



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:57 AM EDT

PDB ID : 1FDH / pdb_00001fdh
Title : STRUCTURE OF HUMAN FOETAL DEOXYHAEMOGLOBIN
Authors : Frierjunior, J.A.
Deposited on : 1976-08-18
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

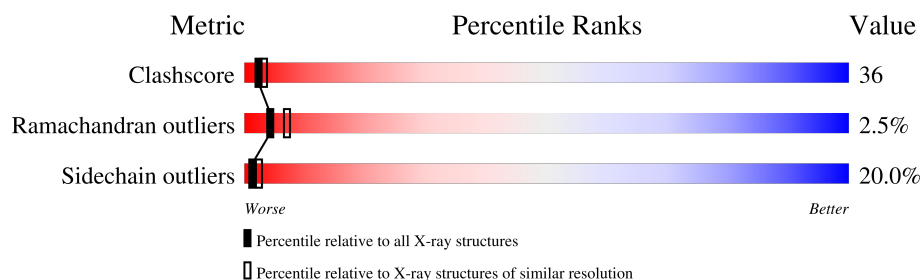
1 Overall quality at a glance

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	141	37% 39% 19% 5%
1	B	141	36% 41% 18% 5%
2	G	147	31% 31% 30% 8%
2	H	147	34% 29% 28% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4576 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.

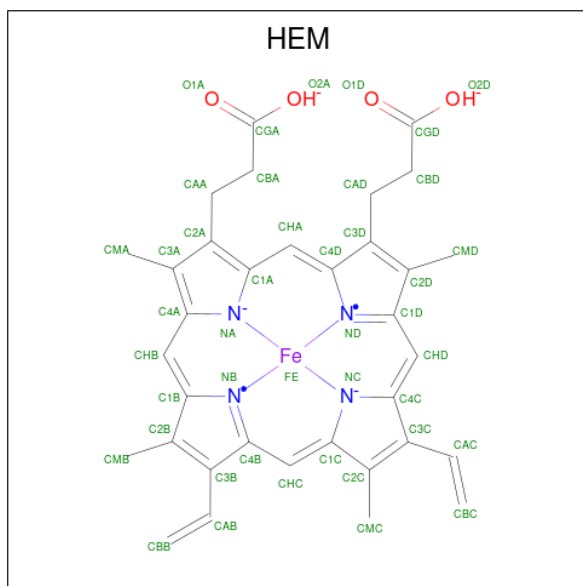
- Molecule 1 is a protein called HEMOGLOBIN F (DEOXY) (ALPHA CHAIN).

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

- Molecule 2 is a protein called HEMOGLOBIN F (DEOXY) (GAMMA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	147	Total	C	N	O	S	0	0	0
			1133	725	193	212	3			
2	H	147	Total	C	N	O	S	0	0	0
			1133	725	193	212	3			

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



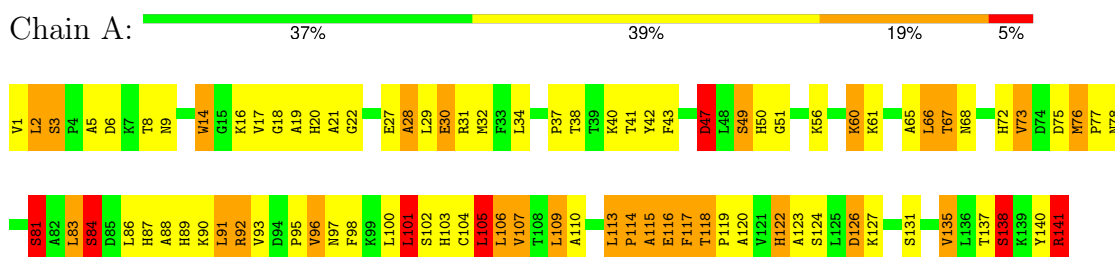
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

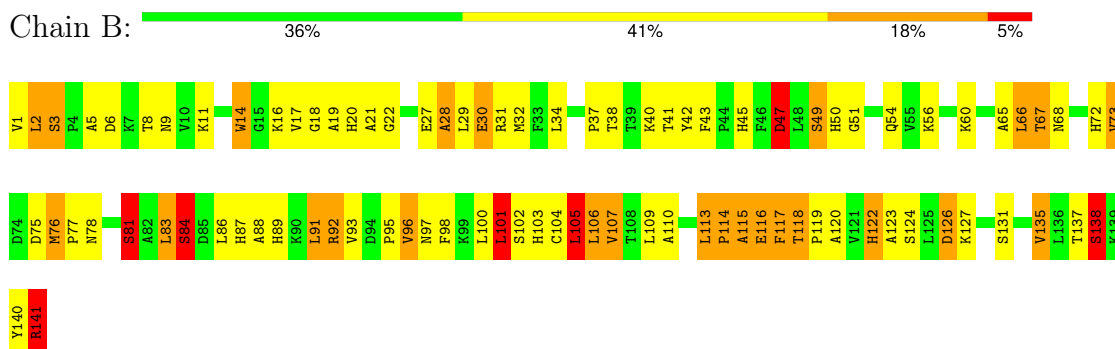
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

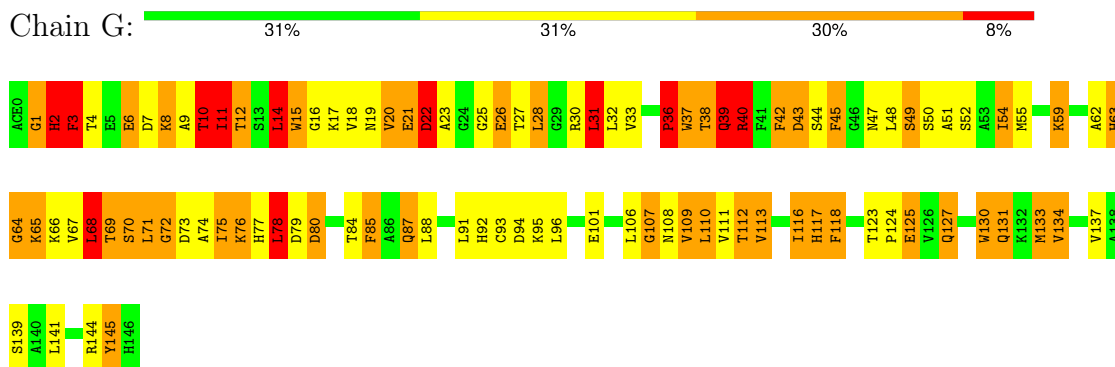
- Molecule 1: HEMOGLOBIN F (DEOXY) (ALPHA CHAIN)



- Molecule 1: HEMOGLOBIN F (DEOXY) (ALPHA CHAIN)

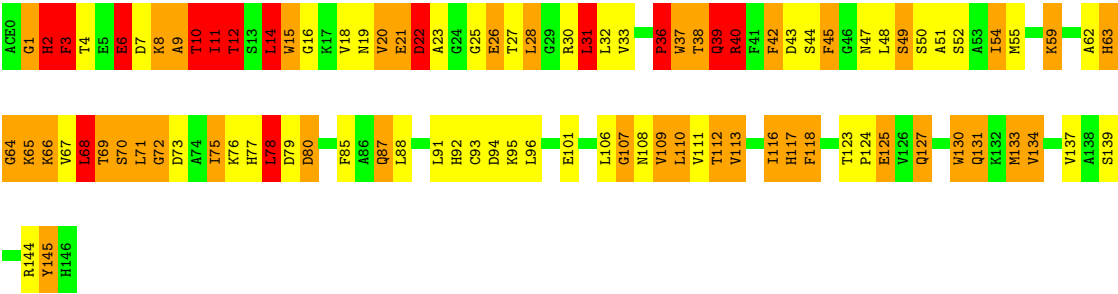


- Molecule 2: HEMOGLOBIN F (DEOXY) (GAMMA CHAIN)



- Molecule 2: HEMOGLOBIN F (DEOXY) (GAMMA CHAIN)

Chain H: 34% 29% 28% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.80Å 95.10Å 102.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4576	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: ACE, 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	0.95	1/1097 (0.1%)	2.14	54/1491 (3.6%)
1	B	0.95	1/1097 (0.1%)	2.14	54/1491 (3.6%)
2	G	1.06	3/1157 (0.3%)	2.43	73/1565 (4.7%)
2	H	1.06	3/1157 (0.3%)	2.43	73/1565 (4.7%)
All	All	1.01	8/4508 (0.2%)	2.29	254/6112 (4.2%)

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	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	130	TRP	NE1-CE2	-8.71	1.27	1.37
2	H	130	TRP	NE1-CE2	-8.67	1.27	1.37
1	B	14	TRP	NE1-CE2	-8.62	1.27	1.37
2	H	15	TRP	NE1-CE2	-8.61	1.27	1.37
1	A	14	TRP	NE1-CE2	-8.61	1.27	1.37
2	G	15	TRP	NE1-CE2	-8.59	1.27	1.37
2	G	37	TRP	NE1-CE2	-8.51	1.28	1.37
2	H	37	TRP	NE1-CE2	-8.49	1.28	1.37

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	GLY	N-CA-C	-26.03	37.82	113.30
2	H	1	GLY	N-CA-C	-26.02	37.85	113.30
1	B	116	GLU	N-CA-C	-23.75	84.59	114.04
1	A	116	GLU	N-CA-C	-23.72	84.62	114.04
2	H	49	SER	N-CA-C	22.15	139.99	113.18
2	G	49	SER	N-CA-C	22.13	139.95	113.18
2	H	42	PHE	N-CA-C	20.58	136.34	110.61
2	G	42	PHE	N-CA-C	20.56	136.31	110.61
2	G	44	SER	N-CA-C	-20.34	88.49	113.50
2	H	44	SER	N-CA-C	-20.30	88.53	113.50
1	B	138	SER	N-CA-C	19.54	134.98	111.33
1	A	138	SER	N-CA-C	19.49	134.91	111.33
2	G	3	PHE	N-CA-C	19.39	141.62	109.24
2	H	3	PHE	N-CA-C	19.39	141.62	109.24
2	H	45	PHE	N-CA-C	16.95	133.68	113.18
2	G	45	PHE	N-CA-C	16.92	133.65	113.18
1	A	47	ASP	N-CA-C	-15.00	84.91	109.07
1	B	47	ASP	N-CA-C	-14.99	84.93	109.07
1	B	5	ALA	N-CA-C	-13.39	95.36	112.23
1	A	5	ALA	N-CA-C	-13.37	95.39	112.23
2	G	9	ALA	N-CA-C	-13.02	95.67	111.69
2	H	9	ALA	N-CA-C	-12.98	95.72	111.69
2	H	38	THR	N-CA-C	-12.81	97.35	113.23
2	G	38	THR	N-CA-C	-12.78	97.39	113.23
1	B	21	ALA	N-CA-C	12.23	126.13	111.33
1	B	126	ASP	N-CA-C	-12.23	97.98	111.07
1	A	21	ALA	N-CA-C	12.22	126.12	111.33
1	A	126	ASP	N-CA-C	-12.19	98.02	111.07
1	A	49	SER	N-CA-C	-10.82	95.25	110.50
1	B	49	SER	N-CA-C	-10.81	95.26	110.50
2	G	94	ASP	N-CA-C	10.80	123.05	111.28
2	G	10	THR	N-CA-C	10.76	122.58	111.07
2	H	94	ASP	N-CA-C	10.73	122.98	111.28
2	H	10	THR	N-CA-C	10.73	122.55	111.07
1	A	91	LEU	N-CA-C	10.54	122.77	111.28
1	B	91	LEU	N-CA-C	10.54	122.77	111.28
1	B	89	HIS	N-CA-C	10.36	127.23	113.97
1	A	89	HIS	N-CA-C	10.34	127.21	113.97
1	A	115	ALA	N-CA-C	10.26	128.44	109.56
1	B	115	ALA	N-CA-C	10.26	128.44	109.56
2	G	39	GLN	N-CA-C	-10.19	99.00	111.33
2	H	39	GLN	N-CA-C	-10.15	99.05	111.33
2	G	14	LEU	N-CA-C	-10.10	100.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	14	LEU	N-CA-C	-10.08	100.37	111.36
2	H	70	SER	N-CA-C	-10.02	100.36	111.28
2	G	70	SER	N-CA-C	-9.98	100.40	111.28
2	G	50	SER	N-CA-C	-9.84	94.38	109.24
1	B	76	MET	N-CA-C	9.81	127.09	113.45
1	A	76	MET	N-CA-C	9.80	127.07	113.45
2	H	50	SER	N-CA-C	-9.79	94.46	109.24
1	B	22	GLY	N-CA-C	-9.60	99.45	113.86
1	A	22	GLY	N-CA-C	-9.59	99.48	113.86
2	G	131	GLN	N-CA-C	-9.54	100.21	112.23
2	H	131	GLN	N-CA-C	-9.53	100.22	112.23
1	B	81	SER	N-CA-C	9.44	122.54	111.02
2	G	109	VAL	N-CA-C	-9.42	101.20	110.72
2	H	109	VAL	N-CA-C	-9.41	101.22	110.72
1	A	81	SER	N-CA-C	9.37	122.45	111.02
1	A	84	SER	N-CA-C	-9.36	101.15	111.36
1	B	84	SER	N-CA-C	-9.36	101.16	111.36
1	B	17	VAL	N-CA-C	-9.31	101.79	110.82
2	G	8	LYS	N-CA-C	9.31	124.44	112.34
2	H	8	LYS	N-CA-C	9.31	124.44	112.34
1	A	17	VAL	N-CA-C	-9.28	101.82	110.82
2	G	111	VAL	N-CA-C	-8.93	99.93	111.09
2	H	111	VAL	N-CA-C	-8.93	99.93	111.09
1	B	138	SER	CB-CA-C	-8.89	95.56	110.68
1	A	138	SER	CB-CA-C	-8.85	95.64	110.68
2	G	16	GLY	N-CA-C	-8.80	104.99	114.67
2	H	42	PHE	CB-CA-C	-8.79	96.23	111.35
2	H	16	GLY	N-CA-C	-8.78	105.01	114.67
2	G	42	PHE	CB-CA-C	-8.76	96.29	111.35
1	A	3	SER	N-CA-C	-8.75	96.03	109.41
2	G	49	SER	CB-CA-C	-8.75	92.55	109.95
2	H	49	SER	CB-CA-C	-8.75	92.55	109.95
1	B	107	VAL	N-CA-C	8.73	119.52	110.62
1	A	107	VAL	N-CA-C	8.72	119.52	110.62
1	B	3	SER	N-CA-C	-8.72	96.07	109.41
2	H	62	ALA	N-CA-C	8.59	120.42	111.14
2	G	62	ALA	N-CA-C	8.55	120.37	111.14
1	A	106	LEU	N-CA-C	-8.52	101.95	111.07
2	G	20	VAL	N-CA-C	8.52	118.60	110.42
1	B	106	LEU	N-CA-C	-8.52	101.95	111.07
2	H	20	VAL	N-CA-C	8.46	118.54	110.42
1	A	122	HIS	N-CA-C	-8.34	102.19	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	HIS	N-CA-C	-8.34	102.19	111.28
2	H	3	PHE	CB-CA-C	-8.19	93.13	109.35
2	G	3	PHE	CB-CA-C	-8.17	93.17	109.35
1	B	8	THR	N-CA-C	-7.99	102.52	111.07
1	A	8	THR	N-CA-C	-7.98	102.53	111.07
2	H	40	ARG	N-CA-C	7.89	127.60	110.80
2	G	76	LYS	N-CA-C	7.88	122.67	112.89
2	H	25	GLY	N-CA-C	-7.88	102.80	113.37
2	G	25	GLY	N-CA-C	-7.88	102.81	113.37
2	H	76	LYS	N-CA-C	7.87	122.65	112.89
1	B	88	ALA	N-CA-C	7.86	119.85	111.28
2	G	40	ARG	N-CA-C	7.85	127.51	110.80
1	B	60	LYS	N-CA-C	-7.83	102.06	111.69
1	A	88	ALA	N-CA-C	7.82	119.80	111.28
1	A	60	LYS	N-CA-C	-7.81	102.08	111.69
2	H	19	ASN	N-CA-C	-7.75	94.35	107.99
2	G	26	GLU	N-CA-C	7.74	121.20	111.69
2	H	26	GLU	N-CA-C	7.73	121.19	111.69
2	H	31	LEU	N-CA-C	-7.68	102.84	111.14
2	G	31	LEU	N-CA-C	-7.66	102.87	111.14
2	G	72	GLY	N-CA-C	-7.65	103.63	112.50
2	H	72	GLY	N-CA-C	-7.64	103.64	112.50
2	G	117	HIS	N-CA-C	7.55	119.30	111.14
2	H	117	HIS	N-CA-C	7.54	119.28	111.14
1	A	19	ALA	N-CA-C	7.39	122.48	113.17
1	B	19	ALA	N-CA-C	7.38	122.47	113.17
1	A	9	ASN	N-CA-C	7.37	119.31	111.28
1	B	92	ARG	N-CA-C	7.36	121.30	111.30
2	H	69	THR	N-CA-C	-7.34	102.98	112.23
1	B	9	ASN	N-CA-C	7.33	119.28	111.28
1	A	92	ARG	N-CA-C	7.31	121.24	111.30
1	A	113	LEU	N-CA-C	-7.29	95.70	108.97
2	G	69	THR	N-CA-C	-7.29	103.04	112.23
2	H	6	GLU	N-CA-C	-7.29	103.64	112.54
2	G	6	GLU	N-CA-C	-7.29	103.65	112.54
1	B	113	LEU	N-CA-C	-7.29	95.71	108.97
2	H	15	TRP	N-CA-C	7.24	121.37	112.54
2	G	15	TRP	N-CA-C	7.22	121.35	112.54
2	G	66	LYS	N-CA-C	-7.22	103.35	111.07
2	H	66	LYS	N-CA-C	-7.21	103.35	111.07
2	G	19	ASN	N-CA-C	-7.21	94.34	107.75
2	G	75	ILE	N-CA-C	-7.18	102.08	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	75	ILE	N-CA-C	-7.18	102.08	111.05
1	A	29	LEU	N-CA-C	7.16	119.09	111.28
1	B	29	LEU	N-CA-C	7.10	119.02	111.28
2	G	36	PRO	N-CA-C	7.08	127.06	112.47
2	H	36	PRO	N-CA-C	7.07	127.03	112.47
2	H	33	VAL	N-CA-C	7.05	119.05	111.58
2	H	85	PHE	N-CA-C	7.03	121.94	112.88
1	B	47	ASP	CB-CA-C	7.03	121.87	109.72
1	A	47	ASP	CB-CA-C	7.02	121.87	109.72
2	G	33	VAL	N-CA-C	7.02	119.02	111.58
2	G	85	PHE	N-CA-C	7.00	121.91	112.88
1	A	20	HIS	N-CA-C	-6.99	104.49	113.16
1	B	20	HIS	N-CA-C	-6.99	104.50	113.16
1	A	65	ALA	N-CA-C	-6.98	103.73	111.82
1	B	65	ALA	N-CA-C	-6.98	103.73	111.82
2	G	59	LYS	N-CA-C	-6.96	103.12	111.69
2	H	59	LYS	N-CA-C	-6.96	103.13	111.69
1	B	56	LYS	N-CA-C	-6.94	103.79	111.36
1	A	56	LYS	N-CA-C	-6.94	103.80	111.36
1	A	100	LEU	N-CA-C	6.93	118.91	111.36
1	B	97	ASN	N-CA-C	6.89	121.43	112.89
1	B	100	LEU	N-CA-C	6.88	118.86	111.36
1	A	97	ASN	N-CA-C	6.83	121.36	112.89
2	H	77	HIS	N-CA-C	-6.83	100.19	109.54
2	G	77	HIS	N-CA-C	-6.81	100.21	109.54
2	H	22	ASP	N-CA-C	6.79	121.30	112.89
1	B	98	PHE	N-CA-C	-6.74	103.73	112.23
1	A	98	PHE	N-CA-C	-6.74	103.74	112.23
2	G	22	ASP	N-CA-C	6.74	121.24	112.89
1	A	95	PRO	N-CA-C	6.65	122.56	113.98
1	B	140	TYR	N-CA-C	6.61	118.49	111.28
1	B	95	PRO	N-CA-C	6.61	122.50	113.98
1	A	140	TYR	N-CA-C	6.61	118.48	111.28
2	H	71	LEU	N-CA-C	6.50	119.69	111.69
2	G	71	LEU	N-CA-C	6.48	119.66	111.69
1	A	51	GLY	N-CA-C	6.43	123.91	115.36
1	B	51	GLY	N-CA-C	6.43	123.91	115.36
2	G	73	ASP	N-CA-C	6.43	120.22	112.38
2	H	73	ASP	N-CA-C	6.42	120.22	112.38
2	H	28	LEU	N-CA-C	-6.41	104.38	111.36
2	G	95	LYS	N-CA-C	6.36	121.56	113.55
2	G	28	LEU	N-CA-C	-6.33	104.45	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	95	LYS	N-CA-C	6.32	121.52	113.55
2	H	18	VAL	N-CA-C	6.31	117.22	108.89
1	A	41	THR	N-CA-C	6.28	120.50	112.34
2	G	18	VAL	N-CA-C	6.28	117.18	108.89
1	A	116	GLU	CB-CA-C	6.23	120.24	109.15
1	B	116	GLU	CB-CA-C	6.23	120.24	109.15
2	G	101	GLU	N-CA-C	-6.22	104.56	111.71
2	H	101	GLU	N-CA-C	-6.20	104.58	111.71
1	B	41	THR	N-CA-C	6.20	120.40	112.34
1	A	123	ALA	N-CA-C	6.17	118.09	111.36
2	G	91	LEU	N-CA-C	6.17	118.98	111.82
1	B	92	ARG	CB-CA-C	-6.16	102.71	111.95
2	H	91	LEU	N-CA-C	6.14	118.94	111.82
1	A	92	ARG	CB-CA-C	-6.14	102.75	111.95
1	B	123	ALA	N-CA-C	6.13	118.05	111.36
2	H	54	ILE	CB-CA-C	-6.10	104.07	112.24
2	G	54	ILE	CB-CA-C	-6.09	104.08	112.24
2	H	45	PHE	CB-CA-C	-6.08	97.86	109.95
2	G	79	ASP	N-CA-C	6.07	119.94	112.54
2	G	45	PHE	CB-CA-C	-6.05	97.92	109.95
2	H	63	HIS	N-CA-C	-6.03	105.42	112.89
2	G	63	HIS	N-CA-C	-6.02	105.42	112.89
2	G	78	LEU	N-CA-C	-5.96	105.28	112.54
2	H	78	LEU	N-CA-C	-5.95	105.28	112.54
2	G	54	ILE	N-CA-C	5.90	117.43	111.00
2	H	54	ILE	N-CA-C	5.86	117.39	111.00
2	H	44	SER	CB-CA-C	5.76	119.78	109.29
2	H	144	ARG	N-CA-C	5.74	123.04	110.80
2	G	144	ARG	N-CA-C	5.73	123.00	110.80
2	G	110	LEU	N-CA-C	5.72	118.29	111.71
2	H	79	ASP	N-CA-C	5.72	119.98	112.89
2	H	110	LEU	N-CA-C	5.72	118.28	111.71
2	G	44	SER	CB-CA-C	5.71	119.69	109.29
2	H	40	ARG	CB-CA-C	-5.71	99.05	110.42
2	G	40	ARG	CB-CA-C	-5.70	99.07	110.42
1	B	43	PHE	N-CA-C	5.63	119.46	110.73
1	A	43	PHE	N-CA-C	5.63	119.46	110.73
2	H	68	LEU	N-CA-C	5.61	119.22	112.38
2	G	68	LEU	N-CA-C	5.58	119.19	112.38
2	H	127	GLN	N-CA-C	-5.57	105.29	111.36
1	A	21	ALA	N-CA-CB	-5.52	101.78	110.06
2	H	64	GLY	N-CA-C	-5.51	106.11	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	64	GLY	N-CA-C	-5.50	106.12	112.50
1	B	21	ALA	N-CA-CB	-5.50	101.81	110.06
1	A	76	MET	CB-CA-C	-5.45	100.47	111.80
2	H	145	TYR	N-CA-C	-5.44	101.41	110.17
1	B	76	MET	CB-CA-C	-5.44	100.48	111.80
2	G	127	GLN	N-CA-C	-5.44	105.27	111.14
2	G	145	TYR	N-CA-C	-5.42	101.45	110.17
2	H	107	GLY	N-CA-C	-5.40	106.25	112.73
2	G	107	GLY	N-CA-C	-5.39	106.26	112.73
1	B	105	LEU	N-CA-C	-5.36	105.09	111.69
2	G	12	THR	N-CA-C	5.35	118.03	111.82
1	A	105	LEU	N-CA-C	-5.35	105.11	111.69
2	H	43	ASP	N-CA-C	-5.34	107.31	112.97
2	H	12	THR	N-CA-C	5.29	117.96	111.82
1	B	96	VAL	N-CA-C	-5.28	104.49	111.09
1	A	104	CYS	N-CA-C	-5.27	106.35	112.89
2	G	43	ASP	N-CA-C	-5.26	107.39	112.97
1	B	30	GLU	N-CA-C	-5.26	105.55	111.28
1	A	30	GLU	N-CA-C	-5.24	105.56	111.28
1	A	96	VAL	N-CA-C	-5.24	104.54	111.09
1	A	115	ALA	N-CA-CB	-5.23	100.64	111.36
1	B	104	CYS	N-CA-C	-5.23	106.40	112.89
1	B	115	ALA	N-CA-CB	-5.22	100.67	111.36
1	B	101	LEU	N-CA-C	-5.18	105.70	112.23
1	A	101	LEU	N-CA-C	-5.17	105.72	112.23
2	G	116	ILE	CA-CB-CG2	-5.17	101.71	110.50
1	A	141	ARG	N-CA-C	-5.16	96.56	111.00
2	H	108	ASN	N-CA-C	5.16	118.73	112.23
2	H	116	ILE	CA-CB-CG2	-5.15	101.74	110.50
1	B	141	ARG	N-CA-C	-5.15	96.58	111.00
2	H	54	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	A	28	ALA	N-CA-C	-5.12	105.60	111.07
1	B	28	ALA	N-CA-C	-5.11	105.60	111.07
2	G	75	ILE	CA-CB-CG2	-5.11	101.81	110.50
2	G	108	ASN	N-CA-C	5.11	118.67	112.23
2	H	75	ILE	CA-CB-CG2	-5.11	101.82	110.50
2	H	11	ILE	CA-CB-CG2	-5.09	101.85	110.50
1	B	81	SER	CB-CA-C	-5.09	102.83	110.92
2	G	11	ILE	CA-CB-CG2	-5.09	101.85	110.50
2	G	118	PHE	N-CA-C	5.07	119.56	113.17
1	A	81	SER	CB-CA-C	-5.06	102.87	110.92
2	G	54	ILE	CA-CB-CG2	-5.06	101.89	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	118	PHE	N-CA-C	5.05	119.53	113.17

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	B	141	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	82	18
1	B	1069	0	1073	81	23
2	G	1133	0	1125	93	15
2	H	1133	0	1125	91	18
3	A	43	0	30	7	0
3	B	43	0	30	6	0
3	G	43	0	30	10	0
3	H	43	0	30	10	0
All	All	4576	0	4516	325	37

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 36.

All (325) 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:B:34:LEU:CD1	2:H:125:GLU:OE2	1.81	1.29
1:A:34:LEU:CD1	2:G:125:GLU:OE2	1.81	1.29
1:B:34:LEU:HD13	2:H:125:GLU:OE2	1.12	1.28
2:G:21:GLU:OE2	2:G:65:LYS:HG3	1.26	1.27
2:H:21:GLU:OE2	2:H:65:LYS:HG3	1.26	1.27
1:A:34:LEU:HD13	2:G:125:GLU:OE2	1.12	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:78:LEU:HD11	2:H:133:MET:HE3	1.21	1.18
2:G:78:LEU:HD11	2:G:133:MET:CE	1.74	1.16
2:H:78:LEU:HD11	2:H:133:MET:CE	1.74	1.15
2:G:22:ASP:OD2	2:G:22:ASP:C	1.90	1.15
2:G:21:GLU:OE2	2:G:65:LYS:CG	1.97	1.13
2:G:113:VAL:HA	2:G:116:ILE:HD12	1.31	1.12
2:H:21:GLU:OE2	2:H:65:LYS:CG	1.97	1.11
2:G:78:LEU:HD11	2:G:133:MET:HE3	1.21	1.10
2:H:113:VAL:HA	2:H:116:ILE:HD12	1.31	1.10
2:H:22:ASP:OD2	2:H:22:ASP:C	1.90	1.08
3:H:147:HEM:HBC2	3:H:147:HEM:HMC2	1.31	1.06
3:G:147:HEM:HMC2	3:G:147:HEM:HBC2	1.31	1.06
1:A:2:LEU:N	1:A:2:LEU:HD23	1.74	1.02
1:B:2:LEU:HD23	1:B:2:LEU:N	1.74	1.01
1:B:118:THR:HG23	1:B:119:PRO:HD2	1.44	0.99
1:A:118:THR:HG23	1:A:119:PRO:HD2	1.44	0.98
1:A:93:VAL:HG11	3:A:142:HEM:HAC	1.48	0.94
2:H:1:GLY:O	2:H:2:HIS:HB3	1.68	0.93
1:B:93:VAL:HG11	3:B:142:HEM:HAC	1.48	0.92
1:A:126:ASP:OD2	1:B:141:ARG:NH2	2.02	0.92
1:A:141:ARG:NH2	1:B:126:ASP:OD2	2.01	0.92
2:G:7:ASP:O	2:G:10:THR:HB	1.69	0.92
2:H:7:ASP:O	2:H:10:THR:HB	1.69	0.91
2:G:78:LEU:CD1	2:G:133:MET:CE	2.48	0.91
2:H:78:LEU:CD1	2:H:133:MET:CE	2.48	0.90
2:G:1:GLY:O	2:G:2:HIS:HB3	1.68	0.89
2:G:78:LEU:CD1	2:G:133:MET:HE3	2.03	0.88
2:H:78:LEU:CD1	2:H:133:MET:HE3	2.03	0.86
2:H:123:THR:HB	2:H:124:PRO:HD2	1.58	0.85
1:A:93:VAL:CG1	3:A:142:HEM:HAC	2.07	0.84
1:B:93:VAL:CG1	3:B:142:HEM:HAC	2.07	0.83
2:H:11:ILE:HD12	2:H:75:ILE:HD12	1.59	0.82
1:A:93:VAL:HG11	3:A:142:HEM:CAC	2.10	0.82
2:G:123:THR:HB	2:G:124:PRO:HD2	1.59	0.82
1:A:113:LEU:O	1:A:114:PRO:C	2.22	0.82
1:B:6:ASP:OD1	1:B:124:SER:OG	1.98	0.82
2:G:11:ILE:HD12	2:G:75:ILE:HD12	1.59	0.81
1:B:93:VAL:HG11	3:B:142:HEM:CAC	2.09	0.81
1:B:113:LEU:O	1:B:114:PRO:C	2.22	0.81
2:G:78:LEU:HD11	2:G:133:MET:HE2	1.63	0.81
2:G:21:GLU:OE2	2:G:65:LYS:CD	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:GLU:OE2	2:H:65:LYS:CD	2.30	0.79
1:A:6:ASP:OD1	1:A:124:SER:OG	1.98	0.79
2:H:78:LEU:HD11	2:H:133:MET:HE2	1.63	0.79
1:B:2:LEU:N	1:B:2:LEU:CD2	2.47	0.78
2:G:4:THR:O	2:G:7:ASP:HB2	1.84	0.77
2:H:4:THR:O	2:H:7:ASP:HB2	1.83	0.77
3:G:147:HEM:HBC2	3:G:147:HEM:CMC	2.15	0.75
1:B:34:LEU:HD11	2:H:125:GLU:OE2	1.85	0.75
1:A:2:LEU:N	1:A:2:LEU:CD2	2.47	0.75
2:G:11:ILE:HD11	2:G:78:LEU:HD21	1.69	0.75
1:A:16:LYS:HE3	1:A:116:GLU:OE2	1.87	0.75
3:H:147:HEM:HBC2	3:H:147:HEM:CMC	2.15	0.74
2:H:11:ILE:HD11	2:H:78:LEU:HD21	1.69	0.74
1:A:141:ARG:OXT	1:B:127:LYS:HD2	1.88	0.74
1:A:127:LYS:HD2	1:B:141:ARG:OXT	1.88	0.74
1:A:113:LEU:HB3	1:A:116:GLU:HG3	1.68	0.74
1:B:16:LYS:HE3	1:B:116:GLU:OE2	1.87	0.73
1:B:113:LEU:HB3	1:B:116:GLU:HG3	1.69	0.73
2:G:11:ILE:HD12	2:G:75:ILE:CD1	2.20	0.72
2:H:11:ILE:HD12	2:H:75:ILE:CD1	2.20	0.72
1:A:34:LEU:HD11	2:G:125:GLU:OE2	1.85	0.72
2:G:22:ASP:OD2	2:G:23:ALA:N	2.23	0.72
2:H:78:LEU:CD1	2:H:133:MET:HE2	2.19	0.72
1:B:27:GLU:O	1:B:31:ARG:HG3	1.90	0.71
1:A:27:GLU:O	1:A:31:ARG:HG3	1.90	0.71
1:A:101:LEU:HD22	1:A:101:LEU:O	1.90	0.71
2:G:78:LEU:CD1	2:G:133:MET:HE2	2.19	0.71
1:B:101:LEU:O	1:B:101:LEU:HD22	1.90	0.70
2:H:22:ASP:OD2	2:H:23:ALA:N	2.23	0.70
2:G:1:GLY:O	2:G:2:HIS:CB	2.40	0.70
2:G:36:PRO:O	2:G:39:GLN:HB2	1.93	0.69
1:B:6:ASP:OD2	1:B:127:LYS:HE2	1.93	0.68
2:H:36:PRO:O	2:H:39:GLN:HB2	1.93	0.67
1:A:6:ASP:OD2	1:A:127:LYS:HE2	1.93	0.66
2:H:1:GLY:O	2:H:2:HIS:CB	2.40	0.66
2:G:54:ILE:HG13	2:G:55:MET:N	2.11	0.65
2:H:3:PHE:N	2:H:3:PHE:CD2	2.63	0.65
2:H:8:LYS:O	2:H:8:LYS:HG2	1.96	0.65
1:A:75:ASP:OD1	1:A:78:ASN:OD1	2.15	0.65
1:A:113:LEU:O	1:A:115:ALA:N	2.30	0.65
2:H:107:GLY:HA3	2:H:134:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:HD21	3:B:142:HEM:HMA3	1.79	0.65
2:G:3:PHE:N	2:G:3:PHE:CD2	2.63	0.64
1:A:83:LEU:HD21	3:A:142:HEM:HMA3	1.79	0.64
1:B:75:ASP:OD1	1:B:78:ASN:OD1	2.15	0.64
2:H:54:ILE:HG13	2:H:55:MET:N	2.12	0.64
2:G:107:GLY:HA3	2:G:134:VAL:HG13	1.78	0.64
2:G:8:LYS:O	2:G:8:LYS:HG2	1.96	0.64
2:G:37:TRP:HB2	1:B:92:ARG:HB3	1.79	0.63
1:B:113:LEU:O	1:B:115:ALA:N	2.30	0.63
2:H:15:TRP:HH2	2:H:68:LEU:CD1	2.12	0.63
1:B:87:HIS:HA	1:B:91:LEU:HB2	1.81	0.63
1:A:92:ARG:HB3	2:H:37:TRP:HB2	1.79	0.63
1:A:127:LYS:HD2	1:B:141:ARG:HG3	1.81	0.63
1:A:87:HIS:HA	1:A:91:LEU:HB2	1.81	0.62
2:G:11:ILE:HD13	2:G:133:MET:HG3	1.81	0.62
2:G:80:ASP:CG	2:G:80:ASP:O	2.43	0.62
2:G:15:TRP:HH2	2:G:68:LEU:CD1	2.12	0.61
2:H:80:ASP:CG	2:H:80:ASP:O	2.43	0.61
2:H:11:ILE:HD13	2:H:133:MET:HG3	1.81	0.61
1:A:141:ARG:HG3	1:B:127:LYS:HD2	1.81	0.61
1:A:118:THR:HG23	1:A:119:PRO:CD	2.26	0.61
2:G:88:LEU:HD11	3:G:147:HEM:HMA1	1.82	0.61
3:H:147:HEM:HMC2	3:H:147:HEM:CBC	2.19	0.60
2:G:22:ASP:OD2	2:G:22:ASP:O	2.20	0.60
2:H:88:LEU:HD11	3:H:147:HEM:HMA1	1.82	0.60
1:A:47:ASP:OD1	1:A:49:SER:OG	2.18	0.60
2:H:65:LYS:O	2:H:69:THR:OG1	2.14	0.60
1:B:101:LEU:O	1:B:101:LEU:CD2	2.50	0.60
1:B:141:ARG:OXT	1:B:141:ARG:HG3	2.02	0.60
1:B:118:THR:HG23	1:B:119:PRO:CD	2.26	0.59
1:A:122:HIS:CE1	2:G:112:THR:HG21	2.37	0.59
1:A:2:LEU:HD23	1:A:2:LEU:H	1.64	0.59
2:G:55:MET:HE3	2:G:55:MET:HA	1.84	0.59
2:H:15:TRP:HH2	2:H:68:LEU:HD13	1.68	0.59
1:B:122:HIS:CE1	2:H:112:THR:HG21	2.37	0.59
1:A:75:ASP:CG	1:A:78:ASN:OD1	2.46	0.59
1:A:101:LEU:HD22	1:A:101:LEU:C	2.27	0.59
1:A:141:ARG:OXT	1:A:141:ARG:HG3	2.02	0.59
1:B:2:LEU:HD23	1:B:2:LEU:H	1.64	0.59
1:A:101:LEU:O	1:A:101:LEU:CD2	2.50	0.59
2:G:65:LYS:O	2:G:69:THR:OG1	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:15:TRP:HH2	2:G:68:LEU:HD13	1.68	0.58
1:A:37:PRO:O	1:A:40:LYS:HB2	2.03	0.58
1:B:103:HIS:HE1	2:H:131:GLN:OE1	1.87	0.58
2:H:14:LEU:HD22	2:H:118:PHE:CZ	2.39	0.58
2:H:55:MET:HE3	2:H:55:MET:HA	1.84	0.58
2:G:38:THR:O	2:G:39:GLN:C	2.47	0.58
1:B:75:ASP:CG	1:B:78:ASN:OD1	2.46	0.58
1:B:101:LEU:HD22	1:B:101:LEU:C	2.28	0.58
1:A:1:VAL:C	1:A:2:LEU:HD23	2.29	0.58
2:G:47:ASN:ND2	2:G:49:SER:OG	2.37	0.57
2:H:47:ASN:ND2	2:H:49:SER:OG	2.37	0.57
1:A:103:HIS:HE1	2:G:131:GLN:OE1	1.87	0.57
1:B:1:VAL:C	1:B:2:LEU:HD23	2.29	0.57
1:B:37:PRO:O	1:B:40:LYS:HB2	2.04	0.57
2:G:14:LEU:HD22	2:G:118:PHE:CZ	2.39	0.57
2:G:28:LEU:HD22	2:G:64:GLY:HA2	1.87	0.56
2:H:22:ASP:OD2	2:H:22:ASP:O	2.20	0.56
2:H:28:LEU:HD22	2:H:64:GLY:HA2	1.87	0.56
3:G:147:HEM:HMC2	3:G:147:HEM:CBC	2.19	0.56
2:H:38:THR:O	2:H:39:GLN:C	2.47	0.56
2:G:8:LYS:O	2:G:8:LYS:CG	2.53	0.56
1:B:2:LEU:HD21	1:B:131:SER:OG	2.06	0.56
1:A:2:LEU:HD21	1:A:131:SER:OG	2.06	0.56
1:A:113:LEU:HB3	1:A:116:GLU:CG	2.36	0.55
2:H:8:LYS:O	2:H:8:LYS:CG	2.53	0.55
2:G:88:LEU:HD21	3:G:147:HEM:CMA	2.37	0.55
1:A:118:THR:HG22	1:A:120:ALA:H	1.72	0.54
2:G:51:ALA:O	2:G:54:ILE:HG12	2.07	0.54
1:B:118:THR:HG22	1:B:120:ALA:H	1.73	0.54
2:H:51:ALA:O	2:H:54:ILE:HG12	2.07	0.54
1:A:31:ARG:HG2	2:G:124:PRO:HB3	1.90	0.54
1:B:113:LEU:HB3	1:B:116:GLU:CG	2.36	0.54
2:H:28:LEU:CD2	2:H:64:GLY:HA2	2.38	0.54
1:A:106:LEU:HD21	1:A:126:ASP:HB2	1.90	0.54
2:H:88:LEU:HD21	3:H:147:HEM:CMA	2.37	0.54
1:A:101:LEU:C	1:A:101:LEU:CD2	2.80	0.54
2:G:15:TRP:CH2	2:G:68:LEU:CD1	2.91	0.54
1:B:31:ARG:HG2	2:H:124:PRO:HB3	1.90	0.54
2:G:28:LEU:HD21	2:G:63:HIS:HD2	1.73	0.54
2:H:28:LEU:HD21	2:H:63:HIS:HD2	1.73	0.54
2:G:70:SER:OG	3:G:147:HEM:HMB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:TRP:CH2	2:H:68:LEU:HD13	2.43	0.54
2:H:70:SER:OG	3:H:147:HEM:HMB2	2.08	0.54
2:H:15:TRP:CH2	2:H:68:LEU:CD1	2.91	0.53
2:G:28:LEU:CD2	2:G:64:GLY:HA2	2.38	0.53
2:H:11:ILE:CD1	2:H:75:ILE:HD12	2.36	0.53
2:H:93:CYS:SG	2:H:145:TYR:HA	2.48	0.53
1:B:101:LEU:CD2	1:B:101:LEU:C	2.80	0.53
2:H:51:ALA:O	2:H:55:MET:HG2	2.09	0.53
2:G:15:TRP:CH2	2:G:68:LEU:HD13	2.43	0.53
1:B:75:ASP:C	1:B:77:PRO:HD2	2.33	0.53
1:B:3:SER:O	1:B:6:ASP:HB2	2.09	0.53
1:B:76:MET:HE1	1:B:131:SER:HB3	1.91	0.53
1:A:28:ALA:CB	1:A:105:LEU:HD12	2.39	0.53
2:G:93:CYS:SG	2:G:145:TYR:HA	2.48	0.53
2:H:113:VAL:CA	2:H:116:ILE:HD12	2.22	0.53
1:A:3:SER:O	1:A:6:ASP:HB2	2.09	0.53
1:B:106:LEU:HD21	1:B:126:ASP:HB2	1.89	0.53
2:G:51:ALA:O	2:G:55:MET:HG2	2.09	0.52
1:B:118:THR:CG2	1:B:119:PRO:HD2	2.28	0.52
1:A:75:ASP:C	1:A:77:PRO:HD2	2.33	0.52
1:A:110:ALA:HB1	2:G:116:ILE:HG13	1.92	0.52
1:B:28:ALA:CB	1:B:105:LEU:HD12	2.39	0.52
2:H:63:HIS:HE1	3:H:147:HEM:C4D	2.28	0.52
1:B:47:ASP:OD1	1:B:49:SER:OG	2.18	0.52
1:A:126:ASP:OD2	1:B:141:ARG:CZ	2.58	0.51
1:A:14:TRP:NE1	1:A:67:THR:OG1	2.31	0.51
1:A:76:MET:HE1	1:A:131:SER:HB3	1.91	0.51
1:A:118:THR:CG2	1:A:119:PRO:HD2	2.28	0.51
2:H:42:PHE:O	2:H:45:PHE:HB2	2.10	0.51
2:G:11:ILE:CD1	2:G:75:ILE:HD12	2.36	0.51
2:G:63:HIS:HE1	3:G:147:HEM:C4D	2.28	0.51
1:B:110:ALA:HB1	2:H:116:ILE:HG13	1.92	0.50
1:B:6:ASP:OD2	1:B:127:LYS:CE	2.59	0.50
1:B:87:HIS:O	1:B:92:ARG:N	2.41	0.50
1:A:118:THR:HG22	1:A:120:ALA:N	2.27	0.50
1:B:118:THR:O	1:B:122:HIS:N	2.38	0.50
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.47	0.50
1:B:42:TYR:CE1	1:B:93:VAL:HA	2.46	0.50
2:G:42:PHE:O	2:G:45:PHE:HB2	2.10	0.50
2:G:107:GLY:HA3	2:G:134:VAL:CG1	2.42	0.50
2:H:123:THR:CB	2:H:124:PRO:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:N	1:A:77:PRO:HD2	2.27	0.49
2:H:7:ASP:O	2:H:10:THR:N	2.45	0.49
2:G:7:ASP:O	2:G:10:THR:N	2.45	0.49
1:A:87:HIS:O	1:A:92:ARG:N	2.41	0.49
1:B:118:THR:HG22	1:B:120:ALA:N	2.27	0.49
2:H:109:VAL:O	2:H:112:THR:HB	2.12	0.49
1:A:141:ARG:CZ	1:B:126:ASP:OD2	2.58	0.49
2:H:11:ILE:CD1	2:H:78:LEU:HD21	2.41	0.49
2:H:107:GLY:HA3	2:H:134:VAL:CG1	2.42	0.49
2:G:109:VAL:O	2:G:112:THR:HB	2.12	0.49
2:G:113:VAL:CA	2:G:116:ILE:HD12	2.22	0.49
1:B:76:MET:N	1:B:77:PRO:HD2	2.27	0.48
2:G:7:ASP:O	2:G:10:THR:CB	2.53	0.48
1:A:6:ASP:OD2	1:A:127:LYS:CE	2.59	0.48
1:B:30:GLU:CD	1:B:50:HIS:HD1	2.21	0.48
3:B:142:HEM:HBD2	3:B:142:HEM:HHA	1.95	0.48
3:A:142:HEM:HBD2	3:A:142:HEM:HHA	1.95	0.48
2:G:11:ILE:CD1	2:G:78:LEU:HD21	2.41	0.48
1:A:30:GLU:CD	1:A:50:HIS:HD1	2.21	0.48
1:B:141:ARG:OXT	1:B:141:ARG:CG	2.62	0.48
1:B:30:GLU:OE1	1:B:50:HIS:ND1	2.43	0.47
2:G:2:HIS:C	2:G:2:HIS:CD2	2.92	0.47
1:A:30:GLU:OE1	1:A:50:HIS:ND1	2.43	0.47
2:H:55:MET:HE3	2:H:55:MET:CA	2.44	0.47
1:A:141:ARG:OXT	1:A:141:ARG:CG	2.62	0.47
1:A:118:THR:O	1:A:122:HIS:N	2.38	0.47
1:B:113:LEU:C	1:B:115:ALA:N	2.71	0.47
1:A:42:TYR:CD1	1:A:93:VAL:HG22	2.49	0.47
1:B:14:TRP:NE1	1:B:67:THR:OG1	2.31	0.47
1:B:42:TYR:CD1	1:B:93:VAL:HG22	2.49	0.47
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.75	0.47
2:H:2:HIS:C	2:H:2:HIS:CD2	2.92	0.47
2:G:28:LEU:HD21	2:G:63:HIS:CD2	2.50	0.47
2:G:27:THR:CG2	2:G:113:VAL:HG21	2.46	0.46
2:G:27:THR:HG21	2:G:110:LEU:HD12	1.97	0.46
2:H:63:HIS:CE1	3:H:147:HEM:C4D	3.04	0.46
2:H:27:THR:CG2	2:H:113:VAL:HG21	2.46	0.46
1:A:113:LEU:C	1:A:115:ALA:N	2.71	0.46
1:A:135:VAL:O	1:A:138:SER:HB2	2.16	0.46
2:H:28:LEU:HD21	2:H:63:HIS:CD2	2.50	0.46
1:A:68:ASN:O	1:A:72:HIS:HD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:63:HIS:CE1	3:G:147:HEM:C4D	3.04	0.46
2:H:72:GLY:O	2:H:75:ILE:HB	2.16	0.46
1:B:66:LEU:HD12	1:B:66:LEU:HA	1.77	0.46
2:G:72:GLY:O	2:G:75:ILE:HB	2.16	0.45
2:G:92:HIS:CD2	2:G:96:LEU:HD12	2.52	0.45
2:H:92:HIS:CD2	2:H:96:LEU:HD12	2.52	0.45
2:G:123:THR:CB	2:G:124:PRO:HD2	2.33	0.45
2:H:27:THR:HG21	2:H:110:LEU:HD12	1.97	0.45
2:H:88:LEU:HD21	3:H:147:HEM:HMA2	1.99	0.45
1:A:31:ARG:NH2	2:G:127:GLN:OE1	2.46	0.45
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.75	0.45
2:G:31:LEU:HD22	2:G:106:LEU:HD13	1.99	0.45
1:B:31:ARG:NH2	2:H:127:GLN:OE1	2.46	0.45
2:H:38:THR:C	2:H:40:ARG:N	2.70	0.45
1:A:32:MET:SD	1:A:101:LEU:HB2	2.57	0.44
1:B:32:MET:SD	1:B:101:LEU:HB2	2.57	0.44
1:B:68:ASN:O	1:B:72:HIS:HD2	1.99	0.44
1:B:16:LYS:HG3	1:B:116:GLU:CD	2.42	0.44
2:H:7:ASP:O	2:H:10:THR:CB	2.53	0.44
2:H:31:LEU:HD22	2:H:106:LEU:HD13	1.99	0.44
1:A:16:LYS:HG3	1:A:116:GLU:CD	2.42	0.44
1:B:86:LEU:CD2	3:B:142:HEM:HBA2	2.47	0.44
1:B:135:VAL:O	1:B:138:SER:HB2	2.16	0.44
2:G:27:THR:HG23	2:G:113:VAL:HG21	2.00	0.44
2:G:55:MET:HE3	2:G:55:MET:CA	2.44	0.44
2:H:27:THR:HG23	2:H:113:VAL:HG21	2.00	0.44
3:H:147:HEM:CMC	3:H:147:HEM:CBC	2.86	0.44
1:B:118:THR:CG2	1:B:120:ALA:H	2.31	0.44
2:H:15:TRP:HH2	2:H:68:LEU:HD11	1.83	0.44
2:H:21:GLU:OE2	2:H:65:LYS:HD2	2.17	0.43
1:A:86:LEU:CD2	3:A:142:HEM:HBA2	2.47	0.43
2:H:39:GLN:HG3	2:H:48:LEU:HD13	2.00	0.43
2:G:38:THR:C	2:G:40:ARG:N	2.70	0.43
2:G:88:LEU:HD21	3:G:147:HEM:HMA2	1.99	0.43
2:G:21:GLU:OE2	2:G:65:LYS:HD2	2.17	0.43
3:G:147:HEM:CMC	3:G:147:HEM:CBC	2.87	0.43
2:G:15:TRP:CE3	2:G:130:TRP:HH2	2.37	0.42
1:A:81:SER:HA	1:A:84:SER:OG	2.19	0.42
2:H:20:VAL:HG13	2:H:68:LEU:HB3	2.01	0.42
1:B:14:TRP:HE1	1:B:67:THR:HG1	1.58	0.42
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:LEU:HD21	2:G:118:PHE:CG	2.54	0.42
2:G:20:VAL:HG13	2:G:68:LEU:HB3	2.02	0.42
2:G:39:GLN:HG3	2:G:48:LEU:HD13	2.01	0.42
2:G:21:GLU:HA	2:G:65:LYS:HB2	2.02	0.42
2:G:28:LEU:HD23	2:G:64:GLY:CA	2.50	0.42
2:H:78:LEU:HD12	2:H:78:LEU:HA	1.72	0.42
2:G:11:ILE:CD1	2:G:75:ILE:CD1	2.94	0.42
2:G:15:TRP:HH2	2:G:68:LEU:HD11	1.83	0.42
1:A:118:THR:CG2	1:A:120:ALA:H	2.31	0.41
1:A:127:LYS:CD	1:B:141:ARG:OXT	2.65	0.41
1:B:81:SER:HA	1:B:84:SER:OG	2.19	0.41
2:H:14:LEU:HD21	2:H:118:PHE:CG	2.54	0.41
2:H:14:LEU:HD21	2:H:118:PHE:CD1	2.55	0.41
2:H:21:GLU:HA	2:H:65:LYS:HB2	2.02	0.41
2:G:78:LEU:HA	2:G:78:LEU:HD12	1.72	0.41
2:H:15:TRP:CE3	2:H:130:TRP:HH2	2.37	0.41
1:B:103:HIS:O	1:B:107:VAL:HG23	2.21	0.41
2:G:14:LEU:HD21	2:G:118:PHE:CD1	2.55	0.41
2:H:28:LEU:HD23	2:H:64:GLY:CA	2.50	0.41
1:A:103:HIS:O	1:A:107:VAL:HG23	2.21	0.41
1:A:117:PHE:CD2	2:G:30:ARG:NH1	2.88	0.41
1:A:127:LYS:NZ	1:B:141:ARG:OXT	2.44	0.41
1:A:93:VAL:HG11	3:A:142:HEM:C3C	2.56	0.41
1:A:141:ARG:OXT	1:B:127:LYS:CD	2.65	0.41
1:A:141:ARG:OXT	1:B:127:LYS:NZ	2.44	0.41
2:G:74:ALA:C	2:G:76:LYS:N	2.76	0.41
1:B:117:PHE:CD2	2:H:30:ARG:NH1	2.88	0.41
2:G:141:LEU:HD23	2:G:141:LEU:HA	1.84	0.41
2:H:8:LYS:O	2:H:12:THR:HB	2.21	0.41
2:H:112:THR:O	2:H:116:ILE:HG13	2.20	0.41
2:G:112:THR:O	2:G:116:ILE:HG13	2.20	0.41
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.82	0.40

All (37) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LYS:CE	2:H:87:GLN:OE1[3_756]	0.79	1.41
1:A:60:LYS:NZ	1:B:54:GLN:CB[2_665]	0.95	1.25
2:G:87:GLN:OE1	2:H:10:THR:CA[4_456]	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:84:THR:O	2:H:6:GLU:CG[4_456]	1.25	0.95
1:B:75:ASP:OD2	2:H:66:LYS:CE[3_756]	1.42	0.78
1:A:60:LYS:CE	1:B:54:GLN:CD[2_665]	1.44	0.76
1:A:60:LYS:NZ	1:B:54:GLN:CA[2_665]	1.44	0.76
1:A:60:LYS:CE	1:B:54:GLN:CG[2_665]	1.45	0.75
1:B:11:LYS:NZ	2:H:87:GLN:OE1[3_756]	1.45	0.75
1:B:75:ASP:OD2	2:H:66:LYS:NZ[3_756]	1.48	0.72
1:A:60:LYS:NZ	1:B:54:GLN:CG[2_665]	1.52	0.68
2:G:17:LYS:CE	2:H:117:HIS:O[1_455]	1.53	0.67
1:A:61:LYS:CE	1:B:45:HIS:CD2[2_665]	1.60	0.60
2:G:17:LYS:NZ	2:H:117:HIS:O[1_455]	1.60	0.60
1:A:90:LYS:CE	2:G:43:ASP:OD2[2_665]	1.63	0.57
1:A:90:LYS:NZ	2:G:43:ASP:OD1[2_665]	1.63	0.57
2:G:117:HIS:O	1:B:114:PRO:CG[1_455]	1.63	0.57
2:G:87:GLN:OE1	2:H:10:THR:N[4_456]	1.71	0.49
1:A:60:LYS:CE	1:B:54:GLN:OE1[2_665]	1.79	0.41
1:B:75:ASP:CG	2:H:66:LYS:CE[3_756]	1.82	0.38
1:A:60:LYS:CG	1:B:54:GLN:NE2[2_665]	1.83	0.37
1:A:90:LYS:CE	2:G:43:ASP:CG[2_665]	1.83	0.37
1:A:90:LYS:CE	2:G:43:ASP:OD1[2_665]	1.88	0.32
1:B:11:LYS:NZ	2:H:87:GLN:CD[3_756]	1.89	0.31
1:A:60:LYS:CE	1:B:54:GLN:CB[2_665]	1.90	0.30
1:A:90:LYS:CD	2:G:43:ASP:OD2[2_665]	1.94	0.26
1:B:11:LYS:CE	2:H:87:GLN:CD[3_756]	1.97	0.23
1:A:60:LYS:CD	1:B:54:GLN:CD[2_665]	1.98	0.22
1:A:60:LYS:CD	1:B:54:GLN:CG[2_665]	2.04	0.16
1:B:11:LYS:CD	2:H:87:GLN:OE1[3_756]	2.06	0.14
2:G:85:PHE:C	2:H:6:GLU:OE2[4_456]	2.09	0.11
1:B:75:ASP:OD1	2:H:66:LYS:CE[3_756]	2.09	0.11
1:A:60:LYS:CD	1:B:54:GLN:NE2[2_665]	2.10	0.10
1:A:60:LYS:NZ	1:B:54:GLN:N[2_665]	2.11	0.09
2:G:87:GLN:OE1	2:H:9:ALA:C[4_456]	2.13	0.07
2:G:85:PHE:CA	2:H:6:GLU:OE2[4_456]	2.19	0.01
2:G:87:GLN:OE1	2:H:9:ALA:O[4_456]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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%)	129 (93%)	6 (4%)	4 (3%)	3	5
1	B	139/141 (99%)	129 (93%)	6 (4%)	4 (3%)	3	5
2	G	145/147 (99%)	134 (92%)	8 (6%)	3 (2%)	5	9
2	H	145/147 (99%)	134 (92%)	8 (6%)	3 (2%)	5	9
All	All	568/576 (99%)	526 (93%)	28 (5%)	14 (2%)	4	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	2	HIS
2	G	40	ARG
2	H	2	HIS
2	H	40	ARG
1	A	18	GLY
2	G	36	PRO
1	B	18	GLY
2	H	36	PRO
1	A	117	PHE
1	B	117	PHE
1	A	114	PRO
1	B	114	PRO
1	A	73	VAL
1	B	73	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	95 (84%)	18 (16%)	2	5
1	B	113/113 (100%)	95 (84%)	18 (16%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	122/122 (100%)	93 (76%)	29 (24%)	1	1
2	H	122/122 (100%)	93 (76%)	29 (24%)	1	1
All	All	470/470 (100%)	376 (80%)	94 (20%)	1	2

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	38	THR
1	A	47	ASP
1	A	66	LEU
1	A	67	THR
1	A	73	VAL
1	A	81	SER
1	A	83	LEU
1	A	84	SER
1	A	96	VAL
1	A	101	LEU
1	A	102	SER
1	A	105	LEU
1	A	109	LEU
1	A	118	THR
1	A	135	VAL
1	A	137	THR
1	A	138	SER
2	G	2	HIS
2	G	3	PHE
2	G	6	GLU
2	G	10	THR
2	G	11	ILE
2	G	12	THR
2	G	14	LEU
2	G	21	GLU
2	G	22	ASP
2	G	26	GLU
2	G	31	LEU
2	G	32	LEU
2	G	39	GLN
2	G	52	SER
2	G	59	LYS
2	G	65	LYS

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Mol	Chain	Res	Type
2	G	67	VAL
2	G	68	LEU
2	G	71	LEU
2	G	78	LEU
2	G	80	ASP
2	G	87	GLN
2	G	112	THR
2	G	113	VAL
2	G	125	GLU
2	G	133	MET
2	G	134	VAL
2	G	137	VAL
2	G	139	SER
1	B	2	LEU
1	B	38	THR
1	B	47	ASP
1	B	66	LEU
1	B	67	THR
1	B	73	VAL
1	B	81	SER
1	B	83	LEU
1	B	84	SER
1	B	96	VAL
1	B	101	LEU
1	B	102	SER
1	B	105	LEU
1	B	109	LEU
1	B	118	THR
1	B	135	VAL
1	B	137	THR
1	B	138	SER
2	H	2	HIS
2	H	3	PHE
2	H	6	GLU
2	H	10	THR
2	H	11	ILE
2	H	12	THR
2	H	14	LEU
2	H	21	GLU
2	H	22	ASP
2	H	26	GLU
2	H	31	LEU

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Mol	Chain	Res	Type
2	H	32	LEU
2	H	39	GLN
2	H	52	SER
2	H	59	LYS
2	H	65	LYS
2	H	67	VAL
2	H	68	LEU
2	H	71	LEU
2	H	78	LEU
2	H	80	ASP
2	H	87	GLN
2	H	112	THR
2	H	113	VAL
2	H	125	GLU
2	H	133	MET
2	H	134	VAL
2	H	137	VAL
2	H	139	SER

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

Mol	Chain	Res	Type
1	A	58	HIS
1	A	72	HIS
1	A	97	ASN
1	A	103	HIS
2	G	2	HIS
2	G	47	ASN
2	G	63	HIS
2	G	77	HIS
2	G	102	ASN
2	G	117	HIS
2	G	131	GLN
1	B	58	HIS
1	B	72	HIS
1	B	97	ASN
1	B	103	HIS
2	H	2	HIS
2	H	47	ASN
2	H	63	HIS
2	H	102	ASN
2	H	117	HIS

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Mol	Chain	Res	Type
2	H	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	G	147	2	50,50,50	1.46	6 (12%)	67,82,82	0.95	3 (4%)
3	HEM	A	142	1	50,50,50	1.67	6 (12%)	67,82,82	0.95	3 (4%)
3	HEM	H	147	2	50,50,50	1.46	6 (12%)	67,82,82	0.95	3 (4%)
3	HEM	B	142	1	50,50,50	1.67	6 (12%)	67,82,82	0.95	3 (4%)

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	G	147	2	-	6/14/54/54	-
3	HEM	A	142	1	-	9/14/54/54	-
3	HEM	H	147	2	-	6/14/54/54	-
3	HEM	B	142	1	-	9/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	142	HEM	FE-NA	5.92	2.14	1.95
3	A	142	HEM	FE-NA	5.91	2.14	1.95
3	B	142	HEM	FE-ND	4.87	2.09	1.94
3	A	142	HEM	FE-ND	4.87	2.09	1.94
3	A	142	HEM	FE-NB	4.58	2.09	1.94
3	B	142	HEM	FE-NB	4.55	2.08	1.94
3	H	147	HEM	FE-NB	4.20	2.07	1.94
3	G	147	HEM	FE-NB	4.20	2.07	1.94
3	A	142	HEM	O2A-CGA	-3.86	1.18	1.30
3	G	147	HEM	O2A-CGA	-3.85	1.18	1.30
3	B	142	HEM	O2A-CGA	-3.85	1.18	1.30
3	H	147	HEM	O2A-CGA	-3.84	1.18	1.30
3	H	147	HEM	FE-NA	3.57	2.06	1.95
3	G	147	HEM	FE-NA	3.55	2.06	1.95
3	G	147	HEM	FE-ND	3.45	2.05	1.94
3	H	147	HEM	FE-ND	3.45	2.05	1.94
3	G	147	HEM	FE-NC	3.41	2.06	1.95
3	H	147	HEM	FE-NC	3.41	2.06	1.95
3	A	142	HEM	FE-NC	2.73	2.04	1.95
3	B	142	HEM	FE-NC	2.72	2.04	1.95
3	A	142	HEM	O2D-CGD	-2.45	1.22	1.30
3	H	147	HEM	O2D-CGD	-2.44	1.22	1.30
3	B	142	HEM	O2D-CGD	-2.44	1.22	1.30
3	G	147	HEM	O2D-CGD	-2.42	1.22	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	147	HEM	CAA-CBA-CGA	-2.23	107.76	113.67
3	A	142	HEM	CAD-CBD-CGD	-2.23	107.76	113.67
3	H	147	HEM	CAA-CBA-CGA	-2.21	107.79	113.67
3	H	147	HEM	CAD-CBD-CGD	-2.21	107.82	113.67
3	A	142	HEM	CAA-CBA-CGA	-2.20	107.83	113.67
3	B	142	HEM	CAD-CBD-CGD	-2.20	107.84	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	142	HEM	CAA-CBA-CGA	-2.18	107.87	113.67
3	G	147	HEM	CAD-CBD-CGD	-2.18	107.88	113.67
3	B	142	HEM	O2A-CGA-CBA	2.12	120.70	114.00
3	H	147	HEM	O2A-CGA-CBA	2.11	120.65	114.00
3	A	142	HEM	O2A-CGA-CBA	2.10	120.64	114.00
3	G	147	HEM	O2A-CGA-CBA	2.10	120.64	114.00

There are no chirality outliers.

All (30) torsion outliers are listed below:

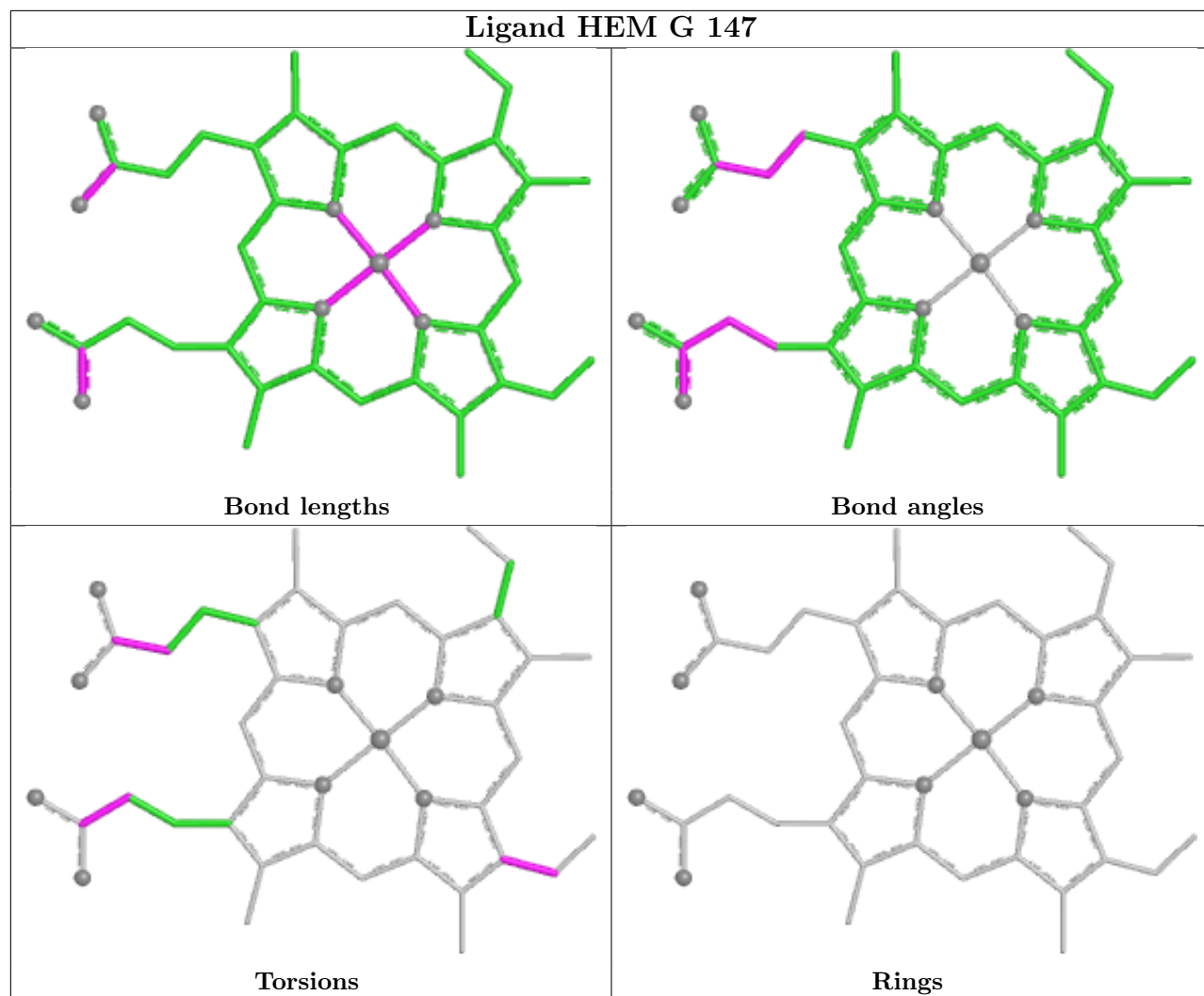
Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C2B-C3B-CAB-CBB
3	A	142	HEM	C2C-C3C-CAC-CBC
3	A	142	HEM	C4C-C3C-CAC-CBC
3	G	147	HEM	C2B-C3B-CAB-CBB
3	G	147	HEM	C4B-C3B-CAB-CBB
3	B	142	HEM	C2B-C3B-CAB-CBB
3	B	142	HEM	C2C-C3C-CAC-CBC
3	B	142	HEM	C4C-C3C-CAC-CBC
3	H	147	HEM	C2B-C3B-CAB-CBB
3	H	147	HEM	C4B-C3B-CAB-CBB
3	A	142	HEM	C4B-C3B-CAB-CBB
3	B	142	HEM	C4B-C3B-CAB-CBB
3	A	142	HEM	C4D-C3D-CAD-CBD
3	B	142	HEM	C4D-C3D-CAD-CBD
3	A	142	HEM	C2D-C3D-CAD-CBD
3	B	142	HEM	C2D-C3D-CAD-CBD
3	G	147	HEM	CAA-CBA-CGA-O1A
3	H	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	B	142	HEM	CAD-CBD-CGD-O1D
3	H	147	HEM	CAA-CBA-CGA-O2A
3	G	147	HEM	CAA-CBA-CGA-O2A
3	B	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	142	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	H	147	HEM	CAD-CBD-CGD-O1D
3	G	147	HEM	CAD-CBD-CGD-O1D
3	G	147	HEM	CAD-CBD-CGD-O2D
3	H	147	HEM	CAD-CBD-CGD-O2D

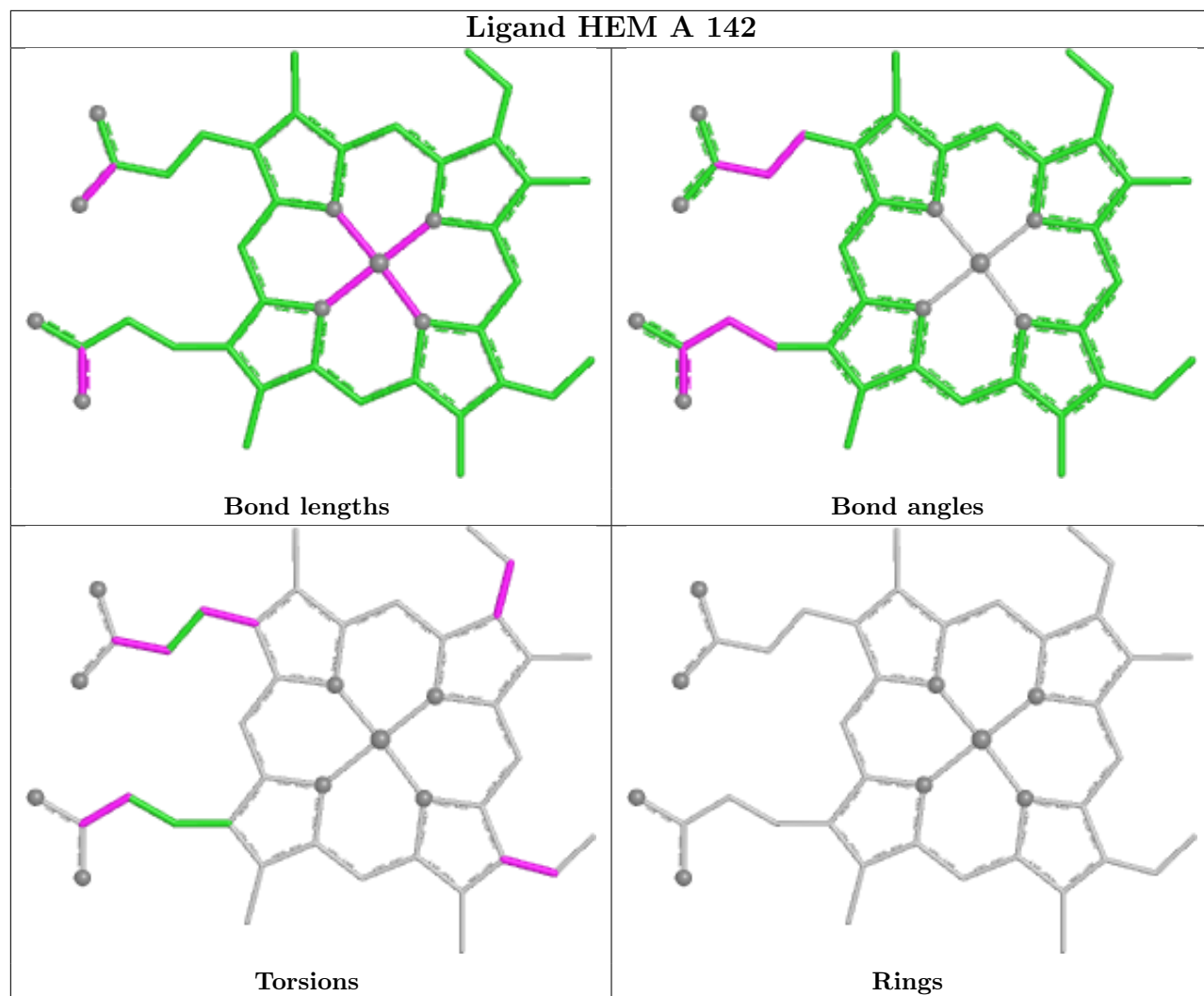
There are no ring outliers.

4 monomers are involved in 33 short contacts:

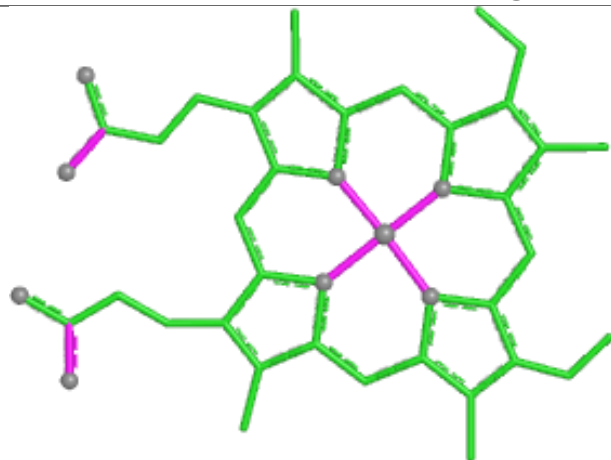
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	147	HEM	10	0
3	A	142	HEM	7	0
3	H	147	HEM	10	0
3	B	142	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

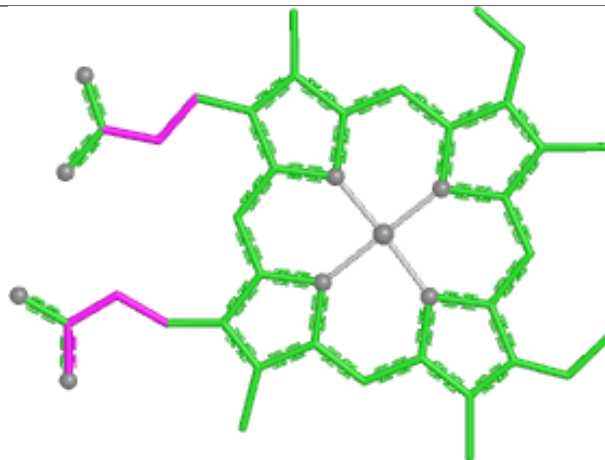




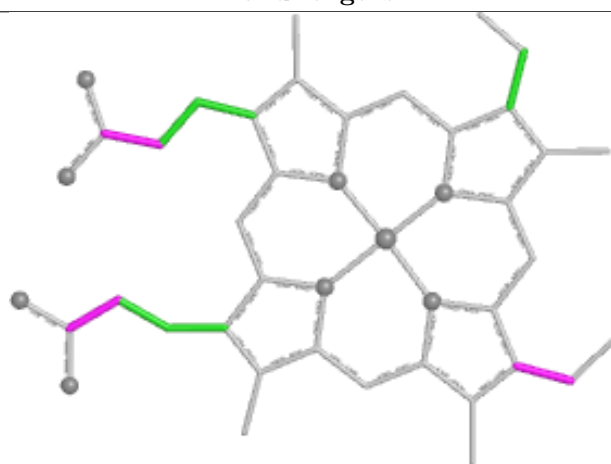
Ligand HEM H 147



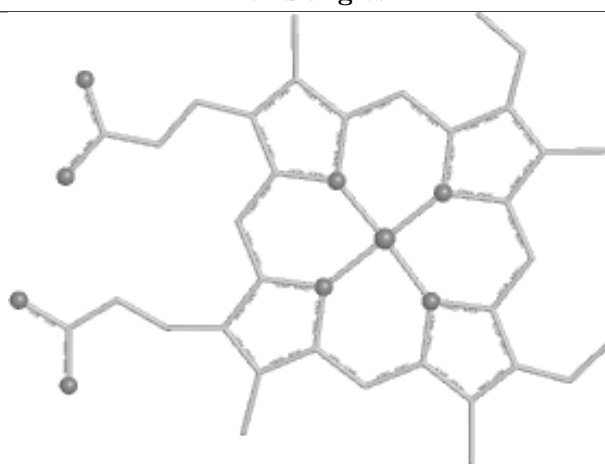
Bond lengths



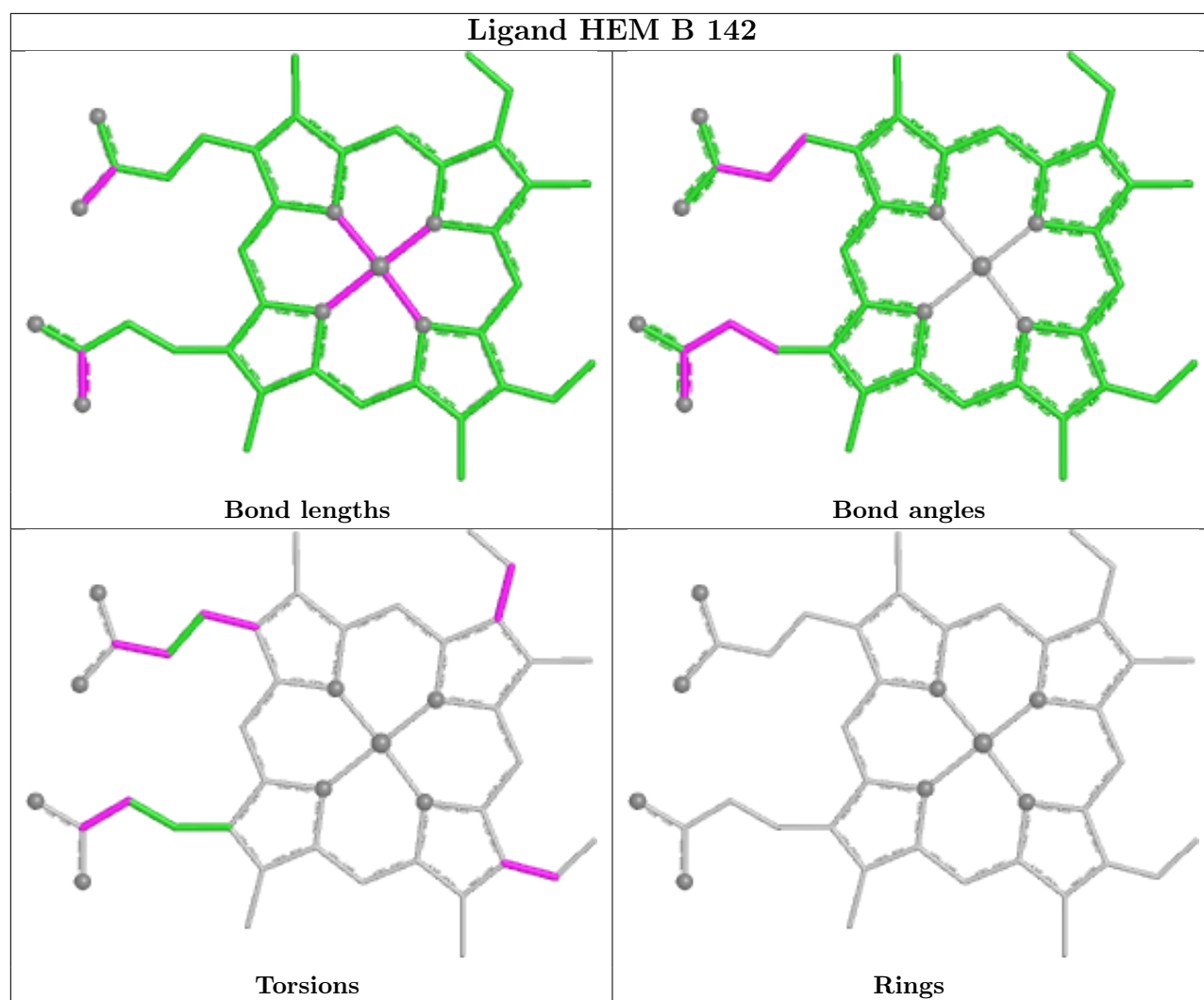
Bond angles



Torsions



Rings



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.