



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 07:19 PM EST

PDB ID : 4NWW
Title : Crystal structure of an N-terminally truncated capsid protein mutant of Orsay virus
Authors : Tao, Y.J.; Guo, Y.R.
Deposited on : 2013-12-06
Resolution : 3.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

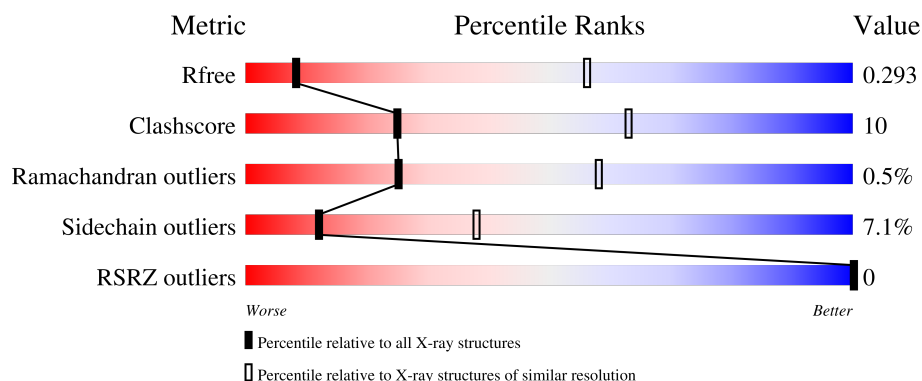
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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}	164625	1256 (3.92-3.60)
Clashscore	180529	1321 (3.92-3.60)
Ramachandran outliers	177936	1293 (3.92-3.60)
Sidechain outliers	177891	1288 (3.92-3.60)
RSRZ outliers	164620	1256 (3.92-3.60)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	358	72% 22% • 5%
1	B	358	73% 21% • •
1	C	358	74% 20% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8019 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2650	1703	443	498	6			
1	B	345	Total	C	N	O	S	0	0	0
			2683	1726	447	504	6			
1	C	345	Total	C	N	O	S	0	0	0
			2683	1726	447	504	6			

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLY	-	expression tag	UNP E9KNV5
A	42	THR	-	expression tag	UNP E9KNV5
A	43	THR	-	expression tag	UNP E9KNV5
A	44	SER	-	expression tag	UNP E9KNV5
A	45	SER	-	expression tag	UNP E9KNV5
A	46	ASN	-	expression tag	UNP E9KNV5
A	47	SER	-	expression tag	UNP E9KNV5
A	48	ILE	-	expression tag	UNP E9KNV5
A	49	LEU	-	expression tag	UNP E9KNV5
A	50	LEU	-	expression tag	UNP E9KNV5
A	51	LYS	-	expression tag	UNP E9KNV5
A	52	GLY	-	expression tag	UNP E9KNV5
A	53	CYS	-	expression tag	UNP E9KNV5
A	54	ASP	-	expression tag	UNP E9KNV5
A	55	ARG	-	expression tag	UNP E9KNV5
A	56	ILE	-	expression tag	UNP E9KNV5
A	57	VAL	-	expression tag	UNP E9KNV5
A	58	THR	-	expression tag	UNP E9KNV5
A	59	VAL	-	expression tag	UNP E9KNV5
A	60	VAL	-	expression tag	UNP E9KNV5
A	61	ASP	-	expression tag	UNP E9KNV5
A	62	ALA	-	expression tag	UNP E9KNV5
A	63	SER	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	64	THR	-	expression tag	UNP E9KNV5
A	65	TYR	-	expression tag	UNP E9KNV5
A	66	ASP	-	expression tag	UNP E9KNV5
A	67	ALA	-	expression tag	UNP E9KNV5
A	68	GLY	-	expression tag	UNP E9KNV5
A	69	SER	-	expression tag	UNP E9KNV5
A	70	ALA	-	expression tag	UNP E9KNV5
A	71	ILE	-	expression tag	UNP E9KNV5
A	72	VAL	-	expression tag	UNP E9KNV5
A	73	SER	-	expression tag	UNP E9KNV5
A	74	ILE	-	expression tag	UNP E9KNV5
A	75	PRO	-	expression tag	UNP E9KNV5
A	76	ILE	-	expression tag	UNP E9KNV5
A	77	THR	-	expression tag	UNP E9KNV5
A	78	PRO	-	expression tag	UNP E9KNV5
A	79	ASP	-	expression tag	UNP E9KNV5
A	80	ILE	-	expression tag	UNP E9KNV5
A	81	ALA	-	expression tag	UNP E9KNV5
A	82	TYR	-	expression tag	UNP E9KNV5
A	83	ARG	-	expression tag	UNP E9KNV5
A	84	LEU	-	expression tag	UNP E9KNV5
A	85	GLY	-	expression tag	UNP E9KNV5
A	86	SER	-	expression tag	UNP E9KNV5
A	87	THR	-	expression tag	UNP E9KNV5
A	88	ALA	-	expression tag	UNP E9KNV5
A	89	ARG	-	expression tag	UNP E9KNV5
A	90	THR	-	expression tag	UNP E9KNV5
A	91	PHE	-	expression tag	UNP E9KNV5
A	92	GLN	-	expression tag	UNP E9KNV5
A	93	ARG	-	expression tag	UNP E9KNV5
A	94	ILE	-	expression tag	UNP E9KNV5
A	95	LYS	-	expression tag	UNP E9KNV5
A	96	TYR	-	expression tag	UNP E9KNV5
A	97	ARG	-	expression tag	UNP E9KNV5
A	98	SER	-	expression tag	UNP E9KNV5
A	99	LEU	-	expression tag	UNP E9KNV5
A	100	LYS	-	expression tag	UNP E9KNV5
A	101	PHE	-	expression tag	UNP E9KNV5
A	102	ARG	-	expression tag	UNP E9KNV5
A	103	VAL	-	expression tag	UNP E9KNV5
A	104	ASN	-	expression tag	UNP E9KNV5
A	105	ALA	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLN	-	expression tag	UNP E9KNV5
A	107	CYS	-	expression tag	UNP E9KNV5
A	108	ALA	-	expression tag	UNP E9KNV5
A	109	THR	-	expression tag	UNP E9KNV5
A	110	THR	-	expression tag	UNP E9KNV5
A	111	THR	-	expression tag	UNP E9KNV5
A	112	ALA	-	expression tag	UNP E9KNV5
A	113	GLY	-	expression tag	UNP E9KNV5
A	114	GLY	-	expression tag	UNP E9KNV5
A	115	TYR	-	expression tag	UNP E9KNV5
A	116	VAL	-	expression tag	UNP E9KNV5
A	117	ALA	-	expression tag	UNP E9KNV5
A	118	GLY	-	expression tag	UNP E9KNV5
A	119	PHE	-	expression tag	UNP E9KNV5
A	120	VAL	-	expression tag	UNP E9KNV5
A	121	LYS	-	expression tag	UNP E9KNV5
A	122	ASP	-	expression tag	UNP E9KNV5
A	123	ALA	-	expression tag	UNP E9KNV5
A	124	ALA	-	expression tag	UNP E9KNV5
A	125	ASP	-	expression tag	UNP E9KNV5
A	126	VAL	-	expression tag	UNP E9KNV5
A	127	LEU	-	expression tag	UNP E9KNV5
A	128	PRO	-	expression tag	UNP E9KNV5
A	129	THR	-	expression tag	UNP E9KNV5
A	130	GLY	-	expression tag	UNP E9KNV5
A	131	THR	-	expression tag	UNP E9KNV5
A	132	ALA	-	expression tag	UNP E9KNV5
A	133	SER	-	expression tag	UNP E9KNV5
A	134	ILE	-	expression tag	UNP E9KNV5
A	135	PRO	-	expression tag	UNP E9KNV5
A	136	TYR	-	expression tag	UNP E9KNV5
A	137	LEU	-	expression tag	UNP E9KNV5
A	392	GLY	-	expression tag	UNP E9KNV5
A	393	HIS	-	expression tag	UNP E9KNV5
A	394	HIS	-	expression tag	UNP E9KNV5
A	395	HIS	-	expression tag	UNP E9KNV5
A	396	HIS	-	expression tag	UNP E9KNV5
A	397	HIS	-	expression tag	UNP E9KNV5
A	398	HIS	-	expression tag	UNP E9KNV5
B	41	GLY	-	expression tag	UNP E9KNV5
B	42	THR	-	expression tag	UNP E9KNV5
B	43	THR	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	44	SER	-	expression tag	UNP E9KNV5
B	45	SER	-	expression tag	UNP E9KNV5
B	46	ASN	-	expression tag	UNP E9KNV5
B	47	SER	-	expression tag	UNP E9KNV5
B	48	ILE	-	expression tag	UNP E9KNV5
B	49	LEU	-	expression tag	UNP E9KNV5
B	50	LEU	-	expression tag	UNP E9KNV5
B	51	LYS	-	expression tag	UNP E9KNV5
B	52	GLY	-	expression tag	UNP E9KNV5
B	53	CYS	-	expression tag	UNP E9KNV5
B	54	ASP	-	expression tag	UNP E9KNV5
B	55	ARG	-	expression tag	UNP E9KNV5
B	56	ILE	-	expression tag	UNP E9KNV5
B	57	VAL	-	expression tag	UNP E9KNV5
B	58	THR	-	expression tag	UNP E9KNV5
B	59	VAL	-	expression tag	UNP E9KNV5
B	60	VAL	-	expression tag	UNP E9KNV5
B	61	ASP	-	expression tag	UNP E9KNV5
B	62	ALA	-	expression tag	UNP E9KNV5
B	63	SER	-	expression tag	UNP E9KNV5
B	64	THR	-	expression tag	UNP E9KNV5
B	65	TYR	-	expression tag	UNP E9KNV5
B	66	ASP	-	expression tag	UNP E9KNV5
B	67	ALA	-	expression tag	UNP E9KNV5
B	68	GLY	-	expression tag	UNP E9KNV5
B	69	SER	-	expression tag	UNP E9KNV5
B	70	ALA	-	expression tag	UNP E9KNV5
B	71	ILE	-	expression tag	UNP E9KNV5
B	72	VAL	-	expression tag	UNP E9KNV5
B	73	SER	-	expression tag	UNP E9KNV5
B	74	ILE	-	expression tag	UNP E9KNV5
B	75	PRO	-	expression tag	UNP E9KNV5
B	76	ILE	-	expression tag	UNP E9KNV5
B	77	THR	-	expression tag	UNP E9KNV5
B	78	PRO	-	expression tag	UNP E9KNV5
B	79	ASP	-	expression tag	UNP E9KNV5
B	80	ILE	-	expression tag	UNP E9KNV5
B	81	ALA	-	expression tag	UNP E9KNV5
B	82	TYR	-	expression tag	UNP E9KNV5
B	83	ARG	-	expression tag	UNP E9KNV5
B	84	LEU	-	expression tag	UNP E9KNV5
B	85	GLY	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	86	SER	-	expression tag	UNP E9KNV5
B	87	THR	-	expression tag	UNP E9KNV5
B	88	ALA	-	expression tag	UNP E9KNV5
B	89	ARG	-	expression tag	UNP E9KNV5
B	90	THR	-	expression tag	UNP E9KNV5
B	91	PHE	-	expression tag	UNP E9KNV5
B	92	GLN	-	expression tag	UNP E9KNV5
B	93	ARG	-	expression tag	UNP E9KNV5
B	94	ILE	-	expression tag	UNP E9KNV5
B	95	LYS	-	expression tag	UNP E9KNV5
B	96	TYR	-	expression tag	UNP E9KNV5
B	97	ARG	-	expression tag	UNP E9KNV5
B	98	SER	-	expression tag	UNP E9KNV5
B	99	LEU	-	expression tag	UNP E9KNV5
B	100	LYS	-	expression tag	UNP E9KNV5
B	101	PHE	-	expression tag	UNP E9KNV5
B	102	ARG	-	expression tag	UNP E9KNV5
B	103	VAL	-	expression tag	UNP E9KNV5
B	104	ASN	-	expression tag	UNP E9KNV5
B	105	ALA	-	expression tag	UNP E9KNV5
B	106	GLN	-	expression tag	UNP E9KNV5
B	107	CYS	-	expression tag	UNP E9KNV5
B	108	ALA	-	expression tag	UNP E9KNV5
B	109	THR	-	expression tag	UNP E9KNV5
B	110	THR	-	expression tag	UNP E9KNV5
B	111	THR	-	expression tag	UNP E9KNV5
B	112	ALA	-	expression tag	UNP E9KNV5
B	113	GLY	-	expression tag	UNP E9KNV5
B	114	GLY	-	expression tag	UNP E9KNV5
B	115	TYR	-	expression tag	UNP E9KNV5
B	116	VAL	-	expression tag	UNP E9KNV5
B	117	ALA	-	expression tag	UNP E9KNV5
B	118	GLY	-	expression tag	UNP E9KNV5
B	119	PHE	-	expression tag	UNP E9KNV5
B	120	VAL	-	expression tag	UNP E9KNV5
B	121	LYS	-	expression tag	UNP E9KNV5
B	122	ASP	-	expression tag	UNP E9KNV5
B	123	ALA	-	expression tag	UNP E9KNV5
B	124	ALA	-	expression tag	UNP E9KNV5
B	125	ASP	-	expression tag	UNP E9KNV5
B	126	VAL	-	expression tag	UNP E9KNV5
B	127	LEU	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	128	PRO	-	expression tag	UNP E9KNV5
B	129	THR	-	expression tag	UNP E9KNV5
B	130	GLY	-	expression tag	UNP E9KNV5
B	131	THR	-	expression tag	UNP E9KNV5
B	132	ALA	-	expression tag	UNP E9KNV5
B	133	SER	-	expression tag	UNP E9KNV5
B	134	ILE	-	expression tag	UNP E9KNV5
B	135	PRO	-	expression tag	UNP E9KNV5
B	136	TYR	-	expression tag	UNP E9KNV5
B	137	LEU	-	expression tag	UNP E9KNV5
B	392	GLY	-	expression tag	UNP E9KNV5
B	393	HIS	-	expression tag	UNP E9KNV5
B	394	HIS	-	expression tag	UNP E9KNV5
B	395	HIS	-	expression tag	UNP E9KNV5
B	396	HIS	-	expression tag	UNP E9KNV5
B	397	HIS	-	expression tag	UNP E9KNV5
B	398	HIS	-	expression tag	UNP E9KNV5
C	41	GLY	-	expression tag	UNP E9KNV5
C	42	THR	-	expression tag	UNP E9KNV5
C	43	THR	-	expression tag	UNP E9KNV5
C	44	SER	-	expression tag	UNP E9KNV5
C	45	SER	-	expression tag	UNP E9KNV5
C	46	ASN	-	expression tag	UNP E9KNV5
C	47	SER	-	expression tag	UNP E9KNV5
C	48	ILE	-	expression tag	UNP E9KNV5
C	49	LEU	-	expression tag	UNP E9KNV5
C	50	LEU	-	expression tag	UNP E9KNV5
C	51	LYS	-	expression tag	UNP E9KNV5
C	52	GLY	-	expression tag	UNP E9KNV5
C	53	CYS	-	expression tag	UNP E9KNV5
C	54	ASP	-	expression tag	UNP E9KNV5
C	55	ARG	-	expression tag	UNP E9KNV5
C	56	ILE	-	expression tag	UNP E9KNV5
C	57	VAL	-	expression tag	UNP E9KNV5
C	58	THR	-	expression tag	UNP E9KNV5
C	59	VAL	-	expression tag	UNP E9KNV5
C	60	VAL	-	expression tag	UNP E9KNV5
C	61	ASP	-	expression tag	UNP E9KNV5
C	62	ALA	-	expression tag	UNP E9KNV5
C	63	SER	-	expression tag	UNP E9KNV5
C	64	THR	-	expression tag	UNP E9KNV5
C	65	TYR	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	66	ASP	-	expression tag	UNP E9KNV5
C	67	ALA	-	expression tag	UNP E9KNV5
C	68	GLY	-	expression tag	UNP E9KNV5
C	69	SER	-	expression tag	UNP E9KNV5
C	70	ALA	-	expression tag	UNP E9KNV5
C	71	ILE	-	expression tag	UNP E9KNV5
C	72	VAL	-	expression tag	UNP E9KNV5
C	73	SER	-	expression tag	UNP E9KNV5
C	74	ILE	-	expression tag	UNP E9KNV5
C	75	PRO	-	expression tag	UNP E9KNV5
C	76	ILE	-	expression tag	UNP E9KNV5
C	77	THR	-	expression tag	UNP E9KNV5
C	78	PRO	-	expression tag	UNP E9KNV5
C	79	ASP	-	expression tag	UNP E9KNV5
C	80	ILE	-	expression tag	UNP E9KNV5
C	81	ALA	-	expression tag	UNP E9KNV5
C	82	TYR	-	expression tag	UNP E9KNV5
C	83	ARG	-	expression tag	UNP E9KNV5
C	84	LEU	-	expression tag	UNP E9KNV5
C	85	GLY	-	expression tag	UNP E9KNV5
C	86	SER	-	expression tag	UNP E9KNV5
C	87	THR	-	expression tag	UNP E9KNV5
C	88	ALA	-	expression tag	UNP E9KNV5
C	89	ARG	-	expression tag	UNP E9KNV5
C	90	THR	-	expression tag	UNP E9KNV5
C	91	PHE	-	expression tag	UNP E9KNV5
C	92	GLN	-	expression tag	UNP E9KNV5
C	93	ARG	-	expression tag	UNP E9KNV5
C	94	ILE	-	expression tag	UNP E9KNV5
C	95	LYS	-	expression tag	UNP E9KNV5
C	96	TYR	-	expression tag	UNP E9KNV5
C	97	ARG	-	expression tag	UNP E9KNV5
C	98	SER	-	expression tag	UNP E9KNV5
C	99	LEU	-	expression tag	UNP E9KNV5
C	100	LYS	-	expression tag	UNP E9KNV5
C	101	PHE	-	expression tag	UNP E9KNV5
C	102	ARG	-	expression tag	UNP E9KNV5
C	103	VAL	-	expression tag	UNP E9KNV5
C	104	ASN	-	expression tag	UNP E9KNV5
C	105	ALA	-	expression tag	UNP E9KNV5
C	106	GLN	-	expression tag	UNP E9KNV5
C	107	CYS	-	expression tag	UNP E9KNV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	108	ALA	-	expression tag	UNP E9KNV5
C	109	THR	-	expression tag	UNP E9KNV5
C	110	THR	-	expression tag	UNP E9KNV5
C	111	THR	-	expression tag	UNP E9KNV5
C	112	ALA	-	expression tag	UNP E9KNV5
C	113	GLY	-	expression tag	UNP E9KNV5
C	114	GLY	-	expression tag	UNP E9KNV5
C	115	TYR	-	expression tag	UNP E9KNV5
C	116	VAL	-	expression tag	UNP E9KNV5
C	117	ALA	-	expression tag	UNP E9KNV5
C	118	GLY	-	expression tag	UNP E9KNV5
C	119	PHE	-	expression tag	UNP E9KNV5
C	120	VAL	-	expression tag	UNP E9KNV5
C	121	LYS	-	expression tag	UNP E9KNV5
C	122	ASP	-	expression tag	UNP E9KNV5
C	123	ALA	-	expression tag	UNP E9KNV5
C	124	ALA	-	expression tag	UNP E9KNV5
C	125	ASP	-	expression tag	UNP E9KNV5
C	126	VAL	-	expression tag	UNP E9KNV5
C	127	LEU	-	expression tag	UNP E9KNV5
C	128	PRO	-	expression tag	UNP E9KNV5
C	129	THR	-	expression tag	UNP E9KNV5
C	130	GLY	-	expression tag	UNP E9KNV5
C	131	THR	-	expression tag	UNP E9KNV5
C	132	ALA	-	expression tag	UNP E9KNV5
C	133	SER	-	expression tag	UNP E9KNV5
C	134	ILE	-	expression tag	UNP E9KNV5
C	135	PRO	-	expression tag	UNP E9KNV5
C	136	TYR	-	expression tag	UNP E9KNV5
C	137	LEU	-	expression tag	UNP E9KNV5
C	392	GLY	-	expression tag	UNP E9KNV5
C	393	HIS	-	expression tag	UNP E9KNV5
C	394	HIS	-	expression tag	UNP E9KNV5
C	395	HIS	-	expression tag	UNP E9KNV5
C	396	HIS	-	expression tag	UNP E9KNV5
C	397	HIS	-	expression tag	UNP E9KNV5
C	398	HIS	-	expression tag	UNP E9KNV5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	404.92Å 375.15Å 412.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.75 30.00 – 3.75	Depositor EDS
% Data completeness (in resolution range)	64.2 (30.00-3.75) 49.2 (30.00-3.75)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.299 , 0.301 0.290 , 0.293	Depositor DCC
R_{free} test set	10134 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.015 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.22	EDS
Total number of atoms	8019	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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](#)

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

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	0.32	0/2725	0.56	0/3738
1	B	0.31	0/2760	0.55	0/3787
1	C	0.32	0/2760	0.56	0/3787
All	All	0.32	0/8245	0.56	0/11312

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	2650	0	2602	52	0
1	B	2683	0	2634	49	0
1	C	2683	0	2636	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	8019	0	7872	151	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 10.

All (151) 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:C:228:HIS:HB3	1:C:249:PRO:HA	1.52	0.91
1:C:228:HIS:CB	1:C:249:PRO:HA	2.05	0.86
1:C:169:THR:HG21	1:C:213:ARG:HH21	1.45	0.80
1:C:107:CYS:SG	1:C:148:TRP:HB3	2.23	0.78
1:A:234:GLY:HA2	1:A:242:VAL:HG22	1.75	0.68
1:B:81:ALA:HB3	1:B:84:LEU:HB3	1.77	0.67
1:C:259:PRO:HB2	1:C:270:PRO:HG2	1.78	0.66
1:C:305:VAL:HG21	1:C:312:ASP:HB2	1.79	0.64
1:C:92:GLN:HE21	1:C:211:THR:HB	1.63	0.64
1:C:247:ILE:HD11	1:C:257:LEU:HG	1.79	0.64
1:B:121:LYS:HG2	1:C:209:ASP:HB3	1.80	0.63
1:A:164:TYR:CE2	1:C:176:ARG:HG2	2.35	0.61
1:A:105:ALA:HB1	1:A:107:CYS:SG	2.40	0.61
1:A:56:ILE:HG13	1:A:80:ILE:HG21	1.81	0.61
1:C:107:CYS:HG	1:C:195:CYS:HG	1.39	0.60
1:A:123:ALA:O	1:B:170:ARG:NH1	2.34	0.60
1:C:107:CYS:CB	1:C:195:CYS:HG	2.13	0.60
1:C:191:PRO:HB3	1:C:195:CYS:SG	2.41	0.60
1:C:277:ARG:HB3	1:C:363:VAL:HG13	1.85	0.59
1:A:247:ILE:HD11	1:A:257:LEU:HA	1.84	0.59
1:C:258:THR:OG1	1:C:261:ARG:NH1	2.35	0.58
1:B:134:ILE:HD13	1:B:186:LEU:HD23	1.85	0.58
1:C:107:CYS:HB3	1:C:195:CYS:HG	1.69	0.58
1:A:92:GLN:OE1	1:C:122:ASP:HB2	2.05	0.57
1:C:262:PHE:CD2	1:C:270:PRO:HG3	2.39	0.57
1:C:223:ALA:HB3	1:C:358:HIS:HA	1.87	0.57
1:B:211:THR:HG22	1:B:212:PHE:N	2.20	0.57
1:C:169:THR:CG2	1:C:213:ARG:HH21	2.18	0.56
1:A:63:SER:HA	1:A:191:PRO:HG2	1.88	0.56
1:C:92:GLN:NE2	1:C:211:THR:HB	2.21	0.55
1:A:62:ALA:HB1	1:A:65:TYR:CD2	2.41	0.54
1:C:228:HIS:HB2	1:C:249:PRO:HA	1.87	0.54
1:C:247:ILE:HD13	1:C:261:ARG:HG2	1.90	0.54
1:A:92:GLN:HE21	1:A:211:THR:CB	2.22	0.53
1:B:121:LYS:HB2	1:C:92:GLN:HG3	1.90	0.53
1:A:74:ILE:HD12	1:A:80:ILE:HD13	1.91	0.52
1:B:121:LYS:CG	1:C:209:ASP:HB3	2.39	0.52
1:A:124:ALA:HB1	1:B:168:PRO:HA	1.91	0.52
1:C:116:VAL:HG21	1:C:134:ILE:HG23	1.91	0.52
1:B:352:ASP:OD2	1:C:294:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PRO:HB2	1:A:329:ILE:HD13	1.91	0.51
1:B:134:ILE:HB	1:B:135:PRO:CD	2.41	0.51
1:C:59:VAL:HA	1:C:198:THR:HG22	1.92	0.51
1:C:67:ALA:HA	1:C:187:VAL:HG23	1.92	0.51
1:B:124:ALA:O	1:C:169:THR:HG23	2.11	0.51
1:B:108:ALA:O	1:B:111:THR:HG23	2.10	0.51
1:B:277:ARG:HB3	1:B:363:VAL:HG13	1.91	0.51
1:C:262:PHE:CG	1:C:270:PRO:HG3	2.45	0.51
1:A:92:GLN:HE21	1:A:211:THR:HB	1.75	0.50
1:B:49:LEU:HD12	1:B:205:VAL:O	2.12	0.50
1:C:258:THR:N	1:C:259:PRO:HA	2.27	0.50
1:C:105:ALA:HB1	1:C:148:TRP:O	2.12	0.50
1:B:323:HIS:O	1:B:368:GLN:NE2	2.44	0.49
1:C:57:VAL:HG12	1:C:199:VAL:HB	1.93	0.49
1:A:126:VAL:HG12	1:B:169:THR:HB	1.94	0.49
1:C:74:ILE:O	1:C:74:ILE:HG23	2.12	0.49
1:C:106:GLN:HB2	1:C:196:PRO:HG2	1.94	0.49
1:B:57:VAL:HG11	1:B:72:VAL:HG22	1.96	0.48
1:B:286:LEU:HB3	1:B:346:PHE:CD1	2.48	0.48
1:C:56:ILE:CG1	1:C:201:LEU:HB2	2.43	0.48
1:C:223:ALA:HB2	1:C:265:PHE:CZ	2.49	0.48
1:C:191:PRO:CB	1:C:195:CYS:SG	3.01	0.48
1:B:77:THR:O	1:B:80:ILE:HG22	2.15	0.47
1:B:137:LEU:HD12	1:B:140:ASN:HD21	1.78	0.47
1:C:107:CYS:SG	1:C:195:CYS:CB	3.03	0.47
1:A:211:THR:OG1	1:C:140:ASN:ND2	2.48	0.47
1:A:158:ILE:N	1:A:159:PRO:CD	2.77	0.47
1:B:121:LYS:CB	1:C:92:GLN:HG3	2.45	0.46
1:A:50:LEU:HD11	1:A:87:THR:HG21	1.98	0.46
1:C:158:ILE:HD12	1:C:180:PRO:HB2	1.96	0.46
1:C:367:PHE:O	1:C:368:GLN:HB2	2.15	0.46
1:A:148:TRP:CD1	1:A:191:PRO:HB3	2.50	0.46
1:B:241:ARG:NH1	1:B:256:ASP:HB3	2.30	0.46
1:C:217:ASP:O	1:C:373:PRO:HA	2.16	0.46
1:B:57:VAL:HA	1:B:388:PRO:HD3	1.98	0.46
1:B:137:LEU:HD22	1:B:186:LEU:HD22	1.98	0.46
1:C:247:ILE:HD12	1:C:255:LYS:O	2.16	0.46
1:C:95:LYS:HB2	1:C:162:LEU:HD23	1.97	0.45
1:C:231:ASN:HB3	1:C:355:VAL:HA	1.98	0.45
1:A:278:ILE:HD13	1:A:300:ILE:HG13	1.98	0.45
1:A:281:PRO:HB3	1:A:296:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:HG23	1:A:74:ILE:HD11	1.97	0.45
1:A:105:ALA:HB3	1:A:148:TRP:O	2.17	0.45
1:A:158:ILE:CD1	1:A:180:PRO:HB2	2.47	0.45
1:A:111:THR:HG22	1:A:193:GLN:HB2	1.98	0.45
1:A:158:ILE:HD13	1:A:180:PRO:HB2	1.98	0.45
1:A:247:ILE:HD11	1:A:257:LEU:HD23	1.99	0.45
1:B:57:VAL:HG22	1:B:199:VAL:HB	1.97	0.45
1:B:60:VAL:O	1:B:196:PRO:HA	2.16	0.45
1:B:107:CYS:SG	1:B:111:THR:HG21	2.56	0.45
1:C:223:ALA:HB2	1:C:265:PHE:CE2	2.52	0.45
1:C:304:LEU:HB3	1:C:308:GLY:HA2	1.98	0.45
1:A:93:ARG:HH11	1:A:93:ARG:HG2	1.81	0.45
1:C:229:THR:HB	1:C:356:TRP:O	2.16	0.45
1:B:166:GLU:OE1	1:B:213:ARG:HG3	2.16	0.45
1:C:98:SER:HB3	1:C:204:VAL:CG1	2.46	0.45
1:A:81:ALA:HB3	1:A:84:LEU:HB3	1.98	0.44
1:C:57:VAL:CG1	1:C:199:VAL:HB	2.47	0.44
1:A:233:TYR:HB2	1:B:338:VAL:HG12	2.00	0.44
1:B:84:LEU:HB2	1:B:203:TRP:CE2	2.52	0.44
1:C:187:VAL:HG23	1:C:187:VAL:O	2.17	0.44
1:A:134:ILE:HD11	1:A:188:ASP:HA	1.99	0.44
1:B:111:THR:HB	1:B:193:GLN:HG2	1.99	0.44
1:C:59:VAL:HG22	1:C:198:THR:CG2	2.48	0.44
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.94	0.43
1:A:232:VAL:HG23	1:A:356:TRP:HZ3	1.84	0.43
1:A:61:ASP:HB2	1:A:195:CYS:H	1.82	0.43
1:A:276:VAL:CG2	1:A:362:PHE:HB3	2.49	0.43
1:B:137:LEU:CD2	1:B:186:LEU:HD22	2.48	0.43
1:A:235:LEU:HB3	1:A:236:PRO:HD3	2.01	0.43
1:C:96:TYR:HB2	1:C:158:ILE:HG21	1.99	0.43
1:A:98:SER:HB3	1:A:204:VAL:HG13	2.00	0.43
1:A:309:LEU:HD12	1:A:310:GLY:N	2.34	0.43
1:B:276:VAL:CG1	1:B:362:PHE:HB3	2.49	0.43
1:A:60:VAL:O	1:A:61:ASP:C	2.57	0.43
1:A:50:LEU:HB3	1:A:203:TRP:HZ3	1.83	0.43
1:B:214:LYS:O	1:B:215:GLU:C	2.56	0.42
1:B:263:ALA:HA	1:B:268:PHE:O	2.19	0.42
1:B:247:ILE:HD12	1:B:261:ARG:HB3	2.02	0.42
1:B:277:ARG:CB	1:B:363:VAL:HG13	2.50	0.42
1:C:231:ASN:HD21	1:C:248:SER:HB2	1.83	0.42
1:A:94:ILE:HB	1:A:165:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:HB3	1:B:213:ARG:HH21	1.84	0.42
1:C:257:LEU:N	1:C:257:LEU:HD12	2.35	0.42
1:A:194:ILE:HG22	1:A:196:PRO:HD3	2.02	0.42
1:A:134:ILE:N	1:A:135:PRO:HD2	2.35	0.42
1:B:52:GLY:HA3	1:B:203:TRP:CZ2	2.55	0.42
1:A:287:THR:OG1	1:A:288:GLY:N	2.52	0.42
1:C:231:ASN:ND2	1:C:233:TYR:OH	2.53	0.41
1:B:71:ILE:HG13	1:B:72:VAL:HG23	2.02	0.41
1:B:148:TRP:CE2	1:B:191:PRO:HG3	2.56	0.41
1:B:58:THR:HG23	1:B:387:LEU:HB2	2.02	0.41
1:C:221:ILE:HG22	1:C:222:SER:N	2.36	0.41
1:A:330:PRO:HG3	1:A:349:ALA:HB2	2.03	0.41
1:B:51:LYS:HG2	1:B:204:VAL:HG22	2.02	0.41
1:B:116:VAL:HG21	1:B:134:ILE:HG23	2.03	0.41
1:A:247:ILE:HD13	1:A:261:ARG:CD	2.51	0.41
1:A:305:VAL:HG12	1:A:310:GLY:HA3	2.03	0.41
1:B:211:THR:CG2	1:B:212:PHE:N	2.84	0.41
1:A:76:ILE:HA	1:A:80:ILE:HD11	2.03	0.41
1:B:48:ILE:HD11	1:B:207:LEU:HD12	2.03	0.41
1:B:363:VAL:HA	1:B:364:PRO:HD3	1.97	0.41
1:C:269:LEU:HA	1:C:270:PRO:HD3	1.96	0.41
1:B:134:ILE:HB	1:B:135:PRO:HD3	2.03	0.41
1:A:305:VAL:HG13	1:A:306:ASN:N	2.36	0.40
1:C:146:GLN:HG3	1:C:150:LYS:HB3	2.03	0.40
1:C:213:ARG:HH11	1:C:213:ARG:HG3	1.86	0.40
1:C:122:ASP:OD1	1:C:176:ARG:NH1	2.54	0.40
1:A:92:GLN:HE21	1:A:211:THR:CG2	2.35	0.40
1:A:174:ALA:HB3	1:A:177:GLU:CD	2.42	0.40
1:B:95:LYS:HB2	1:B:162:LEU:HD23	2.04	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	339/358 (95%)	316 (93%)	21 (6%)	2 (1%)	22	55
1	B	343/358 (96%)	327 (95%)	14 (4%)	2 (1%)	22	55
1	C	343/358 (96%)	329 (96%)	13 (4%)	1 (0%)	37	68
All	All	1025/1074 (95%)	972 (95%)	48 (5%)	5 (0%)	25	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	GLY
1	B	209	ASP
1	C	209	ASP
1	A	61	ASP
1	B	250	ILE

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	293/308 (95%)	276 (94%)	17 (6%)	17	44
1	B	297/308 (96%)	272 (92%)	25 (8%)	9	33
1	C	297/308 (96%)	276 (93%)	21 (7%)	12	38
All	All	887/924 (96%)	824 (93%)	63 (7%)	12	38

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	58	THR
1	A	106	GLN
1	A	182	GLN
1	A	187	VAL
1	A	204	VAL
1	A	214	LYS
1	A	219	THR

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Mol	Chain	Res	Type
1	A	221	ILE
1	A	230	LEU
1	A	241	ARG
1	A	247	ILE
1	A	252	GLN
1	A	293	GLN
1	A	296	GLU
1	A	343	THR
1	A	372	ILE
1	B	50	LEU
1	B	59	VAL
1	B	102	ARG
1	B	106	GLN
1	B	110	THR
1	B	111	THR
1	B	121	LYS
1	B	144	PHE
1	B	169	THR
1	B	182	GLN
1	B	186	LEU
1	B	193	GLN
1	B	214	LYS
1	B	221	ILE
1	B	241	ARG
1	B	252	GLN
1	B	273	LYS
1	B	292	TYR
1	B	293	GLN
1	B	298	THR
1	B	324	THR
1	B	343	THR
1	B	357	THR
1	B	368	GLN
1	B	372	ILE
1	C	50	LEU
1	C	84	LEU
1	C	131	THR
1	C	145	THR
1	C	157	LYS
1	C	169	THR
1	C	189	SER
1	C	192	SER

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Mol	Chain	Res	Type
1	C	204	VAL
1	C	207	LEU
1	C	231	ASN
1	C	241	ARG
1	C	247	ILE
1	C	255	LYS
1	C	261	ARG
1	C	273	LYS
1	C	276	VAL
1	C	343	THR
1	C	363	VAL
1	C	368	GLN
1	C	387	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	106	GLN
1	A	184	HIS
1	A	252	GLN
1	A	319	ASN
1	A	354	HIS
1	B	228	HIS
1	B	319	ASN
1	B	368	GLN
1	C	92	GLN
1	C	140	ASN
1	C	182	GLN
1	C	231	ASN
1	C	326	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Warning: The R factor obtained from EDS is 0.4708, which does not match the depositor's R factor of 0.2988. Please interpret the results in this section carefully.

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	341/358 (95%)	-0.66	0 100 100	25, 60, 107, 156	0
1	B	345/358 (96%)	-0.76	0 100 100	30, 66, 113, 159	0
1	C	345/358 (96%)	-0.69	0 100 100	30, 68, 122, 175	0
All	All	1031/1074 (95%)	-0.71	0 100 100	25, 64, 117, 175	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	B	401	1/1	0.99	0.05	40,40,40,40	0
2	CA	A	401	1/1	1.00	0.07	49,49,49,49	0
2	CA	C	401	1/1	1.00	0.03	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.