



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:56 AM UTC

PDB ID : 5AQ5 / pdb_00005aq5
Title : Structure of the Carboxy-Terminal Domain of the Bacteriophage T5 L- Shaped Tail Fibre
Authors : Garcia-Doval, C.; Granell, M.; van Raaij, M.J.
Deposited on : 2015-09-19
Resolution : 2.30 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
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

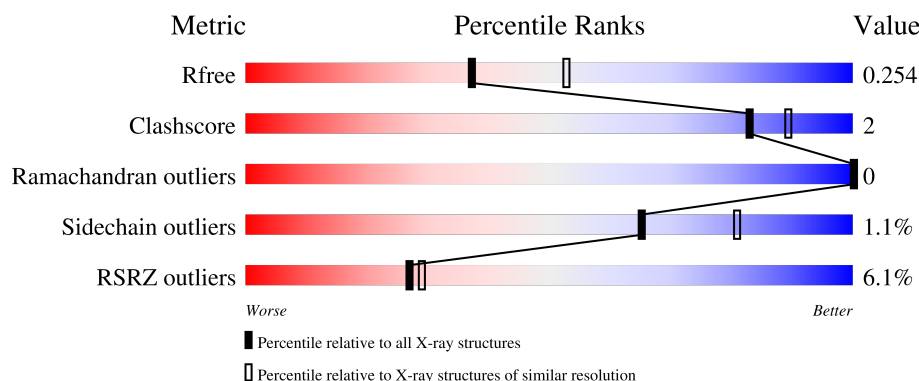
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



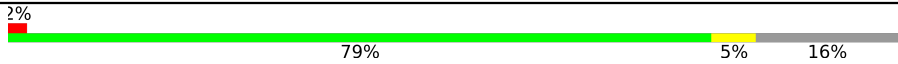
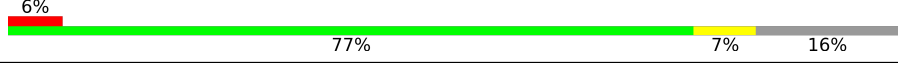
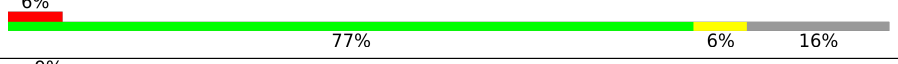
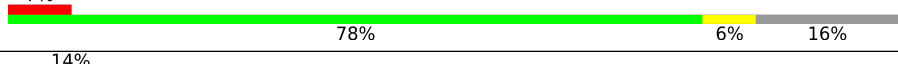
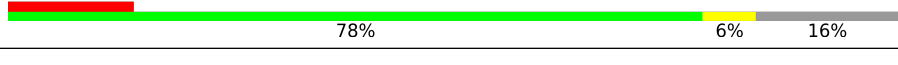
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	328	3% 80% 16%
1	B	328	% 79% 5% 16%
1	C	328	3% 77% 6% 16%
1	D	328	2% 77% 7% 16%
1	E	328	3% 78% 6% 16%

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Mol	Chain	Length	Quality of chain
1	F	328	 2% 79% 5% 16%
1	G	328	 5% 78% 6% 16%
1	H	328	 6% 77% 7% 16%
1	I	328	 6% 77% 6% 16%
1	J	328	 9% 78% 6% 16%
1	K	328	 7% 78% 6% 16%
1	L	328	 14% 78% 6% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25344 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 L-SHAPED TAIL FIBER PROTEIN PB8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	B	276	Total	C	N	O	S	0	0	0
			2048	1271	373	396	8			
1	C	276	Total	C	N	O	S	0	0	0
			2048	1271	373	396	8			
1	D	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	E	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	F	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	G	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	H	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	I	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	J	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	K	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			
1	L	275	Total	C	N	O	S	0	0	0
			2039	1266	372	393	8			

There are 408 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	936	MET	-	expression tag	UNP Q66LT2
A	937	GLY	-	expression tag	UNP Q66LT2
A	938	SER	-	expression tag	UNP Q66LT2
A	939	SER	-	expression tag	UNP Q66LT2
A	940	HIS	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	941	HIS	-	expression tag	UNP Q66LT2
A	942	HIS	-	expression tag	UNP Q66LT2
A	943	HIS	-	expression tag	UNP Q66LT2
A	944	HIS	-	expression tag	UNP Q66LT2
A	945	HIS	-	expression tag	UNP Q66LT2
A	946	SER	-	expression tag	UNP Q66LT2
A	947	SER	-	expression tag	UNP Q66LT2
A	948	GLY	-	expression tag	UNP Q66LT2
A	949	LEU	-	expression tag	UNP Q66LT2
A	950	VAL	-	expression tag	UNP Q66LT2
A	951	PRO	-	expression tag	UNP Q66LT2
A	952	ARG	-	expression tag	UNP Q66LT2
A	953	GLY	-	expression tag	UNP Q66LT2
A	954	SER	-	expression tag	UNP Q66LT2
A	955	HIS	-	expression tag	UNP Q66LT2
A	956	MET	-	expression tag	UNP Q66LT2
A	957	ALA	-	expression tag	UNP Q66LT2
A	958	SER	-	expression tag	UNP Q66LT2
A	959	MET	-	expression tag	UNP Q66LT2
A	960	THR	-	expression tag	UNP Q66LT2
A	961	SER	-	expression tag	UNP Q66LT2
A	962	SER	-	expression tag	UNP Q66LT2
A	963	GLN	-	expression tag	UNP Q66LT2
A	964	GLN	-	expression tag	UNP Q66LT2
A	965	MET	-	expression tag	UNP Q66LT2
A	966	GLY	-	expression tag	UNP Q66LT2
A	967	ARG	-	expression tag	UNP Q66LT2
A	968	GLY	-	expression tag	UNP Q66LT2
A	969	SER	-	expression tag	UNP Q66LT2
B	936	MET	-	expression tag	UNP Q66LT2
B	937	GLY	-	expression tag	UNP Q66LT2
B	938	SER	-	expression tag	UNP Q66LT2
B	939	SER	-	expression tag	UNP Q66LT2
B	940	HIS	-	expression tag	UNP Q66LT2
B	941	HIS	-	expression tag	UNP Q66LT2
B	942	HIS	-	expression tag	UNP Q66LT2
B	943	HIS	-	expression tag	UNP Q66LT2
B	944	HIS	-	expression tag	UNP Q66LT2
B	945	HIS	-	expression tag	UNP Q66LT2
B	946	SER	-	expression tag	UNP Q66LT2
B	947	SER	-	expression tag	UNP Q66LT2
B	948	GLY	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	949	LEU	-	expression tag	UNP Q66LT2
B	950	VAL	-	expression tag	UNP Q66LT2
B	951	PRO	-	expression tag	UNP Q66LT2
B	952	ARG	-	expression tag	UNP Q66LT2
B	953	GLY	-	expression tag	UNP Q66LT2
B	954	SER	-	expression tag	UNP Q66LT2
B	955	HIS	-	expression tag	UNP Q66LT2
B	956	MET	-	expression tag	UNP Q66LT2
B	957	ALA	-	expression tag	UNP Q66LT2
B	958	SER	-	expression tag	UNP Q66LT2
B	959	MET	-	expression tag	UNP Q66LT2
B	960	THR	-	expression tag	UNP Q66LT2
B	961	SER	-	expression tag	UNP Q66LT2
B	962	SER	-	expression tag	UNP Q66LT2
B	963	GLN	-	expression tag	UNP Q66LT2
B	964	GLN	-	expression tag	UNP Q66LT2
B	965	MET	-	expression tag	UNP Q66LT2
B	966	GLY	-	expression tag	UNP Q66LT2
B	967	ARG	-	expression tag	UNP Q66LT2
B	968	GLY	-	expression tag	UNP Q66LT2
B	969	SER	-	expression tag	UNP Q66LT2
C	936	MET	-	expression tag	UNP Q66LT2
C	937	GLY	-	expression tag	UNP Q66LT2
C	938	SER	-	expression tag	UNP Q66LT2
C	939	SER	-	expression tag	UNP Q66LT2
C	940	HIS	-	expression tag	UNP Q66LT2
C	941	HIS	-	expression tag	UNP Q66LT2
C	942	HIS	-	expression tag	UNP Q66LT2
C	943	HIS	-	expression tag	UNP Q66LT2
C	944	HIS	-	expression tag	UNP Q66LT2
C	945	HIS	-	expression tag	UNP Q66LT2
C	946	SER	-	expression tag	UNP Q66LT2
C	947	SER	-	expression tag	UNP Q66LT2
C	948	GLY	-	expression tag	UNP Q66LT2
C	949	LEU	-	expression tag	UNP Q66LT2
C	950	VAL	-	expression tag	UNP Q66LT2
C	951	PRO	-	expression tag	UNP Q66LT2
C	952	ARG	-	expression tag	UNP Q66LT2
C	953	GLY	-	expression tag	UNP Q66LT2
C	954	SER	-	expression tag	UNP Q66LT2
C	955	HIS	-	expression tag	UNP Q66LT2
C	956	MET	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	957	ALA	-	expression tag	UNP Q66LT2
C	958	SER	-	expression tag	UNP Q66LT2
C	959	MET	-	expression tag	UNP Q66LT2
C	960	THR	-	expression tag	UNP Q66LT2
C	961	SER	-	expression tag	UNP Q66LT2
C	962	SER	-	expression tag	UNP Q66LT2
C	963	GLN	-	expression tag	UNP Q66LT2
C	964	GLN	-	expression tag	UNP Q66LT2
C	965	MET	-	expression tag	UNP Q66LT2
C	966	GLY	-	expression tag	UNP Q66LT2
C	967	ARG	-	expression tag	UNP Q66LT2
C	968	GLY	-	expression tag	UNP Q66LT2
C	969	SER	-	expression tag	UNP Q66LT2
D	936	MET	-	expression tag	UNP Q66LT2
D	937	GLY	-	expression tag	UNP Q66LT2
D	938	SER	-	expression tag	UNP Q66LT2
D	939	SER	-	expression tag	UNP Q66LT2
D	940	HIS	-	expression tag	UNP Q66LT2
D	941	HIS	-	expression tag	UNP Q66LT2
D	942	HIS	-	expression tag	UNP Q66LT2
D	943	HIS	-	expression tag	UNP Q66LT2
D	944	HIS	-	expression tag	UNP Q66LT2
D	945	HIS	-	expression tag	UNP Q66LT2
D	946	SER	-	expression tag	UNP Q66LT2
D	947	SER	-	expression tag	UNP Q66LT2
D	948	GLY	-	expression tag	UNP Q66LT2
D	949	LEU	-	expression tag	UNP Q66LT2
D	950	VAL	-	expression tag	UNP Q66LT2
D	951	PRO	-	expression tag	UNP Q66LT2
D	952	ARG	-	expression tag	UNP Q66LT2
D	953	GLY	-	expression tag	UNP Q66LT2
D	954	SER	-	expression tag	UNP Q66LT2
D	955	HIS	-	expression tag	UNP Q66LT2
D	956	MET	-	expression tag	UNP Q66LT2
D	957	ALA	-	expression tag	UNP Q66LT2
D	958	SER	-	expression tag	UNP Q66LT2
D	959	MET	-	expression tag	UNP Q66LT2
D	960	THR	-	expression tag	UNP Q66LT2
D	961	SER	-	expression tag	UNP Q66LT2
D	962	SER	-	expression tag	UNP Q66LT2
D	963	GLN	-	expression tag	UNP Q66LT2
D	964	GLN	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	965	MET	-	expression tag	UNP Q66LT2
D	966	GLY	-	expression tag	UNP Q66LT2
D	967	ARG	-	expression tag	UNP Q66LT2
D	968	GLY	-	expression tag	UNP Q66LT2
D	969	SER	-	expression tag	UNP Q66LT2
E	936	MET	-	expression tag	UNP Q66LT2
E	937	GLY	-	expression tag	UNP Q66LT2
E	938	SER	-	expression tag	UNP Q66LT2
E	939	SER	-	expression tag	UNP Q66LT2
E	940	HIS	-	expression tag	UNP Q66LT2
E	941	HIS	-	expression tag	UNP Q66LT2
E	942	HIS	-	expression tag	UNP Q66LT2
E	943	HIS	-	expression tag	UNP Q66LT2
E	944	HIS	-	expression tag	UNP Q66LT2
E	945	HIS	-	expression tag	UNP Q66LT2
E	946	SER	-	expression tag	UNP Q66LT2
E	947	SER	-	expression tag	UNP Q66LT2
E	948	GLY	-	expression tag	UNP Q66LT2
E	949	LEU	-	expression tag	UNP Q66LT2
E	950	VAL	-	expression tag	UNP Q66LT2
E	951	PRO	-	expression tag	UNP Q66LT2
E	952	ARG	-	expression tag	UNP Q66LT2
E	953	GLY	-	expression tag	UNP Q66LT2
E	954	SER	-	expression tag	UNP Q66LT2
E	955	HIS	-	expression tag	UNP Q66LT2
E	956	MET	-	expression tag	UNP Q66LT2
E	957	ALA	-	expression tag	UNP Q66LT2
E	958	SER	-	expression tag	UNP Q66LT2
E	959	MET	-	expression tag	UNP Q66LT2
E	960	THR	-	expression tag	UNP Q66LT2
E	961	SER	-	expression tag	UNP Q66LT2
E	962	SER	-	expression tag	UNP Q66LT2
E	963	GLN	-	expression tag	UNP Q66LT2
E	964	GLN	-	expression tag	UNP Q66LT2
E	965	MET	-	expression tag	UNP Q66LT2
E	966	GLY	-	expression tag	UNP Q66LT2
E	967	ARG	-	expression tag	UNP Q66LT2
E	968	GLY	-	expression tag	UNP Q66LT2
E	969	SER	-	expression tag	UNP Q66LT2
F	936	MET	-	expression tag	UNP Q66LT2
F	937	GLY	-	expression tag	UNP Q66LT2
F	938	SER	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	939	SER	-	expression tag	UNP Q66LT2
F	940	HIS	-	expression tag	UNP Q66LT2
F	941	HIS	-	expression tag	UNP Q66LT2
F	942	HIS	-	expression tag	UNP Q66LT2
F	943	HIS	-	expression tag	UNP Q66LT2
F	944	HIS	-	expression tag	UNP Q66LT2
F	945	HIS	-	expression tag	UNP Q66LT2
F	946	SER	-	expression tag	UNP Q66LT2
F	947	SER	-	expression tag	UNP Q66LT2
F	948	GLY	-	expression tag	UNP Q66LT2
F	949	LEU	-	expression tag	UNP Q66LT2
F	950	VAL	-	expression tag	UNP Q66LT2
F	951	PRO	-	expression tag	UNP Q66LT2
F	952	ARG	-	expression tag	UNP Q66LT2
F	953	GLY	-	expression tag	UNP Q66LT2
F	954	SER	-	expression tag	UNP Q66LT2
F	955	HIS	-	expression tag	UNP Q66LT2
F	956	MET	-	expression tag	UNP Q66LT2
F	957	ALA	-	expression tag	UNP Q66LT2
F	958	SER	-	expression tag	UNP Q66LT2
F	959	MET	-	expression tag	UNP Q66LT2
F	960	THR	-	expression tag	UNP Q66LT2
F	961	SER	-	expression tag	UNP Q66LT2
F	962	SER	-	expression tag	UNP Q66LT2
F	963	GLN	-	expression tag	UNP Q66LT2
F	964	GLN	-	expression tag	UNP Q66LT2
F	965	MET	-	expression tag	UNP Q66LT2
F	966	GLY	-	expression tag	UNP Q66LT2
F	967	ARG	-	expression tag	UNP Q66LT2
F	968	GLY	-	expression tag	UNP Q66LT2
F	969	SER	-	expression tag	UNP Q66LT2
G	936	MET	-	expression tag	UNP Q66LT2
G	937	GLY	-	expression tag	UNP Q66LT2
G	938	SER	-	expression tag	UNP Q66LT2
G	939	SER	-	expression tag	UNP Q66LT2
G	940	HIS	-	expression tag	UNP Q66LT2
G	941	HIS	-	expression tag	UNP Q66LT2
G	942	HIS	-	expression tag	UNP Q66LT2
G	943	HIS	-	expression tag	UNP Q66LT2
G	944	HIS	-	expression tag	UNP Q66LT2
G	945	HIS	-	expression tag	UNP Q66LT2
G	946	SER	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	947	SER	-	expression tag	UNP Q66LT2
G	948	GLY	-	expression tag	UNP Q66LT2
G	949	LEU	-	expression tag	UNP Q66LT2
G	950	VAL	-	expression tag	UNP Q66LT2
G	951	PRO	-	expression tag	UNP Q66LT2
G	952	ARG	-	expression tag	UNP Q66LT2
G	953	GLY	-	expression tag	UNP Q66LT2
G	954	SER	-	expression tag	UNP Q66LT2
G	955	HIS	-	expression tag	UNP Q66LT2
G	956	MET	-	expression tag	UNP Q66LT2
G	957	ALA	-	expression tag	UNP Q66LT2
G	958	SER	-	expression tag	UNP Q66LT2
G	959	MET	-	expression tag	UNP Q66LT2
G	960	THR	-	expression tag	UNP Q66LT2
G	961	SER	-	expression tag	UNP Q66LT2
G	962	SER	-	expression tag	UNP Q66LT2
G	963	GLN	-	expression tag	UNP Q66LT2
G	964	GLN	-	expression tag	UNP Q66LT2
G	965	MET	-	expression tag	UNP Q66LT2
G	966	GLY	-	expression tag	UNP Q66LT2
G	967	ARG	-	expression tag	UNP Q66LT2
G	968	GLY	-	expression tag	UNP Q66LT2
G	969	SER	-	expression tag	UNP Q66LT2
H	936	MET	-	expression tag	UNP Q66LT2
H	937	GLY	-	expression tag	UNP Q66LT2
H	938	SER	-	expression tag	UNP Q66LT2
H	939	SER	-	expression tag	UNP Q66LT2
H	940	HIS	-	expression tag	UNP Q66LT2
H	941	HIS	-	expression tag	UNP Q66LT2
H	942	HIS	-	expression tag	UNP Q66LT2
H	943	HIS	-	expression tag	UNP Q66LT2
H	944	HIS	-	expression tag	UNP Q66LT2
H	945	HIS	-	expression tag	UNP Q66LT2
H	946	SER	-	expression tag	UNP Q66LT2
H	947	SER	-	expression tag	UNP Q66LT2
H	948	GLY	-	expression tag	UNP Q66LT2
H	949	LEU	-	expression tag	UNP Q66LT2
H	950	VAL	-	expression tag	UNP Q66LT2
H	951	PRO	-	expression tag	UNP Q66LT2
H	952	ARG	-	expression tag	UNP Q66LT2
H	953	GLY	-	expression tag	UNP Q66LT2
H	954	SER	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	955	HIS	-	expression tag	UNP Q66LT2
H	956	MET	-	expression tag	UNP Q66LT2
H	957	ALA	-	expression tag	UNP Q66LT2
H	958	SER	-	expression tag	UNP Q66LT2
H	959	MET	-	expression tag	UNP Q66LT2
H	960	THR	-	expression tag	UNP Q66LT2
H	961	SER	-	expression tag	UNP Q66LT2
H	962	SER	-	expression tag	UNP Q66LT2
H	963	GLN	-	expression tag	UNP Q66LT2
H	964	GLN	-	expression tag	UNP Q66LT2
H	965	MET	-	expression tag	UNP Q66LT2
H	966	GLY	-	expression tag	UNP Q66LT2
H	967	ARG	-	expression tag	UNP Q66LT2
H	968	GLY	-	expression tag	UNP Q66LT2
H	969	SER	-	expression tag	UNP Q66LT2
I	936	MET	-	expression tag	UNP Q66LT2
I	937	GLY	-	expression tag	UNP Q66LT2
I	938	SER	-	expression tag	UNP Q66LT2
I	939	SER	-	expression tag	UNP Q66LT2
I	940	HIS	-	expression tag	UNP Q66LT2
I	941	HIS	-	expression tag	UNP Q66LT2
I	942	HIS	-	expression tag	UNP Q66LT2
I	943	HIS	-	expression tag	UNP Q66LT2
I	944	HIS	-	expression tag	UNP Q66LT2
I	945	HIS	-	expression tag	UNP Q66LT2
I	946	SER	-	expression tag	UNP Q66LT2
I	947	SER	-	expression tag	UNP Q66LT2
I	948	GLY	-	expression tag	UNP Q66LT2
I	949	LEU	-	expression tag	UNP Q66LT2
I	950	VAL	-	expression tag	UNP Q66LT2
I	951	PRO	-	expression tag	UNP Q66LT2
I	952	ARG	-	expression tag	UNP Q66LT2
I	953	GLY	-	expression tag	UNP Q66LT2
I	954	SER	-	expression tag	UNP Q66LT2
I	955	HIS	-	expression tag	UNP Q66LT2
I	956	MET	-	expression tag	UNP Q66LT2
I	957	ALA	-	expression tag	UNP Q66LT2
I	958	SER	-	expression tag	UNP Q66LT2
I	959	MET	-	expression tag	UNP Q66LT2
I	960	THR	-	expression tag	UNP Q66LT2
I	961	SER	-	expression tag	UNP Q66LT2
I	962	SER	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	963	GLN	-	expression tag	UNP Q66LT2
I	964	GLN	-	expression tag	UNP Q66LT2
I	965	MET	-	expression tag	UNP Q66LT2
I	966	GLY	-	expression tag	UNP Q66LT2
I	967	ARG	-	expression tag	UNP Q66LT2
I	968	GLY	-	expression tag	UNP Q66LT2
I	969	SER	-	expression tag	UNP Q66LT2
J	936	MET	-	expression tag	UNP Q66LT2
J	937	GLY	-	expression tag	UNP Q66LT2
J	938	SER	-	expression tag	UNP Q66LT2
J	939	SER	-	expression tag	UNP Q66LT2
J	940	HIS	-	expression tag	UNP Q66LT2
J	941	HIS	-	expression tag	UNP Q66LT2
J	942	HIS	-	expression tag	UNP Q66LT2
J	943	HIS	-	expression tag	UNP Q66LT2
J	944	HIS	-	expression tag	UNP Q66LT2
J	945	HIS	-	expression tag	UNP Q66LT2
J	946	SER	-	expression tag	UNP Q66LT2
J	947	SER	-	expression tag	UNP Q66LT2
J	948	GLY	-	expression tag	UNP Q66LT2
J	949	LEU	-	expression tag	UNP Q66LT2
J	950	VAL	-	expression tag	UNP Q66LT2
J	951	PRO	-	expression tag	UNP Q66LT2
J	952	ARG	-	expression tag	UNP Q66LT2
J	953	GLY	-	expression tag	UNP Q66LT2
J	954	SER	-	expression tag	UNP Q66LT2
J	955	HIS	-	expression tag	UNP Q66LT2
J	956	MET	-	expression tag	UNP Q66LT2
J	957	ALA	-	expression tag	UNP Q66LT2
J	958	SER	-	expression tag	UNP Q66LT2
J	959	MET	-	expression tag	UNP Q66LT2
J	960	THR	-	expression tag	UNP Q66LT2
J	961	SER	-	expression tag	UNP Q66LT2
J	962	SER	-	expression tag	UNP Q66LT2
J	963	GLN	-	expression tag	UNP Q66LT2
J	964	GLN	-	expression tag	UNP Q66LT2
J	965	MET	-	expression tag	UNP Q66LT2
J	966	GLY	-	expression tag	UNP Q66LT2
J	967	ARG	-	expression tag	UNP Q66LT2
J	968	GLY	-	expression tag	UNP Q66LT2
J	969	SER	-	expression tag	UNP Q66LT2
K	936	MET	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	937	GLY	-	expression tag	UNP Q66LT2
K	938	SER	-	expression tag	UNP Q66LT2
K	939	SER	-	expression tag	UNP Q66LT2
K	940	HIS	-	expression tag	UNP Q66LT2
K	941	HIS	-	expression tag	UNP Q66LT2
K	942	HIS	-	expression tag	UNP Q66LT2
K	943	HIS	-	expression tag	UNP Q66LT2
K	944	HIS	-	expression tag	UNP Q66LT2
K	945	HIS	-	expression tag	UNP Q66LT2
K	946	SER	-	expression tag	UNP Q66LT2
K	947	SER	-	expression tag	UNP Q66LT2
K	948	GLY	-	expression tag	UNP Q66LT2
K	949	LEU	-	expression tag	UNP Q66LT2
K	950	VAL	-	expression tag	UNP Q66LT2
K	951	PRO	-	expression tag	UNP Q66LT2
K	952	ARG	-	expression tag	UNP Q66LT2
K	953	GLY	-	expression tag	UNP Q66LT2
K	954	SER	-	expression tag	UNP Q66LT2
K	955	HIS	-	expression tag	UNP Q66LT2
K	956	MET	-	expression tag	UNP Q66LT2
K	957	ALA	-	expression tag	UNP Q66LT2
K	958	SER	-	expression tag	UNP Q66LT2
K	959	MET	-	expression tag	UNP Q66LT2
K	960	THR	-	expression tag	UNP Q66LT2
K	961	SER	-	expression tag	UNP Q66LT2
K	962	SER	-	expression tag	UNP Q66LT2
K	963	GLN	-	expression tag	UNP Q66LT2
K	964	GLN	-	expression tag	UNP Q66LT2
K	965	MET	-	expression tag	UNP Q66LT2
K	966	GLY	-	expression tag	UNP Q66LT2
K	967	ARG	-	expression tag	UNP Q66LT2
K	968	GLY	-	expression tag	UNP Q66LT2
K	969	SER	-	expression tag	UNP Q66LT2
L	936	MET	-	expression tag	UNP Q66LT2
L	937	GLY	-	expression tag	UNP Q66LT2
L	938	SER	-	expression tag	UNP Q66LT2
L	939	SER	-	expression tag	UNP Q66LT2
L	940	HIS	-	expression tag	UNP Q66LT2
L	941	HIS	-	expression tag	UNP Q66LT2
L	942	HIS	-	expression tag	UNP Q66LT2
L	943	HIS	-	expression tag	UNP Q66LT2
L	944	HIS	-	expression tag	UNP Q66LT2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	945	HIS	-	expression tag	UNP Q66LT2
L	946	SER	-	expression tag	UNP Q66LT2
L	947	SER	-	expression tag	UNP Q66LT2
L	948	GLY	-	expression tag	UNP Q66LT2
L	949	LEU	-	expression tag	UNP Q66LT2
L	950	VAL	-	expression tag	UNP Q66LT2
L	951	PRO	-	expression tag	UNP Q66LT2
L	952	ARG	-	expression tag	UNP Q66LT2
L	953	GLY	-	expression tag	UNP Q66LT2
L	954	SER	-	expression tag	UNP Q66LT2
L	955	HIS	-	expression tag	UNP Q66LT2
L	956	MET	-	expression tag	UNP Q66LT2
L	957	ALA	-	expression tag	UNP Q66LT2
L	958	SER	-	expression tag	UNP Q66LT2
L	959	MET	-	expression tag	UNP Q66LT2
L	960	THR	-	expression tag	UNP Q66LT2
L	961	SER	-	expression tag	UNP Q66LT2
L	962	SER	-	expression tag	UNP Q66LT2
L	963	GLN	-	expression tag	UNP Q66LT2
L	964	GLN	-	expression tag	UNP Q66LT2
L	965	MET	-	expression tag	UNP Q66LT2
L	966	GLY	-	expression tag	UNP Q66LT2
L	967	ARG	-	expression tag	UNP Q66LT2
L	968	GLY	-	expression tag	UNP Q66LT2
L	969	SER	-	expression tag	UNP Q66LT2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	112	Total O 112 112	0	0
2	B	95	Total O 95 95	0	0
2	C	81	Total O 81 81	0	0
2	D	119	Total O 119 119	0	0
2	E	112	Total O 112 112	0	0
2	F	83	Total O 83 83	0	0
2	G	39	Total O 39 39	0	0

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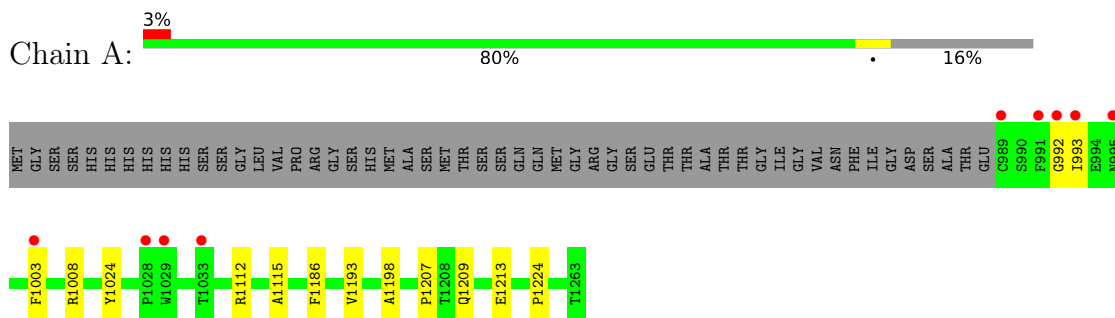
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	43	Total 43	O 43	0	0
2	I	40	Total 40	O 40	0	0
2	J	33	Total 33	O 33	0	0
2	K	25	Total 25	O 25	0	0
2	L	76	Total 76	O 76	0	0

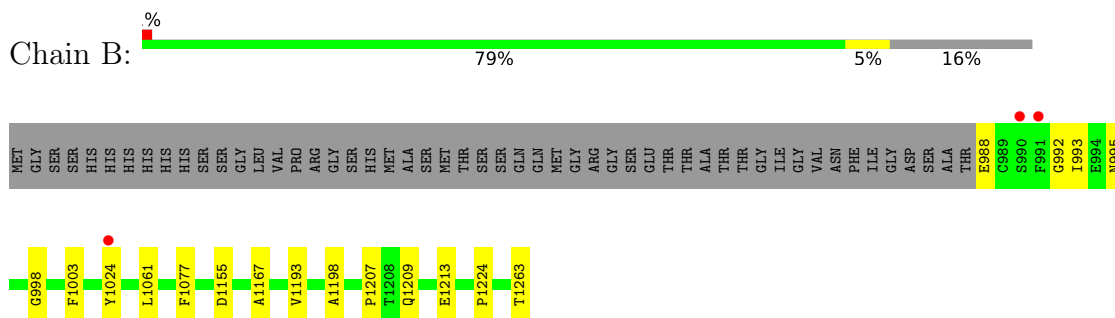
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

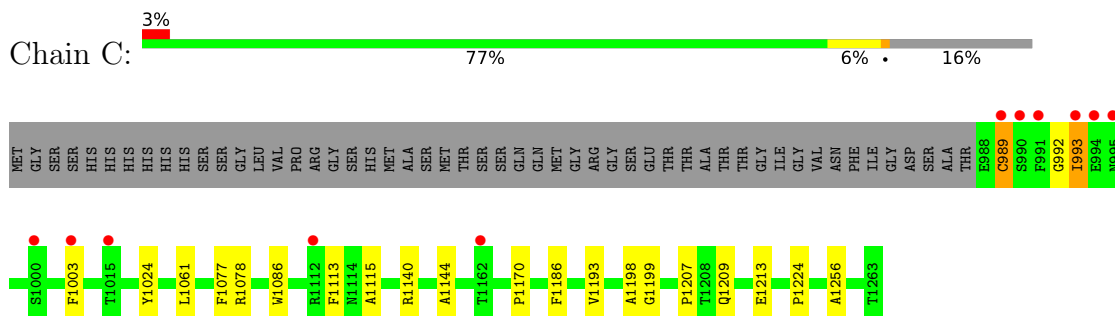
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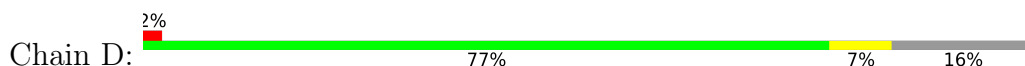
- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

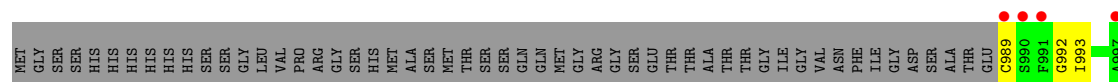


- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

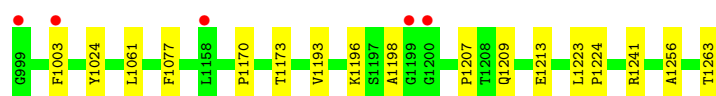
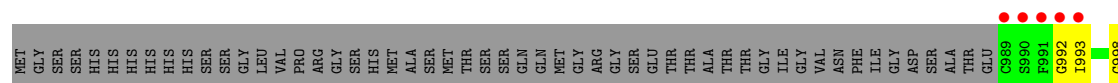
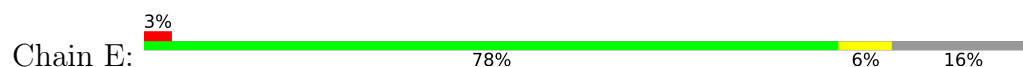


- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

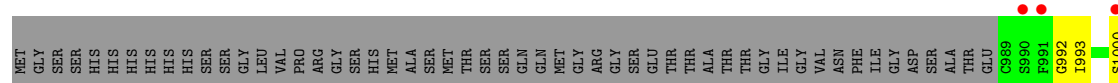
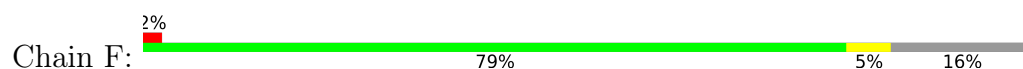




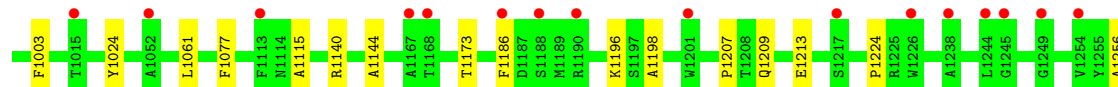
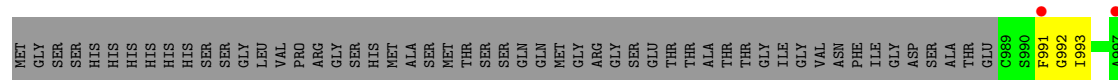
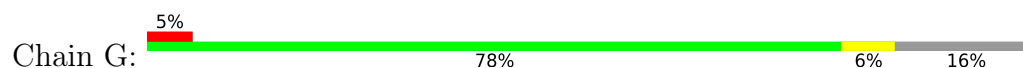
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



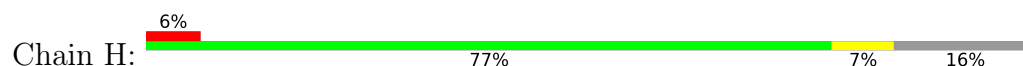
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

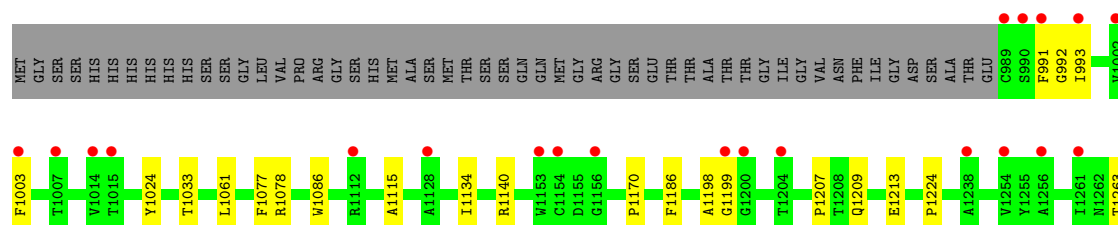


• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

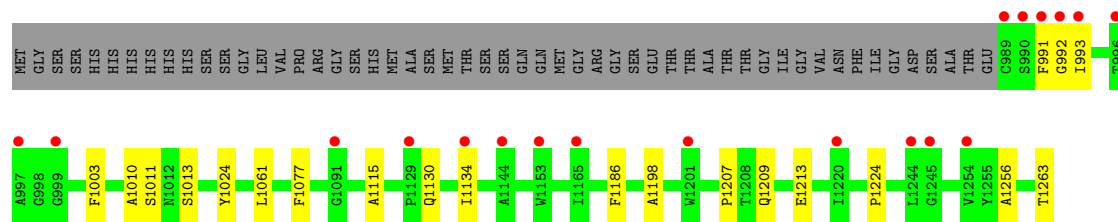
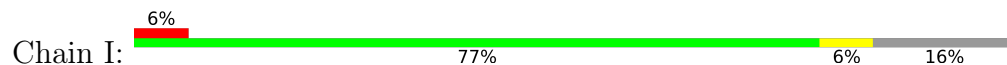


• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

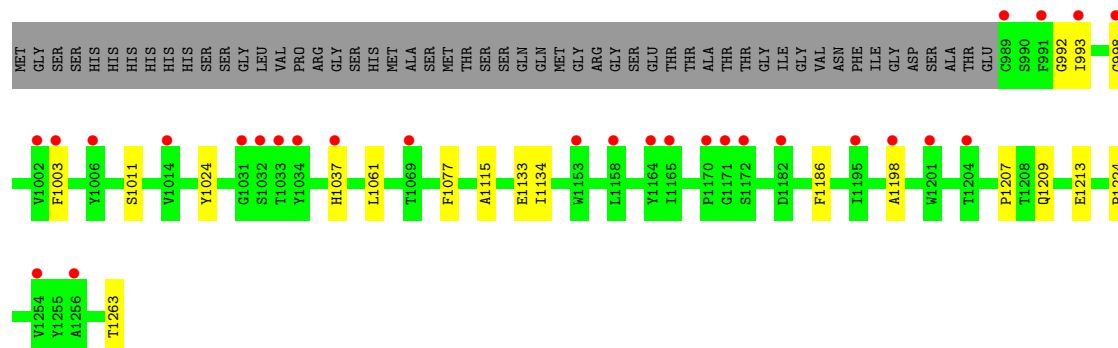
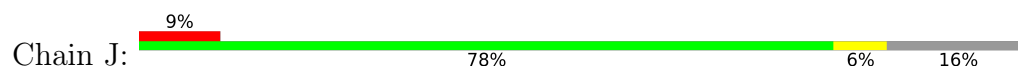




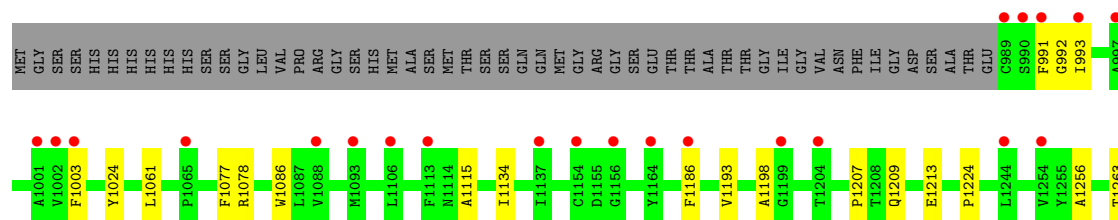
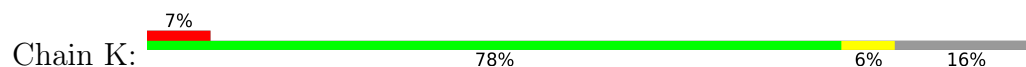
- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



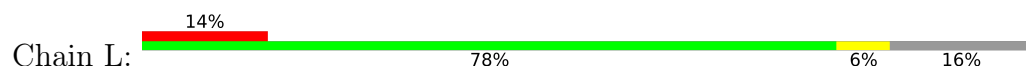
- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

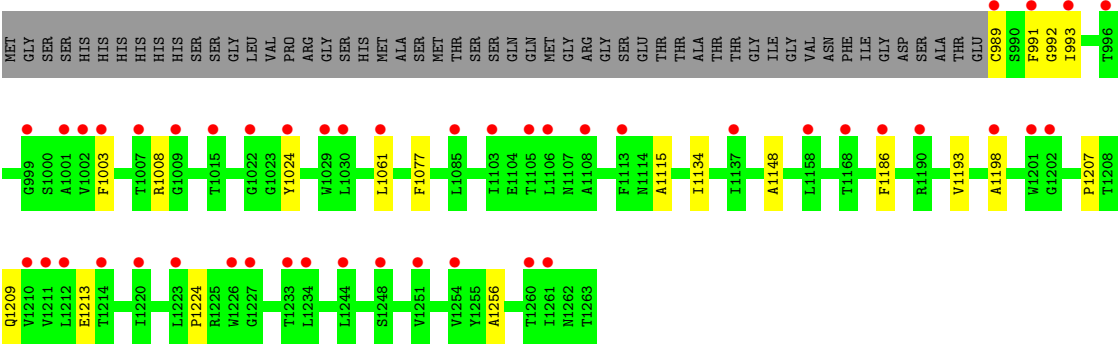


- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



- Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.62Å 95.03Å 127.75Å 68.24° 70.20° 83.63°	Depositor
Resolution (Å)	23.00 – 2.30 23.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (23.00-2.30) 90.9 (23.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.223 , 0.252 0.223 , 0.254	Depositor DCC
R_{free} test set	2924 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25344	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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	0.72	0/2088	0.90	1/2840 (0.0%)
1	B	0.72	0/2097	0.89	1/2852 (0.0%)
1	C	0.72	0/2097	0.91	2/2852 (0.1%)
1	D	0.74	0/2088	0.91	1/2840 (0.0%)
1	E	0.73	0/2088	0.90	1/2840 (0.0%)
1	F	0.73	0/2088	0.90	1/2840 (0.0%)
1	G	0.58	0/2088	0.84	1/2840 (0.0%)
1	H	0.58	0/2088	0.85	1/2840 (0.0%)
1	I	0.57	0/2088	0.86	1/2840 (0.0%)
1	J	0.58	0/2088	0.85	1/2840 (0.0%)
1	K	0.57	0/2088	0.85	1/2840 (0.0%)
1	L	0.57	0/2088	0.85	1/2840 (0.0%)
All	All	0.66	0/25074	0.87	13/34104 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	992	GLY	N-CA-C	7.93	122.12	110.38
1	E	992	GLY	N-CA-C	7.67	121.74	110.38
1	D	992	GLY	N-CA-C	7.66	122.33	110.91
1	C	992	GLY	N-CA-C	7.66	122.32	110.91
1	J	992	GLY	N-CA-C	7.64	122.30	110.91
1	B	992	GLY	N-CA-C	7.59	122.22	110.91
1	F	992	GLY	N-CA-C	7.42	121.96	110.91
1	G	992	GLY	N-CA-C	7.42	121.96	110.91
1	A	992	GLY	N-CA-C	7.34	121.85	110.91
1	I	992	GLY	N-CA-C	7.18	121.60	110.91
1	L	992	GLY	N-CA-C	6.99	121.33	110.91
1	H	992	GLY	N-CA-C	6.89	121.18	110.91
1	C	1113	PHE	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

There are no planarity outliers.

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	2039	0	1971	9	0
1	B	2048	0	1977	10	0
1	C	2048	0	1977	14	0
1	D	2039	0	1971	15	0
1	E	2039	0	1971	16	0
1	F	2039	0	1971	11	0
1	G	2039	0	1971	14	0
1	H	2039	0	1971	14	0
1	I	2039	0	1971	16	0
1	J	2039	0	1971	13	0
1	K	2039	0	1971	14	0
1	L	2039	0	1971	17	0
2	A	112	0	0	2	0
2	B	95	0	0	0	0
2	C	81	0	0	0	0
2	D	119	0	0	0	0
2	E	112	0	0	0	0
2	F	83	0	0	0	0
2	G	39	0	0	0	0
2	H	43	0	0	0	0
2	I	40	0	0	0	0
2	J	33	0	0	0	0
2	K	25	0	0	0	0
2	L	76	0	0	0	0
All	All	25344	0	23664	116	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 2.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1170:PRO:HB2	1:H:1033:THR:HG21	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1223:LEU:HD23	1:I:1013:SER:HB3	1.62	0.82
1:E:1241:ARG:NH1	1:I:1011:SER:OG	2.16	0.79
1:G:991:PHE:CZ	1:L:991:PHE:CZ	2.77	0.72
1:B:995:ASN:ND2	1:C:989:CYS:HB2	2.05	0.71
1:A:1112:ARG:HD2	1:J:1011:SER:HB3	1.72	0.70
1:G:991:PHE:HZ	1:L:991:PHE:HZ	1.42	0.66
1:A:1213:GLU:HG2	1:A:1224:PRO:HA	1.78	0.65
2:A:2001:HOH:O	1:C:993:ILE:HG23	1.95	0.65
1:I:991:PHE:CZ	1:K:991:PHE:CZ	2.84	0.65
1:D:1213:GLU:HG2	1:D:1224:PRO:HA	1.78	0.63
1:B:995:ASN:HD22	1:C:989:CYS:HB2	1.65	0.61
1:E:1213:GLU:HG2	1:E:1224:PRO:HA	1.83	0.61
1:G:1213:GLU:HG2	1:G:1224:PRO:HA	1.83	0.60
1:H:1213:GLU:HG2	1:H:1224:PRO:HA	1.84	0.59
1:B:1213:GLU:HG2	1:B:1224:PRO:HA	1.85	0.59
1:D:989:CYS:HA	1:F:1000:SER:O	2.03	0.58
1:A:1112:ARG:NH1	1:J:1011:SER:HA	2.18	0.58
1:B:1061:LEU:HB2	1:B:1077:PHE:HB3	1.84	0.58
1:E:1241:ARG:CZ	1:I:1011:SER:OG	2.52	0.58
1:K:1213:GLU:HG2	1:K:1224:PRO:HA	1.85	0.58
1:L:1213:GLU:HG2	1:L:1224:PRO:HA	1.85	0.58
1:I:1213:GLU:HG2	1:I:1224:PRO:HA	1.85	0.57
1:J:1213:GLU:HG2	1:J:1224:PRO:HA	1.87	0.56
1:F:1198:ALA:HB3	1:F:1207:PRO:HB2	1.87	0.56
1:C:1061:LEU:HB2	1:C:1077:PHE:HB3	1.87	0.56
1:F:1213:GLU:HG2	1:F:1224:PRO:HA	1.88	0.56
1:D:1246:TRP:HZ3	1:J:1037:HIS:CE1	2.23	0.55
1:E:1223:LEU:CD2	1:I:1013:SER:HB3	2.34	0.55
1:K:1061:LEU:HB2	1:K:1077:PHE:HB3	1.90	0.54
2:A:2001:HOH:O	1:C:993:ILE:CG2	2.53	0.53
1:I:1061:LEU:HB2	1:I:1077:PHE:HB3	1.88	0.53
1:D:1246:TRP:CZ3	1:J:1037:HIS:CE1	2.97	0.53
1:G:1061:LEU:HB2	1:G:1077:PHE:HB3	1.90	0.53
1:G:991:PHE:HZ	1:L:991:PHE:CZ	2.18	0.53
1:L:1061:LEU:HB2	1:L:1077:PHE:HB3	1.90	0.53
1:H:991:PHE:CZ	1:K:991:PHE:CZ	2.97	0.52
1:L:1198:ALA:HB3	1:L:1207:PRO:HB2	1.91	0.52
1:C:1213:GLU:HG2	1:C:1224:PRO:HA	1.90	0.52
1:E:1223:LEU:HD23	1:I:1013:SER:CB	2.37	0.52
1:C:1198:ALA:HB3	1:C:1207:PRO:HB2	1.92	0.52
1:E:1198:ALA:HB3	1:E:1207:PRO:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1223:LEU:HD22	1:I:1010:ALA:O	2.11	0.51
1:I:1198:ALA:HB3	1:I:1207:PRO:HB2	1.93	0.51
1:G:991:PHE:CZ	1:L:991:PHE:HZ	2.19	0.51
1:K:1198:ALA:HB3	1:K:1207:PRO:HB2	1.92	0.50
1:H:1061:LEU:HB2	1:H:1077:PHE:HB3	1.92	0.50
1:E:1061:LEU:HB2	1:E:1077:PHE:HB3	1.93	0.50
1:D:1198:ALA:HB3	1:D:1207:PRO:HB2	1.93	0.50
1:A:1198:ALA:HB3	1:A:1207:PRO:HB2	1.93	0.50
1:H:991:PHE:HZ	1:K:991:PHE:HZ	1.60	0.50
1:G:991:PHE:CZ	1:L:991:PHE:CE1	3.01	0.49
1:B:1198:ALA:HB3	1:B:1207:PRO:HB2	1.95	0.49
1:G:1198:ALA:HB3	1:G:1207:PRO:HB2	1.94	0.49
1:J:1061:LEU:HB2	1:J:1077:PHE:HB3	1.93	0.49
1:H:1198:ALA:HB3	1:H:1207:PRO:HB2	1.95	0.48
1:J:1198:ALA:HB3	1:J:1207:PRO:HB2	1.95	0.48
1:D:1008:ARG:O	1:E:998:GLY:HA2	2.14	0.48
1:G:991:PHE:CE1	1:L:991:PHE:CZ	3.01	0.48
1:H:1003:PHE:CD2	1:H:1024:TYR:HE2	2.34	0.46
1:F:1003:PHE:CD2	1:F:1024:TYR:HE2	2.34	0.45
1:B:1003:PHE:CD2	1:B:1024:TYR:HE2	2.35	0.45
1:H:991:PHE:HZ	1:K:991:PHE:CZ	2.32	0.45
1:K:1003:PHE:CD2	1:K:1024:TYR:HE2	2.35	0.45
1:J:1115:ALA:HA	1:J:1186:PHE:HB2	1.99	0.45
1:D:1078:ARG:HB2	1:D:1086:TRP:HB2	1.98	0.45
1:E:1003:PHE:CD2	1:E:1024:TYR:HE2	2.35	0.45
1:J:1003:PHE:CD2	1:J:1024:TYR:HE2	2.34	0.45
1:D:1263:THR:HA	1:E:1256:ALA:O	2.17	0.45
1:D:1256:ALA:HB3	1:F:1261:ILE:HG21	1.99	0.44
1:D:1173:THR:HG22	1:D:1196:LYS:HG2	1.99	0.44
1:A:1003:PHE:CD2	1:A:1024:TYR:HE2	2.35	0.44
1:A:1193:VAL:HG11	1:C:1193:VAL:HG21	1.99	0.44
1:C:1003:PHE:CD2	1:C:1024:TYR:HE2	2.36	0.44
1:G:1003:PHE:CD2	1:G:1024:TYR:HE2	2.35	0.44
1:L:1003:PHE:CD2	1:L:1024:TYR:HE2	2.35	0.44
1:I:1003:PHE:CD2	1:I:1024:TYR:HE2	2.36	0.44
1:J:998:GLY:HA2	1:L:1008:ARG:O	2.17	0.44
1:H:1140:ARG:O	1:I:1130:GLN:HG2	2.17	0.44
1:H:1263:THR:HA	1:I:1256:ALA:O	2.17	0.43
1:C:1078:ARG:HB2	1:C:1086:TRP:HB2	2.01	0.43
1:G:1173:THR:HG22	1:G:1196:LYS:HG2	2.00	0.43
1:B:1263:THR:HA	1:C:1256:ALA:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1263:THR:HA	1:K:1256:ALA:O	2.18	0.43
1:K:1263:THR:HA	1:L:1256:ALA:O	2.19	0.43
1:D:1003:PHE:CD2	1:D:1024:TYR:HE2	2.37	0.42
1:D:998:GLY:HA2	1:F:1008:ARG:O	2.20	0.42
1:A:1115:ALA:HA	1:A:1186:PHE:HB2	2.02	0.42
1:D:1061:LEU:HB2	1:D:1077:PHE:HB3	2.01	0.42
1:G:1115:ALA:HA	1:G:1186:PHE:HB2	2.02	0.42
1:A:1008:ARG:O	1:B:998:GLY:HA2	2.20	0.42
1:C:1170:PRO:HB3	1:C:1199:GLY:HA2	2.01	0.42
1:G:1256:ALA:O	1:I:1263:THR:HA	2.20	0.42
1:D:1193:VAL:HG11	1:F:1193:VAL:HG21	2.01	0.41
1:H:1115:ALA:HA	1:H:1186:PHE:HB2	2.02	0.41
1:K:1193:VAL:HG21	1:L:1193:VAL:HG11	2.02	0.41
1:K:1134:ILE:HG21	1:L:1134:ILE:HD11	2.02	0.41
1:E:1263:THR:HA	1:F:1256:ALA:O	2.20	0.41
1:F:1170:PRO:HB3	1:F:1199:GLY:HA2	2.01	0.41
1:H:1078:ARG:HB2	1:H:1086:TRP:HB2	2.02	0.41
1:H:1134:ILE:HG21	1:I:1134:ILE:HD11	2.02	0.41
1:B:1155:ASP:HB2	1:B:1167:ALA:O	2.20	0.41
1:E:1193:VAL:HG21	1:F:1193:VAL:HG11	2.03	0.41
1:C:1115:ALA:HA	1:C:1186:PHE:HB2	2.03	0.41
1:E:1173:THR:HG22	1:E:1196:LYS:HG2	2.02	0.41
1:G:1140:ARG:HG3	1:G:1144:ALA:HA	2.02	0.41
1:I:1115:ALA:HA	1:I:1186:PHE:HB2	2.03	0.41
1:J:1134:ILE:HD11	1:L:1134:ILE:HG21	2.03	0.41
1:D:1130:GLN:HG2	1:F:1140:ARG:O	2.21	0.41
1:L:1115:ALA:HA	1:L:1186:PHE:HB2	2.03	0.40
1:C:1140:ARG:HG3	1:C:1144:ALA:HA	2.03	0.40
1:H:1170:PRO:HB3	1:H:1199:GLY:HA2	2.03	0.40
1:A:1193:VAL:HG21	1:B:1193:VAL:HG11	2.03	0.40
1:J:1133:GLU:HG2	1:L:1148:ALA:HB3	2.03	0.40
1:K:1078:ARG:HB2	1:K:1086:TRP:HB2	2.04	0.40
1:K:1115:ALA:HA	1:K:1186:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	273/328 (83%)	267 (98%)	6 (2%)	0	100	100
1	B	274/328 (84%)	268 (98%)	6 (2%)	0	100	100
1	C	274/328 (84%)	264 (96%)	10 (4%)	0	100	100
1	D	273/328 (83%)	264 (97%)	9 (3%)	0	100	100
1	E	273/328 (83%)	265 (97%)	8 (3%)	0	100	100
1	F	273/328 (83%)	263 (96%)	10 (4%)	0	100	100
1	G	273/328 (83%)	267 (98%)	6 (2%)	0	100	100
1	H	273/328 (83%)	265 (97%)	8 (3%)	0	100	100
1	I	273/328 (83%)	265 (97%)	8 (3%)	0	100	100
1	J	273/328 (83%)	267 (98%)	6 (2%)	0	100	100
1	K	273/328 (83%)	265 (97%)	8 (3%)	0	100	100
1	L	273/328 (83%)	267 (98%)	6 (2%)	0	100	100
All	All	3278/3936 (83%)	3187 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	B	213/254 (84%)	210 (99%)	3 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	213/254 (84%)	210 (99%)	3 (1%)	59	76
1	D	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	E	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	F	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	G	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	H	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	I	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	J	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	K	212/254 (84%)	210 (99%)	2 (1%)	70	84
1	L	212/254 (84%)	209 (99%)	3 (1%)	59	76
All	All	2546/3048 (84%)	2519 (99%)	27 (1%)	65	81

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	993	ILE
1	A	1209	GLN
1	B	988	GLU
1	B	993	ILE
1	B	1209	GLN
1	C	989	CYS
1	C	993	ILE
1	C	1209	GLN
1	D	993	ILE
1	D	1209	GLN
1	E	993	ILE
1	E	1209	GLN
1	F	993	ILE
1	F	1209	GLN
1	G	993	ILE
1	G	1209	GLN
1	H	993	ILE
1	H	1209	GLN
1	I	993	ILE
1	I	1209	GLN
1	J	993	ILE
1	J	1209	GLN
1	K	993	ILE

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Mol	Chain	Res	Type
1	K	1209	GLN
1	L	989	CYS
1	L	993	ILE
1	L	1209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1209	GLN
1	B	1209	GLN
1	B	1262	ASN
1	C	1209	GLN
1	C	1253	GLN
1	D	1209	GLN
1	E	1005	ASN
1	E	1209	GLN
1	F	1037	HIS
1	F	1209	GLN
1	G	1209	GLN
1	H	1209	GLN
1	I	1043	HIS
1	I	1209	GLN
1	J	1209	GLN
1	K	1209	GLN
1	L	1209	GLN

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 oligosaccharides 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, 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	275/328 (83%)	0.27	9 (3%) 49 51	30, 46, 72, 95	0
1	B	276/328 (84%)	0.22	3 (1%) 78 79	31, 47, 76, 89	0
1	C	276/328 (84%)	0.24	11 (3%) 42 44	32, 45, 79, 116	0
1	D	275/328 (83%)	0.27	7 (2%) 58 60	29, 46, 74, 85	0
1	E	275/328 (83%)	0.25	10 (3%) 46 48	29, 42, 75, 104	0
1	F	275/328 (83%)	0.23	6 (2%) 62 64	28, 44, 70, 96	0
1	G	275/328 (83%)	0.92	18 (6%) 25 27	54, 79, 101, 111	0
1	H	275/328 (83%)	0.82	21 (7%) 20 21	47, 73, 102, 118	0
1	I	275/328 (83%)	0.79	19 (6%) 23 25	45, 69, 100, 126	0
1	J	275/328 (83%)	0.92	28 (10%) 12 13	57, 75, 104, 120	0
1	K	275/328 (83%)	0.95	22 (8%) 18 20	59, 77, 102, 118	0
1	L	275/328 (83%)	1.24	46 (16%) 4 5	62, 87, 104, 113	0
All	All	3302/3936 (83%)	0.59	200 (6%) 27 29	28, 62, 98, 126	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	991	PHE	5.7
1	F	991	PHE	5.4
1	C	991	PHE	5.0
1	K	991	PHE	5.0
1	L	1210	VAL	4.8
1	E	991	PHE	4.8
1	H	991	PHE	4.8
1	J	991	PHE	4.5
1	I	991	PHE	4.4
1	F	1003	PHE	4.4
1	L	1103	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	993	ILE	4.1
1	D	1199	GLY	4.1
1	D	991	PHE	4.1
1	A	991	PHE	4.0
1	K	1244	LEU	3.9
1	H	1003	PHE	3.8
1	B	991	PHE	3.7
1	D	990	SER	3.6
1	L	1003	PHE	3.5
1	J	1254	VAL	3.5
1	L	1201	TRP	3.5
1	L	993	ILE	3.5
1	E	990	SER	3.4
1	I	990	SER	3.4
1	J	1170	PRO	3.4
1	I	993	ILE	3.4
1	L	1106	LEU	3.4
1	J	1032	SER	3.4
1	L	989	CYS	3.4
1	J	1204	THR	3.3
1	I	989	CYS	3.3
1	J	993	ILE	3.2
1	A	1003	PHE	3.2
1	C	1003	PHE	3.2
1	I	1254	VAL	3.2
1	J	1003	PHE	3.2
1	J	1256	ALA	3.2
1	E	1200	GLY	3.1
1	K	1254	VAL	3.1
1	L	1244	LEU	3.1
1	E	1199	GLY	3.1
1	J	1031	GLY	3.1
1	K	1113	PHE	3.1
1	G	997	ALA	3.1
1	A	993	ILE	3.0
1	J	1171	GLY	3.0
1	L	1212	LEU	2.9
1	I	1244	LEU	2.9
1	H	1014	VAL	2.9
1	F	1000	SER	2.9
1	L	991	PHE	2.9
1	L	1226	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	1153	TRP	2.8
1	H	1007	THR	2.8
1	J	1034	TYR	2.8
1	J	1158	LEU	2.8
1	J	1014	VAL	2.8
1	J	1069	THR	2.7
1	H	1156	GLY	2.7
1	A	989	CYS	2.7
1	J	989	CYS	2.7
1	H	1200	GLY	2.7
1	J	998	GLY	2.7
1	D	989	CYS	2.7
1	E	989	CYS	2.7
1	H	989	CYS	2.7
1	L	1001	ALA	2.7
1	E	993	ILE	2.7
1	G	1201	TRP	2.7
1	D	997	ALA	2.6
1	I	997	ALA	2.6
1	G	1113	PHE	2.6
1	H	993	ILE	2.6
1	B	990	SER	2.6
1	I	1153	TRP	2.6
1	L	1190	ARG	2.6
1	H	1199	GLY	2.6
1	H	1261	ILE	2.6
1	K	1003	PHE	2.6
1	K	990	SER	2.6
1	L	1261	ILE	2.6
1	H	1002	VAL	2.6
1	L	1234	LEU	2.5
1	K	1186	PHE	2.5
1	J	1002	VAL	2.5
1	K	1164	TYR	2.5
1	C	989	CYS	2.5
1	K	1065	PRO	2.5
1	F	1002	VAL	2.5
1	H	1256	ALA	2.5
1	A	992	GLY	2.5
1	C	1162	THR	2.5
1	H	1254	VAL	2.5
1	L	1248	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	993	ILE	2.5
1	K	1001	ALA	2.5
1	L	1260	THR	2.4
1	I	1165	ILE	2.4
1	K	1137	ILE	2.4
1	E	992	GLY	2.4
1	I	992	GLY	2.4
1	L	1022	GLY	2.4
1	J	1033	THR	2.4
1	L	1061	LEU	2.4
1	C	995	ASN	2.4
1	C	994	GLU	2.4
1	I	1144	ALA	2.4
1	L	1227	GLY	2.4
1	F	990	SER	2.4
1	G	1244	LEU	2.4
1	G	1226	TRP	2.4
1	E	999	GLY	2.4
1	D	1003	PHE	2.4
1	H	990	SER	2.3
1	H	1015	THR	2.3
1	H	1112	ARG	2.3
1	G	1168	THR	2.3
1	G	1190	ARG	2.3
1	G	1217	SER	2.3
1	K	1002	VAL	2.3
1	L	1211	VAL	2.3
1	L	1158	LEU	2.3
1	G	1249	GLY	2.3
1	I	1245	GLY	2.3
1	G	1167	ALA	2.3
1	H	1204	THR	2.3
1	L	1214	THR	2.3
1	H	1154	CYS	2.2
1	L	999	GLY	2.2
1	G	1052	ALA	2.2
1	J	1164	TYR	2.2
1	L	996	THR	2.2
1	L	1007	THR	2.2
1	I	1129	PRO	2.2
1	I	1091	GLY	2.2
1	K	997	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	1029	TRP	2.2
1	I	1220	ILE	2.2
1	J	1165	ILE	2.2
1	E	1003	PHE	2.2
1	G	1245	GLY	2.2
1	H	1238	ALA	2.2
1	J	1198	ALA	2.2
1	G	1188	SER	2.2
1	L	1015	THR	2.2
1	L	1108	ALA	2.2
1	I	999	GLY	2.2
1	K	1156	GLY	2.2
1	L	1202	GLY	2.2
1	L	1198	ALA	2.2
1	L	1220	ILE	2.1
1	J	1201	TRP	2.1
1	L	1186	PHE	2.1
1	L	1105	THR	2.1
1	C	1112	ARG	2.1
1	L	1024	TYR	2.1
1	J	1195	ILE	2.1
1	L	1085	LEU	2.1
1	L	1223	LEU	2.1
1	L	1251	VAL	2.1
1	L	1168	THR	2.1
1	G	1238	ALA	2.1
1	H	1128	ALA	2.1
1	L	1137	ILE	2.1
1	G	1254	VAL	2.1
1	K	1088	VAL	2.1
1	L	1254	VAL	2.1
1	G	1015	THR	2.1
1	L	1233	THR	2.1
1	K	1106	LEU	2.1
1	J	1006	TYR	2.1
1	L	1002	VAL	2.1
1	G	1186	PHE	2.1
1	K	1199	GLY	2.1
1	H	1153	TRP	2.1
1	A	1033	THR	2.0
1	C	990	SER	2.0
1	I	996	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	1172	SER	2.0
1	K	1204	THR	2.0
1	D	1052	ALA	2.0
1	K	1154	CYS	2.0
1	J	1037	HIS	2.0
1	A	995	ASN	2.0
1	B	1024	TYR	2.0
1	L	1009	GLY	2.0
1	L	1113	PHE	2.0
1	A	1029	TRP	2.0
1	I	1201	TRP	2.0
1	K	1093	MET	2.0
1	C	1000	SER	2.0
1	C	1015	THR	2.0
1	K	989	CYS	2.0
1	E	1158	LEU	2.0
1	J	1182	ASP	2.0
1	L	1030	LEU	2.0
1	A	1028	PRO	2.0
1	F	1028	PRO	2.0
1	I	1134	ILE	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.