



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:55 AM UTC

PDB ID : 5UDO / pdb_00005udo
Title : Crystal structure of the coiled-coil domain from Listeria Innocua Phage Integrase (Tetragonal Form II)
Authors : Gupta, K.; Yuan, J.B.; Sharp, R.; Van Duyne, G.D.
Deposited on : 2016-12-28
Resolution : 2.54 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

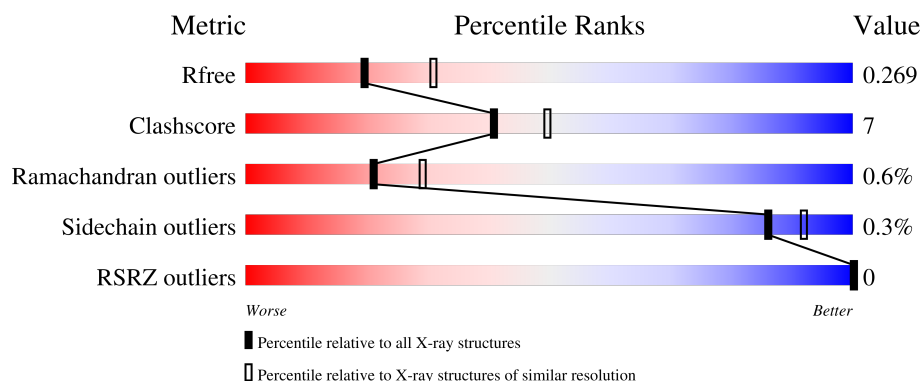
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	328	
1	B	328	
1	C	328	
1	D	328	
1	E	328	

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Mol	Chain	Length	Quality of chain
1	F	328	 10% • 85%
1	G	328	 12% • 87%
1	H	328	 15% • 85%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3881 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 A118 serine integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	48	Total	C	N	O	S	0	0	0
			398	251	64	81	2			
1	B	49	Total	C	N	O	S	0	0	0
			406	257	65	82	2			
1	C	44	Total	C	N	O	S	0	0	0
			359	228	58	71	2			
1	D	48	Total	C	N	O	S	0	0	0
			398	252	64	80	2			
1	E	47	Total	C	N	O	S	0	0	0
			392	249	63	78	2			
1	F	48	Total	C	N	O	S	0	0	0
			398	252	64	80	2			
1	G	42	Total	C	N	O	S	0	0	0
			353	224	57	70	2			
1	H	48	Total	C	N	O	S	0	0	0
			398	251	64	81	2			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	453	LEU	-	expression tag	UNP Q928V6
A	454	GLU	-	expression tag	UNP Q928V6
A	455	HIS	-	expression tag	UNP Q928V6
A	456	HIS	-	expression tag	UNP Q928V6
A	457	HIS	-	expression tag	UNP Q928V6
A	458	HIS	-	expression tag	UNP Q928V6
A	459	HIS	-	expression tag	UNP Q928V6
A	460	HIS	-	expression tag	UNP Q928V6
B	453	LEU	-	expression tag	UNP Q928V6
B	454	GLU	-	expression tag	UNP Q928V6
B	455	HIS	-	expression tag	UNP Q928V6
B	456	HIS	-	expression tag	UNP Q928V6
B	457	HIS	-	expression tag	UNP Q928V6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	458	HIS	-	expression tag	UNP Q928V6
B	459	HIS	-	expression tag	UNP Q928V6
B	460	HIS	-	expression tag	UNP Q928V6
C	453	LEU	-	expression tag	UNP Q928V6
C	454	GLU	-	expression tag	UNP Q928V6
C	455	HIS	-	expression tag	UNP Q928V6
C	456	HIS	-	expression tag	UNP Q928V6
C	457	HIS	-	expression tag	UNP Q928V6
C	458	HIS	-	expression tag	UNP Q928V6
C	459	HIS	-	expression tag	UNP Q928V6
C	460	HIS	-	expression tag	UNP Q928V6
D	453	LEU	-	expression tag	UNP Q928V6
D	454	GLU	-	expression tag	UNP Q928V6
D	455	HIS	-	expression tag	UNP Q928V6
D	456	HIS	-	expression tag	UNP Q928V6
D	457	HIS	-	expression tag	UNP Q928V6
D	458	HIS	-	expression tag	UNP Q928V6
D	459	HIS	-	expression tag	UNP Q928V6
D	460	HIS	-	expression tag	UNP Q928V6
E	453	LEU	-	expression tag	UNP Q928V6
E	454	GLU	-	expression tag	UNP Q928V6
E	455	HIS	-	expression tag	UNP Q928V6
E	456	HIS	-	expression tag	UNP Q928V6
E	457	HIS	-	expression tag	UNP Q928V6
E	458	HIS	-	expression tag	UNP Q928V6
E	459	HIS	-	expression tag	UNP Q928V6
E	460	HIS	-	expression tag	UNP Q928V6
F	453	LEU	-	expression tag	UNP Q928V6
F	454	GLU	-	expression tag	UNP Q928V6
F	455	HIS	-	expression tag	UNP Q928V6
F	456	HIS	-	expression tag	UNP Q928V6
F	457	HIS	-	expression tag	UNP Q928V6
F	458	HIS	-	expression tag	UNP Q928V6
F	459	HIS	-	expression tag	UNP Q928V6
F	460	HIS	-	expression tag	UNP Q928V6
G	453	LEU	-	expression tag	UNP Q928V6
G	454	GLU	-	expression tag	UNP Q928V6
G	455	HIS	-	expression tag	UNP Q928V6
G	456	HIS	-	expression tag	UNP Q928V6
G	457	HIS	-	expression tag	UNP Q928V6
G	458	HIS	-	expression tag	UNP Q928V6
G	459	HIS	-	expression tag	UNP Q928V6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	460	HIS	-	expression tag	UNP Q928V6
H	453	LEU	-	expression tag	UNP Q928V6
H	454	GLU	-	expression tag	UNP Q928V6
H	455	HIS	-	expression tag	UNP Q928V6
H	456	HIS	-	expression tag	UNP Q928V6
H	457	HIS	-	expression tag	UNP Q928V6
H	458	HIS	-	expression tag	UNP Q928V6
H	459	HIS	-	expression tag	UNP Q928V6
H	460	HIS	-	expression tag	UNP Q928V6

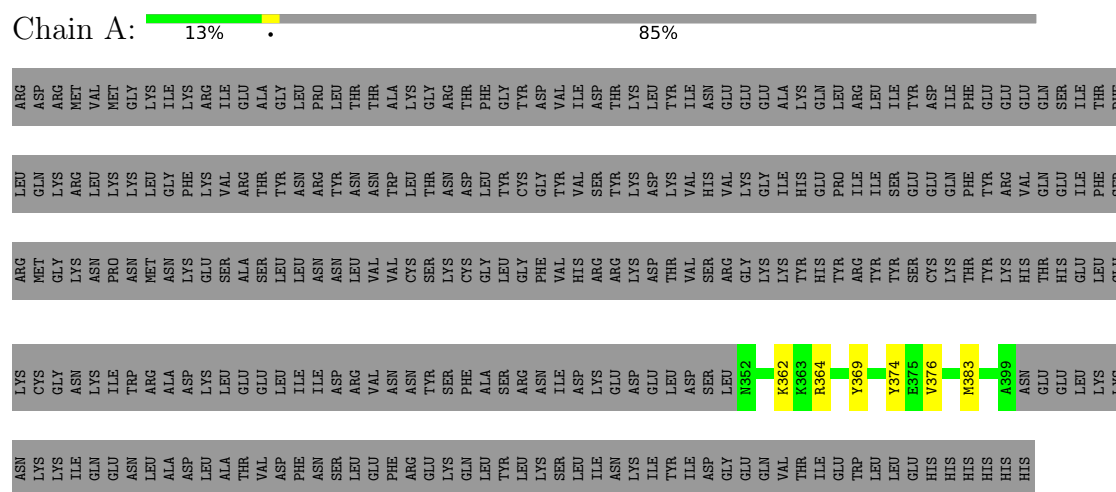
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total 115	O 115	0	0
2	B	101	Total 101	O 101	0	0
2	C	87	Total 87	O 87	0	0
2	D	94	Total 94	O 94	0	0
2	E	102	Total 102	O 102	0	0
2	F	92	Total 92	O 92	0	0
2	G	86	Total 86	O 86	0	0
2	H	102	Total 102	O 102	0	0

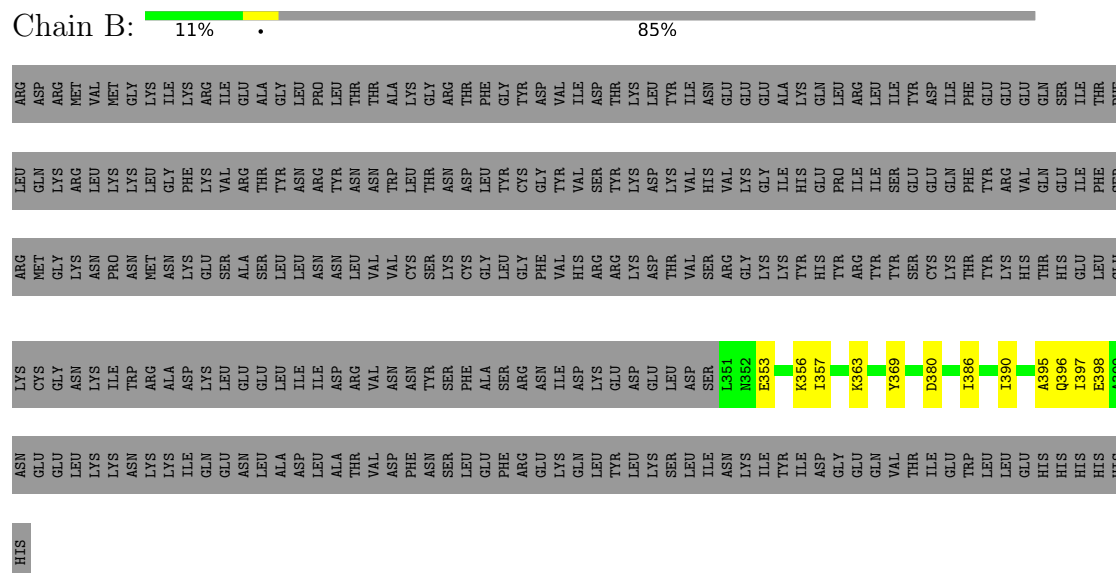
3 Residue-property plots

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: A118 serine integrase

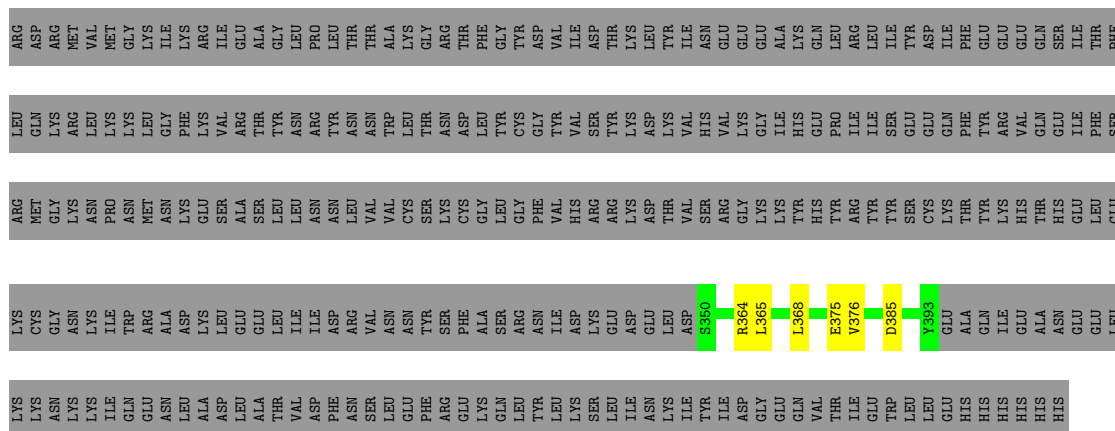


- Molecule 1: A118 serine integrase

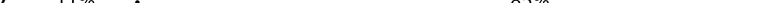


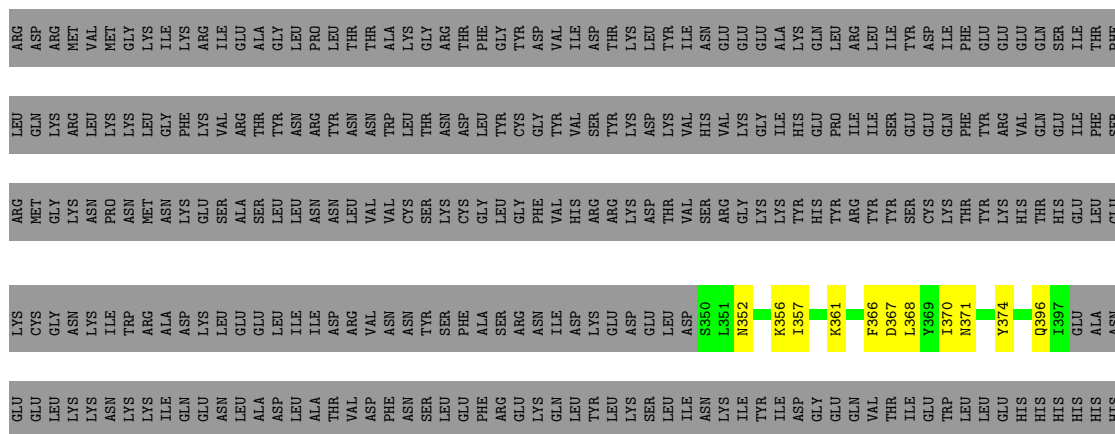
- Molecule 1: A118 serine integrase

Chain C: 12% . 87%

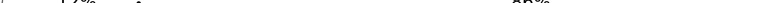


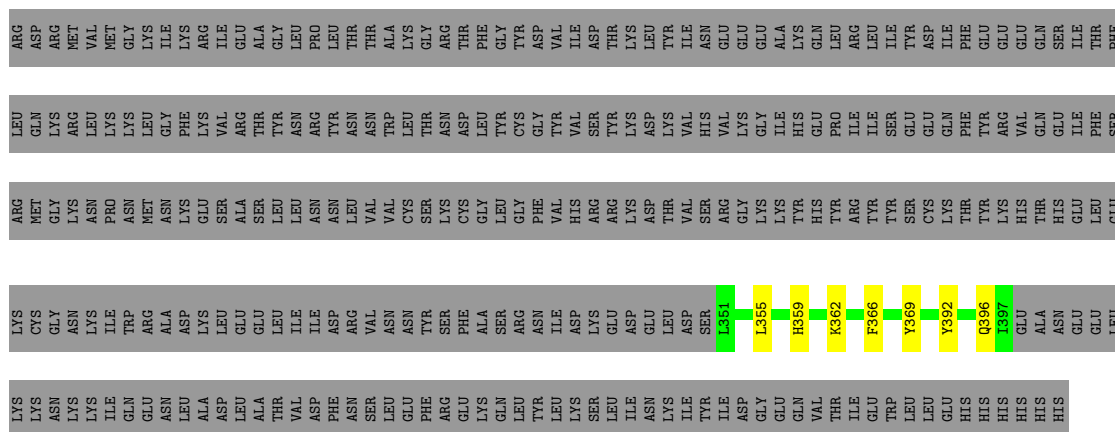
- Molecule 1: A118 serine integrase

Chain D:  11% . 85%



- Molecule 1: A118 serine integrase

Chain E:  12% . 86%



- Molecule 1: A118 serine integrase

HIS	A395	LYS	ARG	LEU	ARG
	Q396	CYS	MET	GLN	ASP
	I397	GLY	GLY	GLY	ARG
	GLU	ASN	LYS	ASN	MET
	ALA	LYS	ASN	LEU	VAL
	ASN	ILE	PRO	LYS	MET
	GLU	TRP	ASN	LYS	GLY
	GLU	ARG	MET	LEU	LYS
	LEU	ALA	ASN	PHE	ILE
	LEU	ASP	LYS	GLY	LYS
HIS	ASN	LYS	GLU	VAL	ARG
	ASN	LEU	ALA	ARG	ILE
	LYS	GLU	SER	THR	GLU
	LYS	GLU	LEU	THR	ALA
	ILE	LEU	LEU	ASN	GLY
	GLN	ILE	LEU	ASN	LEU
	GLU	ILE	ASN	TYR	PRO
	ASN	ASP	ASN	TYR	LEU
	LEU	ARG	LEU	ASN	THR
	ALA	VAL	VAL	ASN	THR
HIS	ASP	ASN	VAL	ASN	ALA
	ASP	ASN	VAL	TRP	ALA
	LEU	ASN	CYS	LEU	LYS
	ALA	TYR	SER	THR	GLY
	THR	SER	LYS	ASN	ARG
	VAL	PHE	CYS	ASP	THR
	ASP	ALA	GLY	LEU	PHE
	PHE	SER	LEU	TYR	GLY
	ASN	ARG	PHE	CYS	TYR
	SER	ASN	PHE	GLY	ASP
HIS	LEU	ILE	VAL	TYR	VAL
	LEU	ASP	HIS	VAL	ILE
	PHE	LYS	ARG	SER	ASP
	ARG	GLU	ARG	TYR	THR
	GLU	ASP	LYS	LYS	LYS
	LYS	GLU	ASP	ASP	LEU
	GLN	LEU	THR	LYS	TYR
	LEU	ASP	VAL	VAL	ILE
	TYR	S350	SER	HIS	ASN
	LEU	L351	ARG	VAL	GLU
HIS	LYS	GLY	LYS	GLU	GLU
	SER	K354	LYS	GLY	GLU
	LEU	K362	TYR	ILE	ALA
	ILE	ASN	HIS	HIS	LYS
	LYS	F366	TYR	PRO	GLN
	ILE	D367	ARG	ILE	LEU
	TYR	L368	TYR	SER	LEU
	ILE	Y369	TYR	ILE	ILE
	ASP	I370	SER	GLU	TYR
	GLY	K373	CYS	GLU	ASP
HIS	GLU	Y374	LYS	GLN	ILE
	GLN	E375	THR	PHE	PHE
	VAL	K378	TYR	TYR	GLU
	THR	ILE	LYS	ARG	GLU
	ILE	GLU	HIS	VAL	GLU
	GLU	Q389	THR	GLN	GLN
	TRP	I390	GLU	GLU	SER
	LEU	N391	LEU	ILE	ILE
	GLU	THR	THR	PHE	THR
	THR	GLN	GLU	STR	PHE

Chain G: 12% . 87%

[illegible]

Chain H: 15% 85%

LYS	CYS	ARG	LEU	ARG
GLY	GLY	MET	GLN	ASP
ASN	ASN	ARG	LYS	ARG
LYS	ASN	VAL	LEU	MET
ILE	PRO	ASN	LYS	MET
TRP	ASN	ASN	LYS	GLY
ARG	MET	ASN	LEU	LYS
ALA	ASN	ASN	GLY	ILE
ASP	LYS	LYS	PHE	LYS
LYS	GLU	SER	VAL	ARG
LEU	LEU	ALA	ARG	ILE
GLU	GLU	SER	THR	GLU
GLU	LEU	LEU	THR	ALA
ILE	LEU	LEU	ASN	GLY
ILE	ASN	ASN	ASN	LEU
ASP	LEU	ASN	THR	LEU
ARG	VAL	VAL	ASN	THR
VAL	ASN	VAL	ASN	THR
ASN	ASN	CYS	TRP	ALA
ASN	CYS	CYS	LEU	LYS
THR	LYS	SER	THR	GLY
SER	LYS	ASN	ASN	ARG
PHE	CYS	CYS	ASP	THR
ALA	GLY	GLY	LEU	PHE
SER	LEU	LEU	THR	GLY
ARG	PHE	GLY	CYS	THR
ASN	PHE	VAL	GLY	ASP
ILE	VAL	VAL	THR	VAL
ASP	HIS	VAL	VAL	ILE
LYS	LYS	ARG	SER	ASP
GLU	GLU	ARG	THR	THR
ASP	ASP	LYS	LYS	LYS
GLU	GLU	THR	ASP	LEU
LEU	ASP	VAL	LYS	THR
SER	SER	VAL	VAL	ILE
SER	SER	ARG	HIS	ASN
LEU	ARG	GLY	VAL	GLN
ILE	LYS	LYS	LYS	GLU
ILE	LYS	LYS	ILE	GLY
LYS	THR	THR	ILE	THR
LYS	THR	THR	SER	ILE
ASN	SER	SER	GLU	THR
LYS	CYS	CYS	GLN	ASP
LYS	LYS	LYS	GLN	ILE
ILE	ILE	THR	PHE	PHE
GLN	GLN	THR	THR	GLU
GLU	LYS	LYS	ARG	GLU
ASN	HIS	VAL	VAL	GLU
LEU	THR	THR	GLN	GLN
ALA	HIS	GLU	ILE	SER
ASP	GLU	GLU	ILE	ILE
LEU	LEU	THR	PHE	ILE
ILE	GLU	LEU	THR	THR
ALA	GLU	THR	SER	PHE

THR	VAL	ASP	PHE	ASN	SER	LEU	GLU	PHE	ARG	GLU	LYS	GLN	LEU	TYR	LEU	LYS	SER	LEU	ILE	ASN	LYS	ILE	TYR	ILE	ASP	GLY	GLU	GLN	VAL	THR	ILE	GLU	TRP	LEU	LEU	GLU	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	98.02Å 98.02Å 52.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.85 – 2.54 35.85 – 2.54	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.85-2.54) 95.3 (35.85-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.252 , 0.265 0.256 , 0.269	Depositor DCC
R_{free} test set	800 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	79.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 141.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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	0.24	0/403	0.67	0/539
1	B	0.24	0/411	0.68	0/550
1	C	0.24	0/364	0.68	0/488
1	D	0.24	0/403	0.66	0/539
1	E	0.24	0/397	0.66	0/531
1	F	0.25	0/403	0.69	0/539
1	G	0.24	0/358	0.67	0/478
1	H	0.24	0/403	0.64	0/539
All	All	0.24	0/3142	0.67	0/4203

There are no bond length outliers.

There are no bond angle outliers.

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	398	0	385	6	0
1	B	406	0	396	8	0
1	C	359	0	345	6	0
1	D	398	0	390	12	0
1	E	392	0	385	6	0
1	F	398	0	390	10	0
1	G	353	0	344	3	0
1	H	398	0	385	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	115	0	0	0	0
2	B	101	0	0	2	0
2	C	87	0	0	0	0
2	D	94	0	0	2	0
2	E	102	0	0	2	0
2	F	92	0	0	3	1
2	G	86	0	0	1	1
2	H	102	0	0	0	0
All	All	3881	0	3020	40	1

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 7.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ASP:O	1:D:371:ASN:ND2	2.26	0.69
1:A:364:ARG:NH1	1:B:369:TYR:O	2.29	0.62
1:B:363:LYS:NZ	2:B:502:HOH:O	2.32	0.62
1:C:364:ARG:NH2	1:D:374:TYR:O	2.36	0.59
1:B:398:GLU:OE1	1:F:350:SER:N	2.36	0.59
1:D:352:ASN:ND2	2:D:502:HOH:O	2.36	0.58
1:E:362:LYS:NZ	2:E:505:HOH:O	2.37	0.56
1:A:374:TYR:OH	1:B:380:ASP:OD1	2.23	0.53
1:F:368:LEU:O	1:F:373:SER:OG	2.27	0.52
1:A:369:TYR:HB3	1:D:361:LYS:HE2	1.92	0.51
1:F:366:PHE:O	1:F:370:ILE:HG12	2.11	0.51
1:C:385:ASP:OD1	1:G:384:ASN:ND2	2.42	0.50
1:F:375:GLU:N	1:F:378:GLU:OE1	2.45	0.48
1:F:389:GLN:NE2	2:F:503:HOH:O	2.42	0.48
1:F:362:LYS:NZ	2:F:502:HOH:O	2.34	0.48
1:A:376:VAL:HG11	1:D:357:ILE:HD13	1.95	0.48
1:E:355:LEU:O	1:E:359:HIS:ND1	2.46	0.47
1:G:354:LYS:NZ	2:G:506:HOH:O	2.36	0.47
1:F:354:LYS:NZ	2:F:505:HOH:O	2.48	0.46
1:D:356:LYS:HG2	1:E:392:TYR:HB2	1.98	0.46
1:B:353:GLU:O	1:B:357:ILE:HG12	2.16	0.46
1:F:391:ASN:O	1:F:395:ALA:N	2.49	0.45
1:B:356:LYS:NZ	2:B:505:HOH:O	2.49	0.45
1:A:362:LYS:HG2	1:D:368:LEU:HD21	1.98	0.45
1:D:356:LYS:NZ	2:D:504:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:HD13	1:D:366:PHE:CE1	2.52	0.44
1:C:364:ARG:HG2	1:D:370:ILE:HA	1.99	0.44
1:F:350:SER:O	1:F:354:LYS:N	2.51	0.44
1:C:375:GLU:HG2	1:C:376:VAL:H	1.83	0.44
1:D:357:ILE:HG22	1:D:361:LYS:HE3	2.01	0.43
1:B:395:ALA:O	1:B:397:ILE:N	2.51	0.43
1:E:366:PHE:HA	1:E:369:TYR:HD2	1.84	0.43
1:F:351:LEU:H	1:F:351:LEU:HD23	1.83	0.42
1:E:396:GLN:OE1	1:E:396:GLN:N	2.52	0.42
1:D:357:ILE:O	1:D:361:LYS:HG3	2.20	0.42
1:E:392:TYR:OH	2:E:501:HOH:O	2.21	0.41
1:B:386:ILE:O	1:B:390:ILE:HG13	2.20	0.41
1:A:362:LYS:HG3	1:A:383:MET:SD	2.60	0.41
1:G:358:GLU:HB3	1:G:386:ILE:HG23	2.03	0.40
1:C:365:LEU:HA	1:C:368:LEU:HD12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:508:HOH:O	2:G:516:HOH:O[3_565]	2.08	0.12

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	46/328 (14%)	43 (94%)	3 (6%)	0	100	100
1	B	47/328 (14%)	43 (92%)	3 (6%)	1 (2%)	5	5
1	C	42/328 (13%)	39 (93%)	3 (7%)	0	100	100
1	D	46/328 (14%)	44 (96%)	1 (2%)	1 (2%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	45/328 (14%)	43 (96%)	2 (4%)	0	100	100
1	F	46/328 (14%)	45 (98%)	1 (2%)	0	100	100
1	G	40/328 (12%)	40 (100%)	0	0	100	100
1	H	46/328 (14%)	45 (98%)	1 (2%)	0	100	100
All	All	358/2624 (14%)	342 (96%)	14 (4%)	2 (1%)	21	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLN
1	D	396	GLN

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	43/302 (14%)	43 (100%)	0	100	100
1	B	44/302 (15%)	44 (100%)	0	100	100
1	C	39/302 (13%)	39 (100%)	0	100	100
1	D	44/302 (15%)	44 (100%)	0	100	100
1	E	43/302 (14%)	43 (100%)	0	100	100
1	F	44/302 (15%)	43 (98%)	1 (2%)	44	62
1	G	39/302 (13%)	39 (100%)	0	100	100
1	H	43/302 (14%)	43 (100%)	0	100	100
All	All	339/2416 (14%)	338 (100%)	1 (0%)	86	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	390	ILE

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

Mol	Chain	Res	Type
1	E	371	ASN
1	E	389	GLN
1	H	384	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	48/328 (14%)	-1.44	0 100 100	76, 103, 139, 147	0
1	B	49/328 (14%)	-1.49	0 100 100	76, 100, 132, 162	0
1	C	44/328 (13%)	-1.54	0 100 100	78, 95, 111, 125	0
1	D	48/328 (14%)	-1.51	0 100 100	74, 90, 100, 101	0
1	E	47/328 (14%)	-1.47	0 100 100	78, 98, 120, 127	0
1	F	48/328 (14%)	-1.52	0 100 100	84, 99, 122, 131	0
1	G	42/328 (12%)	-1.39	0 100 100	80, 108, 128, 131	0
1	H	48/328 (14%)	-1.41	0 100 100	82, 91, 117, 135	0
All	All	374/2624 (14%)	-1.47	0 100 100	74, 96, 128, 162	0

There are no RSRZ outliers to report.

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.