



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:26 PM UTC

PDB ID : 8ZJB / pdb_00008zjb
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 ⓘ 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

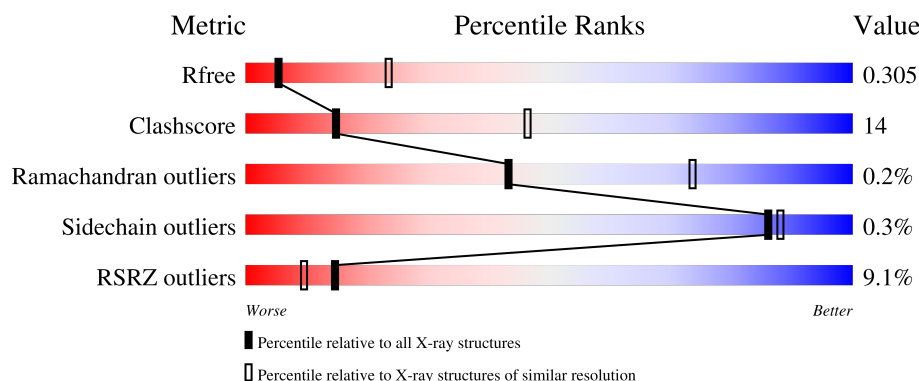
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	247	
1	B	247	
1	C	247	
1	D	247	
1	E	247	

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Mol	Chain	Length	Quality of chain
1	F	247	14% 47% 19% 34%

2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1731	1102	303	318	8			
1	B	228	Total	C	N	O	S	0	0	0
			1741	1107	303	323	8			
1	C	229	Total	C	N	O	S	0	0	0
			1762	1120	310	324	8			
1	D	228	Total	C	N	O	S	0	0	0
			1719	1095	296	320	8			
1	E	165	Total	C	N	O	S	0	0	0
			1140	721	201	213	5			
1	F	163	Total	C	N	O	S	0	0	0
			1075	677	188	206	4			

There are 342 discrepancies between the modelled and reference sequences:

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	235	VAL	-	expression tag	UNP G4Z7E8
B	236	LYS	-	expression tag	UNP G4Z7E8
B	237	GLN	-	expression tag	UNP G4Z7E8
B	238	ALA	-	expression tag	UNP G4Z7E8
B	239	ARG	-	expression tag	UNP G4Z7E8
B	240	ALA	-	expression tag	UNP G4Z7E8
B	241	ALA	-	expression tag	UNP G4Z7E8
B	242	ALA	-	expression tag	UNP G4Z7E8
B	243	ALA	-	expression tag	UNP G4Z7E8
B	244	ALA	-	expression tag	UNP G4Z7E8
B	245	LYS	-	expression tag	UNP G4Z7E8
B	246	ALA	-	expression tag	UNP G4Z7E8
B	247	ALA	-	expression tag	UNP G4Z7E8
C	?	-	VAL	deletion	UNP G4Z7E8
C	?	-	ARG	deletion	UNP G4Z7E8
C	?	-	TYR	deletion	UNP G4Z7E8
C	?	-	ARG	deletion	UNP G4Z7E8
C	?	-	SER	deletion	UNP G4Z7E8
C	?	-	ASP	deletion	UNP G4Z7E8
C	?	-	ILE	deletion	UNP G4Z7E8
C	?	-	PHE	deletion	UNP G4Z7E8
C	?	-	ILE	deletion	UNP G4Z7E8
C	?	-	PHE	deletion	UNP G4Z7E8
C	?	-	TYR	deletion	UNP G4Z7E8
C	?	-	ARG	deletion	UNP G4Z7E8
C	?	-	TRP	deletion	UNP G4Z7E8
C	?	-	SER	deletion	UNP G4Z7E8
C	?	-	VAL	deletion	UNP G4Z7E8
C	?	-	LEU	deletion	UNP G4Z7E8
C	?	-	THR	deletion	UNP G4Z7E8
C	?	-	LEU	deletion	UNP G4Z7E8
C	?	-	VAL	deletion	UNP G4Z7E8
C	?	-	MET	deletion	UNP G4Z7E8
C	?	-	ALA	deletion	UNP G4Z7E8
C	?	-	LEU	deletion	UNP G4Z7E8
C	?	-	GLN	deletion	UNP G4Z7E8
C	214	LEU	-	expression tag	UNP G4Z7E8
C	215	PRO	-	expression tag	UNP G4Z7E8
C	216	TRP	-	expression tag	UNP G4Z7E8
C	217	ASP	-	expression tag	UNP G4Z7E8
C	218	ASP	-	expression tag	UNP G4Z7E8
C	219	ALA	-	expression tag	UNP G4Z7E8

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

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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 G4Z7E8
D	242	ALA	-	expression tag	UNP G4Z7E8
D	243	ALA	-	expression tag	UNP G4Z7E8
D	244	ALA	-	expression tag	UNP G4Z7E8
D	245	LYS	-	expression tag	UNP G4Z7E8
D	246	ALA	-	expression tag	UNP G4Z7E8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	247	ALA	-	expression tag	UNP G4Z7E8
E	?	-	VAL	deletion	UNP G4Z7E8
E	?	-	ARG	deletion	UNP G4Z7E8
E	?	-	TYR	deletion	UNP G4Z7E8
E	?	-	ARG	deletion	UNP G4Z7E8
E	?	-	SER	deletion	UNP G4Z7E8
E	?	-	ASP	deletion	UNP G4Z7E8
E	?	-	ILE	deletion	UNP G4Z7E8
E	?	-	PHE	deletion	UNP G4Z7E8
E	?	-	ILE	deletion	UNP G4Z7E8
E	?	-	PHE	deletion	UNP G4Z7E8
E	?	-	TYR	deletion	UNP G4Z7E8
E	?	-	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
E	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
E	233	GLU	-	expression tag	UNP G4Z7E8
E	234	ILE	-	expression tag	UNP G4Z7E8
E	235	VAL	-	expression tag	UNP G4Z7E8
E	236	LYS	-	expression tag	UNP G4Z7E8
E	237	GLN	-	expression tag	UNP G4Z7E8
E	238	ALA	-	expression tag	UNP G4Z7E8
E	239	ARG	-	expression tag	UNP G4Z7E8
E	240	ALA	-	expression tag	UNP G4Z7E8
E	241	ALA	-	expression tag	UNP G4Z7E8
E	242	ALA	-	expression tag	UNP G4Z7E8
E	243	ALA	-	expression tag	UNP G4Z7E8
E	244	ALA	-	expression tag	UNP G4Z7E8
E	245	LYS	-	expression tag	UNP G4Z7E8
E	246	ALA	-	expression tag	UNP G4Z7E8
E	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

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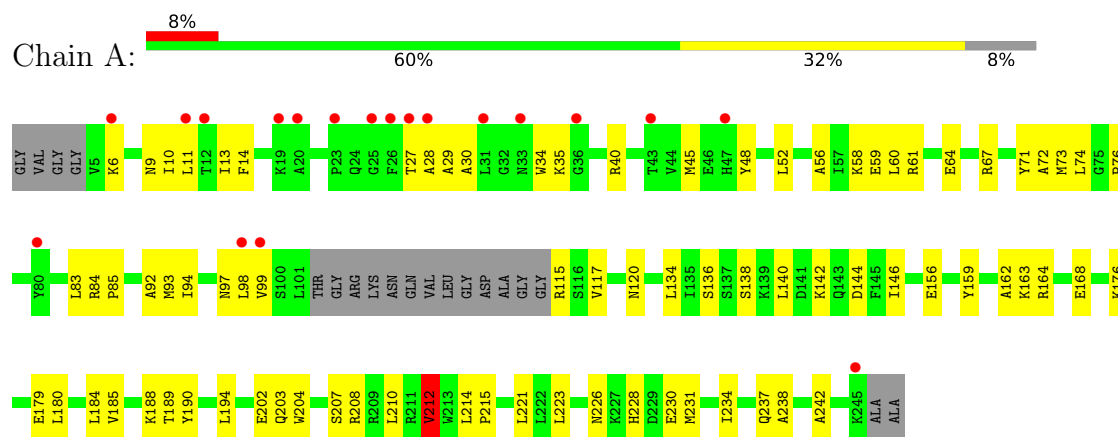
Continued from previous page...

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

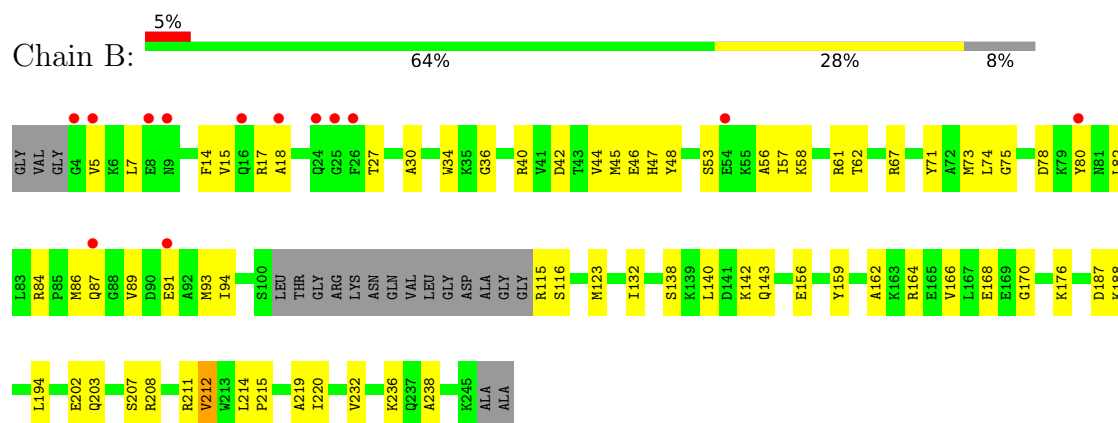
3 Residue-property plots [i](#)

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.

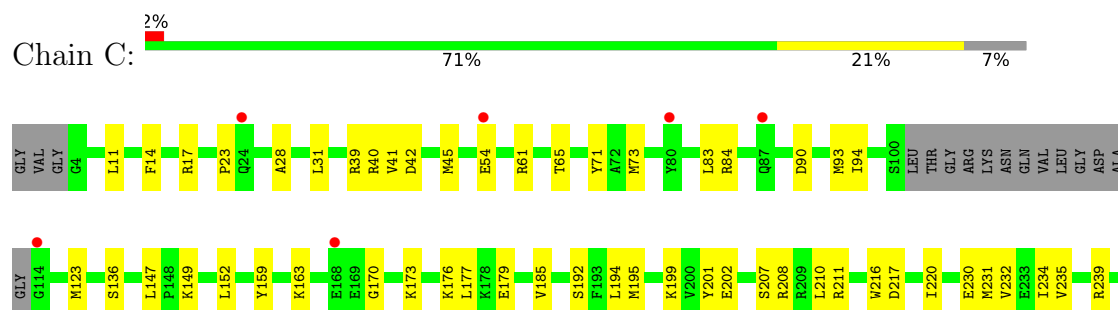
- Molecule 1: Nudix hydrolase domain-containing protein



- Molecule 1: Nudix hydrolase domain-containing protein



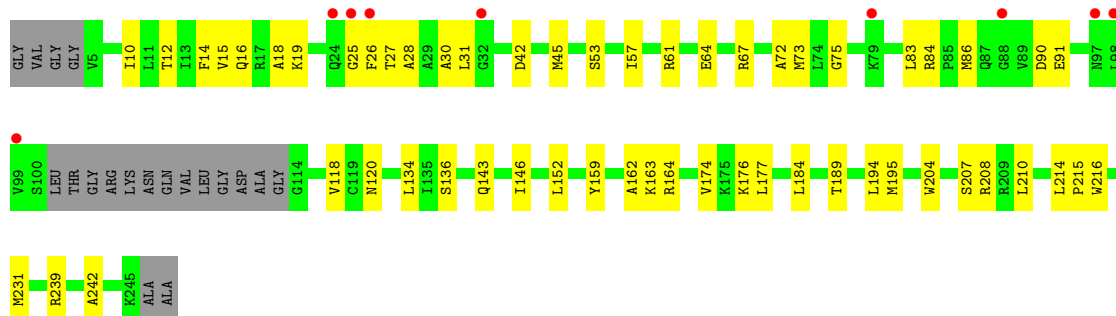
- Molecule 1: Nudix hydrolase domain-containing protein





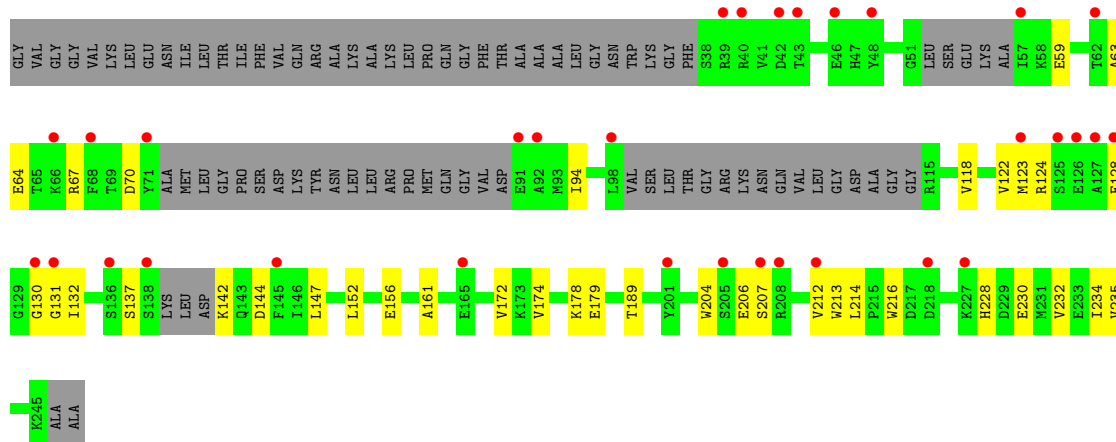
- Molecule 1: Nudix hydrolase domain-containing protein

Chain D: 4% 70% 23% 8%



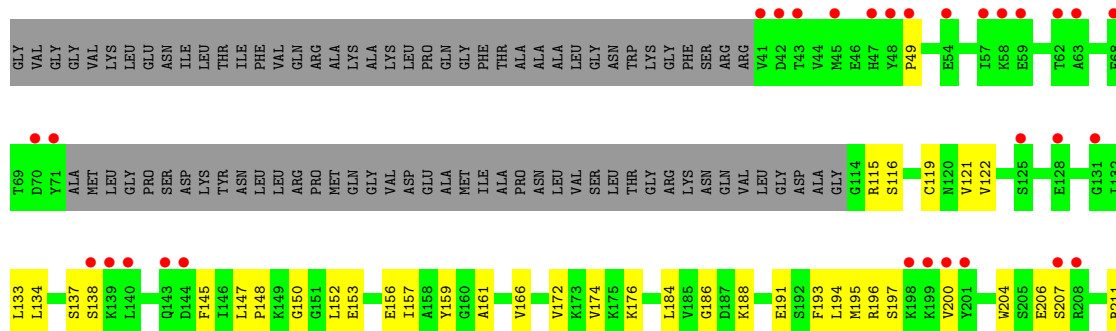
- Molecule 1: Nudix hydrolase domain-containing protein

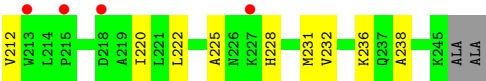
Chain E: 13% 51% 15% 33%



- Molecule 1: Nudix hydrolase domain-containing protein

Chain F: 14% 47% 19% 34%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.36Å 164.50Å 169.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.35 – 3.19 39.35 – 3.19	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.35-3.19) 95.5 (39.35-3.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.256 , 0.311 0.252 , 0.305	Depositor DCC
R_{free} test set	1998 reflections (5.72%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	2/1758 (0.1%)	0.80	0/2369
1	B	0.62	1/1768 (0.1%)	0.81	0/2383
1	C	0.60	0/1789	0.83	2/2408 (0.1%)
1	D	0.52	0/1746	0.73	1/2357 (0.0%)
1	E	0.42	0/1153	0.73	0/1562
1	F	0.40	0/1088	0.74	0/1488
All	All	0.55	3/9302 (0.0%)	0.78	3/12567 (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	E	0	1
1	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	PRO	C-O	-6.97	1.15	1.23
1	B	215	PRO	C-O	-5.54	1.17	1.23
1	A	212	VAL	C-O	-5.39	1.18	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	PRO	CB-CA-C	-5.58	104.25	111.39
1	D	25	GLY	N-CA-C	5.58	126.41	113.18
1	C	152	LEU	CA-CB-CG	5.32	134.90	116.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1731	0	1738	64	0
1	B	1741	0	1754	45	0
1	C	1762	0	1796	40	0
1	D	1719	0	1709	38	0
1	E	1140	0	1018	27	0
1	F	1075	0	914	43	0
All	All	9168	0	8929	250	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 14.

All (250) 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: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: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:A:223:LEU:HD22	1:A:231:MET:HE3	1.69	0.73
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:C:123:MET:HE2	1:C:194:LEU:HD11	1.72	0.71
1:C:147:LEU:HB2	1:C:231:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLU:OE1	1:E:67:ARG:HD2	1.92	0.70
1:C:28:ALA:HA	1:C:73:MET:HE3	1.74	0.70
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:B:93:MET:HE3	1:B:202:GLU:HG3	1.81	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: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:D:45:MET:HE2	1:D:64:GLU:HG3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:GLU:OE1	1:F:161:ALA:N	2.36	0.59
1:A:92:ALA:O	1:A:93:MET:HE2	2.03	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
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:A:58:LYS:HD3	1:A:58:LYS:C	2.30	0.57
1:C:93:MET:HE3	1:C:202:GLU:HB2	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:D:120:ASN:OD1	1:D:162:ALA:HB1	2.09	0.52
1:F:159:TYR:HE1	1:F:195:MET:HE2	1.74	0.52
1:F:204:TRP:CD1	1:F:206:GLU:HB3	2.44	0.52
1:F:159:TYR:CE1	1:F:195:MET:HE2	2.45	0.52
1:B:34:TRP:CD1	1:B:36:GLY:H	2.28	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:45:MET:HE3	1:D:61:ARG:HA	1.92	0.51
1:F:153:GLU:H	1:F:156:GLU:CG	2.20	0.51
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:A:184:LEU:HD12	1:F:191:GLU:HB2	1.94	0.50
1:C:149:LYS:HD3	1:C:231:MET:HE3	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: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:B:45:MET:HE2	1:B:61:ARG:HB2	1.95	0.48
1:D:28:ALA:HB2	1:D:73:MET:HE2	1.97	0.47
1:A:10:ILE:HA	1:A:13:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:124:ARG:HH11	1:E:213:TRP:CG	2.33	0.47
1:F:220:ILE:HG23	1:F:232:VAL:HG23	1.95	0.47
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:D:84:ARG:HD3	1:D:86:MET:HE2	1.97	0.47
1:A:45:MET:HE2	1:A:61:ARG:HB2	1.98	0.46
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:149:LYS:HD3	1:C:231:MET:CE	2.45	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:C:123:MET:HE2	1:C:194:LEU:CD1	2.44	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:B:5:VAL:HG21	1:B:47:HIS:HD1	1.81	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:C:159:TYR:HE1	1:C:195:MET:HE2	1.81	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:E:213:TRP:C	1:E:214:LEU:HD22	2.43	0.44
1:D:64:GLU:OE1	1:D:67:ARG:HD2	2.17	0.44
1:E:123:MET:HE2	1:E:216:TRP:CZ2	2.52	0.44
1:A:228:HIS:HB3	1:A:231:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:123:MET:HE2	1:E:216:TRP:HZ2	1.83	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:A:34:TRP:CD1	1:A:35:LYS:H	2.37	0.43
1:F:49:PRO:HG3	1:F:225:ALA:HB1	2.00	0.43
1:F:228:HIS:HB3	1:F:231:MET:HE2	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:A:146:ILE:CB	1:A:231:MET:HE1	2.48	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
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:B:123:MET:HE2	1:B:123:MET:HB3	1.87	0.42
1:F:119:CYS:SG	1:F:147:LEU:HD11	2.58	0.42
1:A:73:MET:HE3	1:A:73:MET:HB3	1.59	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: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:D:215:PRO:O	1:D:216:TRP:C	2.61	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:E:156:GLU:CD	1:E:161:ALA:HB2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:146:ILE:HB	1:A:231:MET:HE1	2.02	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:146:ILE:HB	1:D:231:MET:HE1	2.03	0.40
1:D:177:LEU:HA	1:D:177:LEU:HD12	1.86	0.40
1:F:193:PHE:CB	1:F:195:MET:HE3	2.51	0.40
1:C:147:LEU:HD11	1:C:235:VAL:HG23	2.02	0.40
1:C:83:LEU:C	1:C:83:LEU:HD23	2.47	0.40
1:F:174:VAL:HG13	1:F:196:ARG:C	2.45	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
1:A:52:LEU:HD23	1:A:221:LEU:HD23	2.03	0.40
1:D:45:MET:CE	1:D:61:ARG:HA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/247 (91%)	206 (92%)	18 (8%)	0	100	100
1	B	224/247 (91%)	208 (93%)	16 (7%)	0	100	100
1	C	225/247 (91%)	207 (92%)	18 (8%)	0	100	100
1	D	224/247 (91%)	207 (92%)	17 (8%)	0	100	100
1	E	155/247 (63%)	139 (90%)	15 (10%)	1 (1%)	21	56
1	F	159/247 (64%)	131 (82%)	27 (17%)	1 (1%)	21	56
All	All	1211/1482 (82%)	1098 (91%)	111 (9%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

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

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	173/198 (87%)	171 (99%)	2 (1%)	63	79
1	B	177/198 (89%)	176 (99%)	1 (1%)	78	84
1	C	181/198 (91%)	181 (100%)	0	100	100
1	D	171/198 (86%)	171 (100%)	0	100	100
1	E	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%)	86	88

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

Mol	Chain	Res	Type
1	A	210	LEU
1	A	212	VAL
1	B	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	HIS
1	C	81	ASN
1	C	226	ASN
1	D	47	HIS

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	228/247 (92%)	0.68	19 (8%)	17 11	15, 24, 53, 69	0
1	B	228/247 (92%)	0.41	13 (5%)	29 19	12, 16, 35, 44	0
1	C	229/247 (92%)	0.21	6 (2%)	57 37	10, 13, 30, 40	0
1	D	228/247 (92%)	0.55	9 (3%)	43 27	19, 26, 40, 54	0
1	E	165/247 (66%)	1.25	32 (19%)	3 2	26, 48, 74, 81	0
1	F	163/247 (65%)	1.23	34 (20%)	2 2	16, 45, 64, 68	0
All	All	1241/1482 (83%)	0.67	113 (9%)	15 9	10, 26, 62, 81	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	TYR	4.0
1	F	125	SER	4.0
1	E	123	MET	3.8
1	F	201	TYR	3.7
1	E	127	ALA	3.7
1	F	42	ASP	3.6
1	B	25	GLY	3.6
1	F	71	TYR	3.5
1	F	138	SER	3.5
1	A	99	VAL	3.5
1	D	99	VAL	3.4
1	E	125	SER	3.3
1	E	42	ASP	3.3
1	C	87	GLN	3.3
1	B	16	GLN	3.2
1	E	126	GLU	3.2
1	F	54	GLU	3.2
1	F	47	HIS	3.2
1	D	25	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	63	ALA	3.2
1	E	205	SER	3.1
1	D	26	PHE	3.1
1	A	23	PRO	3.1
1	F	43	THR	3.1
1	E	48	TYR	3.1
1	E	57	ILE	3.0
1	B	80	TYR	3.0
1	E	128	GLU	3.0
1	A	31	LEU	2.9
1	B	91	GLU	2.9
1	F	213	TRP	2.9
1	A	33	ASN	2.9
1	F	128	GLU	2.9
1	E	68	PHE	2.9
1	E	138	SER	2.8
1	B	54	GLU	2.8
1	F	62	THR	2.8
1	A	26	PHE	2.8
1	A	12	THR	2.8
1	E	91	GLU	2.8
1	F	68	PHE	2.8
1	F	41	VAL	2.8
1	F	143	GLN	2.7
1	E	201	TYR	2.7
1	A	11	LEU	2.7
1	E	136	SER	2.7
1	F	227	LYS	2.7
1	D	24	GLN	2.7
1	E	98	LEU	2.7
1	F	70	ASP	2.7
1	F	144	ASP	2.7
1	F	59	GLU	2.6
1	B	5	VAL	2.6
1	F	45	MET	2.6
1	E	207	SER	2.6
1	B	9	ASN	2.5
1	A	27	THR	2.5
1	E	39	ARG	2.5
1	A	19	LYS	2.5
1	B	87	GLN	2.5
1	F	200	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	208	ARG	2.5
1	A	20	ALA	2.4
1	C	114	GLY	2.4
1	E	227	LYS	2.4
1	A	25	GLY	2.4
1	D	32	GLY	2.4
1	E	130	GLY	2.4
1	A	28	ALA	2.4
1	A	6	LYS	2.4
1	A	98	LEU	2.4
1	E	165	GLU	2.4
1	E	212	VAL	2.4
1	E	131	GLY	2.4
1	F	48	TYR	2.4
1	A	245	LYS	2.3
1	E	145	PHE	2.3
1	A	36	GLY	2.3
1	E	40	ARG	2.3
1	F	131	GLY	2.3
1	E	218	ASP	2.3
1	D	79	LYS	2.3
1	E	208	ARG	2.3
1	B	8	GLU	2.3
1	C	80	TYR	2.2
1	E	66	LYS	2.2
1	F	218	ASP	2.2
1	B	24	GLN	2.2
1	B	26	PHE	2.2
1	A	47	HIS	2.2
1	E	62	THR	2.2
1	F	207	SER	2.2
1	D	97	ASN	2.2
1	F	139	LYS	2.2
1	F	58	LYS	2.2
1	C	24	GLN	2.1
1	B	4	GLY	2.1
1	C	54	GLU	2.1
1	F	49	PRO	2.1
1	F	140	LEU	2.1
1	A	43	THR	2.1
1	E	43	THR	2.1
1	E	71	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	46	GLU	2.1
1	F	215	PRO	2.1
1	D	98	LEU	2.0
1	B	18	ALA	2.0
1	E	92	ALA	2.0
1	C	168	GLU	2.0
1	F	198	LYS	2.0
1	F	199	LYS	2.0
1	D	88	GLY	2.0
1	F	57	ILE	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.