



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:02 PM GMT

PDB ID : 4AMU  
Title : Structure of ornithine carbamoyltransferase from Mycoplasma penetrans with a P321 space group  
Authors : Gallego, P.; Benach, J.; Planell, R.; Querol, E.; Perez-Pons, J.A.; Reverter, D.  
Deposited on : 2012-03-13  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

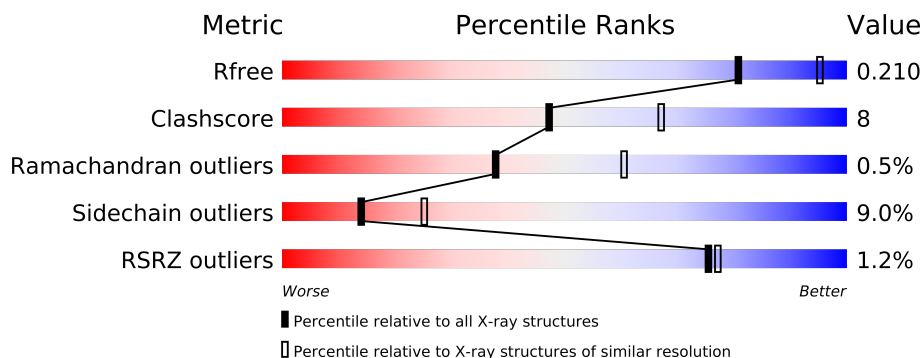
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	365	
1	B	365	
1	C	365	
1	D	365	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11190 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ORNITHINE CARBAMOYLTRANSFERASE,CATABOLIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2693	1713	457	508	15			
1	B	344	Total	C	N	O	S	0	0	0
			2693	1713	457	508	15			
1	C	344	Total	C	N	O	S	0	0	0
			2693	1713	457	508	15			
1	D	344	Total	C	N	O	S	0	0	0
			2693	1713	457	508	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
A	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
A	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
A	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
A	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
A	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
A	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
A	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
A	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
A	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
B	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
B	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
B	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
B	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
B	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
B	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
B	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
B	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
B	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
C	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
C	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
C	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
C	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
C	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
C	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
C	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
D	-21	GLY	-	EXPRESSION TAG	UNP Q8EVF5
D	-20	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-19	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-18	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-17	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-16	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-15	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-14	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-13	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-12	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-11	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-10	SER	-	EXPRESSION TAG	UNP Q8EVF5
D	-9	SER	-	EXPRESSION TAG	UNP Q8EVF5
D	-8	GLY	-	EXPRESSION TAG	UNP Q8EVF5
D	-7	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-6	ILE	-	EXPRESSION TAG	UNP Q8EVF5
D	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
D	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
D	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5

- Molecule 2 is water.

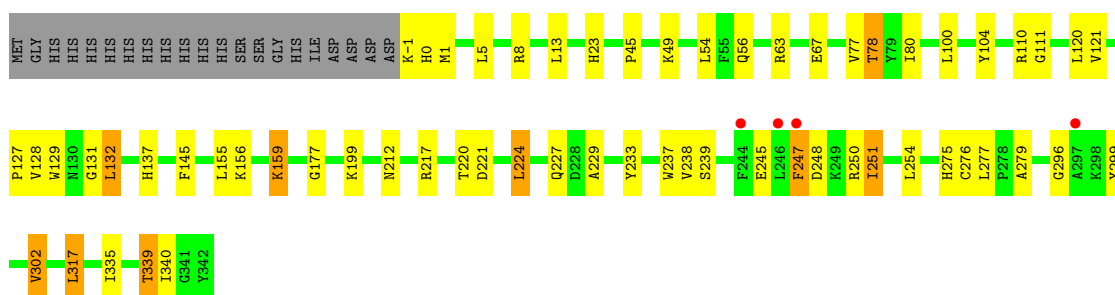
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		
2	B	122	Total	O	0	0
			122	122		
2	C	77	Total	O	0	0
			77	77		
2	D	95	Total	O	0	0
			95	95		

### 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 errors 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.

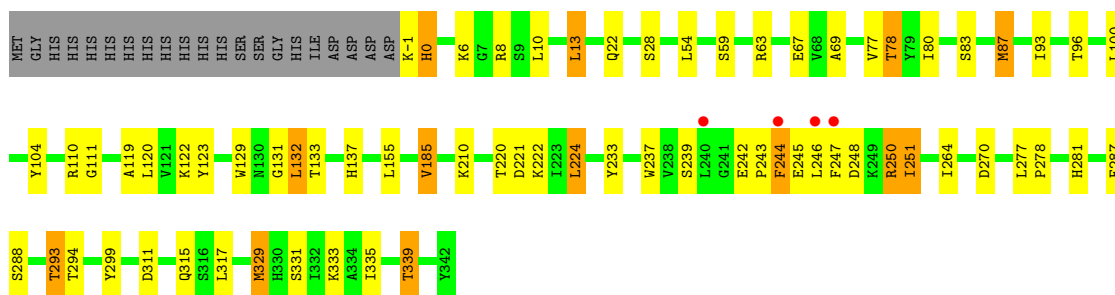
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE,CATABOLIC

Chain A: 



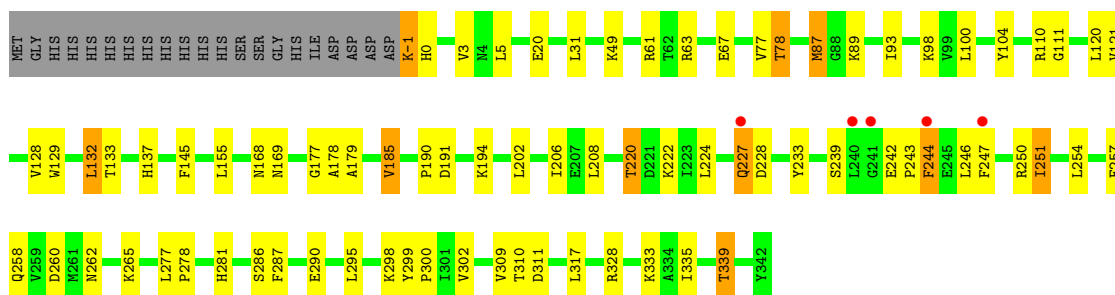
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE,CATABOLIC

Chain B: 



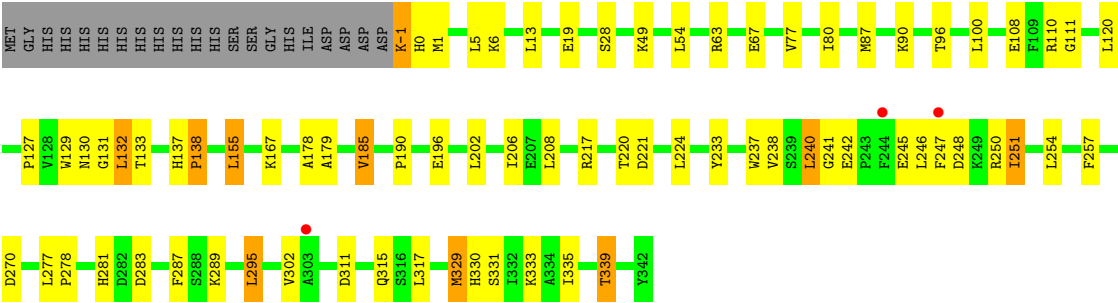
#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE,CATABOLIC

Chain C: 



#### • Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE,CATABOLIC

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.65Å 183.65Å 117.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.42 – 2.50 49.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.42-2.50) 91.5 (49.42-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.170 , 0.215 0.167 , 0.210	Depositor DCC
$R_{free}$ test set	3628 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.3	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 72155 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 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	0.42	0/2744	0.58	0/3696
1	B	0.45	0/2744	0.60	1/3696 (0.0%)
1	C	0.40	0/2744	0.57	0/3696
1	D	0.41	0/2744	0.58	0/3696
All	All	0.42	0/10976	0.58	1/14784 (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	185	VAL	CB-CA-C	-5.19	101.53	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2693	0	2692	39	0
1	B	2693	0	2692	44	0
1	C	2693	0	2692	44	0
1	D	2693	0	2692	50	0
2	A	124	0	0	5	0
2	B	122	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	77	0	0	1	0
2	D	95	0	0	1	0
All	All	11190	0	10768	173	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:329:MET:HE3	1:D:333:LYS:HE3	1.24	1.14
1:B:129:TRP:HE1	1:B:339:THR:HG21	1.16	1.09
1:D:129:TRP:HE1	1:D:339:THR:HG21	1.26	1.00
1:C:129:TRP:HE1	1:C:339:THR:HG21	1.29	0.96
1:B:329:MET:HE3	1:B:333:LYS:HE3	1.47	0.94
1:A:251:ILE:HD12	1:A:302:VAL:HG11	1.54	0.90
1:C:243:PRO:HD2	1:C:246:LEU:HD13	1.55	0.87
1:A:129:TRP:HE1	1:A:339:THR:HG21	1.41	0.85
1:B:129:TRP:NE1	1:B:339:THR:HG21	1.93	0.83
1:C:129:TRP:NE1	1:C:339:THR:HG21	2.01	0.76
1:B:329:MET:CE	1:B:333:LYS:HE3	2.17	0.73
1:B:250:ARG:HH11	1:B:250:ARG:HB2	1.53	0.73
1:D:129:TRP:NE1	1:D:339:THR:HG21	2.02	0.72
1:A:335:ILE:O	1:A:339:THR:HB	1.89	0.72
1:A:296:GLY:HA2	1:A:299:TYR:O	1.88	0.72
1:D:335:ILE:O	1:D:339:THR:HB	1.91	0.69
1:A:129:TRP:NE1	1:A:339:THR:HG21	2.11	0.66
1:D:248:ASP:HA	1:D:251:ILE:HG23	1.78	0.66
1:B:335:ILE:O	1:B:339:THR:HB	1.96	0.66
1:D:329:MET:O	1:D:329:MET:HE2	1.96	0.66
1:A:1:MET:HE2	1:C:98:LYS:HG2	1.79	0.65
1:A:54:LEU:HD22	1:A:80:ILE:HD12	1.77	0.64
1:A:54:LEU:CD2	1:A:80:ILE:HD12	2.28	0.64
1:B:69:ALA:HA	1:B:329:MET:HE3	1.80	0.63
1:C:202:LEU:O	1:C:206:ILE:HG12	1.97	0.63
1:C:335:ILE:O	1:C:339:THR:HB	1.99	0.62
1:C:251:ILE:HD12	1:C:302:VAL:HG11	1.81	0.62
1:C:277:LEU:HB3	1:C:278:PRO:HA	1.82	0.61
1:C:246:LEU:H	1:C:246:LEU:HD12	1.64	0.61
1:D:-1:LYS:HB3	1:D:-1:LYS:NZ	2.15	0.60
1:B:69:ALA:HB2	1:B:329:MET:HE2	1.84	0.60
1:D:167:LYS:HD2	1:D:196:GLU:HG3	1.84	0.60
1:D:127:PRO:HB3	1:D:339:THR:HG23	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:190:PRO:HD3	1:C:257:PHE:CE2	2.38	0.59
1:B:87:MET:HE3	1:B:96:THR:HG21	1.85	0.58
1:B:87:MET:CE	1:B:96:THR:HG21	2.34	0.58
1:B:78:THR:HG21	1:B:104:TYR:OH	2.02	0.57
1:B:111:GLY:O	1:B:133:THR:HA	2.04	0.57
1:D:28:SER:OG	1:D:331:SER:HA	2.05	0.57
1:B:244:PHE:HA	1:B:247:PHE:HB2	1.87	0.56
1:A:238:VAL:HG22	1:A:239:SER:N	2.20	0.56
1:A:317:LEU:HD13	1:A:317:LEU:H	1.71	0.55
1:C:286:SER:O	1:C:290:GLU:HG2	2.06	0.55
1:D:281:HIS:O	1:D:311:ASP:HB2	2.07	0.55
1:D:90:LYS:O	1:D:90:LYS:HG2	2.07	0.55
1:C:87:MET:HG2	1:C:93:ILE:HG13	1.88	0.55
1:A:127:PRO:HB3	1:A:339:THR:HG23	1.88	0.55
1:D:-1:LYS:HG3	1:D:19:GLU:OE2	2.08	0.55
1:B:244:PHE:HB3	2:B:2100:HOH:O	2.06	0.54
1:C:260:ASP:OD1	1:C:262:ASN:HB2	2.07	0.54
1:A:251:ILE:CD1	1:A:302:VAL:HG11	2.35	0.54
1:D:190:PRO:HD3	1:D:257:PHE:CE2	2.43	0.54
1:B:122:LYS:HE2	1:B:123:TYR:OH	2.08	0.53
1:B:87:MET:HE2	1:B:87:MET:HA	1.91	0.53
1:D:-1:LYS:HZ3	1:D:-1:LYS:HB3	1.74	0.53
1:B:122:LYS:HE2	1:B:123:TYR:CZ	2.44	0.52
1:B:281:HIS:O	1:B:311:ASP:HB2	2.09	0.52
1:A:145:PHE:CE1	1:A:177:GLY:HA3	2.45	0.52
1:D:248:ASP:HB3	1:D:295:LEU:HD21	1.92	0.52
1:B:22:GLN:HG2	2:B:2016:HOH:O	2.08	0.52
1:B:10:LEU:HD22	1:B:335:ILE:HD13	1.92	0.52
1:D:111:GLY:O	1:D:133:THR:HA	2.10	0.52
1:A:217:ARG:HD3	2:A:2095:HOH:O	2.09	0.52
1:D:238:VAL:HG11	1:D:287:PHE:HZ	1.75	0.51
1:C:145:PHE:CE1	1:C:177:GLY:HA3	2.45	0.51
1:A:159:LYS:HE3	1:A:227:GLN:O	2.10	0.51
1:C:298:LYS:O	1:C:300:PRO:HD3	2.11	0.51
1:D:221:ASP:OD2	1:D:224:LEU:HD22	2.12	0.50
1:B:293:THR:HG22	1:B:294:THR:N	2.25	0.50
1:A:1:MET:CE	1:C:98:LYS:HG2	2.42	0.50
1:B:6:LYS:HE2	1:D:6:LYS:HE2	1.94	0.50
1:D:302:VAL:O	1:D:302:VAL:HG23	2.11	0.50
1:D:-1:LYS:NZ	1:D:0:HIS:CD2	2.80	0.49
1:C:87:MET:HG3	2:C:2042:HOH:O	2.12	0.49
1:D:108:GLU:OE2	1:D:131:GLY:HA3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:220:THR:CG2	1:C:220:THR:O	2.61	0.49
1:A:159:LYS:HG2	1:A:229:ALA:HA	1.96	0.48
1:D:237:TRP:O	1:D:250:ARG:HD3	2.13	0.48
1:D:202:LEU:O	1:D:206:ILE:HG12	2.13	0.48
1:C:5:LEU:HD21	1:C:20:GLU:HG2	1.96	0.48
1:A:78:THR:HG21	1:A:104:TYR:OH	2.13	0.48
1:C:78:THR:HG23	1:C:104:TYR:HE1	1.79	0.48
1:C:281:HIS:O	1:C:311:ASP:HB2	2.14	0.48
1:C:78:THR:HG21	1:C:104:TYR:OH	2.14	0.47
1:D:54:LEU:CD2	1:D:80:ILE:HD12	2.45	0.47
1:B:329:MET:O	1:B:329:MET:HE2	2.15	0.47
1:C:78:THR:HG23	1:C:104:TYR:CE1	2.48	0.47
1:B:311:ASP:O	1:B:315:GLN:HG2	2.14	0.47
1:A:56:GLN:HG2	1:A:111:GLY:HA2	1.97	0.47
1:A:251:ILE:HD12	1:A:302:VAL:CG1	2.36	0.47
1:D:246:LEU:O	1:D:250:ARG:HG3	2.15	0.47
1:D:178:ALA:HB1	1:D:185:VAL:HG22	1.96	0.47
1:A:121:VAL:HG22	1:A:128:VAL:HB	1.96	0.47
1:B:8:ARG:HD2	2:B:2010:HOH:O	2.14	0.47
1:D:238:VAL:HG11	1:D:247:PHE:CE2	2.50	0.47
1:A:131:GLY:O	1:A:132:LEU:CB	2.63	0.47
1:C:239:SER:O	1:C:242:GLU:HG2	2.15	0.47
1:B:247:PHE:O	1:B:251:ILE:HG23	2.15	0.47
1:D:221:ASP:OD2	1:D:224:LEU:HD13	2.15	0.47
1:D:220:THR:O	1:D:220:THR:HG22	2.15	0.47
1:D:247:PHE:O	1:D:251:ILE:HG22	2.14	0.46
1:A:23:HIS:HE1	2:A:2122:HOH:O	1.97	0.46
1:A:-1:LYS:N	2:A:2001:HOH:O	2.48	0.46
1:C:31:LEU:HD13	1:C:333:LYS:HG2	1.97	0.46
1:B:329:MET:CE	1:B:333:LYS:HB2	2.46	0.46
1:A:238:VAL:HG21	1:A:247:PHE:CE2	2.51	0.46
1:B:13:LEU:HA	1:B:13:LEU:HD23	1.85	0.46
1:C:227:GLN:O	1:C:228:ASP:HB2	2.15	0.45
1:B:239:SER:O	1:B:242:GLU:HG2	2.16	0.45
1:C:3:VAL:HG23	1:C:3:VAL:O	2.16	0.45
1:B:54:LEU:HD22	1:B:80:ILE:HD12	1.98	0.45
1:A:248:ASP:OD1	1:A:299:TYR:HE2	2.00	0.45
1:C:247:PHE:O	1:C:251:ILE:HG23	2.16	0.45
1:C:121:VAL:HG22	1:C:128:VAL:HB	1.98	0.45
1:C:251:ILE:HD11	1:C:299:TYR:CD2	2.52	0.45
1:A:275:HIS:CD2	1:A:279:ALA:HB2	2.52	0.45
1:A:0:HIS:HB3	1:C:98:LYS:HD3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:131:GLY:O	1:D:132:LEU:CB	2.64	0.45
1:D:127:PRO:CB	1:D:339:THR:HG23	2.46	0.45
1:D:240:LEU:HA	1:D:241:GLY:HA2	1.65	0.45
1:D:329:MET:HE1	1:D:330:HIS:HA	1.99	0.44
1:A:237:TRP:O	1:A:250:ARG:HD3	2.18	0.44
1:B:251:ILE:HD11	1:B:299:TYR:CG	2.53	0.44
1:C:309:VAL:HG22	1:C:310:THR:N	2.33	0.44
1:D:329:MET:O	1:D:329:MET:CE	2.65	0.44
1:B:247:PHE:CE2	1:B:287:PHE:HZ	2.36	0.44
1:D:54:LEU:HD22	1:D:80:ILE:HD12	2.00	0.44
1:B:237:TRP:O	1:B:250:ARG:HG2	2.17	0.43
1:D:87:MET:CE	1:D:96:THR:HG21	2.48	0.43
1:A:49:LYS:HE3	2:A:2043:HOH:O	2.18	0.43
1:C:179:ALA:HB1	1:C:208:LEU:HB2	2.01	0.43
1:A:250:ARG:NH1	1:A:250:ARG:HG2	2.33	0.43
1:B:54:LEU:HD23	1:B:54:LEU:N	2.33	0.43
1:B:243:PRO:O	1:B:245:GLU:N	2.46	0.43
1:A:276:CYS:O	1:A:277:LEU:HB2	2.18	0.43
1:A:8:ARG:HD2	2:A:2011:HOH:O	2.18	0.43
1:C:-1:LYS:HD2	1:C:-1:LYS:C	2.39	0.43
1:D:311:ASP:O	1:D:315:GLN:HG2	2.19	0.43
1:A:127:PRO:CB	1:A:339:THR:HG23	2.49	0.42
1:A:245:GLU:CD	1:A:245:GLU:H	2.23	0.42
1:B:131:GLY:O	1:B:132:LEU:CB	2.68	0.42
1:A:199:LYS:HE3	1:A:199:LYS:HB2	1.84	0.42
1:A:127:PRO:HG2	1:A:340:ILE:HD13	2.00	0.42
1:C:168:ASN:C	1:C:168:ASN:OD1	2.58	0.42
1:B:224:LEU:HD12	1:B:224:LEU:HA	1.89	0.42
1:C:111:GLY:O	1:C:133:THR:HA	2.20	0.42
1:D:220:THR:O	1:D:220:THR:CG2	2.68	0.41
1:D:49:LYS:HE3	2:D:2032:HOH:O	2.20	0.41
1:B:93:ILE:HD13	1:B:119:ALA:HB3	2.02	0.41
1:D:-1:LYS:O	1:D:-1:LYS:HG2	2.18	0.41
1:C:244:PHE:CE1	1:C:295:LEU:HD21	2.55	0.41
1:B:28:SER:OG	1:B:331:SER:HA	2.21	0.41
1:C:277:LEU:HA	1:C:278:PRO:C	2.41	0.41
1:B:247:PHE:CE2	1:B:287:PHE:CZ	3.07	0.41
1:D:155:LEU:HA	1:D:155:LEU:HD12	1.81	0.41
1:D:283:ASP:O	1:D:289:LYS:HE3	2.21	0.41
1:C:178:ALA:HB1	1:C:185:VAL:HG22	2.03	0.41
1:D:329:MET:CE	1:D:333:LYS:HB2	2.50	0.41
1:B:-1:LYS:HZ3	1:B:0:HIS:CG	2.38	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:277:LEU:HA	1:B:278:PRO:C	2.41	0.41
1:C:247:PHE:HE2	1:C:287:PHE:HZ	1.68	0.41
1:A:156:LYS:HE3	1:A:212:ASN:O	2.20	0.41
1:A:221:ASP:OD2	1:A:224:LEU:HD22	2.21	0.41
1:C:246:LEU:O	1:C:250:ARG:HG3	2.21	0.41
1:D:248:ASP:OD1	1:D:248:ASP:N	2.54	0.41
1:C:220:THR:O	1:C:220:THR:HG22	2.20	0.41
1:B:221:ASP:OD2	1:B:224:LEU:HD22	2.21	0.41
1:D:130:ASN:HB3	1:D:138:PRO:HG2	2.03	0.41
1:B:210:LYS:HE3	1:B:210:LYS:HB2	1.81	0.40
1:D:277:LEU:HA	1:D:278:PRO:C	2.42	0.40
1:C:191:ASP:O	1:C:194:LYS:HG2	2.22	0.40
1:C:132:LEU:HD11	1:C:169:ASN:ND2	2.36	0.40
1:D:179:ALA:HB1	1:D:208:LEU:HB2	2.02	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	342/365 (94%)	325 (95%)	15 (4%)	2 (1%)	33	55
1	B	342/365 (94%)	330 (96%)	10 (3%)	2 (1%)	33	55
1	C	342/365 (94%)	327 (96%)	13 (4%)	2 (1%)	33	55
1	D	342/365 (94%)	327 (96%)	14 (4%)	1 (0%)	50	73
All	All	1368/1460 (94%)	1309 (96%)	52 (4%)	7 (0%)	38	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	B	132	LEU
1	C	132	LEU
1	D	132	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	244	PHE
1	C	244	PHE
1	A	302	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	293/312 (94%)	272 (93%)	21 (7%)	21	36
1	B	293/312 (94%)	263 (90%)	30 (10%)	11	19
1	C	293/312 (94%)	265 (90%)	28 (10%)	12	22
1	D	293/312 (94%)	267 (91%)	26 (9%)	14	26
All	All	1172/1248 (94%)	1067 (91%)	105 (9%)	14	25

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	13	LEU
1	A	45	PRO
1	A	63	ARG
1	A	67	GLU
1	A	77	VAL
1	A	78	THR
1	A	100	LEU
1	A	110	ARG
1	A	120	LEU
1	A	137	HIS
1	A	155	LEU
1	A	159	LYS
1	A	220	THR
1	A	224	LEU
1	A	233	TYR
1	A	247	PHE
1	A	251	ILE
1	A	254	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	317	LEU
1	A	339	THR
1	B	0	HIS
1	B	13	LEU
1	B	59	SER
1	B	63	ARG
1	B	67	GLU
1	B	77	VAL
1	B	78	THR
1	B	83	SER
1	B	87	MET
1	B	100	LEU
1	B	110	ARG
1	B	120	LEU
1	B	137	HIS
1	B	155	LEU
1	B	185	VAL
1	B	220	THR
1	B	222	LYS
1	B	224	LEU
1	B	233	TYR
1	B	246	LEU
1	B	248	ASP
1	B	250	ARG
1	B	251	ILE
1	B	264	ILE
1	B	270	ASP
1	B	288	SER
1	B	293	THR
1	B	317	LEU
1	B	329	MET
1	B	339	THR
1	C	-1	LYS
1	C	0	HIS
1	C	49	LYS
1	C	61	ARG
1	C	63	ARG
1	C	67	GLU
1	C	77	VAL
1	C	78	THR
1	C	87	MET
1	C	89	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	100	LEU
1	C	110	ARG
1	C	120	LEU
1	C	137	HIS
1	C	155	LEU
1	C	185	VAL
1	C	220	THR
1	C	222	LYS
1	C	224	LEU
1	C	227	GLN
1	C	233	TYR
1	C	251	ILE
1	C	254	LEU
1	C	258	GLN
1	C	265	LYS
1	C	317	LEU
1	C	328	ARG
1	C	339	THR
1	D	-1	LYS
1	D	1	MET
1	D	5	LEU
1	D	13	LEU
1	D	63	ARG
1	D	67	GLU
1	D	77	VAL
1	D	100	LEU
1	D	110	ARG
1	D	120	LEU
1	D	137	HIS
1	D	138	PRO
1	D	155	LEU
1	D	185	VAL
1	D	217	ARG
1	D	233	TYR
1	D	240	LEU
1	D	242	GLU
1	D	245	GLU
1	D	251	ILE
1	D	254	LEU
1	D	270	ASP
1	D	295	LEU
1	D	317	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	329	MET
1	D	339	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	D	0	HIS
1	D	37	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	344/365 (94%)	-0.53	4 (1%) 75 77	20, 33, 61, 87	0
1	B	344/365 (94%)	-0.52	4 (1%) 75 77	17, 30, 56, 91	0
1	C	344/365 (94%)	-0.41	5 (1%) 70 72	21, 37, 68, 100	0
1	D	344/365 (94%)	-0.43	3 (0%) 81 82	20, 35, 65, 98	0
All	All	1376/1460 (94%)	-0.47	16 (1%) 75 77	17, 34, 65, 100	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	PHE	3.3
1	A	244	PHE	3.2
1	C	247	PHE	3.0
1	C	240	LEU	2.9
1	D	247	PHE	2.8
1	A	297	ALA	2.8
1	B	247	PHE	2.4
1	B	244	PHE	2.4
1	A	247	PHE	2.3
1	D	244	PHE	2.2
1	D	303	ALA	2.2
1	C	227	GLN	2.1
1	C	241	GLY	2.1
1	B	246	LEU	2.1
1	A	246	LEU	2.1
1	B	240	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.