



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 10:01 AM EDT

PDB ID : 5FIR / pdb_00005fir
Title : Crystal structure of *C. elegans* XRN2 in complex with the XRN2-binding domain of PAXT-1
Authors : Richter, H.; Katic, I.; Gut, H.; Grosshans, H.
Deposited on : 2015-10-02
Resolution : 2.84 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

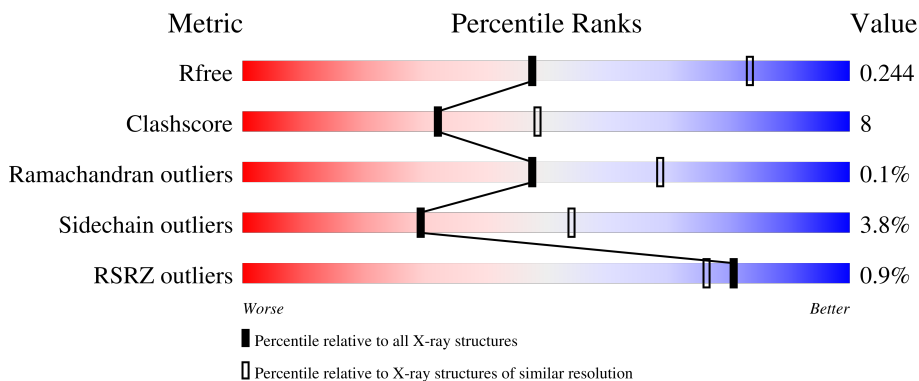
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


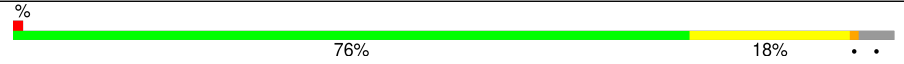
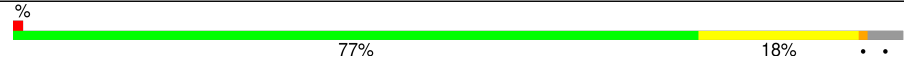
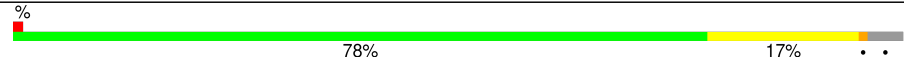
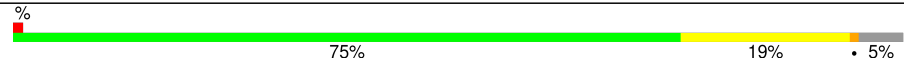
The reported resolution of this entry is 2.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	636	
1	C	636	
1	E	636	
1	G	636	
1	I	636	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	636	
2	B	78	
2	D	78	
2	F	78	
2	H	78	
2	J	78	
2	L	78	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	I	1788	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 33550 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 5'-3' EXORIBONUCLEASE 2 HOMOLOG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	610	4997	3197	855	918	11	16	0	0	0
1	C	608	4993	3195	856	915	11	16	0	1	0
1	E	608	4983	3189	853	914	11	16	0	0	0
1	G	610	5008	3202	858	921	11	16	0	1	0
1	I	606	4968	3180	851	910	11	16	0	0	0
1	K	610	4996	3196	855	918	11	16	0	0	0

There are 912 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	CYS	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	CYS	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	TYR	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	HIS	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	CYS	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	TYR	deletion	UNP Q9U299
A	?	-	CYS	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299
A	?	-	TYR	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	PHE	deletion	UNP Q9U299
A	?	-	VAL	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	HIS	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	ILE	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299
A	?	-	HIS	deletion	UNP Q9U299
A	?	-	HIS	deletion	UNP Q9U299
A	?	-	SER	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	SER	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	SER	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	MET	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	PHE	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	THR	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	ASN	deletion	UNP Q9U299
A	?	-	VAL	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	SER	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	ILE	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	SER	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	ARG	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299
A	?	-	ALA	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLN	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	LEU	deletion	UNP Q9U299
A	?	-	ILE	deletion	UNP Q9U299
A	?	-	LYS	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	ASP	deletion	UNP Q9U299
A	?	-	GLU	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299
A	?	-	PRO	deletion	UNP Q9U299
C	1	MSE	-	initiating methionine	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	CYS	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	CYS	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	TYR	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	HIS	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	CYS	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	TYR	deletion	UNP Q9U299
C	?	-	CYS	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	TYR	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	PHE	deletion	UNP Q9U299
C	?	-	VAL	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	HIS	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	ILE	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	HIS	deletion	UNP Q9U299
C	?	-	HIS	deletion	UNP Q9U299
C	?	-	SER	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	SER	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	SER	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	MET	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	PHE	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	THR	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	ASN	deletion	UNP Q9U299
C	?	-	VAL	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	SER	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	ILE	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	SER	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	ARG	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	ALA	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLN	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	LEU	deletion	UNP Q9U299
C	?	-	ILE	deletion	UNP Q9U299
C	?	-	LYS	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	ASP	deletion	UNP Q9U299
C	?	-	GLU	deletion	UNP Q9U299
C	?	-	GLY	deletion	UNP Q9U299
C	?	-	PRO	deletion	UNP Q9U299
E	1	MSE	-	initiating methionine	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	CYS	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	CYS	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	TYR	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	HIS	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	CYS	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	TYR	deletion	UNP Q9U299
E	?	-	CYS	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	MET	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	MET	deletion	UNP Q9U299
E	?	-	TYR	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	PHE	deletion	UNP Q9U299
E	?	-	VAL	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	HIS	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	ILE	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	MET	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	MET	deletion	UNP Q9U299
E	?	-	HIS	deletion	UNP Q9U299
E	?	-	HIS	deletion	UNP Q9U299
E	?	-	SER	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	SER	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	MET	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	SER	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	MET	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	PHE	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	THR	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	ASN	deletion	UNP Q9U299
E	?	-	VAL	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	SER	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	ILE	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	SER	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	ARG	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	ALA	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLN	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	LEU	deletion	UNP Q9U299
E	?	-	ILE	deletion	UNP Q9U299
E	?	-	LYS	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	ASP	deletion	UNP Q9U299
E	?	-	GLU	deletion	UNP Q9U299
E	?	-	GLY	deletion	UNP Q9U299
E	?	-	PRO	deletion	UNP Q9U299
G	1	MSE	-	initiating methionine	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	CYS	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	CYS	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	TYR	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	HIS	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	CYS	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	TYR	deletion	UNP Q9U299
G	?	-	CYS	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	TYR	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	PHE	deletion	UNP Q9U299
G	?	-	VAL	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	HIS	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	ILE	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	HIS	deletion	UNP Q9U299
G	?	-	HIS	deletion	UNP Q9U299
G	?	-	SER	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	SER	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	SER	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	MET	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	PHE	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	THR	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	ASN	deletion	UNP Q9U299
G	?	-	VAL	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	SER	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299
G	?	-	ILE	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	SER	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	ARG	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	ALA	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLN	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	LEU	deletion	UNP Q9U299
G	?	-	ILE	deletion	UNP Q9U299
G	?	-	LYS	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	ASP	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	GLU	deletion	UNP Q9U299
G	?	-	GLY	deletion	UNP Q9U299
G	?	-	PRO	deletion	UNP Q9U299
I	1	MSE	-	initiating methionine	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	CYS	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	CYS	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	TYR	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	HIS	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	CYS	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	TYR	deletion	UNP Q9U299
I	?	-	CYS	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	MET	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	MET	deletion	UNP Q9U299
I	?	-	TYR	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	PHE	deletion	UNP Q9U299
I	?	-	VAL	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	HIS	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	ILE	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	MET	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	MET	deletion	UNP Q9U299
I	?	-	HIS	deletion	UNP Q9U299
I	?	-	HIS	deletion	UNP Q9U299
I	?	-	SER	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	SER	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	MET	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	SER	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	MET	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	PHE	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	THR	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	ASN	deletion	UNP Q9U299
I	?	-	VAL	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	SER	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	ILE	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	SER	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	ARG	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	ALA	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLN	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	LEU	deletion	UNP Q9U299
I	?	-	ILE	deletion	UNP Q9U299
I	?	-	LYS	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	ASP	deletion	UNP Q9U299
I	?	-	GLU	deletion	UNP Q9U299
I	?	-	GLY	deletion	UNP Q9U299
I	?	-	PRO	deletion	UNP Q9U299
K	1	MSE	-	initiating methionine	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	CYS	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	CYS	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	TYR	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	HIS	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	CYS	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	TYR	deletion	UNP Q9U299
K	?	-	CYS	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	TYR	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	PHE	deletion	UNP Q9U299
K	?	-	VAL	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	HIS	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	ILE	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	HIS	deletion	UNP Q9U299
K	?	-	HIS	deletion	UNP Q9U299
K	?	-	SER	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	SER	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	SER	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	GLN	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	MET	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	PHE	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	THR	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	ASN	deletion	UNP Q9U299
K	?	-	VAL	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	SER	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	ILE	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	SER	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	ARG	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	ALA	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLN	deletion	UNP Q9U299

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	LEU	deletion	UNP Q9U299
K	?	-	ILE	deletion	UNP Q9U299
K	?	-	LYS	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	ASP	deletion	UNP Q9U299
K	?	-	GLU	deletion	UNP Q9U299
K	?	-	GLY	deletion	UNP Q9U299
K	?	-	PRO	deletion	UNP Q9U299

- Molecule 2 is a protein called PAXT-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	73	Total 589	C 376	N 98	O 110	S 2	Se 3	0	0	0
2	D	71	Total 573	C 367	N 93	O 108	S 2	Se 3	0	0	0
2	F	72	Total 584	C 373	N 97	O 109	S 2	Se 3	0	0	0
2	H	69	Total 564	C 362	N 91	O 106	S 2	Se 3	0	0	0
2	J	67	Total 543	C 348	N 88	O 102	S 2	Se 3	0	0	0
2	L	69	Total 564	C 362	N 91	O 106	S 2	Se 3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

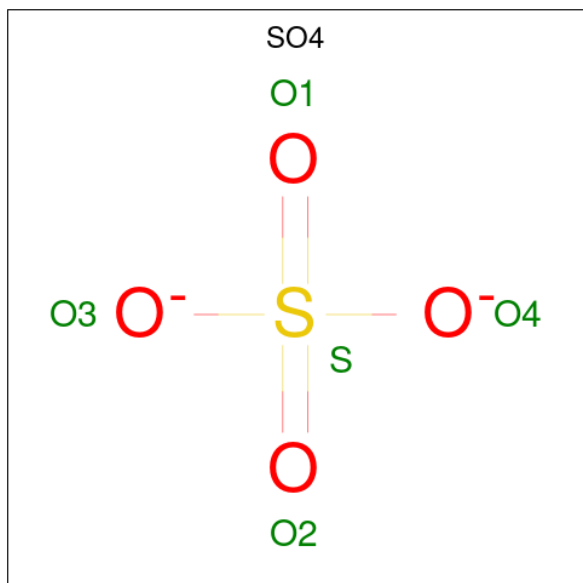
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q21738
B	-1	GLY	-	expression tag	UNP Q21738
B	0	GLY	-	expression tag	UNP Q21738
B	1	ARG	-	expression tag	UNP Q21738
D	-2	GLY	-	expression tag	UNP Q21738
D	-1	GLY	-	expression tag	UNP Q21738
D	0	GLY	-	expression tag	UNP Q21738
D	1	ARG	-	expression tag	UNP Q21738
F	-2	GLY	-	expression tag	UNP Q21738

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP Q21738
F	0	GLY	-	expression tag	UNP Q21738
F	1	ARG	-	expression tag	UNP Q21738
H	-2	GLY	-	expression tag	UNP Q21738
H	-1	GLY	-	expression tag	UNP Q21738
H	0	GLY	-	expression tag	UNP Q21738
H	1	ARG	-	expression tag	UNP Q21738
J	-2	GLY	-	expression tag	UNP Q21738
J	-1	GLY	-	expression tag	UNP Q21738
J	0	GLY	-	expression tag	UNP Q21738
J	1	ARG	-	expression tag	UNP Q21738
L	-2	GLY	-	expression tag	UNP Q21738
L	-1	GLY	-	expression tag	UNP Q21738
L	0	GLY	-	expression tag	UNP Q21738
L	1	ARG	-	expression tag	UNP Q21738

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

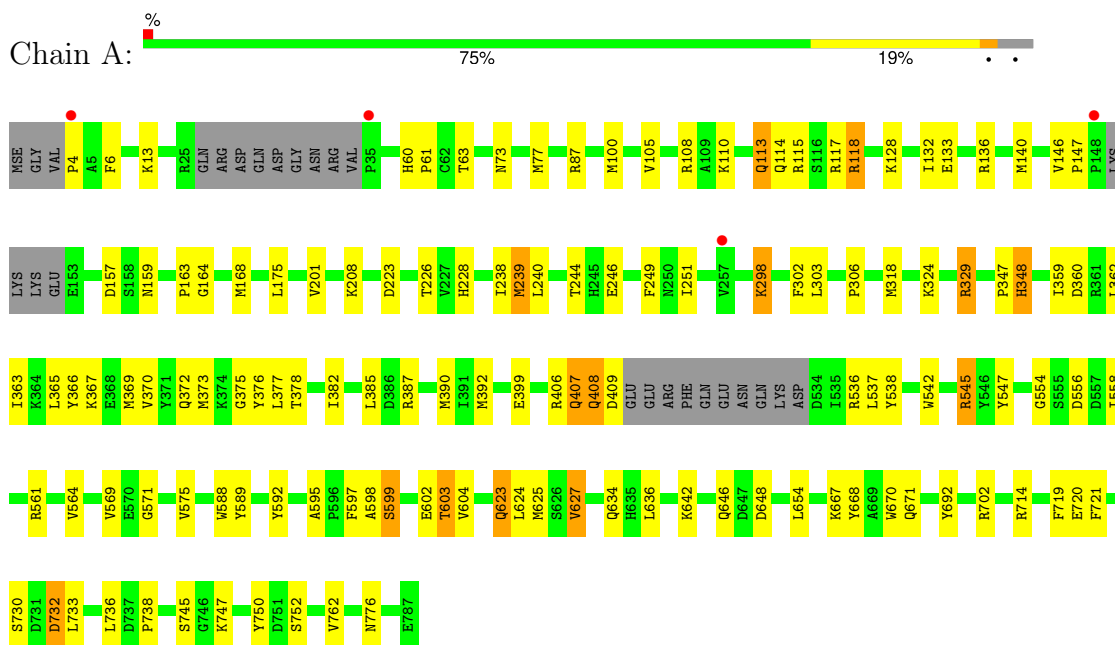
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	2	Total	O	0	0
			2	2		
4	C	8	Total	O	0	0
			8	8		
4	E	14	Total	O	0	0
			14	14		
4	F	1	Total	O	0	0
			1	1		
4	G	5	Total	O	0	0
			5	5		
4	I	7	Total	O	0	0
			7	7		
4	K	7	Total	O	0	0
			7	7		

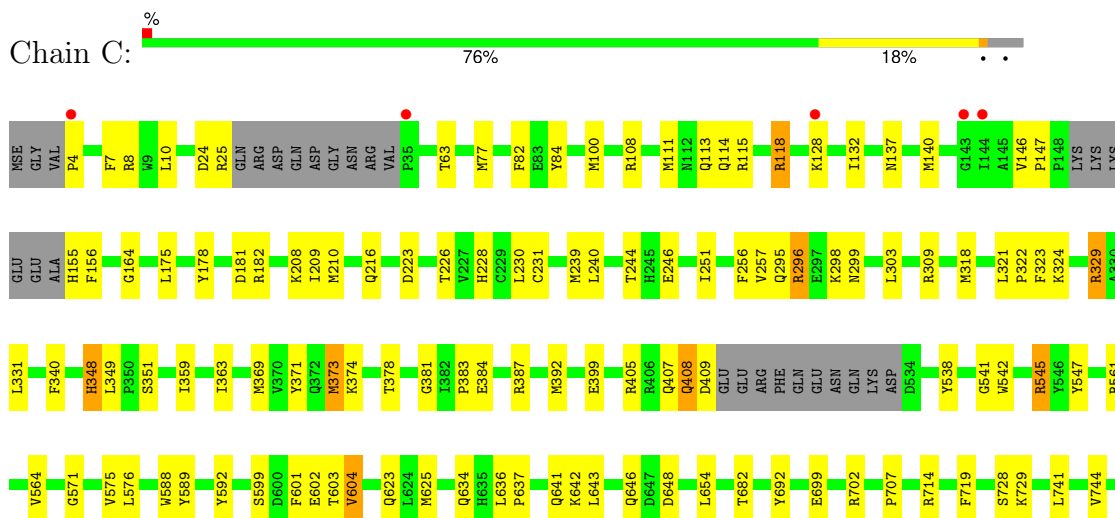
3 Residue-property plots [i](#)

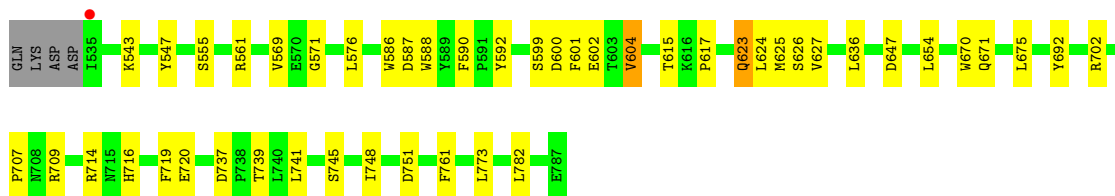
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

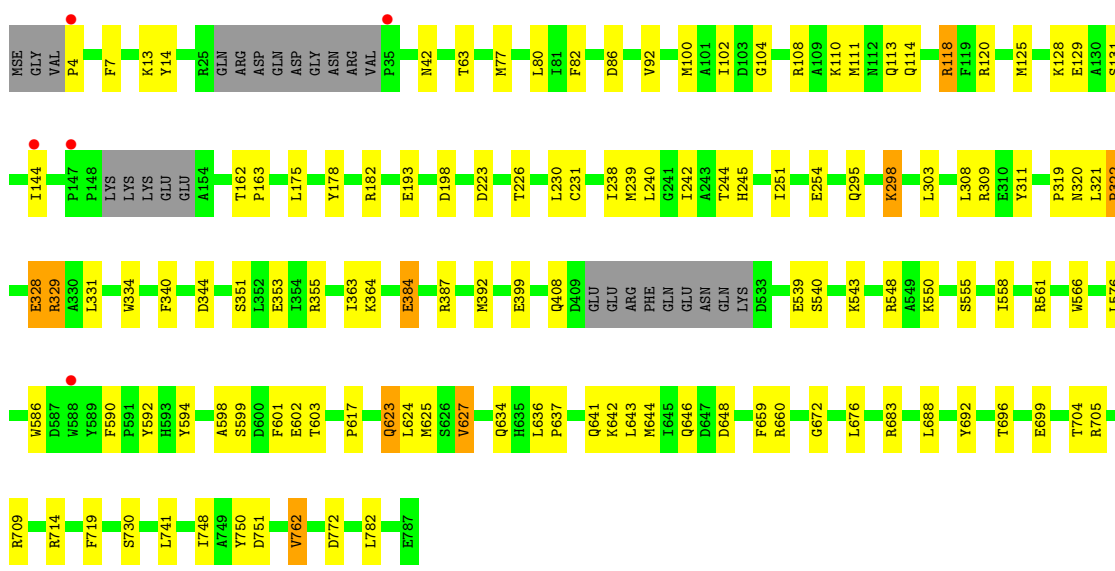
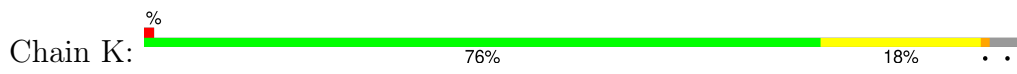


• Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

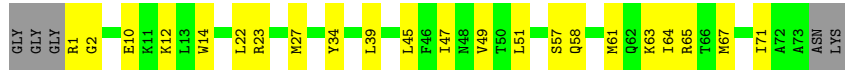




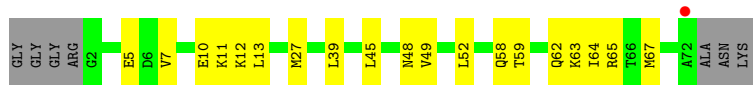
● Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG



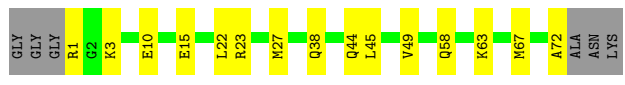
● Molecule 2: PAXT-1



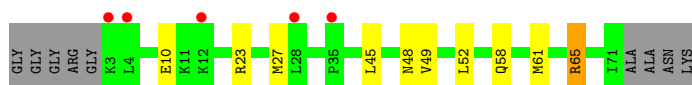
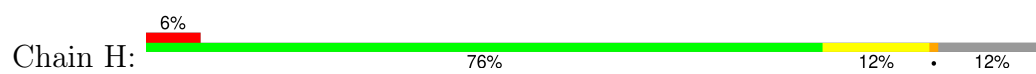
● Molecule 2: PAXT-1



● Molecule 2: PAXT-1



● Molecule 2: PAXT-1



- Molecule 2: PAXT-1



- Molecule 2: PAXT-1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.21Å 200.77Å 202.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.84 49.39 – 2.84	Depositor EDS
% Data completeness (in resolution range)	94.6 (49.39-2.84) 94.5 (49.39-2.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.238 0.196 , 0.244	Depositor DCC
R_{free} test set	3903 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	72.5	Xtrriage
Anisotropy	0.397	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.015 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33550	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	0/5118	0.67	0/6916
1	C	0.52	0/5115	0.71	1/6912 (0.0%)
1	E	0.53	1/5104 (0.0%)	0.70	0/6897
1	G	0.54	1/5129 (0.0%)	0.70	1/6930 (0.0%)
1	I	0.47	0/5088	0.67	0/6874
1	K	0.46	0/5117	0.66	0/6915
2	B	0.47	0/596	0.71	0/796
2	D	0.47	0/580	0.70	0/775
2	F	0.38	0/591	0.61	0/789
2	H	0.31	0/571	0.56	0/763
2	J	0.35	0/550	0.56	0/736
2	L	0.32	0/571	0.58	0/763
All	All	0.49	2/34130 (0.0%)	0.68	2/46066 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	218	GLY	C-N	-7.33	1.18	1.33
1	E	218	GLY	C-N	-5.54	1.22	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	76	GLU	CB-CG-CD	-6.61	101.37	112.60
1	C	208	LYS	CB-CG-CD	-5.39	98.89	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	539	GLU	Peptide

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	4997	0	4837	96	0
1	C	4993	0	4832	80	0
1	E	4983	0	4826	70	0
1	G	5008	0	4840	70	0
1	I	4968	0	4815	90	0
1	K	4996	0	4835	80	0
2	B	589	0	592	18	0
2	D	573	0	571	11	0
2	F	584	0	587	9	0
2	H	564	0	563	5	0
2	J	543	0	538	9	0
2	L	564	0	563	11	0
3	A	40	0	0	2	0
3	C	15	0	0	0	0
3	E	25	0	0	1	0
3	G	20	0	0	3	0
3	I	15	0	0	2	0
3	K	20	0	0	0	0
4	A	9	0	0	0	0
4	B	2	0	0	1	0
4	C	8	0	0	0	0
4	E	14	0	0	0	0
4	F	1	0	0	1	0
4	G	5	0	0	0	0
4	I	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	7	0	0	0	0
All	All	33550	0	32399	528	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 8.

The worst 5 of 528 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:K:543:LYS:NZ	1:K:599:SER:HB2	1.80	0.96
1:A:730:SER:OG	1:A:732:ASP:OD1	1.86	0.94
2:L:21:GLU:OE2	2:L:24:LYS:NZ	2.00	0.94
1:K:543:LYS:HZ1	1:K:599:SER:HB2	1.27	0.92
2:J:6:ASP:OD2	2:J:31:TYR:OH	1.85	0.92

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	602/636 (95%)	583 (97%)	18 (3%)	1 (0%)	43	62
1	C	601/636 (94%)	584 (97%)	17 (3%)	0	100	100
1	E	600/636 (94%)	583 (97%)	15 (2%)	2 (0%)	36	55
1	G	603/636 (95%)	586 (97%)	16 (3%)	1 (0%)	43	62
1	I	598/636 (94%)	580 (97%)	17 (3%)	1 (0%)	43	62
1	K	602/636 (95%)	584 (97%)	17 (3%)	1 (0%)	43	62
2	B	71/78 (91%)	68 (96%)	3 (4%)	0	100	100
2	D	69/78 (88%)	64 (93%)	5 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	70/78 (90%)	67 (96%)	3 (4%)	0	100	100
2	H	67/78 (86%)	64 (96%)	3 (4%)	0	100	100
2	J	65/78 (83%)	62 (95%)	3 (5%)	0	100	100
2	L	67/78 (86%)	63 (94%)	4 (6%)	0	100	100
All	All	4015/4284 (94%)	3888 (97%)	121 (3%)	6 (0%)	48	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	555	SER
1	E	555	SER
1	I	555	SER
1	E	380	ASP
1	A	324	LYS

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	538/545 (99%)	511 (95%)	27 (5%)	22	44
1	C	538/545 (99%)	513 (95%)	25 (5%)	24	48
1	E	537/545 (98%)	519 (97%)	18 (3%)	32	57
1	G	539/545 (99%)	522 (97%)	17 (3%)	34	59
1	I	535/545 (98%)	518 (97%)	17 (3%)	34	59
1	K	538/545 (99%)	518 (96%)	20 (4%)	30	55
2	B	62/61 (102%)	61 (98%)	1 (2%)	55	76
2	D	61/61 (100%)	58 (95%)	3 (5%)	22	45
2	F	62/61 (102%)	59 (95%)	3 (5%)	23	46
2	H	61/61 (100%)	59 (97%)	2 (3%)	33	58
2	J	58/61 (95%)	56 (97%)	2 (3%)	32	57
2	L	61/61 (100%)	59 (97%)	2 (3%)	33	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3590/3636 (99%)	3453 (96%)	137 (4%)	29 54

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	80	LEU
1	K	320	ASN
1	K	648	ASP
1	C	634	GLN
1	C	623	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	30	HIS
1	G	771	GLN
1	K	320	ASN
2	F	40	GLN
1	G	299	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	1789	-	4,4,4	0.28	0	6,6,6	0.44	0
3	SO4	A	1794	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	A	1795	-	4,4,4	0.29	0	6,6,6	0.26	0
3	SO4	G	1788	-	4,4,4	0.34	0	6,6,6	0.34	0
3	SO4	I	1789	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	C	1788	-	4,4,4	0.25	0	6,6,6	0.34	0
3	SO4	A	1790	-	4,4,4	0.28	0	6,6,6	0.21	0
3	SO4	E	1788	-	4,4,4	0.24	0	6,6,6	0.43	0
3	SO4	A	1791	-	4,4,4	0.24	0	6,6,6	0.33	0
3	SO4	I	1788	-	4,4,4	0.36	0	6,6,6	0.25	0
3	SO4	K	1788	-	4,4,4	0.19	0	6,6,6	0.43	0
3	SO4	E	1791	-	4,4,4	0.24	0	6,6,6	0.33	0
3	SO4	C	1790	-	4,4,4	0.26	0	6,6,6	0.16	0
3	SO4	G	1791	-	4,4,4	0.33	0	6,6,6	0.42	0
3	SO4	G	1790	-	4,4,4	0.32	0	6,6,6	0.31	0
3	SO4	A	1788	-	4,4,4	0.21	0	6,6,6	0.55	0
3	SO4	E	1790	-	4,4,4	0.28	0	6,6,6	0.37	0
3	SO4	K	1791	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	K	1790	-	4,4,4	0.28	0	6,6,6	0.28	0
3	SO4	K	1789	-	4,4,4	0.26	0	6,6,6	0.41	0
3	SO4	I	1790	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	A	1789	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	G	1789	-	4,4,4	0.26	0	6,6,6	0.17	0
3	SO4	A	1792	-	4,4,4	0.24	0	6,6,6	0.26	0
3	SO4	A	1793	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	E	1789	-	4,4,4	0.33	0	6,6,6	0.38	0
3	SO4	E	1792	-	4,4,4	0.23	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1788	SO4	1	0
3	E	1788	SO4	1	0
3	I	1788	SO4	2	0
3	G	1791	SO4	1	0
3	G	1790	SO4	1	0
3	A	1788	SO4	1	0
3	A	1789	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	218:GLY	C	219:ASN	N	1.18

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/636 (93%)	-0.35	4 (0%) 84 80	44, 75, 142, 177	0
1	C	592/636 (93%)	-0.48	5 (0%) 82 78	28, 66, 119, 197	1 (0%)
1	E	592/636 (93%)	-0.51	4 (0%) 84 80	39, 67, 124, 154	0
1	G	594/636 (93%)	-0.44	4 (0%) 84 80	33, 71, 126, 170	1 (0%)
1	I	590/636 (92%)	-0.21	4 (0%) 84 80	40, 91, 152, 189	0
1	K	594/636 (93%)	-0.31	5 (0%) 82 78	40, 82, 143, 179	0
2	B	70/78 (89%)	-0.09	0 100 100	69, 89, 117, 134	0
2	D	68/78 (87%)	-0.09	1 (1%) 72 65	69, 98, 144, 182	0
2	F	69/78 (88%)	-0.11	0 100 100	80, 103, 130, 149	0
2	H	66/78 (84%)	0.59	5 (7%) 20 15	107, 151, 187, 203	0
2	J	64/78 (82%)	0.43	2 (3%) 51 42	114, 147, 185, 211	0
2	L	66/78 (84%)	0.48	1 (1%) 72 65	119, 154, 185, 197	0
All	All	3959/4284 (92%)	-0.32	35 (0%) 81 76	28, 77, 148, 211	2 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	PRO	5.1
1	I	535	ILE	4.7
1	G	144	ILE	4.1
1	G	4	PRO	4.0
1	C	143	GLY	3.8

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	1789	5/5	0.64	0.10	141,146,147,147	0
3	SO4	A	1794	5/5	0.67	0.09	155,157,158,159	0
3	SO4	A	1795	5/5	0.69	0.15	119,131,132,135	0
3	SO4	G	1790	5/5	0.69	0.10	132,133,135,136	0
3	SO4	K	1791	5/5	0.76	0.10	138,139,139,140	0
3	SO4	C	1789	5/5	0.78	0.11	106,121,126,134	0
3	SO4	E	1792	5/5	0.78	0.09	141,144,144,148	0
3	SO4	A	1791	5/5	0.78	0.08	146,146,150,151	0
3	SO4	I	1789	5/5	0.78	0.07	156,156,158,159	0
3	SO4	A	1792	5/5	0.78	0.08	143,147,147,149	0
3	SO4	K	1789	5/5	0.79	0.13	131,148,151,151	0
3	SO4	K	1790	5/5	0.81	0.08	108,119,122,125	0
3	SO4	E	1790	5/5	0.81	0.09	126,134,136,144	0
3	SO4	E	1789	5/5	0.82	0.08	117,120,126,127	0
3	SO4	I	1790	5/5	0.85	0.11	140,143,144,144	0
3	SO4	A	1793	5/5	0.85	0.09	125,125,126,133	0
3	SO4	E	1791	5/5	0.86	0.09	107,119,122,122	0
3	SO4	G	1791	5/5	0.87	0.10	114,125,128,130	0
3	SO4	C	1790	5/5	0.87	0.13	153,154,155,156	0
3	SO4	A	1790	5/5	0.91	0.11	112,116,120,122	0
3	SO4	G	1789	5/5	0.92	0.12	110,115,118,120	0
3	SO4	K	1788	5/5	0.95	0.09	78,80,84,96	0
3	SO4	I	1788	5/5	0.96	0.07	83,85,88,91	0
3	SO4	C	1788	5/5	0.97	0.05	55,68,79,81	0
3	SO4	G	1788	5/5	0.97	0.06	65,66,77,83	0
3	SO4	A	1788	5/5	0.97	0.05	71,72,74,76	0
3	SO4	E	1788	5/5	0.99	0.05	61,67,73,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.