



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 04:50 PM EDT

PDB ID : 1GBV / pdb_00001gbv
Title : (ALPHA-OXY, BETA-(C112G)DEOXY) T-STATE HUMAN
HEMOGLOBIN
Authors : Vasquez, G.B.; Ji, X.; Pechik, I.; Fronticelli, C.; Gilliland, G.L.
Deposited on : 1995-12-20
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) : 2.50

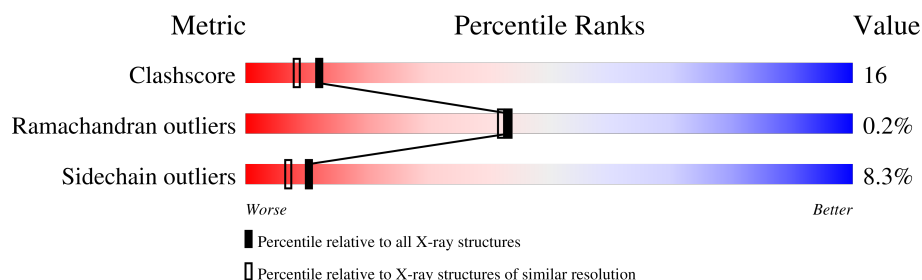
1 Overall quality at a glance

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	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4923 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.

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			

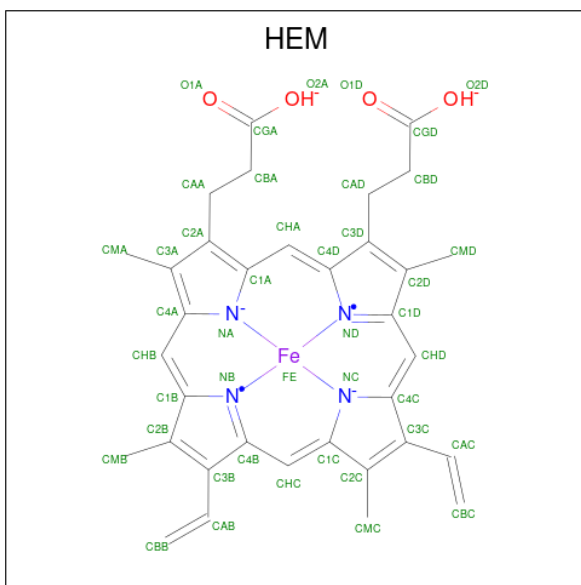
- Molecule 2 is a protein called HEMOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1121	723	195	201	2			
2	D	146	Total	C	N	O	S	0	0	0
			1121	723	195	201	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	GLY	CYS	engineered mutation	UNP P68871
D	112	GLY	CYS	engineered mutation	UNP P68871

- 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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



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

- Molecule 5 is water.

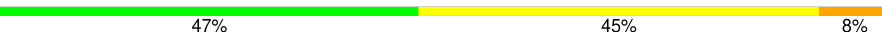
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	94	Total	O	0	0
			94	94		
5	C	95	Total	O	0	0
			95	95		
5	D	80	Total	O	0	0
			80	80		

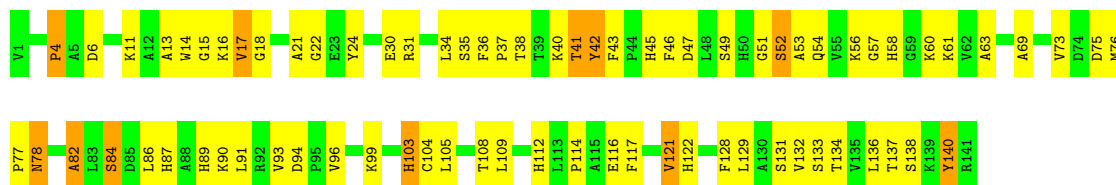
3 Residue-property plots

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.

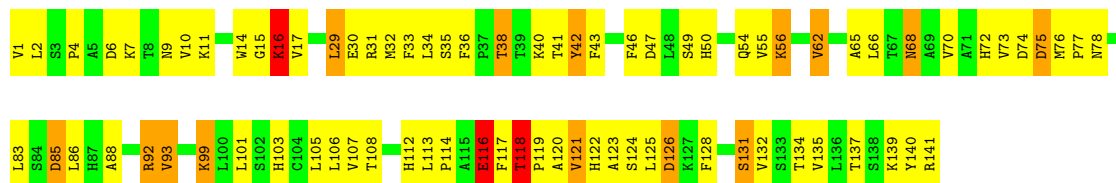
• Molecule 1: HEMOGLOBIN

Chain A: 



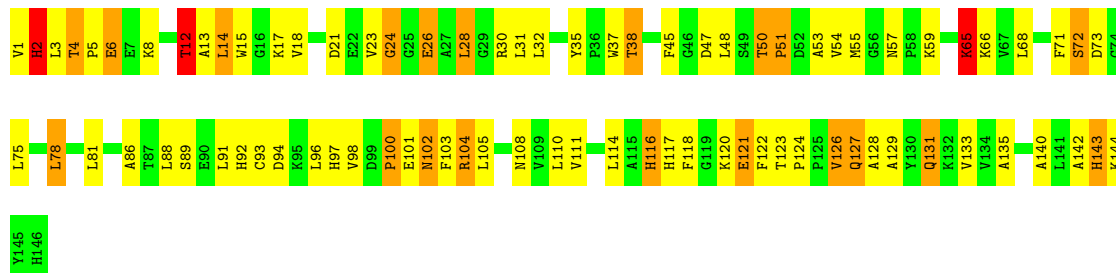
• Molecule 1: HEMOGLOBIN

Chain C: 

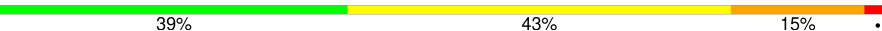


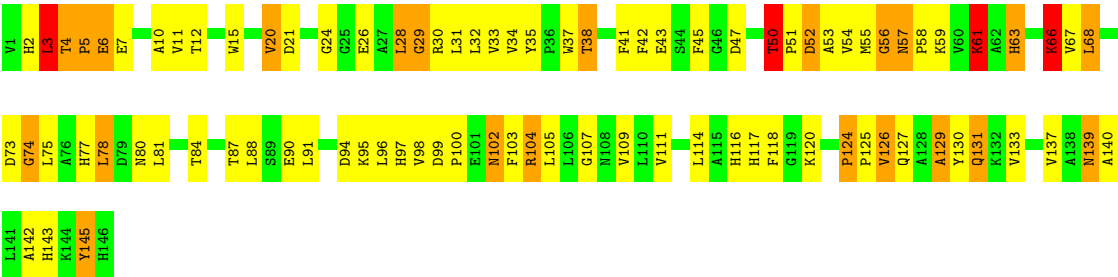
• Molecule 2: HEMOGLOBIN

Chain B: 



• Molecule 2: HEMOGLOBIN

Chain D: 



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	63.18Å 83.56Å 53.73Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	92.8 (6.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, GPRLSA	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4923	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.46	4/1097 (0.4%)	2.34	52/1491 (3.5%)
1	C	1.54	9/1097 (0.8%)	2.38	64/1491 (4.3%)
2	B	1.45	6/1151 (0.5%)	2.35	76/1563 (4.9%)
2	D	1.44	5/1151 (0.4%)	2.40	83/1563 (5.3%)
All	All	1.48	24/4496 (0.5%)	2.37	275/6108 (4.5%)

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	C	0	3
2	B	0	3
2	D	0	1
All	All	0	7

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	PHE	CA-C	7.30	1.62	1.52
1	C	31	ARG	N-CA	7.02	1.54	1.46
1	C	43	PHE	N-CA	6.81	1.54	1.46
2	D	127	GLN	C-O	6.05	1.31	1.24
1	C	40	LYS	N-CA	6.01	1.54	1.46
1	A	94	ASP	N-CA	6.00	1.54	1.46
1	C	108	THR	CA-CB	6.00	1.62	1.53
2	D	126	VAL	N-CA	5.94	1.53	1.46
1	C	55	VAL	N-CA	5.91	1.53	1.46
2	B	35	TYR	CA-C	5.90	1.59	1.52
2	B	98	VAL	N-CA	5.87	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	38	THR	CA-CB	5.73	1.62	1.53
2	D	111	VAL	N-CA	5.69	1.53	1.46
1	A	104	CYS	N-CA	5.67	1.53	1.46
2	D	130	TYR	N-CA	5.50	1.53	1.46
1	C	121	VAL	C-N	-5.41	1.26	1.33
2	B	100	PRO	C-N	-5.41	1.27	1.33
1	C	134	THR	CA-CB	5.21	1.61	1.53
1	C	35	SER	N-CA	5.19	1.52	1.46
2	B	110	LEU	CA-C	5.14	1.59	1.52
2	B	71	PHE	N-CA	5.08	1.52	1.46
1	A	38	THR	CA-CB	5.06	1.61	1.53
1	A	24	TYR	N-CA	5.05	1.52	1.46
2	D	30	ARG	N-CA	5.03	1.52	1.46

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	GLY	CA-C-N	11.50	132.47	119.94
2	D	24	GLY	C-N-CA	11.50	132.47	119.94
1	A	121	VAL	N-CA-C	-11.08	100.11	110.53
1	A	6	ASP	O-C-N	11.00	133.53	122.09
2	B	45	PHE	CA-CB-CG	11.00	124.80	113.80
2	D	57	ASN	CA-CB-CG	10.15	122.75	112.60
1	C	29	LEU	CA-C-O	9.72	130.86	120.55
1	C	126	ASP	CB-CA-C	9.38	126.36	110.79
1	C	42	TYR	CA-C-N	-9.25	112.85	122.28
1	C	42	TYR	C-N-CA	-9.25	112.85	122.28
2	D	124	PRO	CB-CA-C	9.24	122.20	110.92
1	A	6	ASP	CA-C-O	-9.12	111.14	120.90
1	A	47	ASP	CA-CB-CG	8.70	121.30	112.60
2	B	129	ALA	O-C-N	8.67	131.11	122.09
2	B	73	ASP	CA-CB-CG	8.64	121.24	112.60
2	D	139	ASN	CA-CB-CG	-8.45	104.15	112.60
2	D	103	PHE	CA-C-N	8.41	132.06	120.63
2	D	103	PHE	C-N-CA	8.41	132.06	120.63
1	C	105	LEU	CA-CB-CG	8.39	145.66	116.30
2	B	2	HIS	CA-CB-CG	-8.32	105.48	113.80
2	B	103	PHE	O-C-N	8.24	130.85	122.12
1	A	6	ASP	N-CA-CB	8.22	122.18	109.94
1	A	121	VAL	CB-CA-C	8.20	122.77	112.02
1	C	17	VAL	N-CA-C	-8.10	102.64	110.42
1	C	88	ALA	O-C-N	8.07	131.94	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	ASN	CA-CB-CG	8.07	120.67	112.60
1	C	85	ASP	CA-CB-CG	8.07	120.67	112.60
1	C	118	THR	CA-CB-CG2	7.97	124.05	110.50
2	B	124	PRO	CB-CA-C	7.92	120.58	110.92
2	B	126	VAL	CB-CA-C	7.84	122.29	112.02
2	D	63	HIS	CA-CB-CG	-7.84	105.96	113.80
2	B	30	ARG	CD-NE-CZ	7.74	135.24	124.40
2	B	35	TYR	O-C-N	7.71	128.38	121.36
1	A	122	HIS	CA-CB-CG	7.71	121.50	113.80
2	D	94	ASP	N-CA-C	7.60	120.45	111.71
1	C	47	ASP	N-CA-C	-7.51	97.01	108.96
1	A	96	VAL	CA-C-O	7.46	128.71	120.95
1	A	47	ASP	N-CA-C	-7.44	97.13	108.96
1	A	24	TYR	O-C-N	7.41	129.97	122.12
2	B	129	ALA	CA-C-O	-7.16	113.24	120.90
2	D	6	GLU	CB-CG-CD	7.15	124.75	112.60
1	C	112	HIS	CA-CB-CG	-7.12	106.68	113.80
2	D	50	THR	CB-CA-C	7.11	120.72	109.55
2	B	126	VAL	CA-C-N	7.07	130.06	120.38
2	B	126	VAL	C-N-CA	7.07	130.06	120.38
2	D	99	ASP	O-C-N	7.06	127.45	121.31
1	A	96	VAL	CA-CB-CG2	7.02	122.33	110.40
1	A	53	ALA	CA-C-O	6.98	128.00	119.97
1	A	54	GLN	O-C-N	6.97	129.25	122.07
1	A	116	GLU	CG-CD-OE1	6.95	134.40	118.40
2	D	105	LEU	N-CA-CB	6.95	120.48	110.06
1	A	17	VAL	N-CA-C	-6.83	103.86	110.42
2	B	24	GLY	CA-C-N	6.81	127.49	120.00
2	B	24	GLY	C-N-CA	6.81	127.49	120.00
1	C	46	PHE	O-C-N	6.79	130.91	123.10
2	B	32	LEU	O-C-N	6.79	130.62	122.27
2	D	61	LYS	N-CA-CB	6.79	120.05	109.94
1	A	47	ASP	O-C-N	6.77	130.92	123.13
2	D	57	ASN	CA-C-O	6.76	124.67	119.46
1	C	126	ASP	CA-CB-CG	6.75	119.36	112.60
2	D	142	ALA	CA-C-N	6.75	130.00	120.28
2	D	142	ALA	C-N-CA	6.75	130.00	120.28
1	C	55	VAL	CA-C-O	6.72	128.29	121.17
2	D	56	GLY	CA-C-N	6.70	130.58	121.20
2	D	56	GLY	C-N-CA	6.70	130.58	121.20
1	C	34	LEU	O-C-N	6.70	130.93	122.23
1	A	31	ARG	NE-CZ-NH2	6.60	125.14	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	ASN	CA-C-N	6.60	129.12	120.28
2	B	102	ASN	C-N-CA	6.60	129.12	120.28
1	A	108	THR	CA-C-O	-6.58	113.51	120.55
1	C	73	VAL	CA-C-O	-6.58	113.53	120.57
2	D	97	HIS	CA-CB-CG	-6.57	107.23	113.80
2	B	28	LEU	CB-CA-C	6.55	121.17	110.88
2	D	100	PRO	CB-CA-C	6.53	121.15	111.62
2	D	111	VAL	CB-CA-C	6.53	120.33	111.97
1	C	135	VAL	O-C-N	6.51	128.29	121.91
2	B	57	ASN	OD1-CG-ND2	6.47	129.07	122.60
2	B	30	ARG	NE-CZ-NH1	6.46	127.96	121.50
2	D	20	VAL	CB-CA-C	6.42	122.12	112.16
1	C	118	THR	N-CA-CB	-6.41	100.81	110.05
1	C	140	TYR	CA-C-O	-6.35	112.92	120.10
1	A	103	HIS	N-CA-CB	6.35	119.22	110.01
2	B	72	SER	CB-CA-C	6.34	121.31	110.79
1	C	131	SER	N-CA-CB	6.33	119.53	110.16
2	D	137	VAL	CA-C-O	-6.33	114.03	121.05
2	D	105	LEU	CA-C-O	-6.31	113.82	120.63
2	D	114	LEU	CA-C-N	6.29	128.62	120.44
2	D	114	LEU	C-N-CA	6.29	128.62	120.44
1	C	62	VAL	N-CA-CB	-6.28	103.20	110.55
2	B	13	ALA	N-CA-C	6.26	118.19	111.36
2	B	121	GLU	OE1-CD-OE2	6.24	137.88	122.90
2	B	131	GLN	N-CA-CB	6.23	119.81	110.22
1	C	42	TYR	O-C-N	6.22	130.57	122.42
2	D	133	VAL	O-C-N	6.22	128.35	121.94
2	B	124	PRO	CA-C-N	6.21	125.78	119.19
2	B	124	PRO	C-N-CA	6.21	125.78	119.19
1	A	36	PHE	O-C-N	6.21	127.01	121.36
2	D	31	LEU	CA-C-N	6.21	129.75	120.31
2	D	31	LEU	C-N-CA	6.21	129.75	120.31
2	B	65	LYS	CA-CB-CG	6.20	126.50	114.10
1	A	17	VAL	O-C-N	6.18	127.97	121.91
1	C	135	VAL	CA-C-O	-6.18	114.62	121.17
1	A	37	PRO	CB-CA-C	6.16	120.59	111.85
2	B	143	HIS	N-CA-CB	6.15	120.60	110.39
2	D	131	GLN	OE1-CD-NE2	6.14	128.74	122.60
1	A	132	VAL	N-CA-C	-6.13	104.36	110.30
1	C	72	HIS	CA-CB-CG	-6.12	107.68	113.80
1	C	75	ASP	CA-C-N	6.11	127.72	120.09
1	C	75	ASP	C-N-CA	6.11	127.72	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	PHE	N-CA-C	6.11	117.94	111.28
1	A	41	THR	OG1-CB-CG2	6.07	121.44	109.30
2	D	118	PHE	CA-C-N	6.07	129.84	120.07
2	D	118	PHE	C-N-CA	6.07	129.84	120.07
2	D	140	ALA	O-C-N	6.04	129.29	122.22
1	A	108	THR	N-CA-C	-6.02	104.06	111.40
1	A	43	PHE	CA-C-O	-6.01	115.30	121.07
2	D	32	LEU	CA-C-O	-6.00	113.06	119.97
1	C	34	LEU	CA-C-N	-5.99	112.30	120.44
1	C	34	LEU	C-N-CA	-5.99	112.30	120.44
2	D	129	ALA	CA-C-O	-5.98	114.21	120.55
2	B	89	SER	O-C-N	5.98	128.23	122.07
2	D	84	THR	CA-CB-CG2	5.96	120.63	110.50
2	D	87	THR	CA-CB-OG1	-5.96	100.66	109.60
2	B	89	SER	N-CA-C	-5.95	104.70	111.07
1	C	17	VAL	CB-CA-C	5.92	119.55	111.97
2	B	94	ASP	CA-CB-CG	-5.92	106.68	112.60
2	B	91	LEU	N-CA-C	5.92	117.40	111.07
2	D	109	VAL	CA-C-O	-5.92	114.80	120.95
1	A	31	ARG	CA-C-N	5.91	128.12	120.44
1	A	31	ARG	C-N-CA	5.91	128.12	120.44
2	B	24	GLY	CA-C-O	5.91	126.59	120.80
2	D	29	GLY	CA-C-O	5.89	127.37	121.00
1	C	123	ALA	CA-C-O	-5.88	113.71	120.24
2	D	80	ASN	CA-CB-CG	-5.88	106.72	112.60
2	D	102	ASN	CA-CB-CG	5.88	118.48	112.60
2	B	50	THR	O-C-N	5.85	128.04	121.32
1	A	140	TYR	CA-C-O	-5.82	113.53	120.10
2	D	129	ALA	O-C-N	5.81	128.28	122.12
1	C	118	THR	OG1-CB-CG2	5.81	120.92	109.30
1	C	128	PHE	CA-C-O	-5.81	114.72	120.82
2	B	117	HIS	CA-CB-CG	-5.81	107.99	113.80
2	D	11	VAL	CA-C-N	5.80	128.33	120.38
2	D	11	VAL	C-N-CA	5.80	128.33	120.38
2	D	50	THR	CA-CB-CG2	5.80	120.36	110.50
1	C	93	VAL	CA-C-O	-5.79	114.43	121.04
1	A	11	LYS	N-CA-CB	5.78	119.28	110.14
1	C	16	LYS	N-CA-C	-5.78	106.06	113.23
1	C	36	PHE	O-C-N	5.77	126.61	121.36
2	B	86	ALA	N-CA-C	5.77	117.57	111.28
2	B	135	ALA	CA-C-N	5.77	126.35	120.00
2	B	135	ALA	C-N-CA	5.77	126.35	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	GLN	N-CA-CB	5.75	118.69	110.06
2	D	107	GLY	CA-C-O	-5.75	115.16	120.80
2	B	122	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	112	HIS	CA-CB-CG	-5.71	108.09	113.80
2	B	133	VAL	CA-C-O	-5.71	115.34	121.27
2	D	96	LEU	CA-C-O	-5.69	112.94	119.60
2	D	120	LYS	CB-CA-C	-5.69	101.30	110.74
1	C	6	ASP	CB-CG-OD2	-5.67	105.37	118.40
2	B	93	CYS	O-C-N	5.65	128.81	122.32
2	B	114	LEU	O-C-N	5.64	128.10	122.12
2	D	111	VAL	CA-C-N	5.63	126.34	120.03
2	D	111	VAL	C-N-CA	5.63	126.34	120.03
2	D	126	VAL	CB-CA-C	5.63	119.39	112.02
2	B	78	LEU	CA-C-N	5.61	128.57	120.38
2	B	78	LEU	C-N-CA	5.61	128.57	120.38
1	C	41	THR	CA-CB-CG2	5.61	120.04	110.50
1	A	46	PHE	CA-CB-CG	5.61	119.41	113.80
1	C	66	LEU	CB-CA-C	5.61	120.10	110.79
1	A	30	GLU	CA-CB-CG	5.60	125.31	114.10
2	D	81	LEU	CB-CA-C	5.60	119.67	110.88
1	C	54	GLN	O-C-N	5.59	128.53	122.15
2	D	80	ASN	OD1-CG-ND2	5.58	128.18	122.60
2	D	28	LEU	CA-C-N	5.58	126.13	119.94
2	D	28	LEU	C-N-CA	5.58	126.13	119.94
2	D	99	ASP	CA-C-O	-5.58	114.05	119.51
1	A	133	SER	CA-C-O	-5.57	114.61	120.63
1	C	126	ASP	CA-C-N	5.56	127.67	120.44
1	C	126	ASP	C-N-CA	5.56	127.67	120.44
2	D	4	THR	O-C-N	5.56	127.65	121.53
2	B	71	PHE	N-CA-C	-5.55	104.44	111.11
2	B	97	HIS	O-C-N	5.55	129.24	122.58
2	D	47	ASP	CA-CB-CG	-5.53	107.07	112.60
2	D	3	LEU	O-C-N	5.52	130.03	123.24
2	B	142	ALA	CA-C-O	-5.52	112.89	119.35
2	D	74	GLY	N-CA-C	-5.50	105.83	112.49
1	C	137	THR	CA-CB-CG2	5.50	119.84	110.50
2	B	103	PHE	CA-C-O	-5.49	114.73	120.55
1	C	6	ASP	O-C-N	5.49	128.41	122.15
2	B	123	THR	CA-CB-OG1	-5.49	101.36	109.60
2	D	47	ASP	CA-C-O	-5.48	114.44	120.69
1	C	134	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	121	VAL	CA-C-O	-5.47	115.05	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	HIS	CA-C-N	5.46	127.87	120.44
2	B	116	HIS	C-N-CA	5.46	127.87	120.44
1	A	89	HIS	N-CA-C	5.45	120.21	113.50
1	C	9	ASN	OD1-CG-ND2	5.44	128.04	122.60
2	B	38	THR	CA-CB-OG1	-5.44	101.44	109.60
2	D	26	GLU	CB-CA-C	-5.43	102.32	110.90
1	A	69	ALA	N-CA-C	-5.42	105.27	111.07
1	C	78	ASN	N-CA-CB	5.41	117.82	109.98
1	C	141	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	A	42	TYR	N-CA-CB	5.40	118.94	110.46
2	D	12	THR	CA-CB-OG1	-5.39	101.51	109.60
2	D	111	VAL	N-CA-C	-5.38	105.25	110.42
2	B	12	THR	N-CA-CB	5.38	118.12	110.06
1	C	121	VAL	N-CA-C	-5.37	105.30	110.72
1	A	54	GLN	CA-C-O	-5.35	115.20	120.82
1	A	134	THR	CA-C-O	-5.34	114.75	120.42
2	B	26	GLU	CA-CB-CG	-5.34	103.42	114.10
2	D	117	HIS	CA-CB-CG	-5.33	108.47	113.80
2	B	30	ARG	CA-C-O	-5.33	114.77	120.42
2	B	123	THR	O-C-N	5.33	127.25	121.60
2	D	131	GLN	N-CA-CB	5.33	118.42	110.22
1	C	93	VAL	O-C-N	5.32	128.47	122.67
2	D	73	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	108	ASN	OD1-CG-ND2	5.31	127.91	122.60
1	A	87	HIS	N-CA-CB	5.30	118.01	110.16
2	B	126	VAL	CA-C-O	-5.30	115.16	121.05
2	D	34	VAL	O-C-N	5.30	127.29	121.83
2	D	143	HIS	N-CA-C	5.29	117.79	111.71
2	B	32	LEU	CA-C-O	-5.27	113.91	119.97
2	B	4	THR	O-C-N	5.26	127.18	121.60
2	B	37	TRP	N-CA-C	-5.24	106.15	112.54
2	D	50	THR	O-C-N	5.24	125.52	121.85
1	A	138	SER	CA-C-O	-5.24	113.43	119.61
2	D	52	ASP	CA-C-O	5.22	126.31	120.82
2	B	53	ALA	CA-C-O	5.22	126.08	120.55
1	C	4	PRO	N-CA-C	-5.22	106.24	113.81
1	C	132	VAL	CA-C-O	-5.22	115.64	121.17
1	C	121	VAL	CA-C-N	5.22	127.27	120.28
1	C	121	VAL	C-N-CA	5.22	127.27	120.28
1	A	4	PRO	CA-C-N	5.21	127.53	120.38
1	A	4	PRO	C-N-CA	5.21	127.53	120.38
1	A	35	SER	CA-C-O	5.20	126.12	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	LEU	CB-CA-C	5.20	118.34	109.24
1	A	82	ALA	CA-C-O	-5.19	115.03	120.63
2	D	15	TRP	CA-C-O	-5.19	115.05	120.55
2	B	30	ARG	NH1-CZ-NH2	-5.19	112.56	119.30
1	C	116	GLU	CA-C-N	5.19	131.86	122.27
1	C	116	GLU	C-N-CA	5.19	131.86	122.27
2	D	38	THR	CA-CB-OG1	-5.17	101.84	109.60
2	B	111	VAL	CB-CA-C	5.16	118.58	111.97
2	B	30	ARG	O-C-N	5.16	128.03	122.15
2	B	126	VAL	N-CA-C	-5.16	105.68	110.53
2	D	30	ARG	CA-C-O	-5.16	114.04	119.97
2	B	50	THR	CA-CB-OG1	-5.15	101.88	109.60
2	B	57	ASN	CB-CG-ND2	-5.14	108.69	116.40
1	C	86	LEU	CA-C-O	5.14	126.22	120.82
2	B	128	ALA	CA-C-N	5.13	127.47	120.54
2	B	128	ALA	C-N-CA	5.13	127.47	120.54
2	D	21	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	104	CYS	CB-CA-C	5.11	119.28	110.79
1	A	114	PRO	CA-C-N	5.11	127.64	120.28
1	A	114	PRO	C-N-CA	5.11	127.64	120.28
1	C	139	LYS	CB-CA-C	-5.10	102.80	111.02
1	A	13	ALA	O-C-N	5.09	127.32	122.07
2	D	81	LEU	N-CA-C	-5.09	105.62	111.07
2	D	41	PHE	N-CA-CB	5.09	118.45	110.46
1	C	85	ASP	CA-C-N	5.09	127.05	120.44
1	C	85	ASP	C-N-CA	5.09	127.05	120.44
2	D	66	LYS	N-CA-CB	5.08	117.68	110.16
2	B	51	PRO	N-CA-C	-5.08	106.47	113.53
2	B	104	ARG	N-CA-C	-5.07	105.66	111.14
1	A	45	HIS	CB-CA-C	-5.07	102.86	111.02
1	C	6	ASP	OD1-CG-OD2	5.07	135.06	122.90
2	D	145	TYR	O-C-N	5.06	129.03	122.81
2	D	35	TYR	O-C-N	5.05	125.95	121.36
1	A	30	GLU	CB-CG-CD	5.04	121.17	112.60
1	A	78	ASN	O-C-N	5.04	127.27	122.03
2	B	105	LEU	CB-CA-C	5.03	118.86	110.81
2	D	61	LYS	CA-CB-CG	5.03	124.16	114.10
1	C	49	SER	N-CA-C	-5.02	103.86	110.43
2	D	129	ALA	N-CA-C	-5.02	105.81	111.28
2	B	26	GLU	CG-CD-OE1	-5.00	106.90	118.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	104	ARG	Sidechain,Mainchain
2	B	126	VAL	Mainchain
1	C	101	LEU	Mainchain
1	C	120	ALA	Mainchain
1	C	92	ARG	Sidechain
2	D	104	ARG	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	1069	0	1073	31	0
1	C	1069	0	1073	30	0
2	B	1121	0	1116	34	0
2	D	1121	0	1116	41	0
3	A	43	0	30	3	0
3	B	43	0	30	4	0
3	C	43	0	30	2	0
3	D	43	0	30	3	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	98	0	0	4	0
5	B	94	0	0	2	0
5	C	95	0	0	8	0
5	D	80	0	0	2	0
All	All	4923	0	4498	141	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 16.

All (141) 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:118:THR:HG22	1:C:121:VAL:H	1.35	0.91
3:D:147:HEM:HHH	3:D:147:HEM:HBB2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:147:HEM:HMB1	3:B:147:HEM:HBB2	1.62	0.82
2:D:104:ARG:HH21	2:D:139:ASN:HD21	1.26	0.81
2:D:75:LEU:O	2:D:78:LEU:HD22	1.87	0.73
2:B:24:GLY:HA2	2:B:68:LEU:HG	1.72	0.71
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.73	0.69
1:A:73:VAL:HG23	1:A:76:MET:HE2	1.74	0.68
2:D:50:THR:HG22	2:D:53:ALA:H	1.59	0.68
1:A:76:MET:N	1:A:77:PRO:HD2	2.09	0.67
3:B:147:HEM:HBB2	3:B:147:HEM:CMB	2.23	0.67
2:D:104:ARG:HH21	2:D:139:ASN:ND2	1.92	0.67
1:C:7:LYS:HE3	1:C:74:ASP:OD1	1.95	0.66
2:B:50:THR:O	2:B:54:VAL:HG23	1.96	0.66
1:C:16:LYS:HE3	1:C:16:LYS:N	2.11	0.65
1:C:113:LEU:HB3	1:C:116:GLU:HG2	1.80	0.64
2:B:143:HIS:CD2	2:B:144:LYS:HD3	2.33	0.63
1:C:118:THR:HG22	1:C:121:VAL:N	2.12	0.62
2:B:140:ALA:O	2:B:143:HIS:ND1	2.31	0.60
3:C:142:HEM:HMB2	3:C:142:HEM:HBB2	1.83	0.60
2:B:1:VAL:HB	2:B:2:HIS:CE1	2.38	0.58
3:C:142:HEM:HBB2	3:C:142:HEM:CMB	2.34	0.58
3:A:142:HEM:HMB2	3:A:142:HEM:HBB2	1.86	0.57
2:B:88:LEU:HD22	2:B:92:HIS:HE1	1.69	0.57
2:D:4:THR:O	2:D:7:GLU:N	2.37	0.57
1:A:51:GLY:O	1:A:56:LYS:HE2	2.05	0.56
2:B:21:ASP:CG	2:B:65:LYS:HD3	2.31	0.56
2:B:51:PRO:O	2:B:55:MET:HG2	2.04	0.56
1:C:15:GLY:C	1:C:16:LYS:HE3	2.30	0.56
2:D:63:HIS:ND1	2:D:66:LYS:HD2	2.21	0.55
2:D:10:ALA:HB1	2:D:126:VAL:HG22	1.88	0.55
1:A:86:LEU:HD12	1:A:90:LYS:HB2	1.89	0.55
2:D:50:THR:HG22	2:D:53:ALA:HB2	1.88	0.55
3:B:147:HEM:HMC2	3:B:147:HEM:HBC2	1.89	0.54
1:A:84:SER:HB3	1:A:136:LEU:HA	1.90	0.54
1:C:106:LEU:HD21	1:C:126:ASP:HB2	1.90	0.54
1:A:57:GLY:O	1:A:61:LYS:HG3	2.08	0.54
2:D:63:HIS:O	2:D:67:VAL:HG23	2.08	0.54
1:A:14:TRP:O	1:A:15:GLY:C	2.51	0.53
2:D:57:ASN:O	2:D:61:LYS:HD3	2.08	0.53
2:D:42:PHE:O	2:D:45:PHE:HB2	2.09	0.53
2:D:63:HIS:O	2:D:66:LYS:HG3	2.08	0.53
2:D:50:THR:O	2:D:54:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG23	1:A:76:MET:CE	2.39	0.52
1:C:68:ASN:HB2	5:C:203:HOH:O	2.11	0.51
1:A:61:LYS:HE3	5:A:192:HOH:O	2.09	0.51
1:C:76:MET:N	1:C:77:PRO:CD	2.74	0.51
2:D:38:THR:HG22	2:D:102:ASN:OD1	2.11	0.51
1:A:16:LYS:NZ	5:A:229:HOH:O	2.43	0.51
1:C:99:LYS:HD2	5:C:153:HOH:O	2.09	0.50
2:D:104:ARG:NH2	2:D:139:ASN:OD1	2.44	0.50
1:A:77:PRO:HG2	1:A:78:ASN:H	1.75	0.50
2:D:3:LEU:HD13	2:D:7:GLU:HB3	1.93	0.50
2:D:57:ASN:OD1	2:D:59:LYS:HB2	2.12	0.50
2:B:8:LYS:O	2:B:12:THR:HG23	2.11	0.50
2:B:4:THR:OG1	2:B:6:GLU:HG2	2.12	0.49
2:D:51:PRO:O	2:D:55:MET:HG2	2.11	0.49
1:C:92:ARG:HD2	5:C:196:HOH:O	2.13	0.49
2:B:1:VAL:HG13	2:B:81:LEU:HD12	1.94	0.49
1:A:117:PHE:HB3	2:B:116:HIS:CD2	2.47	0.49
2:D:50:THR:HG22	2:D:53:ALA:CB	2.42	0.49
2:D:88:LEU:HG	5:D:150:HOH:O	2.12	0.49
1:C:85:ASP:HB3	5:C:171:HOH:O	2.12	0.48
1:A:76:MET:HE1	1:A:128:PHE:CD1	2.47	0.48
1:A:14:TRP:O	1:A:17:VAL:HB	2.13	0.48
1:A:75:ASP:C	1:A:77:PRO:HD2	2.39	0.48
2:B:38:THR:HG22	2:B:102:ASN:OD1	2.14	0.47
1:C:117:PHE:HB3	2:D:116:HIS:CD2	2.48	0.47
2:D:52:ASP:O	2:D:56:GLY:N	2.43	0.47
1:C:103:HIS:O	1:C:107:VAL:HG23	2.15	0.47
2:D:104:ARG:NH2	2:D:139:ASN:ND2	2.61	0.46
2:B:6:GLU:H	2:B:6:GLU:CD	2.23	0.46
2:B:102:ASN:N	5:C:177:HOH:O	2.48	0.46
1:C:30:GLU:OE2	1:C:50:HIS:ND1	2.49	0.46
3:A:142:HEM:HBB2	3:A:142:HEM:CMB	2.46	0.46
1:A:34:LEU:HD13	5:B:196:HOH:O	2.16	0.46
2:B:127:GLN:O	2:B:131:GLN:HG2	2.16	0.46
1:C:122:HIS:O	1:C:122:HIS:HD2	1.99	0.45
2:B:75:LEU:O	2:B:78:LEU:HG	2.17	0.45
2:B:1:VAL:HG13	2:B:81:LEU:CD1	2.46	0.45
1:C:119:PRO:HD3	5:D:195:HOH:O	2.15	0.45
1:A:42:TYR:CE2	1:A:93:VAL:HA	2.52	0.45
1:C:62:VAL:O	1:C:65:ALA:HB3	2.17	0.45
1:A:40:LYS:O	1:A:42:TYR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ALA:HB3	5:A:173:HOH:O	2.16	0.44
2:B:18:VAL:HG13	2:B:23:VAL:HG21	2.00	0.44
1:A:40:LYS:C	1:A:42:TYR:N	2.75	0.44
1:A:49:SER:O	1:A:52:SER:HB3	2.16	0.44
2:B:100:PRO:HD2	1:C:38:THR:HB	1.99	0.44
2:B:15:TRP:CZ2	2:B:72:SER:HB2	2.53	0.44
2:B:31:LEU:HD11	2:B:38:THR:HG21	1.98	0.44
2:D:124:PRO:N	2:D:125:PRO:HD2	2.32	0.44
1:C:76:MET:N	1:C:77:PRO:HD3	2.33	0.43
2:D:20:VAL:HG13	2:D:68:LEU:HB3	2.00	0.43
2:B:24:GLY:CA	2:B:68:LEU:HG	2.45	0.43
2:D:28:LEU:CD2	2:D:63:HIS:HB3	2.47	0.43
2:D:29:GLY:O	2:D:33:VAL:HG23	2.18	0.43
2:D:91:LEU:CD1	2:D:95:LYS:HD2	2.49	0.43
2:D:4:THR:O	2:D:5:PRO:C	2.62	0.43
1:A:140:TYR:HD2	2:D:37:TRP:CE3	2.37	0.43
2:B:47:ASP:O	2:B:48:LEU:HD23	2.19	0.43
3:B:147:HEM:HBB1	5:B:188:HOH:O	2.19	0.43
1:C:114:PRO:HB3	5:C:151:HOH:O	2.19	0.43
1:A:22:GLY:HA2	1:A:60:LYS:HA	2.00	0.42
2:D:4:THR:OG1	2:D:6:GLU:HB2	2.19	0.42
2:D:7:GLU:HG2	2:D:129:ALA:HB2	2.00	0.42
2:B:101:GLU:HB3	5:C:177:HOH:O	2.20	0.42
1:A:52:SER:O	1:A:56:LYS:HG3	2.19	0.42
1:C:7:LYS:O	1:C:11:LYS:HG3	2.19	0.42
1:C:56:LYS:HG2	5:C:202:HOH:O	2.20	0.42
1:C:75:ASP:OD1	1:C:77:PRO:HD2	2.18	0.42
1:A:51:GLY:O	1:A:52:SER:C	2.62	0.42
1:C:42:TYR:CE2	1:C:93:VAL:HA	2.54	0.42
2:D:2:HIS:O	2:D:3:LEU:HD23	2.19	0.42
1:A:58:HIS:HA	1:A:61:LYS:HD3	2.00	0.42
2:B:21:ASP:HA	2:B:65:LYS:HB3	2.02	0.41
1:A:91:LEU:HD13	3:A:142:HEM:C4D	2.56	0.41
1:A:129:LEU:HA	1:A:129:LEU:HD23	1.81	0.41
1:C:29:LEU:HD23	1:C:32:MET:CE	2.51	0.41
2:B:26:GLU:O	2:B:26:GLU:HG3	2.21	0.41
3:D:147:HEM:HBB2	3:D:147:HEM:CHC	2.36	0.41
2:B:100:PRO:HG2	1:C:38:THR:HG21	2.01	0.41
2:D:50:THR:HG22	2:D:53:ALA:N	2.32	0.41
2:B:1:VAL:HG23	2:B:3:LEU:HD12	2.03	0.41
2:D:2:HIS:C	2:D:3:LEU:HD23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:GLU:OE1	2:D:43:GLU:HA	2.21	0.41
2:D:98:VAL:O	2:D:145:TYR:OH	2.32	0.41
1:C:10:VAL:HG22	1:C:125:LEU:HD23	2.03	0.41
2:D:50:THR:O	2:D:53:ALA:HB3	2.21	0.41
1:A:103:HIS:NE2	2:B:131:GLN:OE1	2.40	0.40
1:C:14:TRP:CD1	1:C:70:VAL:HG21	2.55	0.40
2:D:57:ASN:HA	2:D:58:PRO:HD3	1.62	0.40
2:D:74:GLY:O	2:D:77:HIS:N	2.42	0.40
3:D:147:HEM:HHA	3:D:147:HEM:HAA1	1.90	0.40
1:A:15:GLY:O	1:A:18:GLY:N	2.54	0.40
5:A:190:HOH:O	2:B:120:LYS:HD2	2.21	0.40
2:B:5:PRO:HG2	2:B:6:GLU:OE1	2.21	0.40
2:B:14:LEU:HD21	2:B:118:PHE:CG	2.56	0.40
2:B:131:GLN:HE21	2:B:131:GLN:HB3	1.65	0.40
1:C:122:HIS:CD2	1:C:122:HIS:C	2.99	0.40
2:D:75:LEU:HD23	2:D:75:LEU:HA	1.88	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%)	127 (91%)	11 (8%)	1 (1%)	18	14
1	C	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
2	B	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
2	D	144/146 (99%)	136 (94%)	8 (6%)	0	100	100
All	All	566/574 (99%)	532 (94%)	33 (6%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR

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%)	104 (92%)	9 (8%)	11	8
1	C	113/113 (100%)	103 (91%)	10 (9%)	9	6
2	B	117/117 (100%)	107 (92%)	10 (8%)	10	7
2	D	117/117 (100%)	108 (92%)	9 (8%)	12	8
All	All	460/460 (100%)	422 (92%)	38 (8%)	10	7

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	52	SER
1	A	84	SER
1	A	99	LYS
1	A	105	LEU
1	A	109	LEU
1	A	121	VAL
1	A	131	SER
1	A	137	THR
2	B	2	HIS
2	B	6	GLU
2	B	12	THR
2	B	14	LEU
2	B	17	LYS
2	B	28	LEU
2	B	59	LYS
2	B	65	LYS
2	B	66	LYS
2	B	121	GLU
1	C	1	VAL
1	C	2	LEU

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Mol	Chain	Res	Type
1	C	16	LYS
1	C	56	LYS
1	C	83	LEU
1	C	99	LYS
1	C	116	GLU
1	C	118	THR
1	C	124	SER
1	C	131	SER
2	D	3	LEU
2	D	5	PRO
2	D	50	THR
2	D	61	LYS
2	D	66	LYS
2	D	68	LEU
2	D	78	LEU
2	D	90	GLU
2	D	131	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	39	GLN
2	B	97	HIS
1	C	72	HIS
2	D	2	HIS
2	D	117	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

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	$\# Z > 2$
3	HEM	D	147	2	50,50,50	1.47	7 (14%)	67,82,82	1.59	12 (17%)
3	HEM	C	142	1,4	50,50,50	1.57	8 (16%)	67,82,82	1.54	10 (14%)
4	OXY	A	143	3	1,1,1	0.39	0	-		
3	HEM	A	142	1,4	50,50,50	1.65	13 (26%)	67,82,82	1.55	12 (17%)
3	HEM	B	147	2	50,50,50	1.67	11 (22%)	67,82,82	1.40	12 (17%)
4	OXY	C	143	3	1,1,1	0.07	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	C	142	1,4	-	2/14/54/54	-
3	HEM	A	142	1,4	-	7/14/54/54	-
3	HEM	B	147	2	-	0/14/54/54	-
3	HEM	D	147	2	-	9/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	FE-NB	4.47	2.08	1.94
3	D	147	HEM	FE-NB	4.29	2.08	1.94
3	B	147	HEM	CAB-C3B	4.10	1.58	1.47
3	C	142	HEM	FE-ND	3.85	2.06	1.94
3	C	142	HEM	CAB-C3B	3.81	1.57	1.47
3	A	142	HEM	FE-NC	3.65	2.07	1.95
3	A	142	HEM	CAB-C3B	3.56	1.56	1.47
3	B	147	HEM	FE-ND	3.53	2.05	1.94
3	D	147	HEM	FE-ND	3.40	2.05	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	CMC-C2C	3.17	1.57	1.50
3	A	142	HEM	FE-NB	3.16	2.04	1.94
3	D	147	HEM	CAB-C3B	3.04	1.55	1.47
3	C	142	HEM	CAA-C2A	3.02	1.59	1.51
3	B	147	HEM	FE-NA	2.87	2.04	1.95
3	C	142	HEM	C2A-C3A	-2.86	1.31	1.38
3	A	142	HEM	CBD-CGD	2.83	1.57	1.50
3	C	142	HEM	CMC-C2C	2.77	1.56	1.50
3	B	147	HEM	CAA-C2A	2.76	1.58	1.51
3	C	142	HEM	FE-NB	2.73	2.03	1.94
3	D	147	HEM	CAC-C3C	2.59	1.54	1.47
3	A	142	HEM	CAC-C3C	2.56	1.54	1.47
3	A	142	HEM	C3B-C2B	-2.47	1.32	1.37
3	A	142	HEM	FE-ND	2.42	2.02	1.94
3	A	142	HEM	C2A-C3A	-2.40	1.32	1.38
3	B	147	HEM	C1C-NC	2.33	1.44	1.39
3	A	142	HEM	CAD-C3D	2.23	1.57	1.51
3	D	147	HEM	C2A-C3A	-2.22	1.33	1.38
3	C	142	HEM	CAC-C3C	2.17	1.53	1.47
3	C	142	HEM	CAD-C3D	2.17	1.56	1.51
3	B	147	HEM	C1B-NB	-2.16	1.36	1.40
3	A	142	HEM	CHB-C1B	2.16	1.42	1.38
3	B	147	HEM	CBD-CGD	2.16	1.55	1.50
3	A	142	HEM	C1B-NB	-2.15	1.36	1.40
3	B	147	HEM	C3D-C2D	-2.13	1.32	1.36
3	A	142	HEM	C4A-C3A	2.07	1.48	1.43
3	B	147	HEM	CMC-C2C	2.07	1.55	1.50
3	B	147	HEM	C2A-C3A	-2.06	1.33	1.38
3	D	147	HEM	C4D-ND	-2.05	1.36	1.40
3	D	147	HEM	CMC-C2C	2.03	1.54	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	CBA-CAA-C2A	5.39	127.45	112.53
3	A	142	HEM	O2D-CGD-O1D	4.84	135.78	123.33
3	C	142	HEM	C1C-CHC-C4B	4.55	135.70	126.02
3	D	147	HEM	CHA-C4D-ND	3.87	129.15	124.37
3	A	142	HEM	O1D-CGD-CBD	-3.85	110.87	123.09
3	C	142	HEM	CHC-C4B-NB	-3.65	120.49	124.42
3	C	142	HEM	CHC-C1C-NC	-3.54	120.60	124.45
3	B	147	HEM	O2D-CGD-O1D	3.38	132.03	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	O1D-CGD-CBD	-3.21	112.90	123.09
3	B	147	HEM	CBB-CAB-C3B	-3.12	111.94	127.53
3	C	142	HEM	C4B-C3B-C2B	3.09	110.12	107.28
3	C	142	HEM	CHC-C4B-C3B	3.02	131.10	125.07
3	A	142	HEM	CHC-C1C-NC	-3.00	121.19	124.45
3	C	142	HEM	O1A-CGA-CBA	-2.91	113.86	123.09
3	C	142	HEM	O2A-CGA-O1A	2.91	130.81	123.33
3	B	147	HEM	O1D-CGD-CBD	-2.82	114.14	123.09
3	A	142	HEM	C4A-CHB-C1B	-2.77	119.73	126.25
3	A	142	HEM	O1A-CGA-CBA	-2.73	114.42	123.09
3	D	147	HEM	C4D-ND-C1D	2.72	108.42	105.21
3	D	147	HEM	CBC-CAC-C3C	-2.71	114.00	127.53
3	A	142	HEM	C1C-CHC-C4B	2.69	131.73	126.02
3	B	147	HEM	CMA-C3A-C2A	2.66	131.27	125.62
3	D	147	HEM	C3D-C4D-ND	-2.59	107.33	110.17
3	B	147	HEM	C4A-CHB-C1B	-2.56	120.22	126.25
3	D	147	HEM	O2D-CGD-O1D	2.51	129.79	123.33
3	C	142	HEM	C1A-C2A-C3A	2.45	110.66	106.87
3	B	147	HEM	CHB-C4A-NA	2.44	128.29	123.86
3	A	142	HEM	CAD-CBD-CGD	-2.42	107.26	113.67
3	D	147	HEM	C4A-CHB-C1B	-2.41	120.57	126.25
3	B	147	HEM	C3C-C2C-C1C	2.38	109.30	107.05
3	D	147	HEM	O1A-CGA-CBA	-2.38	115.56	123.09
3	A	142	HEM	CAA-CBA-CGA	-2.34	107.46	113.67
3	C	142	HEM	CBB-CAB-C3B	-2.33	115.86	127.53
3	A	142	HEM	C3D-C4D-ND	-2.33	107.61	110.17
3	B	147	HEM	C3B-C4B-NB	-2.32	107.81	109.47
3	B	147	HEM	CHB-C4A-C3A	-2.31	120.73	127.43
3	D	147	HEM	C4C-CHD-C1D	-2.26	121.22	126.02
3	C	142	HEM	CMA-C3A-C2A	2.19	130.28	125.62
3	A	142	HEM	CMA-C3A-C2A	2.16	130.21	125.62
3	A	142	HEM	O2A-CGA-O1A	2.11	128.76	123.33
3	D	147	HEM	CAD-C3D-C4D	-2.07	121.08	124.70
3	B	147	HEM	C1B-NB-C4B	2.06	107.65	105.21
3	D	147	HEM	O2A-CGA-O1A	2.06	128.63	123.33
3	B	147	HEM	CAA-CBA-CGA	2.03	119.06	113.67
3	A	142	HEM	CAA-C2A-C1A	-2.02	120.98	124.94
3	B	147	HEM	C3D-C4D-ND	-2.01	107.97	110.17

There are no chirality outliers.

All (18) torsion outliers are listed below:

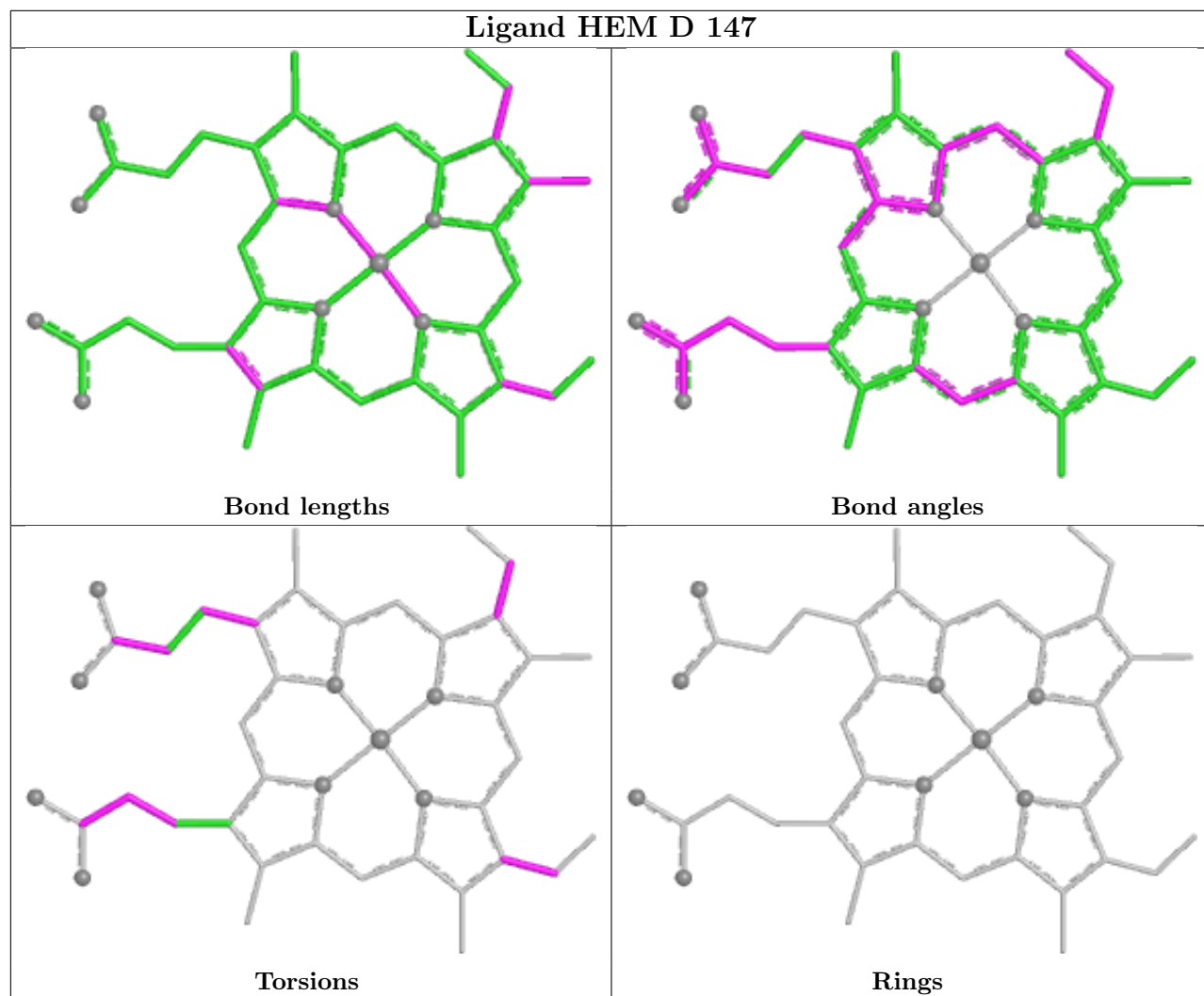
Mol	Chain	Res	Type	Atoms
3	D	147	HEM	C2A-CAA-CBA-CGA
3	A	142	HEM	C3A-C2A-CAA-CBA
3	D	147	HEM	C2C-C3C-CAC-CBC
3	D	147	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	C4C-C3C-CAC-CBC
3	D	147	HEM	C2D-C3D-CAD-CBD
3	A	142	HEM	C2C-C3C-CAC-CBC
3	A	142	HEM	C1A-C2A-CAA-CBA
3	D	147	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAD-CBD-CGD-O2D

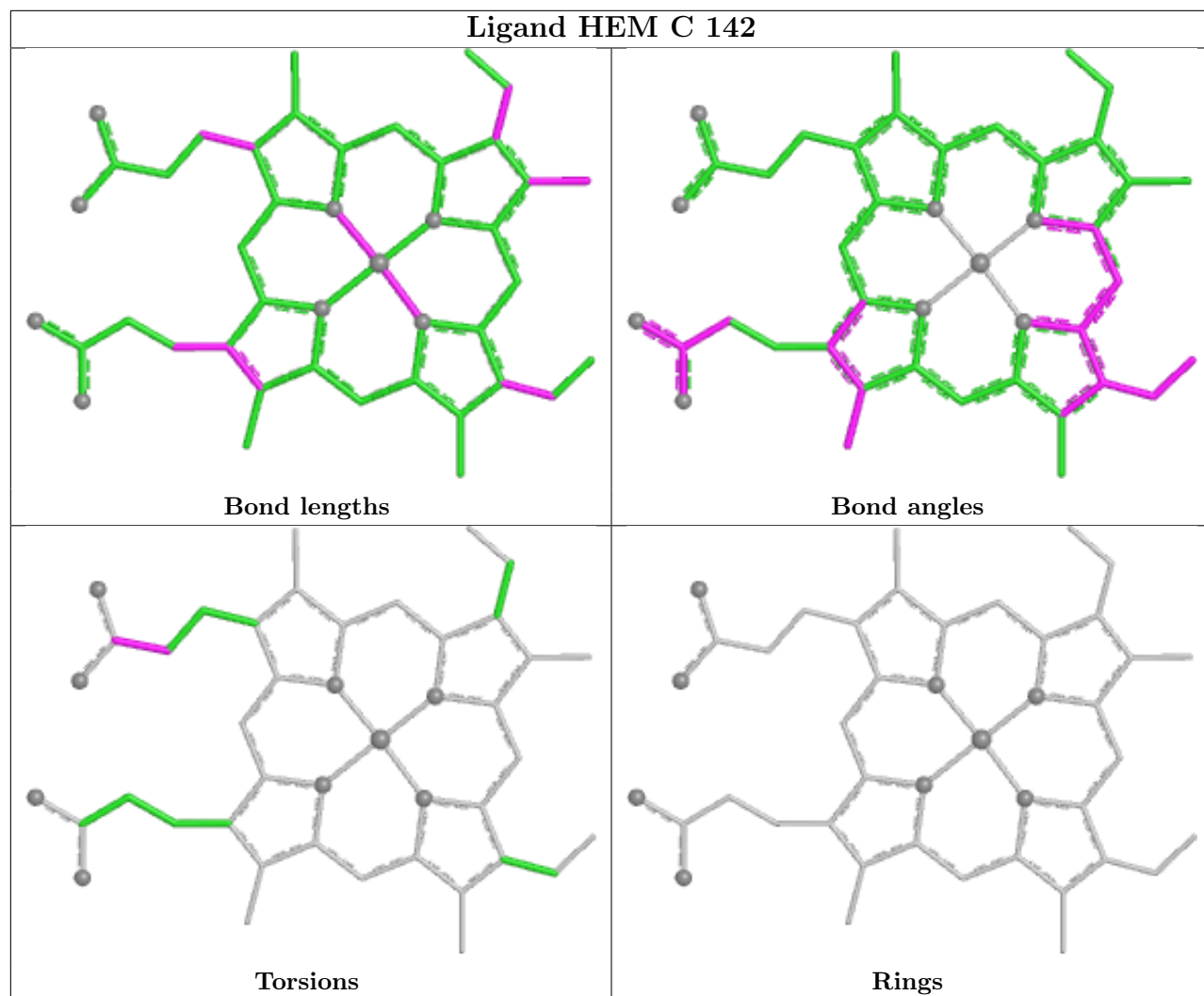
There are no ring outliers.

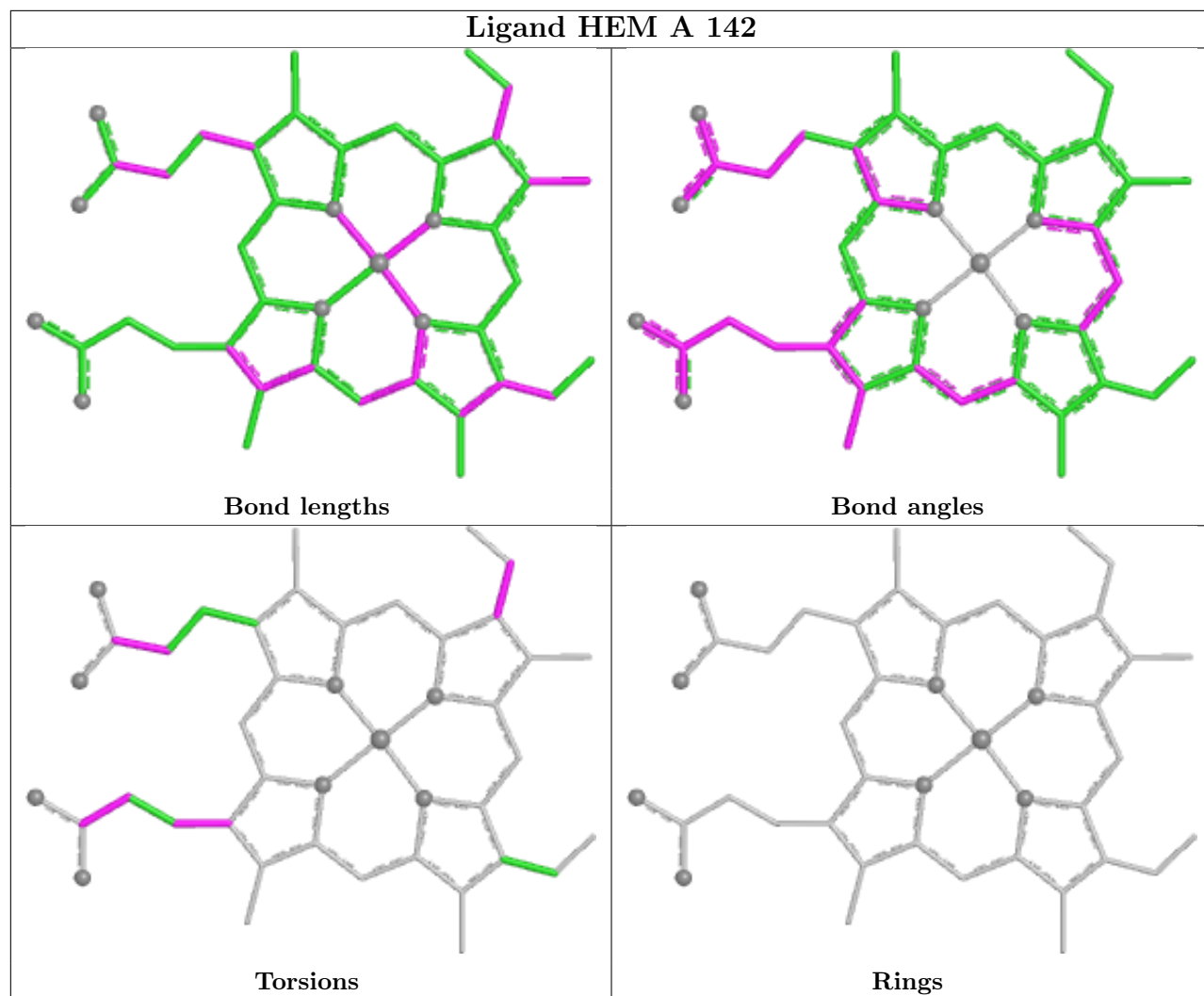
4 monomers are involved in 12 short contacts:

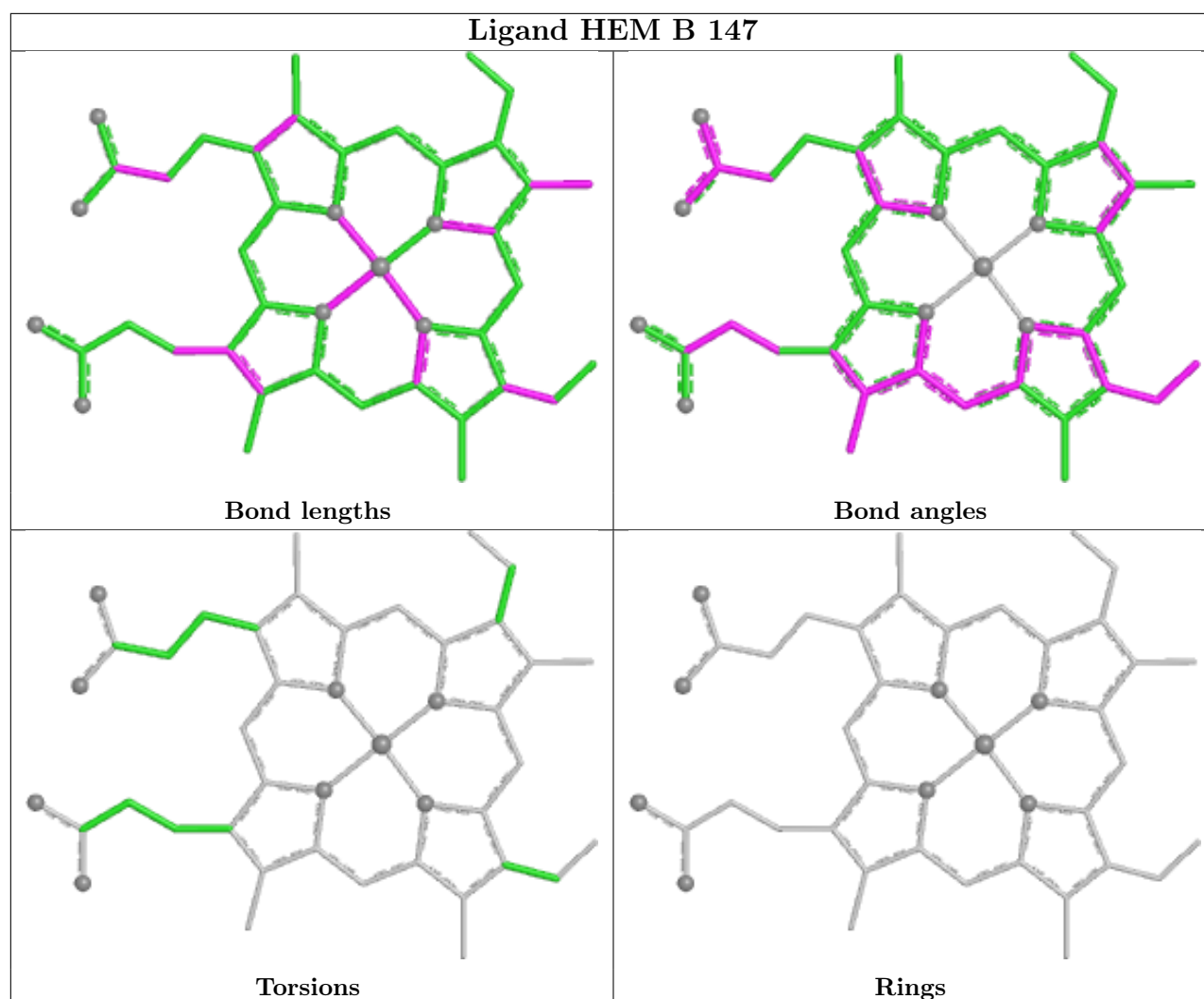
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	147	HEM	3	0
3	C	142	HEM	2	0
3	A	142	HEM	3	0
3	B	147	HEM	4	0

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.