



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:56 PM UTC

PDB ID : 1Z7D / pdb_00001z7d
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

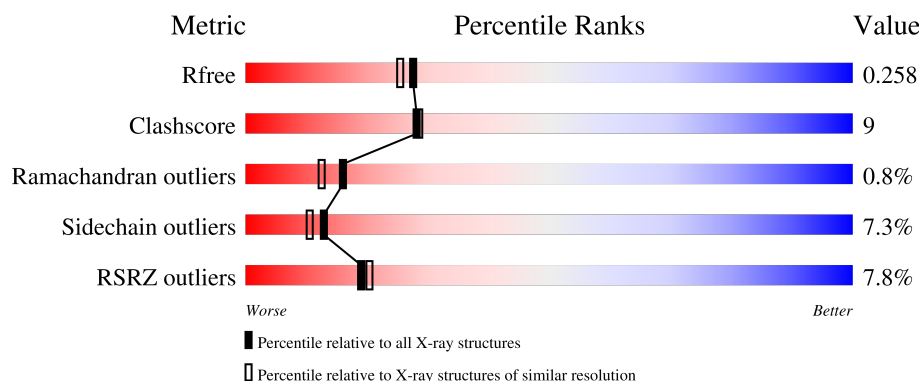
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	433	3% 70% 14% • 13%
1	B	433	7% 68% 16% • 13%
1	C	433	9% 65% 17% • 15%
1	D	433	5% 67% 16% • 13%
1	E	433	9% 70% 15% • 14%

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Mol	Chain	Length	Quality of chain
1	F	433	7% 67% 16% • • 13%

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

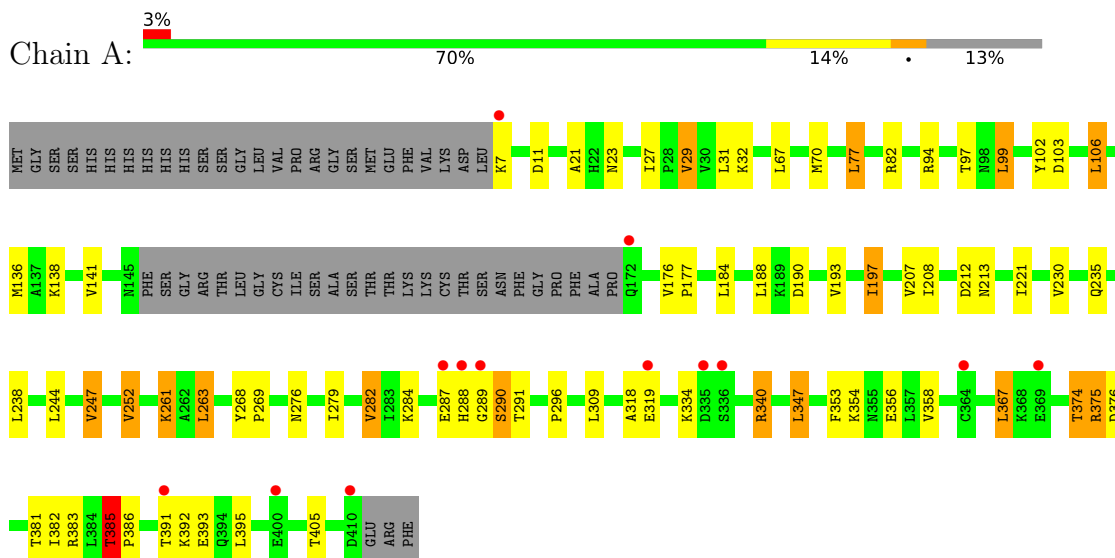
- Molecule 2 is water.

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

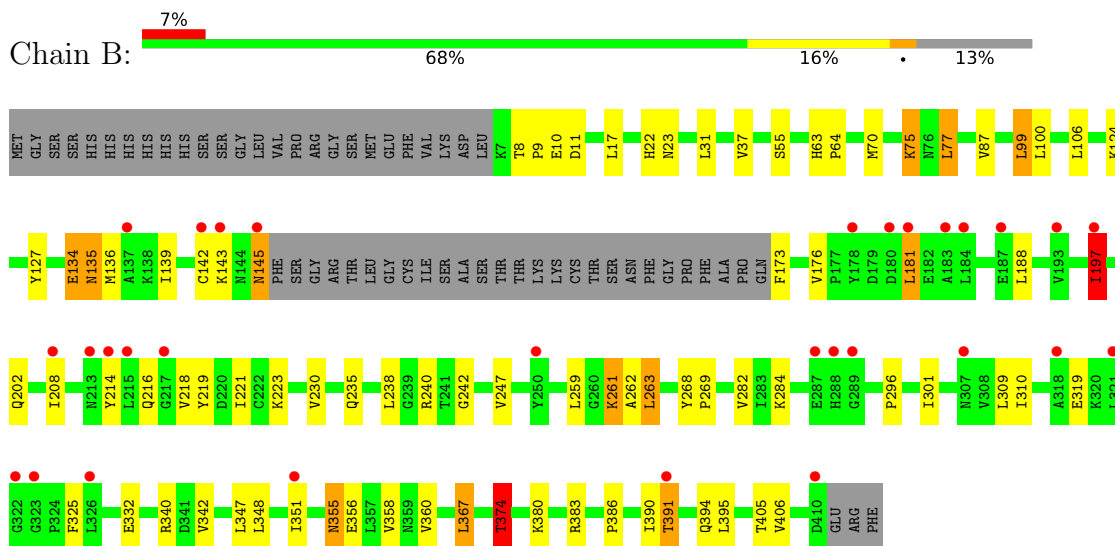
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ornithine aminotransferase

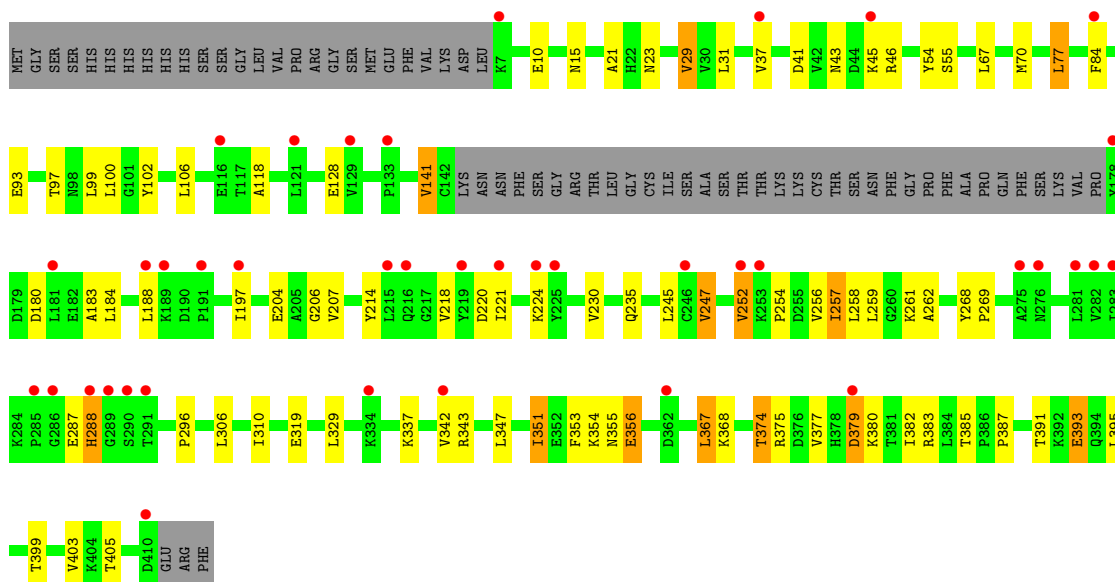


- Molecule 1: ornithine aminotransferase

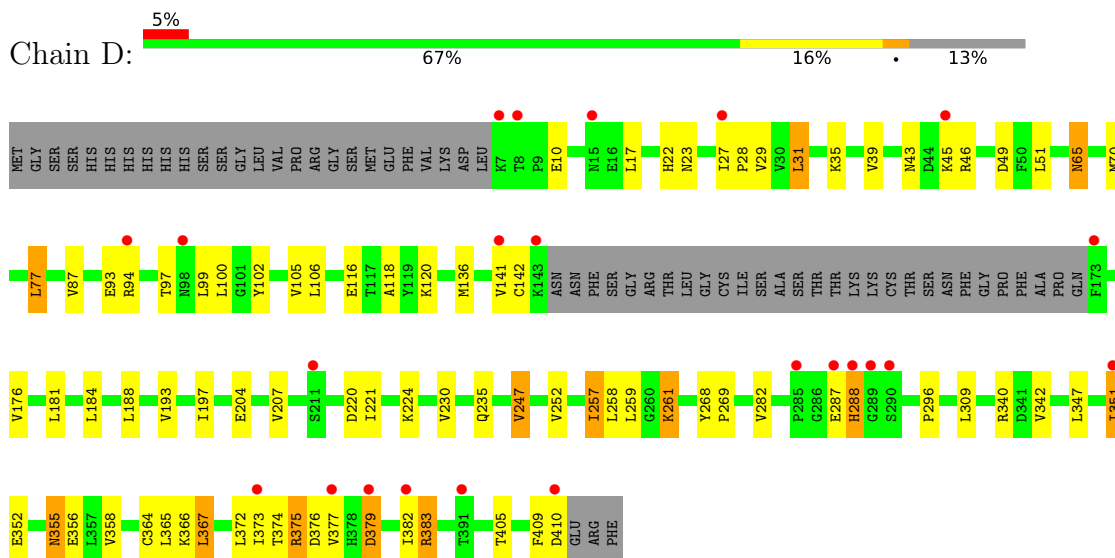


- Molecule 1: ornithine aminotransferase

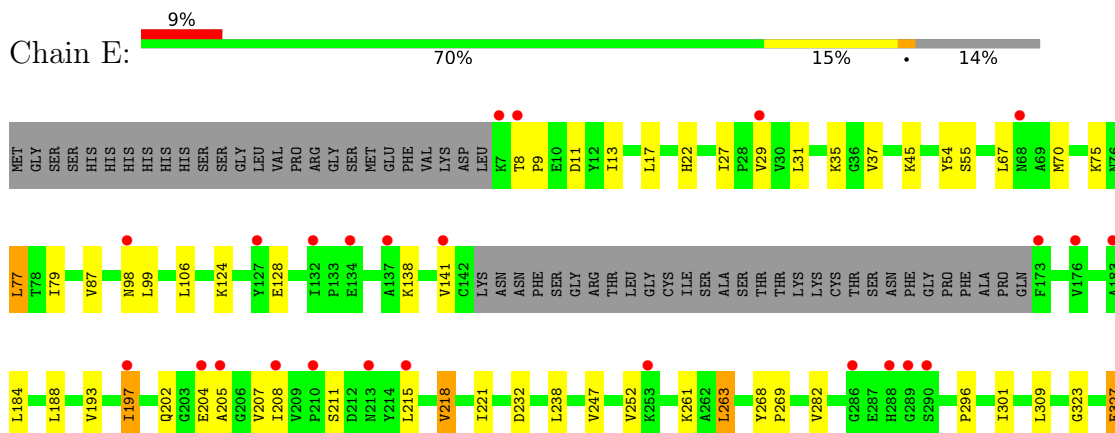


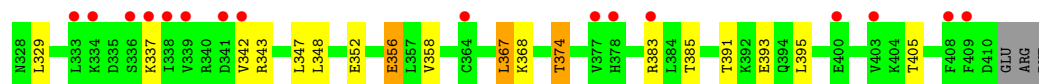


- Molecule 1: ornithine aminotransferase

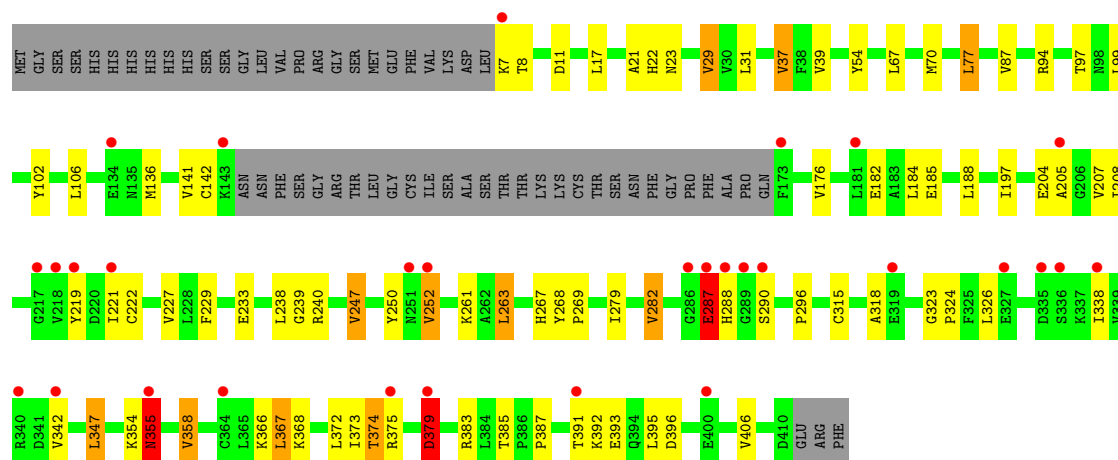


- Molecule 1: ornithine aminotransferase





- 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 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.74-2.10) 99.8 (49.74-2.10)	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	7970 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.76	1/3023 (0.0%)	0.94	2/4092 (0.0%)
1	B	0.69	2/3014 (0.1%)	0.93	1/4080 (0.0%)
1	C	0.62	0/2947	0.89	0/3990
1	D	0.68	1/2998 (0.0%)	0.91	0/4058
1	E	0.67	1/2989 (0.0%)	0.90	0/4047
1	F	0.71	1/2998 (0.0%)	0.93	0/4058
All	All	0.69	6/17969 (0.0%)	0.92	3/24325 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	THR	CA-CB	7.93	1.63	1.53
1	E	87	VAL	CA-CB	5.54	1.56	1.54
1	B	87	VAL	CA-CB	5.52	1.56	1.54
1	B	197	ILE	CA-CB	5.46	1.61	1.54
1	F	87	VAL	CA-CB	5.46	1.57	1.54
1	D	87	VAL	CA-CB	5.03	1.57	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	PRO	CA-C-N	-5.50	114.11	119.78
1	A	386	PRO	C-N-CA	-5.50	114.11	119.78
1	B	374	THR	CB-CA-C	-5.26	100.97	113.02

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	2969	0	3015	59	0
1	B	2960	0	3007	58	0
1	C	2895	0	2939	67	0
1	D	2944	0	2995	63	0
1	E	2935	0	2982	41	0
1	F	2944	0	2995	60	0
2	A	127	0	0	4	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	316	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 (316) 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:E:70:MET:HE3	1:F:70:MET:HE3	1.56	0.86
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:A:70:MET:HE3	1:B:70:MET:HE3	1.63	0.80
1:D:375:ARG:HH11	1:D:375:ARG:CG	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:C:70:MET:HE3	1:D:70:MET:HE3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ARG:HH11	1:D:375:ARG:HG2	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:HD13	1:B:181:LEU:H	1.52	0.75
1:C:43:ASN:HD22	1:C:45:LYS:HE2	1.50	0.75
1:D:65:ASN:HD22	1:D:65:ASN:H	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:B:127:TYR:OH	1:B:135:ASN:HA	1.89	0.72
1:D:287:GLU:HG3	1:D:288:HIS:H	1.54	0.72
1:F:287:GLU:CD	1:F:288:HIS:H	1.98	0.72
1:E:323:GLY:O	1:E:327:GLU:HG2	1.90	0.71
1:C:43:ASN:HB2	1:C:45:LYS:HE2	1.73	0.70
1:F:375:ARG:NH2	2:F:427:HOH:O	2.25	0.70
1:A:385:THR:HG22	1:A:385:THR:O	1.93	0.69
1:A:106:LEU:HD11	1:B:23:ASN:ND2	2.08	0.69
1:B:235:GLN:HE22	1:B:261:LYS:NZ	1.90	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: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: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:HD22	1:D:65:ASN:N	1.95	0.63
1:A:23:ASN:CG	1:B:106:LEU:HD21	2.23	0.63
1:C:235:GLN:HE22	1:C:261:LYS:HZ1	1.46	0.63
1:F:374:THR:HG22	1:F:375:ARG:H	1.63	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:C:10:GLU:CD	1:C:10:GLU:H	2.08	0.61
1:B:17:LEU:O	1:B:22:HIS:HE1	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:235:GLN:NE2	1:A:261:LYS:HE3	2.15	0.60
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: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:E:207:VAL:O	1:E:343:ARG:HD2	2.03	0.58
1:E:8:THR:HG22	1:E:11:ASP:CG	2.28	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:247:VAL:HG22	1:C:252:VAL:HG13	1.85	0.56
1:B:77:LEU:HD13	1:B:296:PRO:HG3	1.87	0.56
1:E:197:ILE:HD11	1:E:232:ASP:HB2	1.88	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: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:C:399:THR:O	1:C:403:VAL:HG23	2.08	0.54
1:E:238:LEU:HB3	1:E:309:LEU:HD11	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:A:77:LEU:HD13	1:A:296:PRO:HG3	1.90	0.54
1:B:360:VAL:HG21	1:B:380:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.53
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:C:37:VAL:HG13	1:C:387:PRO:HD2	1.91	0.53
1:D:247:VAL:HG13	1:D:252:VAL:O	2.08	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:C:356:GLU:CD	1:C:356:GLU:H	2.16	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:B:10:GLU:H	1:B:10:GLU:CD	2.19	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:C:141:VAL:HG23	1:C:197:ILE:HG23	1.94	0.50
1:F:7:LYS:HE3	1:F:11:ASP:HB3	1.93	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:E:67:LEU:HD12	1:E:70:MET:HE2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:54:TYR:O	1:C:55:SER:HB2	2.11	0.49
1:A:67:LEU:HD12	1:A:70:MET:HE2	1.95	0.49
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:A:70:MET:HE3	1:B:70:MET:CE	2.40	0.48
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:N	1:D:65:ASN:ND2	2.61	0.48
1:C:180:ASP:OD2	1:C:183:ALA:HB3	2.13	0.48
1:E:269:PRO:HG2	1:F:269:PRO:HG2	1.96	0.48
1:B:240:ARG:NH1	1:B:386:PRO:O	2.39	0.48
1:E:106:LEU:HD11	1:F:23:ASN:HD21	1.70	0.48
1:C:220:ASP:O	1:C:224:LYS:HG2	2.14	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:A:247:VAL:HG13	1:A:252:VAL:O	2.14	0.48
1:A:353:PHE:HE1	1:A:382:ILE:HD12	1.79	0.48
1:D:118:ALA:HB2	1:D:258:LEU:HD21	1.96	0.48
1:D:136:MET:HA	1:D:136:MET:HE2	1.95	0.48
1:A:136:MET:HE2	1:A:136:MET:HA	1.95	0.47
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:B:391:THR:CG2	1:B:394:GLN:H	2.28	0.47
1:B:181:LEU:H	1:B:181:LEU:CD1	2.25	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:287:GLU:CG	1:D:288:HIS:H	2.24	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: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:F:385:THR:O	1:F:385:THR:CG2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:CD1	1:C:259:LEU:HD11	2.45	0.47
1:A:367:LEU:HD13	1:A:405:THR:HG21	1.96	0.47
1:B:75:LYS:HE3	1:B:75:LYS:HB2	1.41	0.47
1:D:77:LEU:HD13	1:D:296:PRO:HG3	1.96	0.47
1:B:202:GLN:HB2	1:B:208:ILE:HB	1.97	0.47
1:E:138:LYS:HD2	1:E:193:VAL:HG22	1.96	0.47
1:F:8:THR:HG22	1:F:11:ASP:CG	2.40	0.47
1:B:240:ARG:HG3	1:B:348:LEU:HB2	1.97	0.46
1:D:342:VAL:HG13	1:D:351:ILE:HG22	1.96	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:B:235:GLN:HE22	1:B:261:LYS:HZ3	1.60	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:E:356:GLU:CD	1:E:356:GLU:H	2.22	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:D:100:LEU:HD11	1:D:259:LEU:HD11	1.97	0.45
1:F:205:ALA:HB1	1:F:208:ILE:HD12	1.98	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:HG12	1:D:207:VAL:O	2.17	0.45
1:C:67:LEU:HD12	1:C:70:MET:HE2	1.99	0.45
1:D:375:ARG:HG2	1:D:375:ARG:NH1	2.24	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:B:235:GLN:HE22	1:B:261:LYS:HZ1	1.60	0.44
1:C:55:SER:O	1:C:262:ALA:HB2	2.18	0.44
1:C:118:ALA:HB2	1:C:258:LEU:HD21	1.98	0.44
1:C:380:LYS:HD3	2:C:452:HOH:O	2.17	0.44
1:D:39:VAL:HG21	1:D:373:ILE:HD11	1.99	0.44
1:A:268:TYR:CZ	1:B:269:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:HB	1:A:102:TYR:O	2.17	0.44
1:A:340:ARG:NH1	1:A:354:LYS:HE2	2.32	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: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:HG12	1:C:37:VAL:O	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:HD2	1:B:143:LYS:HA	1.87	0.44
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:A:353:PHE:CE1	1:A:382:ILE:HD12	2.52	0.43
1:B:219:TYR:CZ	1:B:223:LYS:HE3	2.53	0.43
1:B:355:ASN:HD22	1:B:355:ASN:HA	1.58	0.43
1:D:97:THR:HB	1:D:102:TYR:O	2.17	0.43
1:F:39:VAL:HG21	1:F:373:ILE:HD11	2.01	0.43
1:C:77:LEU:HD13	1:C:296:PRO:HG3	1.99	0.43
1:B:284:LYS:HE3	2:B:454:HOH:O	2.19	0.43
1:C:342:VAL:HG13	1:C:351:ILE:CG2	2.46	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:F:37:VAL:HA	1:F:387:PRO:HG2	2.00	0.43
1:F:67:LEU:HD12	1:F:70:MET:HE2	2.01	0.43
1:C:391:THR:OG1	1:C:393:GLU:HG2	2.19	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: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:C:15:ASN:OD1	1:D:94:ARG:NE	2.46	0.43
1:F:141:VAL:HG22	1:F:197:ILE:CG2	2.47	0.43
1:A:32:LYS:NZ	2:A:501:HOH:O	2.51	0.43
1:D:372:LEU:HD23	1:D:374:THR:HG23	2.00	0.43
1:F:239:GLY:HA2	1:F:315:CYS:SG	2.59	0.43
1:B:70:MET:HG3	1:B:301:ILE:HD11	2.00	0.42
1:D:27:ILE:HG13	1:D:28:PRO:CD	2.45	0.42
1:D:141:VAL:CG1	1:D:142:CYS:N	2.82	0.42
1:A:99:LEU:CD2	1:A:244:LEU:HD13	2.49	0.42
1:A:391:THR:HG22	1:A:392:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD21	1:A:244:LEU:HD11	2.01	0.42
1:A:106:LEU:HD11	1:B:23:ASN:HD21	1.80	0.42
1:C:100:LEU:HD11	1:C:259:LEU:HD11	2.01	0.42
1:C:245:LEU:HD13	1:C:257:ILE:CD1	2.49	0.42
1:C:269:PRO:HD3	1:D:268:TYR:CZ	2.54	0.42
1:C:375:ARG:NH2	2:C:427:HOH:O	2.51	0.42
1:F:279:ILE:O	1:F:282:VAL:HB	2.19	0.42
1:B:139:ILE:O	1:B:173:PHE:HA	2.19	0.42
1:D:39:VAL:HG21	1:D:373:ILE:CD1	2.49	0.42
1:B:342:VAL:HG22	1:B:351:ILE:HG22	2.02	0.42
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:D:197:ILE:HG12	1:D:230:VAL:HB	2.02	0.41
1:E:141:VAL:HG23	1:E:197:ILE:HG23	2.02	0.41
1:D:29:VAL:HG12	1:D:31:LEU:HD13	2.01	0.41
1:F:54:TYR:OH	1:F:375:ARG:HD2	2.20	0.41
1:A:376:ASP:HA	1:A:381:THR:O	2.20	0.41
1:F:391:THR:CG2	1:F:392:LYS:N	2.83	0.41
1:A:289:GLY:O	1:A:290:SER:CB	2.68	0.41
1:B:8:THR:HG22	1:B:11:ASP:CG	2.45	0.41
1:B:242:GLY:CA	1:B:319:GLU:HG2	2.44	0.41
1:C:204:GLU:N	1:C:204:GLU:CD	2.78	0.41
1:D:364:CYS:SG	1:D:382:ILE:HG12	2.60	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: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:136:MET:HA	1:F:136:MET:HE2	2.01	0.41
1:E:77:LEU:HD13	1:E:296:PRO:HG3	2.02	0.41
1:E:348:LEU:HA	1:E:385:THR:HG22	2.01	0.41
1:F:338:ILE:HD11	1:F:406:VAL:HG13	2.02	0.41
1:A:103:ASP:HB2	1:A:276:ASN:HA	2.02	0.41
1:A:269:PRO:HG2	1:B:269:PRO:HG2	2.03	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:C:23:ASN:CG	1:D:106:LEU:HD21	2.46	0.41
1:D:100:LEU:CD1	1:D:259:LEU:HD11	2.50	0.41
1:B:63:HIS:HA	1:B:64:PRO:HD3	1.89	0.40
1:B:391:THR:HG22	1:B:394:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:97:THR:HG23	2.20	0.40
1:C:188:LEU:HD12	1:C:221:ILE:CG2	2.51	0.40
1:E:13:ILE:O	1:E:17:LEU:HG	2.21	0.40
1:E:205:ALA:CB	1:E:208:ILE:CD1	2.99	0.40
1:F:97:THR:HB	1:F:102:TYR:O	2.21	0.40
1:A:138:LYS:NZ	1:A:190:ASP:OD2	2.46	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	11	8
1	B	373/433 (86%)	353 (95%)	18 (5%)	2 (0%)	24	22
1	C	365/433 (84%)	350 (96%)	13 (4%)	2 (0%)	24	22
1	D	371/433 (86%)	352 (95%)	16 (4%)	3 (1%)	16	12
1	E	370/433 (86%)	350 (95%)	19 (5%)	1 (0%)	36	36
1	F	371/433 (86%)	348 (94%)	18 (5%)	5 (1%)	9	6
All	All	2224/2598 (86%)	2109 (95%)	98 (4%)	17 (1%)	16	12

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	SER
1	C	288	HIS

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Mol	Chain	Res	Type
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%)	305 (92%)	26 (8%)	11	9
1	B	330/378 (87%)	307 (93%)	23 (7%)	14	11
1	C	322/378 (85%)	300 (93%)	22 (7%)	14	12
1	D	328/378 (87%)	305 (93%)	23 (7%)	14	11
1	E	327/378 (86%)	301 (92%)	26 (8%)	11	8
1	F	328/378 (87%)	304 (93%)	24 (7%)	13	10
All	All	1966/2268 (87%)	1822 (93%)	144 (7%)	13	10

All (144) 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

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	106	LEU
1	A	141	VAL
1	A	184	LEU
1	A	197	ILE
1	A	208	ILE
1	A	247	VAL
1	A	252	VAL
1	A	263	LEU
1	A	282	VAL
1	A	284	LYS
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
1	A	375	ARG
1	A	385	THR
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	263	LEU
1	B	309	LEU
1	B	332	GLU
1	B	340	ARG
1	B	347	LEU
1	B	355	ASN
1	B	356	GLU

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Mol	Chain	Res	Type
1	B	358	VAL
1	B	367	LEU
1	B	374	THR
1	B	391	THR
1	C	29	VAL
1	C	31	LEU
1	C	46	ARG
1	C	77	LEU
1	C	99	LEU
1	C	128	GLU
1	C	141	VAL
1	C	184	LEU
1	C	247	VAL
1	C	252	VAL
1	C	257	ILE
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
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	347	LEU
1	D	351	ILE

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Mol	Chain	Res	Type
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	37	VAL
1	E	45	LYS
1	E	75	LYS
1	E	77	LEU
1	E	79	ILE
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	218	VAL
1	E	247	VAL
1	E	252	VAL
1	E	263	LEU
1	E	282	VAL
1	E	327	GLU
1	E	337	LYS
1	E	347	LEU
1	E	356	GLU
1	E	358	VAL
1	E	367	LEU
1	E	374	THR
1	E	395	LEU
1	F	29	VAL
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

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Mol	Chain	Res	Type
1	F	185	GLU
1	F	204	GLU
1	F	247	VAL
1	F	252	VAL
1	F	263	LEU
1	F	282	VAL
1	F	287	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	145	ASN
1	A	235	GLN
1	A	317	ASN
1	A	370	ASN
1	A	378	HIS
1	B	22	HIS
1	B	145	ASN
1	B	216	GLN
1	B	235	GLN
1	B	355	ASN
1	B	370	ASN
1	B	378	HIS
1	C	43	ASN
1	C	73	GLN
1	C	235	GLN
1	C	355	ASN
1	C	370	ASN
1	D	22	HIS
1	D	65	ASN
1	D	109	ASN
1	D	192	ASN
1	D	235	GLN

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Mol	Chain	Res	Type
1	D	355	ASN
1	D	370	ASN
1	E	22	HIS
1	E	235	GLN
1	E	267	HIS
1	E	288	HIS
1	E	307	ASN
1	E	328	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 oligosaccharides 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	378/433 (87%)	0.26	13 (3%)	48	50	16, 34, 57, 71	0
1	B	377/433 (87%)	0.63	30 (7%)	18	19	20, 38, 63, 71	0
1	C	369/433 (85%)	0.84	39 (10%)	11	12	27, 43, 72, 81	0
1	D	375/433 (86%)	0.64	23 (6%)	27	29	23, 40, 57, 83	0
1	E	374/433 (86%)	0.76	41 (10%)	10	11	23, 43, 68, 81	0
1	F	375/433 (86%)	0.47	30 (8%)	18	19	20, 36, 58, 71	0
All	All	2248/2598 (86%)	0.60	176 (7%)	19	20	16, 39, 64, 83	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	GLY	6.9
1	B	181	LEU	6.8
1	D	289	GLY	5.8
1	D	288	HIS	5.4
1	B	289	GLY	4.9
1	F	289	GLY	4.9
1	A	287	GLU	4.7
1	E	141	VAL	4.3
1	A	289	GLY	4.3
1	B	391	THR	4.3
1	F	379	ASP	4.2
1	A	319	GLU	4.1
1	B	213	ASN	4.0
1	F	181	LEU	3.9
1	E	290	SER	3.9
1	E	197	ILE	3.8
1	B	143	LYS	3.6
1	F	286	GLY	3.6
1	A	7	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	339	VAL	3.5
1	A	288	HIS	3.5
1	D	7	LYS	3.5
1	F	7	LYS	3.5
1	D	379	ASP	3.4
1	F	219	TYR	3.4
1	C	224	LYS	3.4
1	B	180	ASP	3.4
1	F	340	ARG	3.4
1	B	183	ALA	3.3
1	E	288	HIS	3.3
1	E	213	ASN	3.3
1	E	338	ILE	3.3
1	D	373	ILE	3.2
1	C	191	PRO	3.1
1	E	183	ALA	3.1
1	C	275	ALA	3.1
1	C	281	LEU	3.1
1	D	173	PHE	3.0
1	C	225	TYR	3.0
1	C	379	ASP	3.0
1	E	137	ALA	3.0
1	E	289	GLY	3.0
1	D	143	LYS	3.0
1	F	134	GLU	2.9
1	B	326	LEU	2.9
1	E	7	LYS	2.9
1	E	204	GLU	2.9
1	F	290	SER	2.9
1	E	333	LEU	2.9
1	C	129	VAL	2.9
1	C	178	TYR	2.9
1	E	205	ALA	2.9
1	C	282	VAL	2.8
1	C	286	GLY	2.8
1	B	287	GLU	2.8
1	B	145	ASN	2.8
1	D	98	ASN	2.8
1	E	286	GLY	2.8
1	F	251	ASN	2.7
1	B	323	GLY	2.7
1	E	409	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	246	CYS	2.7
1	D	27	ILE	2.7
1	F	217	GLY	2.7
1	D	287	GLU	2.7
1	C	283	ILE	2.7
1	C	84	PHE	2.6
1	C	188	LEU	2.6
1	D	290	SER	2.6
1	D	410	ASP	2.6
1	C	7	LYS	2.6
1	C	197	ILE	2.6
1	E	364	CYS	2.6
1	A	369	GLU	2.6
1	C	288	HIS	2.6
1	E	8	THR	2.6
1	E	210	PRO	2.6
1	D	211	SER	2.6
1	F	319	GLU	2.6
1	B	307	ASN	2.6
1	F	355	ASN	2.6
1	D	391	THR	2.6
1	F	288	HIS	2.6
1	C	276	ASN	2.6
1	B	197	ILE	2.5
1	D	285	PRO	2.5
1	F	143	LYS	2.5
1	A	335	ASP	2.5
1	B	318	ALA	2.5
1	E	29	VAL	2.5
1	F	218	VAL	2.5
1	C	291	THR	2.5
1	E	336	SER	2.5
1	E	134	GLU	2.4
1	B	214	TYR	2.4
1	C	290	SER	2.4
1	C	121	LEU	2.4
1	F	338	ILE	2.4
1	F	400	GLU	2.4
1	D	94	ARG	2.4
1	C	181	LEU	2.4
1	E	68	ASN	2.4
1	C	45	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	8	THR	2.4
1	F	375	ARG	2.4
1	B	137	ALA	2.4
1	F	336	SER	2.4
1	B	288	HIS	2.4
1	D	351	ILE	2.3
1	E	403	VAL	2.3
1	F	342	VAL	2.3
1	D	15	ASN	2.3
1	C	37	VAL	2.3
1	A	172	GLN	2.3
1	C	285	PRO	2.3
1	E	378	HIS	2.3
1	E	173	PHE	2.3
1	E	208	ILE	2.3
1	E	337	LYS	2.3
1	F	205	ALA	2.3
1	B	215	LEU	2.3
1	E	215	LEU	2.3
1	C	221	ILE	2.2
1	E	98	ASN	2.2
1	C	253	LYS	2.2
1	A	400	GLU	2.2
1	E	342	VAL	2.2
1	E	341	ASP	2.2
1	E	127	TYR	2.2
1	D	45	LYS	2.2
1	B	351	ILE	2.2
1	C	133	PRO	2.2
1	C	362	ASP	2.2
1	C	215	LEU	2.2
1	B	250	TYR	2.2
1	B	208	ILE	2.1
1	F	173	PHE	2.1
1	F	221	ILE	2.1
1	F	252	VAL	2.1
1	C	216	GLN	2.1
1	C	219	TYR	2.1
1	A	410	ASP	2.1
1	B	187	GLU	2.1
1	F	391	THR	2.1
1	B	193	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	322	GLY	2.1
1	D	141	VAL	2.1
1	D	377	VAL	2.1
1	E	176	VAL	2.1
1	B	321	LEU	2.1
1	A	364	CYS	2.1
1	F	364	CYS	2.1
1	F	335	ASP	2.1
1	E	383	ARG	2.1
1	E	408	PHE	2.1
1	C	342	VAL	2.1
1	E	334	LYS	2.1
1	B	184	LEU	2.1
1	E	400	GLU	2.1
1	C	189	LYS	2.1
1	C	334	LYS	2.1
1	D	382	ILE	2.1
1	C	116	GLU	2.0
1	F	287	GLU	2.0
1	F	327	GLU	2.0
1	C	410	ASP	2.0
1	E	253	LYS	2.0
1	B	217	GLY	2.0
1	E	132	ILE	2.0
1	C	252	VAL	2.0
1	E	377	VAL	2.0
1	A	336	SER	2.0
1	B	410	ASP	2.0
1	B	142	CYS	2.0
1	A	391	THR	2.0
1	B	178	TYR	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 oligosaccharides 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.