B	20	VAL	N-CA-C	5.08	115.70	110.36
2	D	127	GLN	N-CA-CB	5.08	117.32	109.91
2	B	43	GLU	CG-CD-OE1	5.07	130.07	118.40
1	A	8	THR	CA-CB-CG2	5.07	119.12	110.50
2	B	80	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	85	ASP	CA-C-O	-5.02	115.23	120.55
2	B	54	VAL	CA-C-O	-5.02	116.19	121.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	PHE	Mainchain
1	A	92	ARG	Sidechain
1	C	92	ARG	Sidechain

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	13	0
1	C	1069	0	1073	21	0
2	B	1123	0	1116	23	0
2	D	1123	0	1116	17	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	4	0
3	D	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	1	0
4	D	5	0	0	0	0
5	A	110	0	0	1	0
5	B	112	0	0	0	0
5	C	120	0	0	3	0
5	D	92	0	0	0	0
All	All	5000	0	4498	76	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 8.

All (76) 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:C:113:LEU:HB3	1:C:116:GLU:HG2	1.65	0.76
1:A:16:LYS:HG3	1:A:116:GLU:HG2	1.68	0.75
2:D:20:VAL:HG13	2:D:68:LEU:HB3	1.68	0.74
2:D:50:THR:HG23	2:D:53:ALA:H	1.54	0.73
2:D:50:THR:HG22	2:D:53:ALA:HB2	1.74	0.69
1:C:118:THR:HG22	1:C:121:VAL:H	1.59	0.67
2:B:37:TRP:HA	1:C:92:ARG:HD3	1.78	0.65
2:B:58:PRO:HA	2:B:61:LYS:HE3	1.80	0.63
1:A:60:LYS:HZ2	1:A:60:LYS:HB3	1.63	0.62
1:C:109:LEU:HD12	1:C:125:LEU:HD13	1.81	0.61
1:A:60:LYS:HB3	1:A:60:LYS:NZ	2.15	0.61
1:C:66:LEU:O	1:C:70:VAL:HG23	2.01	0.61
2:B:2:HIS:H	2:B:2:HIS:CD2	2.23	0.57
2:D:19:ASN:ND2	2:D:21:ASP:H	2.03	0.56
2:D:19:ASN:HD22	2:D:19:ASN:C	2.12	0.56
1:C:83:LEU:HD11	3:C:142:HEM:HMA1	1.88	0.56
1:C:118:THR:HG21	5:C:205:HOH:O	2.07	0.54
2:B:104:ARG:NH2	2:B:139:ASN:OD1	2.41	0.53
1:A:105:LEU:O	1:A:109:LEU:HD22	2.09	0.52
1:C:16:LYS:HG3	1:C:116:GLU:HG3	1.92	0.51
2:B:58:PRO:HA	2:B:61:LYS:CE	2.40	0.51
2:D:29:GLY:O	2:D:33:VAL:HG23	2.11	0.51
3:B:148:HEM:HMC2	3:B:148:HEM:HBC2	1.94	0.50
1:A:73:VAL:HG22	1:A:73:VAL:O	2.11	0.50
1:A:35:SER:HB3	2:B:131:GLN:HG3	1.95	0.49
2:D:19:ASN:ND2	2:D:19:ASN:C	2.70	0.49
2:B:29:GLY:O	2:B:33:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:CD1	1:C:125:LEU:HD13	2.42	0.48
3:C:142:HEM:HMC1	3:C:142:HEM:HBC2	1.96	0.48
2:B:57:ASN:O	2:B:61:LYS:HG3	2.14	0.48
1:A:16:LYS:HD3	5:A:170:HOH:O	2.14	0.48
2:B:8:LYS:O	2:B:12:THR:HG23	2.13	0.48
2:B:50:THR:O	2:B:54:VAL:HG23	2.14	0.48
1:C:16:LYS:NZ	1:C:116:GLU:OE1	2.39	0.46
1:A:76:MET:N	1:A:77:PRO:HD2	2.30	0.46
1:A:66:LEU:O	1:A:70:VAL:HG23	2.16	0.46
2:B:36:PRO:O	2:B:39:GLN:HG3	2.15	0.46
1:C:87:HIS:HA	1:C:91:LEU:HB2	1.98	0.46
2:B:58:PRO:HA	2:B:61:LYS:HZ2	1.80	0.46
2:D:82:LYS:HE3	2:D:143:HIS:CD2	2.51	0.45
1:C:45:HIS:ND1	1:C:45:HIS:N	2.59	0.45
2:B:109:VAL:O	2:B:113:VAL:HG23	2.16	0.45
1:C:86:LEU:HD21	3:C:142:HEM:HBA2	1.97	0.45
3:C:142:HEM:HBC2	3:C:142:HEM:CMC	2.46	0.45
1:C:106:LEU:CD1	1:C:129:LEU:HD12	2.47	0.45
2:D:17:LYS:NZ	2:D:121:GLU:OE1	2.50	0.45
1:C:92:ARG:NE	5:C:218:HOH:O	2.42	0.44
2:B:50:THR:H	2:B:53:ALA:HB3	1.83	0.44
1:A:80:LEU:O	1:A:81:SER:C	2.61	0.44
2:B:123:THR:OG1	2:B:125:PRO:HD2	2.18	0.44
1:C:32:MET:HE3	1:C:39:THR:HB	1.99	0.44
1:A:16:LYS:HE2	1:A:116:GLU:CG	2.47	0.44
2:D:68:LEU:O	2:D:71:PHE:HB3	2.19	0.43
2:D:50:THR:CG2	2:D:53:ALA:HB2	2.47	0.43
2:D:123:THR:O	2:D:124:PRO:C	2.62	0.43
2:D:19:ASN:HD22	2:D:20:VAL:N	2.17	0.43
2:D:50:THR:HG23	2:D:53:ALA:N	2.30	0.42
2:B:1:VAL:N	4:B:147:SO4:O4	2.53	0.42
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.50	0.42
2:B:58:PRO:HA	2:B:61:LYS:NZ	2.34	0.42
1:C:43:PHE:HA	1:C:45:HIS:CE1	2.55	0.42
2:B:124:PRO:HD2	2:B:125:PRO:HD3	2.01	0.42
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.90	0.42
1:C:68:ASN:O	1:C:72:HIS:HD2	2.02	0.41
2:B:24:GLY:HA2	2:B:68:LEU:HG	2.02	0.41
2:B:58:PRO:CA	2:B:61:LYS:HE3	2.47	0.41
1:C:7:LYS:NZ	5:C:160:HOH:O	2.49	0.41
2:B:100:PRO:HB3	2:B:142:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:HA	1:C:140:TYR:CD1	2.56	0.41
1:A:133:SER:O	1:A:137:THR:HB	2.21	0.41
3:B:148:HEM:CMB	3:B:148:HEM:HBB2	2.50	0.41
2:D:19:ASN:ND2	2:D:21:ASP:OD1	2.45	0.41
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.83	0.41
2:B:21:ASP:OD2	2:B:65:LYS:HD2	2.20	0.41
2:B:57:ASN:OD1	2:B:59:LYS:HB2	2.20	0.41
2:D:50:THR:O	2:D:53:ALA:HB3	2.21	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%)	133 (96%)	5 (4%)	1 (1%)	18	19
1	C	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	566/574 (99%)	553 (98%)	12 (2%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY

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	113/113 (100%)	105 (93%)	8 (7%)	13	16
1	C	113/113 (100%)	106 (94%)	7 (6%)	16	20
2	B	118/118 (100%)	115 (98%)	3 (2%)	42	56
2	D	118/118 (100%)	109 (92%)	9 (8%)	12	14
All	All	462/462 (100%)	435 (94%)	27 (6%)	18	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	60	LYS
1	A	61	LYS
1	A	78	ASN
1	A	99	LYS
1	A	105	LEU
1	A	109	LEU
1	A	137	THR
2	B	1	VAL
2	B	59	LYS
2	B	68	LEU
1	C	1	VAL
1	C	81	SER
1	C	99	LYS
1	C	105	LEU
1	C	116	GLU
1	C	118	THR
1	C	131	SER
2	D	6	GLU
2	D	19	ASN
2	D	32	LEU
2	D	59	LYS
2	D	61	LYS
2	D	68	LEU
2	D	78	LEU
2	D	79	ASP
2	D	120	LYS

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

Mol	Chain	Res	Type
2	B	2	HIS
2	B	80	ASN
2	B	97	HIS
1	C	20	HIS
1	C	72	HIS
2	D	19	ASN
2	D	116	HIS
2	D	117	HIS
2	D	143	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](#)

6 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	$\# Z > 2$
4	SO4	D	147	-	4,4,4	1.33	1 (25%)	6,6,6	0.85	0
4	SO4	B	147	-	4,4,4	1.50	0	6,6,6	0.34	0
3	HEM	B	148	2	50,50,50	1.42	9 (18%)	67,82,82	1.12	4 (5%)
3	HEM	D	148	2	50,50,50	1.30	7 (14%)	67,82,82	1.34	10 (14%)
3	HEM	A	142	1	50,50,50	1.51	12 (24%)	67,82,82	1.17	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	C	142	1	50,50,50	1.47	11 (22%)	67,82,82	1.21	8 (11%)

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	-	2/14/54/54	-
3	HEM	C	142	1	-	4/14/54/54	-
3	HEM	D	148	2	-	2/14/54/54	-
3	HEM	B	148	2	-	3/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	148	HEM	FE-NB	3.79	2.06	1.94
3	A	142	HEM	FE-NA	3.57	2.07	1.95
3	A	142	HEM	FE-NC	3.46	2.06	1.95
3	A	142	HEM	CAC-C3C	3.41	1.56	1.47
3	D	148	HEM	FE-NB	3.05	2.04	1.94
3	B	148	HEM	CAB-C3B	3.04	1.55	1.47
3	B	148	HEM	FE-NA	3.02	2.05	1.95
3	C	142	HEM	CAB-C3B	2.99	1.55	1.47
3	B	148	HEM	FE-ND	2.94	2.04	1.94
3	D	148	HEM	O1A-CGA	2.87	1.31	1.22
3	A	142	HEM	CMB-C2B	2.85	1.56	1.50
3	C	142	HEM	FE-NA	2.78	2.04	1.95
3	C	142	HEM	CAC-C3C	2.75	1.54	1.47
3	B	148	HEM	C2A-C3A	-2.69	1.31	1.38
3	C	142	HEM	CMD-C2D	2.55	1.56	1.50
3	C	142	HEM	CMB-C2B	2.53	1.56	1.50
3	C	142	HEM	FE-NC	2.51	2.03	1.95
3	A	142	HEM	CMA-C3A	2.40	1.55	1.50
3	D	148	HEM	CAC-C3C	2.36	1.53	1.47
3	A	142	HEM	C2A-C3A	-2.33	1.32	1.38
3	A	142	HEM	CMD-C2D	2.29	1.55	1.50
3	B	148	HEM	CAC-C3C	2.25	1.53	1.47
3	C	142	HEM	C2A-C3A	-2.23	1.33	1.38
3	A	142	HEM	C4A-C3A	2.22	1.48	1.43
3	C	142	HEM	FE-ND	2.20	2.01	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CAB-C3B	2.20	1.53	1.47
3	A	142	HEM	FE-ND	2.18	2.01	1.94
3	B	148	HEM	CMA-C3A	2.18	1.55	1.50
3	C	142	HEM	CMA-C3A	2.16	1.55	1.50
3	C	142	HEM	CAA-C2A	2.09	1.56	1.51
3	A	142	HEM	CAD-C3D	2.09	1.56	1.51
3	A	142	HEM	FE-NB	2.07	2.01	1.94
3	C	142	HEM	FE-NB	2.07	2.01	1.94
3	D	148	HEM	CMB-C2B	2.06	1.55	1.50
3	B	148	HEM	C1B-NB	-2.05	1.36	1.40
3	D	148	HEM	FE-NC	2.03	2.01	1.95
3	B	148	HEM	CMB-C2B	2.02	1.54	1.50
3	D	148	HEM	CAB-C3B	2.01	1.52	1.47
3	D	148	HEM	CMC-C2C	2.01	1.54	1.50
4	D	147	SO4	O2-S	2.00	1.56	1.44

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	HEM	O2A-CGA-O1A	3.47	132.25	123.33
3	C	142	HEM	CHB-C1B-NB	3.19	128.31	124.37
3	A	142	HEM	O1D-CGD-CBD	-3.14	113.12	123.09
3	A	142	HEM	CHB-C1B-NB	3.02	128.10	124.37
3	A	142	HEM	CHD-C1D-ND	2.93	127.58	124.42
3	D	148	HEM	CHC-C1C-NC	2.90	127.61	124.45
3	D	148	HEM	C1C-CHC-C4B	-2.76	120.16	126.02
3	D	148	HEM	CHC-C4B-NB	2.72	127.34	124.42
3	C	142	HEM	CMA-C3A-C2A	2.71	131.38	125.62
3	D	148	HEM	O2D-CGD-CBD	2.69	122.49	114.00
3	D	148	HEM	CBA-CAA-C2A	2.60	119.71	112.53
3	B	148	HEM	O1D-CGD-CBD	-2.59	114.89	123.09
3	A	142	HEM	CHA-C4D-ND	2.57	127.54	124.37
3	D	148	HEM	CMA-C3A-C4A	-2.52	121.58	125.42
3	D	148	HEM	CMA-C3A-C2A	2.51	130.94	125.62
3	C	142	HEM	CMA-C3A-C4A	-2.41	121.75	125.42
3	C	142	HEM	CHD-C4C-NC	2.38	127.05	124.45
3	C	142	HEM	O1A-CGA-CBA	-2.36	115.60	123.09
3	B	148	HEM	C3B-C4B-NB	-2.33	107.80	109.47
3	D	148	HEM	O1A-CGA-CBA	-2.31	115.76	123.09
3	D	148	HEM	CHB-C1B-NB	2.22	127.11	124.37
3	C	142	HEM	O2A-CGA-CBA	2.16	120.83	114.00
3	B	148	HEM	CMA-C3A-C2A	2.13	130.14	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	C4C-CHD-C1D	-2.07	121.63	126.02
3	C	142	HEM	CAA-C2A-C1A	-2.04	120.95	124.94
3	C	142	HEM	O2D-CGD-CBD	2.00	120.33	114.00
3	B	148	HEM	C3D-C4D-ND	-2.00	107.97	110.17

There are no chirality outliers.

All (11) torsion outliers are listed below:

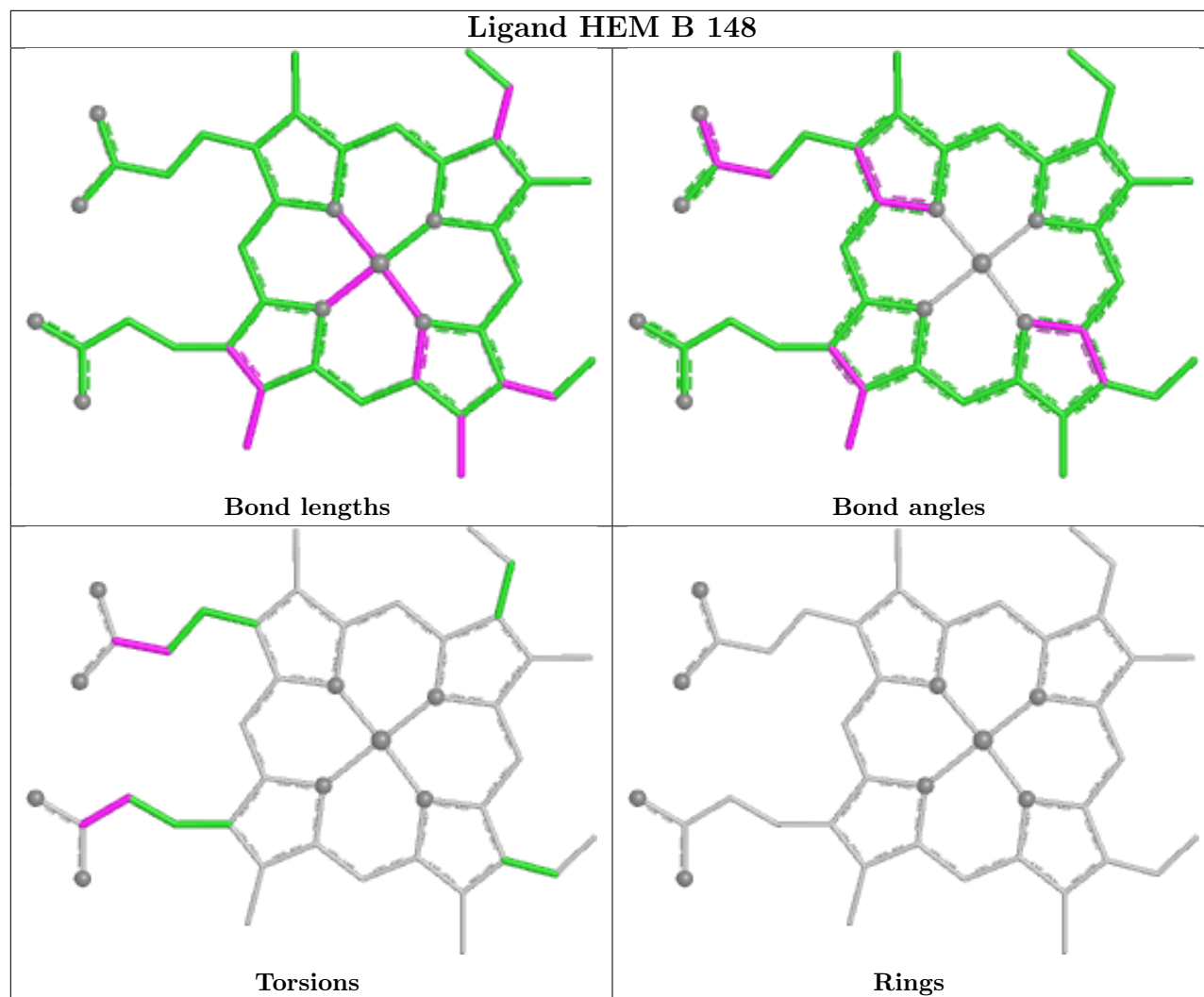
Mol	Chain	Res	Type	Atoms
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAD-CBD-CGD-O1D
3	D	148	HEM	CAD-CBD-CGD-O1D
3	D	148	HEM	CAD-CBD-CGD-O2D
3	B	148	HEM	CAD-CBD-CGD-O2D
3	B	148	HEM	CAA-CBA-CGA-O2A
3	B	148	HEM	CAA-CBA-CGA-O1A

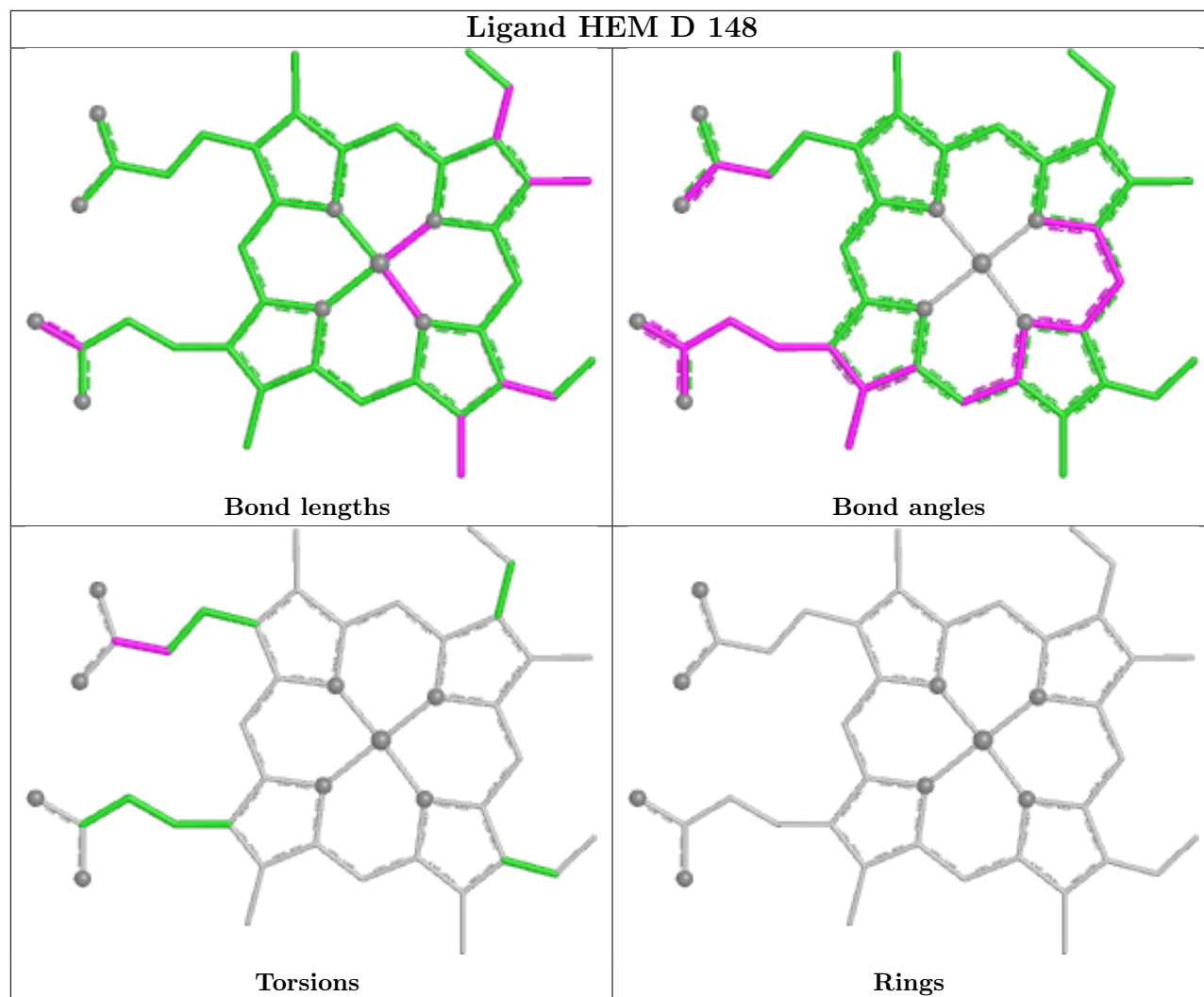
There are no ring outliers.

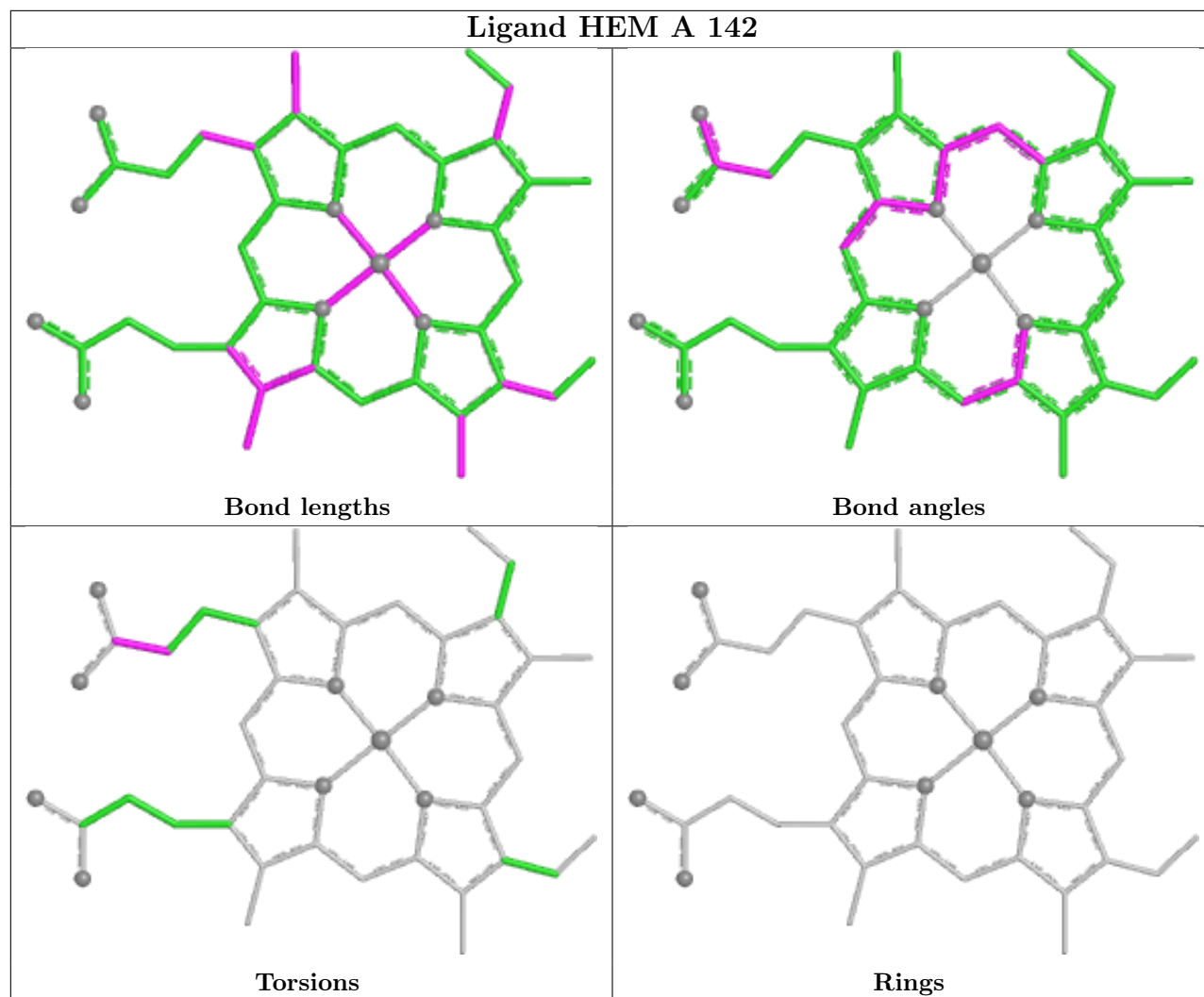
3 monomers are involved in 7 short contacts:

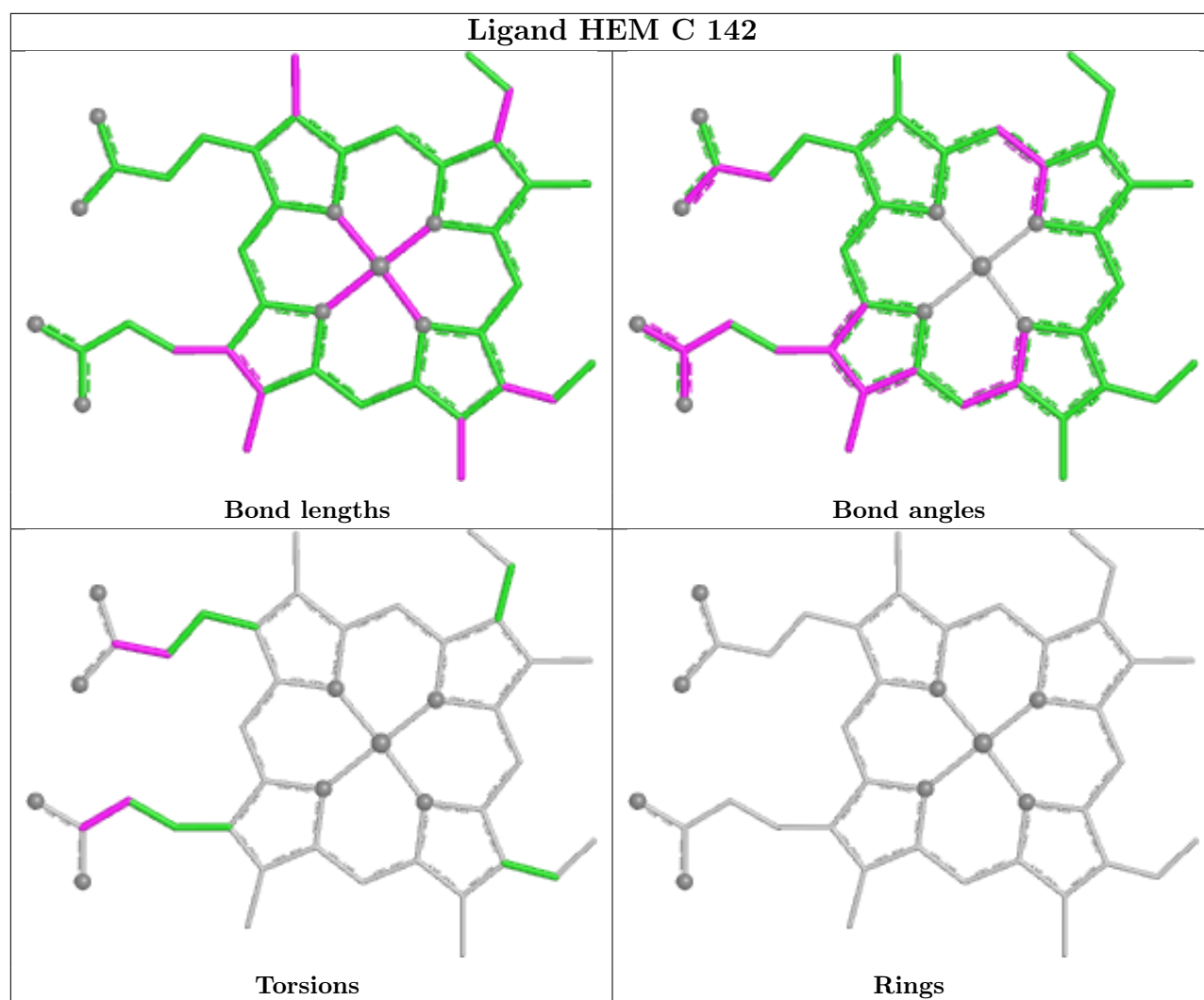
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	147	SO4	1	0
3	B	148	HEM	2	0
3	C	142	HEM	4	0

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.