Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 12:43 AM EST

PDB ID	:	1PYA
Title	:	REFINED STRUCTURE OF THE PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE FROM LACTOBACILLUS 30A
Authors	:	Gallagher, T.; Rozwarski, D.A.; Ernst, S.R.; Hackert, M.L.
Deposited on	:	1992-12-18
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
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:

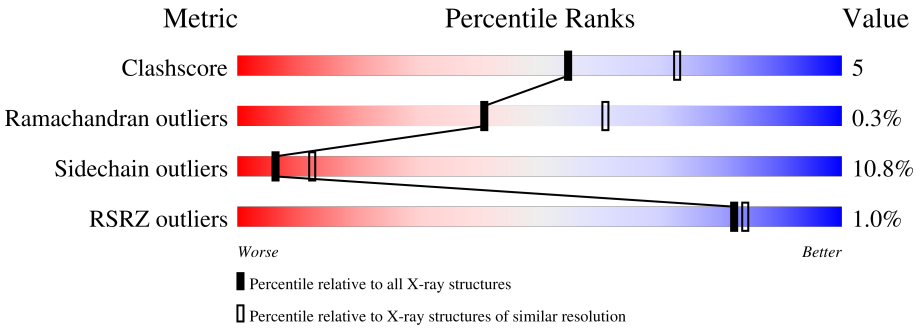
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	81	79% 12% 6% •
1	C	81	85% 11% • •
1	E	81	78% 15% 5% •
2	B	229	2% 77% 21% ••
2	D	229	% 76% 20% • •
2	F	229	% 72% 22% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10140 atoms, of which 2478 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 PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	H	N	O	S	0	0	0
			770	384	149	107	128	2			
1	C	81	Total	C	H	N	O	S	0	0	0
			770	384	149	107	128	2			
1	E	81	Total	C	H	N	O	S	0	0	0
			770	384	149	107	128	2			

- Molecule 2 is a protein called PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	229	Total	C	H	N	O	S	0	0	0
			2139	1127	363	286	352	11			
2	D	229	Total	C	H	N	O	S	0	0	0
			2139	1127	363	286	352	11			
2	F	229	Total	C	H	N	O	S	0	0	0
			2139	1127	363	286	352	11			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	54	Total	H	O	0	0
			162	108	54		
3	B	106	Total	H	O	0	0
			318	212	106		
3	C	61	Total	H	O	0	0
			183	122	61		
3	D	92	Total	H	O	0	0
			276	184	92		
3	E	58	Total	H	O	0	0
			174	116	58		

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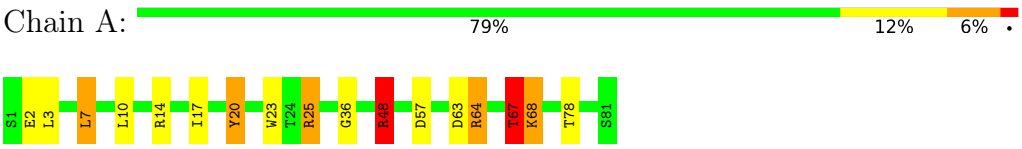
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	100	Total 300	H 200	O 100	0	0

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.

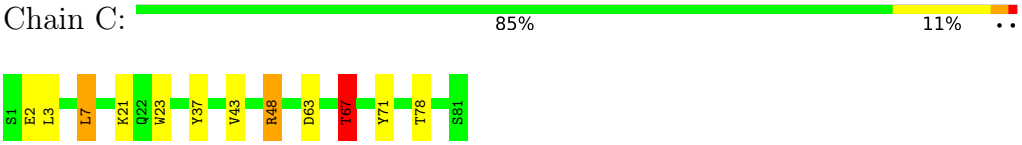
• Molecule 1: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain A:



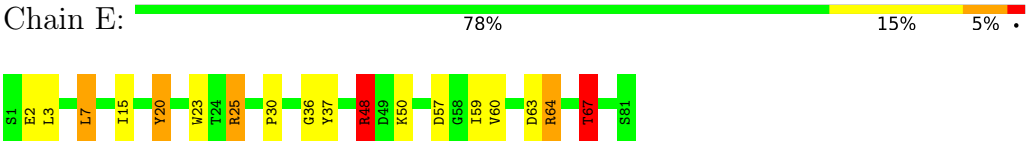
• Molecule 1: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain C:



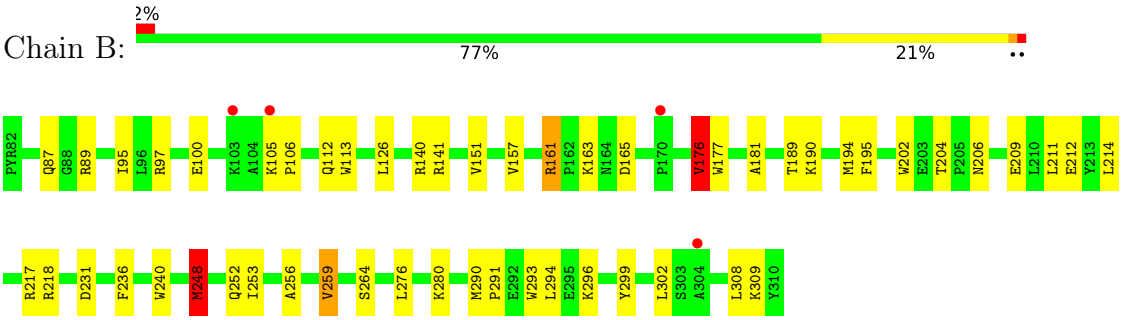
• Molecule 1: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain E:



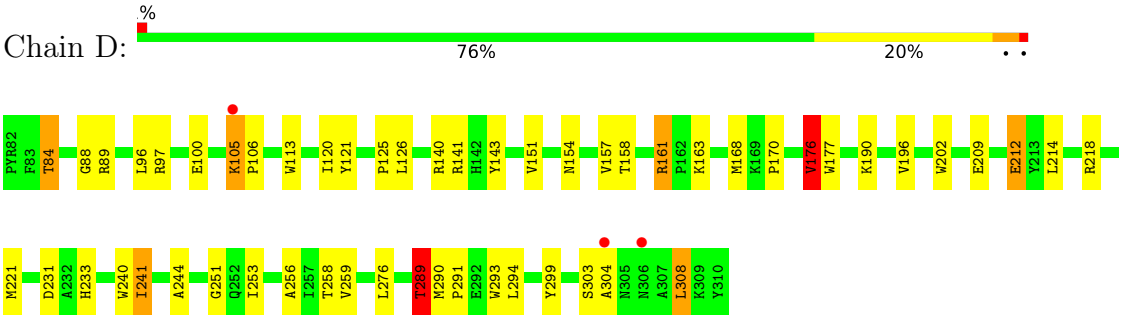
• Molecule 2: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain B:



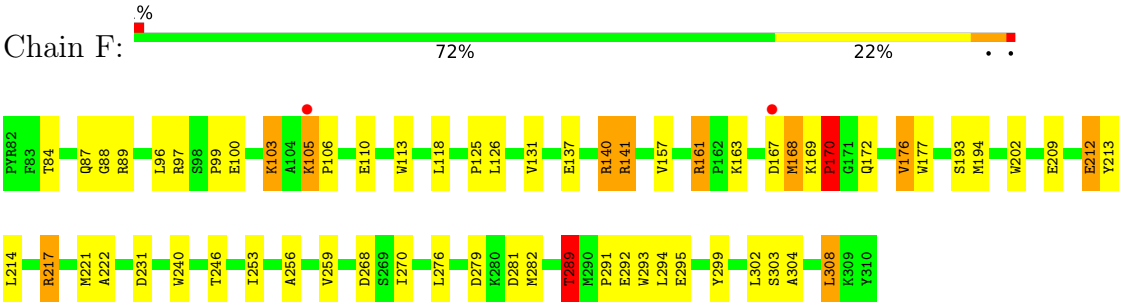
• Molecule 2: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain D:



• Molecule 2: PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE (L-HISTIDINE CARBOXYLASE)

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	221.70Å 221.70Å 107.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 49.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50) 99.5 (49.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.150 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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	0.77	0/629	1.74	10/848 (1.2%)
1	C	0.75	0/629	1.57	10/848 (1.2%)
1	E	0.73	0/629	1.55	11/848 (1.3%)
2	B	0.81	1/1816 (0.1%)	1.51	26/2463 (1.1%)
2	D	0.80	0/1816	1.55	28/2463 (1.1%)
2	F	0.81	0/1816	1.55	29/2463 (1.2%)
All	All	0.79	1/7335 (0.0%)	1.56	114/9933 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	259	VAL	CA-CB	5.12	1.65	1.54

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	89	ARG	NE-CZ-NH2	-17.26	111.67	120.30
1	A	25	ARG	NE-CZ-NH2	-16.05	112.28	120.30
2	D	89	ARG	NE-CZ-NH1	14.55	127.58	120.30
1	A	25	ARG	NE-CZ-NH1	14.04	127.32	120.30
2	F	89	ARG	NE-CZ-NH1	13.10	126.85	120.30
2	F	89	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	A	48	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	C	48	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	E	48	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	A	48	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	B	299	TYR	CB-CG-CD2	-9.41	115.35	121.00
1	C	23	TRP	CD1-CG-CD2	9.15	113.62	106.30
2	F	194	MET	CG-SD-CE	-8.87	86.01	100.20
2	D	177	TRP	CD1-CG-CD2	8.77	113.32	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	141	ARG	NE-CZ-NH1	8.60	124.60	120.30
2	F	177	TRP	CD1-CG-CD2	8.59	113.17	106.30
2	B	202	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	E	64	ARG	NE-CZ-NH2	-8.29	116.15	120.30
2	B	177	TRP	CD1-CG-CD2	8.21	112.87	106.30
2	F	293	TRP	CD1-CG-CD2	8.16	112.83	106.30
2	D	161	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	C	48	ARG	NE-CZ-NH2	-8.07	116.26	120.30
2	D	293	TRP	CD1-CG-CD2	8.02	112.72	106.30
2	F	113	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	23	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	C	67	THR	N-CA-CB	-7.92	95.26	110.30
1	E	23	TRP	CD1-CG-CD2	7.91	112.63	106.30
2	B	161	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	20	TYR	CB-CG-CD2	-7.90	116.26	121.00
2	F	202	TRP	CD1-CG-CD2	7.90	112.62	106.30
2	F	221	MET	CG-SD-CE	-7.80	87.72	100.20
2	F	141	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	23	TRP	CE2-CD2-CG	-7.72	101.12	107.30
2	F	177	TRP	CE2-CD2-CG	-7.63	101.19	107.30
2	D	121	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	E	48	ARG	NE-CZ-NH2	-7.53	116.54	120.30
2	D	161	ARG	NE-CZ-NH1	7.45	124.02	120.30
2	B	177	TRP	CE2-CD2-CG	-7.39	101.39	107.30
2	B	202	TRP	CE2-CD2-CG	-7.39	101.39	107.30
2	F	212	GLU	CA-CB-CG	7.27	129.39	113.40
2	B	113	TRP	CD1-CG-CD2	7.26	112.11	106.30
2	D	221	MET	CG-SD-CE	-7.25	88.59	100.20
2	F	141	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	23	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	67	THR	N-CA-CB	-7.18	96.66	110.30
2	D	177	TRP	CE2-CD2-CG	-7.14	101.59	107.30
2	D	141	ARG	NE-CZ-NH1	7.11	123.86	120.30
2	D	293	TRP	CE2-CD2-CG	-7.10	101.62	107.30
2	D	97	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	B	293	TRP	CD1-CG-CD2	7.02	111.92	106.30
2	B	194	MET	CA-CB-CG	7.01	125.22	113.30
2	B	97	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	B	218	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	F	202	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	E	23	TRP	CE2-CD2-CG	-6.94	101.75	107.30
2	B	113	TRP	CE2-CD2-CG	-6.90	101.78	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	240	TRP	CE2-CD2-CG	-6.84	101.83	107.30
2	D	202	TRP	CD1-CG-CD2	6.83	111.77	106.30
2	D	113	TRP	CD1-CG-CD2	6.82	111.75	106.30
2	F	113	TRP	CE2-CD2-CG	-6.79	101.87	107.30
2	F	299	TYR	CB-CG-CD2	-6.69	116.99	121.00
2	D	141	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	D	97	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	F	293	TRP	CE2-CD2-CG	-6.65	101.98	107.30
2	F	240	TRP	CE2-CD2-CG	-6.54	102.07	107.30
2	B	293	TRP	CE2-CD2-CG	-6.52	102.09	107.30
2	B	140	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	217	ARG	NE-CZ-NH1	6.41	123.50	120.30
2	D	202	TRP	CE2-CD2-CG	-6.38	102.19	107.30
2	B	240	TRP	CD1-CG-CD2	6.22	111.28	106.30
2	F	279	ASP	CB-CG-OD1	6.21	123.89	118.30
2	B	240	TRP	CE2-CD2-CG	-6.21	102.33	107.30
2	F	161	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	23	TRP	CG-CD1-NE1	-6.13	103.97	110.10
2	D	240	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	E	20	TYR	CB-CG-CD2	-5.97	117.42	121.00
2	F	170	PRO	CA-C-N	5.96	128.12	116.20
1	E	48	ARG	CB-CG-CD	5.94	127.05	111.60
1	E	67	THR	N-CA-CB	-5.91	99.08	110.30
1	E	25	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	D	218	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	E	64	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	23	TRP	CG-CD2-CE3	5.84	139.16	133.90
2	F	240	TRP	CD1-CG-CD2	5.81	110.95	106.30
2	D	113	TRP	CE2-CD2-CG	-5.80	102.66	107.30
2	B	97	ARG	NE-CZ-NH1	5.77	123.18	120.30
2	D	177	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	C	71	TYR	CB-CG-CD2	-5.59	117.64	121.00
2	F	289	THR	N-CA-CB	-5.59	99.68	110.30
1	A	64	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	B	248	MET	CA-CB-CG	5.49	122.64	113.30
2	F	295	GLU	CA-CB-CG	5.44	125.36	113.40
2	F	293	TRP	CG-CD1-NE1	-5.43	104.67	110.10
2	D	299	TYR	CB-CG-CD2	-5.39	117.77	121.00
2	F	177	TRP	CG-CD1-NE1	-5.38	104.72	110.10
1	C	23	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	C	37	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	E	48	ARG	CG-CD-NE	-5.31	100.65	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	241	ILE	CG1-CB-CG2	-5.28	99.78	111.40
2	F	170	PRO	N-CA-C	5.28	125.83	112.10
2	D	176	VAL	N-CA-CB	-5.24	99.97	111.50
2	B	202	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	B	176	VAL	N-CA-CB	-5.22	100.02	111.50
2	B	248	MET	CG-SD-CE	-5.22	91.85	100.20
2	D	240	TRP	CG-CD2-CE3	5.21	138.59	133.90
2	F	113	TRP	CG-CD1-NE1	-5.21	104.89	110.10
2	D	293	TRP	CG-CD1-NE1	-5.19	104.91	110.10
2	F	268	ASP	CB-CG-OD1	5.17	122.96	118.30
2	F	140	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	D	289	THR	N-CA-CB	-5.12	100.56	110.30
1	A	23	TRP	CG-CD1-NE1	-5.11	105.00	110.10
2	B	141	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	B	177	TRP	CG-CD2-CE3	5.01	138.41	133.90
2	B	177	TRP	CB-CG-CD1	-5.00	120.50	127.00

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	621	149	611	10	0
1	C	621	149	611	5	0
1	E	621	149	611	12	0
2	B	1776	363	1704	16	0
2	D	1776	363	1704	19	0
2	F	1776	363	1704	26	0
3	A	54	108	0	1	0
3	B	106	212	0	0	0
3	C	61	122	0	0	0
3	D	92	184	0	3	0
3	E	58	116	0	2	0
3	F	100	200	0	1	0
All	All	7662	2478	6945	73	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 5.

All (73) 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)
2:D:105:LYS:NZ	2:D:106:PRO:O	1.89	1.06
2:B:112:GLN:HE22	2:B:236:PHE:H	1.24	0.82
2:D:289:THR:HG23	2:D:291:PRO:HD2	1.65	0.78
2:F:110:GLU:HG3	2:F:222:ALA:HB1	1.68	0.75
2:F:100:GLU:HB2	2:F:125:PRO:HB3	1.68	0.75
1:C:78:THR:HG22	2:D:151:VAL:HG23	1.72	0.71
2:F:289:THR:HG23	2:F:291:PRO:HD2	1.72	0.71
2:F:105:LYS:NZ	2:F:106:PRO:O	2.24	0.70
1:A:78:THR:HG22	2:B:151:VAL:HG23	1.81	0.62
2:F:176:VAL:HG13	2:F:256:ALA:HB2	1.81	0.61
2:B:231:ASP:HB3	1:C:67:THR:HG21	1.83	0.60
2:F:303:SER:HA	2:F:308:LEU:HD22	1.83	0.60
2:D:231:ASP:HB3	1:E:67:THR:HG21	1.83	0.60
1:A:20:TYR:CE2	1:A:25:ARG:HD2	2.36	0.59
2:D:176:VAL:HG13	2:D:256:ALA:HB2	1.86	0.57
2:D:209:GLU:O	2:D:212:GLU:HG3	2.05	0.57
2:D:157:VAL:HG13	2:D:176:VAL:HG22	1.87	0.56
1:E:3:LEU:HG	1:E:7:LEU:HD22	1.87	0.56
1:A:63:ASP:O	1:A:67:THR:HB	2.06	0.56
2:F:270:ILE:HD13	2:F:281:ASP:HB3	1.87	0.56
2:D:100:GLU:HB2	2:D:125:PRO:HB3	1.88	0.55
2:D:251:GLY:HA2	3:D:394:HOH:O	2.05	0.55
2:B:204:THR:HG21	2:B:209:GLU:OE1	2.06	0.55
2:B:204:THR:HG22	2:B:206:ASN:H	1.72	0.55
1:E:63:ASP:O	1:E:67:THR:HB	2.07	0.54
1:E:57:ASP:HB3	2:F:253:ILE:HG21	1.90	0.54
2:F:213:TYR:CZ	2:F:217:ARG:HD3	2.43	0.54
2:F:105:LYS:HG3	2:F:106:PRO:HD2	1.90	0.53
1:A:67:THR:HG21	2:F:231:ASP:HB3	1.91	0.53
2:B:176:VAL:HG13	2:B:256:ALA:HB2	1.91	0.52
2:D:120:ILE:HG23	2:D:241:ILE:HD13	1.91	0.52
1:A:7:LEU:HD13	2:B:189:THR:HG22	1.95	0.49
2:F:141:ARG:HD2	3:F:336:HOH:O	2.12	0.49
1:E:36:GLY:HA2	2:F:87:GLN:HB3	1.95	0.48
1:C:43:VAL:HG13	2:D:244:ALA:HB2	1.95	0.48
2:F:209:GLU:HA	2:F:212:GLU:HG3	1.95	0.48
2:D:303:SER:HA	2:D:308:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:289:THR:HG22	2:F:292:GLU:H	1.79	0.48
2:F:105:LYS:HG3	2:F:106:PRO:CD	2.44	0.48
2:F:157:VAL:HG13	2:F:176:VAL:HG22	1.96	0.47
2:D:233:HIS:HD2	2:F:137:GLU:OE2	1.97	0.47
2:B:105:LYS:NZ	2:B:106:PRO:O	2.47	0.47
2:F:176:VAL:HG12	2:F:246:THR:HG22	1.97	0.47
2:D:289:THR:HG21	3:D:388:HOH:O	2.14	0.47
1:A:48:ARG:O	2:B:253:ILE:HG22	2.16	0.46
1:E:59:ILE:HG23	3:E:104:HOH:O	2.15	0.46
2:D:140:ARG:HB3	2:D:143:TYR:CE1	2.51	0.46
1:A:20:TYR:CZ	1:A:25:ARG:HD2	2.51	0.46
1:E:25:ARG:NH2	1:E:30:PRO:O	2.49	0.45
1:A:57:ASP:HB3	2:B:253:ILE:HG21	1.97	0.45
2:B:248:MET:HB2	2:B:252:GLN:HB2	1.99	0.45
1:E:67:THR:HG22	3:E:125:HOH:O	2.17	0.45
2:F:168:MET:HG2	2:F:172:GLN:HB3	1.99	0.45
1:E:20:TYR:OH	1:E:25:ARG:NH1	2.50	0.44
1:A:36:GLY:HA2	2:B:87:GLN:HB3	1.98	0.44
2:D:154:ASN:HA	2:D:258:THR:O	2.18	0.43
1:E:37:TYR:O	2:F:88:GLY:HA2	2.18	0.43
1:A:68:LYS:NZ	3:A:133:HOH:O	2.52	0.43
2:B:89:ARG:HD3	2:B:95:ILE:HG23	2.00	0.43
2:F:213:TYR:CE2	2:F:217:ARG:HD3	2.53	0.42
1:C:3:LEU:HG	1:C:7:LEU:HD22	2.01	0.42
1:E:15:ILE:HA	2:F:282:MET:HG3	2.01	0.42
2:F:84:THR:O	2:F:193:SER:HB2	2.19	0.42
2:D:84:THR:HG22	2:D:88:GLY:HA3	2.02	0.41
2:B:181:ALA:O	2:B:195:PHE:HA	2.20	0.41
2:F:169:LYS:O	2:F:172:GLN:HB2	2.21	0.41
1:C:63:ASP:O	1:C:67:THR:HB	2.21	0.40
2:B:290:MET:HB3	2:B:291:PRO:HD3	2.03	0.40
2:D:190:LYS:HD3	3:D:338:HOH:O	2.22	0.40
2:D:290:MET:HB3	2:D:291:PRO:HD3	2.03	0.40
1:E:48:ARG:HD3	1:E:60:VAL:HG11	2.03	0.40
2:B:157:VAL:HG13	2:B:176:VAL:HG22	2.03	0.40
2:F:99:PRO:O	2:F:103:LYS:HG2	2.21	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	79/81 (98%)	73 (92%)	6 (8%)	0	100 100
1	C	79/81 (98%)	75 (95%)	4 (5%)	0	100 100
1	E	79/81 (98%)	75 (95%)	4 (5%)	0	100 100
2	B	227/229 (99%)	219 (96%)	8 (4%)	0	100 100
2	D	227/229 (99%)	219 (96%)	7 (3%)	1 (0%)	34 54
2	F	227/229 (99%)	218 (96%)	7 (3%)	2 (1%)	17 31
All	All	918/930 (99%)	879 (96%)	36 (4%)	3 (0%)	41 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	304	ALA
2	D	304	ALA
2	F	170	PRO

5.3.2 Protein sidechains (i)

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	66/66 (100%)	56 (85%)	10 (15%)	3 5
1	C	66/66 (100%)	61 (92%)	5 (8%)	13 25
1	E	66/66 (100%)	60 (91%)	6 (9%)	9 18
2	B	188/188 (100%)	168 (89%)	20 (11%)	6 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	188/188 (100%)	169 (90%)	19 (10%)	7 14
2	F	188/188 (100%)	166 (88%)	22 (12%)	5 10
All	All	762/762 (100%)	680 (89%)	82 (11%)	6 12

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	LEU
1	A	7	LEU
1	A	10	LEU
1	A	14	ARG
1	A	17	ILE
1	A	48	ARG
1	A	64	ARG
1	A	67	THR
1	A	68	LYS
2	B	100	GLU
2	B	126	LEU
2	B	161	ARG
2	B	163	LYS
2	B	165	ASP
2	B	176	VAL
2	B	190	LYS
2	B	211	LEU
2	B	212	GLU
2	B	214	LEU
2	B	248	MET
2	B	259	VAL
2	B	264	SER
2	B	276	LEU
2	B	280	LYS
2	B	294	LEU
2	B	296	LYS
2	B	302	LEU
2	B	308	LEU
2	B	309	LYS
1	C	2	GLU
1	C	7	LEU
1	C	21	LYS
1	C	48	ARG

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Mol	Chain	Res	Type
1	C	67	THR
2	D	84	THR
2	D	96	LEU
2	D	105	LYS
2	D	126	LEU
2	D	158	THR
2	D	161	ARG
2	D	163	LYS
2	D	168	MET
2	D	170	PRO
2	D	176	VAL
2	D	196	VAL
2	D	212	GLU
2	D	214	LEU
2	D	253	ILE
2	D	259	VAL
2	D	276	LEU
2	D	289	THR
2	D	294	LEU
2	D	308	LEU
1	E	2	GLU
1	E	7	LEU
1	E	48	ARG
1	E	50	LYS
1	E	64	ARG
1	E	67	THR
2	F	96	LEU
2	F	97	ARG
2	F	103	LYS
2	F	105	LYS
2	F	118	LEU
2	F	126	LEU
2	F	131	VAL
2	F	140	ARG
2	F	161	ARG
2	F	163	LYS
2	F	167	ASP
2	F	168	MET
2	F	170	PRO
2	F	176	VAL
2	F	214	LEU
2	F	217	ARG

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Mol	Chain	Res	Type
2	F	259	VAL
2	F	276	LEU
2	F	289	THR
2	F	294	LEU
2	F	302	LEU
2	F	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
2	B	112	GLN
2	B	233	HIS
1	C	69	ASN
2	D	233	HIS
1	E	22	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 monosaccharides 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, 95^{th} 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	81/81 (100%)	-0.38	0	100	100	9, 17, 30, 47	0
1	C	81/81 (100%)	-0.35	0	100	100	10, 16, 32, 45	0
1	E	81/81 (100%)	-0.37	0	100	100	10, 16, 30, 48	0
2	B	228/229 (99%)	-0.29	4 (1%)	68	71	10, 21, 43, 57	0
2	D	228/229 (99%)	-0.29	3 (1%)	77	79	9, 21, 40, 54	0
2	F	228/229 (99%)	-0.44	2 (0%)	84	86	9, 20, 39, 57	0
All	All	927/930 (99%)	-0.35	9 (0%)	82	84	9, 19, 40, 57	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	103	LYS	3.0
2	F	167	ASP	2.7
2	D	306	ASN	2.7
2	D	304	ALA	2.6
2	F	105	LYS	2.3
2	D	105	LYS	2.3
2	B	304	ALA	2.2
2	B	105	LYS	2.2
2	B	170	PRO	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.