

Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2024 – 10:08 AM JST

PDB ID	:	8ZJB
Title	:	Oomycete Nudix effectors display WY-Nudix conformations with mRNA de-
		capping activity
Authors	:	Xing, W.; Xing, W.
Deposited on	:	2024-05-14
Resolution	:	3.19 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.19 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R_{free}	130704	1133 (3.20-3.20)		
Clashscore	141614	1253 (3.20-3.20)		
Ramachandran outliers	138981	1234 (3.20-3.20)		
Sidechain outliers	138945	1233 (3.20-3.20)		
RSRZ outliers	127900	1095 (3.20-3.20)		

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	А	247	^{2%} 63%		29%	• 8%		
1	В	247	67%		25%	8%		
1	С	247	72%		20%	7%		
1	D	247	71%		20%	• 8%		
1	Е	247	2% 53%	14%	33%			
1	F	247	48%	17%	34%			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9168 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	228	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	A	220	1731	1102	303	318	8	0	0	0
1	р	222	Total	С	Ν	0	S	0	0	0
	D	220	1741	1107	303	323	8	0	0	U
1	C	C 229	Total	С	Ν	0	S	0	0	0
			1762	1120	310	324	8	0	0	0
1	П	228	Total	С	Ν	0	S	0	0	0
	D		1719	1095	296	320	8			U
1	Б	165	Total	С	Ν	0	S	0	0	0
		601	1140	721	201	213	5	0	0	0
1	Б	1.00	Total	С	Ν	0	S	0	0	0
	Г	103	1075	677	188	206	4	0	U	U

• Molecule 1 is a protein called Nudix hydrolase domain-containing protein.

There are 342 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	VAL	deletion	UNP G4Z7E8
А	?	-	ARG	deletion	UNP G4Z7E8
А	?	-	TYR	deletion	UNP G4Z7E8
А	?	-	ARG	deletion	UNP G4Z7E8
А	?	-	SER	deletion	UNP G4Z7E8
А	?	-	ASP	deletion	UNP G4Z7E8
А	?	-	ILE	deletion	UNP G4Z7E8
A	?	-	PHE	deletion	UNP G4Z7E8
А	?	-	ILE	deletion	UNP G4Z7E8
А	?	-	PHE	deletion	UNP G4Z7E8
А	?	-	TYR	deletion	UNP G4Z7E8
А	?	-	ARG	deletion	UNP G4Z7E8
A	?	-	TRP	deletion	UNP G4Z7E8
А	?	-	SER	deletion	UNP G4Z7E8
A	?	-	VAL	deletion	UNP G4Z7E8
A	?	_	LEU	deletion	UNP G4Z7E8
А	?	-	THR	deletion	UNP G4Z7E8



Chain	Residue	Modelled	Actual	Comment	Reference
А	?	-	LEU	deletion	UNP G4Z7E8
А	?	-	VAL	deletion	UNP G4Z7E8
А	?	-	MET	deletion	UNP G4Z7E8
А	?	-	ALA	deletion	UNP G4Z7E8
А	?	-	LEU	deletion	UNP G4Z7E8
А	?	-	GLN	deletion	UNP G4Z7E8
А	214	LEU	-	expression tag	UNP G4Z7E8
А	215	PRO	-	expression tag	UNP G4Z7E8
А	216	TRP	-	expression tag	UNP G4Z7E8
А	217	ASP	_	expression tag	UNP G4Z7E8
А	218	ASP	-	expression tag	UNP G4Z7E8
А	219	ALA	-	expression tag	UNP G4Z7E8
А	220	ILE	-	expression tag	UNP G4Z7E8
А	221	LEU	_	expression tag	UNP G4Z7E8
А	222	LEU	-	expression tag	UNP G4Z7E8
А	223	LEU	-	expression tag	UNP G4Z7E8
А	224	LYS	-	expression tag	UNP G4Z7E8
А	225	ALA	-	expression tag	UNP G4Z7E8
А	226	ASN	-	expression tag	UNP G4Z7E8
А	227	LYS	_	expression tag	UNP G4Z7E8
А	228	HIS	-	expression tag	UNP G4Z7E8
А	229	ASP	-	expression tag	UNP G4Z7E8
А	230	GLU	-	expression tag	UNP G4Z7E8
А	231	MET	_	expression tag	UNP G4Z7E8
А	232	VAL	-	expression tag	UNP G4Z7E8
А	233	GLU	-	expression tag	UNP G4Z7E8
А	234	ILE	-	expression tag	UNP G4Z7E8
А	235	VAL	-	expression tag	UNP G4Z7E8
А	236	LYS	-	expression tag	UNP G4Z7E8
А	237	GLN	-	expression tag	UNP G4Z7E8
А	238	ALA	-	expression tag	UNP G4Z7E8
А	239	ARG	-	expression tag	UNP G4Z7E8
А	240	ALA	-	expression tag	UNP G4Z7E8
А	241	ALA	-	expression tag	UNP G4Z7E8
А	242	ALA	-	expression tag	UNP G4Z7E8
А	243	ALA	-	expression tag	UNP G4Z7E8
А	244	ALA	-	expression tag	UNP G4Z7E8
А	245	LYS	-	expression tag	UNP G4Z7E8
А	246	ALA	-	expression tag	UNP G4Z7E8
А	247	ALA	-	expression tag	UNP G4Z7E8
В	?	-	VAL	deletion	UNP G4Z7E8
В	?	-	ARG	deletion	UNP G4Z7E8



Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	TYR	deletion	UNP G4Z7E8
В	?	-	ARG	deletion	UNP G4Z7E8
В	?	-	SER	deletion	UNP G4Z7E8
В	?	-	ASP	deletion	UNP G4Z7E8
В	?	-	ILE	deletion	UNP G4Z7E8
В	?	-	PHE	deletion	UNP G4Z7E8
В	?	-	ILE	deletion	UNP G4Z7E8
В	?	-	PHE	deletion	UNP G4Z7E8
В	?	-	TYR	deletion	UNP G4Z7E8
В	?	-	ARG	deletion	UNP G4Z7E8
В	?	-	TRP	deletion	UNP G4Z7E8
В	?	-	SER	deletion	UNP G4Z7E8
В	?	-	VAL	deletion	UNP G4Z7E8
В	?	-	LEU	deletion	UNP G4Z7E8
В	?	-	THR	deletion	UNP G4Z7E8
В	?	-	LEU	deletion	UNP G4Z7E8
В	?	-	VAL	deletion	UNP G4Z7E8
В	?	-	MET	deletion	UNP G4Z7E8
В	?	-	ALA	deletion	UNP G4Z7E8
В	?	-	LEU	deletion	UNP G4Z7E8
В	?	-	GLN	deletion	UNP G4Z7E8
В	214	LEU	-	expression tag	UNP G4Z7E8
В	215	PRO	-	expression tag	UNP G4Z7E8
В	216	TRP	-	expression tag	UNP G4Z7E8
В	217	ASP	-	expression tag	UNP G4Z7E8
В	218	ASP	-	expression tag	UNP G4Z7E8
В	219	ALA	-	expression tag	UNP G4Z7E8
В	220	ILE	-	expression tag	UNP G4Z7E8
В	221	LEU	-	expression tag	UNP G4Z7E8
В	222	LEU	-	expression tag	UNP G4Z7E8
В	223	LEU	-	expression tag	UNP G4Z7E8
В	224	LYS	-	expression tag	UNP G4Z7E8
В	225	ALA	-	expression tag	UNP G4Z7E8
В	226	ASN	-	expression tag	UNP G4Z7E8
В	227	LYS	-	expression tag	UNP G4Z7E8
В	228	HIS	-	expression tag	UNP G4Z7E8
B	229	ASP	_	expression tag	UNP G4Z7E8
В	230	GLU	-	expression tag	UNP G4Z7E8
В	231	MET	-	expression tag	UNP G4Z7E8
В	232	VAL	-	expression tag	UNP G4Z7E8
В	233	GLU	-	expression tag	UNP G4Z7E8
В	234	ILE	-	expression tag	UNP G4Z7E8



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Residue	Modelled	Actual	Comment	Reference
235	VAL	-	expression tag	UNP G4Z7E8
236	LYS	-	expression tag	UNP G4Z7E8
237	GLN	-	expression tag	UNP G4Z7E8
238	ALA	-	expression tag	UNP G4Z7E8
239	ARG	-	expression tag	UNP G4Z7E8
240	ALA	-	expression tag	UNP G4Z7E8
241	ALA	-	expression tag	UNP G4Z7E8
242	ALA	-	expression tag	UNP G4Z7E8
243	ALA	-	expression tag	UNP G4Z7E8
244	ALA	-	expression tag	UNP G4Z7E8
245	LYS	-	expression tag	UNP G4Z7E8
246	ALA	-	expression tag	UNP G4Z7E8
247	ALA	-	expression tag	UNP G4Z7E8
?	-	VAL	deletion	UNP G4Z7E8
?	-	ARG	deletion	UNP G4Z7E8
?	-	TYR	deletion	UNP G4Z7E8
?	-	ARG	deletion	UNP G4Z7E8
?	-	SER	deletion	UNP G4Z7E8
?	-	ASP	deletion	UNP G4Z7E8
?	-	ILE	deletion	UNP G4Z7E8
?	-	PHE	deletion	UNP G4Z7E8
?	_	ILE	deletion	UNP G4Z7E8
?	-	PHE	deletion	UNP G4Z7E8
?	_	TYR	deletion	UNP G4Z7E8
?	-	ARG	deletion	UNP G4Z7E8
?	_	TRP	deletion	UNP G4Z7E8
?	-	SER	deletion	UNP G4Z7E8
?	-	VAL	deletion	UNP G4Z7E8
?	-	LEU	deletion	UNP G4Z7E8
?	-	THR	deletion	UNP G4Z7E8
?	_	LEU	deletion	UNP G4Z7E8
?	-	VAL	deletion	UNP G4Z7E8
?	-	MET	deletion	UNP G4Z7E8
?	-	ALA	deletion	UNP G4Z7E8
?	-	LEU	deletion	UNP G4Z7E8
?	-	GLN	deletion	UNP G4Z7E8
214	LEU	-	expression tag	UNP G4Z7E8
215	PRO	-	expression tag	UNP G4Z7E8
216	TRP	-	expression tag	UNP G4Z7E8
217	ASP	-	expression tag	UNP G4Z7E8
218	ASP	-	expression tag	UNP G4Z7E8
219	ALA	-	expression tag	UNP G4Z7E8
	Residue 235 236 237 238 239 240 241 242 243 244 245 246 247 ?<	Residue Modelled 235 VAL 236 LYS 237 GLN 238 ALA 239 ARG 240 ALA 241 ALA 242 ALA 243 ALA 244 ALA 245 LYS 246 ALA 247 ALA 247 ALA 247 ALA 247 ALA 247 ALA ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? - ? <td>Residue Modelled Actual 235 VAL - 236 LYS - 237 GLN - 238 ALA - 239 ARG - 240 ALA - 241 ALA - 242 ALA - 243 ALA - 244 ALA - 245 LYS - 246 ALA - 247 ALA - 246 ALA - 247 ALA - ? - VAL ? - RG ? - TYR ? - SER ? - ILE ? - ILE ? - TYR ? - TYR ? - TYR ? -</td> <td>ResidueModelledActualComment235VAL-expression tag236LYS-expression tag237GLN-expression tag238ALA-expression tag239ARG-expression tag240ALA-expression tag241ALA-expression tag242ALA-expression tag243ALA-expression tag244ALA-expression tag245LYS-expression tag246ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag?-VALdeletion?-ARGdeletion?-ARGdeletion?-SERdeletion?-SERdeletion?-TYRdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-KAG</td>	Residue Modelled Actual 235 VAL - 236 LYS - 237 GLN - 238 ALA - 239 ARG - 240 ALA - 241 ALA - 242 ALA - 243 ALA - 244 ALA - 245 LYS - 246 ALA - 247 ALA - 246 ALA - 247 ALA - ? - VAL ? - RG ? - TYR ? - SER ? - ILE ? - ILE ? - TYR ? - TYR ? - TYR ? -	ResidueModelledActualComment235VAL-expression tag236LYS-expression tag237GLN-expression tag238ALA-expression tag239ARG-expression tag240ALA-expression tag241ALA-expression tag242ALA-expression tag243ALA-expression tag244ALA-expression tag245LYS-expression tag246ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag247ALA-expression tag?-VALdeletion?-ARGdeletion?-ARGdeletion?-SERdeletion?-SERdeletion?-TYRdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-TRPdeletion?-KAG



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Chain	Residue	Modelled	Actual	Comment	Reference
С	220	ILE	-	expression tag	UNP G4Z7E8
\mathbf{C}	221	LEU	-	expression tag	UNP G4Z7E8
С	222	LEU	-	expression tag	UNP G4Z7E8
\mathbf{C}	223	LEU	-	expression tag	UNP G4Z7E8
С	224	LYS	-	expression tag	UNP G4Z7E8
С	225	ALA	-	expression tag	UNP G4Z7E8
С	226	ASN	-	expression tag	UNP G4Z7E8
С	227	LYS	-	expression tag	UNP G4Z7E8
С	228	HIS	-	expression tag	UNP G4Z7E8
С	229	ASP	-	expression tag	UNP G4Z7E8
С	230	GLU	-	expression tag	UNP G4Z7E8
С	231	MET	-	expression tag	UNP G4Z7E8
С	232	VAL	-	expression tag	UNP G4Z7E8
С	233	GLU	-	expression tag	UNP G4Z7E8
С	234	ILE	-	expression tag	UNP G4Z7E8
С	235	VAL	-	expression tag	UNP G4Z7E8
С	236	LYS	-	expression tag	UNP G4Z7E8
С	237	GLN	-	expression tag	UNP G4Z7E8
С	238	ALA	-	expression tag	UNP G4Z7E8
С	239	ARG	-	expression tag	UNP G4Z7E8
С	240	ALA	-	expression tag	UNP G4Z7E8
С	241	ALA	-	expression tag	UNP G4Z7E8
С	242	ALA	_	expression tag	UNP G4Z7E8
С	243	ALA	-	expression tag	UNP G4Z7E8
С	244	ALA	-	expression tag	UNP G4Z7E8
С	245	LYS	_	expression tag	UNP G4Z7E8
С	246	ALA	-	expression tag	UNP G4Z7E8
С	247	ALA	_	expression tag	UNP G4Z7E8
D	?	-	VAL	deletion	UNP G4Z7E8
D	?	-	ARG	deletion	UNP G4Z7E8
D	?	_	TYR	deletion	UNP G4Z7E8
D	?	_	ARG	deletion	UNP G4Z7E8
D	?	_	SER	deletion	UNP G4Z7E8
D	?	_	ASP	deletion	UNP G4Z7E8
D	?	-	ILE	deletion	UNP G4Z7E8
D	?	-	PHE	deletion	UNP G4Z7E8
D	?	-	ILE	deletion	UNP G4Z7E8
D	?	-	PHE	deletion	UNP G4Z7E8
D	?	_	TYR	deletion	UNP G4Z7E8
D	?	-	ARG	deletion	UNP G4Z7E8
D	?	_	TRP	deletion	UNP G4Z7E8
D	?	-	SER	deletion	UNP G4Z7E8
	1	1	1		1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP G4Z7E8
D	?	-	LEU	deletion	UNP G4Z7E8
D	?	-	THR	deletion	UNP G4Z7E8
D	?	-	LEU	deletion	UNP G4Z7E8
D	?	-	VAL	deletion	UNP G4Z7E8
D	?	-	MET	deletion	UNP G4Z7E8
D	?	-	ALA	deletion	UNP G4Z7E8
D	?	-	LEU	deletion	UNP G4Z7E8
D	?	-	GLN	deletion	UNP G4Z7E8
D	214	LEU	-	expression tag	UNP G4Z7E8
D	215	PRO	-	expression tag	UNP G4Z7E8
D	216	TRP	-	expression tag	UNP G4Z7E8
D	217	ASP	-	expression tag	UNP G4Z7E8
D	218	ASP	-	expression tag	UNP G4Z7E8
D	219	ALA	-	expression tag	UNP G4Z7E8
D	220	ILE	-	expression tag	UNP G4Z7E8
D	221	LEU	-	expression tag	UNP G4Z7E8
D	222	LEU	-	expression tag	UNP G4Z7E8
D	223	LEU	-	expression tag	UNP G4Z7E8
D	224	LYS	-	expression tag	UNP G4Z7E8
D	225	ALA	-	expression tag	UNP G4Z7E8
D	226	ASN	-	expression tag	UNP G4Z7E8
D	227	LYS	-	expression tag	UNP G4Z7E8
D	228	HIS	-	expression tag	UNP G4Z7E8
D	229	ASP	-	expression tag	UNP G4Z7E8
D	230	GLU	-	expression tag	UNP G4Z7E8
D	231	MET	-	expression tag	UNP G4Z7E8
D	232	VAL	-	expression tag	UNP G4Z7E8
D	233	GLU	-	expression tag	UNP G4Z7E8
D	234	ILE	-	expression tag	UNP G4Z7E8
D	235	VAL	-	expression tag	UNP G4Z7E8
D	236	LYS	-	expression tag	UNP G4Z7E8
D	237	GLN	-	expression tag	UNP G4Z7E8
D	238	ALA	-	expression tag	UNP G4Z7E8
D	239	ARG	-	expression tag	UNP G4Z7E8
D	240	ALA	-	expression tag	UNP G4Z7E8
D	241	ALA	-	expression tag	UNP $\overline{G4Z7E8}$
D	242	ALA	-	expression tag	UNP G4Z7E8
D	243	ALA	-	expression tag	UNP $G4Z7E8$
D	244	ALA	-	expression tag	UNP $G4Z7\overline{E8}$
D	245	LYS	-	expression tag	UNP $G4Z7E8$
D	246	ALA	-	expression tag	UNP $G4Z7\overline{E8}$



Chain	Residue	Modelled	Actual	Comment	Reference
D	247	ALA	-	expression tag	UNP G4Z7E8
Е	?	-	VAL	deletion	UNP G4Z7E8
Е	?	-	ARG	deletion	UNP G4Z7E8
Е	?	_	TYR	deletion	UNP G4Z7E8
Е	?	-	ARG	deletion	UNP G4Z7E8
Е	?	-	SER	deletion	UNP G4Z7E8
Е	?	-	ASP	deletion	UNP G4Z7E8
Е	?	-	ILE	deletion	UNP G4Z7E8
Е	?	-	PHE	deletion	UNP G4Z7E8
Е	?	-	ILE	deletion	UNP G4Z7E8
Е	?	-	PHE	deletion	UNP G4Z7E8
E	?	-	TYR	deletion	UNP G4Z7E8
Е	?	-	ARG	deletion	UNP G4Z7E8
E	?	-	TRP	deletion	UNP G4Z7E8
E	?	-	SER	deletion	UNP G4Z7E8
E	?	-	VAL	deletion	UNP G4Z7E8
E	?	-	LEU	deletion	UNP G4Z7E8
E	?	-	THR	deletion	UNP G4Z7E8
E	?	-	LEU	deletion	UNP G4Z7E8
E	?	-	VAL	deletion	UNP G4Z7E8
E	?	-	MET	deletion	UNP G4Z7E8
E	?	-	ALA	deletion	UNP G4Z7E8
E	?	-	LEU	deletion	UNP G4Z7E8
E	?	-	GLN	deletion	UNP G4Z7E8
Ε	214	LEU	-	expression tag	UNP G4Z7E8
E	215	PRO	-	expression tag	UNP G4Z7E8
E	216	TRP	-	expression tag	UNP G4Z7E8
E	217	ASP	-	expression tag	UNP G4Z7E8
E	218	ASP	-	expression tag	UNP G4Z7E8
E	219	ALA	-	expression tag	UNP G4Z7E8
E	220	ILE	-	expression tag	UNP G4Z7E8
E	221	LEU	-	expression tag	UNP G4Z7E8
E	222	LEU	-	expression tag	UNP G4Z7E8
E	223	LEU	-	expression tag	UNP G4Z7E8
E	224	LYS	-	expression tag	UNP G4Z7E8
E	225	ALA	-	expression tag	UNP G4Z7E8
E	226	ASN	-	expression tag	UNP $G4Z7E8$
E	227	LYS	-	expression tag	UNP G4Z7E8
E	228	HIS	-	expression tag	UNP G4Z7E8
E	229	ASP	-	expression tag	UNP G4Z7E8
E	230	GLU	-	expression tag	UNP G4Z7E8
E	231	MET	-	expression tag	UNP $G4Z7E8$



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Chain	Residue	Modelled	Actual	Comment	Reference
E	232	VAL	-	expression tag	UNP G4Z7E8
Е	233	GLU	-	expression tag	UNP G4Z7E8
Е	234	ILE	-	expression tag	UNP G4Z7E8
Е	235	VAL	-	expression tag	UNP G4Z7E8
Е	236	LYS	-	expression tag	UNP G4Z7E8
Е	237	GLN	-	expression tag	UNP G4Z7E8
Е	238	ALA	_	expression tag	UNP G4Z7E8
Е	239	ARG	-	expression tag	UNP G4Z7E8
Е	240	ALA	-	expression tag	UNP G4Z7E8
Е	241	ALA	-	expression tag	UNP G4Z7E8
Е	242	ALA	-	expression tag	UNP G4Z7E8
Е	243	ALA	-	expression tag	UNP G4Z7E8
Е	244	ALA	-	expression tag	UNP G4Z7E8
Е	245	LYS	-	expression tag	UNP G4Z7E8
Е	246	ALA	-	expression tag	UNP G4Z7E8
Е	247	ALA	-	expression tag	UNP G4Z7E8
F	?	-	VAL	deletion	UNP G4Z7E8
F	?	-	ARG	deletion	UNP G4Z7E8
F	?	-	TYR	deletion	UNP G4Z7E8
F	?	-	ARG	deletion	UNP G4Z7E8
F	?	-	SER	deletion	UNP G4Z7E8
F	?	-	ASP	deletion	UNP G4Z7E8
F	?	-	ILE	deletion	UNP G4Z7E8
F	?	-	PHE	deletion	UNP G4Z7E8
F	?	-	ILE	deletion	UNP G4Z7E8
F	?	-	PHE	deletion	UNP G4Z7E8
F	?	-	TYR	deletion	UNP G4Z7E8
F	?	-	ARG	deletion	UNP G4Z7E8
F	?	-	TRP	deletion	UNP G4Z7E8
F	?	-	SER	deletion	UNP G4Z7E8
F	?	-	VAL	deletion	UNP G4Z7E8
F	?	-	LEU	deletion	UNP G4Z7E8
F	?	-	THR	deletion	UNP G4Z7E8
F	?	-	LEU	deletion	UNP G4Z7E8
F	?	-	VAL	deletion	UNP G4Z7E8
F	?	-	MET	deletion	UNP G4Z7E8
F	?	-	ALA	deletion	UNP G4Z7E8
F	?	-	LEU	deletion	UNP G4Z7E8
F	?	-	GLN	deletion	UNP G4Z7E8
F	214	LEU	-	expression tag	UNP G4Z7E8
F	215	PRO	-	expression tag	UNP G4Z7E8
F	216	TRP	-	expression tag	UNP G4Z7E8



Chain	Residue	Modelled	Actual	Comment	Reference
F	217	ASP	-	expression tag	UNP G4Z7E8
F	218	ASP	-	expression tag	UNP G4Z7E8
F	219	ALA	-	expression tag	UNP G4Z7E8
F	220	ILE	-	expression tag	UNP G4Z7E8
F	221	LEU	-	expression tag	UNP G4Z7E8
F	222	LEU	-	expression tag	UNP G4Z7E8
F	223	LEU	-	expression tag	UNP G4Z7E8
F	224	LYS	-	expression tag	UNP G4Z7E8
F	225	ALA	-	expression tag	UNP G4Z7E8
F	226	ASN	-	expression tag	UNP G4Z7E8
F	227	LYS	-	expression tag	UNP G4Z7E8
F	228	HIS	-	expression tag	UNP G4Z7E8
F	229	ASP	-	expression tag	UNP G4Z7E8
F	230	GLU	-	expression tag	UNP G4Z7E8
F	231	MET	-	expression tag	UNP G4Z7E8
F	232	VAL	-	expression tag	UNP G4Z7E8
F	233	GLU	-	expression tag	UNP G4Z7E8
F	234	ILE	-	expression tag	UNP G4Z7E8
F	235	VAL	-	expression tag	UNP G4Z7E8
F	236	LYS	-	expression tag	UNP G4Z7E8
F	237	GLN	-	expression tag	UNP G4Z7E8
F	238	ALA	-	expression tag	UNP G4Z7E8
F	239	ARG	-	expression tag	UNP G4Z7E8
F	240	ALA	-	expression tag	UNP G4Z7E8
F	241	ALA	-	expression tag	UNP G4Z7E8
F	242	ALA	-	expression tag	UNP G4Z7E8
F	243	ALA	-	expression tag	UNP G4Z7E8
F	244	ALA	-	expression tag	UNP G4Z7E8
F	245	LYS	-	expression tag	UNP G4Z7E8
F	246	ALA	-	expression tag	UNP G4Z7E8
F	247	ALA	-	expression tag	UNP G4Z7E8



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: Nudix hydrolase domain-containing protein



 \bullet Molecule 1: Nudix hydrolase domain-containing protein



• Molecule 1: Nudix hydrolase domain-containing protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.36Å 164.50Å 169.54Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	39.35 - 3.19	Depositor
Resolution (A)	43.92 - 3.19	EDS
% Data completeness	96.3 (39.35-3.19)	Depositor
(in resolution range)	95.6(43.92 - 3.19)	EDS
R _{merge}	0.14	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.81 (at 3.19 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
D D.	0.256 , 0.311	Depositor
Π, Π_{free}	0.255 , 0.311	DCC
R_{free} test set	1998 reflections (5.75%)	wwPDB-VP
Wilson B-factor $(Å^2)$	31.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 33.6	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9168	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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	
10101	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.61	0/1758	0.76	1/2369~(0.0%)
1	В	0.67	0/1768	0.75	0/2383
1	С	0.65	0/1789	0.79	1/2408~(0.0%)
1	D	0.61	2/1746~(0.1%)	0.76	3/2357~(0.1%)
1	Е	0.47	0/1153	0.70	0/1562
1	F	0.43	0/1088	0.70	1/1488~(0.1%)
All	All	0.60	2/9302~(0.0%)	0.75	6/12567~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Е	0	1
1	F	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	D	119	CYS	CB-SG	-6.54	1.71	1.82
1	D	174	VAL	CB-CG1	-6.51	1.39	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	26	PHE	CB-CG-CD2	-11.89	112.48	120.80
1	С	152	LEU	CA-CB-CG	8.52	134.90	115.30
1	F	152	LEU	CA-CB-CG	7.35	132.20	115.30
1	D	26	PHE	CB-CG-CD1	6.74	125.52	120.80
1	D	25	GLY	N-CA-C	5.32	126.41	113.10
1	А	134	LEU	CB-CG-CD2	-5.25	102.07	111.00



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Е	70	ASP	Peptide
1	F	150	GLY	Peptide

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	А	1731	0	1738	57	0
1	В	1741	0	1754	40	0
1	С	1762	0	1796	34	0
1	D	1719	0	1709	35	0
1	Е	1140	0	1018	22	0
1	F	1075	0	914	38	0
All	All	9168	0	8929	219	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 12.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:B:86:MET:SD	1:B:203:GLN:NE2	2.37	0.97
1:F:153:GLU:H	1:F:156:GLU:HG3	1.45	0.81
1:D:75:GLY:O	1:D:208:ARG:NH2	2.13	0.80
1:F:176:LYS:HA	1:F:195:MET:HG2	1.65	0.79
1:C:149:LYS:HD3	1:C:231:MET:HE3	1.65	0.77
1:A:94:ILE:HG22	1:A:203:GLN:HB3	1.65	0.77
1:A:11:LEU:HD12	1:A:71:TYR:CG	2.22	0.74
1:F:122:VAL:HG13	1:F:133:LEU:HB3	1.70	0.73
1:D:134:LEU:HD12	1:D:214:LEU:HD12	1.70	0.73
1:A:6:LYS:CB	1:A:142:LYS:HA	2.19	0.72
1:D:159:TYR:CE1	1:D:176:LYS:HB2	2.25	0.72
1:E:137:SER:HB2	1:E:144:ASP:HB3	1.72	0.72
1:E:64:GLU:OE1	1:E:67:ARG:HD2	1.92	0.70



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:212:VAL:HG13	1:B:214:LEU:HG	1.74	0.69
1:C:136:SER:HB2	1:C:210:LEU:HB2	1.76	0.68
1:D:27:THR:HG23	1:D:30:ALA:H	1.59	0.68
1:D:67:ARG:HH12	1:D:143:GLN:HG3	1.58	0.68
1:C:230:GLU:O	1:C:234:ILE:HD12	1.95	0.67
1:B:14:PHE:HD1	1:B:40:ARG:HD2	1.58	0.67
1:B:220:ILE:HG23	1:B:232:VAL:HG13	1.77	0.66
1:E:59:GLU:HG3	1:E:212:VAL:HB	1.76	0.66
1:C:170:GLY:O	1:C:211:ARG:NH1	2.28	0.66
1:A:180:LEU:HD11	1:A:238:ALA:HB2	1.78	0.66
1:D:136:SER:HB3	1:D:210:LEU:HB2	1.78	0.66
1:E:67:ARG:NH2	1:E:142:LYS:O	2.30	0.65
1:A:10:ILE:HD12	1:A:10:ILE:H	1.62	0.65
1:C:173:LYS:HB3	1:C:199:LYS:HB3	1.77	0.65
1:B:140:LEU:HD21	1:B:208:ARG:O	1.97	0.64
1:E:178:LYS:NZ	1:E:179:GLU:O	2.30	0.64
1:B:84:ARG:H	1:B:207:SER:HB2	1.63	0.63
1:C:41:VAL:O	1:C:45:MET:HG2	1.98	0.63
1:B:5:VAL:HG21	1:B:47:HIS:ND1	2.14	0.63
1:F:153:GLU:HB2	1:F:156:GLU:HG2	1.80	0.63
1:B:80:TYR:CE2	1:C:54:GLU:HG2	2.34	0.62
1:F:174:VAL:HG22	1:F:197:SER:HA	1.80	0.62
1:C:220:ILE:HG23	1:C:232:VAL:HG13	1.80	0.62
1:A:64:GLU:OE2	1:A:67:ARG:NH1	2.32	0.62
1:A:13:ILE:HG13	1:A:40:ARG:HH21	1.65	0.61
1:C:217:ASP:OD1	1:C:239:ARG:NH2	2.32	0.61
1:C:84:ARG:H	1:C:207:SER:HB2	1.64	0.61
1:D:204:TRP:CE2	1:D:207:SER:HA	2.35	0.61
1:B:15:VAL:HA	1:B:18:ALA:HB3	1.81	0.61
1:B:73:MET:HB2	1:B:74:LEU:HD12	1.83	0.60
1:D:45:MET:HE2	1:D:64:GLU:HG3	1.83	0.60
1:E:118:VAL:HG13	1:E:152:LEU:HD21	1.82	0.60
1:A:84:ARG:H	1:A:207:SER:HB2	1.66	0.60
1:C:176:LYS:NZ	1:C:179:GLU:OE2	2.24	0.60
1:E:124:ARG:NE	1:E:128:GLU:O	2.32	0.60
1:C:84:ARG:HB2	1:C:208:ARG:HD2	1.83	0.60
1:B:27:THR:HG23	1:B:30:ALA:H	1.66	0.60
1:B:58:LYS:O	1:B:62:THR:HG23	2.01	0.60
1:F:156:GLU:OE1	1:F:161:ALA:N	2.36	0.59
1:F:204:TRP:HZ3	1:F:211:ARG:HE	1.50	0.59
1:D:10:ILE:HD12	1:D:10:ILE:H	1.67	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:9:ASN:HB2	1:A:10:ILE:HD12	1.84	0.58
1:F:174:VAL:CG1	1:F:195:MET:HB3	2.33	0.58
1:F:174:VAL:HG13	1:F:196:ARG:O	2.04	0.58
1:A:60:LEU:HD23	1:A:212:VAL:HG21	1.86	0.57
1:A:212:VAL:HG13	1:A:214:LEU:HG	1.84	0.57
1:B:232:VAL:HG12	1:B:236:LYS:HE3	1.87	0.57
1:C:136:SER:HB3	1:C:210:LEU:H	1.69	0.56
1:C:61:ARG:O	1:C:65:THR:HG23	2.05	0.56
1:F:122:VAL:HG21	1:F:174:VAL:HG21	1.87	0.56
1:A:84:ARG:HB2	1:A:208:ARG:HD2	1.88	0.56
1:F:232:VAL:O	1:F:236:LYS:HG3	2.05	0.55
1:C:42:ASP:OD1	1:C:61:ARG:NH2	2.36	0.55
1:D:26:PHE:HE1	1:D:31:LEU:HD13	1.70	0.55
1:B:71:TYR:O	1:B:75:GLY:N	2.37	0.55
1:C:17:ARG:HH12	1:C:39:ARG:NH1	2.04	0.55
1:C:93:MET:HB3	1:C:202:GLU:HB3	1.87	0.55
1:F:121:VAL:HG21	1:F:238:ALA:HB1	1.88	0.55
1:E:204:TRP:CE3	1:E:207:SER:HA	2.42	0.54
1:A:115:ARG:HB2	1:A:188:LYS:HG2	1.89	0.54
1:E:204:TRP:HE3	1:E:206:GLU:O	1.90	0.54
1:B:187:ASP:N	1:B:187:ASP:OD1	2.40	0.54
1:B:67:ARG:NH2	1:B:142:LYS:O	2.41	0.53
1:E:118:VAL:CG1	1:E:152:LEU:HD21	2.39	0.53
1:F:121:VAL:HG21	1:F:238:ALA:CB	2.39	0.53
1:C:159:TYR:CZ	1:C:163:LYS:HD3	2.42	0.53
1:A:83:LEU:HD11	1:A:203:GLN:NE2	2.24	0.53
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.74	0.53
1:A:184:LEU:HD23	1:A:189:THR:HG22	1.91	0.53
1:A:58:LYS:HD3	1:A:58:LYS:C	2.30	0.52
1:D:120:ASN:OD1	1:D:162:ALA:HB1	2.09	0.52
1:F:204:TRP:CD1	1:F:206:GLU:HB3	2.44	0.52
1:D:118:VAL:HG13	1:D:152:LEU:HD11	1.92	0.51
1:A:98:LEU:CD1	1:D:83:LEU:HD21	2.40	0.51
1:B:14:PHE:CD1	1:B:40:ARG:HD2	2.42	0.51
1:F:174:VAL:HG11	1:F:195:MET:HB3	1.93	0.51
1:B:132:ILE:HD11	1:B:219:ALA:CB	2.41	0.51
1:C:11:LEU:HD13	1:C:71:TYR:CE1	2.45	0.51
1:D:53:SER:O	1:D:57:ILE:HG13	2.10	0.51
1:C:201:TYR:O	1:C:211:ARG:NH2	2.34	0.51
1:D:15:VAL:HA	1:D:18:ALA:HB3	1.93	0.51
1:F:153:GLU:H	1:F:156:GLU:CG	2.20	0.51



	lo de page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:184:LEU:CD2	1:A:189:THR:HG22	2.41	0.51	
1:F:200:VAL:HB	1:F:211:ARG:HH12	1.75	0.51	
1:A:27:THR:HB	1:A:30:ALA:H	1.75	0.50	
1:C:185:VAL:HG21	1:C:230:GLU:HB2	1.92	0.50	
1:A:11:LEU:HB3	1:A:71:TYR:CE1	2.47	0.50	
1:A:27:THR:HG22	1:A:29:ALA:H	1.77	0.50	
1:A:59:GLU:HG3	1:A:212:VAL:HG22	1.94	0.50	
1:A:14:PHE:HE2	1:A:72:ALA:HB2	1.76	0.50	
1:A:14:PHE:CE2	1:A:72:ALA:HB2	2.47	0.50	
1:C:28:ALA:HA	1:C:73:MET:HE3	1.93	0.50	
1:D:28:ALA:HB2	1:D:73:MET:HE2	1.94	0.50	
1:A:184:LEU:HD12	1:F:191:GLU:HB2	1.94	0.50	
1:D:26:PHE:CE1	1:D:31:LEU:HD13	2.46	0.50	
1:B:87:GLN:O	1:B:89:VAL:N	2.41	0.49	
1:C:192:SER:OG	1:C:234:ILE:HG12	2.12	0.49	
1:D:174:VAL:CG1	1:D:195:MET:HB3	2.42	0.49	
1:D:216:TRP:CD2	1:D:239:ARG:HG2	2.46	0.49	
1:A:159:TYR:CZ	1:A:163:LYS:HD3	2.48	0.49	
1:B:170:GLY:O	1:B:211:ARG:HD3	2.12	0.49	
1:A:11:LEU:HD12	1:A:71:TYR:CD2	2.48	0.49	
1:B:162:ALA:O	1:B:166:VAL:HG12	2.12	0.49	
1:E:132:ILE:H	1:E:214:LEU:H	1.60	0.49	
1:A:11:LEU:HB3	1:A:71:TYR:CZ	2.47	0.49	
1:A:48:TYR:OH	1:A:64:GLU:OE1	2.22	0.48	
1:A:146:ILE:HA	1:A:231:MET:HE3	1.94	0.48	
1:B:14:PHE:HD1	1:B:40:ARG:CD	2.25	0.48	
1:A:97:ASN:HB3	1:A:99:VAL:HG13	1.95	0.48	
1:A:159:TYR:CE1	1:A:176:LYS:HB2	2.48	0.48	
1:C:90:ASP:O	1:C:94:ILE:HG13	2.14	0.48	
1:A:117:VAL:HG11	1:A:190:TYR:CE2	2.49	0.48	
1:D:204:TRP:CZ2	1:D:207:SER:HA	2.49	0.48	
1:A:10:ILE:HA	1:A:13:ILE:HG12	1.97	0.47	
1:B:91:GLU:HA	1:B:94:ILE:HD12	1.96	0.47	
1:B:82:LEU:HD11	1:B:138:SER:HB2	1.97	0.47	
1:B:156:GLU:O	1:F:186:GLY:N	2.46	0.47	
1:D:194:LEU:HD21	1:D:242:ALA:HB2	1.96	0.47	
1:F:174:VAL:HG12	1:F:195:MET:HB3	1.95	0.47	
1:B:116:SER:HB3	1:F:184:LEU:HD13	1.96	0.47	
1:B:159:TYR:CZ	1:B:176:LYS:HB2	2.50	0.47	
1:D:14:PHE:HE2	1:D:72:ALA:HB2	1.79	0.47	
1:F:220:ILE:HG23	1:F:232:VAL:HG23	1.95	0.47	



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:B:84:ARG:HB2	1:B:208:ARG:HG2	1.97	0.47		
1:F:204:TRP:HZ3	1:F:211:ARG:NE	2.13	0.47		
1:F:137:SER:OG	1:F:138:SER:N	2.48	0.46		
1:A:138:SER:O	1:A:140:LEU:HD12	2.15	0.46		
1:C:17:ARG:HH22	1:C:39:ARG:HH12	1.64	0.46		
1:C:123:MET:HE2	1:C:194:LEU:HD11	1.97	0.46		
1:A:156:GLU:OE1	1:A:164:ARG:NH2	2.49	0.46		
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.72	0.45		
1:E:228:HIS:O	1:E:232:VAL:HG23	2.16	0.45		
1:A:185:VAL:HG12	1:F:157:ILE:HG22	1.97	0.45		
1:F:145:PHE:HB2	1:F:222:LEU:HD21	1.98	0.45		
1:F:159:TYR:CE1	1:F:176:LYS:HB3	2.51	0.45		
1:A:71:TYR:OH	1:A:76:PRO:HG3	2.16	0.45		
1:A:234:ILE:O	1:A:237:GLN:HB2	2.16	0.45		
1:D:159:TYR:CZ	1:D:163:LYS:HD2	2.52	0.45		
1:A:134:LEU:HD12	1:A:214:LEU:HD12	1.98	0.45		
1:D:42:ASP:OD1	1:D:61:ARG:NH1	2.39	0.45		
1:F:115:ARG:HA	1:F:188:LYS:HG3	1.99	0.45		
1:F:134:LEU:HD22	1:F:222:LEU:HD23	1.99	0.45		
1:A:93:MET:HB3	1:A:202:GLU:HB2	2.00	0.44		
1:B:53:SER:O	1:B:57:ILE:HG12	2.16	0.44		
1:E:137:SER:CB	1:E:144:ASP:HB3	2.45	0.44		
1:D:64:GLU:OE1	1:D:67:ARG:HD2	2.17	0.44		
1:A:194:LEU:HD21	1:A:242:ALA:HB2	2.00	0.44		
1:A:74:LEU:CD1	1:A:85:PRO:HD2	2.48	0.44		
1:A:71:TYR:CZ	1:A:76:PRO:HG3	2.53	0.44		
1:C:40:ARG:HG3	1:C:40:ARG:NH1	2.32	0.44		
1:E:230:GLU:O	1:E:234:ILE:HG13	2.18	0.44		
1:F:121:VAL:HG23	1:F:194:LEU:HA	1.99	0.43		
1:F:49:PRO:HG3	1:F:225:ALA:HB1	2.00	0.43		
1:B:7:LEU:HD22	1:B:44:VAL:HG12	2.00	0.43		
1:E:122:VAL:O	1:E:132:ILE:HA	2.18	0.43		
1:D:184:LEU:CD2	1:D:189:THR:HG22	2.49	0.43		
1:F:166:VAL:O	1:F:172:VAL:N	2.50	0.43		
1:D:15:VAL:O	1:D:19:LYS:N	2.24	0.43		
1:E:147:LEU:HD11	1:E:235:VAL:HG23	2.00	0.43		
1:A:120:ASN:OD1	1:A:162:ALA:HB1	2.19	0.43		
1:D:164:ARG:HG2	1:D:164:ARG:HH11	1.84	0.43		
1:A:74:LEU:HD13	1:A:85:PRO:HD2	2.00	0.43		
1:A:230:GLU:OE1	1:A:230:GLU:N	2.45	0.43		
1:F:134:LEU:HB2	1:F:212:VAL:HG23	2.01	0.43		



Interatomic Clash					
Atom-1	Atom-2	distance $(Å)$	overlap (Å)		
1:A:14:PHE:HB2	1:A:40:ARG:NE	2.34	0.42		
1:C:17:ARG:NH2	1:C:39:ARG:HH12	2.18	0.42		
1:F:119:CYS:SG	1:F:147:LEU:HD11	2.58	0.42		
1:B:78:ASP:OD2	1:B:80:TYR:HD2	2.01	0.42		
1:C:14:PHE:HZ	1:C:31:LEU:HD11	1.84	0.42		
1:D:45:MET:HE3	1:D:61:ARG:HA	2.01	0.42		
1:B:17:ARG:HG3	1:B:40:ARG:NH2	2.35	0.42		
1:F:121:VAL:HG23	1:F:121:VAL:O	2.19	0.42		
1:A:56:ALA:HB1	1:A:214:LEU:HD22	2.01	0.42		
1:B:115:ARG:HB3	1:B:188:LYS:CD	2.49	0.42		
1:F:49:PRO:HG3	1:F:225:ALA:CB	2.49	0.42		
1:A:168:GLU:O	1:A:204:TRP:HD1	2.03	0.42		
1:A:134:LEU:HA	1:A:134:LEU:HD23	1.85	0.42		
1:B:132:ILE:HD11	1:B:219:ALA:HB1	2.02	0.42		
1:B:164:ARG:O	1:B:168:GLU:HG3	2.20	0.42		
1:E:63:ALA:HB2	1:E:212:VAL:HG11	2.02	0.42		
1:B:115:ARG:HB3	1:B:188:LYS:HE3	2.01	0.42		
1:A:176:LYS:HD2	1:A:179:GLU:CG	2.50	0.41		
1:B:48:TYR:CZ	1:B:143:GLN:NE2	2.88	0.41		
1:E:124:ARG:HD3	1:E:130:GLY:N	2.35	0.41		
1:E:131:GLY:HA3	1:E:213:TRP:HB3	2.02	0.41		
1:A:136:SER:HA	1:A:144:ASP:O	2.20	0.41		
1:B:42:ASP:O	1:B:46:GLU:HG2	2.21	0.41		
1:B:56:ALA:CB	1:B:214:LEU:HD22	2.50	0.41		
1:E:172:VAL:HG23	1:E:174:VAL:HG13	2.01	0.41		
1:A:115:ARG:HD2	1:A:115:ARG:HA	1.54	0.41		
1:A:226:ASN:HB2	1:A:228:HIS:CD2	2.56	0.41		
1:B:194:LEU:HD13	1:B:238:ALA:HB1	2.03	0.41		
1:D:12:THR:O	1:D:16:GLN:HG3	2.21	0.41		
1:D:90:ASP:OD1	1:D:91:GLU:N	2.54	0.41		
1:A:27:THR:HG22	1:A:28:ALA:N	2.36	0.41		
1:C:216:TRP:CE2	1:C:239:ARG:HG3	2.56	0.41		
1:F:116:SER:HB3	1:F:152:LEU:HD23	2.03	0.41		
1:D:45:MET:CE	1:D:61:ARG:HA	2.51	0.40		
1:D:177:LEU:HA	1:D:177:LEU:HD12	1.86	0.40		
1:C:147:LEU:HD11	1:C:235:VAL:HG23	2.02	0.40		
1:C:14:PHE:HD1	1:C:40:ARG:HD2	1.86	0.40		
1:D:12:THR:O	1:D:15:VAL:HG22	2.22	0.40		
1:D:184:LEU:HD11	1:E:189:THR:HG22	2.03	0.40		
1:E:212:VAL:HG23	1:E:214:LEU:CD2	2.52	0.40		
1:F:147:LEU:HB2	1:F:148:PRO:HD2	2.03	0.40		



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Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD23	1:A:221:LEU:HD23	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	Perce	entiles
1	А	224/247~(91%)	206 (92%)	18 (8%)	0	100	100
1	В	224/247~(91%)	208~(93%)	16 (7%)	0	100	100
1	С	225/247~(91%)	207 (92%)	18 (8%)	0	100	100
1	D	224/247~(91%)	207~(92%)	17 (8%)	0	100	100
1	Е	155/247~(63%)	139 (90%)	15 (10%)	1 (1%)	25	64
1	F	159/247~(64%)	131 (82%)	27 (17%)	1 (1%)	25	64
All	All	1211/1482 (82%)	1098 (91%)	111 (9%)	2(0%)	47	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	94	ILE
1	F	207	SER

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	Perce	ntiles
1	А	173/198~(87%)	171~(99%)	2(1%)	71	88
1	В	177/198~(89%)	176~(99%)	1 (1%)	86	94
1	С	181/198 (91%)	181 (100%)	0	100	100
1	D	171/198~(86%)	171 (100%)	0	100	100
1	Ε	93/198~(47%)	93~(100%)	0	100	100
1	F	81/198 (41%)	81 (100%)	0	100	100
All	All	876/1188 (74%)	873 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	210	LEU
1	А	212	VAL
1	В	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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, 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	А	228/247~(92%)	-0.04	6 (2%) 56 40	15, 24, 53, 69	0
1	В	228/247~(92%)	-0.20	1 (0%) 92 89	12, 16, 35, 44	0
1	С	229/247~(92%)	-0.36	0 100 100	10, 13, 30, 40	0
1	D	228/247~(92%)	-0.18	1 (0%) 92 89	19, 26, 40, 54	0
1	Ε	165/247~(66%)	0.26	6 (3%) 42 27	26, 48, 74, 81	0
1	F	163/247~(65%)	0.34	8 (4%) 29 17	16, 45, 64, 68	0
All	All	1241/1482 (83%)	-0.06	22 (1%) 68 55	10, 26, 62, 81	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	63	ALA	3.9
1	F	138	SER	3.3
1	F	213	TRP	3.2
1	Е	130	GLY	2.9
1	А	25	GLY	2.7
1	F	62	THR	2.6
1	В	5	VAL	2.5
1	А	24	GLN	2.5
1	Е	123	MET	2.5
1	Ε	126	GLU	2.5
1	F	48	TYR	2.4
1	F	49	PRO	2.4
1	А	28	ALA	2.4
1	А	18	ALA	2.3
1	Е	125	SER	2.2
1	A	26	PHE	2.2
1	F	208	ARG	2.2
1	D	26	PHE	2.2
1	F	43	THR	2.1



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Mol	Chain	Res	Type	RSRZ
1	Е	131	GLY	2.1
1	Е	127	ALA	2.0
1	А	23	PRO	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 monosaccharides 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.

