



Full wwPDB X-ray Structure Validation Report

May 22, 2020 – 03:06 am BST

PDB ID : 5DVB
Title : Crystal Structure of *S. cerevisiae* TSA2
Authors : Nielsen, M.H.; Kidmose, R.T.; Jenner, L.B.
Deposited on : 2015-09-21
Resolution : 2.20 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

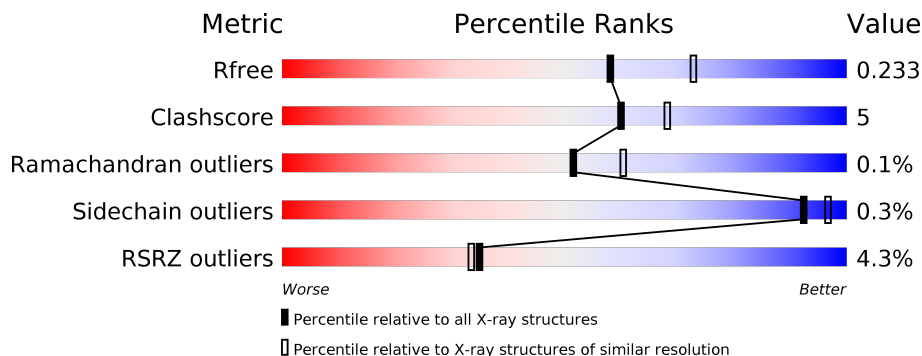
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	

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Mol	Chain	Length	Quality of chain
1	G	217	 <p>4% 72% 7% 21%</p>
1	H	217	 <p>3% 70% 9% 21%</p>
1	I	217	 <p>3% 78% 8% 14%</p>
1	J	217	 <p>4% 70% 10% 21%</p>

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 14334 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 Tsa2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	171	Total 1337	C 868	N 221	O 247	S 1	0	0	0
1	B	176	Total 1369	C 888	N 227	O 252	S 2	0	0	0
1	C	172	Total 1344	C 873	N 222	O 248	S 1	0	0	0
1	A	199	Total 1555	C 1008	N 257	O 288	S 2	0	0	0
1	G	171	Total 1337	C 868	N 221	O 247	S 1	0	0	0
1	I	186	Total 1446	C 940	N 239	O 265	S 2	0	0	0
1	D	170	Total 1330	C 864	N 220	O 245	S 1	0	0	0
1	E	183	Total 1436	C 933	N 237	O 264	S 2	0	2	0
1	J	172	Total 1344	C 873	N 222	O 248	S 1	0	0	0
1	F	176	Total 1373	C 891	N 227	O 253	S 2	0	0	0

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
H	-19	ALA	-	expression tag	UNP A0A0D4RBH7
H	-18	HIS	-	expression tag	UNP A0A0D4RBH7
H	-17	HIS	-	expression tag	UNP A0A0D4RBH7
H	-16	HIS	-	expression tag	UNP A0A0D4RBH7
H	-15	HIS	-	expression tag	UNP A0A0D4RBH7
H	-14	HIS	-	expression tag	UNP A0A0D4RBH7
H	-13	HIS	-	expression tag	UNP A0A0D4RBH7
H	-12	VAL	-	expression tag	UNP A0A0D4RBH7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	ASP	-	expression tag	UNP A0A0D4RBH7
H	-10	ASP	-	expression tag	UNP A0A0D4RBH7
H	-9	ASP	-	expression tag	UNP A0A0D4RBH7
H	-8	ASP	-	expression tag	UNP A0A0D4RBH7
H	-7	LYS	-	expression tag	UNP A0A0D4RBH7
H	-6	GLU	-	expression tag	UNP A0A0D4RBH7
H	-5	ASN	-	expression tag	UNP A0A0D4RBH7
H	-4	LEU	-	expression tag	UNP A0A0D4RBH7
H	-3	TYR	-	expression tag	UNP A0A0D4RBH7
H	-2	PHE	-	expression tag	UNP A0A0D4RBH7
H	-1	GLN	-	expression tag	UNP A0A0D4RBH7
H	0	GLY	-	expression tag	UNP A0A0D4RBH7
H	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
B	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
B	-19	ALA	-	expression tag	UNP A0A0D4RBH7
B	-18	HIS	-	expression tag	UNP A0A0D4RBH7
B	-17	HIS	-	expression tag	UNP A0A0D4RBH7
B	-16	HIS	-	expression tag	UNP A0A0D4RBH7
B	-15	HIS	-	expression tag	UNP A0A0D4RBH7
B	-14	HIS	-	expression tag	UNP A0A0D4RBH7
B	-13	HIS	-	expression tag	UNP A0A0D4RBH7
B	-12	VAL	-	expression tag	UNP A0A0D4RBH7
B	-11	ASP	-	expression tag	UNP A0A0D4RBH7
B	-10	ASP	-	expression tag	UNP A0A0D4RBH7
B	-9	ASP	-	expression tag	UNP A0A0D4RBH7
B	-8	ASP	-	expression tag	UNP A0A0D4RBH7
B	-7	LYS	-	expression tag	UNP A0A0D4RBH7
B	-6	GLU	-	expression tag	UNP A0A0D4RBH7
B	-5	ASN	-	expression tag	UNP A0A0D4RBH7
B	-4	LEU	-	expression tag	UNP A0A0D4RBH7
B	-3	TYR	-	expression tag	UNP A0A0D4RBH7
B	-2	PHE	-	expression tag	UNP A0A0D4RBH7
B	-1	GLN	-	expression tag	UNP A0A0D4RBH7
B	0	GLY	-	expression tag	UNP A0A0D4RBH7
B	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
C	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
C	-19	ALA	-	expression tag	UNP A0A0D4RBH7
C	-18	HIS	-	expression tag	UNP A0A0D4RBH7
C	-17	HIS	-	expression tag	UNP A0A0D4RBH7
C	-16	HIS	-	expression tag	UNP A0A0D4RBH7
C	-15	HIS	-	expression tag	UNP A0A0D4RBH7
C	-14	HIS	-	expression tag	UNP A0A0D4RBH7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP A0A0D4RBH7
C	-12	VAL	-	expression tag	UNP A0A0D4RBH7
C	-11	ASP	-	expression tag	UNP A0A0D4RBH7
C	-10	ASP	-	expression tag	UNP A0A0D4RBH7
C	-9	ASP	-	expression tag	UNP A0A0D4RBH7
C	-8	ASP	-	expression tag	UNP A0A0D4RBH7
C	-7	LYS	-	expression tag	UNP A0A0D4RBH7
C	-6	GLU	-	expression tag	UNP A0A0D4RBH7
C	-5	ASN	-	expression tag	UNP A0A0D4RBH7
C	-4	LEU	-	expression tag	UNP A0A0D4RBH7
C	-3	TYR	-	expression tag	UNP A0A0D4RBH7
C	-2	PHE	-	expression tag	UNP A0A0D4RBH7
C	-1	GLN	-	expression tag	UNP A0A0D4RBH7
C	0	GLY	-	expression tag	UNP A0A0D4RBH7
C	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
A	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
A	-19	ALA	-	expression tag	UNP A0A0D4RBH7
A	-18	HIS	-	expression tag	UNP A0A0D4RBH7
A	-17	HIS	-	expression tag	UNP A0A0D4RBH7
A	-16	HIS	-	expression tag	UNP A0A0D4RBH7
A	-15	HIS	-	expression tag	UNP A0A0D4RBH7
A	-14	HIS	-	expression tag	UNP A0A0D4RBH7
A	-13	HIS	-	expression tag	UNP A0A0D4RBH7
A	-12	VAL	-	expression tag	UNP A0A0D4RBH7
A	-11	ASP	-	expression tag	UNP A0A0D4RBH7
A	-10	ASP	-	expression tag	UNP A0A0D4RBH7
A	-9	ASP	-	expression tag	UNP A0A0D4RBH7
A	-8	ASP	-	expression tag	UNP A0A0D4RBH7
A	-7	LYS	-	expression tag	UNP A0A0D4RBH7
A	-6	GLU	-	expression tag	UNP A0A0D4RBH7
A	-5	ASN	-	expression tag	UNP A0A0D4RBH7
A	-4	LEU	-	expression tag	UNP A0A0D4RBH7
A	-3	TYR	-	expression tag	UNP A0A0D4RBH7
A	-2	PHE	-	expression tag	UNP A0A0D4RBH7
A	-1	GLN	-	expression tag	UNP A0A0D4RBH7
A	0	GLY	-	expression tag	UNP A0A0D4RBH7
A	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
G	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
G	-19	ALA	-	expression tag	UNP A0A0D4RBH7
G	-18	HIS	-	expression tag	UNP A0A0D4RBH7
G	-17	HIS	-	expression tag	UNP A0A0D4RBH7
G	-16	HIS	-	expression tag	UNP A0A0D4RBH7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-15	HIS	-	expression tag	UNP A0A0D4RBH7
G	-14	HIS	-	expression tag	UNP A0A0D4RBH7
G	-13	HIS	-	expression tag	UNP A0A0D4RBH7
G	-12	VAL	-	expression tag	UNP A0A0D4RBH7
G	-11	ASP	-	expression tag	UNP A0A0D4RBH7
G	-10	ASP	-	expression tag	UNP A0A0D4RBH7
G	-9	ASP	-	expression tag	UNP A0A0D4RBH7
G	-8	ASP	-	expression tag	UNP A0A0D4RBH7
G	-7	LYS	-	expression tag	UNP A0A0D4RBH7
G	-6	GLU	-	expression tag	UNP A0A0D4RBH7
G	-5	ASN	-	expression tag	UNP A0A0D4RBH7
G	-4	LEU	-	expression tag	UNP A0A0D4RBH7
G	-3	TYR	-	expression tag	UNP A0A0D4RBH7
G	-2	PHE	-	expression tag	UNP A0A0D4RBH7
G	-1	GLN	-	expression tag	UNP A0A0D4RBH7
G	0	GLY	-	expression tag	UNP A0A0D4RBH7
G	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
I	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
I	-19	ALA	-	expression tag	UNP A0A0D4RBH7
I	-18	HIS	-	expression tag	UNP A0A0D4RBH7
I	-17	HIS	-	expression tag	UNP A0A0D4RBH7
I	-16	HIS	-	expression tag	UNP A0A0D4RBH7
I	-15	HIS	-	expression tag	UNP A0A0D4RBH7
I	-14	HIS	-	expression tag	UNP A0A0D4RBH7
I	-13	HIS	-	expression tag	UNP A0A0D4RBH7
I	-12	VAL	-	expression tag	UNP A0A0D4RBH7
I	-11	ASP	-	expression tag	UNP A0A0D4RBH7
I	-10	ASP	-	expression tag	UNP A0A0D4RBH7
I	-9	ASP	-	expression tag	UNP A0A0D4RBH7
I	-8	ASP	-	expression tag	UNP A0A0D4RBH7
I	-7	LYS	-	expression tag	UNP A0A0D4RBH7
I	-6	GLU	-	expression tag	UNP A0A0D4RBH7
I	-5	ASN	-	expression tag	UNP A0A0D4RBH7
I	-4	LEU	-	expression tag	UNP A0A0D4RBH7
I	-3	TYR	-	expression tag	UNP A0A0D4RBH7
I	-2	PHE	-	expression tag	UNP A0A0D4RBH7
I	-1	GLN	-	expression tag	UNP A0A0D4RBH7
I	0	GLY	-	expression tag	UNP A0A0D4RBH7
I	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
D	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
D	-19	ALA	-	expression tag	UNP A0A0D4RBH7
D	-18	HIS	-	expression tag	UNP A0A0D4RBH7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	HIS	-	expression tag	UNP A0A0D4RBH7
D	-16	HIS	-	expression tag	UNP A0A0D4RBH7
D	-15	HIS	-	expression tag	UNP A0A0D4RBH7
D	-14	HIS	-	expression tag	UNP A0A0D4RBH7
D	-13	HIS	-	expression tag	UNP A0A0D4RBH7
D	-12	VAL	-	expression tag	UNP A0A0D4RBH7
D	-11	ASP	-	expression tag	UNP A0A0D4RBH7
D	-10	ASP	-	expression tag	UNP A0A0D4RBH7
D	-9	ASP	-	expression tag	UNP A0A0D4RBH7
D	-8	ASP	-	expression tag	UNP A0A0D4RBH7
D	-7	LYS	-	expression tag	UNP A0A0D4RBH7
D	-6	GLU	-	expression tag	UNP A0A0D4RBH7
D	-5	ASN	-	expression tag	UNP A0A0D4RBH7
D	-4	LEU	-	expression tag	UNP A0A0D4RBH7
D	-3	TYR	-	expression tag	UNP A0A0D4RBH7
D	-2	PHE	-	expression tag	UNP A0A0D4RBH7
D	-1	GLN	-	expression tag	UNP A0A0D4RBH7
D	0	GLY	-	expression tag	UNP A0A0D4RBH7
D	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
E	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
E	-19	ALA	-	expression tag	UNP A0A0D4RBH7
E	-18	HIS	-	expression tag	UNP A0A0D4RBH7
E	-17	HIS	-	expression tag	UNP A0A0D4RBH7
E	-16	HIS	-	expression tag	UNP A0A0D4RBH7
E	-15	HIS	-	expression tag	UNP A0A0D4RBH7
E	-14	HIS	-	expression tag	UNP A0A0D4RBH7
E	-13	HIS	-	expression tag	UNP A0A0D4RBH7
E	-12	VAL	-	expression tag	UNP A0A0D4RBH7
E	-11	ASP	-	expression tag	UNP A0A0D4RBH7
E	-10	ASP	-	expression tag	UNP A0A0D4RBH7
E	-9	ASP	-	expression tag	UNP A0A0D4RBH7
E	-8	ASP	-	expression tag	UNP A0A0D4RBH7
E	-7	LYS	-	expression tag	UNP A0A0D4RBH7
E	-6	GLU	-	expression tag	UNP A0A0D4RBH7
E	-5	ASN	-	expression tag	UNP A0A0D4RBH7
E	-4	LEU	-	expression tag	UNP A0A0D4RBH7
E	-3	TYR	-	expression tag	UNP A0A0D4RBH7
E	-2	PHE	-	expression tag	UNP A0A0D4RBH7
E	-1	GLN	-	expression tag	UNP A0A0D4RBH7
E	0	GLY	-	expression tag	UNP A0A0D4RBH7
E	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
J	-20	MET	-	initiating methionine	UNP A0A0D4RBH7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-19	ALA	-	expression tag	UNP A0A0D4RBH7
J	-18	HIS	-	expression tag	UNP A0A0D4RBH7
J	-17	HIS	-	expression tag	UNP A0A0D4RBH7
J	-16	HIS	-	expression tag	UNP A0A0D4RBH7
J	-15	HIS	-	expression tag	UNP A0A0D4RBH7
J	-14	HIS	-	expression tag	UNP A0A0D4RBH7
J	-13	HIS	-	expression tag	UNP A0A0D4RBH7
J	-12	VAL	-	expression tag	UNP A0A0D4RBH7
J	-11	ASP	-	expression tag	UNP A0A0D4RBH7
J	-10	ASP	-	expression tag	UNP A0A0D4RBH7
J	-9	ASP	-	expression tag	UNP A0A0D4RBH7
J	-8	ASP	-	expression tag	UNP A0A0D4RBH7
J	-7	LYS	-	expression tag	UNP A0A0D4RBH7
J	-6	GLU	-	expression tag	UNP A0A0D4RBH7
J	-5	ASN	-	expression tag	UNP A0A0D4RBH7
J	-4	LEU	-	expression tag	UNP A0A0D4RBH7
J	-3	TYR	-	expression tag	UNP A0A0D4RBH7
J	-2	PHE	-	expression tag	UNP A0A0D4RBH7
J	-1	GLN	-	expression tag	UNP A0A0D4RBH7
J	0	GLY	-	expression tag	UNP A0A0D4RBH7
J	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7
F	-20	MET	-	initiating methionine	UNP A0A0D4RBH7
F	-19	ALA	-	expression tag	UNP A0A0D4RBH7
F	-18	HIS	-	expression tag	UNP A0A0D4RBH7
F	-17	HIS	-	expression tag	UNP A0A0D4RBH7
F	-16	HIS	-	expression tag	UNP A0A0D4RBH7
F	-15	HIS	-	expression tag	UNP A0A0D4RBH7
F	-14	HIS	-	expression tag	UNP A0A0D4RBH7
F	-13	HIS	-	expression tag	UNP A0A0D4RBH7
F	-12	VAL	-	expression tag	UNP A0A0D4RBH7
F	-11	ASP	-	expression tag	UNP A0A0D4RBH7
F	-10	ASP	-	expression tag	UNP A0A0D4RBH7
F	-9	ASP	-	expression tag	UNP A0A0D4RBH7
F	-8	ASP	-	expression tag	UNP A0A0D4RBH7
F	-7	LYS	-	expression tag	UNP A0A0D4RBH7
F	-6	GLU	-	expression tag	UNP A0A0D4RBH7
F	-5	ASN	-	expression tag	UNP A0A0D4RBH7
F	-4	LEU	-	expression tag	UNP A0A0D4RBH7
F	-3	TYR	-	expression tag	UNP A0A0D4RBH7
F	-2	PHE	-	expression tag	UNP A0A0D4RBH7
F	-1	GLN	-	expression tag	UNP A0A0D4RBH7
F	0	GLY	-	expression tag	UNP A0A0D4RBH7

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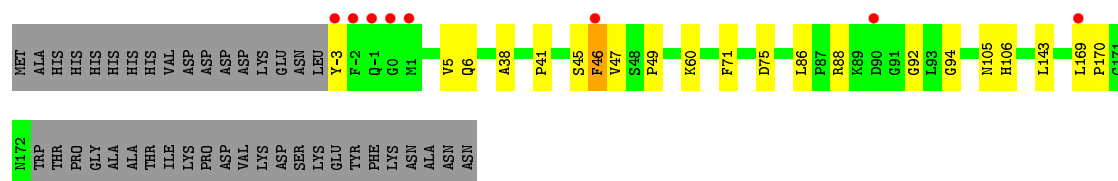
Chain	Residue	Modelled	Actual	Comment	Reference
F	48	SER	CYS	engineered mutation	UNP A0A0D4RBH7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	39	Total O 39 39	0	0
2	B	39	Total O 39 39	0	0
2	C	46	Total O 46 46	0	0
2	A	60	Total O 60 60	0	0
2	G	33	Total O 33 33	0	0
2	I	48	Total O 48 48	0	0
2	D	32	Total O 32 32	0	0
2	E	55	Total O 55 55	0	0
2	J	56	Total O 56 56	0	0
2	F	55	Total O 55 55	0	0

- Molecule 1: Tsa2p

Chain F:  4% 71% 9% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	171.53Å 216.13Å 64.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 2.20 48.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.72-2.20) 95.0 (48.05-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.187 , 0.233 0.187 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtrriage
Anisotropy	0.477	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14334	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	0/1591	0.69	0/2157
1	B	0.69	0/1400	0.74	1/1900 (0.1%)
1	C	0.73	0/1373	0.71	0/1859
1	D	0.64	0/1359	0.63	0/1839
1	E	0.72	0/1470	0.72	1/1997 (0.1%)
1	F	0.71	0/1403	0.71	0/1901
1	G	0.65	0/1366	0.71	0/1849
1	H	0.69	0/1366	0.70	1/1849 (0.1%)
1	I	0.71	0/1480	0.74	0/2009
1	J	0.73	0/1373	0.71	0/1859
All	All	0.70	0/14181	0.71	3/19219 (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	A	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MET	CG-SD-CE	5.44	108.90	100.20
1	H	130	ASP	CB-CG-OD1	5.26	123.03	118.30
1	E	111	ASP	CB-CG-OD1	5.20	122.97	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	SER	Peptide
1	F	45	SER	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	A	1555	0	1573	11	0
1	B	1369	0	1394	8	0
1	C	1344	0	1367	9	0
1	D	1330	0	1351	12	0
1	E	1436	0	1455	25	0
1	F	1373	0	1396	12	0
1	G	1337	0	1358	10	0
1	H	1337	0	1358	16	0
1	I	1446	0	1471	9	0
1	J	1344	0	1367	18	0
2	A	60	0	0	4	0
2	B	39	0	0	4	0
2	C	46	0	0	2	0
2	D	32	0	0	2	0
2	E	55	0	0	5	1
2	F	55	0	0	4	1
2	G	33	0	0	1	0
2	H	39	0	0	7	0
2	I	48	0	0	1	1
2	J	56	0	0	4	1
All	All	14334	0	14090	129	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (129) 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:E:179:THR:O	2:E:201:HOH:O	1.81	0.99
1:F:47:VAL:N	2:F:201:HOH:O	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LYS:O	2:B:201:HOH:O	1.94	0.85
1:C:-3:TYR:OH	2:C:201:HOH:O	1.93	0.84
1:J:146:GLY:N	2:J:201:HOH:O	2.09	0.83
1:J:-3:TYR:N	2:J:202:HOH:O	2.12	0.82
1:E:64:ASP:HB3	1:E:179:THR:HG22	1.62	0.81
1:D:-3:TYR:N	2:D:201:HOH:O	2.12	0.81
1:H:60:LYS:NZ	1:H:64:ASP:OD1	2.15	0.79
1:A:47:VAL:N	2:A:203:HOH:O	2.11	0.79
1:H:1:MET:O	2:H:201:HOH:O	2.01	0.78
1:F:-3:TYR:N	2:F:203:HOH:O	2.17	0.76
1:H:-3:TYR:N	2:H:205:HOH:O	2.19	0.76
1:E:-3:TYR:N	2:E:202:HOH:O	2.07	0.72
1:E:64:ASP:HB3	1:E:179:THR:CG2	2.19	0.72
1:H:167:THR:O	2:H:202:HOH:O	2.06	0.72
1:A:31:LYS:O	2:A:201:HOH:O	2.08	0.71
1:A:31:LYS:NZ	2:A:204:HOH:O	2.24	0.70
1:I:-3:TYR:N	2:I:201:HOH:O	2.25	0.70
1:A:46:PHE:O	2:A:202:HOH:O	2.10	0.69
1:H:166:GLY:O	2:H:203:HOH:O	2.10	0.69
1:E:167:THR:O	2:E:203:HOH:O	2.09	0.69
1:D:86:LEU:O	1:D:92:GLY:HA3	1.94	0.68
1:F:75:ASP:OD1	2:F:202:HOH:O	2.13	0.66
1:H:34:TYR:CE1	1:H:131:PRO:HD3	2.31	0.65
1:H:47:VAL:N	2:H:206:HOH:O	2.25	0.64
1:E:65:GLN:O	1:E:160:GLN:NE2	2.30	0.63
1:G:48:SER:OG	2:G:201:HOH:O	2.17	0.60
1:C:167:THR:HG22	1:C:168:VAL:H	1.66	0.59
1:H:167:THR:O	2:H:204:HOH:O	2.16	0.59
1:B:23:GLU:OE2	2:B:202:HOH:O	2.16	0.59
1:E:45:SER:OG	1:E:47:VAL:HG22	2.03	0.57
1:D:30:TYR:CE1	1:D:68:GLN:HG2	2.41	0.56
1:B:172:ASN:HB3	2:B:219:HOH:O	2.05	0.56
1:A:-2:PHE:CE1	1:A:1:MET:HB2	2.41	0.55
1:E:45:SER:O	2:E:204:HOH:O	2.18	0.54
1:D:152:ALA:O	1:D:156:VAL:HG23	2.08	0.54
1:E:1:MET:HG2	1:E:2:VAL:N	2.23	0.54
1:I:84:THR:HG22	1:I:93:LEU:HD23	1.91	0.53
1:G:47:VAL:HB	1:G:124:ARG:NH2	2.24	0.52
1:J:168:VAL:HG21	2:J:245:HOH:O	2.10	0.52
1:C:42:LEU:O	1:C:45:SER:OG	2.15	0.51
1:H:105:ASN:O	1:H:106:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:THR:O	1:G:167:THR:HG22	2.10	0.51
1:J:40:VAL:HB	1:J:41:PRO:HD2	1.91	0.51
1:H:46:PHE:O	1:H:49:PRO:HD2	2.09	0.51
1:J:5:VAL:O	1:J:6:GLN:HB2	2.11	0.51
1:E:130:ASP:HB2	1:E:131:PRO:CD	2.41	0.50
1:G:51:GLU:OE1	1:G:124:ARG:NH1	2.45	0.50
1:J:40:VAL:HB	1:J:41:PRO:CD	2.42	0.49
1:E:162:THR:HG23	2:E:209:HOH:O	2.12	0.49
1:G:34:TYR:CE1	1:G:131:PRO:HD3	2.47	0.49
1:E:159:PHE:HA	1:E:162:THR:HG22	1.96	0.48
1:A:105:ASN:O	1:A:106:HIS:HB2	2.14	0.48
1:A:16:ALA:HB2	1:A:101:LEU:HD22	1.94	0.48
1:J:52:ILE:HG23	1:J:71:PHE:CE2	2.49	0.48
1:J:159:PHE:HA	1:J:162:THR:HG22	1.96	0.47
1:G:152:ALA:O	1:G:156:VAL:HG23	2.14	0.47
1:D:105:ASN:O	1:D:106:HIS:HB2	2.14	0.47
1:E:55:PHE:HB2	1:E:71:PHE:HZ	1.80	0.47
1:C:34:TYR:CE1	1:C:160:GLN:HG3	2.50	0.46
1:E:64:ASP:O	1:E:179:THR:HG21	2.16	0.46
1:B:161:TRP:CH2	1:B:170:PRO:HD3	2.50	0.46
1:H:167:THR:C	2:H:203:HOH:O	2.53	0.46
1:A:130:ASP:HB2	1:A:131:PRO:CD	2.45	0.46
1:G:130:ASP:HB2	1:G:131:PRO:CD	2.45	0.46
1:E:41[B]:PRO:HD3	1:E:124:ARG:HH12	1.80	0.46
1:J:51:GLU:OE1	1:J:124:ARG:NH1	2.48	0.46
1:F:88:ARG:HH12	1:F:94:GLY:HA3	1.81	0.46
1:B:5:VAL:O	1:B:6:GLN:HB2	2.16	0.45
1:J:168:VAL:O	1:J:168:VAL:HG22	2.16	0.45
1:B:175:PRO:O	2:B:203:HOH:O	2.21	0.45
1:D:5:VAL:O	1:D:6:GLN:HB2	2.16	0.45
1:C:84:THR:HG22	1:C:93:LEU:HD23	1.98	0.45
1:D:48:SER:O	1:D:52:ILE:HD12	2.17	0.45
1:H:47:VAL:HB	1:H:124:ARG:NH2	2.31	0.45
1:F:5:VAL:O	1:F:6:GLN:HB2	2.17	0.45
1:J:65:GLN:OE1	1:J:157:GLU:HG2	2.17	0.44
1:J:167:THR:HG23	2:J:242:HOH:O	2.18	0.44
1:D:130:ASP:HB2	1:D:131:PRO:CD	2.47	0.44
1:E:40[B]:VAL:HB	1:E:41[B]:PRO:CD	2.47	0.44
1:C:31:LYS:O	2:C:202:HOH:O	2.21	0.43
1:E:71:PHE:CE2	1:E:98:VAL:HG21	2.52	0.43
1:H:130:ASP:HB2	1:H:131:PRO:CD	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:GLY:O	1:E:162:THR:HG22	2.18	0.43
1:A:82:ALA:O	1:A:86:LEU:HD13	2.18	0.43
1:C:41:PRO:HD2	1:C:48:SER:OG	2.19	0.43
1:E:41[A]:PRO:CG	1:E:143:LEU:HD22	2.49	0.43
1:F:105:ASN:O	1:F:106:HIS:HB2	2.19	0.43
1:D:65:GLN:O	1:D:160:GLN:NE2	2.51	0.43
1:J:168:VAL:O	1:J:168:VAL:HG13	2.19	0.43
1:J:71:PHE:HB2	1:J:100:LEU:HD23	2.00	0.43
1:D:38:ALA:O	1:D:71:PHE:HA	2.19	0.42
1:I:125:GLY:HA2	1:I:139:THR:O	2.20	0.42
1:B:167:THR:HG22	1:B:168:VAL:N	2.34	0.42
1:E:5:VAL:O	1:E:6:GLN:HB2	2.19	0.42
1:I:130:ASP:HB2	1:I:131:PRO:CD	2.50	0.42
1:G:41:PRO:HG3	1:G:143:LEU:HD22	2.01	0.42
1:E:40[B]:VAL:HB	1:E:41[B]:PRO:HD2	2.02	0.42
1:F:169:LEU:HB3	1:F:170:PRO:HD2	2.02	0.42
1:B:53:VAL:HG13	1:B:88:ARG:NH1	2.35	0.42
1:I:3:ALA:HB1	1:I:135:ILE:CD1	2.49	0.42
1:E:41[B]:PRO:O	1:E:42:LEU:C	2.58	0.42
1:I:5:VAL:O	1:I:6:GLN:HB2	2.20	0.42
1:A:48:SER:O	1:A:52:ILE:HD12	2.20	0.42
1:D:149:VAL:HG12	2:D:228:HOH:O	2.20	0.42
1:J:167:THR:CG2	1:J:168:VAL:N	2.82	0.41
1:I:177:ALA:O	1:I:178:ALA:HB3	2.20	0.41
1:J:71:PHE:CE2	1:J:98:VAL:HG21	2.55	0.41
1:H:152:ALA:O	1:H:156:VAL:HG23	2.20	0.41
1:A:48:SER:N	1:A:49:PRO:CD	2.84	0.41
1:F:60:LYS:NZ	2:F:209:HOH:O	2.50	0.41
1:J:-2:PHE:CZ	1:J:1:MET:HB2	2.56	0.41
1:E:41[B]:PRO:HB3	1:E:124:ARG:NH2	2.36	0.41
1:E:71:PHE:CE2	1:E:98:VAL:CG2	3.03	0.41
1:F:86:LEU:O	1:F:92:GLY:HA3	2.21	0.41
1:G:81:LEU:O	1:G:84:THR:HG22	2.20	0.41
1:D:29:LYS:O	1:D:29:LYS:HG2	2.20	0.41
1:H:151:GLU:HA	1:H:151:GLU:OE1	2.20	0.41
1:C:47:VAL:HB	1:C:124:ARG:NH1	2.35	0.41
1:F:38:ALA:O	1:F:71:PHE:HA	2.20	0.41
1:G:105:ASN:C	1:G:105:ASN:OD1	2.57	0.41
1:C:105:ASN:O	1:C:106:HIS:HB2	2.20	0.40
1:E:101:LEU:N	1:E:101:LEU:HD12	2.35	0.40
1:I:41:PRO:HG3	1:I:143:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:PRO:HG3	1:F:143:LEU:HD22	2.03	0.40
1:I:137:HIS:ND1	1:J:141:ASN:OD1	2.44	0.40
1:F:46:PHE:O	1:F:49:PRO:HD2	2.21	0.40
1:H:58:ALA:O	1:H:59:ALA:C	2.59	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:202:HOH:O	2:F:204:HOH:O[3_548]	1.87	0.33
2:E:253:HOH:O	2:J:201:HOH:O[3_558]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/217 (91%)	190 (96%)	7 (4%)	0	100	100
1	B	174/217 (80%)	166 (95%)	8 (5%)	0	100	100
1	C	170/217 (78%)	161 (95%)	9 (5%)	0	100	100
1	D	168/217 (77%)	158 (94%)	10 (6%)	0	100	100
1	E	183/217 (84%)	173 (94%)	9 (5%)	1 (0%)	29	31
1	F	174/217 (80%)	166 (95%)	8 (5%)	0	100	100
1	G	169/217 (78%)	161 (95%)	8 (5%)	0	100	100
1	H	169/217 (78%)	159 (94%)	10 (6%)	0	100	100
1	I	184/217 (85%)	176 (96%)	7 (4%)	1 (0%)	29	31
1	J	170/217 (78%)	164 (96%)	6 (4%)	0	100	100
All	All	1758/2170 (81%)	1674 (95%)	82 (5%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	42	LEU
1	I	166	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/184 (91%)	167 (100%)	0	100	100
1	B	148/184 (80%)	146 (99%)	2 (1%)	67	80
1	C	144/184 (78%)	143 (99%)	1 (1%)	84	91
1	D	142/184 (77%)	142 (100%)	0	100	100
1	E	154/184 (84%)	154 (100%)	0	100	100
1	F	148/184 (80%)	147 (99%)	1 (1%)	84	91
1	G	143/184 (78%)	143 (100%)	0	100	100
1	H	143/184 (78%)	143 (100%)	0	100	100
1	I	155/184 (84%)	155 (100%)	0	100	100
1	J	144/184 (78%)	144 (100%)	0	100	100
All	All	1488/1840 (81%)	1484 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	2	VAL
1	C	31	LYS
1	F	46	PHE

Some 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 carbohydrates 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	199/217 (91%)	-0.09	6 (3%) 50 48	42, 54, 84, 126	0
1	B	176/217 (81%)	0.06	5 (2%) 53 51	42, 56, 81, 93	0
1	C	172/217 (79%)	0.01	9 (5%) 27 26	43, 57, 88, 124	0
1	D	170/217 (78%)	0.02	12 (7%) 16 14	42, 63, 98, 112	0
1	E	183/217 (84%)	-0.05	8 (4%) 34 32	40, 53, 95, 125	0
1	F	176/217 (81%)	-0.04	8 (4%) 33 32	40, 55, 91, 119	0
1	G	171/217 (78%)	0.17	8 (4%) 31 30	44, 61, 91, 109	0
1	H	171/217 (78%)	-0.06	6 (3%) 44 42	41, 56, 89, 114	0
1	I	186/217 (85%)	-0.06	6 (3%) 47 45	40, 57, 89, 121	0
1	J	172/217 (79%)	0.03	8 (4%) 31 30	43, 56, 80, 118	0
All	All	1776/2170 (81%)	-0.00	76 (4%) 35 33	40, 57, 90, 126	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-2	PHE	9.0
1	I	-2	PHE	8.3
1	E	-2	PHE	6.7
1	E	-3	TYR	6.5
1	A	-2	PHE	6.4
1	J	-2	PHE	5.7
1	C	-1	GLN	5.7
1	E	-1	GLN	5.6
1	G	-2	PHE	5.4
1	J	167	THR	4.6
1	F	-2	PHE	4.4
1	D	166	GLY	4.3
1	D	-2	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	-3	TYR	4.2
1	G	164	LYS	4.1
1	I	-1	GLN	4.1
1	H	167	THR	3.9
1	D	164	LYS	3.9
1	A	-3	TYR	3.8
1	C	46	PHE	3.6
1	F	-1	GLN	3.6
1	G	-3	TYR	3.6
1	J	168	VAL	3.5
1	D	161	TRP	3.4
1	A	-1	GLN	3.4
1	B	21	ILE	3.4
1	D	89	LYS	3.2
1	H	-2	PHE	3.1
1	I	0	GLY	3.0
1	B	1	MET	2.9
1	F	1	MET	2.9
1	B	22	PHE	2.9
1	E	46	PHE	2.9
1	H	-1	GLN	2.9
1	C	167	THR	2.9
1	G	161	TRP	2.9
1	H	46	PHE	2.9
1	I	-3	TYR	2.9
1	I	1	MET	2.8
1	G	166	GLY	2.7
1	C	89	LYS	2.7
1	D	-3	TYR	2.7
1	E	0	GLY	2.7
1	G	1	MET	2.6
1	D	165	ASN	2.6
1	F	90	ASP	2.6
1	C	0	GLY	2.5
1	G	165	ASN	2.5
1	F	46	PHE	2.5
1	I	171	CYS	2.5
1	E	48	SER	2.4
1	J	-1	GLN	2.4
1	D	1	MET	2.4
1	D	162	THR	2.4
1	E	1	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	-3	TYR	2.3
1	J	161	TRP	2.3
1	E	179	THR	2.3
1	D	0	GLY	2.3
1	F	0	GLY	2.3
1	A	46	PHE	2.2
1	B	2	VAL	2.2
1	G	89	LYS	2.2
1	F	169	LEU	2.2
1	A	90	ASP	2.2
1	F	-3	TYR	2.1
1	J	164	LYS	2.1
1	C	90	ASP	2.1
1	C	1	MET	2.1
1	B	18	VAL	2.1
1	H	-3	TYR	2.1
1	D	86	LEU	2.0
1	J	166	GLY	2.0
1	D	90	ASP	2.0
1	H	165	ASN	2.0
1	A	179	THR	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 carbohydrates 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.