



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:22 AM EDT

PDB ID : 1PMB / pdb_00001pmb
Title : THE DETERMINATION OF THE CRYSTAL STRUCTURE OF RECOMBINANT PIG MYOGLOBIN BY MOLECULAR REPLACEMENT AND ITS REFINEMENT
Authors : Smerdon, S.J.; Oldfield, T.J.; Dodson, E.J.; Dodson, G.G.; Hubbard, R.E.; Wilkinson, A.J.
Deposited on : 1989-11-27
Resolution : 2.50 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

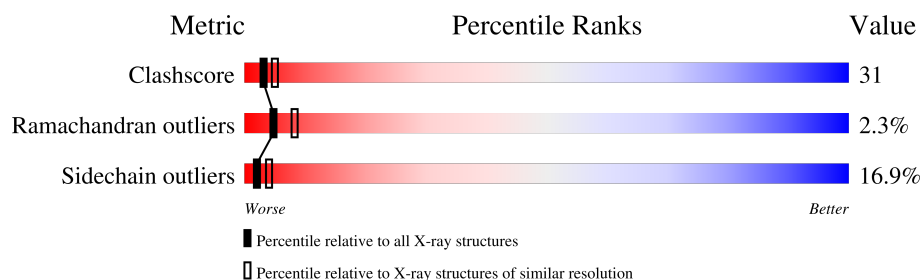
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	153	
1	B	153	

2 Entry composition [i](#)

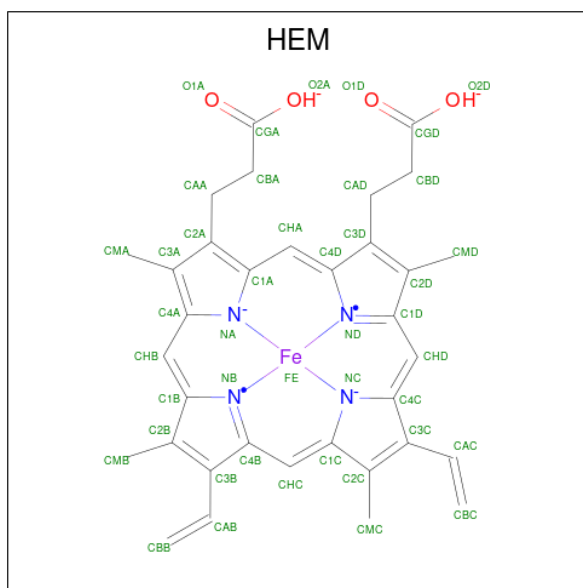
There are 3 unique types of molecules in this entry. The entry contains 2537 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1197	764	208	222	3			
1	B	153	Total	C	N	O	S	0	0	0
			1197	764	208	222	3			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

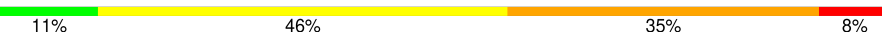
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total 29	O 29	0	0
3	B	28	Total 28	O 28	0	0

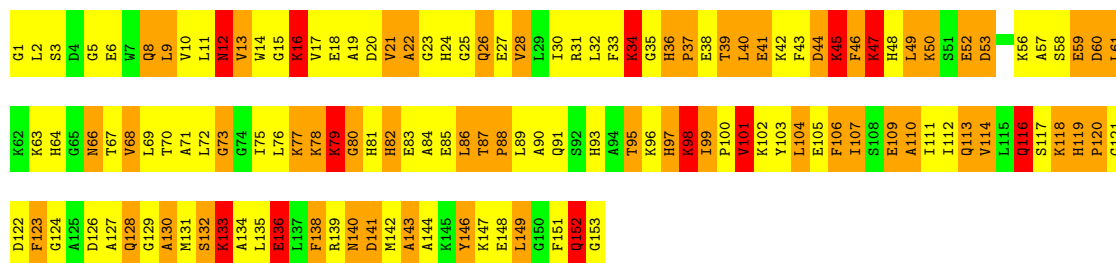
3 Residue-property plots

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.

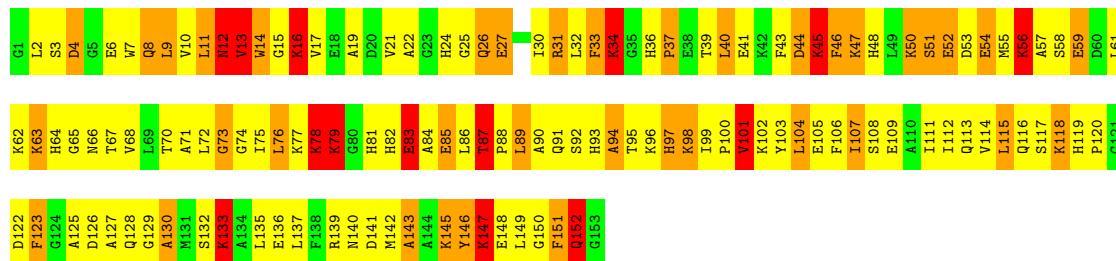
• Molecule 1: MYOGLOBIN

Chain A:  11% 46% 35% 8%



• Molecule 1: MYOGLOBIN

Chain B:  14% 52% 24% 9%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 42.63Å 92.20Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2537	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	4/1222 (0.3%)	3.81	268/1637 (16.4%)
1	B	1.36	1/1222 (0.1%)	3.66	238/1637 (14.5%)
All	All	1.35	5/2444 (0.2%)	3.73	506/3274 (15.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	ILE	CA-CB	6.74	1.60	1.53
1	A	112	ILE	CA-CB	6.23	1.62	1.54
1	A	11	LEU	C-N	-5.73	1.26	1.33
1	B	9	LEU	C-O	-5.60	1.17	1.24
1	A	95	THR	CA-CB	5.20	1.62	1.53

All (506) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	ASN	OD1-CG-ND2	22.69	145.29	122.60
1	B	12	ASN	OD1-CG-ND2	22.57	145.17	122.60
1	A	128	GLN	OE1-CD-NE2	22.27	144.87	122.60
1	A	103	TYR	O-C-N	15.52	139.85	122.15
1	A	109	GLU	CA-CB-CG	14.69	143.47	114.10
1	B	64	HIS	CA-C-N	14.65	136.24	119.98
1	B	64	HIS	C-N-CA	14.65	136.24	119.98
1	B	97	HIS	CA-CB-CG	-14.09	99.71	113.80
1	B	103	TYR	O-C-N	14.07	138.19	122.15
1	A	58	SER	CA-C-N	13.80	138.37	120.44
1	A	58	SER	C-N-CA	13.80	138.37	120.44
1	B	44	ASP	CA-C-O	13.09	135.47	121.07
1	A	73	GLY	CA-C-N	12.98	136.37	120.14
1	A	73	GLY	C-N-CA	12.98	136.37	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	O-C-N	12.97	132.20	121.17
1	B	9	LEU	O-C-N	12.95	135.56	122.09
1	A	83	GLU	CB-CG-CD	12.89	134.51	112.60
1	A	135	LEU	CA-C-O	-12.79	106.86	120.42
1	A	71	ALA	CA-C-O	-12.57	107.62	120.82
1	A	53	ASP	CA-CB-CG	-12.56	100.04	112.60
1	A	25	GLY	CA-C-N	12.41	138.05	120.79
1	A	25	GLY	C-N-CA	12.41	138.05	120.79
1	B	73	GLY	CA-C-N	12.41	133.72	119.94
1	B	73	GLY	C-N-CA	12.41	133.72	119.94
1	B	125	ALA	CA-C-N	12.29	137.35	120.63
1	B	125	ALA	C-N-CA	12.29	137.35	120.63
1	B	146	TYR	O-C-N	12.28	134.86	122.09
1	B	24	HIS	CA-C-N	12.27	133.85	119.99
1	B	24	HIS	C-N-CA	12.27	133.85	119.99
1	A	5	GLY	O-C-N	12.22	136.40	122.34
1	A	75	ILE	CA-C-N	12.06	136.12	120.44
1	A	75	ILE	C-N-CA	12.06	136.12	120.44
1	B	25	GLY	CA-C-N	11.99	136.47	120.65
1	B	25	GLY	C-N-CA	11.99	136.47	120.65
1	B	132	SER	N-CA-CB	-11.98	92.42	110.16
1	B	36	HIS	O-C-N	11.84	131.23	121.17
1	A	44	ASP	CA-C-O	11.77	134.78	121.02
1	B	12	ASN	CA-CB-CG	-11.74	100.86	112.60
1	B	128	GLN	OE1-CD-NE2	11.74	134.34	122.60
1	B	146	TYR	CA-C-O	-11.51	108.59	120.90
1	B	9	LEU	CA-C-O	-11.22	108.90	120.90
1	B	37	PRO	O-C-N	11.12	135.63	122.17
1	A	132	SER	N-CA-CB	-11.00	93.23	110.28
1	A	12	ASN	CB-CG-ND2	-10.96	99.97	116.40
1	A	103	TYR	CA-C-O	-10.90	108.86	120.42
1	A	120	PRO	CA-C-N	10.90	131.99	120.00
1	A	120	PRO	C-N-CA	10.90	131.99	120.00
1	A	78	LYS	N-CA-C	-10.80	99.77	113.16
1	A	71	ALA	CA-C-N	10.63	134.26	120.44
1	A	71	ALA	C-N-CA	10.63	134.26	120.44
1	B	16	LYS	CA-C-O	10.48	131.49	120.70
1	A	19	ALA	CA-C-N	10.45	141.50	121.54
1	A	19	ALA	C-N-CA	10.45	141.50	121.54
1	A	132	SER	CA-C-N	10.43	134.62	120.44
1	A	132	SER	C-N-CA	10.43	134.62	120.44
1	A	77	LYS	CG-CD-CE	10.40	135.21	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	TYR	CA-C-O	-10.35	109.45	120.42
1	B	123	PHE	O-C-N	10.24	135.59	122.28
1	A	97	HIS	CA-CB-CG	-10.19	103.61	113.80
1	A	135	LEU	O-C-N	10.18	133.76	122.15
1	B	52	GLU	CA-C-O	10.18	131.79	120.90
1	B	4	ASP	CA-CB-CG	-10.16	102.44	112.60
1	B	83	GLU	CB-CA-C	-10.16	93.41	110.68
1	B	113	GLN	OE1-CD-NE2	-10.10	112.50	122.60
1	A	149	LEU	N-CA-C	-10.07	100.13	111.71
1	B	72	LEU	CA-C-N	9.81	140.64	121.41
1	B	72	LEU	C-N-CA	9.81	140.64	121.41
1	A	11	LEU	CA-C-N	9.77	133.73	120.44
1	A	11	LEU	C-N-CA	9.77	133.73	120.44
1	A	121	GLY	CA-C-O	-9.71	110.37	120.66
1	A	15	GLY	CA-C-N	9.70	133.63	120.44
1	A	15	GLY	C-N-CA	9.70	133.63	120.44
1	A	147	LYS	CA-C-N	9.68	134.04	120.29
1	A	147	LYS	C-N-CA	9.68	134.04	120.29
1	A	122	ASP	CA-C-O	9.67	130.69	119.18
1	B	19	ALA	CA-C-N	9.63	139.93	121.54
1	B	19	ALA	C-N-CA	9.63	139.93	121.54
1	A	69	LEU	O-C-N	9.62	135.74	122.46
1	B	59	GLU	CA-CB-CG	9.44	132.97	114.10
1	A	143	ALA	CA-C-N	9.36	132.60	120.44
1	A	143	ALA	C-N-CA	9.36	132.60	120.44
1	B	13	VAL	N-CA-C	-9.33	98.94	111.44
1	B	53	ASP	CB-CA-C	9.32	126.53	110.68
1	A	72	LEU	CA-C-N	9.31	139.66	121.41
1	A	72	LEU	C-N-CA	9.31	139.66	121.41
1	A	40	LEU	CA-C-O	9.28	130.59	120.10
1	A	60	ASP	CA-CB-CG	9.12	121.72	112.60
1	B	97	HIS	N-CA-C	9.12	122.20	111.71
1	A	9	LEU	CA-C-N	9.07	132.65	120.77
1	A	9	LEU	C-N-CA	9.07	132.65	120.77
1	B	75	ILE	N-CA-CB	-8.97	95.58	110.56
1	A	132	SER	CA-C-O	8.95	130.27	119.97
1	A	99	ILE	CA-C-O	8.94	124.42	119.15
1	B	106	PHE	O-C-N	8.94	132.34	122.15
1	A	12	ASN	N-CA-CB	-8.90	97.16	110.07
1	B	85	GLU	O-C-N	8.90	131.70	122.09
1	B	108	SER	CA-C-O	8.89	130.15	120.82
1	B	6	GLU	CA-C-O	-8.88	111.50	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	HIS	CA-CB-CG	-8.83	104.97	113.80
1	B	31	ARG	NE-CZ-NH2	8.81	127.13	119.20
1	A	59	GLU	CA-CB-CG	8.80	131.71	114.10
1	A	33	PHE	CA-CB-CG	-8.66	105.14	113.80
1	B	123	PHE	CA-CB-CG	-8.66	105.14	113.80
1	A	59	GLU	CA-C-O	8.63	129.89	120.82
1	A	64	HIS	CA-CB-CG	-8.61	105.19	113.80
1	B	13	VAL	CB-CA-C	8.58	126.14	112.16
1	B	41	GLU	CB-CG-CD	8.54	127.12	112.60
1	A	66	ASN	CA-C-N	8.53	131.52	120.44
1	A	66	ASN	C-N-CA	8.53	131.52	120.44
1	A	99	ILE	O-C-N	-8.47	114.20	121.57
1	B	8	GLN	CB-CG-CD	8.46	126.99	112.60
1	A	12	ASN	N-CA-C	8.45	120.27	111.14
1	B	78	LYS	N-CA-C	-8.39	103.17	113.15
1	B	130	ALA	CA-C-N	8.37	131.84	120.54
1	B	130	ALA	C-N-CA	8.37	131.84	120.54
1	B	103	TYR	N-CA-CB	8.35	122.52	110.16
1	B	115	LEU	O-C-N	-8.31	113.51	122.07
1	A	41	GLU	CB-CG-CD	8.28	126.68	112.60
1	A	140	ASN	CB-CG-ND2	8.27	128.80	116.40
1	B	135	LEU	O-C-N	8.20	132.89	122.23
1	B	152	GLN	CB-CG-CD	8.19	126.52	112.60
1	A	33	PHE	O-C-N	8.14	130.88	122.09
1	B	63	LYS	CA-C-O	-8.14	112.31	120.70
1	B	94	ALA	CA-C-N	8.12	134.26	120.71
1	B	94	ALA	C-N-CA	8.12	134.26	120.71
1	B	51	SER	N-CA-CB	-8.10	98.13	111.66
1	B	117	SER	CB-CA-C	-8.09	98.17	110.88
1	B	87	THR	O-C-N	8.09	125.85	120.27
1	A	52	GLU	CA-C-O	8.08	129.35	120.63
1	A	13	VAL	N-CA-C	-8.05	101.03	111.09
1	A	91	GLN	CG-CD-NE2	8.04	128.46	116.40
1	A	69	LEU	CA-C-O	-8.04	109.35	119.31
1	A	87	THR	O-C-N	8.03	125.81	120.27
1	A	75	ILE	CA-C-O	8.01	129.28	120.71
1	A	70	THR	O-C-N	-7.94	113.52	122.09
1	A	149	LEU	CA-C-N	7.93	136.94	121.41
1	A	149	LEU	C-N-CA	7.93	136.94	121.41
1	B	3	SER	CA-C-O	7.92	131.02	121.99
1	A	139	ARG	CB-CA-C	-7.91	98.47	110.88
1	A	24	HIS	CA-C-O	-7.88	112.58	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	HIS	O-C-N	7.88	133.34	122.46
1	B	12	ASN	CA-C-N	7.87	133.82	120.29
1	B	12	ASN	C-N-CA	7.87	133.82	120.29
1	A	106	PHE	O-C-N	7.86	130.45	122.12
1	A	31	ARG	NE-CZ-NH2	-7.82	112.16	119.20
1	A	45	LYS	N-CA-CB	-7.82	97.27	110.49
1	A	81	HIS	CA-CB-CG	-7.80	106.00	113.80
1	A	91	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	B	112	ILE	CA-C-O	-7.77	112.87	120.95
1	B	8	GLN	CA-C-N	7.76	131.01	120.54
1	B	8	GLN	C-N-CA	7.76	131.01	120.54
1	A	135	LEU	CA-C-N	-7.74	108.54	120.31
1	A	135	LEU	C-N-CA	-7.74	108.54	120.31
1	A	142	MET	N-CA-C	-7.74	102.79	111.07
1	B	141	ASP	CA-C-O	7.70	128.58	120.42
1	A	107	ILE	CA-C-N	7.69	130.59	120.28
1	A	107	ILE	C-N-CA	7.69	130.59	120.28
1	A	61	LEU	N-CA-C	-7.66	102.87	111.14
1	A	37	PRO	O-C-N	7.64	131.03	122.24
1	B	46	PHE	CA-C-O	-7.64	111.21	119.08
1	B	151	PHE	CA-C-N	7.63	136.12	121.54
1	B	151	PHE	C-N-CA	7.63	136.12	121.54
1	A	148	GLU	N-CA-C	7.63	119.67	111.36
1	A	2	LEU	O-C-N	7.62	132.88	123.21
1	B	70	THR	N-CA-C	-7.61	101.88	112.45
1	B	34	LYS	N-CA-CB	7.57	121.95	110.30
1	B	82	HIS	N-CA-CB	-7.56	98.94	111.49
1	A	38	GLU	CA-CB-CG	7.55	129.21	114.10
1	B	140	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	126	ASP	CA-C-O	-7.53	110.89	120.31
1	A	93	HIS	CA-CB-CG	-7.53	106.27	113.80
1	A	111	ILE	CA-C-N	7.50	131.06	120.42
1	A	111	ILE	C-N-CA	7.50	131.06	120.42
1	A	47	LYS	CA-C-O	7.46	128.53	120.10
1	A	124	GLY	CA-C-N	7.45	131.26	120.38
1	A	124	GLY	C-N-CA	7.45	131.26	120.38
1	B	4	ASP	O-C-N	7.45	131.43	122.27
1	A	117	SER	N-CA-CB	7.42	120.78	110.01
1	B	132	SER	CA-CB-OG	-7.42	96.27	111.10
1	A	109	GLU	O-C-N	7.41	130.09	122.09
1	A	49	LEU	CB-CA-C	7.41	121.94	109.80
1	A	127	ALA	N-CA-C	-7.40	103.22	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	LYS	N-CA-CB	7.38	121.58	110.22
1	A	32	LEU	CA-C-N	7.37	130.46	120.44
1	A	32	LEU	C-N-CA	7.37	130.46	120.44
1	B	34	LYS	O-C-N	7.36	132.19	122.33
1	A	142	MET	O-C-N	7.35	129.64	122.07
1	A	138	PHE	CA-CB-CG	-7.33	106.47	113.80
1	A	128	GLN	CG-CD-OE1	-7.30	106.19	120.80
1	A	6	GLU	N-CA-C	-7.25	103.31	111.14
1	A	39	THR	CA-C-O	7.24	128.29	119.38
1	A	5	GLY	CA-C-N	7.23	130.28	120.44
1	A	5	GLY	C-N-CA	7.23	130.28	120.44
1	B	34	LYS	CB-CA-C	-7.21	95.68	110.38
1	B	129	GLY	CA-C-O	7.18	127.83	120.80
1	A	78	LYS	CB-CA-C	-7.17	97.11	110.01
1	A	123	PHE	O-C-N	7.16	132.11	122.59
1	B	66	ASN	CA-C-N	7.15	129.74	120.44
1	B	66	ASN	C-N-CA	7.15	129.74	120.44
1	B	59	GLU	CB-CA-C	-7.15	98.70	110.85
1	B	151	PHE	CA-C-O	7.09	128.69	120.96
1	B	83	GLU	OE1-CD-OE2	7.08	139.88	122.90
1	B	101	VAL	CB-CA-C	7.05	121.95	112.22
1	A	67	THR	CA-C-O	-7.03	113.44	120.82
1	B	85	GLU	N-CA-CB	7.01	120.24	110.07
1	B	75	ILE	CB-CA-C	7.01	121.63	112.24
1	A	14	TRP	CB-CG-CD1	7.00	137.40	126.90
1	A	70	THR	CA-C-N	7.00	129.54	120.44
1	A	70	THR	C-N-CA	7.00	129.54	120.44
1	A	36	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	121	GLY	CA-C-N	6.98	135.04	122.06
1	A	121	GLY	C-N-CA	6.98	135.04	122.06
1	A	22	ALA	CA-C-O	-6.97	113.16	120.55
1	B	64	HIS	O-C-N	-6.96	114.74	122.12
1	B	44	ASP	CA-CB-CG	-6.96	105.64	112.60
1	A	101	VAL	CA-C-O	-6.90	113.53	120.85
1	A	60	ASP	CA-C-N	6.90	129.82	120.44
1	A	60	ASP	C-N-CA	6.90	129.82	120.44
1	B	33	PHE	O-C-N	6.89	129.43	122.12
1	B	56	LYS	CA-C-O	-6.88	110.11	119.05
1	A	114	VAL	O-C-N	-6.87	115.20	121.87
1	B	12	ASN	CB-CG-OD1	-6.86	107.08	120.80
1	B	14	TRP	O-C-N	-6.86	113.83	122.27
1	B	66	ASN	CA-CB-CG	6.85	119.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	LEU	CA-C-O	6.84	127.83	120.10
1	A	24	HIS	O-C-N	6.84	129.48	122.09
1	B	122	ASP	CA-C-O	6.84	127.66	119.59
1	A	100	PRO	CA-C-O	-6.83	113.42	121.95
1	B	152	GLN	CA-C-O	6.82	130.26	120.51
1	B	54	GLU	CA-C-N	6.81	129.30	120.44
1	B	54	GLU	C-N-CA	6.81	129.30	120.44
1	B	31	ARG	O-C-N	-6.80	114.91	122.12
1	A	82	HIS	CA-C-N	6.79	129.86	120.63
1	A	82	HIS	C-N-CA	6.79	129.86	120.63
1	B	83	GLU	N-CA-C	6.77	119.52	111.33
1	B	27	GLU	O-C-N	-6.73	114.35	122.22
1	B	86	LEU	CB-CA-C	6.73	123.34	109.95
1	B	127	ALA	CA-C-N	6.73	130.14	120.79
1	B	127	ALA	C-N-CA	6.73	130.14	120.79
1	B	152	GLN	CA-CB-CG	6.71	127.53	114.10
1	A	61	LEU	CA-C-N	6.66	129.86	120.28
1	A	61	LEU	C-N-CA	6.66	129.86	120.28
1	A	38	GLU	O-C-N	6.64	129.99	122.22
1	A	95	THR	N-CA-C	6.63	121.65	113.50
1	A	6	GLU	CA-CB-CG	-6.62	100.86	114.10
1	B	15	GLY	CA-C-N	6.62	129.44	120.44
1	B	15	GLY	C-N-CA	6.62	129.44	120.44
1	A	21	VAL	CB-CA-C	6.61	120.68	112.02
1	A	83	GLU	CG-CD-OE1	6.60	133.58	118.40
1	A	12	ASN	CA-CB-CG	-6.60	106.00	112.60
1	B	136	GLU	CG-CD-OE2	-6.59	103.23	118.40
1	A	116	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	A	25	GLY	CA-C-O	6.59	127.84	121.05
1	B	139	ARG	CB-CA-C	-6.59	100.54	110.88
1	A	42	LYS	O-C-N	6.58	131.25	122.43
1	A	132	SER	O-C-N	-6.58	114.18	122.27
1	B	136	GLU	CB-CG-CD	-6.57	101.43	112.60
1	B	107	ILE	CA-C-N	6.56	128.97	120.44
1	B	107	ILE	C-N-CA	6.56	128.97	120.44
1	A	148	GLU	N-CA-CB	-6.55	100.46	110.16
1	B	32	LEU	CA-C-N	6.54	129.04	120.28
1	B	32	LEU	C-N-CA	6.54	129.04	120.28
1	B	57	ALA	CA-C-O	6.49	127.45	119.79
1	B	72	LEU	CA-C-O	-6.49	114.00	120.82
1	A	126	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	85	GLU	CB-CA-C	-6.47	100.67	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	O-C-N	6.45	131.01	122.30
1	B	14	TRP	CB-CG-CD1	6.44	136.56	126.90
1	B	109	GLU	OE1-CD-OE2	6.43	138.32	122.90
1	A	61	LEU	N-CA-CB	6.41	119.37	110.07
1	A	79	LYS	CA-CB-CG	6.41	126.92	114.10
1	B	9	LEU	CA-C-N	6.41	128.63	120.56
1	B	9	LEU	C-N-CA	6.41	128.63	120.56
1	B	74	GLY	CA-C-O	6.39	127.91	121.00
1	A	83	GLU	CA-C-N	6.39	129.48	120.28
1	A	83	GLU	C-N-CA	6.39	129.48	120.28
1	B	39	THR	CA-CB-OG1	-6.38	100.03	109.60
1	A	12	ASN	CA-C-N	6.38	130.76	120.30
1	A	12	ASN	C-N-CA	6.38	130.76	120.30
1	B	83	GLU	CB-CG-CD	-6.37	101.77	112.60
1	B	75	ILE	CA-C-O	6.36	127.52	120.71
1	B	152	GLN	CA-C-N	6.36	133.15	121.70
1	B	152	GLN	C-N-CA	6.36	133.15	121.70
1	A	8	GLN	CA-C-O	-6.36	113.75	120.55
1	A	50	LYS	O-C-N	6.35	129.93	122.24
1	B	40	LEU	CA-C-O	6.34	127.27	120.55
1	B	53	ASP	O-C-N	-6.34	115.40	122.12
1	B	12	ASN	N-CA-CB	-6.34	100.75	110.13
1	B	63	LYS	O-C-N	6.34	128.93	122.09
1	B	12	ASN	N-CA-C	6.33	119.13	111.40
1	A	107	ILE	N-CA-C	6.33	117.11	110.72
1	B	53	ASP	N-CA-CB	-6.32	100.58	110.06
1	A	123	PHE	CA-CB-CG	-6.31	107.49	113.80
1	B	86	LEU	CA-C-N	-6.31	112.83	119.83
1	B	86	LEU	C-N-CA	-6.31	112.83	119.83
1	A	16	LYS	N-CA-C	-6.31	104.33	111.14
1	B	27	GLU	CA-C-N	6.30	128.62	120.56
1	B	27	GLU	C-N-CA	6.30	128.62	120.56
1	A	18	GLU	CB-CG-CD	-6.30	101.89	112.60
1	A	57	ALA	CA-C-N	6.30	133.57	121.54
1	A	57	ALA	C-N-CA	6.30	133.57	121.54
1	B	19	ALA	N-CA-C	-6.30	105.56	113.18
1	B	106	PHE	N-CA-CB	6.29	119.47	110.16
1	B	10	VAL	CA-C-O	-6.29	114.51	121.17
1	A	14	TRP	CB-CG-CD2	-6.28	118.01	126.80
1	B	97	HIS	CA-C-O	6.26	127.18	120.10
1	B	102	LYS	CA-C-N	6.25	129.17	120.29
1	B	102	LYS	C-N-CA	6.25	129.17	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	A	36	HIS	CA-C-N	6.24	126.43	119.32
1	A	36	HIS	C-N-CA	6.24	126.43	119.32
1	A	42	LYS	CA-CB-CG	-6.23	101.64	114.10
1	A	24	HIS	N-CA-C	-6.20	104.44	111.14
1	A	122	ASP	CA-C-N	6.19	133.37	121.54
1	A	122	ASP	C-N-CA	6.19	133.37	121.54
1	A	14	TRP	CE2-CD2-CE3	6.19	124.99	118.80
1	B	103	TYR	CB-CA-C	-6.18	100.35	110.85
1	B	46	PHE	O-C-N	6.17	130.37	122.04
1	A	20	ASP	N-CA-CB	-6.17	100.07	110.49
1	B	61	LEU	N-CA-C	-6.17	104.11	111.69
1	A	5	GLY	CA-C-O	-6.17	113.49	120.09
1	B	25	GLY	CA-C-O	6.16	127.40	121.05
1	B	117	SER	N-CA-CB	6.15	118.92	110.01
1	A	101	VAL	CB-CA-C	6.13	120.68	112.22
1	B	85	GLU	CA-C-O	-6.13	114.38	120.70
1	B	103	TYR	CA-CB-CG	-6.12	102.88	113.90
1	B	145	LYS	CA-C-O	6.12	127.03	120.24
1	B	14	TRP	CB-CG-CD2	-6.11	118.24	126.80
1	B	58	SER	CA-C-N	6.11	128.97	120.29
1	B	58	SER	C-N-CA	6.11	128.97	120.29
1	A	149	LEU	CB-CA-C	6.10	121.92	110.63
1	A	31	ARG	N-CA-C	6.10	117.93	111.28
1	A	25	GLY	N-CA-C	6.09	120.01	112.64
1	B	67	THR	CA-CB-OG1	-6.08	100.48	109.60
1	B	146	TYR	CB-CA-C	-6.06	101.12	110.81
1	A	82	HIS	N-CA-CB	-6.03	102.51	111.43
1	B	63	LYS	CG-CD-CE	6.03	125.17	111.30
1	B	63	LYS	CA-C-N	6.01	128.33	120.28
1	B	63	LYS	C-N-CA	6.01	128.33	120.28
1	B	71	ALA	CA-C-O	-6.00	114.06	120.42
1	A	117	SER	CB-CA-C	-5.98	101.49	110.88
1	A	146	TYR	CA-C-N	5.98	129.79	120.82
1	A	146	TYR	C-N-CA	5.98	129.79	120.82
1	B	150	GLY	CA-C-N	5.98	129.60	121.05
1	B	150	GLY	C-N-CA	5.98	129.60	121.05
1	B	64	HIS	CA-CB-CG	-5.98	107.82	113.80
1	A	16	LYS	CA-C-O	5.96	126.84	120.70
1	A	127	ALA	O-C-N	-5.96	115.80	122.12
1	A	104	LEU	N-CA-C	-5.94	104.81	111.28
1	B	126	ASP	N-CA-CB	-5.93	101.37	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	O-C-N	5.92	127.93	121.83
1	A	136	GLU	CA-C-O	5.92	126.78	119.97
1	A	42	LYS	CG-CD-CE	-5.92	97.70	111.30
1	A	118	LYS	N-CA-C	5.91	120.77	113.50
1	A	132	SER	CA-CB-OG	-5.90	99.30	111.10
1	B	76	LEU	O-C-N	5.90	128.38	122.12
1	A	90	ALA	CA-C-O	5.87	126.59	119.31
1	B	147	LYS	CA-C-O	5.86	126.97	120.82
1	B	12	ASN	CB-CG-ND2	-5.86	107.62	116.40
1	A	88	PRO	O-C-N	5.83	128.94	122.24
1	B	148	GLU	N-CA-CB	-5.83	100.72	110.39
1	A	28	VAL	N-CA-C	-5.81	104.85	110.72
1	B	6	GLU	N-CA-C	-5.81	104.85	111.07
1	A	144	ALA	O-C-N	5.79	128.04	122.07
1	A	85	GLU	CA-C-O	-5.79	112.93	120.00
1	B	81	HIS	N-CA-CB	5.79	117.01	110.35
1	B	145	LYS	CA-C-N	5.79	128.35	120.54
1	B	145	LYS	C-N-CA	5.79	128.35	120.54
1	B	87	THR	N-CA-CB	5.78	115.89	110.39
1	A	8	GLN	CA-C-N	5.76	128.31	120.54
1	A	8	GLN	C-N-CA	5.76	128.31	120.54
1	A	119	HIS	O-C-N	5.76	126.03	121.20
1	B	14	TRP	CE2-CD2-CE3	5.75	124.55	118.80
1	A	14	TRP	CG-CD2-CE3	-5.74	128.16	133.90
1	A	42	LYS	CA-C-N	-5.72	114.67	123.14
1	A	42	LYS	C-N-CA	-5.72	114.67	123.14
1	B	61	LEU	CA-C-N	5.72	127.94	120.28
1	B	61	LEU	C-N-CA	5.72	127.94	120.28
1	A	85	GLU	O-C-N	5.71	130.68	122.28
1	B	15	GLY	N-CA-C	-5.71	107.25	114.16
1	A	77	LYS	CA-C-N	5.71	132.72	122.38
1	A	77	LYS	C-N-CA	5.71	132.72	122.38
1	A	36	HIS	CA-C-O	-5.70	114.61	121.22
1	A	28	VAL	N-CA-CB	5.69	119.11	110.58
1	B	135	LEU	CA-C-N	-5.67	111.69	120.31
1	B	135	LEU	C-N-CA	-5.67	111.69	120.31
1	A	61	LEU	CD1-CG-CD2	-5.65	98.36	110.80
1	A	68	VAL	CA-C-O	-5.65	115.08	120.95
1	A	82	HIS	CA-CB-CG	-5.65	108.15	113.80
1	B	105	GLU	N-CA-CB	-5.64	101.54	110.28
1	A	68	VAL	CB-CA-C	5.64	119.75	112.14
1	B	115	LEU	CA-C-O	5.64	126.74	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	PHE	CA-C-O	-5.62	113.29	119.08
1	A	49	LEU	CA-C-O	-5.62	114.19	120.54
1	A	70	THR	N-CA-C	-5.62	105.07	111.14
1	A	93	HIS	CG-CD2-NE2	-5.62	101.58	107.20
1	B	151	PHE	CB-CA-C	5.62	118.28	109.84
1	B	79	LYS	N-CA-C	5.61	122.76	110.80
1	B	24	HIS	N-CA-C	-5.60	105.25	111.36
1	B	8	GLN	CA-C-O	-5.60	114.02	120.24
1	B	22	ALA	CA-C-O	-5.60	114.61	120.55
1	A	2	LEU	N-CA-C	-5.60	100.58	109.59
1	A	59	GLU	N-CA-C	-5.60	105.08	111.07
1	B	11	LEU	CA-C-O	5.59	126.32	119.05
1	A	11	LEU	CA-C-O	5.58	126.40	120.10
1	A	139	ARG	O-C-N	5.56	127.80	122.07
1	B	44	ASP	CA-C-N	5.54	132.13	121.54
1	B	44	ASP	C-N-CA	5.54	132.13	121.54
1	B	111	ILE	N-CA-CB	5.54	116.66	110.51
1	A	30	ILE	CA-C-N	5.54	127.70	120.28
1	A	30	ILE	C-N-CA	5.54	127.70	120.28
1	B	133	LYS	O-C-N	5.53	127.76	122.07
1	B	6	GLU	CB-CG-CD	-5.53	103.21	112.60
1	B	132	SER	CA-C-O	5.53	126.28	120.42
1	A	86	LEU	CA-C-N	-5.52	113.70	119.83
1	A	86	LEU	C-N-CA	-5.52	113.70	119.83
1	A	18	GLU	N-CA-C	5.52	119.63	113.01
1	B	14	TRP	CG-CD2-CE3	-5.51	128.39	133.90
1	B	106	PHE	CA-C-O	-5.50	114.59	120.42
1	B	130	ALA	CB-CA-C	5.49	119.64	110.92
1	B	59	GLU	CG-CD-OE2	-5.47	105.81	118.40
1	B	75	ILE	CA-C-N	5.47	127.61	120.28
1	B	75	ILE	C-N-CA	5.47	127.61	120.28
1	B	146	TYR	N-CA-C	-5.47	104.55	111.11
1	B	33	PHE	CA-CB-CG	-5.47	108.33	113.80
1	B	62	LYS	N-CA-CB	5.46	118.15	110.12
1	A	80	GLY	O-C-N	5.44	127.06	122.71
1	A	6	GLU	CB-CG-CD	-5.43	103.37	112.60
1	B	54	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	118	LYS	CA-C-O	-5.42	113.18	119.14
1	B	59	GLU	O-C-N	5.41	128.32	122.15
1	B	92	SER	O-C-N	-5.41	116.46	122.09
1	A	33	PHE	CB-CA-C	-5.41	102.36	110.90
1	B	93	HIS	CA-CB-CG	-5.40	108.40	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	LYS	CG-CD-CE	5.40	123.72	111.30
1	A	132	SER	N-CA-C	5.39	118.07	111.82
1	A	34	LYS	O-C-N	5.38	128.52	122.22
1	B	24	HIS	CA-C-O	-5.38	114.72	120.42
1	A	17	VAL	N-CA-C	-5.38	105.14	110.62
1	A	84	ALA	O-C-N	5.37	128.50	122.22
1	A	113	GLN	CA-C-O	-5.37	114.86	120.55
1	A	133	LYS	N-CA-CB	-5.36	102.30	110.07
1	B	89	LEU	CB-CA-C	5.35	119.67	110.79
1	A	110	ALA	CA-C-O	5.34	126.62	120.90
1	A	31	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	B	68	VAL	CA-C-O	-5.32	115.53	121.17
1	A	141	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	52	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	34	LYS	CA-C-O	-5.29	113.55	119.79
1	B	116	GLN	CA-C-N	5.28	127.31	120.44
1	B	116	GLN	C-N-CA	5.28	127.31	120.44
1	A	127	ALA	CB-CA-C	5.28	119.56	110.79
1	A	130	ALA	O-C-N	5.28	127.73	122.08
1	A	111	ILE	N-CA-C	5.28	115.90	110.36
1	B	146	TYR	CA-CB-CG	-5.27	104.41	113.90
1	B	58	SER	CA-CB-OG	-5.26	100.58	111.10
1	B	65	GLY	N-CA-C	-5.25	106.43	112.73
1	B	67	THR	CA-C-O	-5.25	115.31	120.82
1	B	139	ARG	O-C-N	5.24	127.47	122.07
1	A	152	GLN	CA-CB-CG	5.24	124.58	114.10
1	A	35	GLY	CA-C-N	5.23	128.28	122.74
1	A	35	GLY	C-N-CA	5.23	128.28	122.74
1	A	89	LEU	CB-CA-C	5.20	119.69	110.85
1	B	6	GLU	CB-CA-C	5.20	119.05	110.88
1	A	35	GLY	CA-C-O	-5.19	111.53	120.57
1	B	143	ALA	O-C-N	5.19	128.29	122.22
1	A	20	ASP	N-CA-C	5.18	121.84	110.80
1	B	14	TRP	N-CA-CB	5.17	118.29	110.28
1	A	64	HIS	CA-C-N	5.16	126.77	120.22
1	A	64	HIS	C-N-CA	5.16	126.77	120.22
1	A	53	ASP	N-CA-CB	-5.15	102.27	109.94
1	A	3	SER	CA-CB-OG	5.14	121.39	111.10
1	A	42	LYS	CB-CG-CD	-5.14	99.47	111.30
1	A	75	ILE	N-CA-CB	-5.14	101.98	110.56
1	A	134	ALA	O-C-N	-5.13	116.69	122.12
1	A	47	LYS	CA-CB-CG	5.12	124.34	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	CA-C-O	5.12	125.98	120.55
1	A	140	ASN	O-C-N	5.12	127.42	122.09
1	A	148	GLU	CA-C-O	5.11	125.84	120.42
1	B	62	LYS	CB-CA-C	-5.11	102.31	110.79
1	A	122	ASP	N-CA-C	5.09	119.49	113.28
1	B	31	ARG	CA-C-O	5.09	125.94	120.55
1	B	86	LEU	N-CA-C	-5.09	107.02	113.18
1	A	91	GLN	O-C-N	-5.09	115.82	122.59
1	B	118	LYS	N-CA-C	5.08	119.55	112.90
1	A	110	ALA	O-C-N	-5.08	116.81	122.09
1	A	39	THR	N-CA-C	-5.07	106.35	112.54
1	A	98	LYS	CA-CB-CG	5.07	124.24	114.10
1	A	140	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	B	53	ASP	CA-C-O	5.06	126.10	120.63
1	B	149	LEU	CA-C-N	5.06	128.66	123.30
1	B	149	LEU	C-N-CA	5.06	128.66	123.30
1	A	2	LEU	N-CA-CB	5.05	118.82	110.69
1	A	116	GLN	CA-C-N	5.05	127.00	120.44
1	A	116	GLN	C-N-CA	5.05	127.00	120.44
1	B	116	GLN	CA-C-O	5.05	126.12	120.82
1	A	142	MET	N-CA-CB	5.04	117.31	110.01
1	A	28	VAL	CA-CB-CG1	5.03	118.95	110.40
1	A	24	HIS	CA-C-N	5.03	125.67	119.99
1	A	24	HIS	C-N-CA	5.03	125.67	119.99
1	B	137	LEU	O-C-N	5.02	127.51	122.09
1	A	64	HIS	N-CA-C	-5.01	105.89	111.36
1	A	153	GLY	N-CA-C	5.01	127.82	113.30
1	B	36	HIS	CA-C-N	5.00	125.27	119.47
1	B	36	HIS	C-N-CA	5.00	125.27	119.47
1	B	74	GLY	O-C-N	-5.00	117.38	122.18

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	1197	0	1205	78	0
1	B	1197	0	1205	75	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
3	A	29	0	0	2	0
3	B	28	0	0	3	0
All	All	2537	0	2470	154	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 31.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HD12	2:A:154:HEM:HAC	1.26	1.13
1:B:2:LEU:HD11	1:B:133:LYS:HB3	1.38	1.05
1:B:52:GLU:HG2	1:B:56:LYS:HE2	1.09	1.04
1:B:52:GLU:CG	1:B:56:LYS:HE2	1.90	1.00
1:B:52:GLU:HG2	1:B:56:LYS:CE	1.97	0.94
1:A:37:PRO:O	1:A:40:LEU:HB3	1.72	0.88
1:B:143:ALA:O	1:B:147:LYS:HE2	1.79	0.82
1:A:99:ILE:CD1	2:A:154:HEM:HAC	2.10	0.81
1:B:44:ASP:HA	1:B:47:LYS:HE3	1.63	0.81
1:A:23:GLY:O	1:A:27:GLU:HG3	1.79	0.80
1:B:59:GLU:O	1:B:63:LYS:HG3	1.83	0.79
1:B:44:ASP:O	1:B:47:LYS:HG2	1.83	0.78
1:A:8:GLN:O	1:A:12:ASN:HB2	1.84	0.77
1:B:8:GLN:O	1:B:12:ASN:HB2	1.83	0.77
1:B:96:LYS:HE2	1:B:97:HIS:CE1	2.21	0.76
1:B:2:LEU:CD1	1:B:133:LYS:HB3	2.19	0.72
1:A:116:GLN:HG2	1:A:123:PHE:HD2	1.54	0.71
1:B:147:LYS:N	1:B:147:LYS:HD3	2.03	0.71
1:A:78:LYS:HA	1:A:78:LYS:HE2	1.73	0.70
1:B:98:LYS:O	1:B:100:PRO:HD3	1.92	0.70
1:B:52:GLU:O	1:B:56:LYS:HG2	1.92	0.69
1:B:90:ALA:HB2	1:B:142:MET:HE3	1.75	0.69
1:A:102:LYS:O	1:A:105:GLU:HB3	1.93	0.68
1:A:101:VAL:H	1:A:152:GLN:HE22	1.42	0.67
1:A:102:LYS:HG3	1:A:106:PHE:CZ	2.30	0.66
1:A:119:HIS:N	1:A:120:PRO:HD3	2.10	0.66
1:B:48:HIS:O	1:B:50:LYS:HD3	1.95	0.65
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ALA:HA	1:A:113:GLN:HE21	1.61	0.65
1:B:96:LYS:HE2	1:B:97:HIS:HE1	1.60	0.63
1:A:96:LYS:O	1:A:98:LYS:HD3	1.99	0.63
1:A:78:LYS:O	1:A:79:LYS:C	2.40	0.62
1:A:101:VAL:HG13	1:A:152:GLN:HE22	1.63	0.62
1:B:99:ILE:HD12	2:B:154:HEM:HAC	1.81	0.61
1:A:46:PHE:HB3	1:A:49:LEU:HD12	1.81	0.61
1:A:44:ASP:HA	1:A:47:LYS:HE2	1.83	0.61
1:B:94:ALA:HA	1:B:151:PHE:CD2	2.37	0.60
1:B:104:LEU:O	1:B:107:ILE:HG22	2.01	0.60
1:A:132:SER:O	1:A:136:GLU:CG	2.51	0.59
2:B:154:HEM:HBC2	2:B:154:HEM:HMC2	1.83	0.59
1:B:90:ALA:CB	1:B:142:MET:HE3	2.33	0.59
1:B:118:LYS:C	1:B:120:PRO:HD3	2.27	0.59
1:A:132:SER:O	1:A:136:GLU:HG2	2.03	0.58
1:A:59:GLU:O	1:A:63:LYS:HG3	2.02	0.58
1:B:119:HIS:N	1:B:120:PRO:HD3	2.19	0.57
1:B:99:ILE:HD12	2:B:154:HEM:CAC	2.35	0.57
1:B:4:ASP:O	1:B:8:GLN:HG2	2.03	0.56
1:B:34:LYS:HD2	1:B:52:GLU:OE2	2.03	0.56
1:B:73:GLY:O	1:B:77:LYS:HG3	2.05	0.56
1:B:84:ALA:O	1:B:88:PRO:HD3	2.06	0.56
1:A:36:HIS:HB2	1:A:39:THR:CG2	2.36	0.56
1:A:116:GLN:HG2	1:A:123:PHE:CD2	2.40	0.55
1:B:87:THR:N	1:B:88:PRO:HD2	2.21	0.55
1:A:95:THR:HG22	1:A:151:PHE:CE2	2.42	0.55
1:B:31:ARG:HD2	3:B:156:HOH:O	2.06	0.55
1:A:99:ILE:HD12	2:A:154:HEM:CAC	2.19	0.54
1:A:13:VAL:HG21	1:A:123:PHE:CD1	2.43	0.53
1:A:36:HIS:CB	1:A:39:THR:HG23	2.38	0.53
1:A:82:HIS:O	1:A:86:LEU:HB2	2.09	0.53
1:B:87:THR:N	1:B:88:PRO:CD	2.71	0.52
1:A:118:LYS:C	1:A:120:PRO:HD3	2.34	0.52
1:A:95:THR:O	1:A:98:LYS:HE2	2.09	0.52
1:A:21:VAL:HG12	1:A:66:ASN:ND2	2.25	0.52
1:A:82:HIS:CD2	1:A:82:HIS:C	2.88	0.52
1:A:86:LEU:HD11	1:A:138:PHE:CE2	2.45	0.52
1:B:151:PHE:CE1	1:B:152:GLN:HG3	2.44	0.51
1:A:10:VAL:HG23	1:A:130:ALA:HB1	1.92	0.51
1:B:44:ASP:HA	1:B:47:LYS:CE	2.39	0.51
1:A:34:LYS:HE2	1:A:52:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:O	1:B:94:ALA:CB	2.59	0.51
1:B:101:VAL:HG13	1:B:152:GLN:HE22	1.75	0.51
1:A:36:HIS:HB2	1:A:39:THR:HG23	1.93	0.50
1:A:40:LEU:O	1:A:40:LEU:HD12	2.11	0.50
1:A:102:LYS:HG3	1:A:106:PHE:CE1	2.46	0.50
1:A:37:PRO:O	1:A:40:LEU:CB	2.54	0.49
1:A:119:HIS:N	1:A:120:PRO:CD	2.75	0.49
1:A:143:ALA:O	1:A:146:TYR:HB2	2.12	0.49
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.94	0.49
1:A:13:VAL:HG21	1:A:123:PHE:HD1	1.76	0.49
1:A:1:GLY:O	1:A:133:LYS:NZ	2.46	0.48
1:B:84:ALA:O	1:B:88:PRO:CD	2.61	0.48
1:B:101:VAL:CG1	1:B:152:GLN:HE22	2.26	0.48
1:A:78:LYS:O	1:A:80:GLY:N	2.46	0.48
1:B:143:ALA:O	1:B:147:LYS:CE	2.59	0.48
1:A:13:VAL:CG1	1:A:131:MET:CE	2.91	0.48
1:B:104:LEU:CD1	1:B:142:MET:HG2	2.44	0.48
1:B:97:HIS:HB2	1:B:99:ILE:HG12	1.95	0.48
1:B:90:ALA:CA	1:B:142:MET:HE3	2.45	0.47
1:A:110:ALA:O	1:A:114:VAL:HG23	2.14	0.47
1:A:132:SER:O	1:A:136:GLU:HG3	2.14	0.47
1:B:146:TYR:HD1	1:B:152:GLN:NE2	2.13	0.47
1:A:43:PHE:O	1:A:44:ASP:C	2.58	0.47
1:B:101:VAL:HG12	1:B:146:TYR:CD1	2.50	0.47
1:A:101:VAL:HG13	1:A:152:GLN:NE2	2.30	0.47
1:B:83:GLU:H	1:B:83:GLU:HG2	1.28	0.46
1:A:22:ALA:O	1:A:26:GLN:HB2	2.16	0.46
1:A:60:ASP:HB2	3:A:168:HOH:O	2.15	0.46
1:A:119:HIS:O	1:A:123:PHE:HB2	2.16	0.46
1:B:13:VAL:O	1:B:16:LYS:HB2	2.16	0.46
1:B:21:VAL:HG23	3:B:171:HOH:O	2.16	0.46
1:A:16:LYS:HD2	1:A:16:LYS:HA	1.63	0.46
1:B:7:TRP:HB3	1:B:79:LYS:HE3	1.97	0.46
1:B:78:LYS:O	1:B:79:LYS:C	2.59	0.46
1:B:130:ALA:O	1:B:133:LYS:HB2	2.15	0.46
1:B:143:ALA:O	1:B:146:TYR:HB2	2.16	0.46
1:A:45:LYS:O	1:A:48:HIS:HE1	1.99	0.45
1:A:97:HIS:HB2	1:A:99:ILE:HG12	1.97	0.45
1:B:7:TRP:CD2	1:B:79:LYS:HG2	2.52	0.45
1:A:13:VAL:CG1	1:A:131:MET:HE2	2.47	0.45
1:A:73:GLY:O	1:A:77:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.82	0.44
1:A:129:GLY:O	1:A:133:LYS:HB2	2.16	0.44
1:B:98:LYS:HE2	1:B:98:LYS:HB3	1.80	0.44
1:B:56:LYS:HG2	1:B:56:LYS:H	1.35	0.44
1:B:85:GLU:O	1:B:88:PRO:HD2	2.18	0.44
1:B:114:VAL:O	1:B:118:LYS:HG3	2.17	0.44
1:A:140:ASN:O	1:A:143:ALA:HB3	2.17	0.44
1:A:104:LEU:O	1:A:107:ILE:HG22	2.18	0.43
1:B:90:ALA:O	1:B:94:ALA:HB3	2.17	0.43
1:B:119:HIS:O	1:B:123:PHE:HB2	2.17	0.43
1:A:82:HIS:NE2	1:A:141:ASP:OD2	2.38	0.43
1:A:107:ILE:O	1:A:110:ALA:HB3	2.17	0.43
1:A:36:HIS:O	1:A:39:THR:HG23	2.19	0.43
1:B:45:LYS:O	1:B:48:HIS:HE1	2.02	0.43
1:B:95:THR:O	1:B:98:LYS:HD2	2.18	0.43
1:A:40:LEU:HD12	1:A:40:LEU:C	2.42	0.43
1:A:77:LYS:C	1:A:79:LYS:H	2.24	0.43
1:A:152:GLN:HE21	1:A:152:GLN:HB3	1.55	0.43
1:A:118:LYS:HB3	1:A:118:LYS:HE3	1.91	0.43
1:B:17:VAL:CG2	1:B:115:LEU:HD21	2.49	0.43
1:B:13:VAL:HG21	1:B:123:PHE:HD1	1.82	0.43
1:A:21:VAL:HG12	1:A:66:ASN:HD22	1.83	0.42
1:A:110:ALA:HA	1:A:113:GLN:NE2	2.30	0.42
1:B:50:LYS:HB2	1:B:54:GLU:OE1	2.20	0.42
1:B:43:PHE:CB	1:B:46:PHE:CD2	3.02	0.42
1:B:43:PHE:N	1:B:43:PHE:CD2	2.86	0.42
1:B:91:GLN:HE21	1:B:91:GLN:HB2	1.52	0.42
1:B:11:LEU:HD21	1:B:76:LEU:O	2.18	0.42
1:B:33:PHE:O	1:B:37:PRO:HA	2.19	0.42
1:A:87:THR:HB	1:A:88:PRO:HD3	2.02	0.41
1:A:68:VAL:HG21	3:A:156:HOH:O	2.21	0.41
1:A:149:LEU:HD23	1:A:149:LEU:HA	1.84	0.41
1:B:16:LYS:HD3	1:B:16:LYS:HA	1.32	0.41
1:A:101:VAL:H	1:A:152:GLN:NE2	2.12	0.41
1:B:26:GLN:HG3	3:B:155:HOH:O	2.21	0.41
1:B:90:ALA:HA	1:B:142:MET:HE3	2.01	0.41
1:A:78:LYS:HA	1:A:78:LYS:CE	2.41	0.41
1:B:47:LYS:HB3	1:B:47:LYS:HE2	1.66	0.41
1:B:97:HIS:CB	1:B:99:ILE:HG12	2.51	0.41
1:B:14:TRP:NE1	1:B:73:GLY:HA2	2.36	0.40
1:A:78:LYS:HE2	1:A:78:LYS:CA	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD23	1:B:9:LEU:HA	1.28	0.40
1:A:43:PHE:N	1:A:43:PHE:CD2	2.90	0.40
1:A:129:GLY:O	1:A:130:ALA:C	2.64	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	151/153 (99%)	138 (91%)	9 (6%)	4 (3%)	4	7
1	B	151/153 (99%)	140 (93%)	8 (5%)	3 (2%)	6	10
All	All	302/306 (99%)	278 (92%)	17 (6%)	7 (2%)	5	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	79	LYS
1	A	45	LYS
1	B	152	GLN
1	A	79	LYS
1	A	128	GLN
1	B	45	LYS

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	124/124 (100%)	104 (84%)	20 (16%)	2	4
1	B	124/124 (100%)	102 (82%)	22 (18%)	2	3
All	All	248/248 (100%)	206 (83%)	42 (17%)	2	4

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	LYS
1	A	26	GLN
1	A	28	VAL
1	A	34	LYS
1	A	41	GLU
1	A	45	LYS
1	A	47	LYS
1	A	50	LYS
1	A	53	ASP
1	A	56	LYS
1	A	61	LEU
1	A	76	LEU
1	A	98	LYS
1	A	101	VAL
1	A	109	GLU
1	A	116	GLN
1	A	133	LYS
1	A	136	GLU
1	A	152	GLN
1	B	12	ASN
1	B	13	VAL
1	B	16	LYS
1	B	26	GLN
1	B	27	GLU
1	B	34	LYS
1	B	40	LEU
1	B	45	LYS
1	B	47	LYS
1	B	50	LYS
1	B	51	SER
1	B	56	LYS
1	B	78	LYS
1	B	83	GLU

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Mol	Chain	Res	Type
1	B	87	THR
1	B	89	LEU
1	B	98	LYS
1	B	101	VAL
1	B	133	LYS
1	B	145	LYS
1	B	147	LYS
1	B	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	26	GLN
1	A	48	HIS
1	A	66	ASN
1	A	113	GLN
1	A	116	GLN
1	A	152	GLN
1	B	91	GLN
1	B	128	GLN
1	B	140	ASN
1	B	152	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	B	154	3,1	50,50,50	1.40	6 (12%)	67,82,82	1.79	16 (23%)
2	HEM	A	154	1	50,50,50	1.44	7 (14%)	67,82,82	1.68	16 (23%)

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
2	HEM	B	154	3,1	-	7/14/54/54	-
2	HEM	A	154	1	-	6/14/54/54	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	FE-NB	4.37	2.08	1.94
2	A	154	HEM	CAB-C3B	3.36	1.56	1.47
2	B	154	HEM	CAC-C3C	3.33	1.56	1.47
2	B	154	HEM	CAB-C3B	3.12	1.55	1.47
2	A	154	HEM	CMB-C2B	3.05	1.57	1.50
2	A	154	HEM	CAC-C3C	2.76	1.54	1.47
2	B	154	HEM	CMB-C2B	2.75	1.56	1.50
2	B	154	HEM	CMD-C2D	2.48	1.55	1.50
2	A	154	HEM	CMC-C2C	2.41	1.55	1.50
2	B	154	HEM	FE-NB	2.40	2.02	1.94
2	A	154	HEM	CMD-C2D	2.19	1.55	1.50
2	A	154	HEM	CAA-C2A	2.05	1.56	1.51
2	B	154	HEM	C1B-NB	-2.04	1.36	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	CHD-C1D-ND	4.65	129.42	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	HEM	O1D-CGD-CBD	-4.33	109.37	123.09
2	A	154	HEM	CAA-CBA-CGA	4.31	125.11	113.67
2	A	154	HEM	O2D-CGD-O1D	4.10	133.86	123.33
2	B	154	HEM	C3D-C4D-ND	-4.03	105.75	110.17
2	A	154	HEM	CHD-C4C-NC	4.03	128.84	124.45
2	B	154	HEM	CMB-C2B-C1B	-3.93	118.90	125.03
2	A	154	HEM	O1D-CGD-CBD	-3.84	110.91	123.09
2	B	154	HEM	O2D-CGD-O1D	3.80	133.09	123.33
2	B	154	HEM	CMD-C2D-C1D	-3.75	119.18	125.03
2	A	154	HEM	CAD-C3D-C4D	-3.43	118.72	124.70
2	A	154	HEM	CAC-C3C-C4C	-3.20	117.17	124.82
2	B	154	HEM	CMD-C2D-C3D	3.08	134.49	126.15
2	A	154	HEM	O1A-CGA-CBA	-2.94	113.75	123.09
2	A	154	HEM	O2A-CGA-CBA	2.89	123.14	114.00
2	B	154	HEM	C4D-ND-C1D	2.78	108.50	105.21
2	B	154	HEM	C4D-C3D-C2D	2.70	110.82	106.89
2	B	154	HEM	CHD-C4C-NC	2.69	127.38	124.45
2	A	154	HEM	CMB-C2B-C1B	-2.67	120.86	125.03
2	B	154	HEM	C3B-C2B-C1B	2.66	108.41	106.41
2	A	154	HEM	CHA-C4D-C3D	2.60	130.02	125.23
2	B	154	HEM	C4C-CHD-C1D	-2.57	120.56	126.02
2	B	154	HEM	CHA-C4D-ND	2.46	127.41	124.37
2	A	154	HEM	CAD-C3D-C2D	2.37	132.31	127.87
2	A	154	HEM	C1A-CHA-C4D	2.37	131.81	126.25
2	A	154	HEM	CHA-C4D-ND	-2.32	121.50	124.37
2	B	154	HEM	CHD-C4C-C3C	-2.31	121.31	125.21
2	B	154	HEM	CMA-C3A-C2A	2.16	130.21	125.62
2	A	154	HEM	CMB-C2B-C3B	2.07	133.43	128.43
2	A	154	HEM	CHD-C4C-C3C	-2.04	121.77	125.21
2	A	154	HEM	CAC-C3C-C2C	2.03	135.02	128.43
2	B	154	HEM	CAC-C3C-C4C	-2.00	120.03	124.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	154	HEM	C2A-CAA-CBA-CGA
2	A	154	HEM	C2C-C3C-CAC-CBC
2	B	154	HEM	C4B-C3B-CAB-CBB
2	A	154	HEM	CAD-CBD-CGD-O1D
2	A	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	CAA-CBA-CGA-O2A

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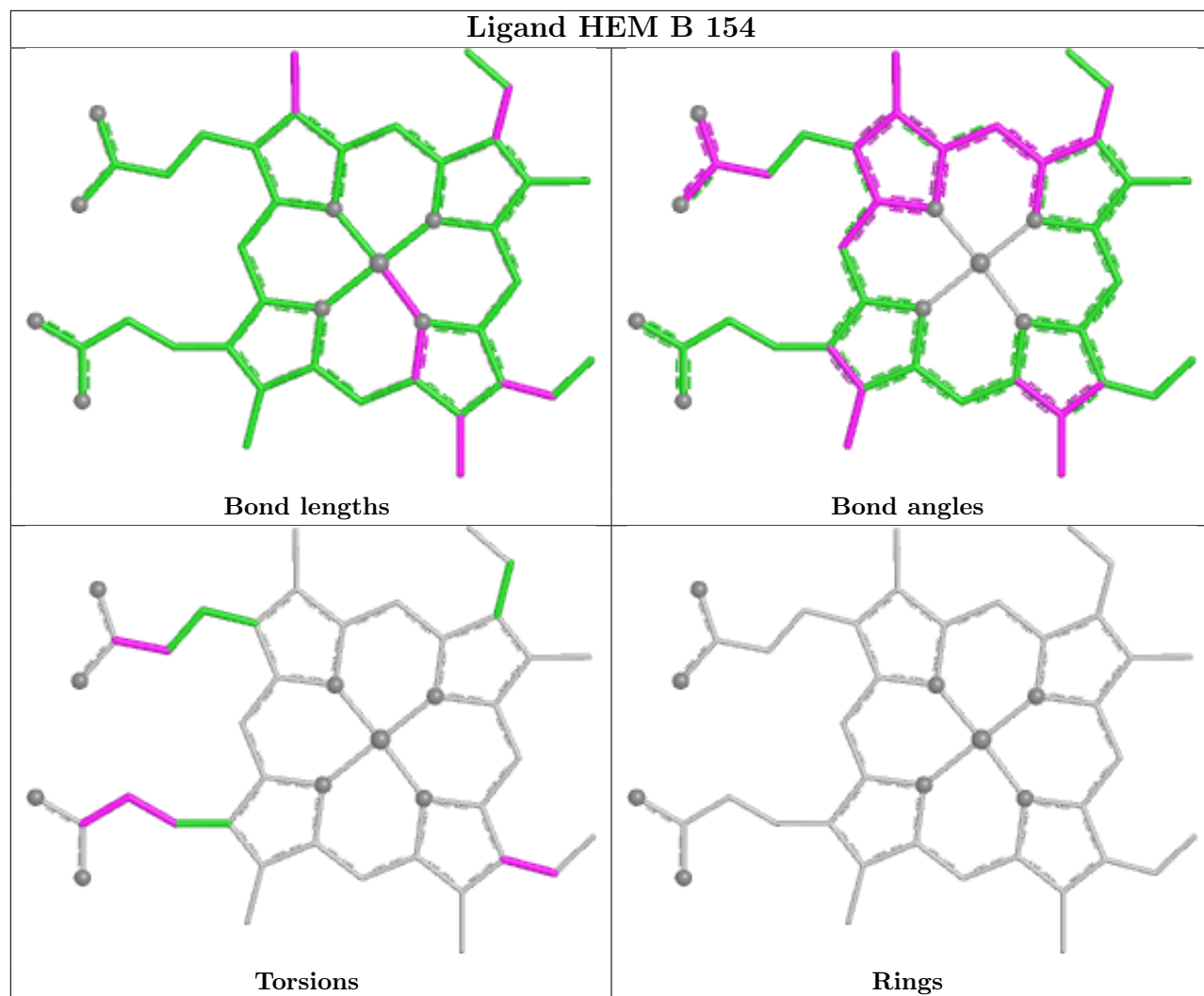
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	CAA-CBA-CGA-O2A
2	B	154	HEM	CAA-CBA-CGA-O1A
2	B	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	C2B-C3B-CAB-CBB
2	A	154	HEM	CAA-CBA-CGA-O1A
2	A	154	HEM	C4C-C3C-CAC-CBC
2	B	154	HEM	CAD-CBD-CGD-O1D

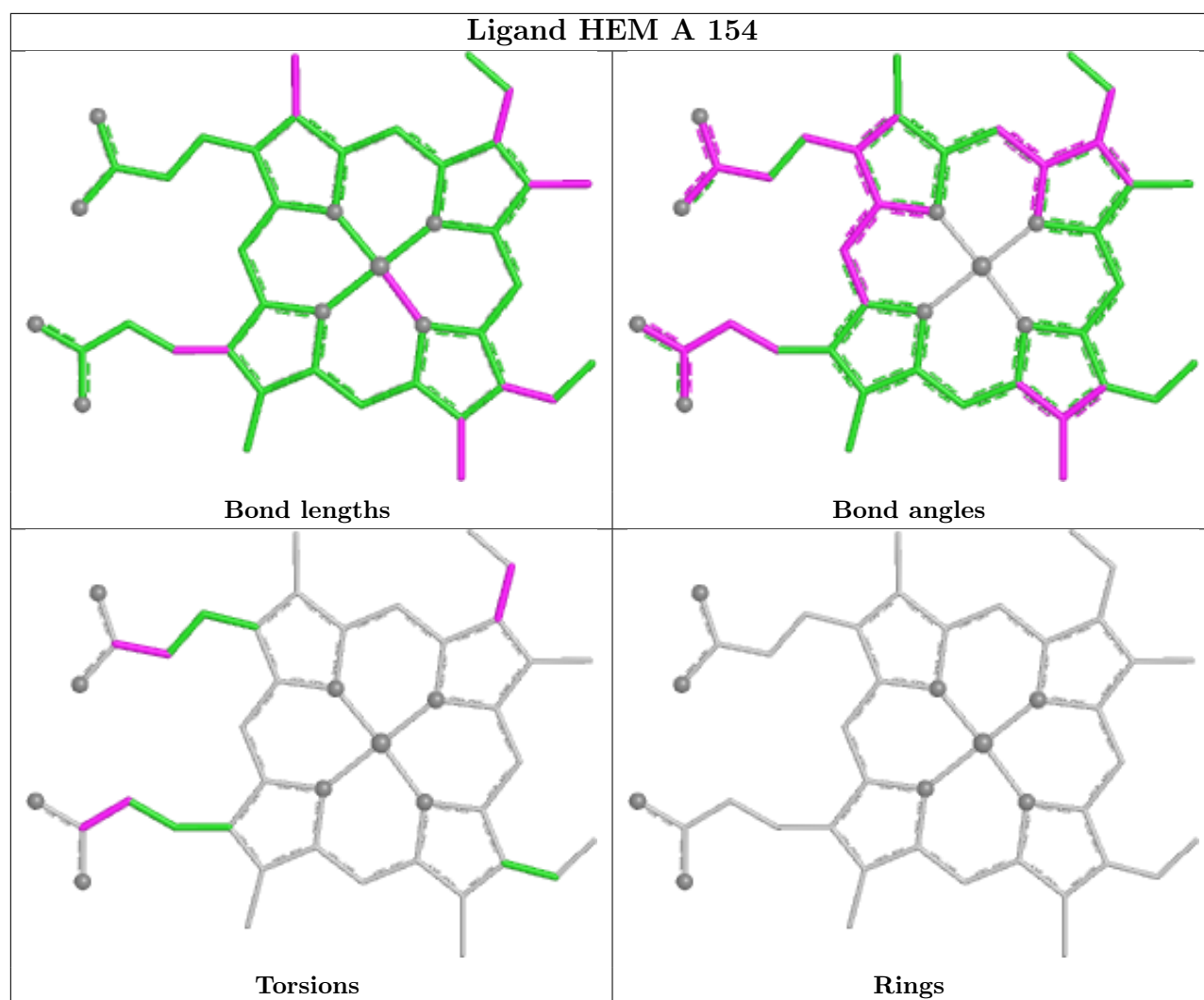
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	HEM	3	0
2	A	154	HEM	3	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.