



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 02:01 am GMT

PDB ID : 5AQ5
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

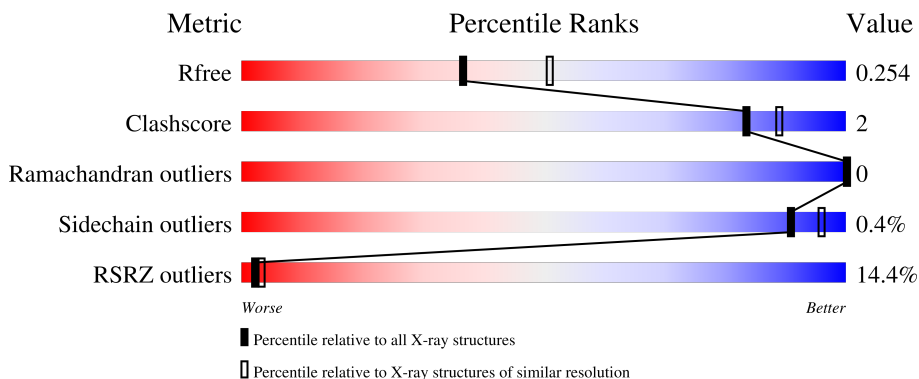
1 Overall quality at a glance

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.



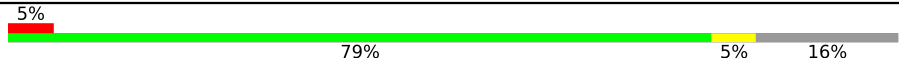
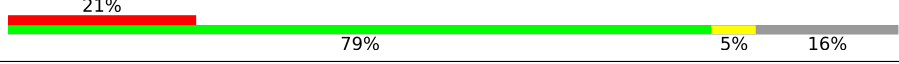
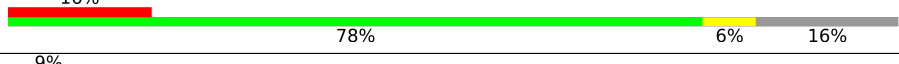
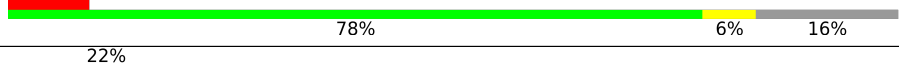

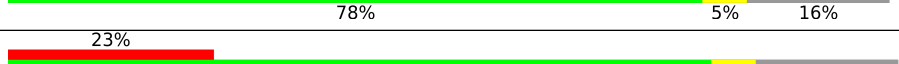
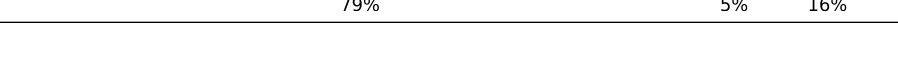
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	 6% 80% 16%
1	B	328	 4% 79% 5% 16%
1	C	328	 5% 78% 6% 16%
1	D	328	 5% 77% 6% 16%
1	E	328	 4% 78% 5% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	328	 5% 79% 5% 16%
1	G	328	 21% 79% 5% 16%
1	H	328	 16% 78% 6% 16%
1	I	328	 9% 78% 6% 16%
1	J	328	 22% 79% 5% 16%
1	K	328	 24% 78% 5% 16%
1	L	328	 23% 79% 5% 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
			Total	C	N	O	S			
1	A	275	2039	1266	372	393	8	0	0	0
1	B	276	2048	1271	373	396	8	0	0	0
1	C	276	2048	1271	373	396	8	0	0	0
1	D	275	2039	1266	372	393	8	0	0	0
1	E	275	2039	1266	372	393	8	0	0	0
1	F	275	2039	1266	372	393	8	0	0	0
1	G	275	2039	1266	372	393	8	0	0	0
1	H	275	2039	1266	372	393	8	0	0	0
1	I	275	2039	1266	372	393	8	0	0	0
1	J	275	2039	1266	372	393	8	0	0	0
1	K	275	2039	1266	372	393	8	0	0	0
1	L	275	2039	1266	372	393	8	0	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

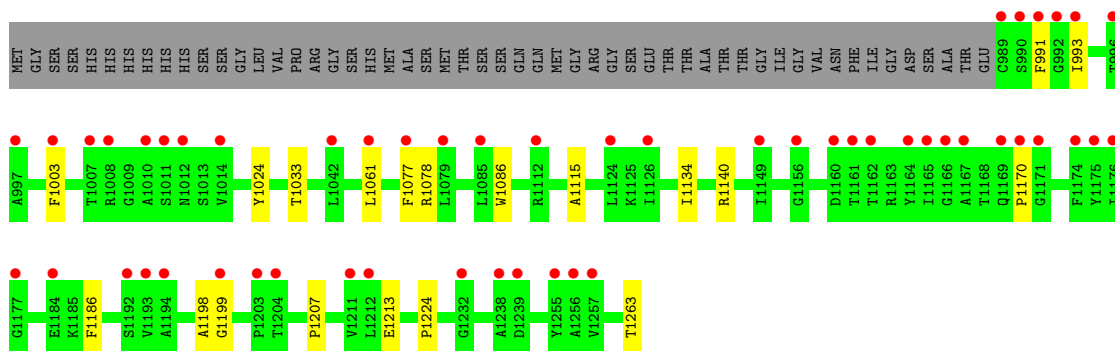
- Molecule 2 is water.

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

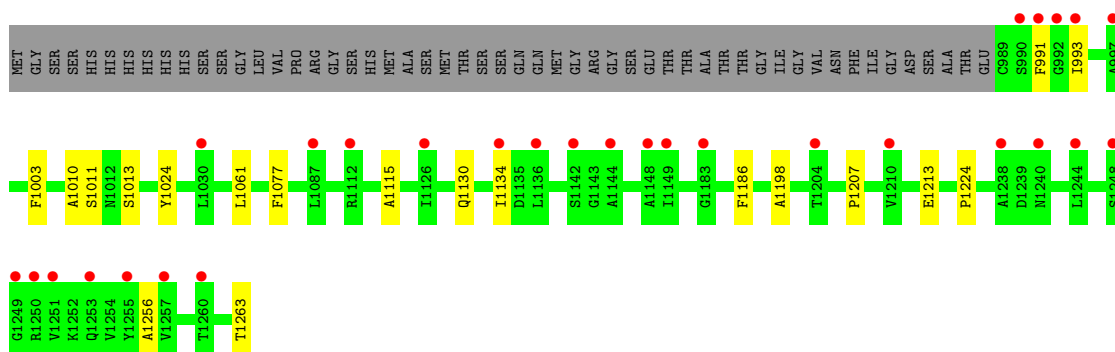
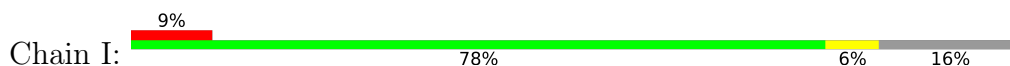
Continued on next page...

Continued from previous page...

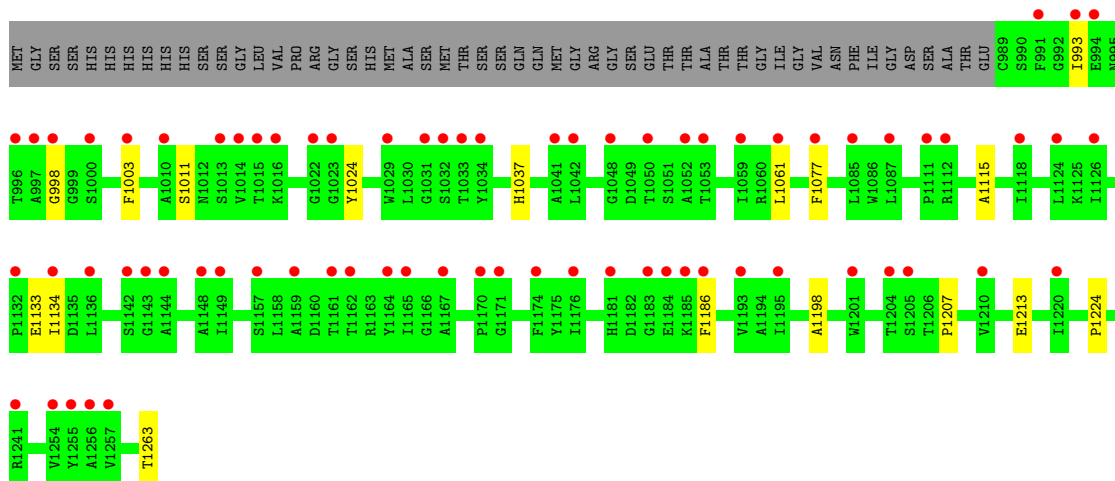
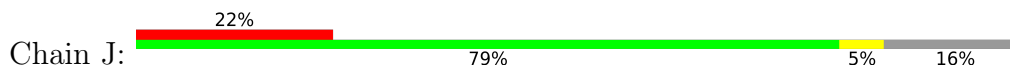
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	43	Total O 43 43	0	0
2	I	40	Total O 40 40	0	0
2	J	33	Total O 33 33	0	0
2	K	25	Total O 25 25	0	0
2	L	76	Total O 76 76	0	0



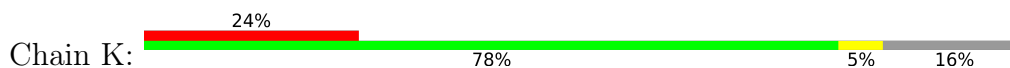
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



• 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 35.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (23.00-2.30) 91.0 (35.19-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.223 , 0.252 0.223 , 0.254	Depositor DCC
R_{free} test set	2910 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtrriage
Anisotropy	0.690	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.55	0/2088	0.68	0/2840
1	B	0.54	0/2097	0.68	0/2852
1	C	0.55	0/2097	0.68	0/2852
1	D	0.56	0/2088	0.70	1/2840 (0.0%)
1	E	0.54	0/2088	0.69	1/2840 (0.0%)
1	F	0.53	0/2088	0.67	0/2840
1	G	0.43	0/2088	0.63	0/2840
1	H	0.43	0/2088	0.63	0/2840
1	I	0.43	0/2088	0.65	0/2840
1	J	0.44	0/2088	0.63	0/2840
1	K	0.44	0/2088	0.63	0/2840
1	L	0.43	0/2088	0.63	0/2840
All	All	0.49	0/25074	0.66	2/34104 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1060	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	1060	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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

The worst 5 of 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
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

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	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/254 (84%)	212 (100%)	0	100	100
1	B	213/254 (84%)	211 (99%)	2 (1%)	78	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	213/254 (84%)	211 (99%)	2 (1%)	78	89
1	D	212/254 (84%)	212 (100%)	0	100	100
1	E	212/254 (84%)	212 (100%)	0	100	100
1	F	212/254 (84%)	211 (100%)	1 (0%)	88	95
1	G	212/254 (84%)	212 (100%)	0	100	100
1	H	212/254 (84%)	211 (100%)	1 (0%)	88	95
1	I	212/254 (84%)	211 (100%)	1 (0%)	88	95
1	J	212/254 (84%)	211 (100%)	1 (0%)	88	95
1	K	212/254 (84%)	211 (100%)	1 (0%)	88	95
1	L	212/254 (84%)	211 (100%)	1 (0%)	88	95
All	All	2546/3048 (84%)	2536 (100%)	10 (0%)	91	96

5 of 10 residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/328 (83%)	0.31	19 (6%) 16 22	30, 46, 72, 95	0
1	B	276/328 (84%)	0.29	14 (5%) 28 35	31, 47, 76, 89	0
1	C	276/328 (84%)	0.32	18 (6%) 18 24	32, 45, 79, 116	0
1	D	275/328 (83%)	0.32	17 (6%) 20 26	29, 46, 74, 85	0
1	E	275/328 (83%)	0.29	14 (5%) 28 35	29, 42, 75, 104	0
1	F	275/328 (83%)	0.24	17 (6%) 20 26	28, 44, 70, 96	0
1	G	275/328 (83%)	1.19	68 (24%) 0 0	54, 79, 101, 111	0
1	H	275/328 (83%)	0.94	53 (19%) 1 1	47, 73, 102, 118	0
1	I	275/328 (83%)	0.64	29 (10%) 6 8	45, 69, 100, 126	0
1	J	275/328 (83%)	1.27	72 (26%) 0 0	57, 75, 104, 120	0
1	K	275/328 (83%)	1.43	79 (28%) 0 0	59, 77, 102, 118	0
1	L	275/328 (83%)	1.46	76 (27%) 0 0	62, 87, 104, 113	0
All	All	3302/3936 (83%)	0.73	476 (14%) 2 3	28, 62, 98, 126	0

The worst 5 of 476 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1031	GLY	9.0
1	K	1010	ALA	8.0
1	J	1256	ALA	7.5
1	J	1204	THR	6.9
1	H	997	ALA	6.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.