



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2024 – 01:48 PM EDT

PDB ID : 4KK0  
Title : Crystal Structure of TSC1 core domain from *S. pombe*  
Authors : Sun, W.; Zhu, Y.; Wang, Z.Z.; Zhong, Q.; Gao, F.; Lou, J.Z.; Gong, W.M.;  
Xu, W.Q.  
Deposited on : 2013-05-05  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

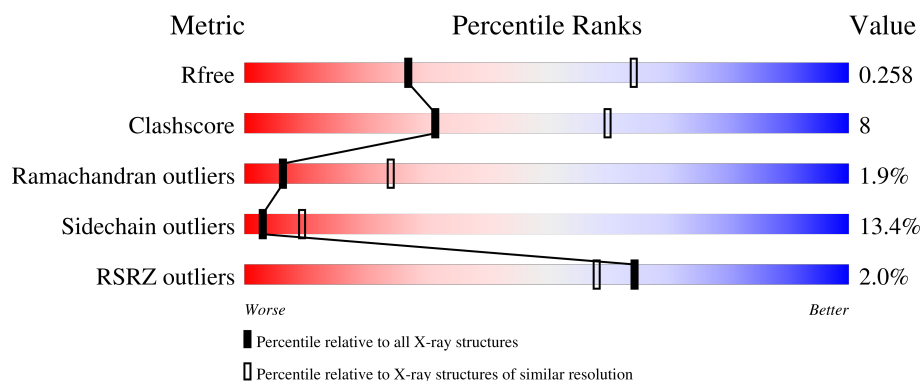
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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  $\geq 3$ , 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	461	<div> <div>2%</div> <div>64% 20% 13%</div> </div>
1	B	461	<div> <div>2%</div> <div>56% 24% 15%</div> </div>
1	C	461	<div> <div>0%</div> <div>60% 20% 5% 15%</div> </div>
1	D	461	<div> <div>2%</div> <div>65% 18% 15%</div> </div>
1	E	461	<div> <div>2%</div> <div>59% 21% 5% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	461	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>62%</div><div>19%</div><div>• •</div><div>15%</div></div></div>
1	G	461	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>62%</div><div>19%</div><div>•</div><div>15%</div></div></div>
1	H	461	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>63%</div><div>18%</div><div>•</div><div>15%</div></div></div>
1	I	461	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>17%</div><div>5%</div><div>15%</div></div></div>
1	J	461	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>%</div><div>61%</div><div>19%</div><div>•</div><div>15%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31897 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 Tuberous sclerosis 1 protein homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	Se	0	0	0
			3268	2116	548	591	8	5			
1	B	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	C	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	D	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	E	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	F	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	G	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	H	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	I	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			
1	J	391	Total	C	N	O	S	Se	0	0	0
			3181	2066	532	570	8	5			

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MSE	-	expression tag	UNP Q09778
A	-28	GLY	-	expression tag	UNP Q09778
A	-27	SER	-	expression tag	UNP Q09778
A	-26	SER	-	expression tag	UNP Q09778
A	-25	HIS	-	expression tag	UNP Q09778
A	-24	HIS	-	expression tag	UNP Q09778
A	-23	HIS	-	expression tag	UNP Q09778
A	-22	HIS	-	expression tag	UNP Q09778
A	-21	HIS	-	expression tag	UNP Q09778

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	HIS	-	expression tag	UNP Q09778
A	-19	SER	-	expression tag	UNP Q09778
A	-18	SER	-	expression tag	UNP Q09778
A	-17	GLY	-	expression tag	UNP Q09778
A	-16	LEU	-	expression tag	UNP Q09778
A	-15	VAL	-	expression tag	UNP Q09778
A	-14	PRO	-	expression tag	UNP Q09778
A	-13	ARG	-	expression tag	UNP Q09778
A	-12	GLY	-	expression tag	UNP Q09778
A	-11	SER	-	expression tag	UNP Q09778
A	-10	HIS	-	expression tag	UNP Q09778
A	-9	SER	-	expression tag	UNP Q09778
A	-8	GLU	-	expression tag	UNP Q09778
A	-7	ASN	-	expression tag	UNP Q09778
A	-6	LEU	-	expression tag	UNP Q09778
A	-5	TYR	-	expression tag	UNP Q09778
A	-4	PHE	-	expression tag	UNP Q09778
A	-3	GLN	-	expression tag	UNP Q09778
A	-2	SER	-	expression tag	UNP Q09778
A	-1	HIS	-	expression tag	UNP Q09778
A	0	MSE	-	expression tag	UNP Q09778
B	-29	MSE	-	expression tag	UNP Q09778
B	-28	GLY	-	expression tag	UNP Q09778
B	-27	SER	-	expression tag	UNP Q09778
B	-26	SER	-	expression tag	UNP Q09778
B	-25	HIS	-	expression tag	UNP Q09778
B	-24	HIS	-	expression tag	UNP Q09778
B	-23	HIS	-	expression tag	UNP Q09778
B	-22	HIS	-	expression tag	UNP Q09778
B	-21	HIS	-	expression tag	UNP Q09778
B	-20	HIS	-	expression tag	UNP Q09778
B	-19	SER	-	expression tag	UNP Q09778
B	-18	SER	-	expression tag	UNP Q09778
B	-17	GLY	-	expression tag	UNP Q09778
B	-16	LEU	-	expression tag	UNP Q09778
B	-15	VAL	-	expression tag	UNP Q09778
B	-14	PRO	-	expression tag	UNP Q09778
B	-13	ARG	-	expression tag	UNP Q09778
B	-12	GLY	-	expression tag	UNP Q09778
B	-11	SER	-	expression tag	UNP Q09778
B	-10	HIS	-	expression tag	UNP Q09778
B	-9	SER	-	expression tag	UNP Q09778

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLU	-	expression tag	UNP Q09778
B	-7	ASN	-	expression tag	UNP Q09778
B	-6	LEU	-	expression tag	UNP Q09778
B	-5	TYR	-	expression tag	UNP Q09778
B	-4	PHE	-	expression tag	UNP Q09778
B	-3	GLN	-	expression tag	UNP Q09778
B	-2	SER	-	expression tag	UNP Q09778
B	-1	HIS	-	expression tag	UNP Q09778
B	0	MSE	-	expression tag	UNP Q09778
C	-29	MSE	-	expression tag	UNP Q09778
C	-28	GLY	-	expression tag	UNP Q09778
C	-27	SER	-	expression tag	UNP Q09778
C	-26	SER	-	expression tag	UNP Q09778
C	-25	HIS	-	expression tag	UNP Q09778
C	-24	HIS	-	expression tag	UNP Q09778
C	-23	HIS	-	expression tag	UNP Q09778
C	-22	HIS	-	expression tag	UNP Q09778
C	-21	HIS	-	expression tag	UNP Q09778
C	-20	HIS	-	expression tag	UNP Q09778
C	-19	SER	-	expression tag	UNP Q09778
C	-18	SER	-	expression tag	UNP Q09778
C	-17	GLY	-	expression tag	UNP Q09778
C	-16	LEU	-	expression tag	UNP Q09778
C	-15	VAL	-	expression tag	UNP Q09778
C	-14	PRO	-	expression tag	UNP Q09778
C	-13	ARG	-	expression tag	UNP Q09778
C	-12	GLY	-	expression tag	UNP Q09778
C	-11	SER	-	expression tag	UNP Q09778
C	-10	HIS	-	expression tag	UNP Q09778
C	-9	SER	-	expression tag	UNP Q09778
C	-8	GLU	-	expression tag	UNP Q09778
C	-7	ASN	-	expression tag	UNP Q09778
C	-6	LEU	-	expression tag	UNP Q09778
C	-5	TYR	-	expression tag	UNP Q09778
C	-4	PHE	-	expression tag	UNP Q09778
C	-3	GLN	-	expression tag	UNP Q09778
C	-2	SER	-	expression tag	UNP Q09778
C	-1	HIS	-	expression tag	UNP Q09778
C	0	MSE	-	expression tag	UNP Q09778
D	-29	MSE	-	expression tag	UNP Q09778
D	-28	GLY	-	expression tag	UNP Q09778
D	-27	SER	-	expression tag	UNP Q09778

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-26	SER	-	expression tag	UNP Q09778
D	-25	HIS	-	expression tag	UNP Q09778
D	-24	HIS	-	expression tag	UNP Q09778
D	-23	HIS	-	expression tag	UNP Q09778
D	-22	HIS	-	expression tag	UNP Q09778
D	-21	HIS	-	expression tag	UNP Q09778
D	-20	HIS	-	expression tag	UNP Q09778
D	-19	SER	-	expression tag	UNP Q09778
D	-18	SER	-	expression tag	UNP Q09778
D	-17	GLY	-	expression tag	UNP Q09778
D	-16	LEU	-	expression tag	UNP Q09778
D	-15	VAL	-	expression tag	UNP Q09778
D	-14	PRO	-	expression tag	UNP Q09778
D	-13	ARG	-	expression tag	UNP Q09778
D	-12	GLY	-	expression tag	UNP Q09778
D	-11	SER	-	expression tag	UNP Q09778
D	-10	HIS	-	expression tag	UNP Q09778
D	-9	SER	-	expression tag	UNP Q09778
D	-8	GLU	-	expression tag	UNP Q09778
D	-7	ASN	-	expression tag	UNP Q09778
D	-6	LEU	-	expression tag	UNP Q09778
D	-5	TYR	-	expression tag	UNP Q09778
D	-4	PHE	-	expression tag	UNP Q09778
D	-3	GLN	-	expression tag	UNP Q09778
D	-2	SER	-	expression tag	UNP Q09778
D	-1	HIS	-	expression tag	UNP Q09778
D	0	MSE	-	expression tag	UNP Q09778
E	-29	MSE	-	expression tag	UNP Q09778
E	-28	GLY	-	expression tag	UNP Q09778
E	-27	SER	-	expression tag	UNP Q09778
E	-26	SER	-	expression tag	UNP Q09778
E	-25	HIS	-	expression tag	UNP Q09778
E	-24	HIS	-	expression tag	UNP Q09778
E	-23	HIS	-	expression tag	UNP Q09778
E	-22	HIS	-	expression tag	UNP Q09778
E	-21	HIS	-	expression tag	UNP Q09778
E	-20	HIS	-	expression tag	UNP Q09778
E	-19	SER	-	expression tag	UNP Q09778
E	-18	SER	-	expression tag	UNP Q09778
E	-17	GLY	-	expression tag	UNP Q09778
E	-16	LEU	-	expression tag	UNP Q09778
E	-15	VAL	-	expression tag	UNP Q09778

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	PRO	-	expression tag	UNP Q09778
E	-13	ARG	-	expression tag	UNP Q09778
E	-12	GLY	-	expression tag	UNP Q09778
E	-11	SER	-	expression tag	UNP Q09778
E	-10	HIS	-	expression tag	UNP Q09778
E	-9	SER	-	expression tag	UNP Q09778
E	-8	GLU	-	expression tag	UNP Q09778
E	-7	ASN	-	expression tag	UNP Q09778
E	-6	LEU	-	expression tag	UNP Q09778
E	-5	TYR	-	expression tag	UNP Q09778
E	-4	PHE	-	expression tag	UNP Q09778
E	-3	GLN	-	expression tag	UNP Q09778
E	-2	SER	-	expression tag	UNP Q09778
E	-1	HIS	-	expression tag	UNP Q09778
E	0	MSE	-	expression tag	UNP Q09778
F	-29	MSE	-	expression tag	UNP Q09778
F	-28	GLY	-	expression tag	UNP Q09778
F	-27	SER	-	expression tag	UNP Q09778
F	-26	SER	-	expression tag	UNP Q09778
F	-25	HIS	-	expression tag	UNP Q09778
F	-24	HIS	-	expression tag	UNP Q09778
F	-23	HIS	-	expression tag	UNP Q09778
F	-22	HIS	-	expression tag	UNP Q09778
F	-21	HIS	-	expression tag	UNP Q09778
F	-20	HIS	-	expression tag	UNP Q09778
F	-19	SER	-	expression tag	UNP Q09778
F	-18	SER	-	expression tag	UNP Q09778
F	-17	GLY	-	expression tag	UNP Q09778
F	-16	LEU	-	expression tag	UNP Q09778
F	-15	VAL	-	expression tag	UNP Q09778
F	-14	PRO	-	expression tag	UNP Q09778
F	-13	ARG	-	expression tag	UNP Q09778
F	-12	GLY	-	expression tag	UNP Q09778
F	-11	SER	-	expression tag	UNP Q09778
F	-10	HIS	-	expression tag	UNP Q09778
F	-9	SER	-	expression tag	UNP Q09778
F	-8	GLU	-	expression tag	UNP Q09778
F	-7	ASN	-	expression tag	UNP Q09778
F	-6	LEU	-	expression tag	UNP Q09778
F	-5	TYR	-	expression tag	UNP Q09778
F	-4	PHE	-	expression tag	UNP Q09778
F	-3	GLN	-	expression tag	UNP Q09778

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	SER	-	expression tag	UNP Q09778
F	-1	HIS	-	expression tag	UNP Q09778
F	0	MSE	-	expression tag	UNP Q09778
G	-29	MSE	-	expression tag	UNP Q09778
G	-28	GLY	-	expression tag	UNP Q09778
G	-27	SER	-	expression tag	UNP Q09778
G	-26	SER	-	expression tag	UNP Q09778
G	-25	HIS	-	expression tag	UNP Q09778
G	-24	HIS	-	expression tag	UNP Q09778
G	-23	HIS	-	expression tag	UNP Q09778
G	-22	HIS	-	expression tag	UNP Q09778
G	-21	HIS	-	expression tag	UNP Q09778
G	-20	HIS	-	expression tag	UNP Q09778
G	-19	SER	-	expression tag	UNP Q09778
G	-18	SER	-	expression tag	UNP Q09778
G	-17	GLY	-	expression tag	UNP Q09778
G	-16	LEU	-	expression tag	UNP Q09778
G	-15	VAL	-	expression tag	UNP Q09778
G	-14	PRO	-	expression tag	UNP Q09778
G	-13	ARG	-	expression tag	UNP Q09778
G	-12	GLY	-	expression tag	UNP Q09778
G	-11	SER	-	expression tag	UNP Q09778
G	-10	HIS	-	expression tag	UNP Q09778
G	-9	SER	-	expression tag	UNP Q09778
G	-8	GLU	-	expression tag	UNP Q09778
G	-7	ASN	-	expression tag	UNP Q09778
G	-6	LEU	-	expression tag	UNP Q09778
G	-5	TYR	-	expression tag	UNP Q09778
G	-4	PHE	-	expression tag	UNP Q09778
G	-3	GLN	-	expression tag	UNP Q09778
G	-2	SER	-	expression tag	UNP Q09778
G	-1	HIS	-	expression tag	UNP Q09778
G	0	MSE	-	expression tag	UNP Q09778
H	-29	MSE	-	expression tag	UNP Q09778
H	-28	GLY	-	expression tag	UNP Q09778
H	-27	SER	-	expression tag	UNP Q09778
H	-26	SER	-	expression tag	UNP Q09778
H	-25	HIS	-	expression tag	UNP Q09778
H	-24	HIS	-	expression tag	UNP Q09778
H	-23	HIS	-	expression tag	UNP Q09778
H	-22	HIS	-	expression tag	UNP Q09778
H	-21	HIS	-	expression tag	UNP Q09778

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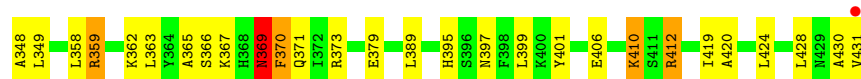
Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	HIS	-	expression tag	UNP Q09778
H	-19	SER	-	expression tag	UNP Q09778
H	-18	SER	-	expression tag	UNP Q09778
H	-17	GLY	-	expression tag	UNP Q09778
H	-16	LEU	-	expression tag	UNP Q09778
H	-15	VAL	-	expression tag	UNP Q09778
H	-14	PRO	-	expression tag	UNP Q09778
H	-13	ARG	-	expression tag	UNP Q09778
H	-12	GLY	-	expression tag	UNP Q09778
H	-11	SER	-	expression tag	UNP Q09778
H	-10	HIS	-	expression tag	UNP Q09778
H	-9	SER	-	expression tag	UNP Q09778
H	-8	GLU	-	expression tag	UNP Q09778
H	-7	ASN	-	expression tag	UNP Q09778
H	-6	LEU	-	expression tag	UNP Q09778
H	-5	TYR	-	expression tag	UNP Q09778
H	-4	PHE	-	expression tag	UNP Q09778
H	-3	GLN	-	expression tag	UNP Q09778
H	-2	SER	-	expression tag	UNP Q09778
H	-1	HIS	-	expression tag	UNP Q09778
H	0	MSE	-	expression tag	UNP Q09778
I	-29	MSE	-	expression tag	UNP Q09778
I	-28	GLY	-	expression tag	UNP Q09778
I	-27	SER	-	expression tag	UNP Q09778
I	-26	SER	-	expression tag	UNP Q09778
I	-25	HIS	-	expression tag	UNP Q09778
I	-24	HIS	-	expression tag	UNP Q09778
I	-23	HIS	-	expression tag	UNP Q09778
I	-22	HIS	-	expression tag	UNP Q09778
I	-21	HIS	-	expression tag	UNP Q09778
I	-20	HIS	-	expression tag	UNP Q09778
I	-19	SER	-	expression tag	UNP Q09778
I	-18	SER	-	expression tag	UNP Q09778
I	-17	GLY	-	expression tag	UNP Q09778
I	-16	LEU	-	expression tag	UNP Q09778
I	-15	VAL	-	expression tag	UNP Q09778
I	-14	PRO	-	expression tag	UNP Q09778
I	-13	ARG	-	expression tag	UNP Q09778
I	-12	GLY	-	expression tag	UNP Q09778
I	-11	SER	-	expression tag	UNP Q09778
I	-10	HIS	-	expression tag	UNP Q09778
I	-9	SER	-	expression tag	UNP Q09778

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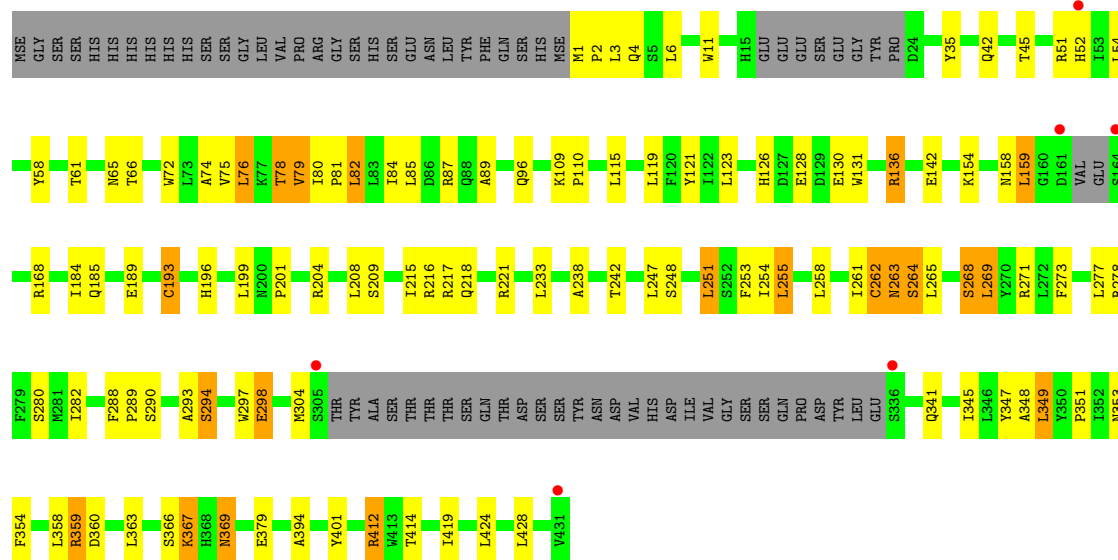
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Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLU	-	expression tag	UNP Q09778
I	-7	ASN	-	expression tag	UNP Q09778
I	-6	LEU	-	expression tag	UNP Q09778
I	-5	TYR	-	expression tag	UNP Q09778
I	-4	PHE	-	expression tag	UNP Q09778
I	-3	GLN	-	expression tag	UNP Q09778
I	-2	SER	-	expression tag	UNP Q09778
I	-1	HIS	-	expression tag	UNP Q09778
I	0	MSE	-	expression tag	UNP Q09778
J	-29	MSE	-	expression tag	UNP Q09778
J	-28	GLY	-	expression tag	UNP Q09778
J	-27	SER	-	expression tag	UNP Q09778
J	-26	SER	-	expression tag	UNP Q09778
J	-25	HIS	-	expression tag	UNP Q09778
J	-24	HIS	-	expression tag	UNP Q09778
J	-23	HIS	-	expression tag	UNP Q09778
J	-22	HIS	-	expression tag	UNP Q09778
J	-21	HIS	-	expression tag	UNP Q09778
J	-20	HIS	-	expression tag	UNP Q09778
J	-19	SER	-	expression tag	UNP Q09778
J	-18	SER	-	expression tag	UNP Q09778
J	-17	GLY	-	expression tag	UNP Q09778
J	-16	LEU	-	expression tag	UNP Q09778
J	-15	VAL	-	expression tag	UNP Q09778
J	-14	PRO	-	expression tag	UNP Q09778
J	-13	ARG	-	expression tag	UNP Q09778
J	-12	GLY	-	expression tag	UNP Q09778
J	-11	SER	-	expression tag	UNP Q09778
J	-10	HIS	-	expression tag	UNP Q09778
J	-9	SER	-	expression tag	UNP Q09778
J	-8	GLU	-	expression tag	UNP Q09778
J	-7	ASN	-	expression tag	UNP Q09778
J	-6	LEU	-	expression tag	UNP Q09778
J	-5	TYR	-	expression tag	UNP Q09778
J	-4	PHE	-	expression tag	UNP Q09778
J	-3	GLN	-	expression tag	UNP Q09778
J	-2	SER	-	expression tag	UNP Q09778
J	-1	HIS	-	expression tag	UNP Q09778
J	0	MSE	-	expression tag	UNP Q09778

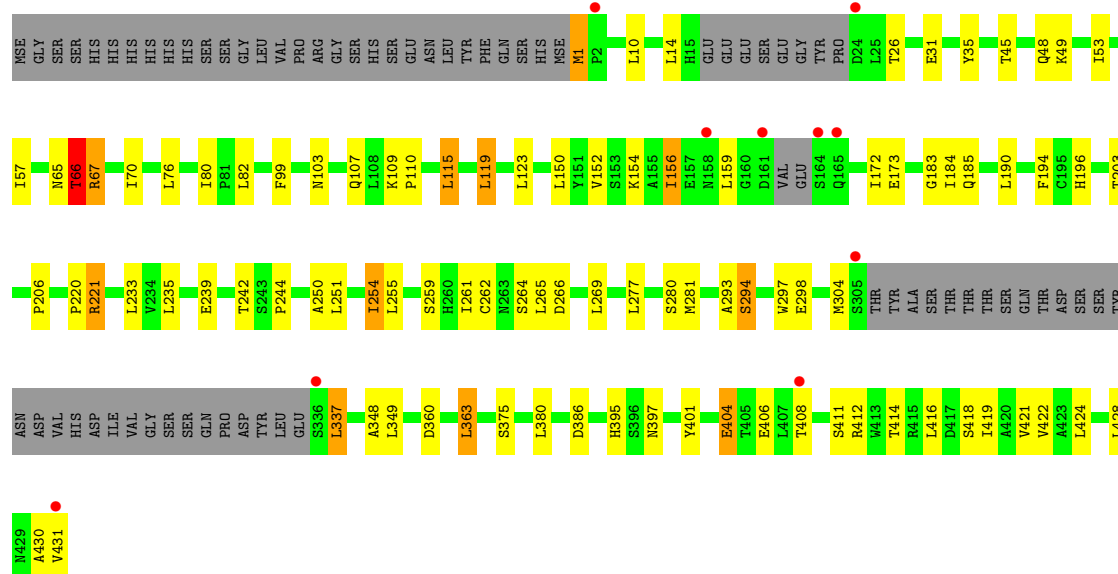




• Molecule 1: Tuberous sclerosis 1 protein homolog

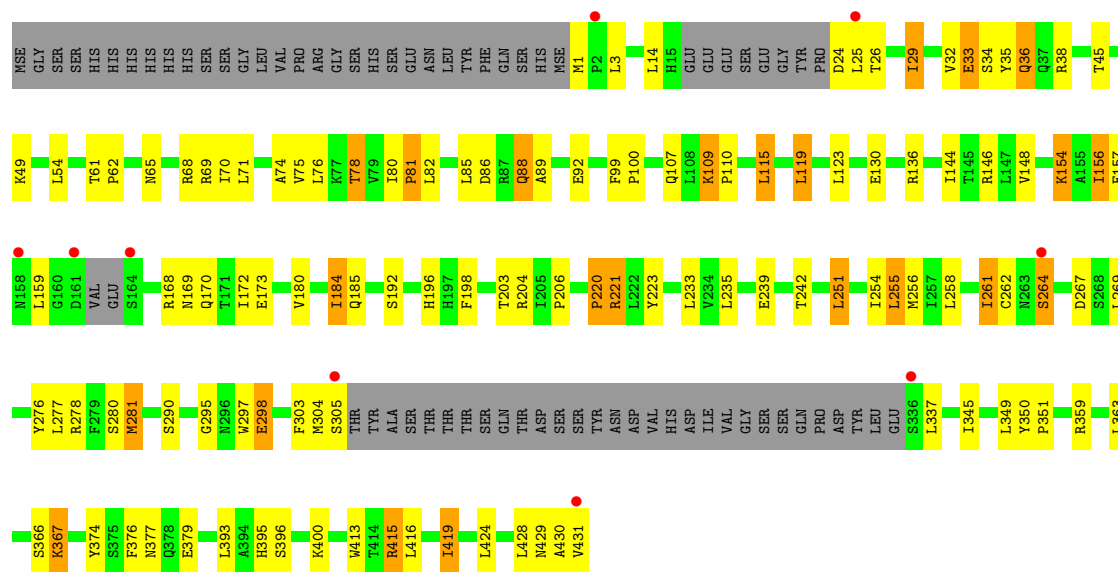


• Molecule 1: Tuberous sclerosis 1 protein homolog

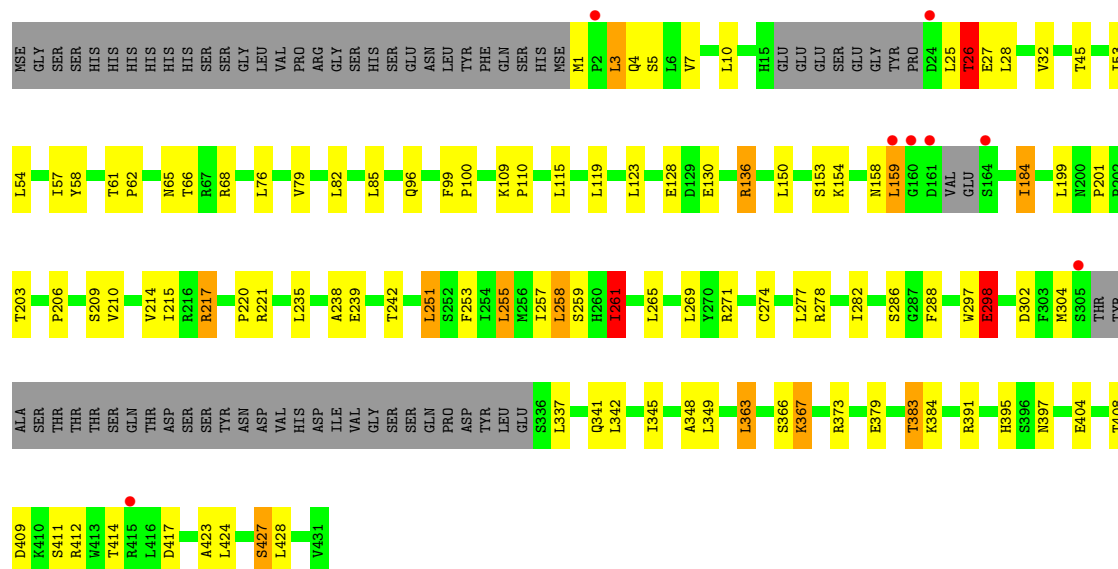


• Molecule 1: Tuberous sclerosis 1 protein homolog

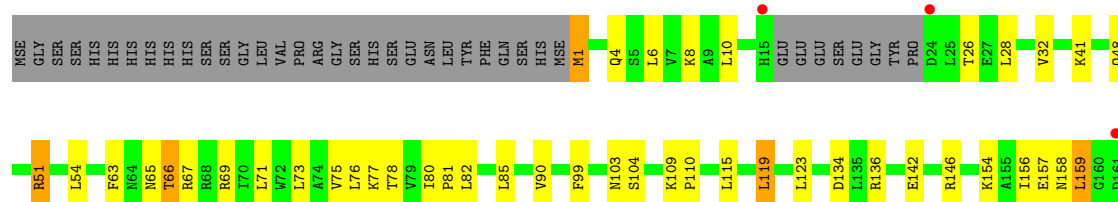


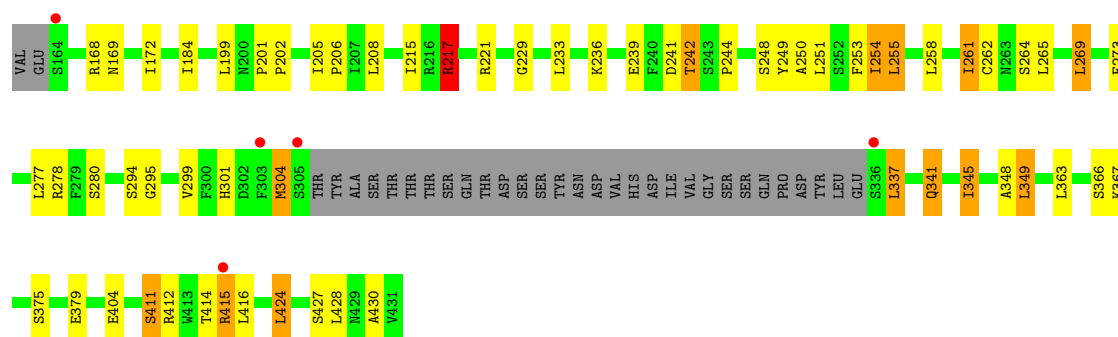


• Molecule 1: Tuberous sclerosis 1 protein homolog

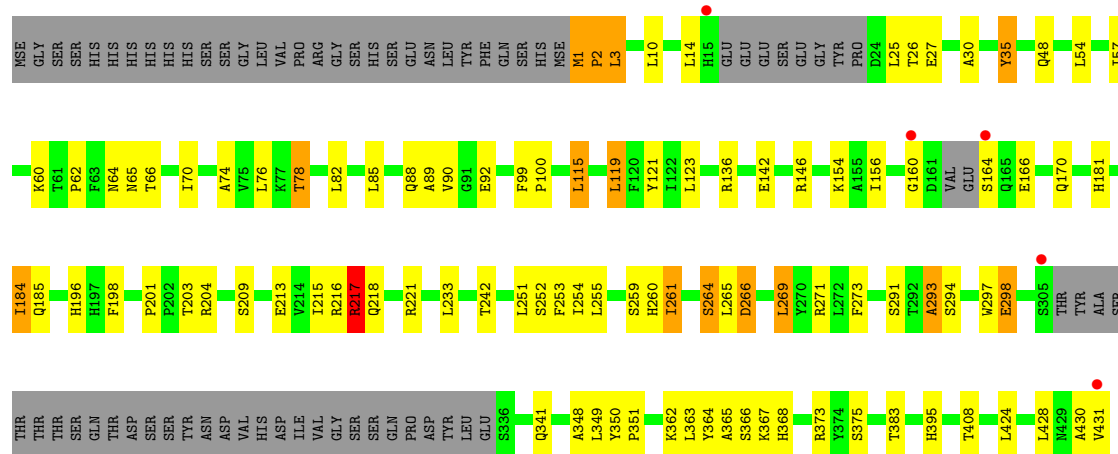


• Molecule 1: Tuberous sclerosis 1 protein homolog

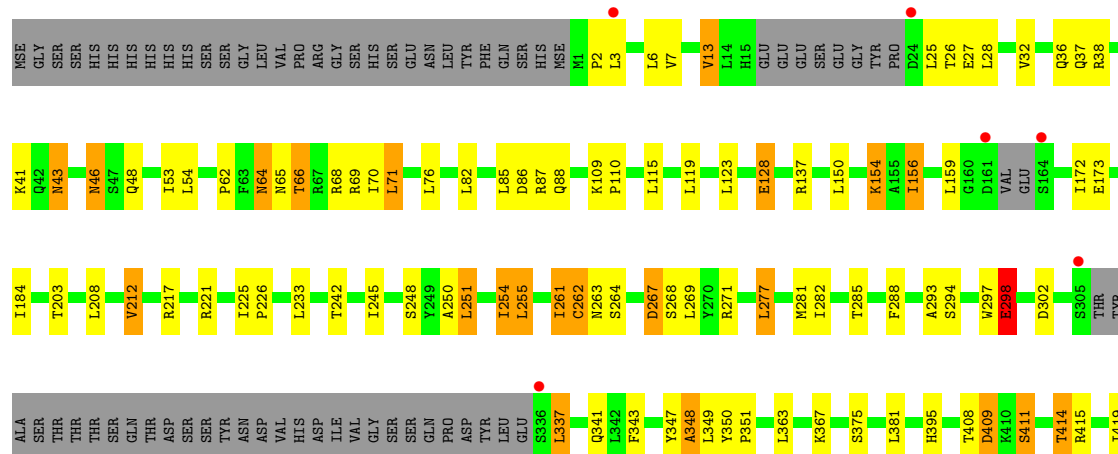




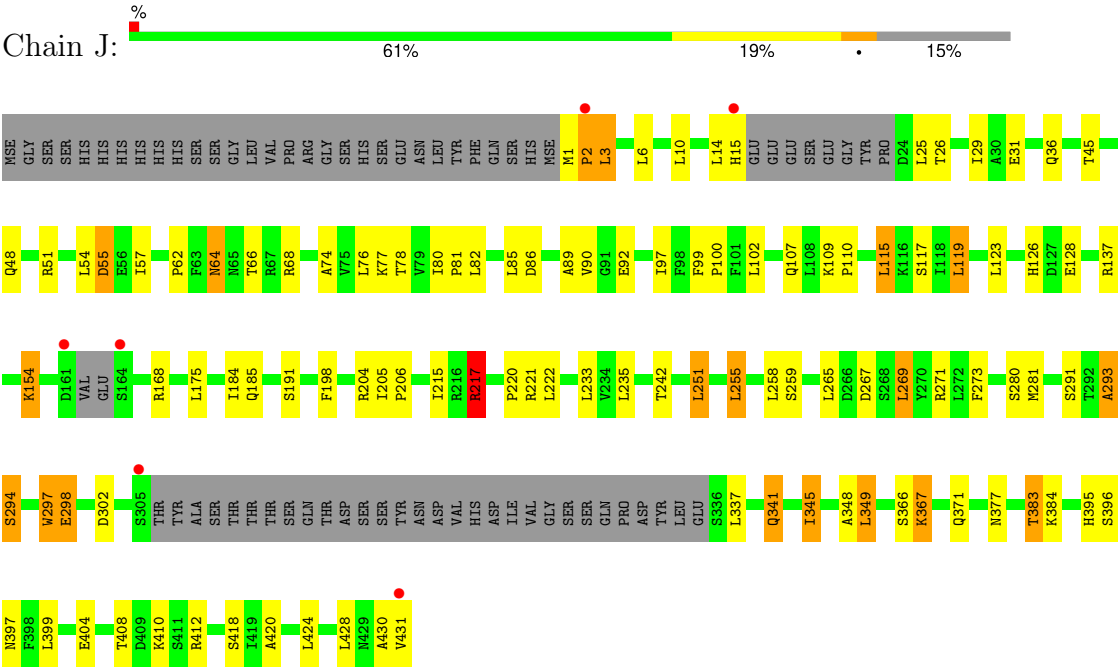
• Molecule 1: Tuberous sclerosis 1 protein homolog



• Molecule 1: Tuberous sclerosis 1 protein homolog



● Molecule 1: Tuberous sclerosis 1 protein homolog





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.38Å 239.79Å 112.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 2.90 29.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.74-2.90) 99.5 (29.74-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.192 , 0.256 0.195 , 0.258	Depositor DCC
$R_{free}$ test set	6917 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 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	0.61	0/3343	0.79	0/4535
1	B	0.57	0/3257	0.78	1/4421 (0.0%)
1	C	0.66	0/3257	0.83	2/4421 (0.0%)
1	D	0.59	0/3257	0.78	1/4421 (0.0%)
1	E	0.65	0/3257	0.85	2/4421 (0.0%)
1	F	0.62	0/3257	0.81	1/4421 (0.0%)
1	G	0.62	0/3257	0.82	4/4421 (0.1%)
1	H	0.58	0/3257	0.79	1/4421 (0.0%)
1	I	0.62	0/3257	0.80	3/4421 (0.1%)
1	J	0.61	0/3257	0.81	1/4421 (0.0%)
All	All	0.61	0/32656	0.81	16/44324 (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	B	0	1
1	E	0	2
1	F	0	1
1	G	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	217	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	J	217	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	I	337	LEU	CA-CB-CG	7.42	132.37	115.30
1	G	217	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	136	ARG	NE-CZ-NH1	7.15	123.87	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	LEU	Peptide
1	E	220	PRO	Peptide
1	E	24	ASP	Peptide
1	F	220	PRO	Peptide
1	G	430	ALA	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	3268	0	3216	59	0
1	B	3181	0	3145	67	0
1	C	3181	0	3145	57	0
1	D	3181	0	3145	50	0
1	E	3181	0	3145	54	0
1	F	3181	0	3145	47	0
1	G	3181	0	3145	53	0
1	H	3181	0	3145	48	0
1	I	3181	0	3145	45	0
1	J	3181	0	3145	52	0
All	All	31897	0	31521	504	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 8.

The worst 5 of 504 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:297:TRP:O	1:C:298:GLU:HB3	1.70	0.90
1:J:251:LEU:HD22	1:J:255:LEU:HD22	1.55	0.88
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.11	0.82
1:J:74:ALA:O	1:J:78:THR:HG22	1.79	0.82
1:E:88:GLN:NE2	1:E:92:GLU:OE2	2.13	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/461 (86%)	361 (91%)	28 (7%)	6 (2%)	8	29
1	B	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	7	25
1	C	383/461 (83%)	348 (91%)	28 (7%)	7 (2%)	7	25
1	D	383/461 (83%)	349 (91%)	30 (8%)	4 (1%)	13	40
1	E	383/461 (83%)	342 (89%)	31 (8%)	10 (3%)	4	17
1	F	383/461 (83%)	355 (93%)	21 (6%)	7 (2%)	7	25
1	G	383/461 (83%)	353 (92%)	25 (6%)	5 (1%)	10	33
1	H	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	7	25
1	I	383/461 (83%)	354 (92%)	17 (4%)	12 (3%)	3	14
1	J	383/461 (83%)	354 (92%)	20 (5%)	9 (2%)	5	20
All	All	3842/4610 (83%)	3508 (91%)	260 (7%)	74 (2%)	6	24

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ALA
1	B	2	PRO
1	C	159	LEU
1	C	262	CYS
1	D	66	THR

### 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	361/421 (86%)	320 (89%)	41 (11%)	4	15
1	B	352/421 (84%)	294 (84%)	58 (16%)	2	6
1	C	352/421 (84%)	300 (85%)	52 (15%)	2	8
1	D	352/421 (84%)	318 (90%)	34 (10%)	6	22
1	E	352/421 (84%)	302 (86%)	50 (14%)	2	8
1	F	352/421 (84%)	306 (87%)	46 (13%)	3	10
1	G	352/421 (84%)	305 (87%)	47 (13%)	3	9
1	H	352/421 (84%)	307 (87%)	45 (13%)	3	11
1	I	352/421 (84%)	301 (86%)	51 (14%)	2	8
1	J	352/421 (84%)	303 (86%)	49 (14%)	3	9
All	All	3529/4210 (84%)	3056 (87%)	473 (13%)	3	9

5 of 473 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	419	ILE
1	J	117	SER
1	G	41	LYS
1	J	77	LYS
1	I	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	169	ASN
1	J	395	HIS
1	I	43	ASN
1	E	107	GLN
1	G	301	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	397/461 (86%)	-0.44	9 (2%) 61 54	39, 63, 108, 136	0
1	B	386/461 (83%)	-0.22	9 (2%) 61 54	42, 75, 119, 152	0
1	C	386/461 (83%)	-0.52	6 (1%) 70 64	39, 59, 93, 130	0
1	D	386/461 (83%)	-0.28	10 (2%) 57 51	37, 71, 131, 172	0
1	E	386/461 (83%)	-0.35	9 (2%) 61 54	37, 60, 117, 152	0
1	F	386/461 (83%)	-0.43	8 (2%) 63 57	41, 63, 103, 149	0
1	G	386/461 (83%)	-0.38	8 (2%) 63 57	39, 67, 103, 134	0
1	H	386/461 (83%)	-0.40	5 (1%) 74 69	42, 67, 106, 141	0
1	I	386/461 (83%)	-0.43	7 (1%) 67 61	42, 64, 109, 140	0
1	J	386/461 (83%)	-0.40	6 (1%) 70 64	38, 65, 109, 146	0
All	All	3871/4610 (83%)	-0.38	77 (1%) 64 58	37, 65, 112, 172	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	305	SER	5.0
1	F	305	SER	4.4
1	E	161	ASP	4.3
1	E	25	LEU	3.9
1	B	305	SER	3.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.