Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:07 PM GMT

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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

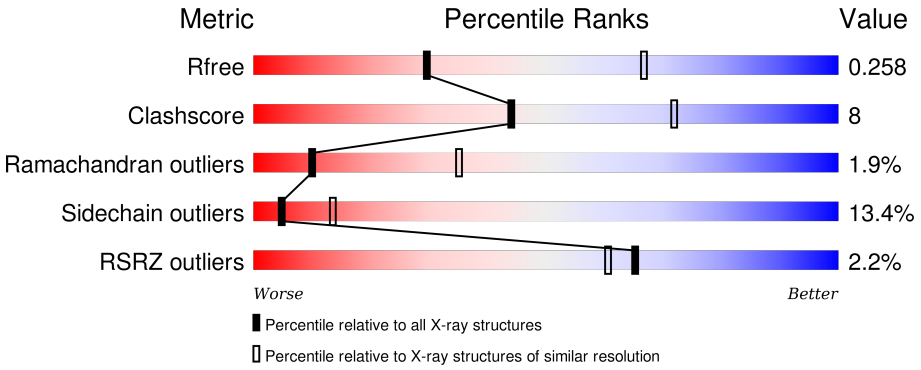
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	3% 64% 20% • 13%
1	B	461	2% 56% 24% • 15%
1	C	461	% 60% 20% 5% 15%
1	D	461	3% 65% 18% • 15%
1	E	461	2% 59% 21% 5% 15%

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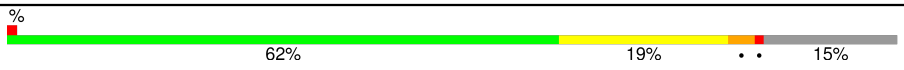
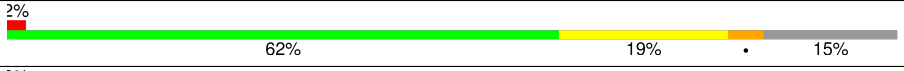
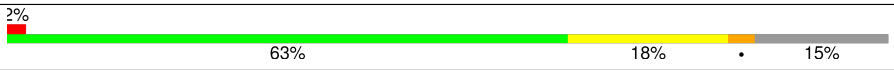
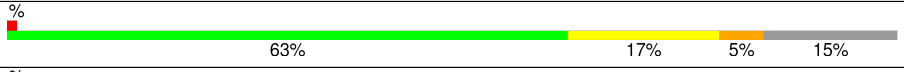
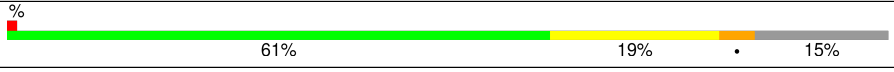
Mol	Chain	Length	Quality of chain
1	F	461	
1	G	461	
1	H	461	
1	I	461	
1	J	461	

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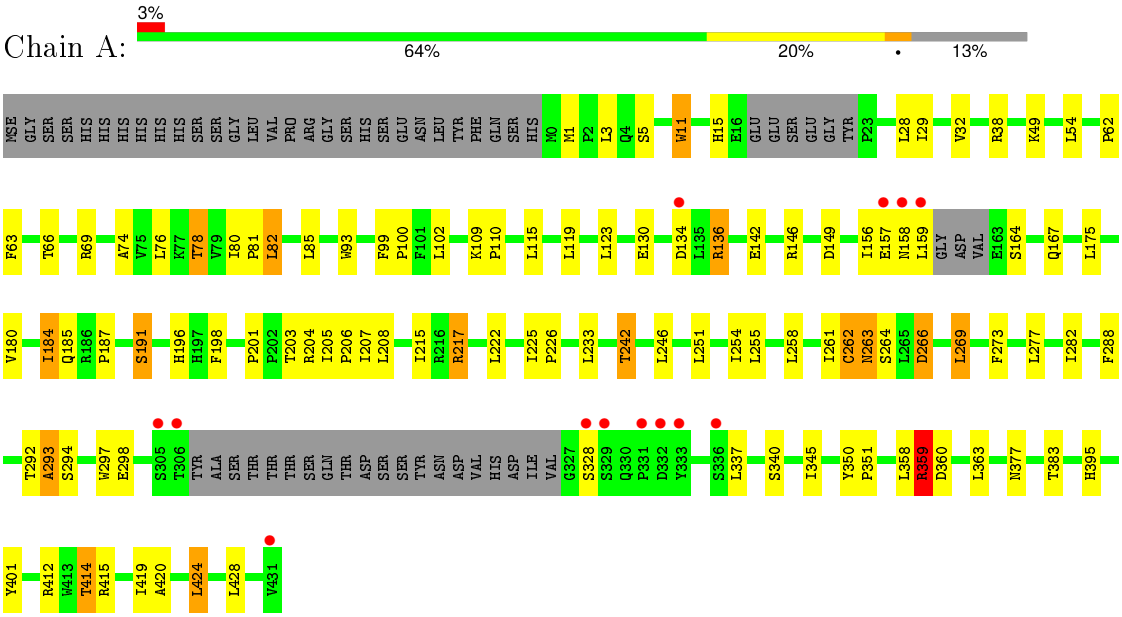
Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLU	-	EXPRESSION TAG	UNP Q09778
I	-7	ASN	-	EXPRESSION TAG	UNP Q09778
I	-6	LEU	-	EXPRESSION TAG	UNP Q09778
I	-5	TYR	-	EXPRESSION TAG	UNP Q09778
I	-4	PHE	-	EXPRESSION TAG	UNP Q09778
I	-3	GLN	-	EXPRESSION TAG	UNP Q09778
I	-2	SER	-	EXPRESSION TAG	UNP Q09778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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

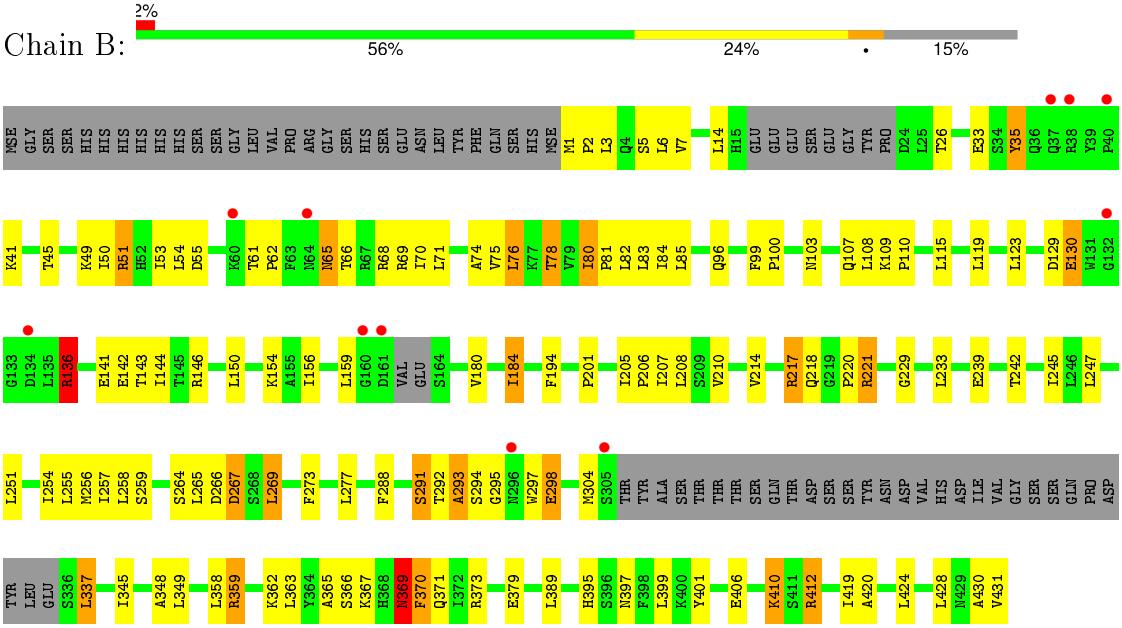
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain A:



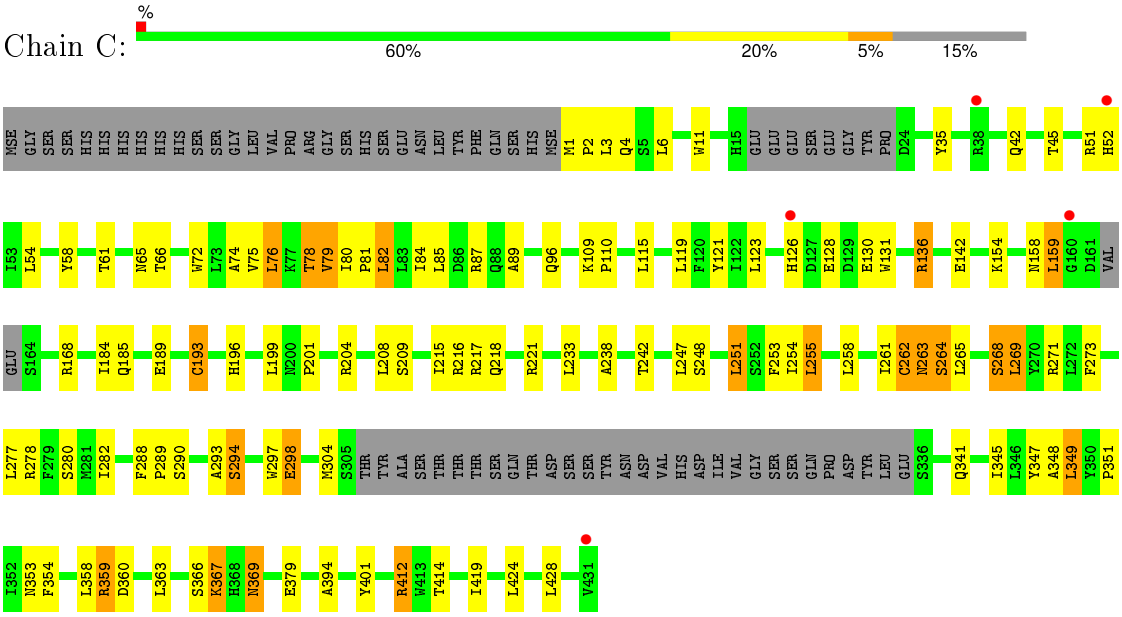
- Molecule 1: Tuberous sclerosis 1 protein homolog

Chain B:



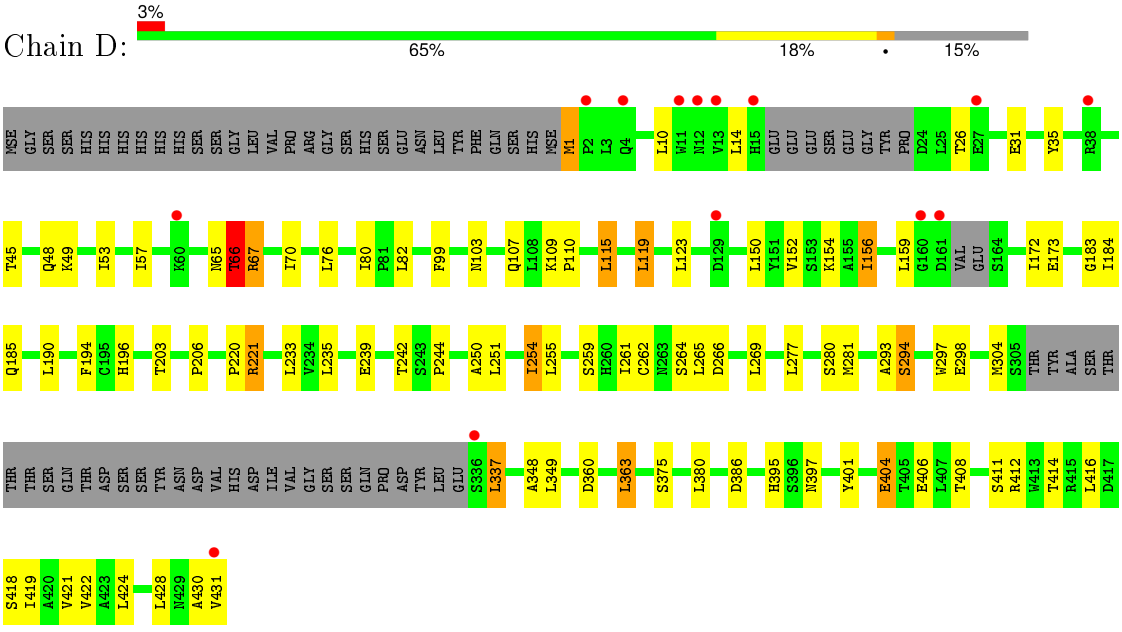
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain C:



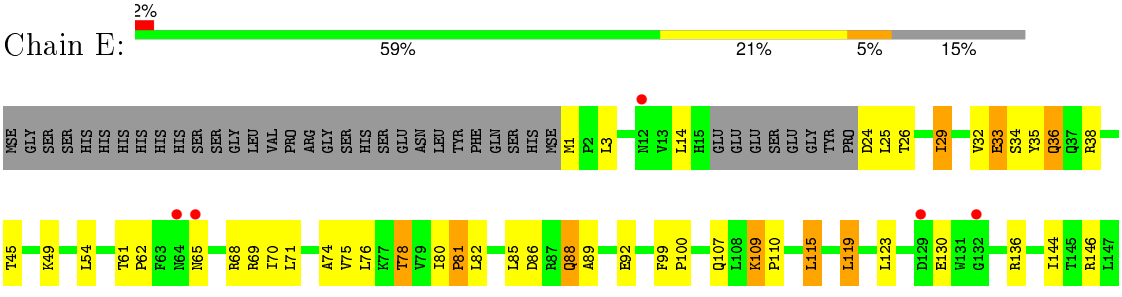
• Molecule 1: Tuberous sclerosis 1 protein homolog

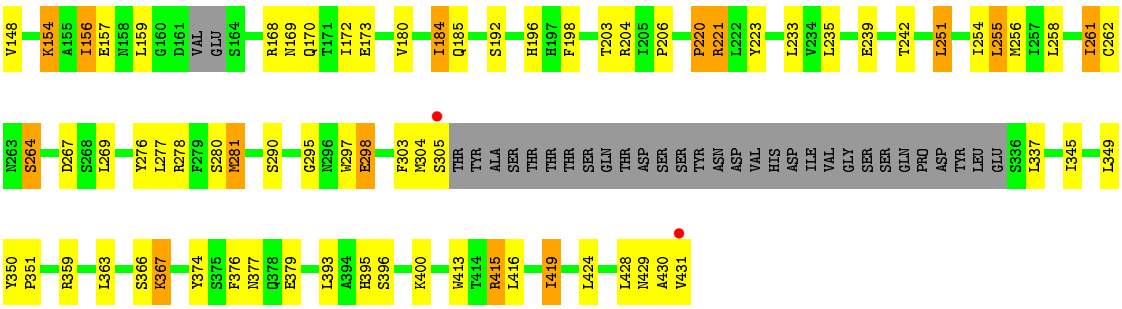
Chain D:



• Molecule 1: Tuberous sclerosis 1 protein homolog

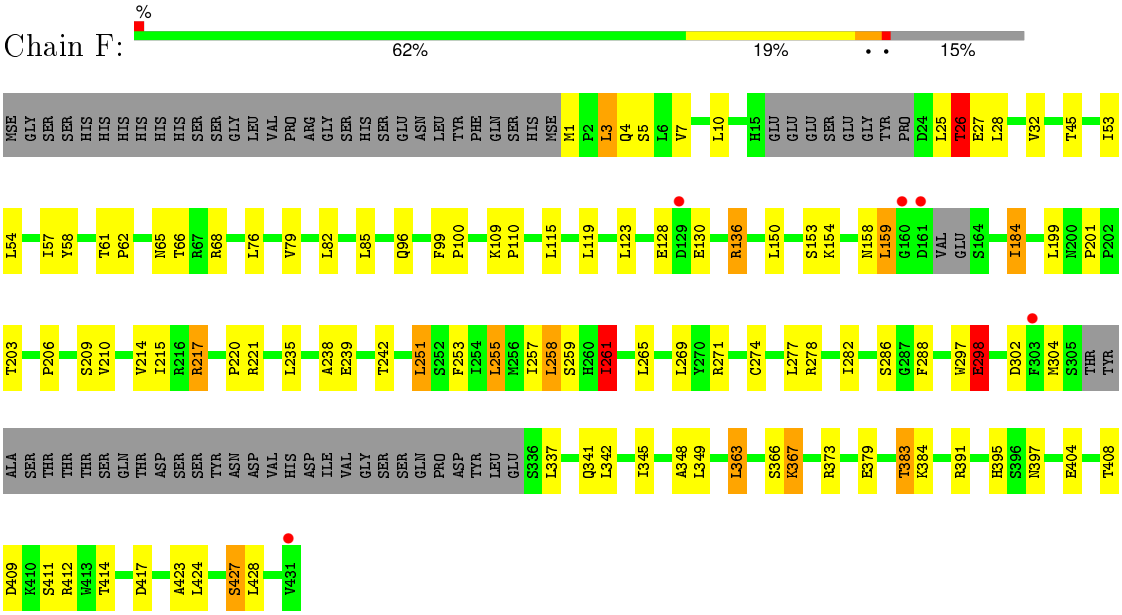
Chain E:





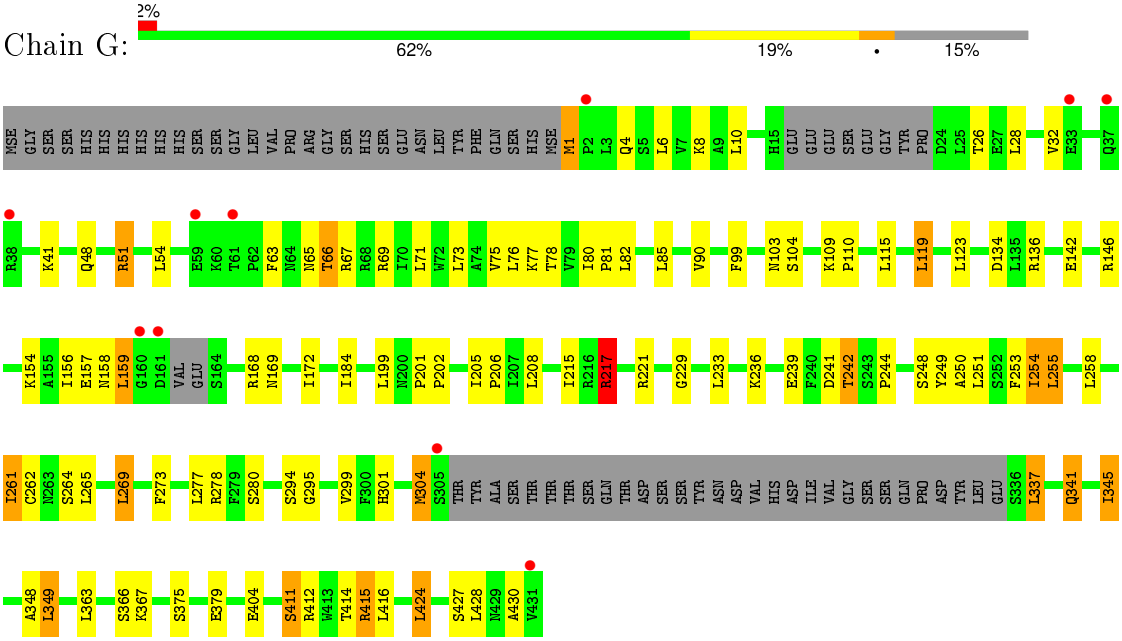
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain F:



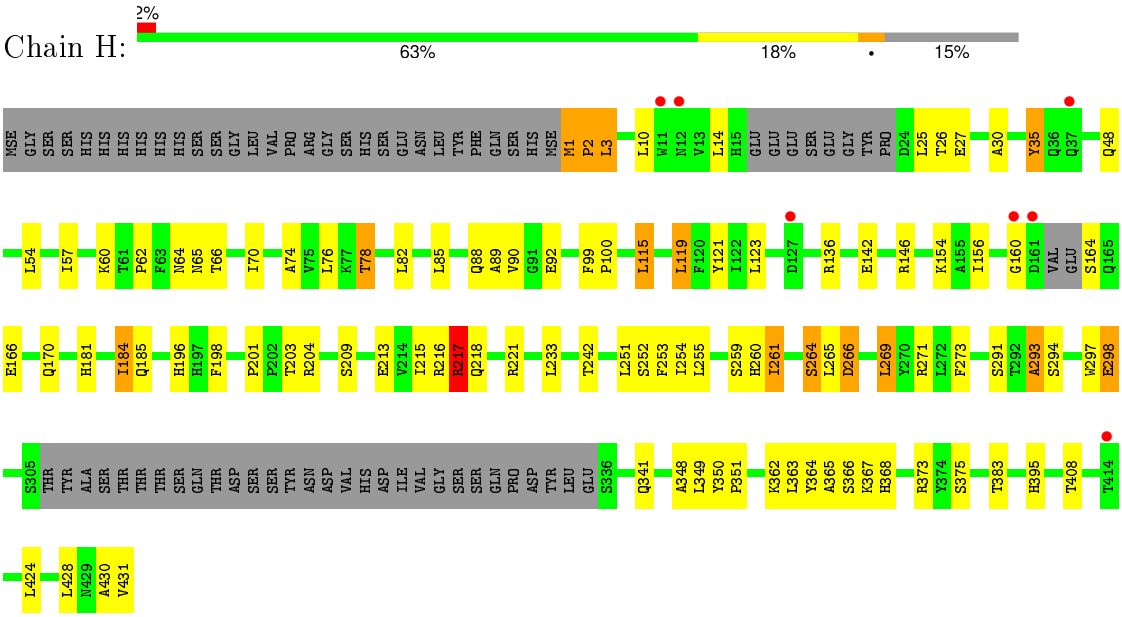
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain G:



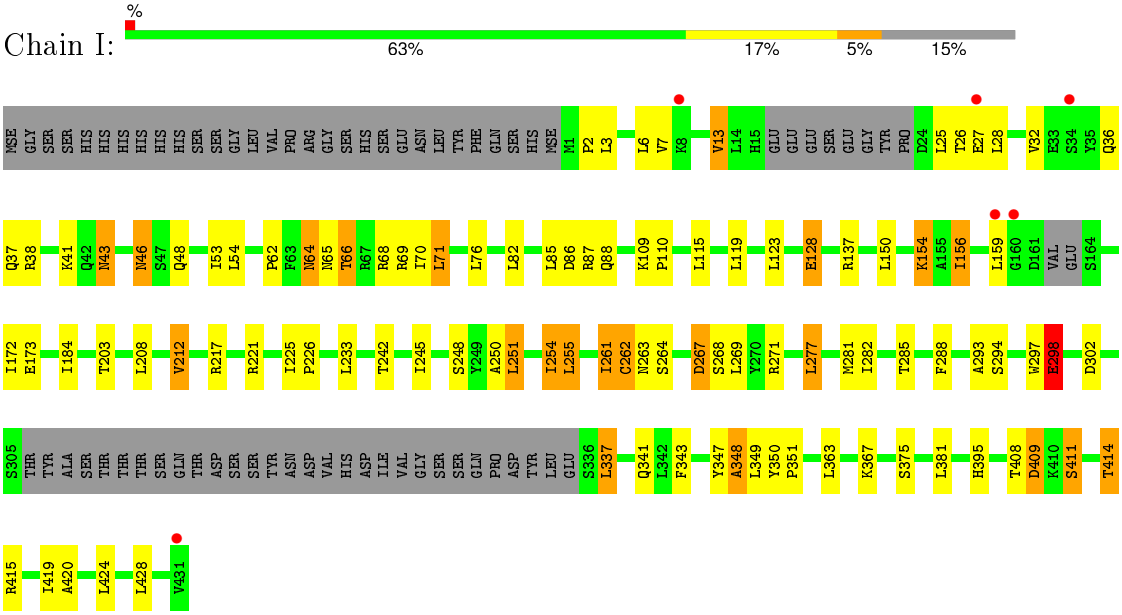
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain H:



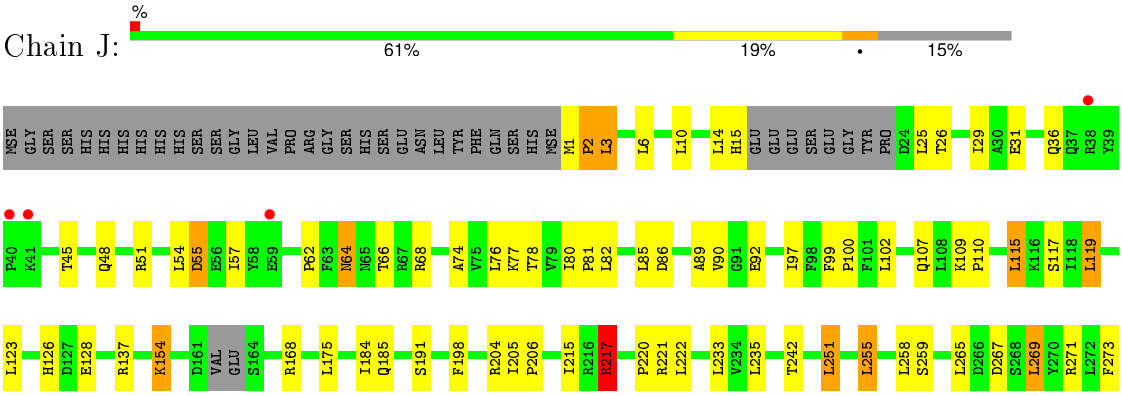
• Molecule 1: Tuberous sclerosis 1 protein homolog

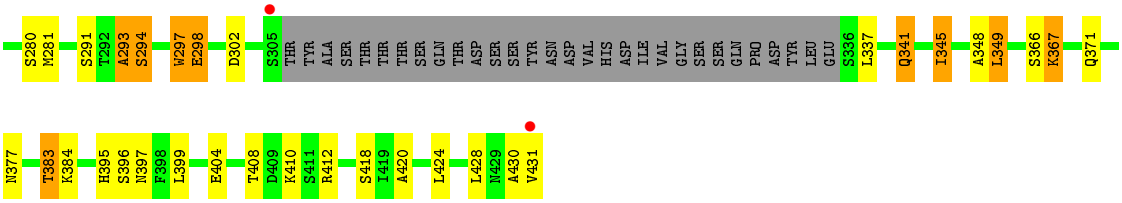
Chain I:



• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain J:




S280 M281 S291 T292 A293 S294 W297 E298 D302 S305 THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 L337 Q341 I345 A348 L349 S366 K367 Q371
N377 T383 K384 H395 S396 N397 F398 L399 E404 T408 D409 K410 S411 R412 S418 I419 A420 L424 L428 N429 A430 V431

4 Data and refinement statistics (i)

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 29.73 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.74-2.90) 98.8 (29.73-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	6917 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.6	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 139494 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	C	278	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	G	337	LEU	CA-CB-CG	5.79	128.60	115.30
1	I	69	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	337	LEU	CA-CB-CG	5.46	127.86	115.30
1	G	217	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	I	156	ILE	CB-CA-C	-5.36	100.88	111.60
1	F	217	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	G	304	MSE	CG-SE-CE	5.15	110.23	98.90
1	E	256	MSE	CG-SE-CE	-5.07	87.74	98.90
1	E	337	LEU	CA-CB-CG	5.03	126.88	115.30
1	C	216	ARG	NE-CZ-NH1	5.01	122.81	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 (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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:J:297:TRP:O	1:J:298:GLU:CB	2.32	0.78
1:F:411:SER:O	1:F:414:THR:HG22	1.83	0.78
1:E:251:LEU:HD22	1:E:255:LEU:HD22	1.65	0.77
1:J:297:TRP:O	1:J:298:GLU:HB2	1.84	0.77
1:E:366:SER:O	1:E:367:LYS:HB2	1.87	0.74
1:J:395:HIS:HD2	1:J:397:ASN:H	1.36	0.74
1:G:51:ARG:HH11	1:G:51:ARG:HG3	1.53	0.74
1:B:348:ALA:O	1:B:349:LEU:HB2	1.88	0.73
1:D:411:SER:O	1:D:414:THR:HG22	1.88	0.73
1:I:297:TRP:O	1:I:298:GLU:HB2	1.88	0.73
1:J:1:MSE:O	1:J:3:LEU:N	2.22	0.72
1:G:348:ALA:O	1:G:349:LEU:HB2	1.90	0.72
1:E:430:ALA:O	1:E:431:VAL:HG23	1.89	0.72
1:H:408:THR:O	1:H:408:THR:HG23	1.87	0.72
1:F:3:LEU:HD22	1:F:7:VAL:HG23	1.72	0.71
1:C:348:ALA:O	1:C:349:LEU:HB2	1.91	0.71
1:B:395:HIS:HD2	1:B:397:ASN:H	1.41	0.69
1:J:348:ALA:O	1:J:349:LEU:HB2	1.93	0.69
1:G:115:LEU:HD13	1:G:119:LEU:HD22	1.74	0.68
1:H:215:ILE:HD11	1:H:253:PHE:CE2	2.28	0.68
1:D:261:ILE:HG22	1:D:262:CYS:N	2.09	0.67
1:F:297:TRP:O	1:F:298:GLU:HB2	1.93	0.67
1:D:395:HIS:HD2	1:D:397:ASN:H	1.39	0.67
1:B:80:ILE:O	1:B:80:ILE:HD13	1.94	0.67
1:F:217:ARG:HH11	1:F:217:ARG:HG2	1.58	0.67
1:H:217:ARG:HH11	1:H:217:ARG:HG2	1.59	0.66
1:D:297:TRP:O	1:D:298:GLU:HB3	1.93	0.66
1:B:150:LEU:O	1:B:154:LYS:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ALA:O	1:B:431:VAL:HB	1.96	0.66
1:G:217:ARG:CG	1:G:217:ARG:HH11	2.09	0.66
1:B:71:LEU:O	1:B:75:VAL:HG23	1.96	0.65
1:F:395:HIS:HD2	1:F:397:ASN:H	1.42	0.65
1:J:341:GLN:O	1:J:345:ILE:HG22	1.96	0.65
1:B:366:SER:O	1:B:367:LYS:HB2	1.96	0.64
1:C:74:ALA:O	1:C:78:THR:HG23	1.98	0.64
1:D:115:LEU:HD22	1:D:119:LEU:HD22	1.79	0.63
1:I:32:VAL:O	1:I:36:GLN:HG2	1.98	0.63
1:I:411:SER:O	1:I:414:THR:HB	1.99	0.63
1:J:215:ILE:HD13	1:J:222:LEU:HD22	1.79	0.62
1:D:280:SER:O	1:D:281:MSE:HE2	2.00	0.61
1:J:64:ASN:OD1	1:J:68:ARG:NH1	2.33	0.61
1:I:64:ASN:OD1	1:I:64:ASN:N	2.34	0.61
1:H:217:ARG:HH11	1:H:217:ARG:CG	2.13	0.61
1:H:115:LEU:HD13	1:H:119:LEU:HD22	1.81	0.61
1:A:359:ARG:HB2	1:J:399:LEU:O	2.01	0.61
1:H:66:THR:O	1:H:70:ILE:HD12	2.01	0.61
1:H:156:ILE:HD11	1:H:203:THR:HG22	1.82	0.60
1:D:220:PRO:HB2	1:D:221:ARG:HG3	1.83	0.60
1:E:419:ILE:HD11	1:F:423:ALA:HB3	1.83	0.60
1:G:241:ASP:O	1:G:278:ARG:NH2	2.34	0.59
1:A:158:ASN:O	1:A:159:LEU:HB2	2.02	0.59
1:E:185:GLN:HG2	1:G:379:GLU:HG2	1.84	0.59
1:F:297:TRP:O	1:F:298:GLU:CB	2.50	0.59
1:B:99:PHE:O	1:B:103:ASN:HB2	2.02	0.59
1:D:242:THR:O	1:D:244:PRO:HD3	2.02	0.58
1:I:261:ILE:HG22	1:I:262:CYS:N	2.18	0.58
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.16	0.58
1:E:280:SER:O	1:E:281:MSE:HE2	2.03	0.58
1:F:65:ASN:HD21	1:F:68:ARG:HD2	1.69	0.58
1:C:130:GLU:OE1	1:C:136:ARG:NH1	2.34	0.58
1:D:380:LEU:HB2	1:F:184:ILE:HD11	1.86	0.58
1:H:297:TRP:O	1:H:298:GLU:CB	2.52	0.58
1:E:144:ILE:O	1:E:148:VAL:HG23	2.04	0.57
1:F:363:LEU:O	1:F:366:SER:O	2.22	0.57
1:E:366:SER:O	1:E:367:LYS:CB	2.52	0.57
1:C:158:ASN:O	1:C:159:LEU:CB	2.52	0.57
1:I:347:TYR:C	1:I:348:ALA:O	2.39	0.57
1:E:261:ILE:HG22	1:E:262:CYS:N	2.18	0.57
1:F:65:ASN:ND2	1:F:68:ARG:HD2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:TRP:O	1:E:298:GLU:CB	2.52	0.57
1:B:369:ASN:OD1	1:B:370:PHE:N	2.37	0.56
1:I:267:ASP:OD1	1:I:267:ASP:N	2.38	0.56
1:A:358:LEU:O	1:A:359:ARG:CB	2.53	0.56
1:B:142:GLU:O	1:B:146:ARG:HG3	2.06	0.56
1:F:235:LEU:O	1:F:239:GLU:HG3	2.05	0.56
1:A:282:ILE:HD12	1:A:288:PHE:CE2	2.40	0.56
1:D:395:HIS:CD2	1:D:397:ASN:H	2.20	0.56
1:F:366:SER:O	1:F:367:LYS:HB2	2.06	0.56
1:E:185:GLN:HA	1:G:379:GLU:HG3	1.88	0.56
1:A:187:PRO:O	1:A:191:SER:OG	2.23	0.56
1:C:348:ALA:O	1:C:349:LEU:CB	2.51	0.56
1:H:1:MSE:O	1:H:3:LEU:N	2.39	0.56
1:B:80:ILE:N	1:B:81:PRO:HD2	2.20	0.56
1:C:215:ILE:HD11	1:C:253:PHE:CE2	2.41	0.56
1:A:63:PHE:CE2	1:A:69:ARG:HG2	2.41	0.56
1:F:379:GLU:HG3	1:H:185:GLN:HA	1.88	0.55
1:B:399:LEU:O	1:C:359:ARG:HB2	2.05	0.55
1:A:293:ALA:O	1:A:294:SER:HB3	2.06	0.55
1:G:345:ILE:O	1:G:348:ALA:O	2.23	0.55
1:J:366:SER:O	1:J:367:LYS:HB2	2.07	0.55
1:B:210:VAL:O	1:B:214:VAL:HG23	2.05	0.55
1:F:409:ASP:OD1	1:F:409:ASP:C	2.45	0.55
1:G:229:GLY:O	1:G:233:LEU:HD13	2.07	0.55
1:A:185:GLN:HG2	1:C:379:GLU:HG2	1.89	0.55
1:C:366:SER:O	1:C:367:LYS:HB2	2.06	0.55
1:E:29:ILE:O	1:E:33:GLU:OE1	2.25	0.54
1:D:348:ALA:O	1:D:349:LEU:HB2	2.08	0.54
1:H:291:SER:HA	1:H:373:ARG:O	2.08	0.54
1:I:156:ILE:HD11	1:I:203:THR:HG22	1.87	0.54
1:D:67:ARG:HA	1:D:70:ILE:HD12	1.89	0.54
1:F:348:ALA:O	1:F:349:LEU:HB2	2.08	0.54
1:I:409:ASP:OD1	1:I:411:SER:HB3	2.08	0.54
1:E:280:SER:C	1:E:281:MSE:HE2	2.28	0.54
1:H:14:LEU:HD13	1:H:57:ILE:HG21	1.89	0.54
1:A:297:TRP:O	1:A:298:GLU:HB3	2.07	0.54
1:C:264:SER:O	1:C:268:SER:OG	2.26	0.54
1:G:348:ALA:O	1:G:349:LEU:CB	2.52	0.54
1:A:63:PHE:CD2	1:A:69:ARG:HG2	2.42	0.54
1:G:115:LEU:CD1	1:G:119:LEU:HD22	2.37	0.54
1:H:293:ALA:O	1:H:294:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:LEU:HD13	1:J:175:LEU:HD21	1.88	0.54
1:G:269:LEU:HD22	1:G:273:PHE:CE1	2.43	0.54
1:D:14:LEU:HD13	1:D:57:ILE:HG21	1.88	0.54
1:A:358:LEU:O	1:A:359:ARG:HB3	2.07	0.53
1:H:269:LEU:HD22	1:H:273:PHE:CE1	2.43	0.53
1:G:261:ILE:HG22	1:G:262:CYS:H	1.73	0.53
1:B:51:ARG:O	1:B:55:ASP:OD2	2.26	0.53
1:B:84:ILE:C	1:B:85:LEU:HD12	2.29	0.53
1:J:348:ALA:O	1:J:349:LEU:CB	2.57	0.53
1:D:99:PHE:CZ	1:D:103:ASN:ND2	2.75	0.53
1:G:205:ILE:HB	1:G:206:PRO:HD3	1.91	0.53
1:C:184:ILE:HD11	1:E:377:ASN:ND2	2.23	0.53
1:E:130:GLU:OE1	1:E:136:ARG:NH1	2.41	0.53
1:A:297:TRP:O	1:A:298:GLU:CB	2.56	0.53
1:J:293:ALA:O	1:J:294:SER:CB	2.57	0.53
1:H:215:ILE:CD1	1:H:253:PHE:CE2	2.92	0.53
1:A:180:VAL:O	1:A:184:ILE:HG23	2.09	0.53
1:F:99:PHE:HB3	1:F:100:PRO:HD3	1.91	0.53
1:F:251:LEU:HD22	1:F:255:LEU:HD22	1.91	0.53
1:H:408:THR:CG2	1:H:408:THR:O	2.56	0.52
1:C:154:LYS:O	1:C:168:ARG:HD3	2.09	0.52
1:C:358:LEU:O	1:C:359:ARG:CB	2.56	0.52
1:A:266:ASP:OD1	1:A:266:ASP:N	2.41	0.52
1:G:217:ARG:HH11	1:G:217:ARG:HG2	1.73	0.52
1:B:74:ALA:O	1:B:78:THR:HG23	2.09	0.52
1:H:366:SER:O	1:H:367:LYS:HB2	2.10	0.52
1:I:46:ASN:N	1:I:46:ASN:OD1	2.42	0.52
1:G:65:ASN:O	1:G:66:THR:HG22	2.09	0.52
1:F:158:ASN:O	1:F:159:LEU:CB	2.58	0.52
1:I:150:LEU:O	1:I:154:LYS:HB2	2.10	0.52
1:B:136:ARG:CG	1:B:136:ARG:HH11	2.23	0.52
1:C:35:TYR:CE2	1:C:82:LEU:HG	2.45	0.51
1:E:156:ILE:O	1:E:157:GLU:C	2.48	0.51
1:B:247:LEU:HD13	1:B:288:PHE:CD1	2.46	0.51
1:H:35:TYR:CD2	1:H:35:TYR:C	2.84	0.51
1:D:408:THR:O	1:D:408:THR:HG23	2.10	0.51
1:C:75:VAL:O	1:C:79:VAL:HG13	2.11	0.51
1:F:277:LEU:HD13	1:F:277:LEU:C	2.31	0.51
1:A:102:LEU:HD13	1:A:175:LEU:HD21	1.92	0.51
1:B:7:VAL:HG13	1:B:53:ILE:HD13	1.93	0.51
1:B:369:ASN:C	1:B:369:ASN:OD1	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ASN:O	1:G:159:LEU:CB	2.59	0.51
1:G:169:ASN:O	1:G:172:ILE:HG13	2.11	0.51
1:H:430:ALA:O	1:H:431:VAL:HG23	2.10	0.51
1:E:172:ILE:HG13	1:E:173:GLU:N	2.25	0.51
1:F:395:HIS:CD2	1:F:397:ASN:H	2.27	0.51
1:A:28:LEU:O	1:A:32:VAL:HG23	2.11	0.51
1:D:183:GLY:HA3	1:D:190:LEU:HD23	1.93	0.51
1:I:217:ARG:HH11	1:I:217:ARG:HG2	1.76	0.51
1:I:7:VAL:HG13	1:I:53:ILE:HD13	1.93	0.51
1:A:156:ILE:HD11	1:A:203:THR:HG22	1.92	0.50
1:J:220:PRO:HB2	1:J:221:ARG:HG3	1.92	0.50
1:A:156:ILE:CD1	1:A:203:THR:HG22	2.41	0.50
1:D:401:TYR:CZ	1:D:412:ARG:HG3	2.46	0.50
1:E:80:ILE:N	1:E:81:PRO:HD2	2.26	0.50
1:C:261:ILE:O	1:C:263:ASN:N	2.44	0.50
1:H:265:LEU:HD23	1:H:350:TYR:HE2	1.76	0.50
1:I:348:ALA:O	1:I:350:TYR:N	2.45	0.50
1:F:217:ARG:HG2	1:F:217:ARG:NH1	2.26	0.50
1:F:130:GLU:OE1	1:F:136:ARG:NH1	2.44	0.50
1:E:180:VAL:O	1:E:184:ILE:HG23	2.11	0.50
1:J:366:SER:O	1:J:367:LYS:CB	2.59	0.50
1:C:261:ILE:C	1:C:263:ASN:H	2.14	0.50
1:J:99:PHE:HB3	1:J:100:PRO:HD3	1.93	0.50
1:E:221:ARG:HB3	1:E:223:TYR:CE2	2.46	0.50
1:J:404:GLU:O	1:J:408:THR:HG23	2.12	0.50
1:E:71:LEU:O	1:E:75:VAL:HG23	2.11	0.50
1:B:3:LEU:O	1:B:3:LEU:HD23	2.12	0.50
1:G:424:LEU:O	1:G:427:SER:OG	2.28	0.50
1:G:261:ILE:HG22	1:G:262:CYS:N	2.27	0.50
1:A:203:THR:O	1:A:207:ILE:HG13	2.12	0.50
1:A:164:SER:HB3	1:A:167:GLN:OE1	2.11	0.49
1:E:220:PRO:HB2	1:E:221:ARG:HG3	1.94	0.49
1:D:261:ILE:HG23	1:D:264:SER:HB2	1.93	0.49
1:C:359:ARG:HG3	1:C:360:ASP:N	2.26	0.49
1:F:109:LYS:HB2	1:F:110:PRO:HD3	1.93	0.49
1:I:250:ALA:O	1:I:254:ILE:HG23	2.13	0.49
1:B:365:ALA:O	1:B:369:ASN:N	2.44	0.49
1:C:185:GLN:HG2	1:E:379:GLU:HG2	1.93	0.49
1:F:1:MSE:HE2	1:F:4:GLN:OE1	2.12	0.49
1:I:414:THR:HG22	1:I:415:ARG:N	2.28	0.49
1:C:358:LEU:O	1:C:359:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:O	1:A:415:ARG:C	2.50	0.49
1:A:395:HIS:CD2	1:B:428:LEU:HD21	2.47	0.49
1:I:261:ILE:O	1:I:263:ASN:N	2.46	0.49
1:H:365:ALA:C	1:H:366:SER:O	2.49	0.49
1:C:217:ARG:O	1:C:218:GLN:C	2.52	0.49
1:G:255:LEU:HD23	1:G:337:LEU:HB3	1.94	0.49
1:E:69:ARG:O	1:E:70:ILE:C	2.51	0.48
1:D:150:LEU:HD11	1:D:154:LYS:HE3	1.95	0.48
1:I:277:LEU:HD13	1:I:277:LEU:C	2.33	0.48
1:J:205:ILE:HB	1:J:206:PRO:HD3	1.96	0.48
1:A:261:ILE:HG22	1:A:262:CYS:N	2.29	0.48
1:F:408:THR:OG1	1:F:408:THR:O	2.27	0.48
1:F:342:LEU:O	1:F:345:ILE:HG22	2.13	0.48
1:H:364:TYR:O	1:H:366:SER:O	2.31	0.48
1:B:406:GLU:O	1:B:412:ARG:NH2	2.45	0.48
1:J:217:ARG:CG	1:J:217:ARG:HH11	2.26	0.48
1:G:65:ASN:OD1	1:G:66:THR:N	2.46	0.48
1:G:156:ILE:HG22	1:G:157:GLU:N	2.26	0.48
1:G:366:SER:O	1:G:367:LYS:HB2	2.14	0.48
1:B:379:GLU:HG2	1:D:185:GLN:HG2	1.95	0.48
1:B:410:LYS:HA	1:B:410:LYS:HE3	1.95	0.48
1:E:109:LYS:N	1:E:110:PRO:HD2	2.28	0.48
1:D:152:VAL:HG12	1:D:156:ILE:HD11	1.95	0.48
1:J:430:ALA:O	1:J:431:VAL:HB	2.13	0.48
1:D:277:LEU:HD13	1:D:277:LEU:C	2.33	0.48
1:C:366:SER:O	1:C:367:LYS:CB	2.61	0.48
1:D:261:ILE:CG2	1:D:264:SER:HB2	2.44	0.48
1:J:185:GLN:O	1:J:221:ARG:NH2	2.44	0.48
1:C:261:ILE:HG22	1:C:262:CYS:N	2.29	0.48
1:B:256:MSE:HE3	1:B:337:LEU:CD2	2.43	0.48
1:I:251:LEU:HD22	1:I:255:LEU:HD13	1.96	0.48
1:A:401:TYR:CZ	1:A:412:ARG:HG2	2.49	0.48
1:H:166:GLU:O	1:H:170:GLN:HG3	2.14	0.47
1:I:351:PRO:HG3	1:I:395:HIS:CG	2.49	0.47
1:B:430:ALA:O	1:B:431:VAL:CB	2.61	0.47
1:C:121:TYR:O	1:C:136:ARG:NH2	2.48	0.47
1:C:215:ILE:HD11	1:C:253:PHE:CZ	2.50	0.47
1:E:154:LYS:O	1:E:168:ARG:HD2	2.15	0.47
1:E:26:THR:HG23	1:G:295:GLY:HA2	1.95	0.47
1:C:366:SER:OG	1:C:366:SER:O	2.20	0.47
1:D:404:GLU:O	1:D:408:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:PHE:C	1:E:305:SER:H	2.18	0.47
1:B:35:TYR:C	1:B:35:TYR:CD2	2.87	0.47
1:C:277:LEU:O	1:C:277:LEU:HD23	2.13	0.47
1:D:406:GLU:O	1:D:412:ARG:NH2	2.42	0.47
1:I:208:LEU:HA	1:I:208:LEU:HD23	1.77	0.47
1:A:11:TRP:CZ3	1:A:15:HIS:CE1	3.02	0.47
1:B:269:LEU:HD22	1:B:273:PHE:CE1	2.50	0.47
1:B:50:ILE:HA	1:B:53:ILE:HD12	1.97	0.47
1:F:53:ILE:O	1:F:57:ILE:HG13	2.15	0.47
1:D:430:ALA:O	1:D:431:VAL:HG23	2.14	0.47
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.97	0.47
1:D:293:ALA:O	1:D:294:SER:CB	2.63	0.47
1:C:238:ALA:HA	1:C:247:LEU:CD2	2.45	0.47
1:I:251:LEU:CD2	1:I:255:LEU:HD13	2.44	0.47
1:D:203:THR:C	1:D:206:PRO:HD2	2.35	0.47
1:G:73:LEU:O	1:G:77:LYS:HB2	2.15	0.47
1:J:14:LEU:HD13	1:J:57:ILE:HG21	1.97	0.47
1:J:99:PHE:N	1:J:100:PRO:CD	2.77	0.46
1:J:97:ILE:C	1:J:100:PRO:HD2	2.34	0.46
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.97	0.46
1:B:297:TRP:O	1:B:298:GLU:CB	2.63	0.46
1:C:293:ALA:O	1:C:294:SER:CB	2.62	0.46
1:E:107:GLN:HE22	1:E:170:GLN:HG2	1.79	0.46
1:F:366:SER:O	1:F:367:LYS:CB	2.63	0.46
1:E:278:ARG:HD2	1:E:374:TYR:CZ	2.51	0.46
1:G:215:ILE:CD1	1:G:253:PHE:CE2	2.99	0.46
1:F:58:TYR:CE2	1:F:96:GLN:HG2	2.50	0.46
1:H:198:PHE:CE1	1:H:204:ARG:HD3	2.49	0.46
1:H:217:ARG:O	1:H:218:GLN:C	2.53	0.46
1:E:235:LEU:O	1:E:239:GLU:HG2	2.16	0.46
1:J:395:HIS:CD2	1:J:397:ASN:H	2.25	0.46
1:F:274:CYS:O	1:F:277:LEU:HB3	2.15	0.46
1:J:109:LYS:N	1:J:110:PRO:CD	2.79	0.46
1:J:128:GLU:OE1	1:J:137:ARG:NH1	2.49	0.46
1:F:257:ILE:HG23	1:F:261:ILE:HD11	1.98	0.46
1:D:190:LEU:HD11	1:D:194:PHE:CE2	2.51	0.46
1:H:142:GLU:OE2	1:H:146:ARG:NH1	2.49	0.46
1:B:180:VAL:O	1:B:184:ILE:HG23	2.15	0.46
1:B:379:GLU:HG3	1:D:185:GLN:HA	1.96	0.46
1:D:65:ASN:O	1:D:66:THR:HG23	2.16	0.46
1:B:292:THR:HG23	1:B:292:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:THR:O	1:G:244:PRO:HD3	2.16	0.46
1:C:282:ILE:HD12	1:C:288:PHE:CE2	2.50	0.46
1:H:260:HIS:C	1:H:261:ILE:HG13	2.37	0.46
1:E:430:ALA:O	1:E:431:VAL:CG2	2.63	0.45
1:A:11:TRP:CE3	1:A:15:HIS:CE1	3.04	0.45
1:G:201:PRO:HB2	1:G:202:PRO:HD3	1.98	0.45
1:D:35:TYR:CD2	1:D:35:TYR:C	2.88	0.45
1:H:217:ARG:CG	1:H:217:ARG:NH1	2.78	0.45
1:I:408:THR:OG1	1:I:408:THR:O	2.30	0.45
1:I:281:MSE:HE3	1:I:381:LEU:HD12	1.98	0.45
1:H:1:MSE:O	1:H:2:PRO:C	2.55	0.45
1:I:281:MSE:HA	1:I:281:MSE:HE2	1.97	0.45
1:E:35:TYR:CD2	1:E:35:TYR:C	2.90	0.45
1:I:208:LEU:O	1:I:212:VAL:HG13	2.16	0.45
1:D:31:GLU:OE2	1:D:31:GLU:HA	2.15	0.45
1:G:51:ARG:NH1	1:G:51:ARG:HG3	2.28	0.45
1:H:27:GLU:O	1:H:30:ALA:HB3	2.17	0.45
1:A:74:ALA:O	1:A:78:THR:CG2	2.65	0.45
1:E:393:LEU:HD12	1:F:427:SER:O	2.17	0.45
1:J:80:ILE:N	1:J:81:PRO:CD	2.80	0.45
1:A:242:THR:HG21	1:I:110:PRO:CG	2.47	0.45
1:E:99:PHE:N	1:E:100:PRO:HD2	2.32	0.45
1:B:292:THR:HG22	1:B:373:ARG:O	2.17	0.45
1:I:282:ILE:HD12	1:I:288:PHE:CE2	2.52	0.45
1:C:269:LEU:HA	1:C:269:LEU:HD23	1.87	0.44
1:F:277:LEU:HD13	1:F:277:LEU:O	2.17	0.44
1:I:109:LYS:HB2	1:I:110:PRO:HD3	1.98	0.44
1:C:80:ILE:N	1:C:81:PRO:HD2	2.32	0.44
1:C:189:GLU:O	1:C:193:CYS:HB2	2.17	0.44
1:J:269:LEU:HD22	1:J:273:PHE:CE1	2.52	0.44
1:D:172:ILE:HD12	1:D:173:GLU:N	2.32	0.44
1:C:204:ARG:CZ	1:C:297:TRP:CZ2	2.99	0.44
1:F:4:GLN:HA	1:F:7:VAL:HB	1.99	0.44
1:C:401:TYR:CZ	1:C:412:ARG:HG3	2.52	0.44
1:E:350:TYR:N	1:E:351:PRO:CD	2.80	0.44
1:A:424:LEU:HD13	1:B:348:ALA:HB1	1.99	0.44
1:I:65:ASN:ND2	1:I:68:ARG:HD2	2.32	0.44
1:D:418:SER:O	1:D:422:VAL:HG23	2.18	0.44
1:C:208:LEU:HD23	1:C:208:LEU:HA	1.77	0.44
1:I:225:ILE:N	1:I:226:PRO:CD	2.80	0.44
1:A:215:ILE:HG13	1:A:222:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:HA	1:B:144:ILE:HG22	1.99	0.44
1:G:28:LEU:O	1:G:32:VAL:HG23	2.17	0.44
1:G:63:PHE:CE2	1:G:69:ARG:HG2	2.51	0.44
1:A:359:ARG:HG3	1:A:360:ASP:N	2.27	0.44
1:H:297:TRP:O	1:H:298:GLU:HB3	2.17	0.44
1:E:297:TRP:O	1:E:298:GLU:HB3	2.17	0.44
1:J:377:ASN:C	1:J:377:ASN:OD1	2.56	0.44
1:F:150:LEU:O	1:F:154:LYS:HB2	2.17	0.44
1:B:217:ARG:HD2	1:J:383:THR:HG21	1.99	0.44
1:I:13:VAL:O	1:I:71:LEU:HD21	2.17	0.44
1:A:420:ALA:HB2	1:B:420:ALA:HB2	2.00	0.44
1:D:109:LYS:HB2	1:D:110:PRO:HD3	1.99	0.44
1:C:199:LEU:O	1:C:201:PRO:HD3	2.18	0.44
1:F:383:THR:HG22	1:F:384:LYS:N	2.33	0.44
1:A:208:LEU:HD12	1:A:246:LEU:HD11	2.00	0.44
1:B:267:ASP:OD1	1:B:267:ASP:N	2.51	0.44
1:F:203:THR:C	1:F:206:PRO:HD2	2.38	0.44
1:I:43:ASN:HB3	1:I:46:ASN:OD1	2.17	0.43
1:D:406:GLU:HG2	1:D:412:ARG:NH2	2.33	0.43
1:I:128:GLU:HB3	1:I:137:ARG:NH1	2.32	0.43
1:I:86:ASP:O	1:I:87:ARG:C	2.55	0.43
1:A:269:LEU:HD22	1:A:273:PHE:CE1	2.53	0.43
1:B:358:LEU:O	1:B:359:ARG:CB	2.65	0.43
1:E:86:ASP:H	1:E:89:ALA:HB3	1.82	0.43
1:A:80:ILE:HD12	1:A:93:TRP:CZ3	2.53	0.43
1:D:250:ALA:O	1:D:254:ILE:HG23	2.18	0.43
1:B:110:PRO:HG2	1:J:242:THR:HG21	1.99	0.43
1:J:280:SER:O	1:J:281:MSE:HE2	2.17	0.43
1:G:366:SER:O	1:G:367:LYS:CB	2.66	0.43
1:B:291:SER:OG	1:B:292:THR:N	2.49	0.43
1:B:107:GLN:O	1:B:108:LEU:HD23	2.19	0.43
1:B:389:LEU:HD11	1:C:394:ALA:HB1	1.98	0.43
1:E:169:ASN:HA	1:E:172:ILE:HG12	2.00	0.43
1:B:220:PRO:HB2	1:B:221:ARG:CG	2.48	0.43
1:C:268:SER:O	1:C:269:LEU:C	2.56	0.43
1:A:80:ILE:HG23	1:A:81:PRO:HD3	2.01	0.43
1:G:299:VAL:HG12	1:G:301:HIS:CE1	2.53	0.43
1:E:32:VAL:O	1:E:36:GLN:HG3	2.18	0.43
1:D:53:ILE:HG22	1:D:57:ILE:HD11	2.01	0.43
1:G:215:ILE:HD12	1:G:253:PHE:CE2	2.53	0.43
1:C:282:ILE:HD12	1:C:288:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:GLY:O	1:H:164:SER:CB	2.67	0.43
1:C:87:ARG:HD3	1:C:142:GLU:OE1	2.18	0.43
1:H:366:SER:O	1:H:368:HIS:N	2.50	0.43
1:B:217:ARG:O	1:B:218:GLN:C	2.57	0.43
1:E:419:ILE:CD1	1:F:423:ALA:HB3	2.47	0.43
1:H:121:TYR:O	1:H:136:ARG:NH2	2.52	0.43
1:I:66:THR:O	1:I:70:ILE:HG13	2.18	0.43
1:E:281:MSE:HG3	1:E:376:PHE:HB2	2.00	0.43
1:H:293:ALA:HB3	1:H:373:ARG:HD3	2.00	0.43
1:G:199:LEU:O	1:G:201:PRO:HD3	2.19	0.43
1:E:351:PRO:HG3	1:E:395:HIS:CE1	2.54	0.43
1:D:386:ASP:OD2	1:E:396:SER:HB3	2.19	0.43
1:G:99:PHE:CZ	1:G:103:ASN:ND2	2.87	0.43
1:H:65:ASN:OD1	1:H:66:THR:N	2.50	0.43
1:E:415:ARG:O	1:E:419:ILE:HG23	2.18	0.43
1:F:25:LEU:O	1:F:26:THR:C	2.58	0.43
1:J:86:ASP:OD1	1:J:89:ALA:N	2.38	0.43
1:A:261:ILE:C	1:A:263:ASN:H	2.22	0.42
1:B:269:LEU:CD2	1:B:273:PHE:CE1	3.02	0.42
1:G:217:ARG:CG	1:G:217:ARG:NH1	2.75	0.42
1:I:28:LEU:O	1:I:32:VAL:HG23	2.19	0.42
1:A:32:VAL:HG13	1:A:82:LEU:HD21	2.00	0.42
1:I:282:ILE:O	1:I:282:ILE:HG23	2.19	0.42
1:C:251:LEU:HD22	1:C:255:LEU:HD22	2.00	0.42
1:A:99:PHE:HB3	1:A:100:PRO:HD3	2.01	0.42
1:F:210:VAL:O	1:F:214:VAL:HG23	2.19	0.42
1:B:69:ARG:O	1:B:70:ILE:C	2.57	0.42
1:B:395:HIS:CD2	1:B:397:ASN:HB2	2.54	0.42
1:D:235:LEU:O	1:D:239:GLU:HG3	2.19	0.42
1:C:353:ASN:O	1:C:354:PHE:C	2.57	0.42
1:G:411:SER:O	1:G:414:THR:HB	2.20	0.42
1:G:236:LYS:HA	1:G:239:GLU:HG2	2.01	0.42
1:G:142:GLU:OE2	1:G:146:ARG:NH1	2.53	0.42
1:B:229:GLY:O	1:B:233:LEU:HD13	2.20	0.42
1:C:184:ILE:HD11	1:E:377:ASN:HD21	1.83	0.42
1:A:242:THR:HG21	1:I:110:PRO:HG2	2.00	0.42
1:I:172:ILE:HD12	1:I:173:GLU:N	2.35	0.42
1:J:154:LYS:O	1:J:168:ARG:NH1	2.51	0.42
1:B:293:ALA:O	1:B:295:GLY:N	2.40	0.42
1:I:277:LEU:C	1:I:277:LEU:CD1	2.88	0.42
1:I:277:LEU:HD13	1:I:277:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:ARG:HD2	1:H:136:ARG:HA	1.86	0.42
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.81	0.42
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.85	0.42
1:D:190:LEU:HD12	1:D:190:LEU:O	2.18	0.42
1:C:262:CYS:SG	1:D:421:VAL:HG21	2.59	0.42
1:E:65:ASN:OD1	1:E:68:ARG:CG	2.68	0.42
1:C:84:ILE:HG23	1:C:131:TRP:HB3	2.01	0.42
1:A:130:GLU:OE1	1:A:136:ARG:NH1	2.52	0.42
1:A:292:THR:O	1:A:293:ALA:HB2	2.20	0.42
1:G:65:ASN:O	1:G:66:THR:CB	2.67	0.42
1:A:215:ILE:CG1	1:A:222:LEU:HD13	2.50	0.42
1:E:203:THR:C	1:E:206:PRO:HD2	2.40	0.42
1:C:288:PHE:O	1:C:289:PRO:C	2.57	0.42
1:G:250:ALA:O	1:G:254:ILE:HG23	2.20	0.42
1:A:157:GLU:HA	1:A:157:GLU:OE1	2.19	0.42
1:F:199:LEU:O	1:F:201:PRO:HD3	2.20	0.42
1:E:115:LEU:HD13	1:E:119:LEU:HD22	2.02	0.42
1:G:80:ILE:N	1:G:81:PRO:CD	2.83	0.42
1:B:65:ASN:ND2	1:B:68:ARG:HG3	2.35	0.42
1:G:1:MSE:HE2	1:G:4:GLN:HB3	2.01	0.42
1:C:293:ALA:O	1:C:294:SER:HB3	2.20	0.41
1:B:110:PRO:CG	1:J:242:THR:HG21	2.49	0.41
1:H:351:PRO:HG3	1:H:395:HIS:CE1	2.54	0.41
1:H:99:PHE:HB3	1:H:100:PRO:HD3	2.01	0.41
1:D:10:LEU:O	1:D:14:LEU:HD12	2.20	0.41
1:A:261:ILE:HG23	1:A:264:SER:H	1.85	0.41
1:E:74:ALA:O	1:E:78:THR:HG22	2.19	0.41
1:B:194:PHE:CD1	1:B:207:ILE:HG12	2.55	0.41
1:C:58:TYR:CE2	1:C:96:GLN:HG2	2.54	0.41
1:H:35:TYR:HD2	1:H:35:TYR:C	2.23	0.41
1:J:217:ARG:HG2	1:J:217:ARG:HH11	1.84	0.41
1:A:109:LYS:N	1:A:110:PRO:CD	2.83	0.41
1:J:25:LEU:O	1:J:29:ILE:HG13	2.19	0.41
1:H:74:ALA:O	1:H:78:THR:HG23	2.20	0.41
1:B:80:ILE:N	1:B:81:PRO:CD	2.83	0.41
1:D:281:MSE:HE2	1:D:281:MSE:HA	2.02	0.41
1:J:383:THR:HG22	1:J:384:LYS:N	2.34	0.41
1:B:194:PHE:CE1	1:B:207:ILE:HG12	2.56	0.41
1:C:72:TRP:O	1:C:76:LEU:HD22	2.21	0.41
1:E:276:TYR:C	1:E:276:TYR:CD1	2.94	0.41
1:A:38:ARG:NH1	1:A:38:ARG:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:ASP:OD1	1:H:266:ASP:N	2.51	0.41
1:H:184:ILE:HD13	1:H:184:ILE:HG21	1.80	0.41
1:G:217:ARG:HH11	1:G:217:ARG:HG3	1.85	0.41
1:H:181:HIS:O	1:H:185:GLN:HG3	2.21	0.41
1:H:269:LEU:CD2	1:H:273:PHE:CE1	3.04	0.41
1:A:80:ILE:HG23	1:A:81:PRO:CD	2.50	0.41
1:B:109:LYS:N	1:B:110:PRO:CD	2.83	0.41
1:A:198:PHE:CE2	1:A:204:ARG:HA	2.55	0.41
1:G:65:ASN:C	1:G:66:THR:HG22	2.41	0.41
1:C:347:TYR:O	1:C:351:PRO:HD3	2.21	0.41
1:G:71:LEU:O	1:G:75:VAL:HG23	2.21	0.41
1:A:377:ASN:C	1:A:377:ASN:OD1	2.59	0.41
1:A:225:ILE:N	1:A:226:PRO:CD	2.83	0.41
1:A:242:THR:O	1:A:242:THR:CG2	2.66	0.41
1:B:348:ALA:O	1:B:349:LEU:CB	2.55	0.41
1:G:414:THR:O	1:G:416:LEU:N	2.54	0.41
1:J:1:MSE:N	1:J:2:PRO:CD	2.84	0.41
1:D:203:THR:O	1:D:206:PRO:HD2	2.21	0.41
1:D:65:ASN:CG	1:D:66:THR:N	2.74	0.41
1:E:413:TRP:O	1:E:416:LEU:HB2	2.20	0.41
1:C:51:ARG:NH2	1:C:89:ALA:HB2	2.36	0.41
1:A:350:TYR:N	1:A:351:PRO:CD	2.83	0.41
1:B:129:ASP:O	1:B:130:GLU:C	2.60	0.41
1:J:1:MSE:O	1:J:2:PRO:C	2.59	0.41
1:C:269:LEU:HD22	1:C:273:PHE:CE1	2.56	0.41
1:I:420:ALA:HB2	1:J:420:ALA:HB2	2.03	0.41
1:F:258:LEU:HA	1:F:258:LEU:HD12	1.90	0.41
1:I:343:PHE:C	1:I:343:PHE:CD2	2.95	0.41
1:G:341:GLN:O	1:G:345:ILE:HG22	2.20	0.40
1:C:215:ILE:CD1	1:C:253:PHE:CE2	3.04	0.40
1:B:401:TYR:CZ	1:B:412:ARG:HG3	2.56	0.40
1:J:281:MSE:HA	1:J:281:MSE:HE2	2.03	0.40
1:I:245:ILE:O	1:I:248:SER:HB3	2.21	0.40
1:G:258:LEU:HA	1:G:258:LEU:HD12	1.89	0.40
1:H:65:ASN:CG	1:H:66:THR:H	2.24	0.40
1:A:293:ALA:O	1:A:294:SER:CB	2.69	0.40
1:J:102:LEU:HA	1:J:102:LEU:HD23	1.89	0.40
1:J:89:ALA:O	1:J:92:GLU:HB2	2.22	0.40
1:B:96:GLN:O	1:B:100:PRO:HG2	2.21	0.40
1:H:348:ALA:O	1:H:349:LEU:HB2	2.21	0.40
1:D:360:ASP:CG	1:D:363:LEU:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MSE:HE3	1:D:1:MSE:O	2.21	0.40
1:J:235:LEU:HD23	1:J:235:LEU:HA	1.97	0.40
1:J:198:PHE:CE2	1:J:204:ARG:HG2	2.56	0.40
1:B:76:LEU:O	1:B:80:ILE:HB	2.21	0.40
1:J:215:ILE:CD1	1:J:222:LEU:HD22	2.49	0.40
1:D:221:ARG:CG	1:D:221:ARG:HH11	2.35	0.40
1:F:28:LEU:O	1:F:32:VAL:HG23	2.22	0.40
1:F:238:ALA:O	1:F:278:ARG:NH1	2.52	0.40
1:E:198:PHE:CE2	1:E:204:ARG:HG2	2.56	0.40
1:F:215:ILE:HG13	1:F:253:PHE:CE2	2.56	0.40
1:B:83:LEU:HD23	1:B:83:LEU:N	2.36	0.40
1:H:89:ALA:O	1:H:92:GLU:N	2.53	0.40
1:J:115:LEU:HD22	1:J:119:LEU:HD22	2.03	0.40
1:F:282:ILE:HD13	1:F:288:PHE:CZ	2.56	0.40
1:G:109:LYS:N	1:G:110:PRO:CD	2.84	0.40
1:G:208:LEU:HB3	1:G:249:TYR:HB3	2.03	0.40
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.95	0.40
1:C:1:MSE:N	1:C:2:PRO:HD3	2.36	0.40
1:C:109:LYS:HB2	1:C:110:PRO:HD3	2.02	0.40
1:J:51:ARG:O	1:J:55:ASP:OD1	2.40	0.40

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%)	13	42
1	B	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	11	37
1	C	383/461 (83%)	348 (91%)	28 (7%)	7 (2%)	11	37
1	D	383/461 (83%)	349 (91%)	30 (8%)	4 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	383/461 (83%)	342 (89%)	31 (8%)	10 (3%)	7 26
1	F	383/461 (83%)	355 (93%)	21 (6%)	7 (2%)	11 37
1	G	383/461 (83%)	353 (92%)	25 (6%)	5 (1%)	15 46
1	H	383/461 (83%)	346 (90%)	30 (8%)	7 (2%)	11 37
1	I	383/461 (83%)	354 (92%)	17 (4%)	12 (3%)	5 21
1	J	383/461 (83%)	354 (92%)	20 (5%)	9 (2%)	8 30
All	All	3842/4610 (83%)	3508 (91%)	260 (7%)	74 (2%)	10 35

All (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
1	E	359	ARG
1	F	26	THR
1	G	66	THR
1	G	159	LEU
1	H	2	PRO
1	H	261	ILE
1	I	337	LEU
1	I	409	ASP
1	J	293	ALA
1	J	294	SER
1	J	297	TRP
1	J	298	GLU
1	A	328	SER
1	B	293	ALA
1	B	369	ASN
1	C	294	SER
1	C	367	LYS
1	D	107	GLN
1	D	159	LEU
1	D	294	SER
1	F	159	LEU
1	F	298	GLU
1	G	415	ARG
1	H	298	GLU

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Mol	Chain	Res	Type
1	I	298	GLU
1	I	348	ALA
1	I	349	LEU
1	J	2	PRO
1	J	107	GLN
1	A	62	PRO
1	C	298	GLU
1	C	369	ASN
1	E	298	GLU
1	F	62	PRO
1	F	367	LYS
1	G	261	ILE
1	G	349	LEU
1	H	264	SER
1	H	293	ALA
1	I	262	CYS
1	I	294	SER
1	A	196	HIS
1	A	262	CYS
1	B	62	PRO
1	B	159	LEU
1	B	294	SER
1	E	264	SER
1	F	302	ASP
1	H	62	PRO
1	J	349	LEU
1	J	367	LYS
1	A	359	ARG
1	B	370	PHE
1	C	349	LEU
1	E	62	PRO
1	E	159	LEU
1	E	367	LYS
1	H	25	LEU
1	I	2	PRO
1	I	62	PRO
1	I	159	LEU
1	E	295	GLY
1	E	415	ARG
1	I	293	ALA
1	E	29	ILE
1	I	261	ILE

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Mol	Chain	Res	Type
1	J	62	PRO
1	E	261	ILE
1	F	261	ILE

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%)	7 21
1	B	352/421 (84%)	294 (84%)	58 (16%)	3 8
1	C	352/421 (84%)	300 (85%)	52 (15%)	4 11
1	D	352/421 (84%)	318 (90%)	34 (10%)	10 30
1	E	352/421 (84%)	302 (86%)	50 (14%)	4 12
1	F	352/421 (84%)	306 (87%)	46 (13%)	5 15
1	G	352/421 (84%)	305 (87%)	47 (13%)	5 13
1	H	352/421 (84%)	307 (87%)	45 (13%)	5 16
1	I	352/421 (84%)	301 (86%)	51 (14%)	4 12
1	J	352/421 (84%)	303 (86%)	49 (14%)	4 12
All	All	3529/4210 (84%)	3056 (87%)	473 (13%)	5 13

All (473) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	LEU
1	A	5	SER
1	A	11	TRP
1	A	29	ILE
1	A	49	LYS
1	A	54	LEU
1	A	66	THR
1	A	76	LEU
1	A	78	THR

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Mol	Chain	Res	Type
1	A	82	LEU
1	A	85	LEU
1	A	115	LEU
1	A	119	LEU
1	A	123	LEU
1	A	134	ASP
1	A	136	ARG
1	A	149	ASP
1	A	184	ILE
1	A	191	SER
1	A	201	PRO
1	A	217	ARG
1	A	233	LEU
1	A	242	THR
1	A	251	LEU
1	A	254	ILE
1	A	255	LEU
1	A	263	ASN
1	A	266	ASP
1	A	269	LEU
1	A	277	LEU
1	A	337	LEU
1	A	340	SER
1	A	345	ILE
1	A	359	ARG
1	A	363	LEU
1	A	383	THR
1	A	414	THR
1	A	419	ILE
1	A	424	LEU
1	A	428	LEU
1	B	1	MSE
1	B	5	SER
1	B	6	LEU
1	B	14	LEU
1	B	26	THR
1	B	33	GLU
1	B	35	TYR
1	B	41	LYS
1	B	45	THR
1	B	49	LYS
1	B	51	ARG

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Mol	Chain	Res	Type
1	B	54	LEU
1	B	61	THR
1	B	65	ASN
1	B	66	THR
1	B	76	LEU
1	B	78	THR
1	B	80	ILE
1	B	82	LEU
1	B	115	LEU
1	B	119	LEU
1	B	123	LEU
1	B	130	GLU
1	B	136	ARG
1	B	143	THR
1	B	156	ILE
1	B	184	ILE
1	B	201	PRO
1	B	217	ARG
1	B	221	ARG
1	B	239	GLU
1	B	242	THR
1	B	245	ILE
1	B	251	LEU
1	B	254	ILE
1	B	255	LEU
1	B	257	ILE
1	B	258	LEU
1	B	259	SER
1	B	264	SER
1	B	265	LEU
1	B	266	ASP
1	B	267	ASP
1	B	269	LEU
1	B	277	LEU
1	B	291	SER
1	B	298	GLU
1	B	304	MSE
1	B	345	ILE
1	B	359	ARG
1	B	362	LYS
1	B	363	LEU
1	B	369	ASN

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Mol	Chain	Res	Type
1	B	371	GLN
1	B	410	LYS
1	B	412	ARG
1	B	419	ILE
1	B	424	LEU
1	C	3	LEU
1	C	4	GLN
1	C	6	LEU
1	C	11	TRP
1	C	42	GLN
1	C	45	THR
1	C	52	HIS
1	C	54	LEU
1	C	61	THR
1	C	65	ASN
1	C	66	THR
1	C	76	LEU
1	C	78	THR
1	C	79	VAL
1	C	82	LEU
1	C	85	LEU
1	C	115	LEU
1	C	119	LEU
1	C	123	LEU
1	C	126	HIS
1	C	128	GLU
1	C	136	ARG
1	C	193	CYS
1	C	196	HIS
1	C	209	SER
1	C	221	ARG
1	C	233	LEU
1	C	242	THR
1	C	248	SER
1	C	251	LEU
1	C	254	ILE
1	C	255	LEU
1	C	258	LEU
1	C	263	ASN
1	C	264	SER
1	C	265	LEU
1	C	268	SER

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Mol	Chain	Res	Type
1	C	269	LEU
1	C	271	ARG
1	C	280	SER
1	C	290	SER
1	C	304	MSE
1	C	341	GLN
1	C	345	ILE
1	C	359	ARG
1	C	363	LEU
1	C	369	ASN
1	C	412	ARG
1	C	414	THR
1	C	419	ILE
1	C	424	LEU
1	C	428	LEU
1	D	1	MSE
1	D	26	THR
1	D	45	THR
1	D	48	GLN
1	D	49	LYS
1	D	66	THR
1	D	67	ARG
1	D	76	LEU
1	D	80	ILE
1	D	82	LEU
1	D	115	LEU
1	D	119	LEU
1	D	123	LEU
1	D	156	ILE
1	D	184	ILE
1	D	196	HIS
1	D	221	ARG
1	D	233	LEU
1	D	251	LEU
1	D	254	ILE
1	D	255	LEU
1	D	259	SER
1	D	265	LEU
1	D	266	ASP
1	D	269	LEU
1	D	304	MSE
1	D	337	LEU

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Mol	Chain	Res	Type
1	D	363	LEU
1	D	375	SER
1	D	404	GLU
1	D	416	LEU
1	D	419	ILE
1	D	424	LEU
1	D	428	LEU
1	E	1	MSE
1	E	3	LEU
1	E	14	LEU
1	E	25	LEU
1	E	33	GLU
1	E	34	SER
1	E	36	GLN
1	E	38	ARG
1	E	45	THR
1	E	49	LYS
1	E	54	LEU
1	E	61	THR
1	E	76	LEU
1	E	78	THR
1	E	81	PRO
1	E	82	LEU
1	E	85	LEU
1	E	88	GLN
1	E	109	LYS
1	E	115	LEU
1	E	119	LEU
1	E	123	LEU
1	E	146	ARG
1	E	154	LYS
1	E	156	ILE
1	E	184	ILE
1	E	192	SER
1	E	196	HIS
1	E	221	ARG
1	E	233	LEU
1	E	242	THR
1	E	251	LEU
1	E	254	ILE
1	E	255	LEU
1	E	258	LEU

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Mol	Chain	Res	Type
1	E	264	SER
1	E	267	ASP
1	E	269	LEU
1	E	277	LEU
1	E	281	MSE
1	E	290	SER
1	E	304	MSE
1	E	345	ILE
1	E	349	LEU
1	E	363	LEU
1	E	400	LYS
1	E	419	ILE
1	E	424	LEU
1	E	428	LEU
1	E	429	ASN
1	F	3	LEU
1	F	5	SER
1	F	10	LEU
1	F	26	THR
1	F	27	GLU
1	F	45	THR
1	F	54	LEU
1	F	61	THR
1	F	66	THR
1	F	76	LEU
1	F	79	VAL
1	F	82	LEU
1	F	85	LEU
1	F	115	LEU
1	F	119	LEU
1	F	123	LEU
1	F	128	GLU
1	F	136	ARG
1	F	153	SER
1	F	184	ILE
1	F	209	SER
1	F	221	ARG
1	F	242	THR
1	F	251	LEU
1	F	255	LEU
1	F	258	LEU
1	F	259	SER

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Mol	Chain	Res	Type
1	F	261	ILE
1	F	265	LEU
1	F	269	LEU
1	F	271	ARG
1	F	286	SER
1	F	298	GLU
1	F	304	MSE
1	F	337	LEU
1	F	341	GLN
1	F	363	LEU
1	F	373	ARG
1	F	383	THR
1	F	391	ARG
1	F	404	GLU
1	F	412	ARG
1	F	417	ASP
1	F	424	LEU
1	F	427	SER
1	F	428	LEU
1	G	1	MSE
1	G	6	LEU
1	G	8	LYS
1	G	10	LEU
1	G	26	THR
1	G	41	LYS
1	G	48	GLN
1	G	51	ARG
1	G	54	LEU
1	G	67	ARG
1	G	76	LEU
1	G	78	THR
1	G	82	LEU
1	G	85	LEU
1	G	90	VAL
1	G	104	SER
1	G	119	LEU
1	G	123	LEU
1	G	134	ASP
1	G	136	ARG
1	G	154	LYS
1	G	168	ARG
1	G	184	ILE

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Mol	Chain	Res	Type
1	G	217	ARG
1	G	221	ARG
1	G	242	THR
1	G	248	SER
1	G	251	LEU
1	G	254	ILE
1	G	255	LEU
1	G	264	SER
1	G	265	LEU
1	G	269	LEU
1	G	277	LEU
1	G	280	SER
1	G	294	SER
1	G	304	MSE
1	G	341	GLN
1	G	345	ILE
1	G	363	LEU
1	G	375	SER
1	G	404	GLU
1	G	411	SER
1	G	412	ARG
1	G	415	ARG
1	G	424	LEU
1	G	428	LEU
1	H	1	MSE
1	H	3	LEU
1	H	10	LEU
1	H	26	THR
1	H	35	TYR
1	H	48	GLN
1	H	54	LEU
1	H	60	LYS
1	H	64	ASN
1	H	76	LEU
1	H	78	THR
1	H	82	LEU
1	H	85	LEU
1	H	88	GLN
1	H	90	VAL
1	H	115	LEU
1	H	119	LEU
1	H	123	LEU

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Mol	Chain	Res	Type
1	H	154	LYS
1	H	184	ILE
1	H	196	HIS
1	H	201	PRO
1	H	209	SER
1	H	213	GLU
1	H	216	ARG
1	H	217	ARG
1	H	221	ARG
1	H	233	LEU
1	H	242	THR
1	H	251	LEU
1	H	252	SER
1	H	254	ILE
1	H	255	LEU
1	H	259	SER
1	H	264	SER
1	H	266	ASP
1	H	269	LEU
1	H	271	ARG
1	H	341	GLN
1	H	362	LYS
1	H	363	LEU
1	H	375	SER
1	H	383	THR
1	H	424	LEU
1	H	428	LEU
1	I	3	LEU
1	I	6	LEU
1	I	13	VAL
1	I	25	LEU
1	I	26	THR
1	I	27	GLU
1	I	37	GLN
1	I	38	ARG
1	I	41	LYS
1	I	43	ASN
1	I	46	ASN
1	I	48	GLN
1	I	54	LEU
1	I	64	ASN
1	I	66	THR

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Mol	Chain	Res	Type
1	I	71	LEU
1	I	76	LEU
1	I	82	LEU
1	I	85	LEU
1	I	88	GLN
1	I	115	LEU
1	I	119	LEU
1	I	123	LEU
1	I	128	GLU
1	I	154	LYS
1	I	184	ILE
1	I	212	VAL
1	I	221	ARG
1	I	233	LEU
1	I	242	THR
1	I	251	LEU
1	I	254	ILE
1	I	255	LEU
1	I	264	SER
1	I	267	ASP
1	I	268	SER
1	I	269	LEU
1	I	271	ARG
1	I	277	LEU
1	I	285	THR
1	I	298	GLU
1	I	302	ASP
1	I	341	GLN
1	I	363	LEU
1	I	367	LYS
1	I	375	SER
1	I	411	SER
1	I	414	THR
1	I	419	ILE
1	I	424	LEU
1	I	428	LEU
1	J	3	LEU
1	J	6	LEU
1	J	10	LEU
1	J	15	HIS
1	J	26	THR
1	J	31	GLU

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Mol	Chain	Res	Type
1	J	36	GLN
1	J	45	THR
1	J	48	GLN
1	J	54	LEU
1	J	55	ASP
1	J	64	ASN
1	J	66	THR
1	J	76	LEU
1	J	77	LYS
1	J	82	LEU
1	J	85	LEU
1	J	90	VAL
1	J	115	LEU
1	J	117	SER
1	J	119	LEU
1	J	123	LEU
1	J	126	HIS
1	J	154	LYS
1	J	184	ILE
1	J	191	SER
1	J	217	ARG
1	J	233	LEU
1	J	251	LEU
1	J	255	LEU
1	J	258	LEU
1	J	259	SER
1	J	265	LEU
1	J	267	ASP
1	J	269	LEU
1	J	271	ARG
1	J	291	SER
1	J	302	ASP
1	J	337	LEU
1	J	341	GLN
1	J	345	ILE
1	J	371	GLN
1	J	383	THR
1	J	396	SER
1	J	410	LYS
1	J	412	ARG
1	J	418	SER
1	J	424	LEU

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Mol	Chain	Res	Type
1	J	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	B	12	ASN
1	B	42	GLN
1	B	395	HIS
1	C	12	ASN
1	C	88	GLN
1	D	395	HIS
1	E	46	ASN
1	E	107	GLN
1	E	169	ASN
1	F	46	ASN
1	F	395	HIS
1	G	227	GLN
1	G	301	HIS
1	H	169	ASN
1	H	341	GLN
1	I	43	ASN
1	J	395	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.32	13 (3%) 50 42	39, 63, 108, 136	0
1	B	386/461 (83%)	-0.18	11 (2%) 56 50	42, 75, 119, 152	0
1	C	386/461 (83%)	-0.31	5 (1%) 79 78	39, 59, 93, 130	0
1	D	386/461 (83%)	-0.23	14 (3%) 46 38	37, 71, 131, 172	0
1	E	386/461 (83%)	-0.23	7 (1%) 71 68	37, 60, 117, 152	0
1	F	386/461 (83%)	-0.27	5 (1%) 79 78	41, 63, 103, 149	0
1	G	386/461 (83%)	-0.26	10 (2%) 59 54	39, 67, 103, 134	0
1	H	386/461 (83%)	-0.29	7 (1%) 71 68	42, 67, 106, 141	0
1	I	386/461 (83%)	-0.31	6 (1%) 74 72	42, 64, 109, 140	0
1	J	386/461 (83%)	-0.32	6 (1%) 74 72	38, 65, 109, 146	0
All	All	3871/4610 (83%)	-0.27	84 (2%) 65 60	37, 65, 112, 172	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	161	ASP	5.3
1	A	305	SER	5.1
1	F	431	VAL	4.7
1	F	160	GLY	4.7
1	D	12	ASN	4.7
1	B	161	ASP	4.5
1	B	37	GLN	4.3
1	A	332	ASP	4.2
1	G	305	SER	4.1
1	F	161	ASP	4.1
1	G	2	PRO	4.0
1	G	160	GLY	4.0
1	A	159	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	160	GLY	3.7
1	D	431	VAL	3.6
1	G	38	ARG	3.6
1	B	64	ASN	3.5
1	D	60	LYS	3.4
1	D	15	HIS	3.3
1	D	11	TRP	3.3
1	G	37	GLN	3.2
1	B	134	ASP	3.2
1	E	431	VAL	3.2
1	I	431	VAL	3.1
1	A	329	SER	3.1
1	I	27	GLU	3.1
1	D	4	GLN	3.1
1	E	65	ASN	3.1
1	I	159	LEU	3.1
1	D	38	ARG	3.0
1	G	61	THR	3.0
1	G	431	VAL	3.0
1	E	64	ASN	2.9
1	I	8	LYS	2.9
1	C	126	HIS	2.9
1	B	132	GLY	2.8
1	B	38	ARG	2.7
1	H	161	ASP	2.7
1	C	38	ARG	2.7
1	A	336	SER	2.6
1	H	37	GLN	2.6
1	H	12	ASN	2.6
1	H	11	TRP	2.6
1	C	160	GLY	2.5
1	A	306	THR	2.5
1	J	40	PRO	2.5
1	A	134	ASP	2.5
1	H	160	GLY	2.5
1	E	305	SER	2.5
1	B	40	PRO	2.5
1	A	158	ASN	2.5
1	D	27	GLU	2.4
1	E	132	GLY	2.4
1	I	34	SER	2.4
1	D	13	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	296	ASN	2.4
1	J	431	VAL	2.4
1	F	129	ASP	2.3
1	J	38	ARG	2.3
1	D	129	ASP	2.3
1	D	336	SER	2.3
1	A	157	GLU	2.3
1	A	328	SER	2.3
1	C	431	VAL	2.3
1	D	2	PRO	2.3
1	A	333	TYR	2.3
1	J	305	SER	2.3
1	J	59	GLU	2.3
1	D	161	ASP	2.2
1	B	305	SER	2.2
1	D	160	GLY	2.2
1	E	129	ASP	2.2
1	G	59	GLU	2.2
1	E	12	ASN	2.2
1	G	33	GLU	2.1
1	C	52	HIS	2.1
1	J	41	LYS	2.1
1	A	431	VAL	2.1
1	I	160	GLY	2.1
1	H	127	ASP	2.1
1	A	331	PRO	2.1
1	F	303	PHE	2.0
1	B	60	LYS	2.0
1	H	414	THR	2.0

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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.