



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:59 PM GMT

PDB ID : 1Z7D
Title : Ornithine aminotransferase PY00104 from Plasmodium Yoelii
Authors : Walker, J.R.; Alam, Z.; Amani, M.; Lew, J.; Wasney, G.; Boulanger, K.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.; Edwards, A.; Bochkarev, A.; Hui, R.; Vedadi, M.; Structural Genomics Consortium (SGC)
Deposited on : 2005-03-24
Resolution : 2.10 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
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

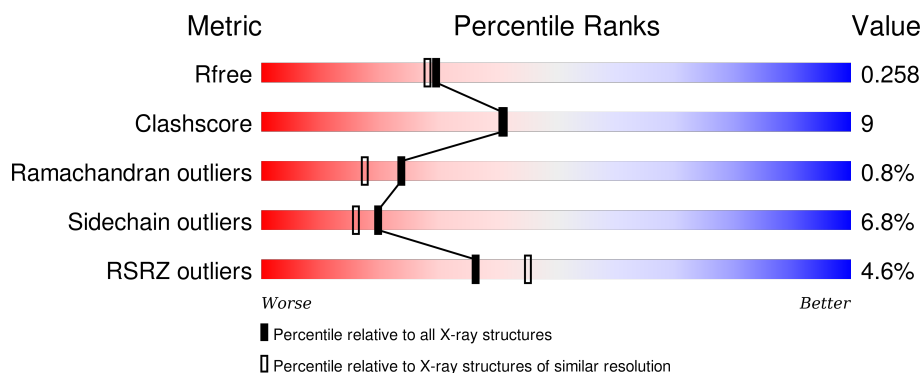
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	433	<div> <div>70%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	B	433	<div> <div>5%</div> <div>68%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	C	433	<div> <div>6%</div> <div>66%</div> <div>17%</div> <div>•</div> <div>15%</div> </div>
1	D	433	<div> <div>3%</div> <div>68%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	E	433	<div> <div>6%</div> <div>71%</div> <div>14%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	433	<div><div></div><div>2%</div><div>68%</div><div>16%</div><div>• •</div><div>13%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18172 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 aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2969	1898	497	555	19			
1	B	377	Total	C	N	O	S	0	0	0
			2960	1893	495	553	19			
1	C	369	Total	C	N	O	S	0	0	0
			2895	1851	483	542	19			
1	D	375	Total	C	N	O	S	0	0	0
			2944	1885	491	549	19			
1	E	374	Total	C	N	O	S	0	0	0
			2935	1879	489	548	19			
1	F	375	Total	C	N	O	S	0	0	0
			2944	1885	491	549	19			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
A	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90
A	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
A	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
A	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
A	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
A	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
A	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
A	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
A	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
A	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
A	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
A	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90
B	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
B	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90
B	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
B	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
B	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
B	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
B	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
B	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
B	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
B	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
B	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
B	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90
B	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
B	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90
C	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
C	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90
C	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
C	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
C	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
C	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
C	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
C	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
C	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
C	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
C	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
C	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90
C	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
C	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90
D	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
D	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
D	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
D	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
D	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
D	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
D	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
D	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
D	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
D	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
D	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90
D	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
D	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90
E	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
E	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90
E	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
E	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
E	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
E	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
E	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
E	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
E	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
E	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
E	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
E	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90
E	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
E	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90
F	-19	MET	-	CLONING ARTIFACT	UNP Q7RT90
F	-18	GLY	-	CLONING ARTIFACT	UNP Q7RT90
F	-17	SER	-	CLONING ARTIFACT	UNP Q7RT90
F	-16	SER	-	CLONING ARTIFACT	UNP Q7RT90
F	-15	HIS	-	CLONING ARTIFACT	UNP Q7RT90
F	-14	HIS	-	CLONING ARTIFACT	UNP Q7RT90

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	HIS	-	CLONING ARTIFACT	UNP Q7RT90
F	-12	HIS	-	CLONING ARTIFACT	UNP Q7RT90
F	-11	HIS	-	CLONING ARTIFACT	UNP Q7RT90
F	-10	HIS	-	CLONING ARTIFACT	UNP Q7RT90
F	-9	SER	-	CLONING ARTIFACT	UNP Q7RT90
F	-8	SER	-	CLONING ARTIFACT	UNP Q7RT90
F	-7	GLY	-	CLONING ARTIFACT	UNP Q7RT90
F	-6	LEU	-	CLONING ARTIFACT	UNP Q7RT90
F	-5	VAL	-	CLONING ARTIFACT	UNP Q7RT90
F	-4	PRO	-	CLONING ARTIFACT	UNP Q7RT90
F	-3	ARG	-	CLONING ARTIFACT	UNP Q7RT90
F	-2	GLY	-	CLONING ARTIFACT	UNP Q7RT90
F	-1	SER	-	CLONING ARTIFACT	UNP Q7RT90

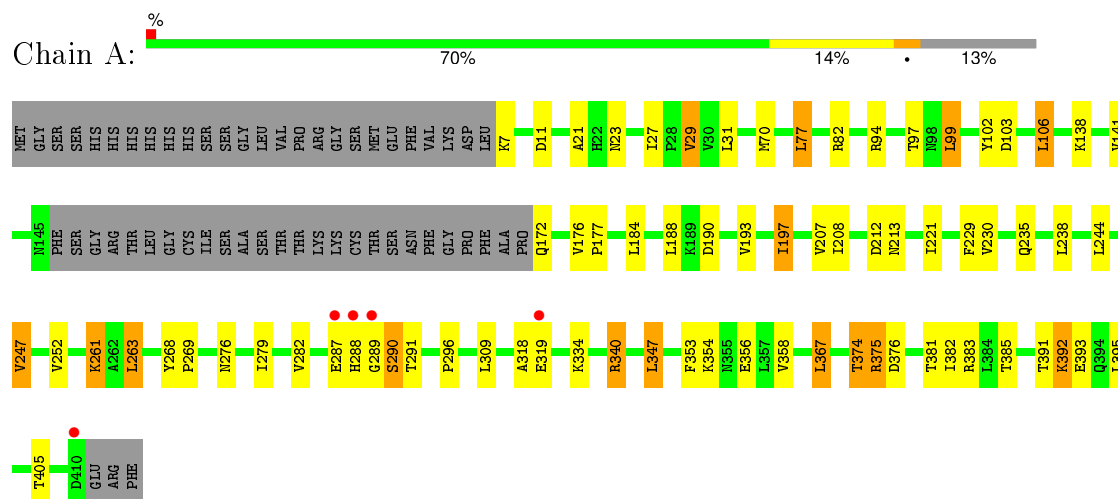
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	127	Total O 127 127	0	0
2	B	87	Total O 87 87	0	0
2	C	56	Total O 56 56	0	0
2	D	82	Total O 82 82	0	0
2	E	67	Total O 67 67	0	0
2	F	106	Total O 106 106	0	0

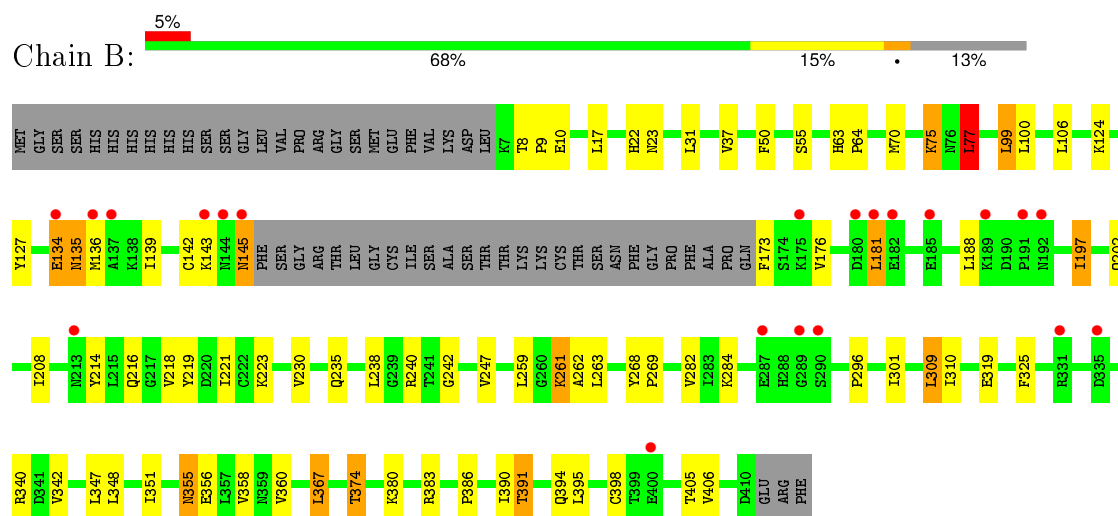
3 Residue-property plots

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 aminotransferase

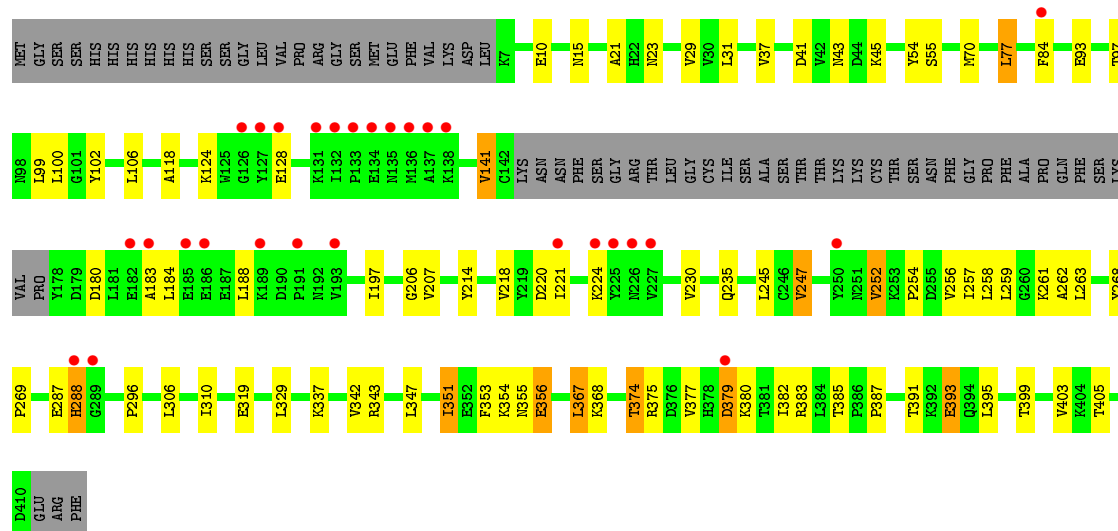


- Molecule 1: ornithine aminotransferase

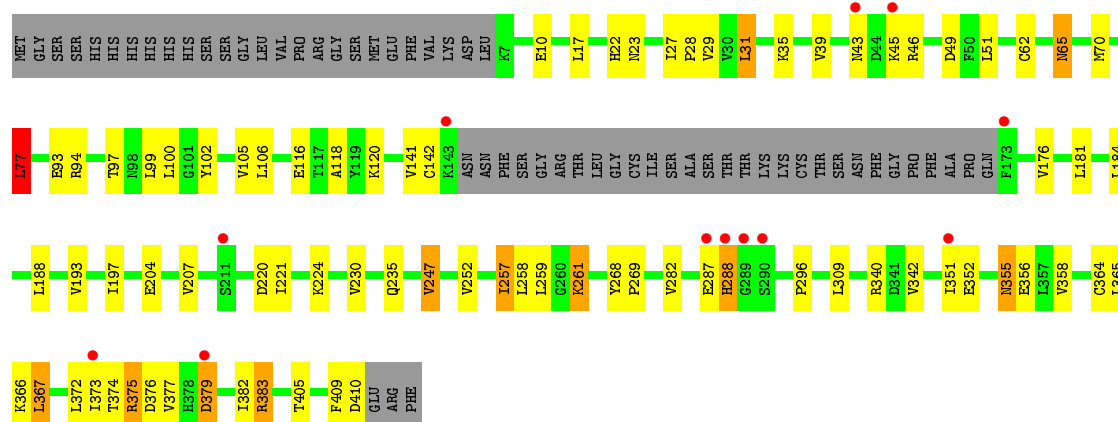


- Molecule 1: ornithine aminotransferase

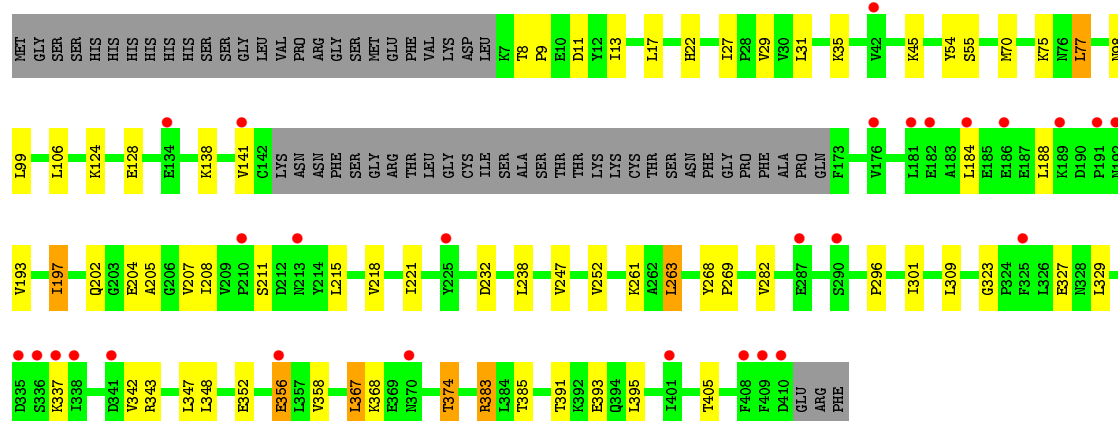




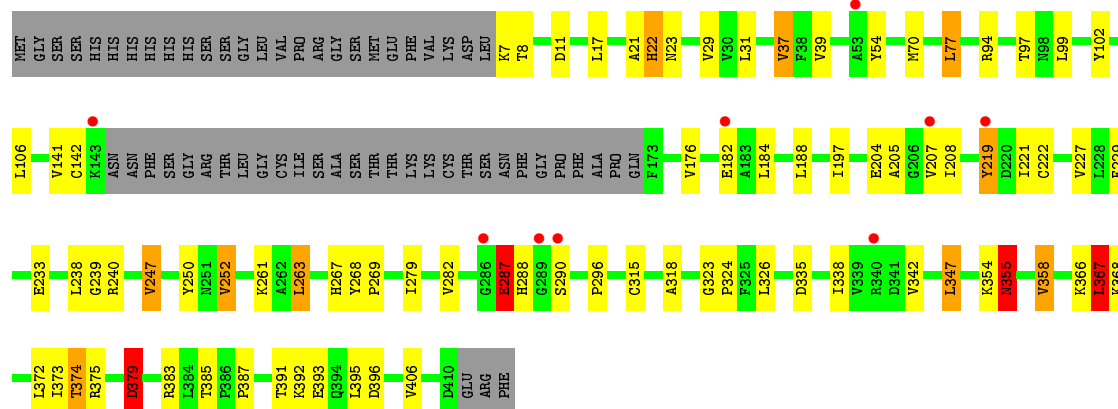
- Molecule 1: ornithine aminotransferase



- Molecule 1: ornithine aminotransferase



• Molecule 1: ornithine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.49Å 221.83Å 114.48Å 90.00° 100.89° 90.00°	Depositor
Resolution (Å)	49.74 – 2.10 49.74 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.74-2.10) 99.1 (49.74-2.09)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.259 0.214 , 0.258	Depositor DCC
R_{free} test set	7912 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 158699 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18172	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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 ⓘ

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	0.61	0/3023	0.69	0/4092
1	B	0.55	0/3014	0.68	2/4080 (0.0%)
1	C	0.50	0/2947	0.63	1/3990 (0.0%)
1	D	0.55	1/2998 (0.0%)	0.67	1/4058 (0.0%)
1	E	0.52	0/2989	0.65	0/4047
1	F	0.58	0/2998	0.70	1/4058 (0.0%)
All	All	0.55	1/17969 (0.0%)	0.67	5/24325 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	CYS	CB-SG	-5.17	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	LEU	CA-CB-CG	6.11	129.35	115.30
1	F	367	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	309	LEU	CA-CB-CG	5.67	128.33	115.30
1	D	77	LEU	CA-CB-CG	5.21	127.27	115.30
1	C	263	LEU	CA-CB-CG	5.01	126.81	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	2969	0	3015	56	0
1	B	2960	0	3007	57	0
1	C	2895	0	2939	64	0
1	D	2944	0	2995	61	0
1	E	2935	0	2982	40	0
1	F	2944	0	2995	58	0
2	A	127	0	0	3	0
2	B	87	0	0	2	0
2	C	56	0	0	4	0
2	D	82	0	0	1	0
2	E	67	0	0	2	0
2	F	106	0	0	4	0
All	All	18172	0	17933	305	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 9.

All (305) 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:F:366:LYS:HD2	2:F:514:HOH:O	1.49	1.10
1:C:374:THR:HG21	1:C:383:ARG:O	1.52	1.09
1:A:21:ALA:HB3	1:B:106:LEU:HD23	1.34	1.07
1:E:98:ASN:HB3	2:E:459:HOH:O	1.58	1.03
1:A:374:THR:HG21	1:A:383:ARG:O	1.60	1.02
1:F:374:THR:HG21	1:F:383:ARG:O	1.58	1.01
1:E:374:THR:HG21	1:E:383:ARG:O	1.67	0.95
1:C:287:GLU:O	1:C:288:HIS:HB2	1.70	0.90
1:E:106:LEU:HD11	1:F:23:ASN:ND2	1.87	0.90
1:B:374:THR:HG21	1:B:383:ARG:O	1.74	0.87
1:A:235:GLN:HE22	1:A:261:LYS:HE3	1.38	0.86
1:A:23:ASN:ND2	1:B:106:LEU:HD21	1.94	0.82
1:D:375:ARG:CG	1:D:375:ARG:HH11	1.96	0.78
1:F:385:THR:HG22	1:F:385:THR:O	1.83	0.78
1:C:206:GLY:O	1:C:343:ARG:NH1	2.16	0.78
1:C:235:GLN:HE22	1:C:261:LYS:NZ	1.81	0.77
1:D:375:ARG:HG2	1:D:375:ARG:HH11	1.49	0.77
1:C:21:ALA:HB3	1:D:106:LEU:HD23	1.67	0.77
1:C:106:LEU:HD11	1:D:23:ASN:ND2	2.00	0.76
1:E:27:ILE:HG22	1:E:29:VAL:HG23	1.67	0.76
1:C:41:ASP:OD2	1:C:45:LYS:HD2	1.86	0.76
1:B:181:LEU:H	1:B:181:LEU:HD13	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ASN:HD22	1:C:45:LYS:HE2	1.50	0.75
1:D:65:ASN:H	1:D:65:ASN:HD22	1.35	0.74
1:B:242:GLY:HA3	1:B:319:GLU:HG2	1.68	0.74
1:F:141:VAL:HG12	1:F:142:CYS:H	1.50	0.74
1:D:27:ILE:HG13	1:D:28:PRO:HD2	1.71	0.72
1:D:287:GLU:HG3	1:D:288:HIS:H	1.54	0.72
1:B:127:TYR:OH	1:B:135:ASN:HA	1.89	0.72
1:E:323:GLY:O	1:E:327:GLU:HG2	1.90	0.71
1:F:375:ARG:NH2	2:F:427:HOH:O	2.25	0.70
1:C:43:ASN:HB2	1:C:45:LYS:HE2	1.73	0.70
1:A:385:THR:HG22	1:A:385:THR:O	1.93	0.69
1:B:235:GLN:HE22	1:B:261:LYS:NZ	1.90	0.69
1:A:106:LEU:HD11	1:B:23:ASN:ND2	2.08	0.69
1:A:291:THR:HG21	1:B:261:LYS:HE3	1.75	0.68
1:A:188:LEU:HD22	1:A:193:VAL:HG11	1.76	0.68
1:F:287:GLU:CD	1:F:288:HIS:H	1.98	0.67
1:D:102:TYR:CZ	1:D:257:ILE:HD13	2.30	0.67
1:A:21:ALA:CB	1:B:106:LEU:HD23	2.19	0.66
1:D:355:ASN:H	1:D:355:ASN:HD22	1.42	0.64
1:E:70:MET:HE3	1:F:70:MET:HG2	1.79	0.64
1:F:247:VAL:HG22	1:F:252:VAL:HG13	1.77	0.64
1:B:145:ASN:H	1:B:145:ASN:HD22	1.45	0.64
1:A:288:HIS:CG	1:A:289:GLY:H	2.16	0.63
1:D:65:ASN:N	1:D:65:ASN:HD22	1.95	0.63
1:F:374:THR:HG22	1:F:375:ARG:H	1.63	0.63
1:C:235:GLN:HE22	1:C:261:LYS:HZ1	1.46	0.63
1:A:70:MET:HE3	1:B:70:MET:HG2	1.81	0.63
1:A:391:THR:HG22	1:A:393:GLU:H	1.63	0.63
1:E:391:THR:HG22	1:E:393:GLU:H	1.64	0.63
1:F:238:LEU:HD11	1:F:263:LEU:HD13	1.81	0.62
1:C:106:LEU:HD11	1:D:23:ASN:HD21	1.63	0.62
1:B:367:LEU:HD13	1:B:405:THR:HG21	1.80	0.62
1:A:94:ARG:HD2	2:A:443:HOH:O	1.99	0.62
1:F:17:LEU:O	1:F:22:HIS:HE1	1.83	0.61
1:B:17:LEU:O	1:B:22:HIS:HE1	1.84	0.61
1:C:21:ALA:CB	1:D:106:LEU:HD23	2.31	0.61
1:C:342:VAL:HG13	1:C:351:ILE:HG22	1.83	0.61
1:F:355:ASN:ND2	1:F:379:ASP:O	2.33	0.61
1:F:141:VAL:HG12	1:F:142:CYS:N	2.16	0.61
1:C:70:MET:HE3	1:D:70:MET:HG2	1.83	0.61
1:A:235:GLN:NE2	1:A:261:LYS:HE3	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ASP:HB2	2:D:493:HOH:O	2.00	0.60
1:F:141:VAL:HG22	1:F:197:ILE:HG23	1.83	0.60
1:E:343:ARG:NH2	1:E:352:GLU:OE1	2.31	0.60
1:D:102:TYR:OH	1:D:257:ILE:HD13	2.01	0.60
1:B:235:GLN:HE22	1:B:261:LYS:HZ1	1.49	0.59
1:B:238:LEU:HD11	1:B:263:LEU:HD13	1.85	0.59
1:D:340:ARG:HB3	1:D:352:GLU:HG2	1.84	0.59
1:A:23:ASN:CG	1:B:106:LEU:HD21	2.23	0.58
1:E:207:VAL:O	1:E:343:ARG:HD2	2.03	0.58
1:E:17:LEU:O	1:E:22:HIS:HE1	1.86	0.58
1:E:8:THR:HG23	1:E:11:ASP:H	1.68	0.58
1:E:215:LEU:HA	1:E:218:VAL:HG13	1.85	0.57
1:A:27:ILE:HG12	1:A:375:ARG:HH12	1.70	0.57
1:B:124:LYS:HE3	1:B:282:VAL:O	2.04	0.57
1:A:82:ARG:NH1	2:A:423:HOH:O	2.28	0.57
1:A:391:THR:CG2	1:A:393:GLU:OE1	2.53	0.57
1:C:10:GLU:CD	1:C:10:GLU:H	2.08	0.57
1:C:247:VAL:HG22	1:C:252:VAL:HG13	1.85	0.56
1:E:197:ILE:HD11	1:E:232:ASP:HB2	1.88	0.56
1:B:77:LEU:HD13	1:B:296:PRO:HG3	1.87	0.56
1:D:188:LEU:HD12	1:D:221:ILE:HG22	1.86	0.56
1:A:374:THR:HG22	1:A:375:ARG:H	1.71	0.56
1:A:99:LEU:HD21	1:A:244:LEU:CD1	2.35	0.56
1:A:212:ASP:O	1:A:213:ASN:HB2	2.07	0.55
2:C:431:HOH:O	1:D:35:LYS:HE2	2.06	0.55
1:C:268:TYR:CZ	1:D:269:PRO:HD3	2.40	0.55
1:C:287:GLU:O	1:C:288:HIS:CB	2.48	0.55
1:C:84:PHE:CZ	1:D:373:ILE:HD12	2.42	0.55
1:E:367:LEU:HD13	1:E:405:THR:HG21	1.89	0.55
1:E:238:LEU:HB3	1:E:309:LEU:HD11	1.89	0.54
1:C:399:THR:O	1:C:403:VAL:HG23	2.08	0.54
1:A:238:LEU:HD11	1:A:263:LEU:HD13	1.89	0.54
1:B:188:LEU:HD12	1:B:221:ILE:HG22	1.90	0.54
1:C:188:LEU:HD12	1:C:221:ILE:HG22	1.89	0.54
1:F:8:THR:CG2	1:F:11:ASP:H	2.20	0.54
1:A:288:HIS:CG	1:A:289:GLY:N	2.73	0.54
1:B:360:VAL:HG21	1:B:380:LYS:HA	1.90	0.54
1:A:77:LEU:HD13	1:A:296:PRO:HG3	1.90	0.54
1:F:8:THR:HG22	1:F:11:ASP:OD2	2.07	0.54
1:C:21:ALA:HB3	1:D:106:LEU:CD2	2.37	0.54
1:F:391:THR:HG22	1:F:392:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:THR:HG22	1:E:11:ASP:CG	2.28	0.54
1:E:106:LEU:HD13	1:F:21:ALA:HB3	1.89	0.53
1:A:7:LYS:HE2	1:A:11:ASP:HB3	1.90	0.53
1:D:409:PHE:O	1:D:410:ASP:HB2	2.08	0.53
1:A:99:LEU:HD21	1:A:244:LEU:HD13	1.91	0.53
1:D:247:VAL:HG13	1:D:252:VAL:O	2.08	0.53
1:C:37:VAL:HG13	1:C:387:PRO:HD2	1.91	0.53
1:E:29:VAL:HG22	1:E:368:LYS:HE2	1.91	0.52
1:C:23:ASN:ND2	1:D:106:LEU:HD21	2.24	0.52
1:F:338:ILE:HG21	1:F:358:VAL:HG13	1.92	0.52
1:E:188:LEU:HD12	1:E:221:ILE:HG22	1.92	0.52
1:E:205:ALA:HB3	1:E:208:ILE:CD1	2.40	0.52
1:C:214:TYR:O	1:C:218:VAL:HG23	2.10	0.51
1:C:43:ASN:HD22	1:C:45:LYS:CE	2.21	0.51
1:C:235:GLN:NE2	1:C:261:LYS:NZ	2.55	0.51
1:E:268:TYR:CZ	1:F:269:PRO:HD3	2.45	0.51
1:C:54:TYR:O	1:C:55:SER:HB2	2.11	0.51
1:F:188:LEU:HD12	1:F:221:ILE:HG22	1.92	0.51
1:A:188:LEU:HD12	1:A:221:ILE:HG22	1.92	0.51
1:A:197:ILE:HB	1:A:230:VAL:HB	1.91	0.51
1:F:29:VAL:HG22	1:F:368:LYS:HE2	1.91	0.51
1:A:318:ALA:HA	1:A:347:LEU:HD22	1.93	0.51
1:B:99:LEU:HD11	1:B:310:ILE:HD11	1.93	0.51
1:E:205:ALA:HB3	1:E:208:ILE:HD13	1.92	0.50
1:F:205:ALA:CB	1:F:208:ILE:HD12	2.41	0.50
1:F:7:LYS:HE3	1:F:11:ASP:HB3	1.93	0.50
1:C:141:VAL:HG23	1:C:197:ILE:HG23	1.94	0.50
1:F:94:ARG:HD2	2:F:467:HOH:O	2.11	0.50
1:A:391:THR:HG21	1:A:393:GLU:OE1	2.11	0.50
1:D:17:LEU:O	1:D:22:HIS:HE1	1.94	0.50
1:C:235:GLN:HE22	1:C:261:LYS:HZ3	1.59	0.50
1:B:55:SER:O	1:B:262:ALA:HB2	2.12	0.50
1:F:54:TYR:OH	1:F:375:ARG:NH1	2.29	0.50
1:C:43:ASN:ND2	1:C:45:LYS:HE2	2.24	0.50
1:E:8:THR:OG1	1:E:9:PRO:HD2	2.11	0.50
1:E:238:LEU:HD11	1:E:263:LEU:HD13	1.94	0.50
1:B:325:PHE:CD1	1:B:395:LEU:HG	2.47	0.49
1:D:207:VAL:HG23	1:D:383:ARG:HD3	1.94	0.49
1:B:214:TYR:O	1:B:218:VAL:HG23	2.12	0.49
1:C:230:VAL:HG22	1:C:256:VAL:HB	1.93	0.49
1:B:134:GLU:O	1:B:136:MET:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLU:O	1:D:120:LYS:HG3	2.12	0.49
1:F:222:CYS:HB3	1:F:227:VAL:O	2.13	0.49
1:D:43:ASN:HB3	1:D:45:LYS:HE3	1.94	0.49
1:B:406:VAL:HA	2:B:483:HOH:O	2.11	0.48
1:A:385:THR:O	1:A:385:THR:CG2	2.61	0.48
1:D:102:TYR:OH	1:D:257:ILE:CD1	2.61	0.48
1:C:353:PHE:CE1	1:C:382:ILE:HD12	2.48	0.48
1:D:65:ASN:ND2	1:D:65:ASN:N	2.61	0.48
1:E:269:PRO:HG2	1:F:269:PRO:HG2	1.96	0.48
1:C:180:ASP:OD2	1:C:183:ALA:HB3	2.13	0.48
1:B:50:PHE:HE1	1:B:398:CYS:HG	1.59	0.48
1:E:106:LEU:HD11	1:F:23:ASN:HD21	1.70	0.48
1:B:240:ARG:NH1	1:B:386:PRO:O	2.39	0.48
1:D:235:GLN:HE22	1:D:261:LYS:NZ	2.12	0.48
1:F:318:ALA:HA	1:F:347:LEU:HD22	1.95	0.48
1:C:220:ASP:O	1:C:224:LYS:HG2	2.14	0.48
1:A:353:PHE:HE1	1:A:382:ILE:HD12	1.79	0.48
1:A:247:VAL:HG13	1:A:252:VAL:O	2.14	0.48
1:D:118:ALA:HB2	1:D:258:LEU:HD21	1.96	0.48
1:C:235:GLN:NE2	1:C:261:LYS:HZ3	2.12	0.47
1:F:8:THR:HG23	1:F:11:ASP:H	1.78	0.47
1:C:356:GLU:H	1:C:356:GLU:CD	2.16	0.47
1:B:391:THR:CG2	1:B:394:GLN:H	2.28	0.47
1:F:385:THR:CG2	1:F:385:THR:O	2.55	0.47
1:B:181:LEU:H	1:B:181:LEU:CD1	2.25	0.47
1:D:287:GLU:CG	1:D:288:HIS:H	2.24	0.47
1:F:219:TYR:CG	1:F:252:VAL:HG23	2.50	0.47
1:F:233:GLU:OE2	1:F:247:VAL:HB	2.14	0.47
1:C:269:PRO:HG2	1:D:269:PRO:HG2	1.97	0.47
1:D:220:ASP:O	1:D:224:LYS:HG3	2.15	0.47
1:D:367:LEU:HD13	1:D:405:THR:HG21	1.95	0.47
1:E:54:TYR:O	1:E:55:SER:HB2	2.15	0.47
1:B:390:ILE:HD13	1:B:395:LEU:HD13	1.96	0.47
1:B:391:THR:HG22	1:B:394:GLN:H	1.79	0.47
1:C:100:LEU:CD1	1:C:259:LEU:HD11	2.45	0.47
1:D:77:LEU:HD13	1:D:296:PRO:HG3	1.96	0.47
1:B:75:LYS:HE3	1:B:75:LYS:HB2	1.41	0.47
1:A:367:LEU:HD13	1:A:405:THR:HG21	1.96	0.47
1:E:138:LYS:HD2	1:E:193:VAL:HG22	1.96	0.47
1:B:202:GLN:HB2	1:B:208:ILE:HB	1.97	0.47
1:B:240:ARG:HG3	1:B:348:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:VAL:HG13	1:D:351:ILE:HG22	1.96	0.46
1:B:10:GLU:CD	1:B:10:GLU:H	2.19	0.46
1:C:43:ASN:CB	1:C:45:LYS:HE2	2.42	0.46
1:D:287:GLU:HG3	1:D:288:HIS:N	2.27	0.46
1:F:250:TYR:HB2	1:F:252:VAL:HG12	1.97	0.46
1:A:291:THR:CG2	1:B:261:LYS:HE3	2.42	0.46
1:F:240:ARG:CZ	1:F:385:THR:HG23	2.44	0.46
1:C:97:THR:HB	1:C:102:TYR:O	2.16	0.46
1:C:367:LEU:HD13	1:C:405:THR:HG21	1.97	0.46
1:C:306:LEU:O	1:C:310:ILE:HG12	2.15	0.46
1:F:268:TYR:CD1	1:F:269:PRO:HD2	2.51	0.46
1:F:326:LEU:HD12	1:F:342:VAL:HG12	1.98	0.46
1:F:205:ALA:HB1	1:F:208:ILE:HD12	1.98	0.45
1:D:100:LEU:HD11	1:D:259:LEU:HD11	1.97	0.45
1:A:279:ILE:O	1:A:282:VAL:HB	2.16	0.45
1:C:45:LYS:HB3	2:C:416:HOH:O	2.15	0.45
1:C:337:LYS:O	1:C:354:LYS:HD2	2.16	0.45
1:C:355:ASN:ND2	1:C:379:ASP:O	2.49	0.45
1:E:8:THR:O	1:E:11:ASP:HB2	2.16	0.45
1:C:207:VAL:HG12	1:C:207:VAL:O	2.16	0.45
1:D:207:VAL:O	1:D:207:VAL:HG12	2.17	0.45
1:D:375:ARG:HG2	1:D:375:ARG:NH1	2.24	0.45
1:A:70:MET:HG2	1:B:70:MET:HE3	1.99	0.45
1:B:8:THR:OG1	1:B:9:PRO:HD2	2.16	0.45
1:A:27:ILE:HG22	1:A:29:VAL:HG23	1.98	0.44
1:A:188:LEU:CD2	1:A:193:VAL:HG11	2.45	0.44
1:D:39:VAL:HG21	1:D:373:ILE:HD11	1.99	0.44
1:C:55:SER:O	1:C:262:ALA:HB2	2.18	0.44
1:C:380:LYS:HD3	2:C:452:HOH:O	2.17	0.44
1:C:118:ALA:HB2	1:C:258:LEU:HD21	1.98	0.44
1:A:268:TYR:CZ	1:B:269:PRO:HD3	2.52	0.44
1:D:188:LEU:HD22	1:D:193:VAL:HG11	1.99	0.44
1:D:366:LYS:CG	1:D:405:THR:HG23	2.48	0.44
1:A:340:ARG:NH1	1:A:354:LYS:HE2	2.32	0.44
1:A:97:THR:HB	1:A:102:TYR:O	2.17	0.44
1:E:188:LEU:HD22	1:E:193:VAL:HG11	1.99	0.44
1:F:367:LEU:HG	1:F:372:LEU:HD22	2.00	0.44
1:C:37:VAL:O	1:C:37:VAL:HG12	2.16	0.44
1:D:204:GLU:O	1:D:377:VAL:HG11	2.18	0.44
1:A:176:VAL:HG12	1:A:177:PRO:O	2.17	0.44
1:B:143:LYS:HA	1:B:143:LYS:HD2	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:VAL:HG22	1:C:368:LYS:HE3	2.00	0.43
2:E:429:HOH:O	1:F:267:HIS:HE1	2.01	0.43
1:F:391:THR:HG22	1:F:393:GLU:H	1.83	0.43
1:D:97:THR:HB	1:D:102:TYR:O	2.17	0.43
1:A:353:PHE:CE1	1:A:382:ILE:HD12	2.52	0.43
1:F:39:VAL:HG21	1:F:373:ILE:HD11	2.01	0.43
1:B:355:ASN:HA	1:B:355:ASN:HD22	1.58	0.43
1:B:219:TYR:CZ	1:B:223:LYS:HE3	2.53	0.43
1:C:77:LEU:HD13	1:C:296:PRO:HG3	1.99	0.43
1:E:70:MET:HG3	1:E:301:ILE:HD11	1.99	0.43
1:F:229:PHE:HE2	1:F:252:VAL:CG2	2.32	0.43
1:C:342:VAL:HG13	1:C:351:ILE:CG2	2.46	0.43
1:B:284:LYS:HE3	2:B:454:HOH:O	2.19	0.43
1:F:37:VAL:HA	1:F:387:PRO:HG2	2.00	0.43
1:D:376:ASP:OD2	1:D:379:ASP:HA	2.17	0.43
1:F:207:VAL:HG12	1:F:207:VAL:O	2.18	0.43
1:C:391:THR:OG1	1:C:393:GLU:HG2	2.19	0.43
1:A:269:PRO:HD3	1:B:268:TYR:CZ	2.53	0.43
1:B:100:LEU:CD1	1:B:259:LEU:HD11	2.49	0.43
1:B:197:ILE:HB	1:B:230:VAL:HB	2.01	0.43
1:F:141:VAL:HG22	1:F:197:ILE:CG2	2.47	0.43
1:C:15:ASN:OD1	1:D:94:ARG:NE	2.46	0.43
1:F:239:GLY:HA2	1:F:315:CYS:SG	2.59	0.43
1:D:372:LEU:HD23	1:D:374:THR:HG23	2.00	0.43
1:D:27:ILE:HG13	1:D:28:PRO:CD	2.45	0.42
1:B:70:MET:HG3	1:B:301:ILE:HD11	2.00	0.42
1:D:141:VAL:CG1	1:D:142:CYS:N	2.82	0.42
1:A:391:THR:HG22	1:A:392:LYS:N	2.34	0.42
1:A:99:LEU:CD2	1:A:244:LEU:HD13	2.49	0.42
1:A:106:LEU:HD11	1:B:23:ASN:HD21	1.80	0.42
1:A:99:LEU:HD21	1:A:244:LEU:HD11	2.01	0.42
1:C:269:PRO:HD3	1:D:268:TYR:CZ	2.54	0.42
1:C:100:LEU:HD11	1:C:259:LEU:HD11	2.01	0.42
1:C:375:ARG:NH2	2:C:427:HOH:O	2.51	0.42
1:C:245:LEU:HD13	1:C:257:ILE:CD1	2.49	0.42
1:F:279:ILE:O	1:F:282:VAL:HB	2.19	0.42
1:D:39:VAL:HG21	1:D:373:ILE:CD1	2.49	0.42
1:F:8:THR:HG22	1:F:11:ASP:CG	2.40	0.42
1:B:139:ILE:O	1:B:173:PHE:HA	2.19	0.42
1:E:356:GLU:CD	1:E:356:GLU:H	2.22	0.42
1:B:342:VAL:HG22	1:B:351:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:GLY:N	1:F:324:PRO:HD2	2.34	0.42
1:E:35:LYS:HE2	2:F:431:HOH:O	2.20	0.42
1:C:45:LYS:H	1:C:45:LYS:HG3	1.67	0.42
1:A:385:THR:HG21	2:A:468:HOH:O	2.20	0.41
1:E:141:VAL:HG23	1:E:197:ILE:HG23	2.02	0.41
1:D:197:ILE:HG12	1:D:230:VAL:HB	2.02	0.41
1:F:54:TYR:OH	1:F:375:ARG:HD2	2.20	0.41
1:D:29:VAL:HG12	1:D:31:LEU:HD13	2.01	0.41
1:F:391:THR:CG2	1:F:392:LYS:N	2.83	0.41
1:A:376:ASP:HA	1:A:381:THR:O	2.20	0.41
1:A:289:GLY:O	1:A:290:SER:CB	2.68	0.41
1:B:242:GLY:CA	1:B:319:GLU:HG2	2.44	0.41
1:E:202:GLN:HB2	1:E:208:ILE:HB	2.02	0.41
1:E:329:LEU:HB3	1:E:342:VAL:HG11	2.02	0.41
1:D:364:CYS:SG	1:D:382:ILE:HG12	2.60	0.41
1:B:142:CYS:O	1:B:145:ASN:ND2	2.54	0.41
1:D:93:GLU:HG2	1:D:105:VAL:HG13	2.03	0.41
1:F:338:ILE:HD11	1:F:406:VAL:HG13	2.02	0.41
1:E:348:LEU:HA	1:E:385:THR:HG22	2.01	0.41
1:E:77:LEU:HD13	1:E:296:PRO:HG3	2.02	0.41
1:C:247:VAL:HG21	1:C:254:PRO:HG3	2.02	0.41
1:D:49:ASP:HA	1:D:373:ILE:HG13	2.03	0.41
1:A:269:PRO:HG2	1:B:269:PRO:HG2	2.03	0.41
1:A:103:ASP:HB2	1:A:276:ASN:HA	2.02	0.41
1:D:100:LEU:CD1	1:D:259:LEU:HD11	2.50	0.41
1:E:13:ILE:O	1:E:17:LEU:HG	2.21	0.40
1:C:188:LEU:HD12	1:C:221:ILE:CG2	2.51	0.40
1:E:205:ALA:CB	1:E:208:ILE:CD1	2.99	0.40
1:B:391:THR:HG22	1:B:394:GLN:HB2	2.02	0.40
1:C:93:GLU:O	1:C:97:THR:HG23	2.20	0.40
1:B:63:HIS:HA	1:B:64:PRO:HD3	1.89	0.40
1:F:97:THR:HB	1:F:102:TYR:O	2.21	0.40
1:D:372:LEU:CD2	1:D:374:THR:HG23	2.51	0.40
1:A:212:ASP:O	1:A:213:ASN:CB	2.68	0.40
1:F:393:GLU:O	1:F:396:ASP:HB2	2.22	0.40
1:F:77:LEU:HD13	1:F:296:PRO:HG3	2.03	0.40
1:A:138:LYS:NZ	1:A:190:ASP:OD2	2.46	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	374/433 (86%)	356 (95%)	14 (4%)	4 (1%)	17	11
1	B	373/433 (86%)	353 (95%)	18 (5%)	2 (0%)	34	30
1	C	365/433 (84%)	350 (96%)	13 (4%)	2 (0%)	34	30
1	D	371/433 (86%)	352 (95%)	16 (4%)	3 (1%)	24	17
1	E	370/433 (86%)	350 (95%)	19 (5%)	1 (0%)	46	45
1	F	371/433 (86%)	348 (94%)	18 (5%)	5 (1%)	15	9
All	All	2224/2598 (86%)	2109 (95%)	98 (4%)	17 (1%)	24	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	C	288	HIS
1	C	379	ASP
1	D	288	HIS
1	D	379	ASP
1	F	287	GLU
1	F	290	SER
1	F	355	ASN
1	A	261	LYS
1	A	287	GLU
1	D	261	LYS
1	B	261	LYS
1	E	261	LYS
1	F	261	LYS
1	B	134	GLU
1	F	379	ASP
1	A	207	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	331/378 (88%)	306 (92%)	25 (8%)	16	12
1	B	330/378 (87%)	309 (94%)	21 (6%)	22	18
1	C	322/378 (85%)	302 (94%)	20 (6%)	23	19
1	D	328/378 (87%)	307 (94%)	21 (6%)	22	18
1	E	327/378 (86%)	304 (93%)	23 (7%)	19	15
1	F	328/378 (87%)	304 (93%)	24 (7%)	17	13
All	All	1966/2268 (87%)	1832 (93%)	134 (7%)	20	16

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	31	LEU
1	A	77	LEU
1	A	99	LEU
1	A	106	LEU
1	A	141	VAL
1	A	172	GLN
1	A	184	LEU
1	A	197	ILE
1	A	208	ILE
1	A	229	PHE
1	A	247	VAL
1	A	263	LEU
1	A	309	LEU
1	A	319	GLU
1	A	334	LYS
1	A	340	ARG
1	A	347	LEU
1	A	356	GLU
1	A	358	VAL
1	A	367	LEU
1	A	374	THR

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	392	LYS
1	A	395	LEU
1	B	31	LEU
1	B	37	VAL
1	B	75	LYS
1	B	77	LEU
1	B	99	LEU
1	B	135	ASN
1	B	145	ASN
1	B	176	VAL
1	B	181	LEU
1	B	197	ILE
1	B	216	GLN
1	B	247	VAL
1	B	309	LEU
1	B	340	ARG
1	B	347	LEU
1	B	355	ASN
1	B	356	GLU
1	B	358	VAL
1	B	367	LEU
1	B	374	THR
1	B	391	THR
1	C	31	LEU
1	C	77	LEU
1	C	99	LEU
1	C	124	LYS
1	C	128	GLU
1	C	141	VAL
1	C	184	LEU
1	C	247	VAL
1	C	252	VAL
1	C	319	GLU
1	C	329	LEU
1	C	347	LEU
1	C	351	ILE
1	C	356	GLU
1	C	367	LEU
1	C	374	THR
1	C	377	VAL
1	C	385	THR

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Mol	Chain	Res	Type
1	C	393	GLU
1	C	395	LEU
1	D	10	GLU
1	D	31	LEU
1	D	46	ARG
1	D	51	LEU
1	D	65	ASN
1	D	77	LEU
1	D	99	LEU
1	D	176	VAL
1	D	181	LEU
1	D	184	LEU
1	D	247	VAL
1	D	257	ILE
1	D	282	VAL
1	D	309	LEU
1	D	355	ASN
1	D	356	GLU
1	D	358	VAL
1	D	365	LEU
1	D	367	LEU
1	D	375	ARG
1	D	383	ARG
1	E	31	LEU
1	E	45	LYS
1	E	75	LYS
1	E	77	LEU
1	E	99	LEU
1	E	124	LYS
1	E	128	GLU
1	E	184	LEU
1	E	197	ILE
1	E	204	GLU
1	E	211	SER
1	E	247	VAL
1	E	252	VAL
1	E	263	LEU
1	E	282	VAL
1	E	337	LYS
1	E	347	LEU
1	E	356	GLU
1	E	358	VAL

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Mol	Chain	Res	Type
1	E	367	LEU
1	E	374	THR
1	E	383	ARG
1	E	395	LEU
1	F	22	HIS
1	F	31	LEU
1	F	37	VAL
1	F	77	LEU
1	F	99	LEU
1	F	106	LEU
1	F	176	VAL
1	F	182	GLU
1	F	184	LEU
1	F	204	GLU
1	F	219	TYR
1	F	247	VAL
1	F	252	VAL
1	F	263	LEU
1	F	287	GLU
1	F	335	ASP
1	F	347	LEU
1	F	354	LYS
1	F	355	ASN
1	F	358	VAL
1	F	367	LEU
1	F	374	THR
1	F	379	ASP
1	F	395	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	235	GLN
1	A	248	HIS
1	A	267	HIS
1	A	370	ASN
1	B	22	HIS
1	B	135	ASN
1	B	145	ASN
1	B	235	GLN
1	B	355	ASN

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Mol	Chain	Res	Type
1	B	370	ASN
1	B	378	HIS
1	C	43	ASN
1	C	235	GLN
1	C	355	ASN
1	C	370	ASN
1	D	22	HIS
1	D	65	ASN
1	D	235	GLN
1	D	267	HIS
1	D	355	ASN
1	D	370	ASN
1	E	22	HIS
1	E	235	GLN
1	E	267	HIS
1	E	307	ASN
1	E	370	ASN
1	F	22	HIS
1	F	235	GLN
1	F	267	HIS
1	F	370	ASN

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

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, 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	378/433 (87%)	0.19	5 (1%) 79 84	16, 34, 57, 71	0
1	B	377/433 (87%)	0.40	21 (5%) 28 36	20, 38, 63, 71	0
1	C	369/433 (85%)	0.43	28 (7%) 17 23	27, 43, 72, 81	0
1	D	375/433 (86%)	0.27	12 (3%) 51 60	23, 40, 57, 83	0
1	E	374/433 (86%)	0.57	28 (7%) 17 23	23, 43, 68, 81	0
1	F	375/433 (86%)	0.30	9 (2%) 62 68	20, 36, 58, 71	0
All	All	2248/2598 (86%)	0.36	103 (4%) 36 45	16, 39, 64, 83	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	HIS	10.5
1	D	287	GLU	5.9
1	D	289	GLY	5.1
1	B	289	GLY	5.0
1	C	135	ASN	4.3
1	C	136	MET	4.2
1	A	287	GLU	4.0
1	E	191	PRO	3.8
1	E	335	ASP	3.7
1	E	287	GLU	3.7
1	E	186	GLU	3.7
1	F	289	GLY	3.5
1	E	338	ILE	3.4
1	B	181	LEU	3.4
1	B	145	ASN	3.4
1	C	134	GLU	3.3
1	C	221	ILE	3.2
1	E	225	TYR	3.2
1	C	224	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	186	GLU	3.0
1	E	134	GLU	3.0
1	E	181	LEU	3.0
1	B	191	PRO	3.0
1	B	134	GLU	3.0
1	C	193	VAL	3.0
1	E	141	VAL	3.0
1	C	225	TYR	3.0
1	C	191	PRO	3.0
1	B	137	ALA	3.0
1	E	184	LEU	2.9
1	E	189	LYS	2.9
1	B	213	ASN	2.9
1	F	286	GLY	2.9
1	F	340	ARG	2.9
1	B	143	LYS	2.8
1	B	331	ARG	2.8
1	C	131	LYS	2.8
1	E	341	ASP	2.8
1	C	132	ILE	2.8
1	C	133	PRO	2.7
1	E	337	LYS	2.7
1	E	401	ILE	2.7
1	A	288	HIS	2.7
1	D	379	ASP	2.6
1	E	192	ASN	2.6
1	E	182	GLU	2.6
1	D	373	ILE	2.6
1	C	138	LYS	2.5
1	F	219	TYR	2.5
1	E	176	VAL	2.5
1	D	43	ASN	2.5
1	E	290	SER	2.5
1	A	410	ASP	2.4
1	C	126	GLY	2.4
1	C	288	HIS	2.4
1	B	185	GLU	2.4
1	F	182	GLU	2.4
1	D	351	ILE	2.4
1	C	226	ASN	2.4
1	C	137	ALA	2.4
1	C	189	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	400	GLU	2.3
1	C	227	VAL	2.3
1	B	136	MET	2.3
1	E	210	PRO	2.3
1	C	289	GLY	2.3
1	E	410	ASP	2.3
1	B	175	LYS	2.3
1	C	185	GLU	2.2
1	B	182	GLU	2.2
1	C	84	PHE	2.2
1	C	127	TYR	2.2
1	E	42	VAL	2.2
1	E	213	ASN	2.2
1	D	290	SER	2.2
1	B	180	ASP	2.2
1	E	370	ASN	2.2
1	C	250	TYR	2.2
1	E	409	PHE	2.2
1	D	143	LYS	2.1
1	E	408	PHE	2.1
1	A	319	GLU	2.1
1	F	53	ALA	2.1
1	C	183	ALA	2.1
1	E	325	PHE	2.1
1	A	289	GLY	2.1
1	E	356	GLU	2.1
1	D	45	LYS	2.1
1	F	143	LYS	2.1
1	B	335	ASP	2.1
1	B	192	ASN	2.1
1	B	287	GLU	2.1
1	B	290	SER	2.1
1	B	189	LYS	2.1
1	B	144	ASN	2.1
1	E	336	SER	2.1
1	C	379	ASP	2.0
1	D	173	PHE	2.0
1	D	211	SER	2.0
1	F	207	VAL	2.0
1	C	128	GLU	2.0
1	C	182	GLU	2.0
1	F	290	SER	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.