Full wwPDB X-ray Structure Validation 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 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:

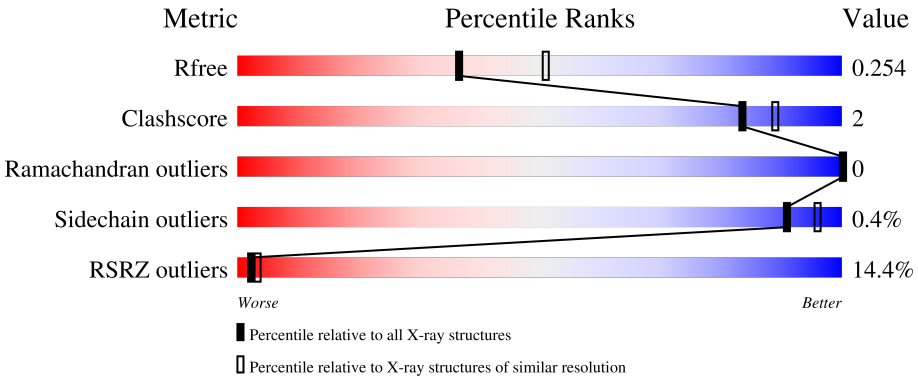
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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 <=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%

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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 (i)

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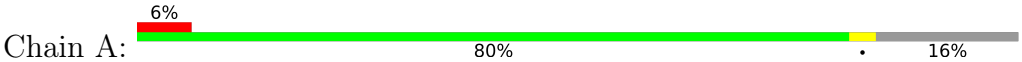
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	43	Total O 43 43	0	0
2	I	40	Total O 40 40	0	0
2	J	33	Total O 33 33	0	0
2	K	25	Total O 25 25	0	0
2	L	76	Total O 76 76	0	0

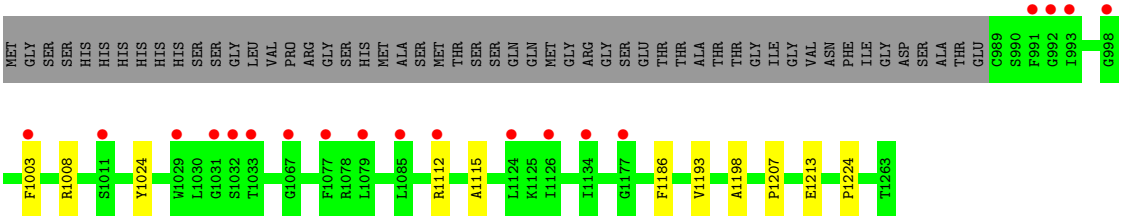
3 Residue-property plots (i)

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.

• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

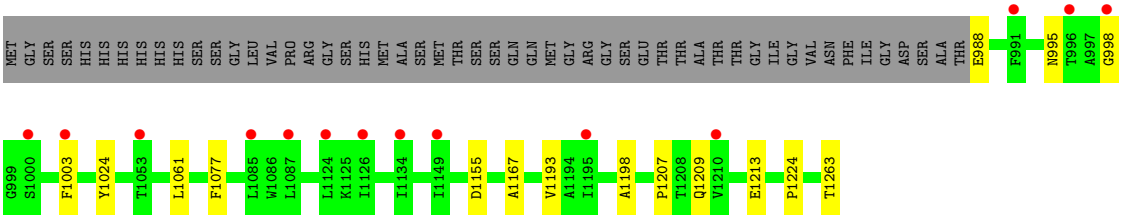
Chain A:





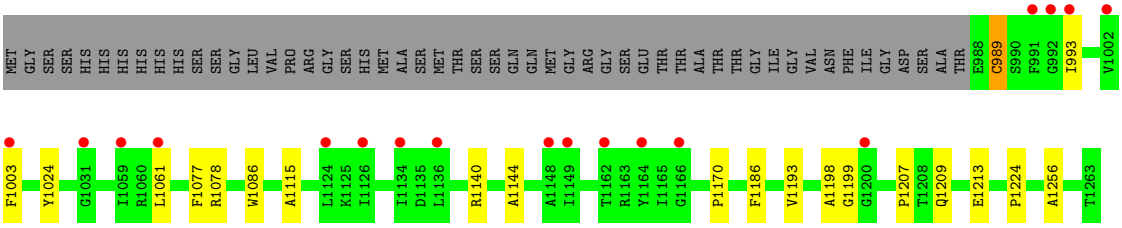
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain B:



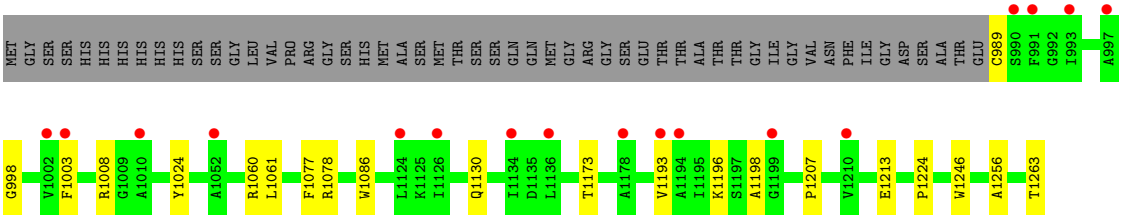
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain C:

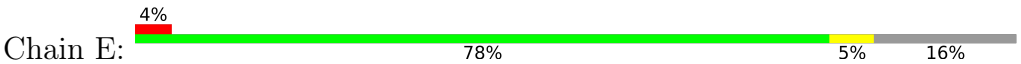


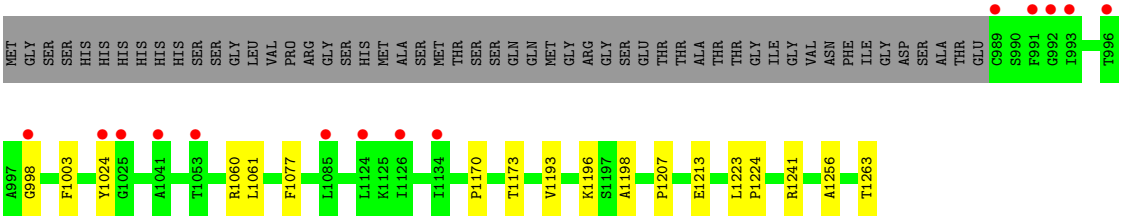
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain D:

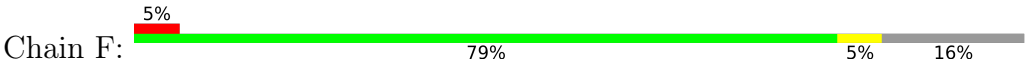


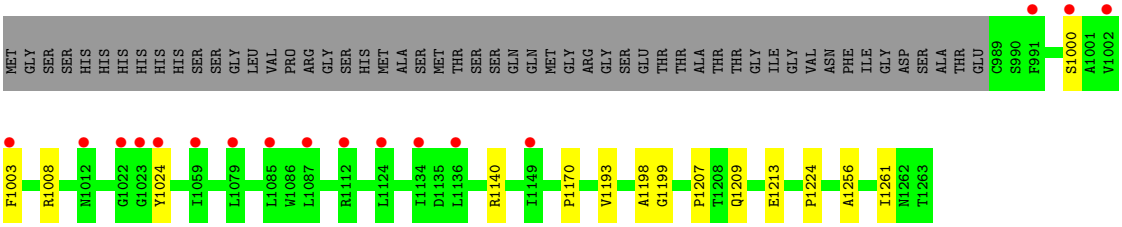
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



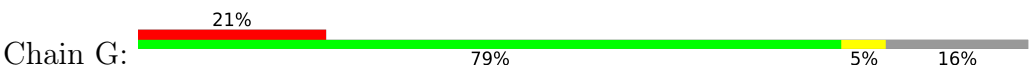


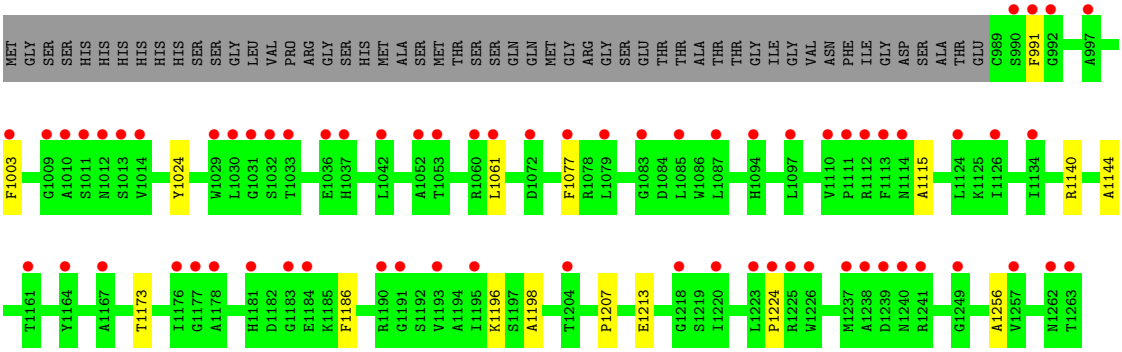
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8



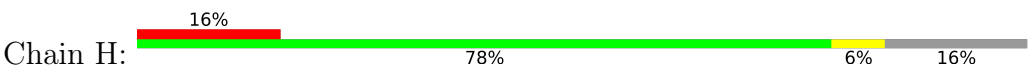


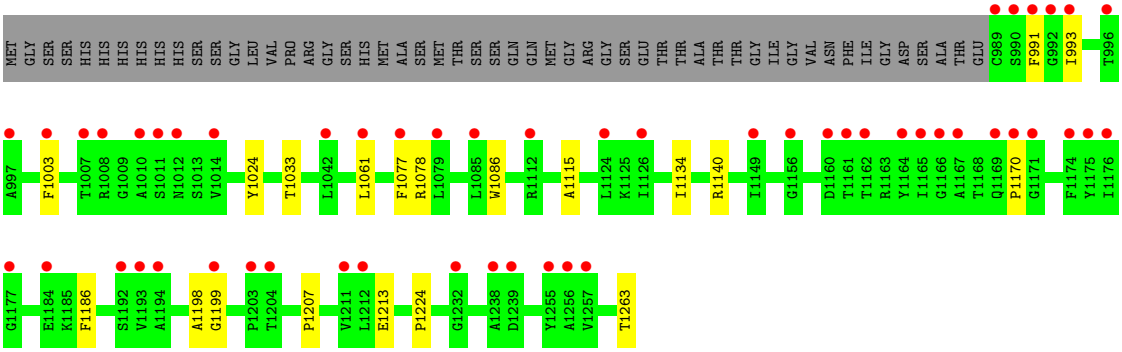
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8





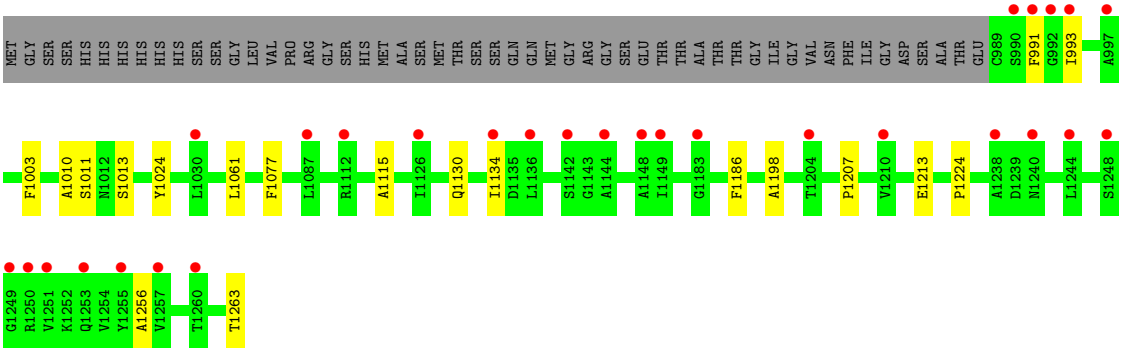
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8





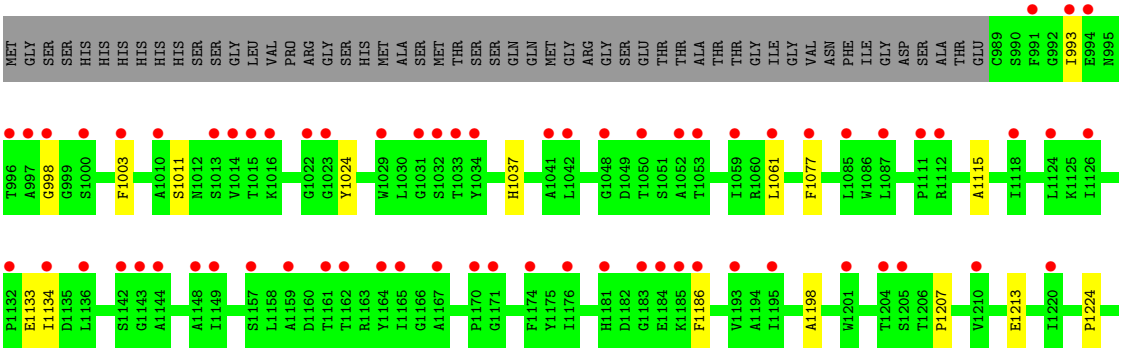
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain I:



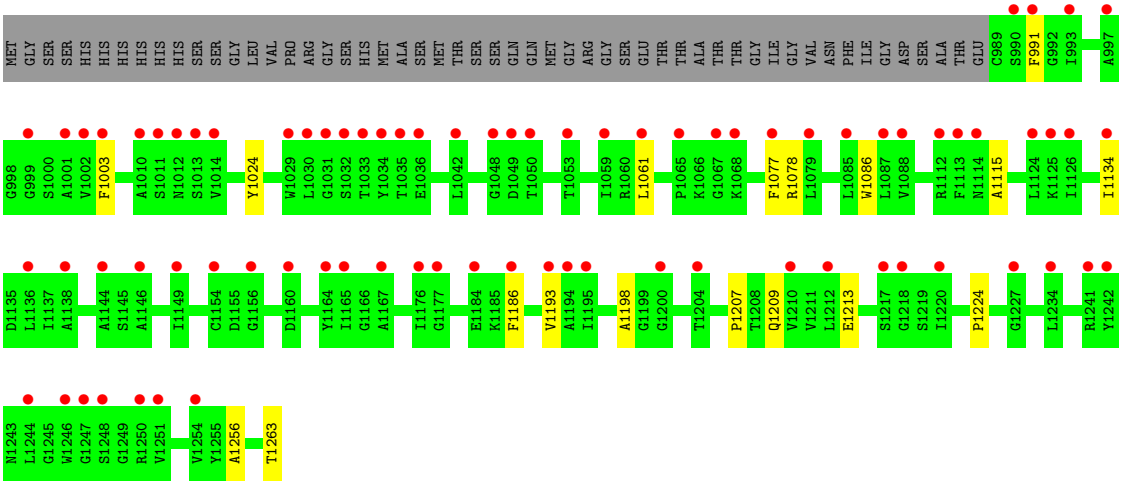
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain J:



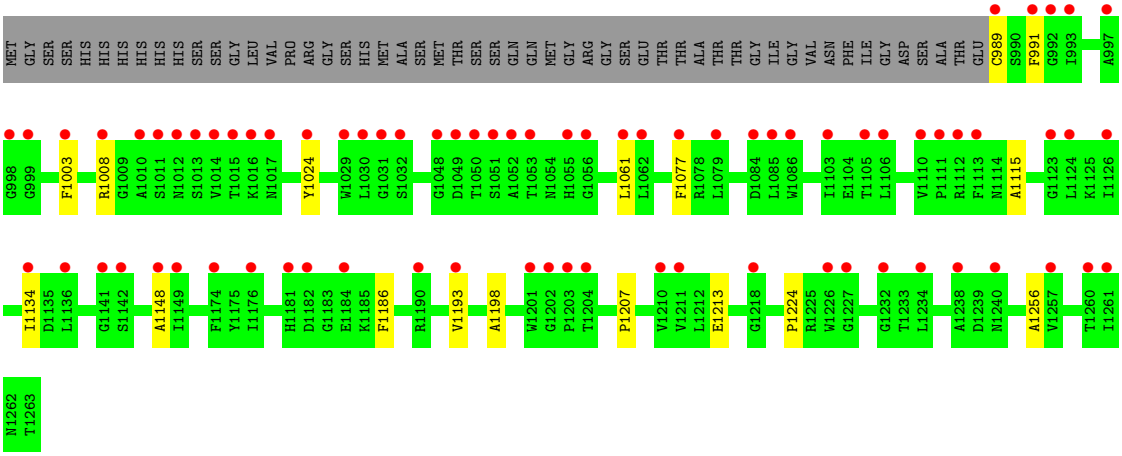
• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain K:



• Molecule 1: L-SHAPED TAIL FIBER PROTEIN PB8

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	2910 reflections (2.02%)	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)	0.29 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.55	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(^{o})	Ideal(^{o})
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

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
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

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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: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
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

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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: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 (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

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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 (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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

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

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

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

All (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
1	L	1103	ILE	6.5
1	L	1012	ASN	6.1
1	F	991	PHE	6.1
1	K	991	PHE	6.1
1	H	1166	GLY	6.0
1	K	1164	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	H	1164	TYR	5.9
1	K	1030	LEU	5.7
1	H	1257	VAL	5.6
1	K	1246	TRP	5.6
1	G	1032	SER	5.5
1	G	1238	ALA	5.5
1	K	1156	GLY	5.4
1	L	1014	VAL	5.4
1	L	1029	TRP	5.4
1	K	1085	LEU	5.3
1	L	1142	SER	5.2
1	K	1033	THR	5.1
1	K	1218	GLY	5.0
1	J	1170	PRO	5.0
1	K	1029	TRP	5.0
1	K	1011	SER	5.0
1	H	1256	ALA	4.9
1	E	991	PHE	4.9
1	K	999	GLY	4.8
1	L	1134	ILE	4.8
1	H	991	PHE	4.8
1	L	1013	SER	4.8
1	G	1010	ALA	4.8
1	L	1110	VAL	4.8
1	I	990	SER	4.8
1	J	1164	TYR	4.6
1	L	1260	THR	4.6
1	K	1247	GLY	4.6
1	L	1257	VAL	4.6
1	H	1156	GLY	4.5
1	J	1176	ILE	4.5
1	G	991	PHE	4.5
1	H	1255	TYR	4.4
1	L	1015	THR	4.3
1	L	992	GLY	4.3
1	A	991	PHE	4.3
1	J	1003	PHE	4.3
1	H	1204	THR	4.3
1	C	991	PHE	4.2
1	G	1097	LEU	4.2
1	H	1199	GLY	4.2
1	L	1226	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	1204	THR	4.2
1	I	1204	THR	4.2
1	L	1032	SER	4.2
1	G	1111	PRO	4.2
1	J	1015	THR	4.1
1	G	1223	LEU	4.1
1	A	1003	PHE	4.1
1	K	1134	ILE	4.1
1	L	1112	ARG	4.1
1	G	1012	ASN	4.1
1	J	1171	GLY	4.1
1	K	1136	LEU	4.1
1	H	1184	GLU	4.0
1	D	997	ALA	4.0
1	K	1034	TYR	4.0
1	G	1077	PHE	4.0
1	H	1112	ARG	4.0
1	G	1262	ASN	4.0
1	J	1010	ALA	3.9
1	G	1164	TYR	3.9
1	G	1011	SER	3.9
1	K	1003	PHE	3.9
1	K	1165	ILE	3.9
1	K	1176	ILE	3.9
1	H	1011	SER	3.9
1	J	1205	SER	3.9
1	K	1032	SER	3.9
1	G	1226	TRP	3.9
1	L	991	PHE	3.9
1	G	1087	LEU	3.9
1	F	1003	PHE	3.8
1	L	1201	TRP	3.8
1	J	1201	TRP	3.8
1	A	1033	THR	3.8
1	L	1184	GLU	3.8
1	H	1176	ILE	3.8
1	K	1220	ILE	3.8
1	L	1111	PRO	3.8
1	J	1052	ALA	3.7
1	J	1181	HIS	3.7
1	G	1113	PHE	3.7
1	J	1161	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	1011	SER	3.7
1	I	1136	LEU	3.7
1	J	1143	GLY	3.7
1	J	1031	GLY	3.7
1	G	1176	ILE	3.6
1	J	1195	ILE	3.6
1	C	1136	LEU	3.6
1	G	1183	GLY	3.6
1	J	1085	LEU	3.6
1	K	1184	GLU	3.6
1	H	1167	ALA	3.6
1	J	1134	ILE	3.5
1	K	1014	VAL	3.5
1	H	1165	ILE	3.5
1	L	1050	THR	3.5
1	K	1204	THR	3.5
1	J	1042	LEU	3.5
1	D	1003	PHE	3.5
1	K	1194	ALA	3.5
1	B	1124	LEU	3.4
1	G	1126	ILE	3.4
1	H	1079	LEU	3.4
1	L	1106	LEU	3.4
1	K	1036	GLU	3.4
1	L	1202	GLY	3.4
1	L	1010	ALA	3.4
1	I	1249	GLY	3.4
1	J	1167	ALA	3.4
1	L	1052	ALA	3.4
1	L	1055	HIS	3.4
1	L	1051	SER	3.4
1	G	1134	ILE	3.4
1	K	1077	PHE	3.4
1	A	1124	LEU	3.3
1	K	1087	LEU	3.3
1	I	991	PHE	3.3
1	B	991	PHE	3.3
1	E	992	GLY	3.3
1	J	1257	VAL	3.3
1	J	1124	LEU	3.3
1	G	992	GLY	3.3
1	G	1037	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	1008	ARG	3.3
1	L	1210	VAL	3.3
1	I	1142	SER	3.2
1	J	993	ILE	3.2
1	A	1031	GLY	3.2
1	E	1124	LEU	3.2
1	G	1030	LEU	3.2
1	K	1149	ILE	3.2
1	D	991	PHE	3.2
1	B	1085	LEU	3.2
1	H	1212	LEU	3.2
1	A	1134	ILE	3.2
1	K	1068	LYS	3.2
1	J	1193	VAL	3.2
1	G	1112	ARG	3.2
1	L	1030	LEU	3.2
1	C	992	GLY	3.2
1	K	1195	ILE	3.2
1	E	989	CYS	3.2
1	G	1053	THR	3.2
1	J	1162	THR	3.2
1	E	1041	ALA	3.2
1	J	1032	SER	3.2
1	G	1029	TRP	3.2
1	K	1079	LEU	3.2
1	J	1126	ILE	3.1
1	H	1010	ALA	3.1
1	L	1136	LEU	3.1
1	J	1142	SER	3.1
1	L	1203	PRO	3.1
1	L	1227	GLY	3.1
1	H	1008	ARG	3.1
1	L	1124	LEU	3.1
1	L	1149	ILE	3.1
1	I	992	GLY	3.1
1	J	997	ALA	3.1
1	H	1003	PHE	3.1
1	I	997	ALA	3.1
1	H	1012	ASN	3.0
1	J	1136	LEU	3.0
1	I	1112	ARG	3.0
1	B	1134	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	989	CYS	3.0
1	J	1185	LYS	3.0
1	H	1171	GLY	3.0
1	J	1220	ILE	3.0
1	L	1003	PHE	3.0
1	H	989	CYS	3.0
1	K	1013	SER	3.0
1	F	1124	LEU	3.0
1	C	1148	ALA	3.0
1	D	1010	ALA	3.0
1	J	1029	TRP	3.0
1	A	992	GLY	3.0
1	G	1220	ILE	3.0
1	E	996	THR	3.0
1	G	1052	ALA	3.0
1	L	997	ALA	3.0
1	D	1126	ILE	3.0
1	D	1199	GLY	3.0
1	K	1242	TYR	2.9
1	K	1244	LEU	2.9
1	G	1239	ASP	2.9
1	B	1053	THR	2.9
1	L	1182	ASP	2.9
1	C	993	ILE	2.9
1	I	1149	ILE	2.9
1	H	1193	VAL	2.9
1	L	1016	LYS	2.9
1	J	1059	ILE	2.9
1	J	1118	ILE	2.9
1	K	1065	PRO	2.9
1	C	1162	THR	2.9
1	J	991	PHE	2.9
1	L	1077	PHE	2.9
1	K	1002	VAL	2.9
1	E	998	GLY	2.9
1	L	1141	GLY	2.9
1	G	1167	ALA	2.9
1	B	1149	ILE	2.9
1	L	1204	THR	2.9
1	L	1126	ILE	2.8
1	K	1254	VAL	2.8
1	J	1159	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1032	SER	2.8
1	A	1126	ILE	2.8
1	G	1263	THR	2.8
1	J	1254	VAL	2.8
1	G	1036	GLU	2.8
1	J	1087	LEU	2.8
1	L	1031	GLY	2.8
1	G	1033	THR	2.8
1	K	1124	LEU	2.8
1	G	1191	GLY	2.8
1	C	1126	ILE	2.8
1	C	1149	ILE	2.8
1	E	1053	THR	2.8
1	I	1250	ARG	2.8
1	I	1248	SER	2.7
1	B	998	GLY	2.7
1	H	1177	GLY	2.7
1	J	1048	GLY	2.7
1	K	1144	ALA	2.7
1	H	1077	PHE	2.7
1	J	1053	THR	2.7
1	G	1061	LEU	2.7
1	D	1134	ILE	2.7
1	H	1149	ILE	2.7
1	L	1232	GLY	2.7
1	G	997	ALA	2.7
1	L	1193	VAL	2.7
1	L	1211	VAL	2.7
1	G	1085	LEU	2.7
1	I	1240	ASN	2.7
1	H	992	GLY	2.7
1	H	1203	PRO	2.7
1	C	1124	LEU	2.7
1	G	1094	HIS	2.7
1	H	996	THR	2.7
1	K	993	ILE	2.7
1	G	1178	ALA	2.7
1	K	997	ALA	2.7
1	J	1165	ILE	2.6
1	L	1176	ILE	2.6
1	C	1031	GLY	2.6
1	G	1009	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	1031	GLY	2.6
1	H	1014	VAL	2.6
1	K	1210	VAL	2.6
1	K	1160	ASP	2.6
1	K	1177	GLY	2.6
1	J	994	GLU	2.6
1	J	996	THR	2.6
1	H	1174	PHE	2.6
1	J	1077	PHE	2.6
1	K	1012	ASN	2.6
1	K	1114	ASN	2.6
1	I	1238	ALA	2.6
1	L	1190	ARG	2.6
1	D	990	SER	2.6
1	I	1244	LEU	2.6
1	J	1034	TYR	2.6
1	B	1126	ILE	2.6
1	K	1217	SER	2.6
1	K	1186	PHE	2.6
1	H	1170	PRO	2.6
1	F	1024	TYR	2.6
1	J	1186	PHE	2.5
1	G	1124	LEU	2.5
1	G	1257	VAL	2.5
1	C	1164	TYR	2.5
1	H	1194	ALA	2.5
1	I	1148	ALA	2.5
1	H	1162	THR	2.5
1	F	1085	LEU	2.5
1	H	1232	GLY	2.5
1	J	1148	ALA	2.5
1	L	1053	THR	2.5
1	D	993	ILE	2.5
1	L	1218	GLY	2.5
1	H	1085	LEU	2.5
1	K	1088	VAL	2.5
1	K	1112	ARG	2.5
1	G	1003	PHE	2.5
1	K	1154	CYS	2.5
1	D	1136	LEU	2.5
1	D	1193	VAL	2.4
1	J	1016	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	1126	ILE	2.4
1	A	1011	SER	2.4
1	E	1085	LEU	2.4
1	G	1013	SER	2.4
1	J	1033	THR	2.4
1	L	1261	ILE	2.4
1	L	1234	LEU	2.4
1	L	1017	ASN	2.4
1	G	1181	HIS	2.4
1	J	1014	VAL	2.4
1	J	1255	TYR	2.4
1	L	1024	TYR	2.4
1	B	1195	ILE	2.4
1	H	1169	GLN	2.4
1	G	1237	MET	2.4
1	J	1210	VAL	2.4
1	K	1126	ILE	2.4
1	F	1087	LEU	2.4
1	H	1042	LEU	2.4
1	F	1112	ARG	2.4
1	G	1225	ARG	2.4
1	J	1023	GLY	2.4
1	L	1123	GLY	2.4
1	I	1253	GLN	2.4
1	G	1195	ILE	2.4
1	J	1149	ILE	2.4
1	G	1241	ARG	2.4
1	A	1085	LEU	2.4
1	H	1238	ALA	2.4
1	I	1260	THR	2.4
1	K	1113	PHE	2.4
1	B	1000	SER	2.4
1	G	1072	ASP	2.3
1	E	993	ILE	2.3
1	G	1177	GLY	2.3
1	I	1255	TYR	2.3
1	K	1125	LYS	2.3
1	H	1160	ASP	2.3
1	F	1023	GLY	2.3
1	E	1134	ILE	2.3
1	J	1132	PRO	2.3
1	L	1079	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	1161	THR	2.3
1	H	1007	THR	2.3
1	H	1161	THR	2.3
1	C	1003	PHE	2.3
1	I	1183	GLY	2.3
1	K	1059	ILE	2.3
1	J	1111	PRO	2.3
1	I	1030	LEU	2.3
1	K	1001	ALA	2.3
1	L	1238	ALA	2.3
1	J	1157	SER	2.3
1	I	1251	VAL	2.3
1	K	1250	ARG	2.3
1	A	993	ILE	2.3
1	C	1134	ILE	2.3
1	L	1085	LEU	2.3
1	J	1013	SER	2.3
1	K	1248	SER	2.3
1	A	1029	TRP	2.3
1	J	1183	GLY	2.3
1	B	1210	VAL	2.3
1	K	1251	VAL	2.3
1	L	1084	ASP	2.3
1	L	993	ILE	2.3
1	B	1087	LEU	2.3
1	H	990	SER	2.3
1	H	1124	LEU	2.3
1	J	1061	LEU	2.3
1	K	1212	LEU	2.3
1	I	1210	VAL	2.3
1	K	1146	ALA	2.3
1	L	1105	THR	2.2
1	L	998	GLY	2.2
1	H	1175	TYR	2.2
1	G	1224	PRO	2.2
1	G	990	SER	2.2
1	G	1190	ARG	2.2
1	I	1144	ALA	2.2
1	C	1166	GLY	2.2
1	J	1050	THR	2.2
1	H	1061	LEU	2.2
1	D	1210	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	1193	VAL	2.2
1	F	1000	SER	2.2
1	C	1059	ILE	2.2
1	K	1053	THR	2.2
1	C	1061	LEU	2.2
1	G	1014	VAL	2.2
1	G	1193	VAL	2.2
1	A	1077	PHE	2.2
1	G	1042	LEU	2.2
1	K	1241	ARG	2.2
1	F	1002	VAL	2.2
1	F	1059	ILE	2.2
1	F	1079	LEU	2.2
1	H	1211	VAL	2.2
1	E	1126	ILE	2.2
1	K	1061	LEU	2.2
1	D	1194	ALA	2.1
1	G	1184	GLU	2.1
1	F	1134	ILE	2.1
1	K	1049	ASP	2.1
1	L	1049	ASP	2.1
1	L	1062	LEU	2.1
1	G	1114	ASN	2.1
1	J	998	GLY	2.1
1	J	1041	ALA	2.1
1	J	1144	ALA	2.1
1	F	1149	ILE	2.1
1	F	1136	LEU	2.1
1	I	1087	LEU	2.1
1	K	1042	LEU	2.1
1	A	998	GLY	2.1
1	L	1240	ASN	2.1
1	G	1110	VAL	2.1
1	K	1035	THR	2.1
1	A	1177	GLY	2.1
1	K	1048	GLY	2.1
1	K	1234	LEU	2.1
1	L	999	GLY	2.1
1	B	1003	PHE	2.1
1	L	1113	PHE	2.1
1	L	1174	PHE	2.1
1	C	1200	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	1067	GLY	2.1
1	K	1227	GLY	2.1
1	L	1056	GLY	2.1
1	L	1061	LEU	2.1
1	A	1112	ARG	2.1
1	D	1178	ALA	2.1
1	K	1138	ALA	2.1
1	I	1257	VAL	2.1
1	E	1025	GLY	2.1
1	H	993	ILE	2.1
1	I	993	ILE	2.1
1	L	1181	HIS	2.1
1	B	996	THR	2.1
1	G	1240	ASN	2.1
1	L	1148	ALA	2.1
1	H	1192	SER	2.1
1	J	1022	GLY	2.1
1	J	1184	GLU	2.0
1	A	1079	LEU	2.0
1	G	1079	LEU	2.0
1	I	1126	ILE	2.0
1	I	1134	ILE	2.0
1	F	1012	ASN	2.0
1	G	1218	GLY	2.0
1	G	1249	GLY	2.0
1	K	1167	ALA	2.0
1	J	1000	SER	2.0
1	K	1200	GLY	2.0
1	L	1048	GLY	2.0
1	C	1002	VAL	2.0
1	H	1239	ASP	2.0
1	E	1024	TYR	2.0
1	J	1174	PHE	2.0
1	D	1124	LEU	2.0
1	A	1067	GLY	2.0
1	F	1022	GLY	2.0
1	K	1050	THR	2.0
1	K	990	SER	2.0
1	G	1060	ARG	2.0
1	J	1241	ARG	2.0
1	D	1002	VAL	2.0
1	L	1086	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	1083	GLY	2.0
1	J	1112	ARG	2.0
1	D	1052	ALA	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 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.