



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

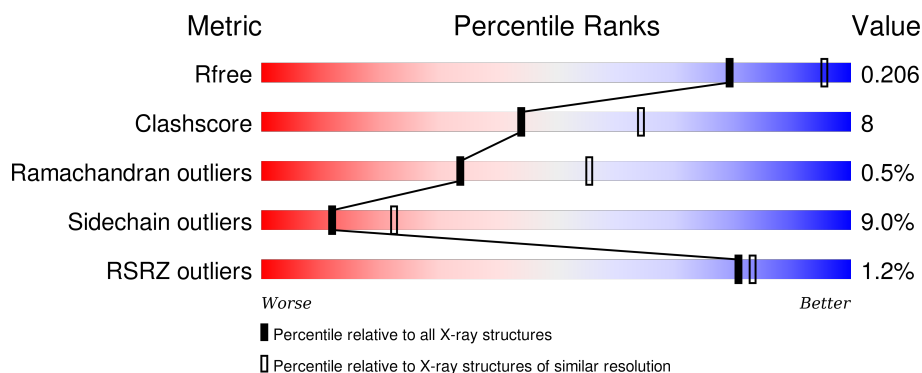
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

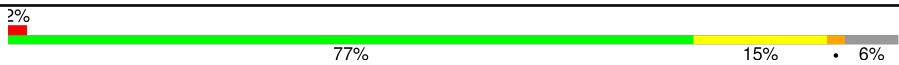



The reported resolution of this entry is 2.50 Å.

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))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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.

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 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 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

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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

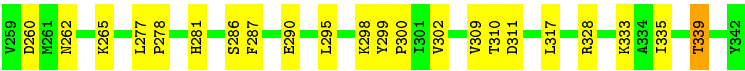
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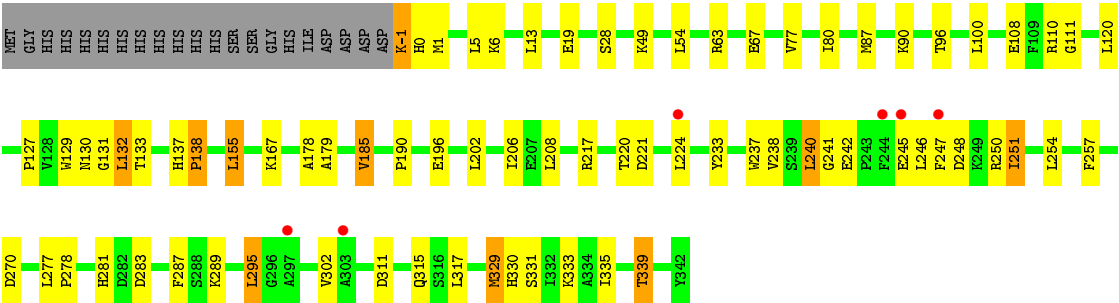
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-4	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-3	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-2	ASP	-	EXPRESSION TAG	UNP Q8EVF5
C	-1	LYS	-	EXPRESSION TAG	UNP Q8EVF5
C	0	HIS	-	EXPRESSION TAG	UNP Q8EVF5
D	-22	MET	-	EXPRESSION TAG	UNP Q8EVF5
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 124 124	0	0
2	B	122	Total O 122 122	0	0
2	C	77	Total O 77 77	0	0
2	D	95	Total O 95 95	0	0



● Molecule 1: ORNITHINE CARBAMOYLTRANSFERASE, CATABOLIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.170 , 0.215 0.158 , 0.206	Depositor DCC
R_{free} test set	3628 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 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	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
2	C	77	0	0	1	0
2	D	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11190	0	10768	173	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 8.

All (173) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLU:OE2	1:D:131:GLY:HA3	2.13	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	30	50
1	B	342/365 (94%)	330 (96%)	10 (3%)	2 (1%)	30	50
1	C	342/365 (94%)	327 (96%)	13 (4%)	2 (1%)	30	50
1	D	342/365 (94%)	327 (96%)	14 (4%)	1 (0%)	46	68
All	All	1368/1460 (94%)	1309 (96%)	52 (4%)	7 (0%)	34	55

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
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%)	18	33
1	B	293/312 (94%)	263 (90%)	30 (10%)	9	17
1	C	293/312 (94%)	265 (90%)	28 (10%)	10	19
1	D	293/312 (94%)	267 (91%)	26 (9%)	12	23
All	All	1172/1248 (94%)	1067 (91%)	105 (9%)	12	22

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

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Mol	Chain	Res	Type
1	A	233	TYR
1	A	247	PHE
1	A	251	ILE
1	A	254	LEU
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

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Mol	Chain	Res	Type
1	C	77	VAL
1	C	78	THR
1	C	87	MET
1	C	89	LYS
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

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Mol	Chain	Res	Type
1	D	254	LEU
1	D	270	ASP
1	D	295	LEU
1	D	317	LEU
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 [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 [i](#)

There are no ligands in this entry.

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	344/365 (94%)	-0.33	6 (1%) 73 76	20, 33, 61, 87	0
1	B	344/365 (94%)	-0.57	2 (0%) 90 91	17, 30, 56, 91	0
1	C	344/365 (94%)	-0.39	3 (0%) 85 88	21, 37, 68, 100	0
1	D	344/365 (94%)	-0.23	6 (1%) 73 76	20, 35, 65, 98	0
All	All	1376/1460 (94%)	-0.38	17 (1%) 81 83	17, 34, 65, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	247	PHE	3.4
1	A	297	ALA	3.4
1	C	244	PHE	3.3
1	A	244	PHE	3.3
1	A	247	PHE	3.0
1	A	294	THR	3.0
1	C	247	PHE	2.7
1	D	297	ALA	2.7
1	D	244	PHE	2.6
1	B	247	PHE	2.5
1	A	296	GLY	2.4
1	A	246	LEU	2.4
1	D	224	LEU	2.3
1	D	303	ALA	2.3
1	C	0	HIS	2.1
1	D	245	GLU	2.1
1	B	297	ALA	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 [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.