



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:09 pm GMT

PDB ID : 1G5U  
Title : LATEX PROFILIN HEVB8  
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Deposited on : 2000-11-02  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

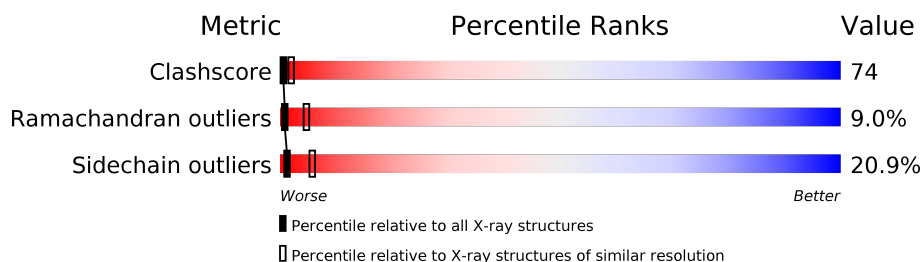
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	131	
1	B	131	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1953 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 PROFILIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			976	614	166	190	6			
1	B	130	Total	C	N	O	S	0	0	0
			976	614	166	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1096	ARG	LYS	CONFLICT	UNP Q9LEI8
B	2096	ARG	LYS	CONFLICT	UNP Q9LEI8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

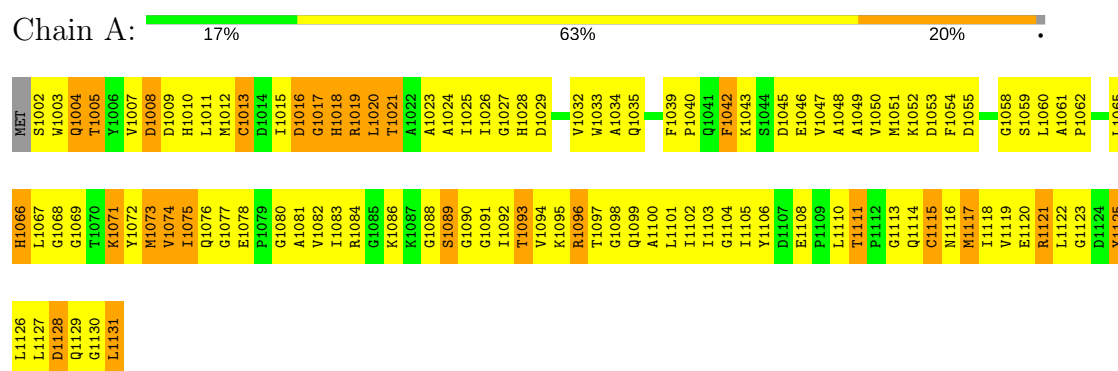
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

### 3 Residue-property plots

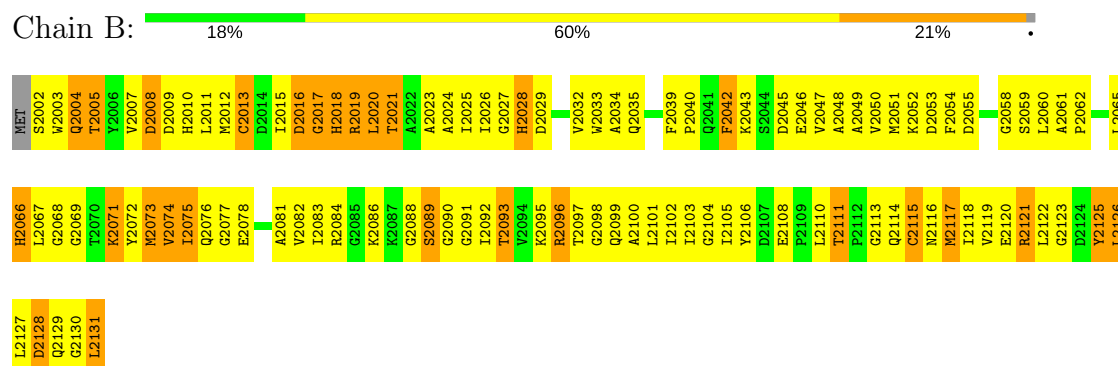
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: PROFILIN



#### • Molecule 1: PROFILIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.88Å 58.88Å 83.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.30 – 3.10	Depositor
% Data completeness (in resolution range)	97.0 (19.30-3.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.259 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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: NA

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	0.52	0/996	0.74	0/1347
1	B	0.52	0/996	0.74	0/1347
All	All	0.52	0/1992	0.74	0/2694

There are no bond length outliers.

There are no bond angle outliers.

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	976	0	955	158	0
1	B	976	0	955	156	0
2	A	1	0	0	0	0
All	All	1953	0	1910	287	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 74.

All (287) 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:2043:LYS:HB3	1:B:2046:GLU:HG3	1.27	1.13
1:A:1043:LYS:HB3	1:A:1046:GLU:HG3	1.30	1.12
1:A:1121:ARG:HG3	1:B:2121:ARG:HG3	1.40	1.03
1:A:1126:LEU:H	1:A:1126:LEU:HD12	1.24	1.00
1:B:2126:LEU:H	1:B:2126:LEU:HD12	1.25	0.96
1:A:1126:LEU:H	1:A:1126:LEU:CD1	1.81	0.93
1:B:2126:LEU:H	1:B:2126:LEU:CD1	1.81	0.92
1:A:1100:ALA:O	1:A:1101:LEU:HD23	1.73	0.88
1:B:2100:ALA:O	1:B:2101:LEU:HD23	1.75	0.86
1:A:1015:ILE:HD12	1:A:1114:GLN:HB3	1.58	0.85
1:B:2061:ALA:CB	1:B:2074:VAL:HG11	2.06	0.85
1:A:1061:ALA:CB	1:A:1074:VAL:HG11	2.07	0.85
1:B:2095:LYS:HD3	1:B:2120:GLU:HA	1.60	0.83
1:B:2015:ILE:HD12	1:B:2114:GLN:HB3	1.59	0.83
1:B:2015:ILE:HD11	1:B:2110:LEU:HD11	1.62	0.82
1:A:1126:LEU:N	1:A:1126:LEU:HD12	1.94	0.80
1:A:1095:LYS:HD3	1:A:1120:GLU:HA	1.62	0.80
1:B:2004:GLN:OE1	1:B:2034:ALA:HB1	1.81	0.80
1:A:1004:GLN:OE1	1:A:1034:ALA:HB1	1.81	0.80
1:B:2043:LYS:HB3	1:B:2046:GLU:CG	2.10	0.80
1:B:2060:LEU:HD21	1:B:2065:LEU:HB2	1.64	0.80
1:A:1015:ILE:HD11	1:A:1110:LEU:HD11	1.62	0.79
1:A:1043:LYS:HB3	1:A:1046:GLU:CG	2.12	0.78
1:B:2126:LEU:HD12	1:B:2126:LEU:N	1.95	0.77
1:A:1116:ASN:HB3	1:A:1120:GLU:OE2	1.83	0.77
1:A:1060:LEU:HD21	1:A:1065:LEU:HB2	1.65	0.77
1:A:1013:CYS:SG	1:A:1118:ILE:HD11	2.25	0.77
1:A:1020:LEU:HD22	1:A:1105:ILE:O	1.84	0.76
1:B:2020:LEU:HD22	1:B:2105:ILE:O	1.84	0.76
1:A:1021:THR:HG1	1:A:1106:TYR:HA	1.50	0.76
1:B:2116:ASN:HB3	1:B:2120:GLU:OE2	1.85	0.76
1:A:1046:GLU:OE1	1:A:1067:LEU:HA	1.87	0.75
1:B:2046:GLU:OE1	1:B:2067:LEU:HA	1.87	0.75
1:A:1046:GLU:CD	1:A:1067:LEU:HA	2.08	0.74
1:B:2046:GLU:CD	1:B:2067:LEU:HA	2.08	0.74
1:A:1021:THR:OG1	1:A:1106:TYR:HA	1.88	0.74
1:A:1111:THR:OG1	1:A:1114:GLN:HG3	1.88	0.74
1:B:2111:THR:OG1	1:B:2114:GLN:HG3	1.87	0.74
1:A:1002:SER:O	1:A:1005:THR:HG23	1.88	0.73
1:B:2021:THR:HG1	1:B:2106:TYR:HA	1.52	0.73
1:A:1035:GLN:OE1	1:A:1039:PHE:HB3	1.89	0.73
1:B:2116:ASN:O	1:B:2120:GLU:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2021:THR:OG1	1:B:2106:TYR:HA	1.87	0.73
1:A:1116:ASN:O	1:A:1120:GLU:HG3	1.88	0.73
1:B:2084:ARG:HG2	1:B:2093:THR:HG23	1.69	0.73
1:A:1084:ARG:HG2	1:A:1093:THR:HG23	1.71	0.71
1:B:2035:GLN:OE1	1:B:2039:PHE:HB3	1.90	0.71
1:A:1113:GLY:HA2	1:A:1116:ASN:HD22	1.54	0.71
1:A:1015:ILE:CD1	1:A:1114:GLN:HB3	2.21	0.71
1:B:2002:SER:O	1:B:2005:THR:HG23	1.90	0.70
1:B:2113:GLY:HA2	1:B:2116:ASN:HD22	1.55	0.70
1:A:1121:ARG:NE	1:B:2121:ARG:HD2	2.07	0.70
1:A:1121:ARG:HD2	1:B:2121:ARG:NE	2.07	0.70
1:B:2025:ILE:C	1:B:2026:ILE:HD12	2.12	0.70
1:B:2015:ILE:CD1	1:B:2114:GLN:HB3	2.22	0.69
1:B:2013:CYS:SG	1:B:2118:ILE:HD11	2.32	0.69
1:B:2040:PRO:HB2	1:B:2068:GLY:CA	2.24	0.68
1:B:2058:GLY:O	1:B:2062:PRO:HD3	1.94	0.68
1:A:1025:ILE:C	1:A:1026:ILE:HD12	2.14	0.68
1:A:1058:GLY:O	1:A:1062:PRO:HD3	1.94	0.67
1:A:1040:PRO:HB2	1:A:1068:GLY:CA	2.24	0.67
1:A:1061:ALA:HB1	1:A:1074:VAL:HG11	1.77	0.66
1:B:2061:ALA:HB1	1:B:2074:VAL:HG11	1.77	0.66
1:A:1071:LYS:HG3	1:A:1072:TYR:N	2.11	0.65
1:B:2071:LYS:HG3	1:B:2072:TYR:N	2.12	0.65
1:A:1125:TYR:HB3	1:A:1126:LEU:HD12	1.79	0.64
1:A:1078:GLU:HB3	1:A:1081:ALA:HB3	1.79	0.64
1:B:2078:GLU:HB3	1:B:2081:ALA:HB3	1.79	0.64
1:B:2125:TYR:HB3	1:B:2126:LEU:HD12	1.80	0.64
1:B:2075:ILE:HG22	1:B:2076:GLN:N	2.13	0.64
1:A:1125:TYR:HE1	1:B:2114:GLN:HG2	1.63	0.63
1:A:1130:GLY:C	1:A:1131:LEU:HD23	2.18	0.63
1:A:1027:GLY:C	1:A:1029:ASP:H	2.02	0.63
1:B:2027:GLY:C	1:B:2029:ASP:H	2.02	0.63
1:B:2095:LYS:HB2	1:B:2119:VAL:HG12	1.80	0.63
1:B:2015:ILE:O	1:B:2017:GLY:N	2.32	0.63
1:A:1015:ILE:O	1:A:1017:GLY:N	2.32	0.62
1:B:2130:GLY:C	1:B:2131:LEU:HD23	2.20	0.62
1:A:1114:GLN:HG2	1:B:2125:TYR:HE1	1.64	0.62
1:A:1046:GLU:O	1:A:1050:VAL:HG23	2.00	0.62
1:A:1095:LYS:HB2	1:A:1119:VAL:HG12	1.80	0.61
1:A:1007:VAL:HG22	1:A:1011:LEU:HD12	1.82	0.61
1:A:1075:ILE:HG22	1:A:1076:GLN:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2046:GLU:O	1:B:2050:VAL:HG23	2.00	0.61
1:A:1104:GLY:C	1:A:1105:ILE:HD12	2.22	0.60
1:A:1058:GLY:O	1:A:1060:LEU:N	2.35	0.60
1:A:1082:VAL:HG12	1:A:1083:ILE:N	2.15	0.60
1:B:2082:VAL:HG12	1:B:2083:ILE:N	2.16	0.60
1:B:2066:HIS:HA	1:B:2071:LYS:HA	1.84	0.60
1:B:2007:VAL:HG22	1:B:2011:LEU:HD12	1.83	0.60
1:B:2058:GLY:O	1:B:2060:LEU:N	2.35	0.60
1:A:1066:HIS:HA	1:A:1071:LYS:HA	1.84	0.59
1:A:1121:ARG:NE	1:B:2121:ARG:CD	2.65	0.59
1:A:1121:ARG:CD	1:B:2121:ARG:NE	2.66	0.59
1:B:2086:LYS:HE2	1:B:2088:GLY:O	2.01	0.59
1:A:1043:LYS:HB2	1:A:1043:LYS:HZ3	1.67	0.59
1:A:1111:THR:HG23	1:A:1114:GLN:OE1	2.03	0.58
1:B:2040:PRO:HB2	1:B:2068:GLY:HA2	1.84	0.58
1:A:1061:ALA:HB2	1:A:1074:VAL:HG11	1.86	0.58
1:A:1011:LEU:HD13	1:A:1023:ALA:HB1	1.86	0.58
1:B:2090:GLY:HA3	1:B:2106:TYR:O	2.03	0.58
1:A:1086:LYS:HE2	1:A:1088:GLY:O	2.03	0.58
1:B:2061:ALA:HB2	1:B:2074:VAL:HG11	1.84	0.58
1:B:2104:GLY:C	1:B:2105:ILE:HD12	2.23	0.58
1:A:1040:PRO:HB2	1:A:1068:GLY:HA2	1.85	0.58
1:B:2118:ILE:HG22	1:B:2119:VAL:N	2.19	0.58
1:A:1053:ASP:HB2	1:A:1060:LEU:HB2	1.85	0.58
1:A:1090:GLY:HA3	1:A:1106:TYR:O	2.03	0.58
1:A:1095:LYS:HG2	1:A:1123:GLY:HA3	1.85	0.58
1:A:1073:MET:HA	1:A:1073:MET:CE	2.34	0.58
1:B:2011:LEU:HD13	1:B:2023:ALA:HB1	1.83	0.58
1:A:1118:ILE:HG22	1:A:1119:VAL:N	2.18	0.58
1:B:2067:LEU:HD23	1:B:2068:GLY:N	2.19	0.57
1:B:2095:LYS:HG2	1:B:2123:GLY:HA3	1.85	0.57
1:B:2122:LEU:H	1:B:2122:LEU:HD12	1.70	0.57
1:B:2026:ILE:HG22	1:B:2027:GLY:N	2.19	0.56
1:B:2053:ASP:HB2	1:B:2060:LEU:HB2	1.86	0.56
1:A:1043:LYS:NZ	1:A:1043:LYS:HB2	2.21	0.56
1:A:1067:LEU:HD23	1:A:1068:GLY:N	2.20	0.56
1:A:1121:ARG:CZ	1:B:2121:ARG:CZ	2.83	0.56
1:B:2045:ASP:O	1:B:2048:ALA:N	2.39	0.56
1:A:1122:LEU:H	1:A:1122:LEU:HD12	1.70	0.56
1:A:1117:MET:O	1:A:1121:ARG:HB2	2.07	0.55
1:B:2111:THR:HG23	1:B:2114:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2073:MET:HA	1:B:2073:MET:CE	2.36	0.55
1:B:2117:MET:O	1:B:2121:ARG:HB2	2.07	0.55
1:B:2043:LYS:NZ	1:B:2043:LYS:HB2	2.21	0.55
1:B:2067:LEU:C	1:B:2069:GLY:N	2.59	0.55
1:B:2005:THR:C	1:B:2007:VAL:H	2.09	0.55
1:B:2039:PHE:CD1	1:B:2040:PRO:HD2	2.42	0.55
1:A:1123:GLY:O	1:A:1127:LEU:HD12	2.07	0.55
1:A:1116:ASN:O	1:A:1117:MET:C	2.46	0.55
1:A:1026:ILE:HG22	1:A:1027:GLY:N	2.22	0.54
1:B:2043:LYS:HG2	1:B:2045:ASP:H	1.72	0.54
1:A:1121:ARG:HD2	1:B:2121:ARG:HE	1.73	0.54
1:A:1045:ASP:O	1:A:1048:ALA:N	2.41	0.54
1:B:2039:PHE:CG	1:B:2040:PRO:HD2	2.43	0.53
1:A:1060:LEU:HD21	1:A:1065:LEU:CB	2.38	0.53
1:B:2042:PHE:CD2	1:B:2043:LYS:N	2.77	0.53
1:A:1131:LEU:N	1:A:1131:LEU:HD23	2.23	0.53
1:B:2026:ILE:CG2	1:B:2027:GLY:N	2.70	0.53
1:B:2116:ASN:O	1:B:2117:MET:C	2.46	0.53
1:B:2131:LEU:N	1:B:2131:LEU:HD23	2.23	0.53
1:A:1043:LYS:HG2	1:A:1045:ASP:H	1.72	0.53
1:A:1026:ILE:CG2	1:A:1027:GLY:N	2.72	0.53
1:A:1117:MET:SD	1:B:2121:ARG:HG2	2.49	0.53
1:A:1042:PHE:CD2	1:A:1043:LYS:N	2.76	0.53
1:B:2043:LYS:HZ3	1:B:2043:LYS:HB2	1.74	0.53
1:B:2067:LEU:C	1:B:2069:GLY:H	2.13	0.53
1:B:2097:THR:HG1	1:B:2100:ALA:H	1.57	0.53
1:A:1008:ASP:N	1:A:1008:ASP:OD1	2.42	0.52
1:A:1039:PHE:CD1	1:A:1040:PRO:HD2	2.44	0.52
1:A:1051:MET:SD	1:A:1101:LEU:HD11	2.50	0.52
1:A:1067:LEU:C	1:A:1069:GLY:H	2.12	0.52
1:A:1005:THR:C	1:A:1007:VAL:H	2.11	0.52
1:A:1058:GLY:O	1:A:1061:ALA:N	2.43	0.52
1:B:2008:ASP:N	1:B:2008:ASP:OD1	2.43	0.52
1:B:2123:GLY:O	1:B:2127:LEU:HD12	2.09	0.52
1:B:2058:GLY:O	1:B:2061:ALA:N	2.43	0.52
1:A:1114:GLN:HG2	1:B:2125:TYR:CE1	2.45	0.52
1:A:1045:ASP:O	1:A:1046:GLU:C	2.48	0.52
1:A:1128:ASP:OD1	1:A:1128:ASP:N	2.43	0.52
1:B:2024:ALA:O	1:B:2103:ILE:HG22	2.10	0.51
1:B:2045:ASP:O	1:B:2046:GLU:C	2.49	0.51
1:A:1102:ILE:HB	1:A:1119:VAL:HG13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:ARG:HG3	1:A:1096:ARG:HH11	1.75	0.51
1:B:2102:ILE:HB	1:B:2119:VAL:HG13	1.92	0.51
1:A:1024:ALA:O	1:A:1103:ILE:HG22	2.11	0.51
1:A:1039:PHE:CG	1:A:1040:PRO:HD2	2.46	0.51
1:A:1122:LEU:O	1:A:1125:TYR:HB3	2.11	0.51
1:A:1067:LEU:C	1:A:1069:GLY:N	2.59	0.51
1:A:1121:ARG:CG	1:B:2121:ARG:HG3	2.29	0.51
1:A:1125:TYR:HB3	1:A:1126:LEU:CD1	2.41	0.51
1:B:2060:LEU:HD21	1:B:2065:LEU:CB	2.37	0.51
1:A:1121:ARG:HG2	1:B:2117:MET:SD	2.51	0.51
1:A:1010:HIS:HB3	1:A:1122:LEU:HD11	1.93	0.51
1:B:2010:HIS:HB3	1:B:2122:LEU:HD11	1.93	0.51
1:A:1125:TYR:CE1	1:B:2114:GLN:HG2	2.44	0.50
1:A:1121:ARG:NE	1:B:2121:ARG:NE	2.59	0.50
1:B:2096:ARG:HH11	1:B:2096:ARG:HG3	1.76	0.50
1:A:1005:THR:C	1:A:1007:VAL:N	2.64	0.50
1:A:1077:GLY:HA2	1:A:1084:ARG:HH12	1.75	0.50
1:B:2051:MET:SD	1:B:2101:LEU:HD11	2.51	0.50
1:B:2005:THR:C	1:B:2007:VAL:N	2.63	0.50
1:B:2077:GLY:HA2	1:B:2084:ARG:HH12	1.77	0.50
1:B:2128:ASP:OD1	1:B:2128:ASP:N	2.44	0.50
1:B:2075:ILE:HD11	1:B:2086:LYS:HB3	1.94	0.50
1:A:1121:ARG:HE	1:B:2121:ARG:HD2	1.74	0.49
1:B:2125:TYR:HB3	1:B:2126:LEU:CD1	2.42	0.49
1:A:1024:ALA:HA	1:A:1035:GLN:HA	1.95	0.49
1:B:2122:LEU:O	1:B:2125:TYR:HB3	2.12	0.49
1:A:1121:ARG:NH1	1:B:2121:ARG:CZ	2.76	0.49
1:A:1016:ASP:HB2	1:B:2125:TYR:OH	2.13	0.49
1:A:1026:ILE:HG22	1:A:1027:GLY:O	2.13	0.48
1:A:1074:VAL:HG22	1:A:1075:ILE:N	2.28	0.48
1:B:2095:LYS:CB	1:B:2119:VAL:HG12	2.44	0.48
1:B:2033:TRP:N	1:B:2033:TRP:CD1	2.81	0.48
1:A:1095:LYS:CB	1:A:1119:VAL:HG12	2.43	0.48
1:B:2042:PHE:HA	1:B:2068:GLY:H	1.79	0.48
1:B:2096:ARG:O	1:B:2096:ARG:HD3	2.14	0.48
1:B:2020:LEU:CD2	1:B:2105:ILE:O	2.58	0.48
1:A:1075:ILE:HD11	1:A:1086:LYS:HB3	1.95	0.48
1:A:1097:THR:OG1	1:A:1100:ALA:N	2.44	0.48
1:A:1121:ARG:CZ	1:B:2121:ARG:NH1	2.78	0.47
1:A:1121:ARG:HG3	1:B:2121:ARG:CG	2.29	0.47
1:B:2024:ALA:HA	1:B:2035:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2049:ALA:O	1:B:2052:LYS:HB3	2.14	0.47
1:B:2027:GLY:C	1:B:2029:ASP:N	2.66	0.47
1:B:2058:GLY:O	1:B:2062:PRO:CD	2.63	0.47
1:B:2074:VAL:HG22	1:B:2075:ILE:N	2.29	0.47
1:A:1046:GLU:OE1	1:A:1067:LEU:HG	2.14	0.47
1:A:1082:VAL:CG1	1:A:1083:ILE:N	2.78	0.47
1:A:1105:ILE:N	1:A:1105:ILE:HD12	2.30	0.47
1:A:1027:GLY:C	1:A:1029:ASP:N	2.66	0.47
1:A:1042:PHE:HA	1:A:1068:GLY:H	1.79	0.47
1:B:2105:ILE:HD12	1:B:2105:ILE:N	2.30	0.47
1:B:2082:VAL:CG1	1:B:2083:ILE:N	2.78	0.47
1:B:2046:GLU:OE1	1:B:2067:LEU:HG	2.15	0.46
1:B:2013:CYS:O	1:B:2019:ARG:HA	2.16	0.46
1:A:1058:GLY:O	1:A:1062:PRO:CD	2.63	0.46
1:B:2026:ILE:HG22	1:B:2027:GLY:O	2.14	0.46
1:A:1125:TYR:OH	1:B:2114:GLN:NE2	2.45	0.46
1:B:2028:HIS:ND1	1:B:2099:GLN:C	2.69	0.46
1:A:1033:TRP:CD1	1:A:1033:TRP:N	2.81	0.46
1:A:1045:ASP:C	1:A:1047:VAL:N	2.66	0.45
1:A:1020:LEU:CD2	1:A:1105:ILE:O	2.59	0.45
1:A:1121:ARG:HH21	1:B:2118:ILE:HG12	1.82	0.45
1:B:2098:GLY:N	1:B:2131:LEU:O	2.49	0.45
1:B:2018:HIS:HE1	1:B:2114:GLN:HE22	1.65	0.45
1:B:2097:THR:OG1	1:B:2100:ALA:N	2.45	0.45
1:A:1092:ILE:HG13	1:A:1104:GLY:O	2.16	0.45
1:A:1028:HIS:ND1	1:A:1099:GLN:C	2.71	0.45
1:A:1097:THR:HG1	1:A:1100:ALA:H	1.59	0.45
1:A:1049:ALA:O	1:A:1052:LYS:HB3	2.16	0.45
1:A:1098:GLY:N	1:A:1131:LEU:O	2.49	0.45
1:A:1054:PHE:HE1	1:A:1081:ALA:C	2.21	0.44
1:B:2073:MET:HA	1:B:2073:MET:HE3	1.98	0.44
1:A:1018:HIS:HE1	1:A:1114:GLN:HE22	1.65	0.44
1:B:2054:PHE:HE1	1:B:2081:ALA:C	2.21	0.44
1:A:1007:VAL:O	1:A:1011:LEU:HB2	2.17	0.44
1:A:1096:ARG:HD3	1:A:1096:ARG:O	2.17	0.44
1:B:2126:LEU:N	1:B:2126:LEU:CD1	2.57	0.44
1:B:2092:ILE:HG13	1:B:2104:GLY:O	2.17	0.44
1:A:1013:CYS:O	1:A:1019:ARG:HA	2.17	0.44
1:B:2007:VAL:O	1:B:2011:LEU:HB2	2.17	0.44
1:A:1125:TYR:OH	1:B:2016:ASP:HB2	2.17	0.43
1:A:1073:MET:HA	1:A:1073:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:VAL:O	1:A:1032:VAL:HG12	2.19	0.43
1:A:1122:LEU:HD12	1:A:1122:LEU:N	2.33	0.43
1:B:2011:LEU:HB3	1:B:2023:ALA:CB	2.49	0.43
1:B:2045:ASP:C	1:B:2047:VAL:N	2.67	0.43
1:A:1118:ILE:HG12	1:B:2121:ARG:HH21	1.82	0.43
1:A:1074:VAL:HG22	1:A:1075:ILE:H	1.83	0.42
1:A:1011:LEU:HG	1:A:1122:LEU:HD22	2.01	0.42
1:A:1114:GLN:NE2	1:B:2125:TYR:OH	2.47	0.42
1:B:2122:LEU:O	1:B:2123:GLY:C	2.56	0.42
1:B:2074:VAL:HG22	1:B:2075:ILE:H	1.84	0.42
1:B:2092:ILE:HD11	1:B:2105:ILE:HD11	2.02	0.42
1:A:1011:LEU:HB3	1:A:1023:ALA:CB	2.50	0.42
1:A:1091:GLY:C	1:A:1106:TYR:CE2	2.93	0.42
1:A:1117:MET:HG3	1:B:2125:TYR:HB2	2.01	0.42
1:B:2122:LEU:N	1:B:2122:LEU:HD12	2.33	0.42
1:B:2011:LEU:C	1:B:2012:MET:HG2	2.39	0.42
1:A:1094:VAL:HG22	1:A:1103:ILE:HG13	2.02	0.42
1:A:1028:HIS:CE1	1:A:1100:ALA:O	2.73	0.42
1:A:1093:THR:OG1	1:A:1115:CYS:SG	2.57	0.41
1:A:1003:TRP:HB3	1:A:1034:ALA:CB	2.50	0.41
1:B:2091:GLY:C	1:B:2106:TYR:CE2	2.94	0.41
1:B:2026:ILE:N	1:B:2026:ILE:HD12	2.36	0.41
1:A:1003:TRP:HB3	1:A:1034:ALA:HB2	2.02	0.41
1:A:1077:GLY:HA2	1:A:1084:ARG:NH1	2.35	0.41
1:A:1054:PHE:O	1:A:1080:GLY:HA2	2.21	0.41
1:B:2032:VAL:HG12	1:B:2032:VAL:O	2.20	0.41
1:B:2003:TRP:HB3	1:B:2034:ALA:HB2	2.02	0.41
1:A:1122:LEU:O	1:A:1123:GLY:C	2.59	0.41
1:A:1115:CYS:O	1:A:1116:ASN:C	2.59	0.41
1:B:2077:GLY:HA2	1:B:2084:ARG:NH1	2.36	0.41
1:B:2003:TRP:HB3	1:B:2034:ALA:CB	2.50	0.41
1:B:2116:ASN:C	1:B:2120:GLU:HG3	2.41	0.41
1:A:1011:LEU:C	1:A:1012:MET:HG2	2.41	0.40
1:A:1122:LEU:O	1:A:1126:LEU:HD13	2.21	0.40
1:B:2115:CYS:O	1:B:2116:ASN:C	2.59	0.40
1:B:2122:LEU:O	1:B:2126:LEU:HD13	2.21	0.40
1:A:1003:TRP:CH2	1:A:1033:TRP:CZ3	3.09	0.40
1:B:2051:MET:SD	1:B:2051:MET:N	2.95	0.40
1:A:1113:GLY:CA	1:A:1116:ASN:HD22	2.30	0.40
1:A:1125:TYR:HB2	1:B:2117:MET:HG3	2.04	0.40

There are no symmetry-related clashes.

## 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	128/131 (98%)	82 (64%)	35 (27%)	11 (9%)	1	5
1	B	128/131 (98%)	82 (64%)	34 (27%)	12 (9%)	1	4
All	All	256/262 (98%)	164 (64%)	69 (27%)	23 (9%)	1	5

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1059	SER
1	A	1129	GLN
1	B	2059	SER
1	B	2125	TYR
1	B	2129	GLN
1	A	1042	PHE
1	A	1125	TYR
1	B	2042	PHE
1	A	1016	ASP
1	A	1075	ILE
1	B	2016	ASP
1	B	2075	ILE
1	A	1089	SER
1	B	2089	SER
1	A	1121	ARG
1	B	2121	ARG
1	A	1019	ARG
1	B	2019	ARG
1	B	2028	HIS
1	B	2074	VAL
1	A	1074	VAL
1	B	2017	GLY
1	A	1017	GLY

### 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	103/104 (99%)	82 (80%)	21 (20%)	1	6
1	B	103/104 (99%)	81 (79%)	22 (21%)	1	5
All	All	206/208 (99%)	163 (79%)	43 (21%)	1	6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	GLN
1	A	1005	THR
1	A	1008	ASP
1	A	1009	ASP
1	A	1013	CYS
1	A	1018	HIS
1	A	1020	LEU
1	A	1021	THR
1	A	1055	ASP
1	A	1066	HIS
1	A	1071	LYS
1	A	1073	MET
1	A	1089	SER
1	A	1093	THR
1	A	1096	ARG
1	A	1108	GLU
1	A	1111	THR
1	A	1115	CYS
1	A	1117	MET
1	A	1128	ASP
1	A	1131	LEU
1	B	2004	GLN
1	B	2005	THR
1	B	2008	ASP
1	B	2009	ASP
1	B	2013	CYS
1	B	2018	HIS

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Mol	Chain	Res	Type
1	B	2020	LEU
1	B	2021	THR
1	B	2055	ASP
1	B	2066	HIS
1	B	2071	LYS
1	B	2073	MET
1	B	2089	SER
1	B	2093	THR
1	B	2096	ARG
1	B	2108	GLU
1	B	2111	THR
1	B	2115	CYS
1	B	2117	MET
1	B	2126	LEU
1	B	2128	ASP
1	B	2131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1018	HIS
1	B	2010	HIS
1	B	2018	HIS
1	B	2129	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 carbohydrates in this entry.



## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.