



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:19 PM 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

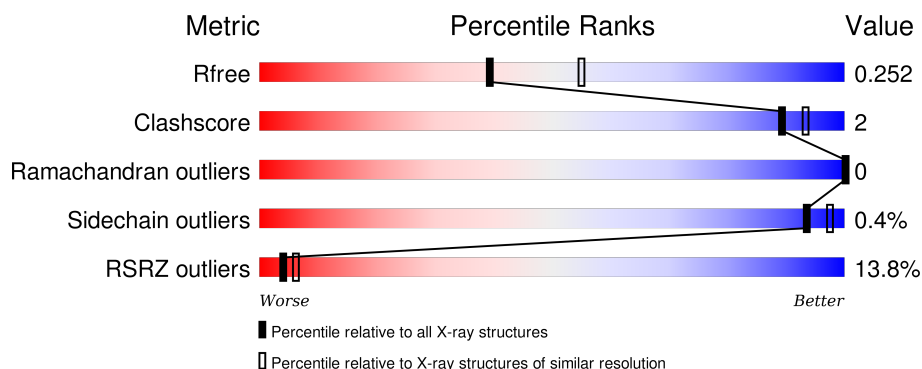
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	<div> <div>5%</div> <div>80%</div> <div>16%</div> </div>
1	B	328	<div> <div>4%</div> <div>79%</div> <div>5%</div> <div>16%</div> </div>
1	C	328	<div> <div>5%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
1	D	328	<div> <div>5%</div> <div>77%</div> <div>6%</div> <div>16%</div> </div>
1	E	328	<div> <div>4%</div> <div>78%</div> <div>5%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	328	
1	G	328	
1	H	328	
1	I	328	
1	J	328	
1	K	328	
1	L	328	

## 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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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

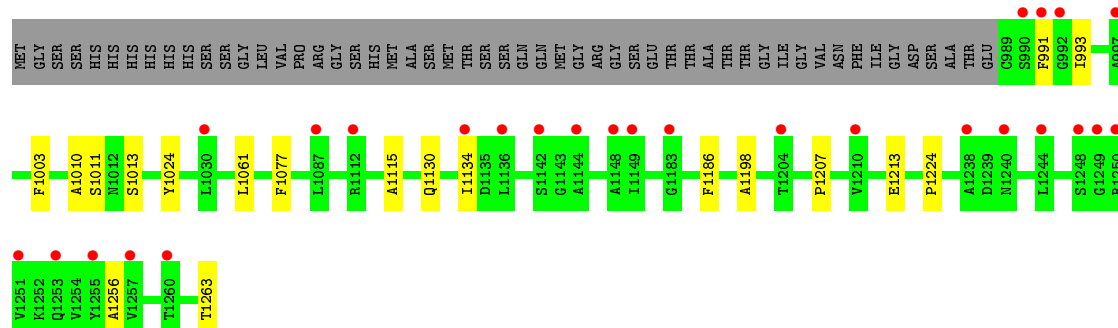
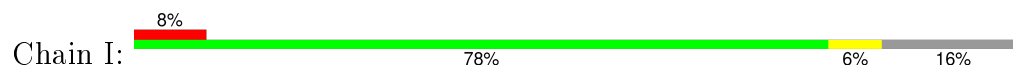




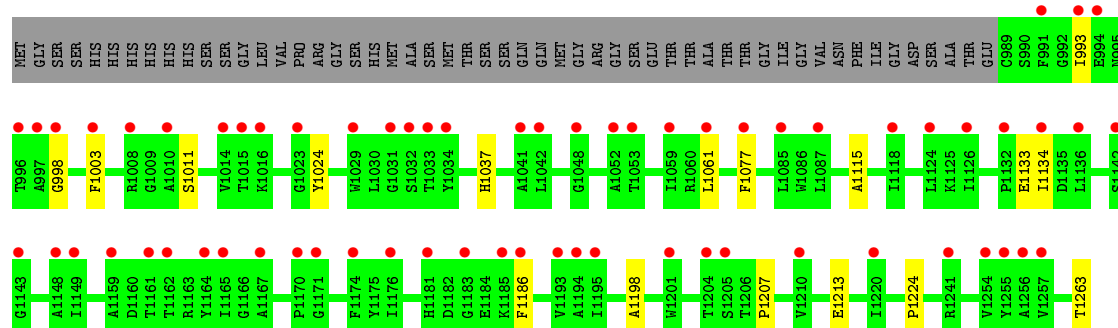
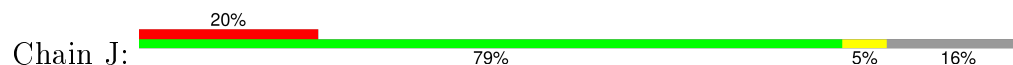




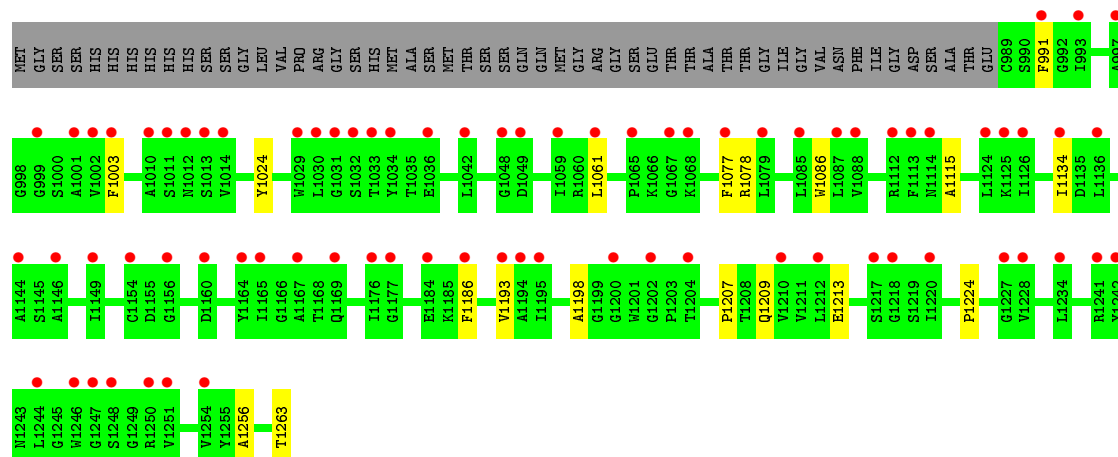
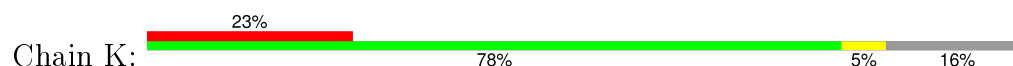
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



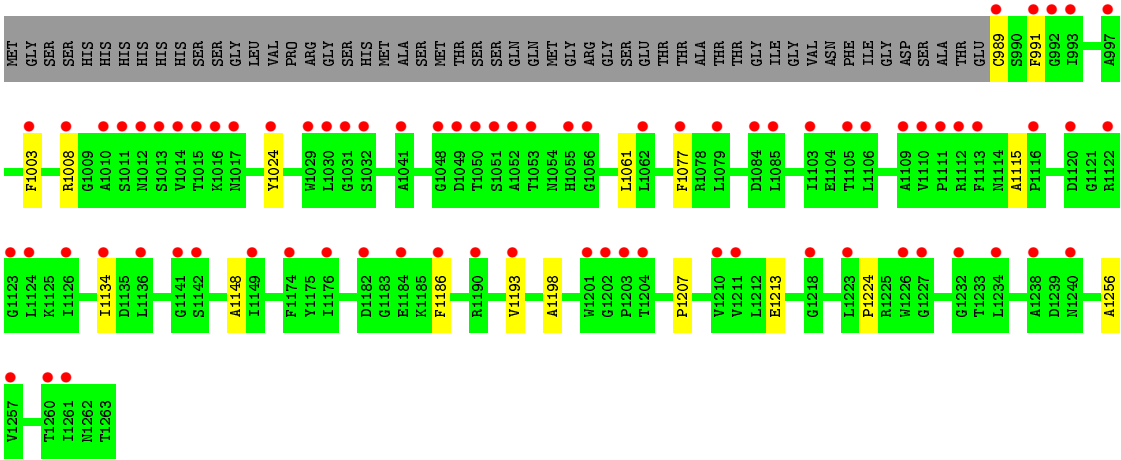
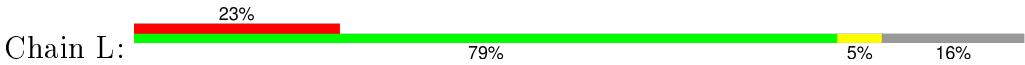
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



• 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, $\alpha$ , $\beta$ , $\gamma$	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) 79.7 (35.19-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.223 , 0.252 0.223 , 0.252	Depositor DCC
$R_{free}$ test set	2920 reflections (2.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 31.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 143912 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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.

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
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
1:I:991:PHE:CZ	1:K:991:PHE:CZ	2.84	0.65
2:A:2001:HOH:O	1:C:993:ILE:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1003:PHE:CD2	1:E:1024:TYR:HE2	2.35	0.45
1:D:1078:ARG:HB2	1:D:1086:TRP:HB2	1.98	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:C:1003:PHE:CD2	1:C:1024:TYR:HE2	2.36	0.44
1:A:1193:VAL:HG11	1:C:1193:VAL:HG21	1.99	0.44
1:A:1003:PHE:CD2	1:A:1024:TYR:HE2	2.35	0.44
1:L:1003:PHE:CD2	1:L:1024:TYR:HE2	2.35	0.44
1:G:1003:PHE:CD2	1:G: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
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:C:1170:PRO:HB3	1:C:1199:GLY:HA2	2.01	0.42
1:A:1008:ARG:O	1:B:998:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1193:VAL:HG21	1:F:1193:VAL:HG11	2.03	0.41
1:B:1155:ASP:HB2	1:B:1167:ALA:O	2.20	0.41
1:J:1134:ILE:HD11	1:L:1134:ILE:HG21	2.03	0.41
1:G:1140:ARG:HG3	1:G:1144:ALA:HA	2.02	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:I:1115:ALA:HA	1:I:1186:PHE:HB2	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: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
1:J:1133:GLU:HG2	1:L:1148:ALA:HB3	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	273/328 (83%)	267 (98%)	6 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	212 (100%)	0	100	100
1	B	213/254 (84%)	211 (99%)	2 (1%)	84	93
1	C	213/254 (84%)	211 (99%)	2 (1%)	84	93
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%)	92	97
1	G	212/254 (84%)	212 (100%)	0	100	100
1	H	212/254 (84%)	211 (100%)	1 (0%)	92	97
1	I	212/254 (84%)	211 (100%)	1 (0%)	92	97
1	J	212/254 (84%)	211 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	212/254 (84%)	211 (100%)	1 (0%)	92	97
1	L	212/254 (84%)	211 (100%)	1 (0%)	92	97
All	All	2546/3048 (84%)	2536 (100%)	10 (0%)	93	97

All (10) residues with a non-rotameric sidechain are listed below:

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

Some 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 [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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	275/328 (83%)	0.29	16 (5%) 26 35	30, 46, 72, 95	0
1	B	276/328 (84%)	0.26	14 (5%) 32 41	31, 47, 76, 89	0
1	C	276/328 (84%)	0.30	16 (5%) 26 35	32, 45, 79, 116	0
1	D	275/328 (83%)	0.32	18 (6%) 22 30	29, 46, 74, 85	0
1	E	275/328 (83%)	0.27	12 (4%) 38 47	29, 42, 75, 104	0
1	F	275/328 (83%)	0.25	16 (5%) 26 35	28, 44, 70, 96	0
1	G	275/328 (83%)	1.15	61 (22%) 1 1	54, 79, 101, 111	0
1	H	275/328 (83%)	0.92	56 (20%) 1 2	47, 73, 102, 118	0
1	I	275/328 (83%)	0.64	27 (9%) 10 14	45, 69, 100, 126	0
1	J	275/328 (83%)	1.18	65 (23%) 1 1	57, 75, 104, 120	0
1	K	275/328 (83%)	1.40	77 (28%) 1 1	59, 77, 102, 118	0
1	L	275/328 (83%)	1.42	77 (28%) 1 1	62, 87, 104, 113	0
All	All	3302/3936 (83%)	0.70	455 (13%) 4 6	28, 62, 98, 126	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	1031	GLY	8.9
1	J	1256	ALA	8.3
1	K	1010	ALA	8.2
1	L	1103	ILE	7.3
1	J	1204	THR	6.8
1	H	997	ALA	6.5
1	K	991	PHE	6.3
1	F	991	PHE	6.3
1	K	1246	TRP	5.8
1	L	1012	ASN	5.7
1	K	1164	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	1164	TYR	5.7
1	H	1166	GLY	5.7
1	K	1030	LEU	5.5
1	G	1032	SER	5.4
1	K	999	GLY	5.3
1	K	1156	GLY	5.2
1	L	1142	SER	5.1
1	H	1257	VAL	5.1
1	K	1085	LEU	5.1
1	L	1014	VAL	5.0
1	K	1011	SER	4.9
1	L	1110	VAL	4.9
1	L	1029	TRP	4.9
1	H	991	PHE	4.9
1	K	1218	GLY	4.8
1	L	1260	THR	4.8
1	E	991	PHE	4.8
1	L	1134	ILE	4.8
1	G	1010	ALA	4.8
1	H	1256	ALA	4.7
1	I	990	SER	4.7
1	G	1238	ALA	4.7
1	K	1247	GLY	4.7
1	K	1033	THR	4.7
1	J	1170	PRO	4.6
1	G	991	PHE	4.6
1	J	1176	ILE	4.5
1	K	1029	TRP	4.5
1	G	1204	THR	4.4
1	L	1257	VAL	4.4
1	L	1013	SER	4.4
1	H	1199	GLY	4.4
1	C	991	PHE	4.3
1	L	1226	TRP	4.3
1	A	991	PHE	4.3
1	H	1204	THR	4.3
1	K	1136	LEU	4.3
1	H	1156	GLY	4.3
1	L	1032	SER	4.3
1	J	1003	PHE	4.2
1	L	992	GLY	4.2
1	G	1012	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	1255	TYR	4.1
1	K	1134	ILE	4.1
1	D	997	ALA	4.0
1	I	1204	THR	4.0
1	G	1011	SER	4.0
1	L	1015	THR	4.0
1	G	1164	TYR	3.9
1	J	1164	TYR	3.9
1	G	1077	PHE	3.9
1	K	1034	TYR	3.9
1	J	1171	GLY	3.9
1	L	1106	LEU	3.9
1	L	1112	ARG	3.9
1	K	1165	ILE	3.9
1	A	1003	PHE	3.9
1	H	1184	GLU	3.9
1	G	1223	LEU	3.9
1	J	1205	SER	3.8
1	K	1176	ILE	3.8
1	H	1011	SER	3.8
1	L	991	PHE	3.8
1	G	1176	ILE	3.8
1	G	1111	PRO	3.8
1	L	1111	PRO	3.8
1	H	1176	ILE	3.7
1	G	1262	ASN	3.7
1	J	1181	HIS	3.7
1	K	1032	SER	3.7
1	I	1136	LEU	3.7
1	J	1052	ALA	3.7
1	K	1220	ILE	3.7
1	A	1033	THR	3.6
1	K	1204	THR	3.6
1	K	1003	PHE	3.6
1	G	1087	LEU	3.6
1	L	1184	GLU	3.6
1	F	1003	PHE	3.6
1	H	1112	ARG	3.6
1	H	1167	ALA	3.6
1	J	1257	VAL	3.6
1	L	1011	SER	3.6
1	J	1195	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	1097	LEU	3.5
1	D	1199	GLY	3.5
1	J	1085	LEU	3.5
1	J	1010	ALA	3.5
1	J	1015	THR	3.5
1	J	1143	GLY	3.5
1	E	996	THR	3.4
1	G	1226	TRP	3.4
1	K	1077	PHE	3.4
1	K	1036	GLU	3.4
1	C	1136	LEU	3.4
1	J	1134	ILE	3.4
1	L	1050	THR	3.4
1	G	1126	ILE	3.4
1	K	1087	LEU	3.4
1	L	1052	ALA	3.4
1	J	1193	VAL	3.3
1	H	1171	GLY	3.3
1	J	1161	THR	3.3
1	B	1124	LEU	3.3
1	I	1112	ARG	3.3
1	A	1124	LEU	3.3
1	E	989	CYS	3.3
1	H	1079	LEU	3.3
1	J	1042	LEU	3.3
1	D	991	PHE	3.3
1	L	1055	HIS	3.3
1	J	1201	TRP	3.3
1	I	1142	SER	3.3
1	K	1194	ALA	3.3
1	L	1051	SER	3.3
1	A	1134	ILE	3.2
1	D	1003	PHE	3.2
1	G	1183	GLY	3.2
1	E	1041	ALA	3.2
1	I	991	PHE	3.2
1	K	1184	GLU	3.2
1	H	1212	LEU	3.2
1	G	1113	PHE	3.2
1	E	1124	LEU	3.2
1	G	1134	ILE	3.2
1	G	1053	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	993	ILE	3.1
1	K	1195	ILE	3.1
1	J	1142	SER	3.1
1	K	1014	VAL	3.1
1	K	1254	VAL	3.1
1	J	1031	GLY	3.1
1	K	1149	ILE	3.1
1	B	991	PHE	3.1
1	K	1068	LYS	3.1
1	I	997	ALA	3.1
1	L	1201	TRP	3.1
1	J	1136	LEU	3.1
1	H	1165	ILE	3.1
1	G	1167	ALA	3.1
1	J	1167	ALA	3.1
1	E	992	GLY	3.1
1	L	1210	VAL	3.1
1	B	1085	LEU	3.1
1	L	1030	LEU	3.1
1	H	1012	ASN	3.1
1	C	992	GLY	3.1
1	I	992	GLY	3.1
1	F	1124	LEU	3.1
1	L	1124	LEU	3.1
1	G	1220	ILE	3.1
1	J	1254	VAL	3.0
1	K	1242	TYR	3.0
1	G	992	GLY	3.0
1	B	1134	ILE	3.0
1	H	1238	ALA	3.0
1	L	1202	GLY	3.0
1	J	991	PHE	3.0
1	L	1003	PHE	3.0
1	I	1249	GLY	3.0
1	G	1029	TRP	3.0
1	J	1124	LEU	3.0
1	L	1008	ARG	3.0
1	C	993	ILE	3.0
1	I	1149	ILE	3.0
1	L	1227	GLY	3.0
1	H	1003	PHE	3.0
1	L	1077	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1162	THR	3.0
1	G	1030	LEU	2.9
1	D	1010	ALA	2.9
1	G	997	ALA	2.9
1	H	1010	ALA	2.9
1	H	1008	ARG	2.9
1	H	1193	VAL	2.9
1	K	1079	LEU	2.9
1	J	1159	ALA	2.9
1	K	1244	LEU	2.9
1	D	1126	ILE	2.9
1	J	1118	ILE	2.9
1	L	1182	ASP	2.9
1	G	1052	ALA	2.9
1	L	1149	ILE	2.9
1	C	1148	ALA	2.9
1	G	1112	ARG	2.9
1	L	1193	VAL	2.8
1	J	1032	SER	2.8
1	J	1220	ILE	2.8
1	L	1126	ILE	2.8
1	L	1016	LYS	2.8
1	A	992	GLY	2.8
1	K	1013	SER	2.8
1	C	1149	ILE	2.8
1	G	1263	THR	2.8
1	J	1185	LYS	2.8
1	L	1136	LEU	2.8
1	L	989	CYS	2.8
1	E	998	GLY	2.8
1	L	1141	GLY	2.8
1	B	1149	ILE	2.8
1	H	1149	ILE	2.8
1	J	1126	ILE	2.8
1	L	997	ALA	2.8
1	J	1162	THR	2.8
1	I	1255	TYR	2.8
1	G	1037	HIS	2.8
1	L	1010	ALA	2.8
1	L	1238	ALA	2.8
1	C	1126	ILE	2.7
1	I	1240	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	1059	ILE	2.7
1	K	1210	VAL	2.7
1	E	1053	THR	2.7
1	L	1105	THR	2.7
1	A	1031	GLY	2.7
1	H	1170	PRO	2.7
1	H	989	CYS	2.7
1	G	1249	GLY	2.7
1	L	1261	ILE	2.7
1	J	1210	VAL	2.7
1	K	1124	LEU	2.7
1	L	1204	THR	2.7
1	K	1177	GLY	2.7
1	D	1134	ILE	2.7
1	L	1176	ILE	2.7
1	J	997	ALA	2.7
1	L	1190	ARG	2.7
1	G	1085	LEU	2.7
1	K	1002	VAL	2.7
1	A	1011	SER	2.7
1	L	1203	PRO	2.7
1	B	1126	ILE	2.7
1	L	1017	ASN	2.7
1	K	1251	VAL	2.7
1	G	1191	GLY	2.7
1	K	1065	PRO	2.6
1	K	997	ALA	2.6
1	H	1077	PHE	2.6
1	H	1177	GLY	2.6
1	L	1211	VAL	2.6
1	D	990	SER	2.6
1	G	1239	ASP	2.6
1	I	1238	ALA	2.6
1	K	1144	ALA	2.6
1	H	1169	GLN	2.6
1	G	1178	ALA	2.6
1	I	1248	SER	2.6
1	K	993	ILE	2.6
1	G	1031	GLY	2.6
1	I	1260	THR	2.6
1	C	1124	LEU	2.6
1	F	1024	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	1144	ALA	2.6
1	G	1033	THR	2.6
1	K	1114	ASN	2.6
1	K	1154	CYS	2.6
1	K	1088	VAL	2.6
1	A	1126	ILE	2.6
1	H	990	SER	2.5
1	H	1203	PRO	2.5
1	G	1013	SER	2.5
1	D	1136	LEU	2.5
1	H	1174	PHE	2.5
1	L	1218	GLY	2.5
1	L	1232	GLY	2.5
1	J	1148	ALA	2.5
1	K	1248	SER	2.5
1	B	1053	THR	2.5
1	H	996	THR	2.5
1	J	1029	TRP	2.5
1	K	1250	ARG	2.5
1	L	1234	LEU	2.5
1	A	1032	SER	2.5
1	J	1255	TYR	2.5
1	K	1241	ARG	2.5
1	F	1085	LEU	2.5
1	I	1030	LEU	2.5
1	J	1087	LEU	2.5
1	G	1257	VAL	2.5
1	H	1014	VAL	2.5
1	J	1053	THR	2.5
1	L	1031	GLY	2.5
1	J	1034	TYR	2.5
1	J	994	GLU	2.5
1	H	992	GLY	2.5
1	H	1126	ILE	2.5
1	J	1165	ILE	2.5
1	G	1003	PHE	2.4
1	H	1194	ALA	2.4
1	H	1232	GLY	2.4
1	I	1250	ARG	2.4
1	G	1061	LEU	2.4
1	G	1009	GLY	2.4
1	L	1053	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1195	ILE	2.4
1	F	1112	ARG	2.4
1	K	1217	SER	2.4
1	G	1124	LEU	2.4
1	G	1177	GLY	2.4
1	I	1253	GLN	2.4
1	K	1212	LEU	2.4
1	I	1183	GLY	2.4
1	H	1239	ASP	2.4
1	K	1186	PHE	2.4
1	D	993	ILE	2.4
1	K	1126	ILE	2.4
1	H	1085	LEU	2.4
1	I	1210	VAL	2.4
1	K	1012	ASN	2.4
1	L	1024	TYR	2.4
1	J	1048	GLY	2.4
1	A	1085	LEU	2.4
1	E	1085	LEU	2.4
1	J	1149	ILE	2.3
1	G	1094	HIS	2.3
1	H	1175	TYR	2.3
1	L	1123	GLY	2.3
1	F	1087	LEU	2.3
1	L	1079	LEU	2.3
1	L	1223	LEU	2.3
1	D	1193	VAL	2.3
1	K	1112	ARG	2.3
1	G	1195	ILE	2.3
1	G	990	SER	2.3
1	J	1077	PHE	2.3
1	L	1113	PHE	2.3
1	C	1134	ILE	2.3
1	K	1059	ILE	2.3
1	I	1257	VAL	2.3
1	H	1200	GLY	2.3
1	J	1183	GLY	2.3
1	K	1200	GLY	2.3
1	E	1134	ILE	2.3
1	L	1240	ASN	2.3
1	I	1148	ALA	2.3
1	H	1042	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	1244	LEU	2.3
1	L	1085	LEU	2.3
1	B	998	GLY	2.3
1	B	1210	VAL	2.3
1	F	1002	VAL	2.3
1	G	1014	VAL	2.3
1	G	1193	VAL	2.3
1	J	1186	PHE	2.3
1	G	1036	GLU	2.3
1	K	1160	ASP	2.3
1	H	1007	THR	2.3
1	H	1162	THR	2.3
1	J	996	THR	2.3
1	K	1061	LEU	2.3
1	F	1023	GLY	2.3
1	G	1225	ARG	2.3
1	L	1084	ASP	2.3
1	L	993	ILE	2.3
1	C	1031	GLY	2.2
1	E	993	ILE	2.2
1	J	1023	GLY	2.2
1	D	1210	VAL	2.2
1	A	1077	PHE	2.2
1	C	1003	PHE	2.2
1	G	1161	THR	2.2
1	K	1042	LEU	2.2
1	G	1241	ARG	2.2
1	J	1016	LYS	2.2
1	F	1000	SER	2.2
1	D	1052	ALA	2.2
1	G	1072	ASP	2.2
1	C	1059	ILE	2.2
1	K	1125	LYS	2.2
1	G	1181	HIS	2.2
1	H	1161	THR	2.2
1	J	1041	ALA	2.2
1	K	1146	ALA	2.2
1	A	993	ILE	2.2
1	F	1059	ILE	2.2
1	C	1061	LEU	2.2
1	I	1087	LEU	2.2
1	F	1012	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	1109	ALA	2.2
1	B	1000	SER	2.2
1	H	1160	ASP	2.2
1	G	1218	GLY	2.2
1	L	1048	GLY	2.2
1	D	1014	VAL	2.1
1	K	1113	PHE	2.1
1	L	1174	PHE	2.1
1	J	1033	THR	2.1
1	H	1261	ILE	2.1
1	I	1134	ILE	2.1
1	C	1002	VAL	2.1
1	L	1049	ASP	2.1
1	B	1212	LEU	2.1
1	J	1132	PRO	2.1
1	A	1177	GLY	2.1
1	G	1190	ARG	2.1
1	J	1174	PHE	2.1
1	J	1241	ARG	2.1
1	A	1079	LEU	2.1
1	F	1079	LEU	2.1
1	L	1056	GLY	2.1
1	L	1116	PRO	2.1
1	L	1120	ASP	2.1
1	D	1002	VAL	2.1
1	K	1001	ALA	2.1
1	K	1193	VAL	2.1
1	L	1041	ALA	2.1
1	L	1186	PHE	2.1
1	E	1025	GLY	2.1
1	K	1202	GLY	2.1
1	H	1061	LEU	2.1
1	A	989	CYS	2.1
1	D	989	CYS	2.1
1	H	1246	TRP	2.1
1	L	1122	ARG	2.1
1	H	1024	TYR	2.1
1	J	998	GLY	2.1
1	F	1149	ILE	2.1
1	G	1042	LEU	2.1
1	K	1234	LEU	2.1
1	G	1168	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	1194	ALA	2.1
1	I	1251	VAL	2.1
1	K	1227	GLY	2.1
1	K	1228	VAL	2.1
1	C	1164	TYR	2.1
1	D	1164	TYR	2.1
1	K	1049	ASP	2.0
1	B	1087	LEU	2.0
1	F	1134	ILE	2.0
1	F	1136	LEU	2.0
1	G	1165	ILE	2.0
1	D	1178	ALA	2.0
1	K	1067	GLY	2.0
1	K	1167	ALA	2.0
1	J	1014	VAL	2.0
1	B	1136	LEU	2.0
1	H	1124	LEU	2.0
1	L	1062	LEU	2.0
1	H	1148	ALA	2.0
1	H	1072	ASP	2.0
1	J	1061	LEU	2.0
1	K	1048	GLY	2.0
1	K	1169	GLN	2.0
1	J	1008	ARG	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 carbohydrates 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.