



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:26 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

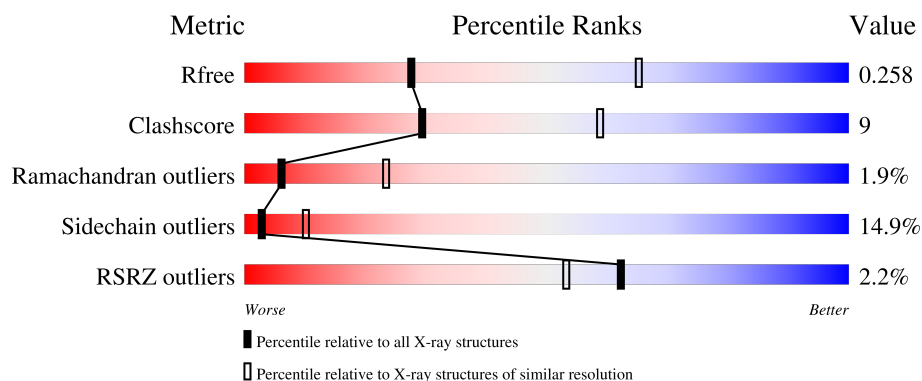
1 Overall quality at a glance

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
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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
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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
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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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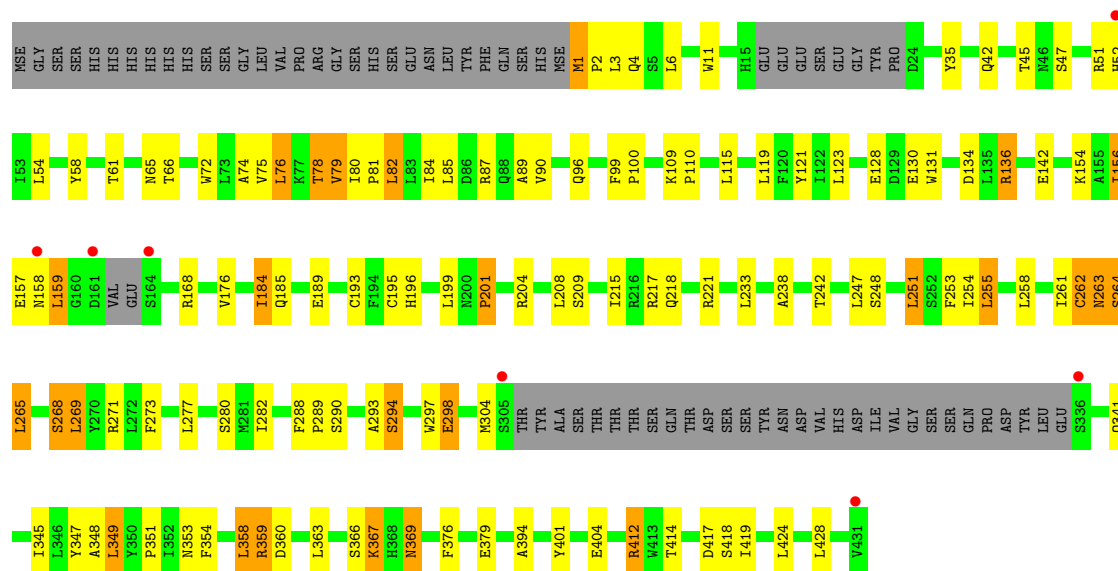
Chain	Residue	Modelled	Actual	Comment	Reference
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H	-19	SER	-	expression tag	UNP Q09778
H	-18	SER	-	expression tag	UNP Q09778
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H	-16	LEU	-	expression tag	UNP Q09778
H	-15	VAL	-	expression tag	UNP Q09778
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
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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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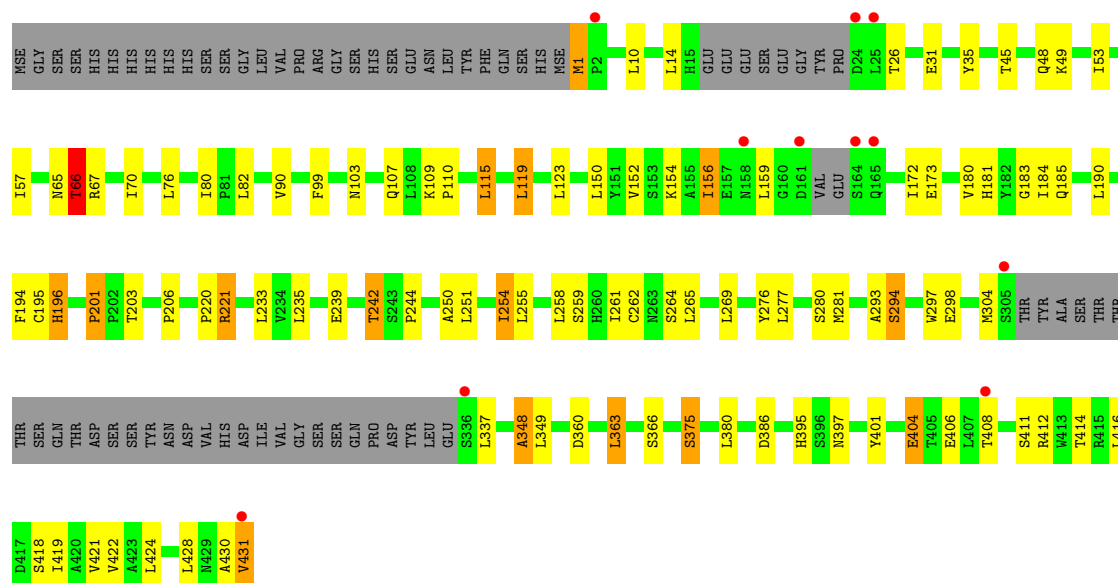
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Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	GLU	-	expression tag	UNP Q09778
I	-7	ASN	-	expression tag	UNP Q09778
I	-6	LEU	-	expression tag	UNP Q09778
I	-5	TYR	-	expression tag	UNP Q09778
I	-4	PHE	-	expression tag	UNP Q09778
I	-3	GLN	-	expression 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

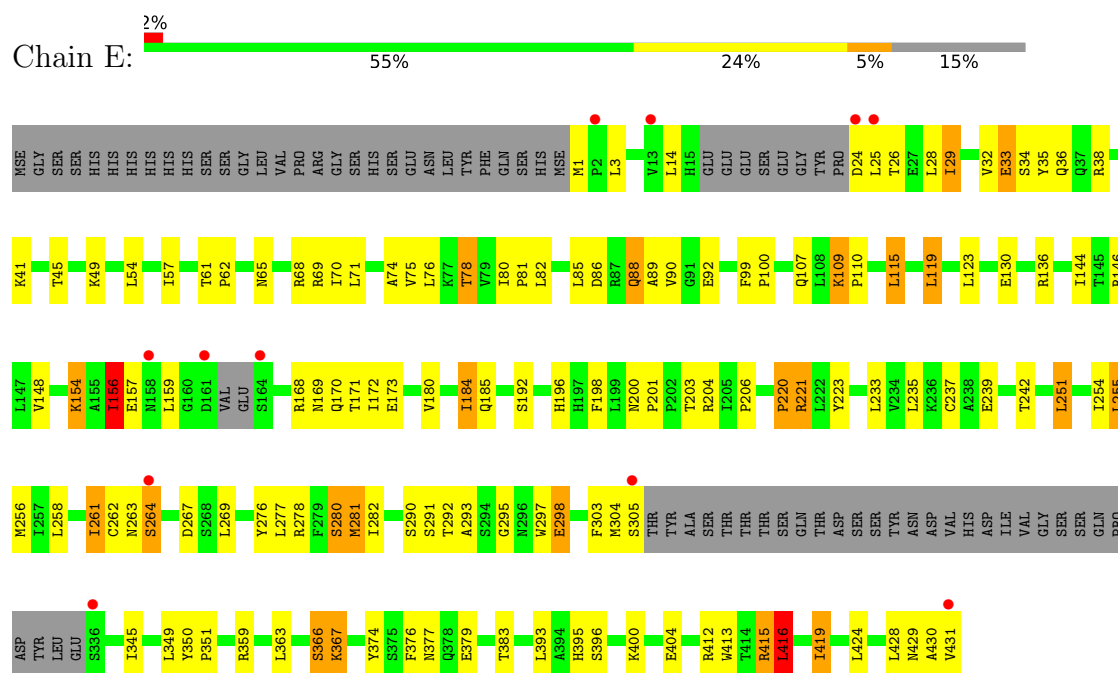
- Molecule 1: Tuberous sclerosis 1 protein homolog



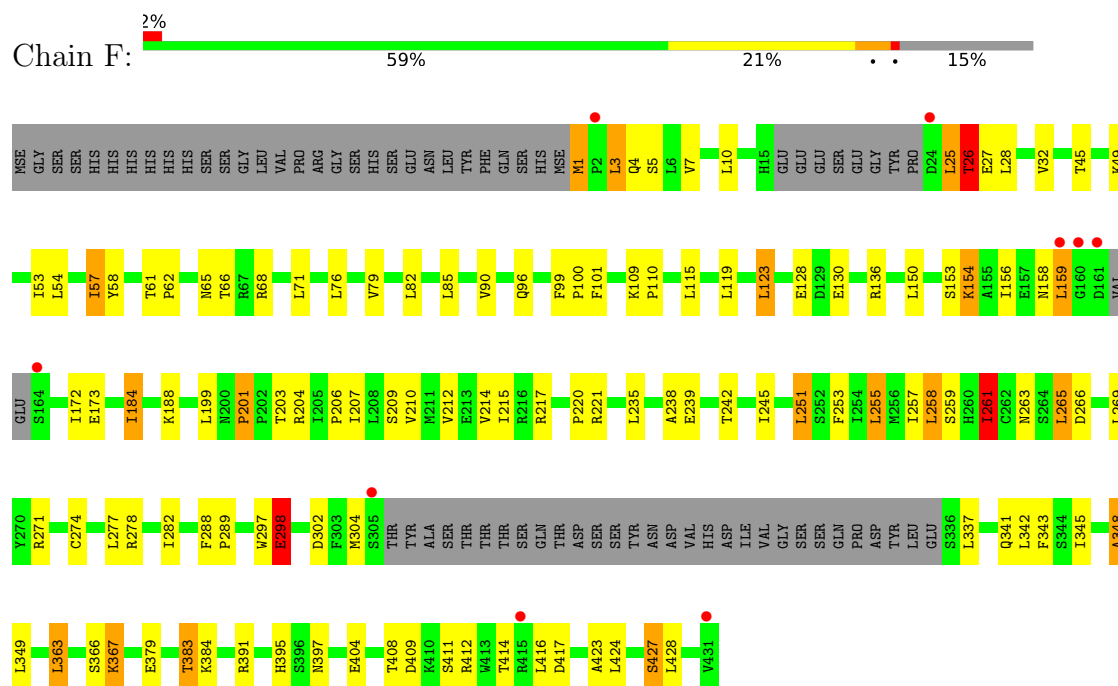
- Molecule 1: Tuberous sclerosis 1 protein homolog



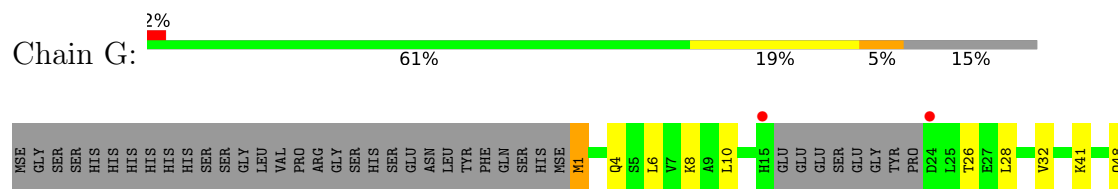
- Molecule 1: Tuberous sclerosis 1 protein homolog

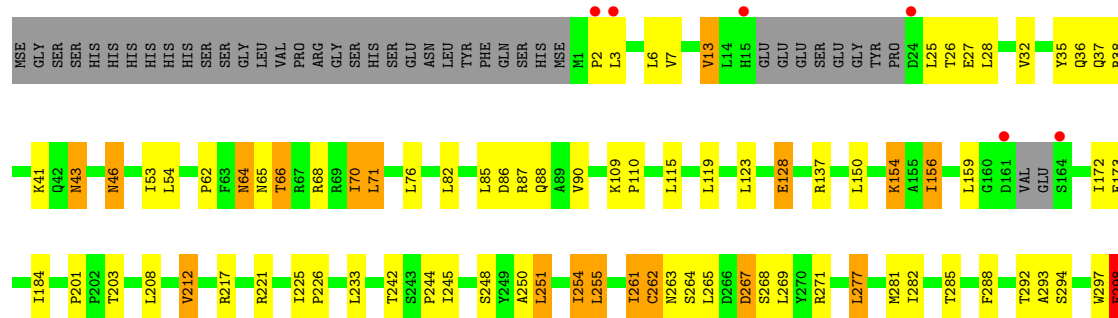


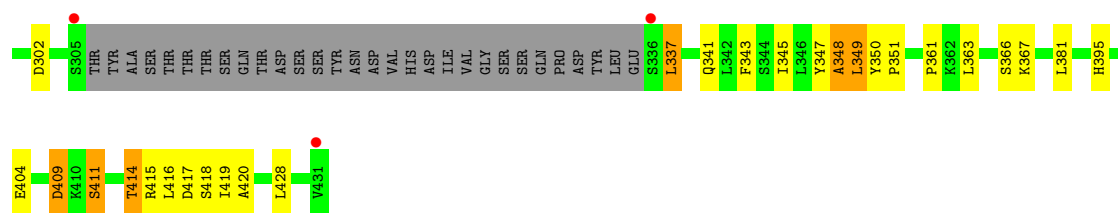
- Molecule 1: Tuberous sclerosis 1 protein homolog



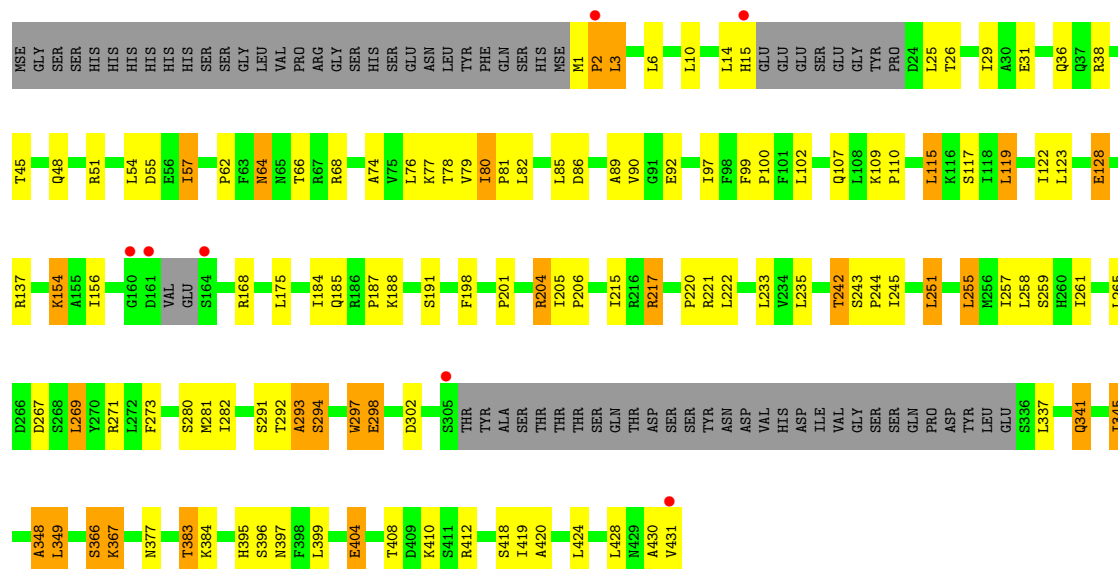
- Molecule 1: Tuberous sclerosis 1 protein homolog







● Molecule 1: Tuberous sclerosis 1 protein homolog



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

All (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
1	G	156	ILE	N-CA-C	7.76	118.30	110.23
1	H	348	ALA	N-CA-C	-7.65	100.71	110.19
1	F	25	LEU	N-CA-C	7.61	121.82	112.54
1	E	366	SER	N-CA-C	-7.43	100.72	110.53
1	B	348	ALA	N-CA-C	-7.37	100.10	110.50
1	C	201	PRO	N-CA-C	7.29	119.59	110.70
1	J	201	PRO	N-CA-C	7.24	119.53	110.70
1	E	201	PRO	N-CA-C	7.19	119.48	110.70
1	F	207	ILE	N-CA-C	7.19	117.32	110.42
1	D	348	ALA	N-CA-C	-7.19	100.58	110.35
1	H	80	ILE	CA-C-N	-7.00	112.49	119.56
1	H	80	ILE	C-N-CA	-7.00	112.49	119.56
1	J	156	ILE	N-CA-C	6.96	117.07	110.53
1	A	201	PRO	N-CA-C	6.90	119.12	110.70
1	J	80	ILE	CA-C-N	-6.82	112.88	120.45
1	J	80	ILE	C-N-CA	-6.82	112.88	120.45
1	B	97	ILE	CB-CA-C	-6.75	105.97	111.71
1	D	201	PRO	N-CA-C	6.61	118.77	110.70
1	I	201	PRO	N-CA-C	6.61	118.76	110.70
1	E	200	ASN	CA-C-N	6.48	127.05	120.38
1	E	200	ASN	C-N-CA	6.48	127.05	120.38
1	A	358	LEU	N-CA-C	-6.27	102.26	110.53
1	J	366	SER	N-CA-C	-6.23	101.71	110.50
1	E	416	LEU	N-CA-C	6.17	117.68	111.07
1	F	212	VAL	N-CA-CB	6.02	119.61	110.58
1	H	200	ASN	CA-C-N	6.00	126.56	120.38
1	H	200	ASN	C-N-CA	6.00	126.56	120.38
1	C	201	PRO	CA-C-N	-5.99	113.64	119.87
1	C	201	PRO	C-N-CA	-5.99	113.64	119.87
1	F	156	ILE	N-CA-C	5.97	117.91	111.58
1	I	156	ILE	N-CA-C	5.97	116.94	111.81
1	A	360	ASP	CA-C-N	5.93	125.14	118.97
1	A	360	ASP	C-N-CA	5.93	125.14	118.97
1	F	348	ALA	N-CA-C	-5.91	102.31	110.35
1	B	156	ILE	CB-CA-C	-5.84	104.27	111.92
1	G	201	PRO	N-CA-C	5.80	117.78	110.70
1	A	378	GLN	N-CA-C	5.77	117.57	111.28
1	A	156	ILE	N-CA-C	5.72	116.93	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	366	SER	N-CA-C	-5.70	102.96	110.43
1	B	201	PRO	CA-C-N	-5.67	114.15	120.45
1	B	201	PRO	C-N-CA	-5.67	114.15	120.45
1	A	415	ARG	CA-C-N	5.64	128.11	120.38
1	A	415	ARG	C-N-CA	5.64	128.11	120.38
1	I	349	LEU	N-CA-C	5.64	122.81	110.80
1	F	201	PRO	CA-C-N	-5.63	113.95	120.04
1	F	201	PRO	C-N-CA	-5.63	113.95	120.04
1	J	348	ALA	N-CA-C	-5.60	102.60	110.50
1	J	156	ILE	CB-CA-C	-5.56	104.74	112.02
1	E	156	ILE	CB-CA-C	-5.54	106.17	111.44
1	F	123	LEU	N-CA-C	5.53	116.99	111.07
1	I	366	SER	N-CA-C	-5.50	103.28	110.53
1	D	195	CYS	N-CA-C	5.49	117.98	111.33
1	C	195	CYS	N-CA-C	5.49	117.69	111.11
1	J	201	PRO	CA-C-N	-5.44	114.17	120.04
1	J	201	PRO	C-N-CA	-5.44	114.17	120.04
1	C	358	LEU	N-CA-C	-5.43	103.32	110.33
1	E	280	SER	N-CA-C	-5.42	106.84	113.50
1	J	292	THR	N-CA-C	-5.40	104.35	111.96
1	D	201	PRO	CA-C-N	-5.38	114.15	120.12
1	D	201	PRO	C-N-CA	-5.38	114.15	120.12
1	B	366	SER	N-CA-C	-5.35	103.46	110.53
1	B	200	ASN	CA-C-N	5.24	125.78	120.38
1	B	200	ASN	C-N-CA	5.24	125.78	120.38
1	E	293	ALA	CB-CA-C	-5.22	110.53	116.54
1	J	79	VAL	CB-CA-C	-5.16	104.40	110.84
1	C	376	PHE	N-CA-C	5.15	116.90	108.76
1	D	196	HIS	N-CA-C	-5.15	105.58	111.14
1	G	304	MSE	CG-SE-CE	5.14	110.23	98.92
1	J	122	ILE	CB-CA-C	-5.12	105.33	112.04
1	C	134	ASP	N-CA-C	-5.11	105.52	112.26
1	G	212	VAL	N-CA-CB	5.10	118.23	110.58
1	E	237	CYS	N-CA-C	-5.08	105.63	111.07
1	E	256	MSE	CG-SE-CE	-5.08	87.74	98.92
1	B	212	VAL	N-CA-CB	5.07	118.19	110.58
1	J	204	ARG	N-CA-C	5.07	116.80	111.28
1	C	47	SER	N-CA-C	-5.05	105.66	111.07
1	D	375	SER	N-CA-C	-5.05	101.73	109.76
1	I	292	THR	N-CA-C	-5.05	107.19	113.55
1	C	156	ILE	CB-CA-C	-5.04	103.02	111.29
1	F	204	ARG	N-CA-C	5.04	116.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	118	ILE	CB-CA-C	-5.03	105.38	111.87

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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:G:51:ARG:HH11	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:HG23	1:H:408:THR:O	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:B:80:ILE:HD13	1:B:80:ILE:O	1.94	0.67
1:D:395:HIS:HD2	1:D:397:ASN:H	1.39	0.67
1:F:217:ARG:HG2	1:F:217:ARG:HH11	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
1:G:217:ARG:HH11	1:G:217:ARG:CG	2.09	0.66
1:B:71:LEU:O	1:B:75:VAL:HG23	1.96	0.65
1:B:430:ALA:O	1:B:431:VAL:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:347:TYR:C	1:I:348:ALA:O	2.39	0.61
1:D:280:SER:O	1:D:281:MSE:HE2	2.00	0.61
1:I:64:ASN:OD1	1:I:64:ASN:N	2.34	0.61
1:J:64:ASN:OD1	1:J:68:ARG:NH1	2.33	0.61
1:H:115:LEU:HD13	1:H:119:LEU:HD22	1.81	0.61
1:H:217:ARG:HH11	1:H:217:ARG:CG	2.13	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:F:409:ASP:OD1	1:F:409:ASP:C	2.45	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:E:280:SER:C	1:E:281:MSE:HE2	2.28	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:CG	1:A:217:ARG:HH11	2.16	0.58
1:E:280:SER:O	1:E:281:MSE:HE2	2.03	0.58
1:B:84:ILE:C	1:B:85:LEU:HD12	2.29	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:C:366:SER:OG	1:C:366:SER:O	2.20	0.57
1:E:261:ILE:HG22	1:E:262:CYS:N	2.18	0.57
1:E:297:TRP:O	1:E:298:GLU:CB	2.52	0.57
1:F:65:ASN:ND2	1:F:68:ARG:HD2	2.20	0.57
1:B:369:ASN:OD1	1:B:370:PHE:N	2.37	0.56
1:I:267:ASP:N	1:I:267:ASP:OD1	2.38	0.56
1:A:282:ILE:HD12	1:A:288:PHE:CE2	2.40	0.56
1:B:142:GLU:O	1:B:146:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:LEU:O	1:F:239:GLU:HG3	2.05	0.56
1:D:395:HIS:CD2	1:D:397:ASN:H	2.20	0.56
1:E:156:ILE:O	1:E:157:GLU:C	2.48	0.56
1:F:366:SER:O	1:F:367:LYS:HB2	2.06	0.56
1:A:187:PRO:O	1:A:191:SER:OG	2.23	0.56
1:E:185:GLN:HA	1:G:379:GLU:HG3	1.88	0.56
1:F:277:LEU:HD13	1:F:277:LEU:C	2.31	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:B:369:ASN:OD1	1:B:369:ASN:C	2.49	0.56
1:A:63:PHE:CE2	1:A:69:ARG:HG2	2.41	0.56
1:C:215:ILE:HD11	1:C:253:PHE:CE2	2.41	0.56
1:H:35:TYR:C	1:H:35:TYR:CD2	2.84	0.56
1:B:399:LEU:O	1:C:359:ARG:HB2	2.05	0.55
1:F:379:GLU:HG3	1:H:185:GLN:HA	1.88	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: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:261:ILE:C	1:C:263:ASN:H	2.14	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:H:14:LEU:HD13	1:H:57:ILE:HG21	1.89	0.54
1:I:409:ASP:OD1	1:I:411:SER:HB3	2.08	0.54
1:A:297:TRP:O	1:A:298:GLU:HB3	2.07	0.54
1:A:358:LEU:O	1:A:359:ARG:CB	2.53	0.54
1:C:264:SER:O	1:C:268:SER:OG	2.26	0.54
1:A:63:PHE:CD2	1:A:69:ARG:HG2	2.42	0.54
1:G:348:ALA:O	1:G:349:LEU:CB	2.52	0.54
1:A:414:THR:O	1:A:415:ARG:C	2.50	0.54
1:G:115:LEU:CD1	1:G:119:LEU:HD22	2.37	0.54
1:G:269:LEU:HD22	1:G:273:PHE:CE1	2.43	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:D:14:LEU:HD13	1:D:57:ILE:HG21	1.88	0.54
1:C:217:ARG:O	1:C:218:GLN:C	2.52	0.53
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:B:51:ARG:O	1:B:55:ASP:OD2	2.26	0.53
1:E:69:ARG:O	1:E:70:ILE:C	2.51	0.53
1:G:261:ILE:HG22	1:G:262:CYS:H	1.73	0.53
1:I:277:LEU:HD13	1:I:277:LEU:C	2.33	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:J:348:ALA:O	1:J:349:LEU:CB	2.57	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:D:277:LEU:HD13	1:D:277:LEU:C	2.33	0.53
1:J:293:ALA:O	1:J:294:SER:CB	2.57	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:215:ILE:CD1	1:H:253:PHE:CE2	2.92	0.53
1:H:408:THR:O	1:H:408:THR:CG2	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:H:365:ALA:C	1:H:366:SER:O	2.49	0.52
1:B:74:ALA:O	1:B:78:THR:HG23	2.09	0.52
1:G:217:ARG:HH11	1:G:217:ARG:HG2	1.73	0.52
1:B:35:TYR:C	1:B:35:TYR:CD2	2.87	0.52
1:E:303:PHE:C	1:E:305:SER:H	2.18	0.52
1:H:366:SER:O	1:H:367:LYS:HB2	2.10	0.52
1:F:158:ASN:O	1:F:159:LEU:CB	2.58	0.52
1:G:65:ASN:O	1:G:66:THR:HG22	2.09	0.52
1:I:46:ASN:OD1	1:I:46:ASN:N	2.42	0.52
1:A:266:ASP:OD1	1:A:266:ASP:N	2.41	0.52
1:I:150:LEU:O	1:I:154:LYS:HB2	2.10	0.52
1:B:136:ARG:HH11	1:B:136:ARG:CG	2.23	0.52
1:B:247:LEU:HD13	1:B:288:PHE:CD1	2.46	0.51
1:C:35:TYR:CE2	1:C:82:LEU:HG	2.45	0.51
1:D:203:THR:C	1:D:206:PRO:HD2	2.35	0.51
1:D:408:THR:HG23	1:D:408:THR:O	2.10	0.51
1:A:102:LEU:HD13	1:A:175:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:VAL:O	1:C:79:VAL:HG13	2.11	0.51
1:J:97:ILE:C	1:J:100:PRO:HD2	2.34	0.51
1:B:7:VAL:HG13	1:B:53:ILE:HD13	1.93	0.51
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: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:F:395:HIS:CD2	1:F:397:ASN:H	2.27	0.51
1:H:217:ARG:O	1:H:218:GLN:C	2.53	0.51
1:E:172:ILE:HG13	1:E:173:GLU:N	2.25	0.51
1:I:7:VAL:HG13	1:I:53:ILE:HD13	1.93	0.51
1:I:217:ARG:HG2	1:I:217:ARG:HH11	1.76	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:C:261:ILE:O	1:C:263:ASN:N	2.44	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:H:260:HIS:C	1:H:261:ILE:HG13	2.37	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:D:35:TYR:C	1:D:35:TYR:CD2	2.88	0.50
1:E:180:VAL:O	1:E:184:ILE:HG23	2.11	0.50
1:F:130:GLU:OE1	1:F:136:ARG:NH1	2.44	0.50
1:F:217:ARG:HG2	1:F:217:ARG:NH1	2.26	0.50
1:E:35:TYR:C	1:E:35:TYR:CD2	2.90	0.50
1:E:221:ARG:HB3	1:E:223:TYR:CE2	2.46	0.50
1:J:99:PHE:HB3	1:J:100:PRO:HD3	1.93	0.50
1:J:366:SER:O	1:J:367:LYS:CB	2.59	0.50
1:B:3:LEU:HD23	1:B:3:LEU:O	2.12	0.50
1:E:71:LEU:O	1:E:75:VAL:HG23	2.11	0.50
1:G:424:LEU:O	1:G:427:SER:OG	2.28	0.50
1:H:1:MSE:O	1:H:2:PRO:C	2.55	0.50
1:J:404:GLU:O	1:J:408:THR:HG23	2.12	0.50
1:A:203:THR:O	1:A:207:ILE:HG13	2.12	0.50
1:G:261:ILE:HG22	1:G:262:CYS:N	2.27	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:C:359:ARG:HG3	1:C:360:ASP:N	2.26	0.49
1:D:261:ILE:HG23	1:D:264:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:358:LEU:O	1:C:359:ARG:HB3	2.12	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: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:F:203:THR:C	1:F:206:PRO:HD2	2.38	0.49
1:G:255:LEU:HD23	1:G:337:LEU:HB3	1.94	0.49
1:D:150:LEU:HD11	1:D:154:LYS:HE3	1.95	0.48
1:A:261:ILE:HG22	1:A:262:CYS:N	2.29	0.48
1:F:342:LEU:O	1:F:345:ILE:HG22	2.13	0.48
1:F:408:THR:O	1:F:408:THR:OG1	2.27	0.48
1:J:205:ILE:HB	1:J:206:PRO:HD3	1.96	0.48
1:B:406:GLU:O	1:B:412:ARG:NH2	2.45	0.48
1:H:364:TYR:O	1:H:366:SER:O	2.31	0.48
1:J:217:ARG:HH11	1:J:217:ARG:CG	2.26	0.48
1:B:379:GLU:HG2	1:D:185:GLN:HG2	1.95	0.48
1:B:410:LYS:HE3	1:B:410:LYS:HA	1.95	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:D:152:VAL:HG12	1:D:156:ILE:HD11	1.95	0.48
1:E:109:LYS:N	1:E:110:PRO:HD2	2.28	0.48
1:J:430:ALA:O	1:J:431:VAL:HB	2.13	0.48
1:C:268:SER:O	1:C:269:LEU:C	2.56	0.48
1:C:366:SER:O	1:C:367:LYS:CB	2.61	0.48
1:I:86:ASP:O	1:I:87:ARG:C	2.55	0.48
1:J:377:ASN:OD1	1:J:377:ASN:C	2.56	0.48
1:A:401:TYR:CZ	1:A:412:ARG:HG2	2.49	0.48
1:B:256:MSE:HE3	1:B:337:LEU:CD2	2.43	0.48
1:C:261:ILE:HG22	1:C:262:CYS:N	2.29	0.48
1:D:261:ILE:CG2	1:D:264:SER:HB2	2.44	0.48
1:I:251:LEU:HD22	1:I:255:LEU:HD13	1.96	0.48
1:J:185:GLN:O	1:J:221:ARG:NH2	2.44	0.48
1:B:217:ARG:O	1:B:218:GLN:C	2.57	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:A:261:ILE:C	1:A:263:ASN:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:ALA:O	1:B:431:VAL:CB	2.61	0.47
1:F:25:LEU:O	1:F:26:THR:C	2.58	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:26:THR:HG23	1:G:295:GLY:HA2	1.95	0.47
1:E:154:LYS:O	1:E:168:ARG:HD2	2.15	0.47
1:B:69:ARG:O	1:B:70:ILE:C	2.57	0.47
1:C:277:LEU:HD23	1:C:277:LEU:O	2.13	0.47
1:D:404:GLU:O	1:D:408:THR:HG22	2.14	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:C:353:ASN:O	1:C:354:PHE:C	2.57	0.47
1:D:406:GLU:O	1:D:412:ARG:NH2	2.42	0.47
1:I:208:LEU:HD23	1:I:208:LEU:HA	1.77	0.47
1:B:50:ILE:HA	1:B:53:ILE:HD12	1.97	0.47
1:B:205:ILE:HB	1:B:206:PRO:HD3	1.97	0.47
1:D:430:ALA:O	1:D:431:VAL:HG23	2.14	0.47
1:F:53:ILE:O	1:F:57:ILE:HG13	2.15	0.47
1:I:277:LEU:C	1:I:277:LEU:CD1	2.88	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:E:203:THR:C	1:E:206:PRO:HD2	2.40	0.47
1:G:73:LEU:O	1:G:77:LYS:HB2	2.15	0.47
1:I:251:LEU:CD2	1:I:255:LEU:HD13	2.44	0.47
1:J:14:LEU:HD13	1:J:57:ILE:HG21	1.97	0.47
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:J:99:PHE:N	1:J:100:PRO:CD	2.77	0.46
1:E:278:ARG:HD2	1:E:374:TYR:CZ	2.51	0.46
1:F:366:SER:O	1:F:367:LYS:CB	2.63	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:35:TYR:C	1:H:35:TYR:HD2	2.23	0.46
1:H:198:PHE:CE1	1:H:204:ARG:HD3	2.49	0.46
1:E:235:LEU:O	1:E:239:GLU:HG2	2.16	0.46
1:E:276:TYR:CD1	1:E:276:TYR:C	2.94	0.46
1:F:257:ILE:HG23	1:F:261:ILE:HD11	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:128:GLU:OE1	1:J:137:ARG:NH1	2.49	0.46
1:J:395:HIS:CD2	1:J:397:ASN:H	2.25	0.46
1:A:377:ASN:C	1:A:377:ASN:OD1	2.59	0.46
1:B:180:VAL:O	1:B:184:ILE:HG23	2.15	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:292:THR:HG23	1:B:292:THR:O	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: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:D:65:ASN:CG	1:D:66:THR:N	2.74	0.45
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:I:343:PHE:C	1:I:343:PHE:CD2	2.95	0.45
1:J:1:MSE:O	1:J:2:PRO:C	2.59	0.45
1:H:217:ARG:CG	1:H:217:ARG:NH1	2.78	0.45
1:I:281:MSE:HE3	1:I:381:LEU:HD12	1.98	0.45
1:I:281:MSE:HE2	1:I:281:MSE:HA	1.97	0.45
1:C:288:PHE:O	1:C:289:PRO:C	2.57	0.45
1:D:31:GLU:OE2	1:D:31:GLU:HA	2.15	0.45
1:D:360:ASP:CG	1:D:363:LEU:HB2	2.42	0.45
1:I:208:LEU:O	1:I:212:VAL:HG13	2.16	0.45
1:A:74:ALA:O	1:A:78:THR:CG2	2.65	0.45
1:B:129:ASP:O	1:B:130:GLU:C	2.60	0.45
1:G:51:ARG:HG3	1:G:51:ARG:NH1	2.28	0.45
1:H:27:GLU:O	1:H:30:ALA:HB3	2.17	0.45
1:H:65:ASN:CG	1:H:66:THR:H	2.24	0.45
1:E:393:LEU:HD12	1:F:427:SER:O	2.17	0.45
1:G:65:ASN:C	1:G:66:THR:HG22	2.41	0.45
1:I:244:PRO:O	1:I:245:ILE:C	2.60	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:C:277:LEU:HD23	1:C:277:LEU:C	2.42	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: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:C:269:LEU:HD23	1:C:269:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ILE:HD12	1:D:173:GLU:N	2.32	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:J:269:LEU:HD22	1:J:273:PHE:CE1	2.52	0.44
1:C:204:ARG:CZ	1:C:297:TRP:CZ2	2.99	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:F:4:GLN:HA	1:F:7:VAL:HB	1.99	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:I:172:ILE:HD12	1:I:172:ILE:C	2.43	0.44
1:J:187:PRO:O	1:J:188:LYS:C	2.60	0.44
1:C:208:LEU:HD23	1:C:208:LEU:HA	1.77	0.44
1:C:261:ILE:C	1:C:263:ASN:N	2.76	0.44
1:D:418:SER:O	1:D:422:VAL:HG23	2.18	0.44
1:F:265:LEU:O	1:F:266:ASP:C	2.58	0.44
1:F:288:PHE:O	1:F:289:PRO:C	2.61	0.44
1:A:215:ILE:HG13	1:A:222:LEU:HD13	2.00	0.44
1:I:225:ILE:N	1:I:226:PRO:CD	2.80	0.44
1:B:141:GLU:HA	1:B:144:ILE:HG22	1.99	0.44
1:C:156:ILE:O	1:C:157:GLU:C	2.61	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:B:217:ARG:HD2	1:J:383:THR:HG21	1.99	0.44
1:C:263:ASN:C	1:C:265:LEU:H	2.26	0.44
1:E:297:TRP:O	1:E:298:GLU:HB3	2.17	0.44
1:F:150:LEU:O	1:F:154:LYS:HB2	2.17	0.44
1:F:261:ILE:C	1:F:263:ASN:H	2.26	0.44
1:F:277:LEU:C	1:F:277:LEU:CD1	2.90	0.44
1:H:297:TRP:O	1:H:298:GLU:HB3	2.17	0.44
1:I:13:VAL:O	1:I:71:LEU:HD21	2.17	0.44
1:A:208:LEU:HD12	1:A:246:LEU:HD11	2.00	0.44
1:A:420:ALA:HB2	1:B:420:ALA:HB2	2.00	0.44
1:B:267:ASP:N	1:B:267:ASP:OD1	2.51	0.44
1:C:199:LEU:O	1:C:201:PRO:HD3	2.18	0.44
1:D:109:LYS:HB2	1:D:110:PRO:HD3	1.99	0.44
1:F:172:ILE:O	1:F:173:GLU:C	2.61	0.44
1:F:383:THR:HG22	1:F:384:LYS:N	2.33	0.44
1:A:80:ILE:HD12	1:A:93:TRP:CZ3	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:GLU:HG2	1:D:412:ARG:NH2	2.33	0.43
1:E:86:ASP:H	1:E:89:ALA:HB3	1.82	0.43
1:I:43:ASN:HB3	1:I:46:ASN:OD1	2.17	0.43
1:I:128:GLU:HB3	1:I:137:ARG:NH1	2.32	0.43
1:B:110:PRO:HG2	1:J:242:THR:HG21	1.99	0.43
1:D:250:ALA:O	1:D:254:ILE:HG23	2.18	0.43
1:F:101:PHE:C	1:F:101:PHE:CD2	2.96	0.43
1:J:280:SER:O	1:J:281:MSE:HE2	2.17	0.43
1:B:107:GLN:O	1:B:108:LEU:HD23	2.19	0.43
1:B:291:SER:OG	1:B:292:THR:N	2.49	0.43
1:B:389:LEU:HD11	1:C:394:ALA:HB1	1.98	0.43
1:B:220:PRO:HB2	1:B:221:ARG:CG	2.48	0.43
1:E:169:ASN:HA	1:E:172:ILE:HG12	2.00	0.43
1:G:366:SER:O	1:G:367:LYS:CB	2.66	0.43
1:A:80:ILE:HG23	1:A:81:PRO:HD3	2.01	0.43
1:E:32:VAL:O	1:E:36:GLN:HG3	2.18	0.43
1:G:299:VAL:HG12	1:G:301:HIS:CE1	2.53	0.43
1:C:87:ARG:HD3	1:C:142:GLU:OE1	2.18	0.43
1:C:282:ILE:HD12	1:C:288:PHE:CZ	2.54	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:H:160:GLY:O	1:H:164:SER:CB	2.67	0.43
1:H:263:ASN:C	1:H:265:LEU:H	2.25	0.43
1:H:366:SER:O	1:H:368:HIS:N	2.50	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:D:386:ASP:OD2	1:E:396:SER:HB3	2.19	0.43
1:E:281:MSE:HG3	1:E:376:PHE:HB2	2.00	0.43
1:E:351:PRO:HG3	1:E:395:HIS:CE1	2.54	0.43
1:G:99:PHE:CZ	1:G:103:ASN:ND2	2.87	0.43
1:G:199:LEU:O	1:G:201:PRO:HD3	2.19	0.43
1:H:24:ASP:C	1:H:26:THR:H	2.27	0.43
1:H:293:ALA:HB3	1:H:373:ARG:HD3	2.00	0.43
1:A:195:CYS:O	1:A:196:HIS:C	2.62	0.43
1:B:86:ASP:O	1:B:87:ARG:C	2.61	0.43
1:E:415:ARG:O	1:E:419:ILE:HG23	2.18	0.43
1:H:65:ASN:OD1	1:H:66:THR:N	2.50	0.43
1:J:86:ASP:OD1	1:J:89:ALA:N	2.38	0.43
1:B:269:LEU:CD2	1:B:273:PHE:CE1	3.02	0.42
1:A:32:VAL:HG13	1:A:82:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HB3	1:A:100:PRO:HD3	2.01	0.42
1:C:251:LEU:HD22	1:C:255:LEU:HD22	2.00	0.42
1:F:99:PHE:C	1:F:99:PHE:CD2	2.98	0.42
1:F:210:VAL:O	1:F:214:VAL:HG23	2.19	0.42
1:G:217:ARG:CG	1:G:217:ARG:NH1	2.75	0.42
1:G:414:THR:C	1:G:416:LEU:H	2.27	0.42
1:I:28:LEU:O	1:I:32:VAL:HG23	2.19	0.42
1:B:229:GLY:O	1:B:233:LEU:HD13	2.20	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:G:142:GLU:OE2	1:G:146:ARG:NH1	2.53	0.42
1:G:236:LYS:HA	1:G:239:GLU:HG2	2.01	0.42
1:G:411:SER:O	1:G:414:THR:HB	2.20	0.42
1:A:242:THR:HG21	1:I:110:PRO:HG2	2.00	0.42
1:B:293:ALA:O	1:B:295:GLY:N	2.40	0.42
1:C:184:ILE:HD11	1:E:377:ASN:HD21	1.83	0.42
1:C:417:ASP:O	1:C:418:SER:C	2.62	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:A:258:LEU:HD12	1:A:258:LEU:HA	1.81	0.42
1:B:25:LEU:O	1:B:26:THR:C	2.61	0.42
1:H:136:ARG:HD2	1:H:136:ARG:HA	1.86	0.42
1:I:265:LEU:C	1:I:265:LEU:HD23	2.45	0.42
1:I:277:LEU:HD13	1:I:277:LEU:O	2.20	0.42
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.85	0.42
1:C:262:CYS:SG	1:D:421:VAL:HG21	2.59	0.42
1:D:180:VAL:O	1:D:181:HIS:C	2.61	0.42
1:D:190:LEU:HD12	1:D:190:LEU:O	2.18	0.42
1:E:65:ASN:OD1	1:E:68:ARG:CG	2.68	0.42
1:G:293:ALA:O	1:G:294:SER:C	2.63	0.42
1:H:419:ILE:HD12	1:H:419:ILE:C	2.44	0.42
1:A:130:GLU:OE1	1:A:136:ARG:NH1	2.52	0.42
1:C:84:ILE:HG23	1:C:131:TRP:HB3	2.01	0.42
1:A:215:ILE:CG1	1:A:222:LEU:HD13	2.50	0.42
1:A:292:THR:O	1:A:293:ALA:HB2	2.20	0.42
1:B:197:HIS:O	1:B:203:THR:OG1	2.33	0.42
1:G:65:ASN:O	1:G:66:THR:CB	2.67	0.42
1:H:360:ASP:CG	1:H:363:LEU:HB2	2.44	0.42
1:A:157:GLU:HA	1:A:157:GLU:OE1	2.19	0.42
1:C:99:PHE:O	1:C:100:PRO:C	2.61	0.42
1:C:263:ASN:C	1:C:265:LEU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LEU:O	1:E:29:ILE:C	2.63	0.42
1:E:261:ILE:C	1:E:263:ASN:H	2.28	0.42
1:G:250:ALA:O	1:G:254:ILE:HG23	2.20	0.42
1:I:282:ILE:O	1:I:282:ILE:HG23	2.19	0.42
1:B:65:ASN:ND2	1:B:68:ARG:HG3	2.35	0.42
1:E:115:LEU:HD13	1:E:119:LEU:HD22	2.02	0.42
1:F:199:LEU:O	1:F:201:PRO:HD3	2.20	0.42
1:G:1:MSE:HE2	1:G:4:GLN:HB3	2.01	0.42
1:G:80:ILE:N	1:G:81:PRO:CD	2.83	0.42
1:B:110:PRO:CG	1:J:242:THR:HG21	2.49	0.41
1:C:293:ALA:O	1:C:294:SER:HB3	2.20	0.41
1:H:99:PHE:HB3	1:H:100:PRO:HD3	2.01	0.41
1:H:351:PRO:HG3	1:H:395:HIS:CE1	2.54	0.41
1:A:261:ILE:HG23	1:A:264:SER:H	1.85	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:D:10:LEU:O	1:D:14:LEU:HD12	2.20	0.41
1:E:74:ALA:O	1:E:78:THR:HG22	2.19	0.41
1:J:243:SER:O	1:J:244:PRO:C	2.63	0.41
1:A:109:LYS:N	1:A:110:PRO:CD	2.83	0.41
1:H:74:ALA:O	1:H:78:THR:HG23	2.20	0.41
1:J:25:LEU:O	1:J:29:ILE:HG13	2.19	0.41
1:J:217:ARG:HH11	1:J:217:ARG:HG2	1.84	0.41
1:A:38:ARG:HB2	1:A:38:ARG:NH1	2.35	0.41
1:B:80:ILE:N	1:B:81:PRO:CD	2.83	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:D:281:MSE:HE2	1:D:281:MSE:HA	2.02	0.41
1:F:343:PHE:CD2	1:F:343:PHE:C	2.99	0.41
1:H:184:ILE:HD13	1:H:184:ILE:HG21	1.80	0.41
1:H:266:ASP:OD1	1:H:266:ASP:N	2.51	0.41
1:J:383:THR:HG22	1:J:384:LYS:N	2.34	0.41
1:A:80:ILE:HG23	1:A:81:PRO:CD	2.50	0.41
1:A:198:PHE:CE2	1:A:204:ARG:HA	2.55	0.41
1:B:109:LYS:N	1:B:110:PRO:CD	2.83	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:225:ILE:N	1:A:226:PRO:CD	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:O	1:A:242:THR:CG2	2.66	0.41
1:I:35:TYR:CD2	1:I:35:TYR:C	2.99	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:A:350:TYR:N	1:A:351:PRO:CD	2.83	0.41
1:C:51:ARG:NH2	1:C:89:ALA:HB2	2.36	0.41
1:D:203:THR:O	1:D:206:PRO:HD2	2.21	0.41
1:E:413:TRP:O	1:E:416:LEU:HB2	2.20	0.41
1:J:1:MSE:N	1:J:2:PRO:CD	2.84	0.41
1:C:269:LEU:HD22	1:C:273:PHE:CE1	2.56	0.41
1:F:258:LEU:HD12	1:F:258:LEU:HA	1.90	0.41
1:I:417:ASP:O	1:I:418:SER:C	2.63	0.41
1:I:420:ALA:HB2	1:J:420:ALA:HB2	2.03	0.41
1:B:401:TYR:CZ	1:B:412:ARG:HG3	2.56	0.40
1:C:215:ILE:CD1	1:C:253:PHE:CE2	3.04	0.40
1:G:341:GLN:O	1:G:345:ILE:HG22	2.20	0.40
1:J:281:MSE:HE2	1:J:281:MSE:HA	2.03	0.40
1:E:291:SER:C	1:E:292:THR:O	2.63	0.40
1:G:258:LEU:HD12	1:G:258:LEU:HA	1.89	0.40
1:I:245:ILE:O	1:I:248:SER:HB3	2.21	0.40
1:A:293:ALA:O	1:A:294:SER:CB	2.69	0.40
1:B:96:GLN:O	1:B:100:PRO:HG2	2.21	0.40
1:D:1:MSE:HE3	1:D:1:MSE:O	2.21	0.40
1:H:348:ALA:O	1:H:349:LEU:HB2	2.21	0.40
1:J:89:ALA:O	1:J:92:GLU:HB2	2.22	0.40
1:J:102:LEU:HD23	1:J:102:LEU:HA	1.89	0.40
1:J:198:PHE:CE2	1:J:204:ARG:HG2	2.56	0.40
1:J:235:LEU:HD23	1:J:235:LEU:HA	1.97	0.40
1:A:359:ARG:HG3	1:A:360:ASP:N	2.27	0.40
1:B:76:LEU:O	1:B:80:ILE:HB	2.21	0.40
1:B:83:LEU:N	1:B:83:LEU:HD23	2.36	0.40
1:D:221:ARG:CG	1:D:221:ARG:HH11	2.35	0.40
1:E:198:PHE:CE2	1:E:204:ARG:HG2	2.56	0.40
1:F:28:LEU:O	1:F:32:VAL:HG23	2.22	0.40
1:F:215:ILE:HG13	1:F:253:PHE:CE2	2.56	0.40
1:F:238:ALA:O	1:F:278:ARG:NH1	2.52	0.40
1:H:89:ALA:O	1:H:92:GLU:N	2.53	0.40
1:J:215:ILE:CD1	1:J:222:LEU:HD22	2.49	0.40
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.95	0.40
1:B:283:ASP:CG	1:B:284:PRO:HD2	2.47	0.40
1:C:1:MSE:N	1:C:2:PRO:HD3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LYS:HB2	1:C:110:PRO:HD3	2.02	0.40
1:D:276:TYR:CD1	1:D:276:TYR:C	2.98	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:G:414:THR:C	1:G:416:LEU:N	2.80	0.40
1:J:51:ARG:O	1:J:55:ASP:OD1	2.40	0.40
1:J:115:LEU:HD22	1:J:119:LEU:HD22	2.03	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%)	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

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
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

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

5.3.2 Protein sidechains ⓘ

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

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

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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

All (525) 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	60	LYS
1	A	66	THR
1	A	76	LEU
1	A	78	THR
1	A	82	LEU
1	A	85	LEU
1	A	90	VAL
1	A	115	LEU
1	A	119	LEU
1	A	123	LEU
1	A	134	ASP
1	A	154	LYS
1	A	184	ILE
1	A	191	SER
1	A	201	PRO

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	217	ARG
1	A	233	LEU
1	A	242	THR
1	A	245	ILE
1	A	251	LEU
1	A	254	ILE
1	A	255	LEU
1	A	257	ILE
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	373	ARG
1	A	383	THR
1	A	404	GLU
1	A	414	THR
1	A	419	ILE
1	A	424	LEU
1	A	428	LEU
1	A	431	VAL
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	38	ARG
1	B	41	LYS
1	B	45	THR
1	B	49	LYS
1	B	51	ARG
1	B	54	LEU
1	B	61	THR
1	B	65	ASN
1	B	66	THR

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Mol	Chain	Res	Type
1	B	76	LEU
1	B	78	THR
1	B	80	ILE
1	B	82	LEU
1	B	90	VAL
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	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
1	B	371	GLN
1	B	379	GLU
1	B	383	THR
1	B	384	LYS

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Mol	Chain	Res	Type
1	B	404	GLU
1	B	410	LYS
1	B	412	ARG
1	B	416	LEU
1	B	419	ILE
1	B	424	LEU
1	C	1	MSE
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	90	VAL
1	C	115	LEU
1	C	119	LEU
1	C	123	LEU
1	C	128	GLU
1	C	136	ARG
1	C	176	VAL
1	C	184	ILE
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

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Mol	Chain	Res	Type
1	C	264	SER
1	C	265	LEU
1	C	268	SER
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	404	GLU
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	76	LEU
1	D	80	ILE
1	D	82	LEU
1	D	90	VAL
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	201	PRO
1	D	221	ARG
1	D	233	LEU
1	D	242	THR
1	D	251	LEU
1	D	254	ILE
1	D	255	LEU

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Mol	Chain	Res	Type
1	D	258	LEU
1	D	259	SER
1	D	265	LEU
1	D	269	LEU
1	D	304	MSE
1	D	337	LEU
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	D	431	VAL
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	38	ARG
1	E	41	LYS
1	E	45	THR
1	E	49	LYS
1	E	54	LEU
1	E	57	ILE
1	E	61	THR
1	E	76	LEU
1	E	78	THR
1	E	82	LEU
1	E	85	LEU
1	E	88	GLN
1	E	90	VAL
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	171	THR
1	E	184	ILE

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Mol	Chain	Res	Type
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
1	E	264	SER
1	E	267	ASP
1	E	269	LEU
1	E	277	LEU
1	E	281	MSE
1	E	282	ILE
1	E	290	SER
1	E	304	MSE
1	E	345	ILE
1	E	349	LEU
1	E	363	LEU
1	E	383	THR
1	E	400	LYS
1	E	404	GLU
1	E	412	ARG
1	E	416	LEU
1	E	419	ILE
1	E	424	LEU
1	E	428	LEU
1	E	429	ASN
1	F	1	MSE
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	49	LYS
1	F	54	LEU
1	F	57	ILE
1	F	61	THR
1	F	66	THR
1	F	71	LEU

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Mol	Chain	Res	Type
1	F	76	LEU
1	F	79	VAL
1	F	82	LEU
1	F	85	LEU
1	F	90	VAL
1	F	115	LEU
1	F	119	LEU
1	F	123	LEU
1	F	128	GLU
1	F	153	SER
1	F	154	LYS
1	F	184	ILE
1	F	209	SER
1	F	221	ARG
1	F	242	THR
1	F	245	ILE
1	F	251	LEU
1	F	255	LEU
1	F	258	LEU
1	F	259	SER
1	F	261	ILE
1	F	265	LEU
1	F	269	LEU
1	F	271	ARG
1	F	298	GLU
1	F	304	MSE
1	F	337	LEU
1	F	341	GLN
1	F	363	LEU
1	F	383	THR
1	F	391	ARG
1	F	404	GLU
1	F	412	ARG
1	F	416	LEU
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

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Mol	Chain	Res	Type
1	G	26	THR
1	G	41	LYS
1	G	48	GLN
1	G	51	ARG
1	G	54	LEU
1	G	57	ILE
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
1	G	215	ILE
1	G	217	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	337	LEU
1	G	341	GLN
1	G	345	ILE
1	G	362	LYS
1	G	363	LEU
1	G	375	SER
1	G	404	GLU
1	G	411	SER

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Mol	Chain	Res	Type
1	G	412	ARG
1	G	414	THR
1	G	415	ARG
1	G	424	LEU
1	G	428	LEU
1	G	431	VAL
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	70	ILE
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
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	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	265	LEU

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Mol	Chain	Res	Type
1	H	266	ASP
1	H	269	LEU
1	H	271	ARG
1	H	285	THR
1	H	341	GLN
1	H	362	LYS
1	H	363	LEU
1	H	375	SER
1	H	383	THR
1	H	404	GLU
1	H	416	LEU
1	H	424	LEU
1	H	428	LEU
1	H	431	VAL
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	54	LEU
1	I	64	ASN
1	I	66	THR
1	I	70	ILE
1	I	71	LEU
1	I	76	LEU
1	I	82	LEU
1	I	85	LEU
1	I	88	GLN
1	I	90	VAL
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

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Mol	Chain	Res	Type
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	337	LEU
1	I	341	GLN
1	I	345	ILE
1	I	361	PRO
1	I	363	LEU
1	I	367	LYS
1	I	404	GLU
1	I	411	SER
1	I	414	THR
1	I	416	LEU
1	I	419	ILE
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
1	J	36	GLN
1	J	38	ARG
1	J	45	THR
1	J	48	GLN
1	J	54	LEU
1	J	57	ILE
1	J	64	ASN
1	J	66	THR
1	J	76	LEU

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Mol	Chain	Res	Type
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	128	GLU
1	J	154	LYS
1	J	184	ILE
1	J	191	SER
1	J	217	ARG
1	J	233	LEU
1	J	242	THR
1	J	245	ILE
1	J	251	LEU
1	J	255	LEU
1	J	257	ILE
1	J	258	LEU
1	J	259	SER
1	J	261	ILE
1	J	265	LEU
1	J	267	ASP
1	J	269	LEU
1	J	271	ARG
1	J	282	ILE
1	J	291	SER
1	J	302	ASP
1	J	337	LEU
1	J	341	GLN
1	J	345	ILE
1	J	383	THR
1	J	396	SER
1	J	404	GLU
1	J	410	LYS
1	J	412	ARG
1	J	418	SER
1	J	419	ILE
1	J	424	LEU
1	J	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	107	GLN
1	A	170	GLN
1	A	369	ASN
1	A	378	GLN
1	B	12	ASN
1	B	42	GLN
1	B	107	GLN
1	B	395	HIS
1	C	12	ASN
1	C	88	GLN
1	C	107	GLN
1	C	185	GLN
1	D	12	ASN
1	D	177	ASN
1	D	395	HIS
1	E	46	ASN
1	E	107	GLN
1	E	169	ASN
1	E	170	GLN
1	E	301	HIS
1	F	52	HIS
1	F	64	ASN
1	F	353	ASN
1	F	378	GLN
1	F	395	HIS
1	G	52	HIS
1	G	103	ASN
1	G	107	GLN
1	G	170	GLN
1	G	227	GLN
1	H	46	ASN
1	H	197	HIS
1	I	88	GLN
1	I	107	GLN
1	I	185	GLN
1	J	36	GLN
1	J	185	GLN
1	J	395	HIS

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	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

All (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
1	F	161	ASP	3.8
1	J	2	PRO	3.7
1	C	431	VAL	3.7
1	H	164	SER	3.7
1	I	431	VAL	3.7
1	I	164	SER	3.5
1	E	431	VAL	3.5
1	B	164	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	164	SER	3.4
1	B	161	ASP	3.3
1	J	164	SER	3.3
1	B	2	PRO	3.2
1	I	3	LEU	3.2
1	D	161	ASP	3.2
1	B	431	VAL	3.2
1	C	164	SER	3.1
1	C	305	SER	3.1
1	G	164	SER	3.1
1	G	15	HIS	3.1
1	I	161	ASP	3.1
1	I	305	SER	3.1
1	A	23	PRO	3.1
1	C	161	ASP	3.0
1	A	329	SER	3.0
1	D	158	ASN	3.0
1	G	415	ARG	3.0
1	A	327	GLY	2.9
1	A	16	GLU	2.9
1	F	2	PRO	2.9
1	I	336	SER	2.9
1	C	52	HIS	2.8
1	H	160	GLY	2.8
1	H	431	VAL	2.8
1	J	305	SER	2.8
1	J	161	ASP	2.8
1	A	163	GLU	2.7
1	B	262	CYS	2.7
1	G	336	SER	2.7
1	A	328	SER	2.7
1	H	305	SER	2.7
1	H	15	HIS	2.6
1	D	165	GLN	2.5
1	F	164	SER	2.5
1	E	336	SER	2.5
1	D	2	PRO	2.4
1	E	305	SER	2.4
1	J	431	VAL	2.4
1	E	158	ASN	2.4
1	F	24	ASP	2.4
1	F	160	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	24	ASP	2.4
1	F	159	LEU	2.4
1	A	262	CYS	2.4
1	A	431	VAL	2.3
1	G	305	SER	2.3
1	B	264	SER	2.3
1	B	336	SER	2.3
1	E	2	PRO	2.3
1	B	24	ASP	2.3
1	G	161	ASP	2.3
1	C	336	SER	2.3
1	D	336	SER	2.3
1	E	164	SER	2.3
1	D	24	ASP	2.2
1	G	303	PHE	2.2
1	F	415	ARG	2.2
1	G	24	ASP	2.2
1	D	431	VAL	2.2
1	A	330	GLN	2.2
1	D	408	THR	2.2
1	E	264	SER	2.2
1	J	15	HIS	2.1
1	J	160	GLY	2.1
1	E	13	VAL	2.1
1	H	158	ASN	2.1
1	D	25	LEU	2.1
1	I	15	HIS	2.1
1	F	431	VAL	2.1
1	C	158	ASN	2.0
1	I	2	PRO	2.0
1	H	415	ARG	2.0
1	E	24	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.