



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:32 am BST

PDB ID : 2PTG  
Title : Crystal structure of Eimeria tenella enoyl reductase  
Authors : Lu, J.Z.; Prigge, S.T.  
Deposited on : 2007-05-08  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

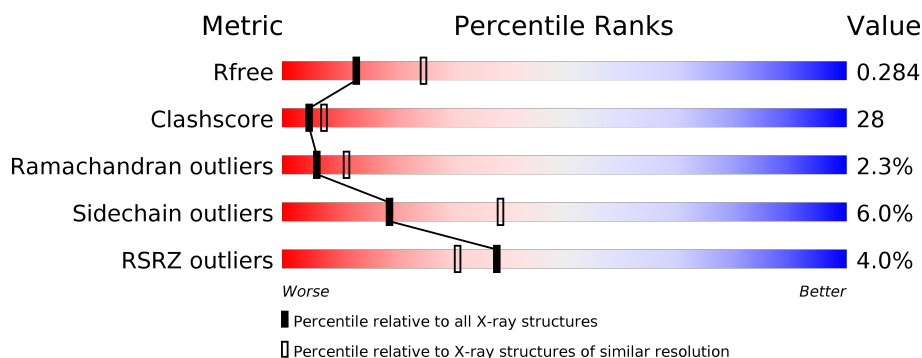
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	319	<div> <div>3%</div> <div> <div></div> <div>38%</div> <div>29%</div> <div>•</div> <div>30%</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>41%</div> <div>26%</div> <div>••</div> <div>30%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3336 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.

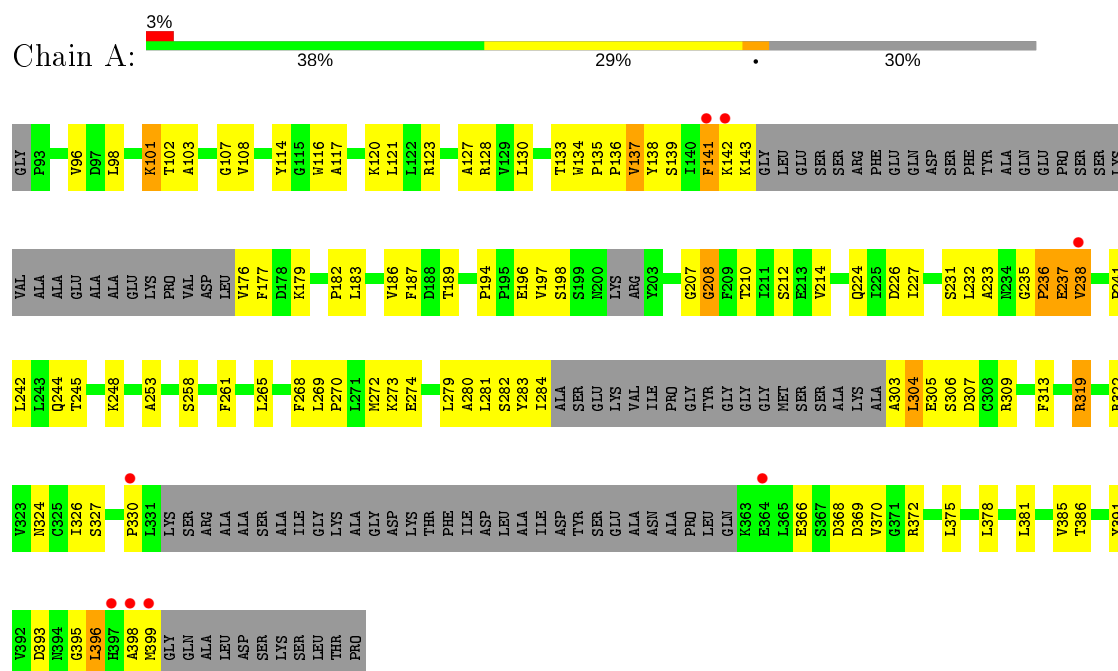
- Molecule 1 is a protein called Enoyl-acyl carrier reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1668	1070	282	311	5			
1	B	224	Total	C	N	O	S	0	0	0
			1668	1070	282	311	5			

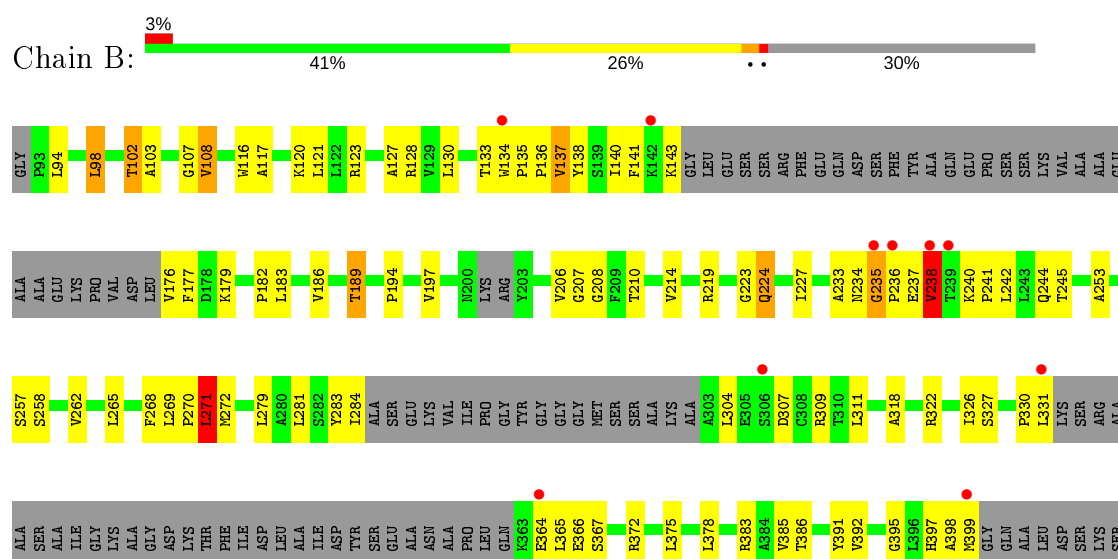
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: Enoyl-acyl carrier reductase



#### • Molecule 1: Enoyl-acyl carrier reductase



LEU  
THR  
PRO

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.26 Å   105.26 Å   92.95 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	27.68 – 2.60 27.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	84.8 (27.68-2.60) 93.2 (27.68-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.265 0.246 , 0.284	Depositor DCC
$R_{free}$ test set	869 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.486 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.43	0/1700	0.67	0/2310
1	B	0.42	0/1700	0.67	1/2310 (0.0%)
All	All	0.42	0/3400	0.67	1/4620 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	LEU	CA-CB-CG	5.92	128.91	115.30

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	1668	0	1679	115	0
1	B	1668	0	1679	83	0
All	All	3336	0	3358	186	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 28.

All (186) 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:309:ARG:HD2	1:B:398:ALA:HB1	1.48	0.95
1:A:233:ALA:HB2	1:A:283:TYR:CZ	2.08	0.89
1:A:319:ARG:HB3	1:A:319:ARG:HH21	1.40	0.84
1:A:242:LEU:O	1:A:245:THR:HG22	1.80	0.82
1:B:108:VAL:O	1:B:133:THR:HG23	1.79	0.81
1:A:176:VAL:HG13	1:A:177:PHE:H	1.46	0.80
1:A:108:VAL:O	1:A:133:THR:HG23	1.80	0.79
1:B:117:ALA:O	1:B:121:LEU:HD23	1.82	0.79
1:A:135:PRO:HG2	1:A:136:PRO:HD3	1.63	0.79
1:A:98:LEU:HB3	1:A:127:ALA:HB2	1.64	0.78
1:A:319:ARG:NH2	1:A:319:ARG:HB3	1.98	0.78
1:A:117:ALA:HA	1:A:120:LYS:HE2	1.66	0.78
1:B:135:PRO:HG2	1:B:136:PRO:HD3	1.69	0.75
1:B:398:ALA:O	1:B:399:MET:HG3	1.86	0.75
1:B:234:ASN:ND2	1:B:257:SER:HB3	2.03	0.73
1:A:381:LEU:HD22	1:B:372:ARG:HD2	1.70	0.73
1:A:258:SER:HB3	1:A:304:LEU:HD21	1.71	0.73
1:A:133:THR:HG22	1:A:137:VAL:HG13	1.72	0.71
1:A:183:LEU:HD13	1:A:214:VAL:HG11	1.72	0.70
1:B:242:LEU:O	1:B:245:THR:HG22	1.91	0.70
1:A:284:ILE:O	1:A:284:ILE:HG13	1.90	0.69
1:A:309:ARG:HD2	1:B:398:ALA:CB	2.22	0.69
1:A:238:VAL:HG13	1:A:253:ALA:HB1	1.75	0.68
1:B:133:THR:HG22	1:B:137:VAL:HG13	1.75	0.68
1:A:279:LEU:HD11	1:A:326:ILE:HG12	1.75	0.68
1:A:395:GLY:O	1:A:399:MET:HB2	1.94	0.67
1:B:98:LEU:HB3	1:B:127:ALA:HB2	1.76	0.66
1:B:102:THR:HB	1:B:128:ARG:HB3	1.77	0.66
1:A:284:ILE:HG22	1:A:330:PRO:HB3	1.78	0.66
1:A:123:ARG:HG2	1:A:123:ARG:HH11	1.61	0.65
1:B:116:TRP:CZ2	1:B:176:VAL:HG21	2.32	0.65
1:B:283:TYR:HD2	1:B:284:ILE:HG23	1.62	0.65
1:A:399:MET:HE3	1:B:386:THR:HG23	1.80	0.64
1:A:281:LEU:HD23	1:A:281:LEU:C	2.19	0.62
1:A:232:LEU:HD23	1:A:232:LEU:O	2.00	0.62
1:A:117:ALA:O	1:A:121:LEU:HD23	2.00	0.61
1:B:241:PRO:HG2	1:B:244:GLN:NE2	2.16	0.61
1:B:258:SER:HB2	1:B:304:LEU:HD11	1.82	0.61
1:B:233:ALA:HB2	1:B:283:TYR:OH	2.01	0.59
1:A:135:PRO:O	1:A:138:TYR:HB3	2.02	0.59
1:B:121:LEU:HB3	1:B:375:LEU:HD22	1.85	0.59
1:B:176:VAL:HG12	1:B:177:PHE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PRO:HG2	1:B:197:VAL:HG23	1.86	0.58
1:A:117:ALA:HA	1:A:120:LYS:CE	2.31	0.57
1:A:283:TYR:HD2	1:A:284:ILE:HG23	1.70	0.57
1:A:233:ALA:HB2	1:A:283:TYR:OH	2.05	0.57
1:B:237:GLU:O	1:B:238:VAL:HG12	2.05	0.57
1:A:398:ALA:O	1:A:399:MET:HG3	2.05	0.56
1:A:196:GLU:HG2	1:A:197:VAL:H	1.70	0.56
1:B:395:GLY:O	1:B:399:MET:HB2	2.06	0.56
1:B:183:LEU:HD13	1:B:214:VAL:HG11	1.87	0.56
1:A:398:ALA:HB1	1:B:309:ARG:HD2	1.86	0.56
1:B:123:ARG:HG2	1:B:123:ARG:HH11	1.70	0.56
1:B:284:ILE:HG22	1:B:330:PRO:HB3	1.87	0.56
1:B:107:GLY:O	1:B:108:VAL:C	2.44	0.55
1:B:224:GLN:HG2	1:B:271:LEU:O	2.06	0.55
1:B:268:PHE:HA	1:B:271:LEU:HD13	1.88	0.55
1:A:241:PRO:HG2	1:A:244:GLN:CD	2.26	0.55
1:A:238:VAL:HG13	1:A:253:ALA:CB	2.37	0.55
1:A:123:ARG:HG2	1:A:123:ARG:NH1	2.21	0.55
1:A:123:ARG:HH12	1:A:176:VAL:N	2.06	0.54
1:A:130:LEU:CD2	1:A:179:LYS:HB3	2.37	0.54
1:A:319:ARG:CB	1:A:319:ARG:HH21	2.18	0.53
1:B:365:LEU:HD11	1:B:392:VAL:HG12	1.90	0.53
1:A:241:PRO:HG2	1:A:244:GLN:NE2	2.23	0.53
1:A:269:LEU:N	1:A:270:PRO:HD2	2.23	0.53
1:A:241:PRO:CG	1:A:244:GLN:NE2	2.71	0.53
1:A:237:GLU:HB3	1:A:253:ALA:HB2	1.91	0.53
1:A:258:SER:CB	1:A:304:LEU:HD21	2.39	0.53
1:A:102:THR:CG2	1:A:128:ARG:HD2	2.39	0.52
1:B:103:ALA:HB2	1:B:227:ILE:HB	1.91	0.52
1:A:138:TYR:CE2	1:A:182:PRO:HD3	2.45	0.52
1:A:189:THR:C	1:A:210:THR:HG21	2.30	0.52
1:B:233:ALA:HB2	1:B:283:TYR:CZ	2.45	0.52
1:B:138:TYR:CE2	1:B:182:PRO:HD3	2.44	0.52
1:A:139:SER:C	1:A:141:PHE:H	2.12	0.52
1:A:327:SER:HB3	1:A:391:TYR:CD1	2.45	0.52
1:B:240:LYS:HD3	1:B:244:GLN:HG2	1.90	0.52
1:B:327:SER:HB3	1:B:391:TYR:CD1	2.45	0.52
1:A:133:THR:HG22	1:A:137:VAL:CG1	2.40	0.51
1:A:102:THR:HG22	1:A:128:ARG:HB3	1.91	0.51
1:B:135:PRO:CG	1:B:136:PRO:HD3	2.40	0.51
1:B:140:ILE:N	1:B:140:ILE:HD12	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:LEU:HD11	1:B:326:ILE:HG12	1.93	0.50
1:A:135:PRO:CG	1:A:136:PRO:HD3	2.36	0.50
1:A:386:THR:HG23	1:B:399:MET:HE1	1.92	0.50
1:B:116:TRP:CD1	1:B:120:LYS:HE2	2.47	0.50
1:A:176:VAL:HG13	1:A:177:PHE:N	2.22	0.50
1:A:309:ARG:CD	1:B:398:ALA:HB1	2.30	0.50
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.27	0.49
1:B:283:TYR:CD2	1:B:284:ILE:HG23	2.44	0.49
1:A:226:ASP:OD2	1:A:273:LYS:HD2	2.11	0.49
1:B:331:LEU:HD21	1:B:367:SER:N	2.28	0.49
1:A:138:TYR:OH	1:A:142:LYS:HD3	2.13	0.49
1:A:395:GLY:HA2	1:A:399:MET:HE3	1.94	0.49
1:A:123:ARG:NH1	1:A:176:VAL:N	2.60	0.48
1:A:227:ILE:HG23	1:A:378:LEU:HD22	1.95	0.48
1:B:189:THR:C	1:B:210:THR:HG21	2.34	0.48
1:B:281:LEU:HD23	1:B:281:LEU:C	2.33	0.48
1:A:114:TYR:CE1	1:A:370:VAL:HG21	2.49	0.48
1:B:262:VAL:HG22	1:B:311:LEU:HD11	1.95	0.48
1:A:114:TYR:HB3	1:A:281:LEU:HD11	1.95	0.48
1:A:268:PHE:O	1:A:272:MET:HG3	2.13	0.48
1:A:187:PHE:HB3	1:A:210:THR:HG22	1.96	0.48
1:A:189:THR:HG22	1:A:212:SER:OG	2.14	0.48
1:A:322:ARG:HD2	1:A:385:VAL:O	2.14	0.48
1:B:322:ARG:HD3	1:B:383:ARG:O	2.14	0.48
1:A:398:ALA:CB	1:B:309:ARG:HD2	2.44	0.47
1:B:135:PRO:O	1:B:138:TYR:HB3	2.14	0.47
1:A:313:PHE:HB2	1:B:399:MET:HG2	1.95	0.47
1:A:142:LYS:O	1:A:142:LYS:HG2	2.14	0.47
1:B:133:THR:HG22	1:B:137:VAL:CG1	2.45	0.47
1:B:120:LYS:HG2	1:B:176:VAL:HG22	1.97	0.47
1:B:141:PHE:C	1:B:143:LYS:H	2.19	0.46
1:B:123:ARG:HG2	1:B:123:ARG:NH1	2.31	0.46
1:B:134:TRP:HB3	1:B:137:VAL:CG1	2.46	0.46
1:A:393:ASP:O	1:A:396:LEU:HB2	2.16	0.46
1:A:281:LEU:CD2	1:A:281:LEU:C	2.84	0.46
1:A:138:TYR:CZ	1:A:182:PRO:HD3	2.50	0.46
1:B:238:VAL:HB	1:B:253:ALA:HB1	1.97	0.46
1:A:399:MET:CE	1:B:386:THR:HG23	2.45	0.46
1:B:269:LEU:N	1:B:270:PRO:HD2	2.31	0.46
1:A:366:GLU:O	1:A:369:ASP:HB2	2.16	0.46
1:A:121:LEU:HB3	1:A:375:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HA	1:A:324:ASN:O	2.17	0.45
1:A:284:ILE:CG1	1:A:284:ILE:O	2.58	0.45
1:A:368:ASP:O	1:A:372:ARG:HG3	2.16	0.45
1:B:258:SER:CB	1:B:304:LEU:HD11	2.45	0.45
1:A:116:TRP:CH2	1:A:176:VAL:HG11	2.51	0.45
1:A:258:SER:HB2	1:A:304:LEU:HD11	1.98	0.45
1:B:392:VAL:HG12	1:B:392:VAL:O	2.17	0.45
1:A:134:TRP:O	1:A:137:VAL:HG13	2.17	0.45
1:A:241:PRO:HG3	1:A:244:GLN:NE2	2.31	0.45
1:A:196:GLU:HG2	1:A:197:VAL:N	2.31	0.44
1:A:261:PHE:CE1	1:A:280:ALA:HB2	2.52	0.44
1:A:281:LEU:HD23	1:A:282:SER:N	2.33	0.44
1:B:364:GLU:HG2	1:B:365:LEU:N	2.32	0.44
1:B:134:TRP:O	1:B:137:VAL:HG13	2.17	0.44
1:A:393:ASP:OD2	1:A:396:LEU:HB3	2.17	0.44
1:A:194:PRO:HG2	1:A:197:VAL:HB	1.99	0.44
1:A:304:LEU:C	1:A:306:SER:N	2.71	0.44
1:A:303:ALA:C	1:A:305:GLU:H	2.20	0.44
1:A:103:ALA:HB2	1:A:227:ILE:HB	2.00	0.44
1:A:134:TRP:HB3	1:A:137:VAL:CG1	2.48	0.43
1:B:395:GLY:HA2	1:B:399:MET:HE1	2.00	0.43
1:B:237:GLU:HB3	1:B:253:ALA:HB2	2.01	0.43
1:A:107:GLY:O	1:A:231:SER:HB3	2.18	0.43
1:A:207:GLY:O	1:A:208:GLY:O	2.37	0.43
1:A:284:ILE:HG22	1:A:330:PRO:CB	2.47	0.43
1:A:130:LEU:HD22	1:A:179:LYS:HB3	2.00	0.43
1:A:116:TRP:CH2	1:A:176:VAL:HG21	2.54	0.43
1:A:139:SER:HB3	1:A:143:LYS:HE2	2.00	0.42
1:A:210:THR:O	1:A:214:VAL:HG12	2.19	0.42
1:A:102:THR:HG21	1:A:128:ARG:HH21	1.82	0.42
1:B:206:VAL:HG23	1:B:207:GLY:N	2.34	0.42
1:B:330:PRO:O	1:B:365:LEU:HD23	2.19	0.42
1:A:381:LEU:CD1	1:B:94:LEU:HD12	2.50	0.42
1:B:102:THR:HB	1:B:128:ARG:HD3	2.00	0.42
1:B:130:LEU:CD2	1:B:179:LYS:HB3	2.49	0.42
1:A:235:GLY:N	1:A:236:PRO:HD2	2.33	0.42
1:A:322:ARG:HG2	1:A:386:THR:HB	2.02	0.42
1:B:322:ARG:HD2	1:B:385:VAL:O	2.20	0.42
1:B:117:ALA:HB2	1:B:367:SER:HB2	2.01	0.42
1:A:101:LYS:HB3	1:A:226:ASP:CG	2.40	0.42
1:B:227:ILE:HG23	1:B:378:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:HIS:O	1:B:398:ALA:HB3	2.19	0.42
1:A:139:SER:HB3	1:A:143:LYS:CE	2.49	0.41
1:B:235:GLY:HA3	1:B:236:PRO:HD2	1.82	0.41
1:A:120:LYS:HE3	1:A:120:LYS:HB2	1.90	0.41
1:A:102:THR:HG22	1:A:128:ARG:HD2	2.03	0.41
1:B:375:LEU:HA	1:B:375:LEU:HD12	1.86	0.41
1:A:133:THR:HG21	1:A:137:VAL:HG22	2.02	0.41
1:A:386:THR:HG23	1:B:399:MET:CE	2.50	0.41
1:A:235:GLY:H	1:A:236:PRO:HD2	1.86	0.41
1:A:237:GLU:HG3	1:A:238:VAL:H	1.86	0.41
1:A:304:LEU:C	1:A:306:SER:H	2.24	0.41
1:B:258:SER:HB2	1:B:304:LEU:CD1	2.49	0.41
1:A:96:VAL:HG13	1:A:381:LEU:HD11	2.03	0.41
1:B:141:PHE:C	1:B:143:LYS:N	2.74	0.41
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.88	0.41
1:A:139:SER:C	1:A:141:PHE:N	2.75	0.40
1:B:219:ARG:O	1:B:223:GLY:HA2	2.22	0.40
1:B:284:ILE:HG22	1:B:330:PRO:HA	2.03	0.40
1:A:261:PHE:CZ	1:A:280:ALA:HB2	2.56	0.40
1:B:331:LEU:CD2	1:B:366:GLU:HA	2.50	0.40
1:B:268:PHE:O	1:B:272:MET:HG3	2.22	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	214/319 (67%)	183 (86%)	26 (12%)	5 (2%)	6	11
1	B	214/319 (67%)	189 (88%)	20 (9%)	5 (2%)	6	11
All	All	428/638 (67%)	372 (87%)	46 (11%)	10 (2%)	6	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	GLY
1	A	236	PRO
1	B	108	VAL
1	B	238	VAL
1	A	237	GLU
1	B	208	GLY
1	A	198	SER
1	B	318	ALA
1	A	238	VAL
1	B	235	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	175/246 (71%)	164 (94%)	11 (6%)	18	36
1	B	175/246 (71%)	165 (94%)	10 (6%)	20	41
All	All	350/492 (71%)	329 (94%)	21 (6%)	19	39

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	137	VAL
1	A	141	PHE
1	A	186	VAL
1	A	224	GLN
1	A	265	LEU
1	A	274	GLU
1	A	304	LEU
1	A	307	ASP
1	A	319	ARG
1	A	396	LEU
1	B	98	LEU
1	B	102	THR

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Mol	Chain	Res	Type
1	B	137	VAL
1	B	186	VAL
1	B	189	THR
1	B	224	GLN
1	B	238	VAL
1	B	265	LEU
1	B	271	LEU
1	B	307	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	230	HIS
1	A	244	GLN
1	B	224	GLN
1	B	230	HIS
1	B	234	ASN
1	B	244	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	224/319 (70%)	-0.12	8 (3%) 42 35	20, 45, 88, 99	0
1	B	224/319 (70%)	-0.14	10 (4%) 33 26	19, 45, 87, 102	0
All	All	448/638 (70%)	-0.13	18 (4%) 38 31	19, 45, 88, 102	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	MET	6.2
1	B	399	MET	4.2
1	A	398	ALA	3.6
1	B	142	LYS	3.6
1	B	238	VAL	3.1
1	A	364	GLU	2.9
1	B	134	TRP	2.8
1	A	397	HIS	2.8
1	B	235	GLY	2.7
1	A	330	PRO	2.6
1	A	141	PHE	2.4
1	B	239	THR	2.3
1	B	364	GLU	2.2
1	B	331	LEU	2.2
1	B	236	PRO	2.1
1	B	306	SER	2.1
1	A	142	LYS	2.0
1	A	238	VAL	2.0

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

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



### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.