



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:23 AM UTC

PDB ID : 4KK0 / pdb_00004kk0
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

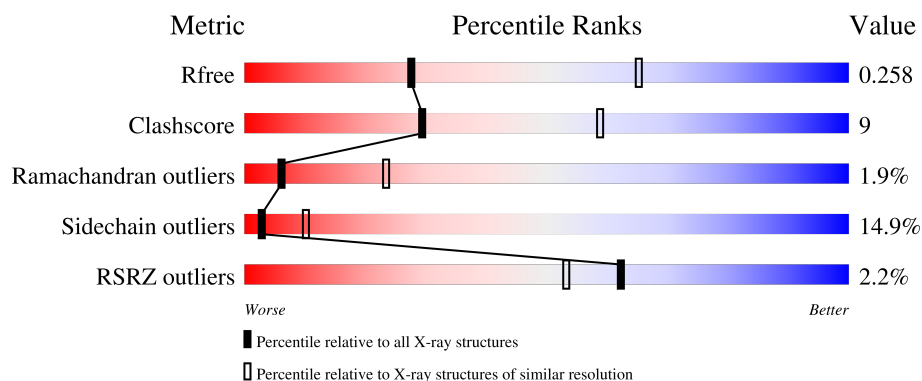
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 ≥ 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	2% 62% 21% . 13%
1	B	461	2% 53% 26% 6% 15%
1	C	461	2% 58% 21% 6% 15%
1	D	461	2% 63% 18% . 15%
1	E	461	2% 55% 24% 5% 15%

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Mol	Chain	Length	Quality of chain
1	F	461	2% 59% 21% • • 15%
1	G	461	2% 61% 19% 5% 15%
1	H	461	2% 61% 19% 5% 15%
1	I	461	2% 61% 18% 5% 15%
1	J	461	2% 59% 20% 6% 15%

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
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G	-14	PRO	-	expression tag	UNP Q09778
G	-13	ARG	-	expression tag	UNP Q09778
G	-12	GLY	-	expression tag	UNP Q09778
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G	-5	TYR	-	expression tag	UNP Q09778
G	-4	PHE	-	expression tag	UNP Q09778
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G	-2	SER	-	expression tag	UNP Q09778
G	-1	HIS	-	expression tag	UNP Q09778
G	0	MSE	-	expression tag	UNP Q09778
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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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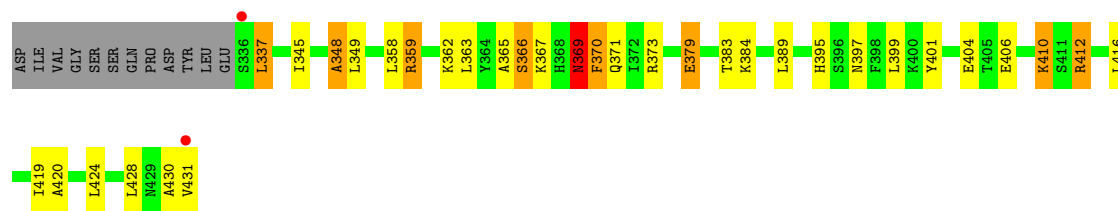
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Chain	Residue	Modelled	Actual	Comment	Reference
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H	-18	SER	-	expression tag	UNP Q09778
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H	-16	LEU	-	expression tag	UNP Q09778
H	-15	VAL	-	expression 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

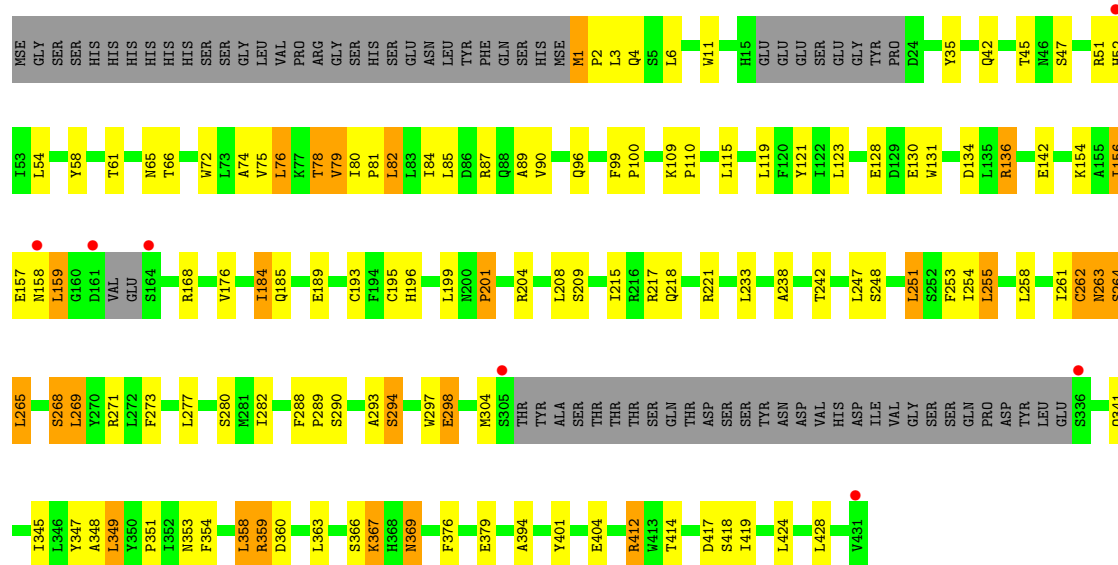
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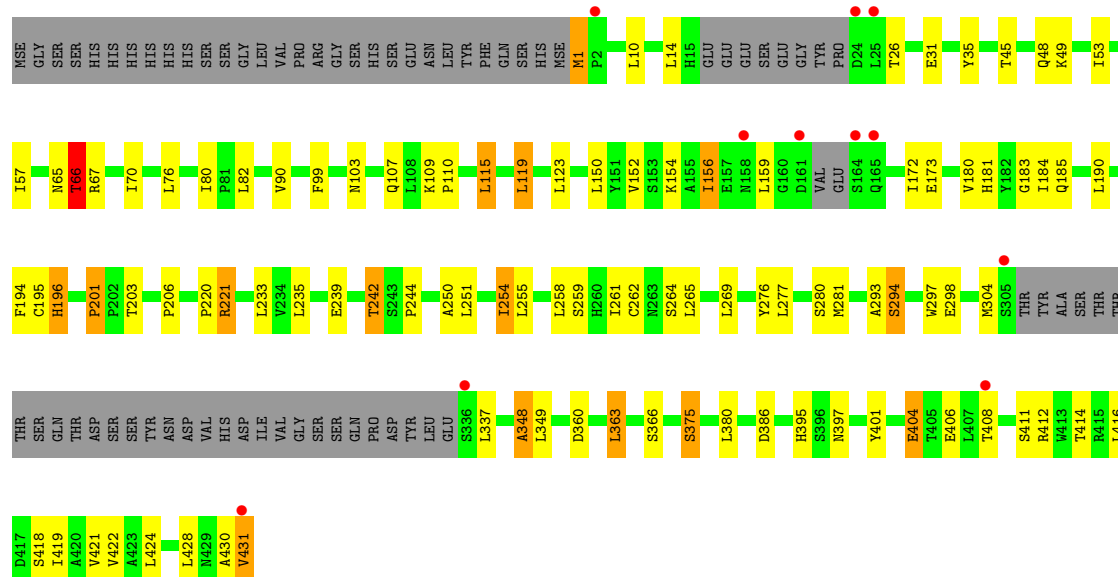
Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLU	-	expression tag	UNP Q09778
I	-7	ASN	-	expression tag	UNP Q09778
I	-6	LEU	-	expression tag	UNP Q09778
I	-5	TYR	-	expression tag	UNP Q09778
I	-4	PHE	-	expression tag	UNP Q09778
I	-3	GLN	-	expression tag	UNP Q09778
I	-2	SER	-	expression tag	UNP Q09778
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



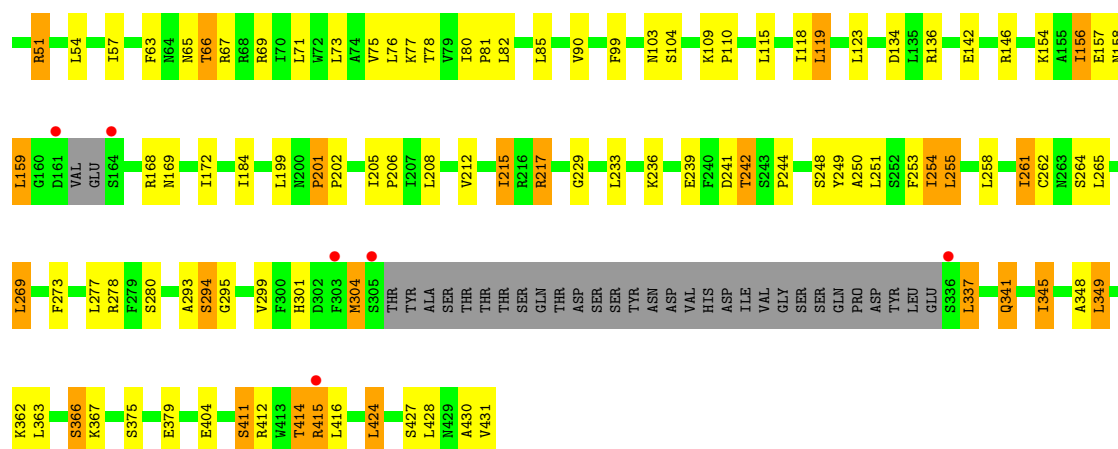
• Molecule 1: Tuberous sclerosis 1 protein homolog



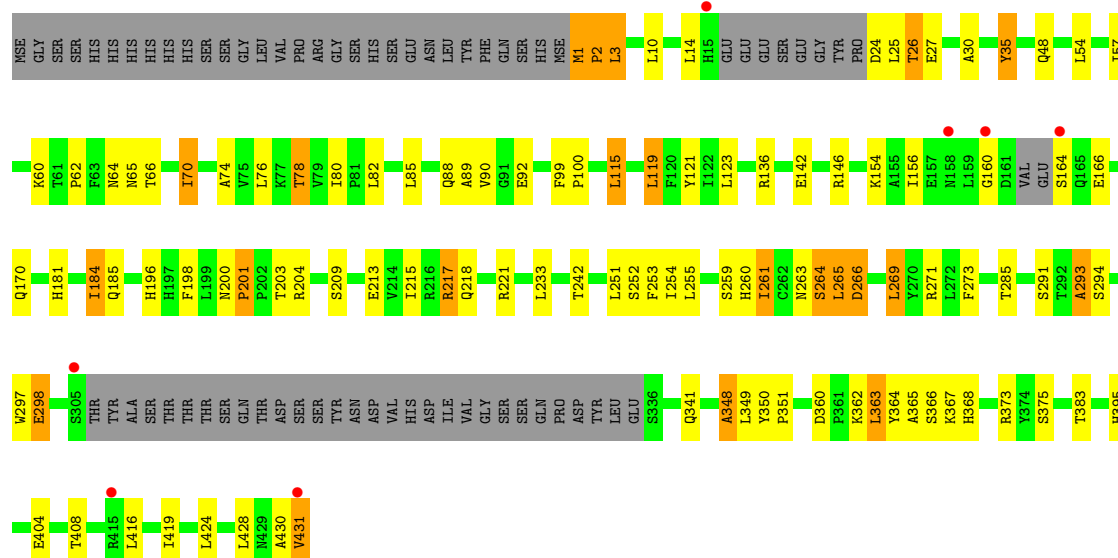
• Molecule 1: Tuberous sclerosis 1 protein homolog



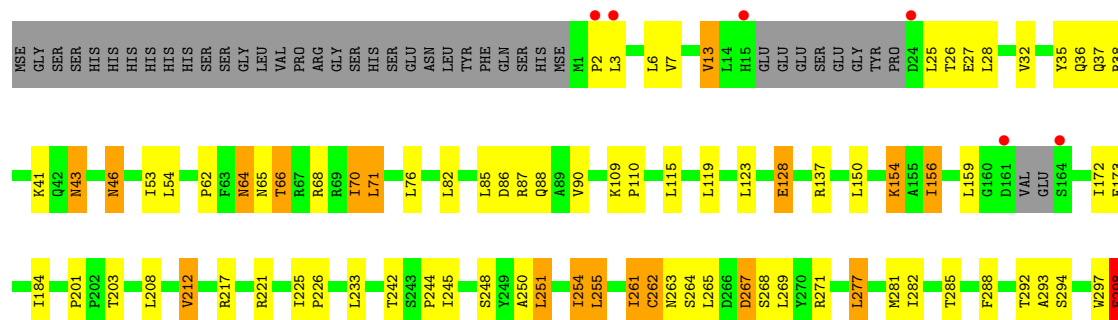
• Molecule 1: Tuberous sclerosis 1 protein homolog

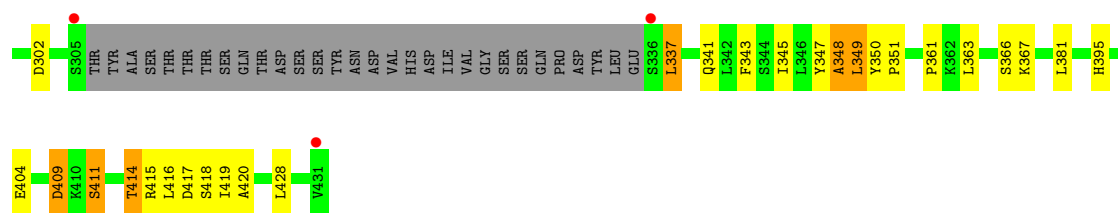


• Molecule 1: Tuberous sclerosis 1 protein homolog

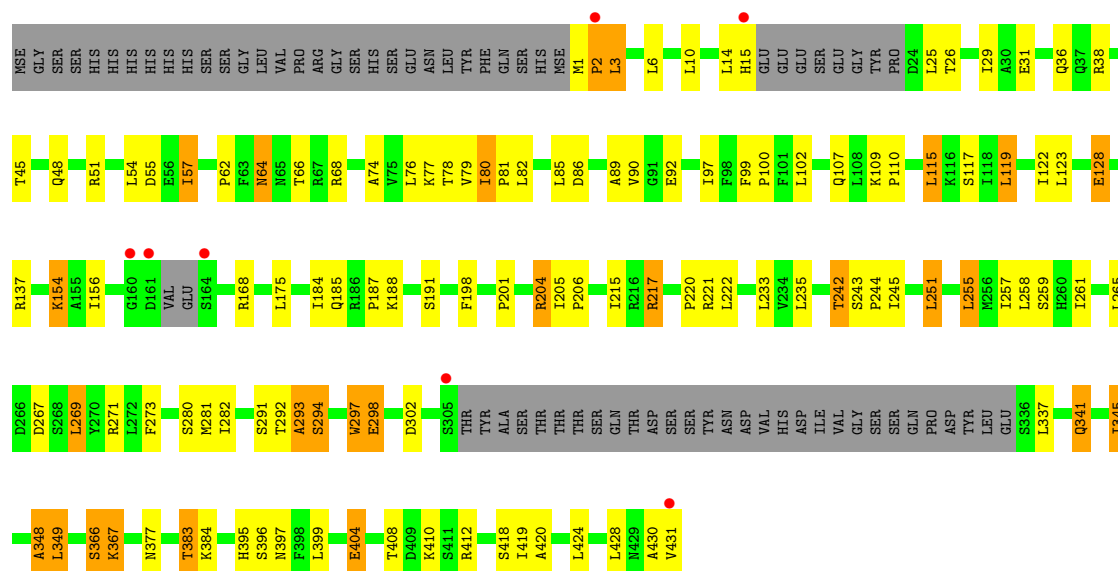


• Molecule 1: Tuberous sclerosis 1 protein homolog





● Molecule 1: Tuberous sclerosis 1 protein homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	6995 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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	0.82	0/3343	1.03	8/4535 (0.2%)
1	B	0.78	0/3257	1.06	10/4421 (0.2%)
1	C	0.90	0/3257	1.07	9/4421 (0.2%)
1	D	0.81	0/3257	1.05	8/4421 (0.2%)
1	E	0.88	0/3257	1.11	10/4421 (0.2%)
1	F	0.86	1/3257 (0.0%)	1.09	10/4421 (0.2%)
1	G	0.84	0/3257	1.07	6/4421 (0.1%)
1	H	0.80	0/3257	1.02	6/4421 (0.1%)
1	I	0.85	0/3257	1.04	6/4421 (0.1%)
1	J	0.83	0/3257	1.09	13/4421 (0.3%)
All	All	0.84	1/32656 (0.0%)	1.06	86/44324 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	188	LYS	N-CA	5.16	1.52	1.46

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	156	ILE	CB-CA-C	-9.28	100.88	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	201	PRO	N-CA-C	9.01	121.69	110.70
1	H	201	PRO	N-CA-C	8.91	121.57	110.70
1	D	366	SER	N-CA-C	-8.22	99.67	110.43
1	B	201	PRO	N-CA-C	7.90	120.34	110.70

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	60	0
1	B	3181	0	3145	71	0
1	C	3181	0	3145	64	0
1	D	3181	0	3145	52	0
1	E	3181	0	3145	57	0
1	F	3181	0	3145	55	0
1	G	3181	0	3145	56	0
1	H	3181	0	3145	52	0
1	I	3181	0	3145	49	0
1	J	3181	0	3145	54	0
All	All	31897	0	31521	542	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 9.

The worst 5 of 542 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	28
1	B	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	6	25
1	C	383/461 (83%)	348 (91%)	28 (7%)	7 (2%)	6	25
1	D	383/461 (83%)	349 (91%)	30 (8%)	4 (1%)	12	39
1	E	383/461 (83%)	342 (89%)	31 (8%)	10 (3%)	4	17
1	F	383/461 (83%)	355 (93%)	21 (6%)	7 (2%)	6	25
1	G	383/461 (83%)	353 (92%)	25 (6%)	5 (1%)	9	32
1	H	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	6	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	19
All	All	3842/4610 (83%)	3508 (91%)	260 (7%)	74 (2%)	6	23

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ALA
1	B	2	PRO
1	C	159	LEU

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Mol	Chain	Res	Type
1	C	262	CYS
1	D	66	THR

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	361/421 (86%)	313 (87%)	48 (13%)	4	12
1	B	352/421 (84%)	288 (82%)	64 (18%)	2	6
1	C	352/421 (84%)	297 (84%)	55 (16%)	2	9
1	D	352/421 (84%)	315 (90%)	37 (10%)	6	22
1	E	352/421 (84%)	295 (84%)	57 (16%)	2	8
1	F	352/421 (84%)	301 (86%)	51 (14%)	3	10
1	G	352/421 (84%)	300 (85%)	52 (15%)	3	10
1	H	352/421 (84%)	302 (86%)	50 (14%)	3	11
1	I	352/421 (84%)	297 (84%)	55 (16%)	2	9
1	J	352/421 (84%)	296 (84%)	56 (16%)	2	8
All	All	3529/4210 (84%)	3004 (85%)	525 (15%)	3	10

5 of 525 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	404	GLU
1	J	38	ARG
1	I	367	LYS
1	J	412	ARG
1	D	304	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	107	GLN

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Mol	Chain	Res	Type
1	I	185	GLN
1	G	170	GLN
1	H	197	HIS
1	J	185	GLN

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 [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, 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	397/461 (86%)	-0.28	9 (2%) 61 52	39, 63, 108, 136	0
1	B	386/461 (83%)	-0.07	9 (2%) 61 52	42, 75, 119, 152	0
1	C	386/461 (83%)	-0.36	7 (1%) 67 59	39, 59, 93, 130	0
1	D	386/461 (83%)	-0.12	11 (2%) 55 46	37, 71, 131, 172	0
1	E	386/461 (83%)	-0.19	11 (2%) 55 46	37, 60, 117, 152	0
1	F	386/461 (83%)	-0.28	9 (2%) 61 52	41, 63, 103, 149	0
1	G	386/461 (83%)	-0.23	8 (2%) 63 54	39, 67, 103, 134	0
1	H	386/461 (83%)	-0.25	7 (1%) 67 59	42, 67, 106, 141	0
1	I	386/461 (83%)	-0.28	9 (2%) 61 52	42, 64, 109, 140	0
1	J	386/461 (83%)	-0.24	7 (1%) 67 59	38, 65, 109, 146	0
All	All	3871/4610 (83%)	-0.23	87 (2%) 62 53	37, 65, 112, 172	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	305	SER	5.0
1	F	305	SER	4.5
1	E	161	ASP	4.3
1	E	25	LEU	4.0
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 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.