



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:13 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

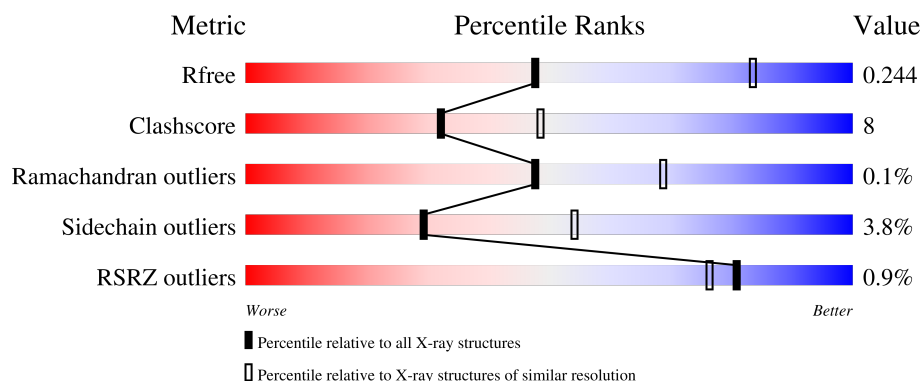
1 Overall quality at a glance

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	 75% 19% • •
1	C	636	 76% 18% • •
1	E	636	 77% 18% • •
1	G	636	 78% 17% • •
1	I	636	 75% 19% • 5%

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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

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

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

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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	?	-	ARG	deletion	UNP Q9U299
A	?	-	GLY	deletion	UNP Q9U299

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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	?	-	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

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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	?	-	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

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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

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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

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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

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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	?	-	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

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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

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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

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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

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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

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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

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

There are 24 discrepancies between the modelled and reference sequences:

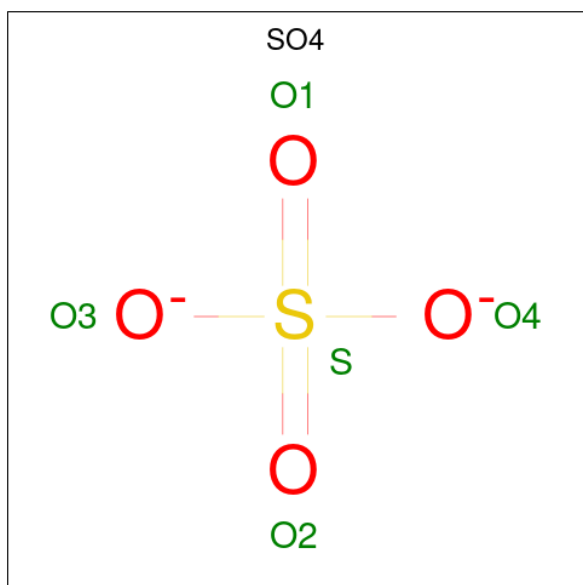
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q21738
B	-1	GLY	-	expression tag	UNP Q21738
B	0	GLY	-	expression tag	UNP Q21738
B	1	ARG	-	expression tag	UNP Q21738
D	-2	GLY	-	expression tag	UNP Q21738
D	-1	GLY	-	expression tag	UNP Q21738
D	0	GLY	-	expression tag	UNP Q21738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

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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	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		

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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	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		

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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		

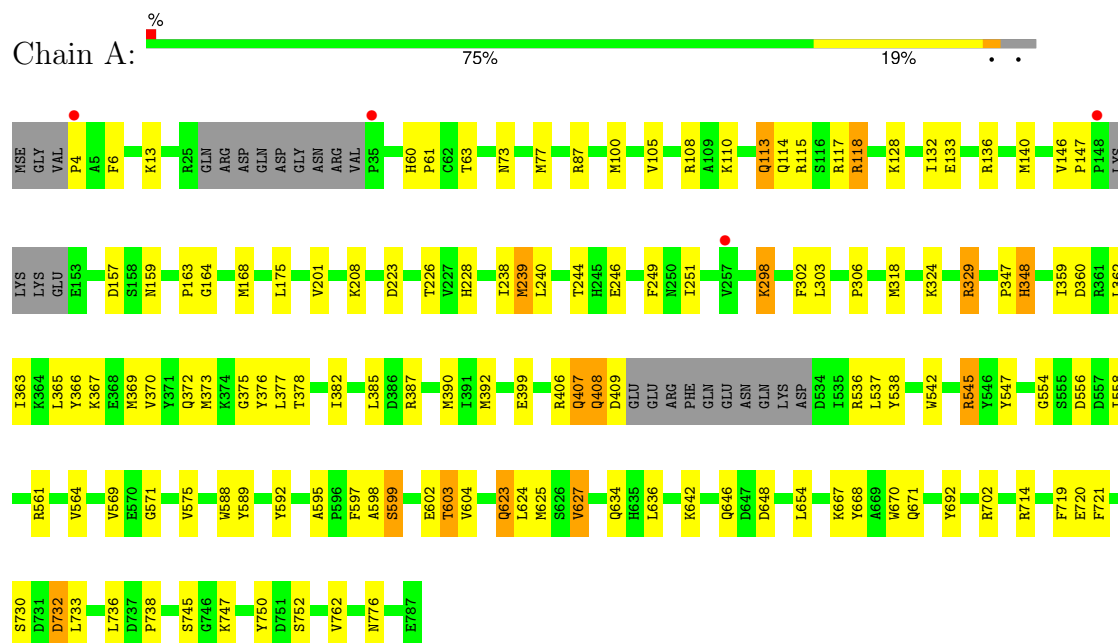
- Molecule 4 is water.

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		

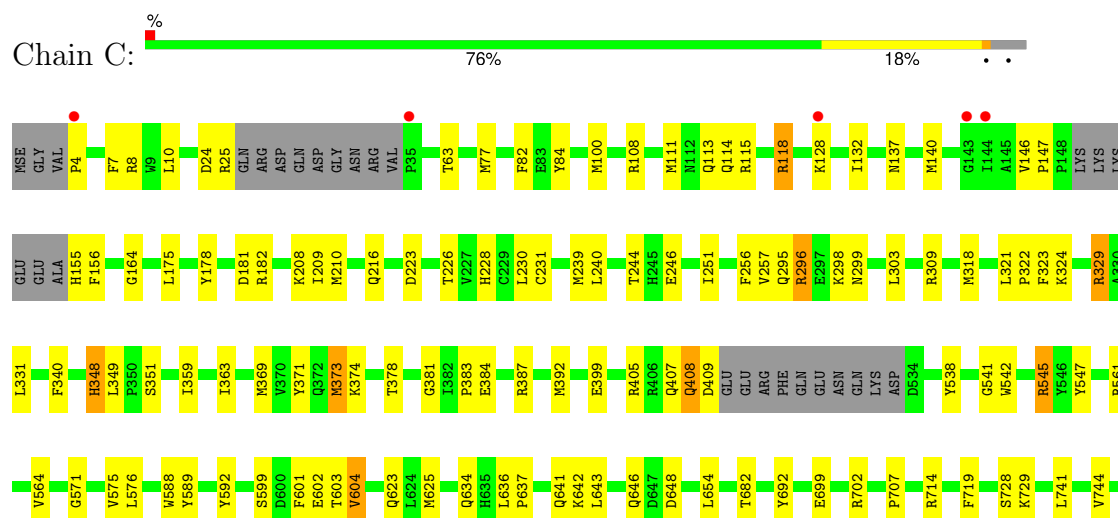
3 Residue-property plots

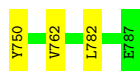
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

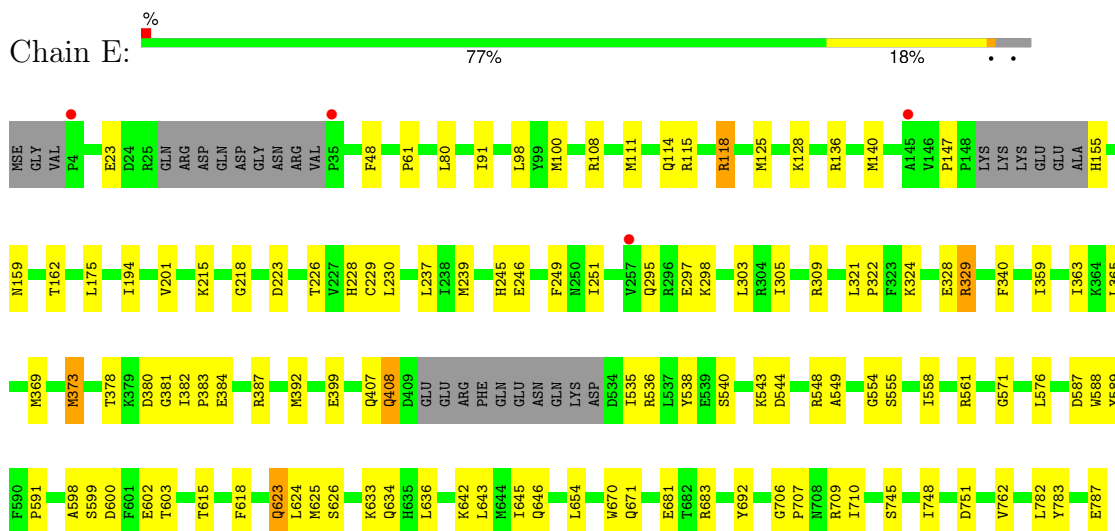


• Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

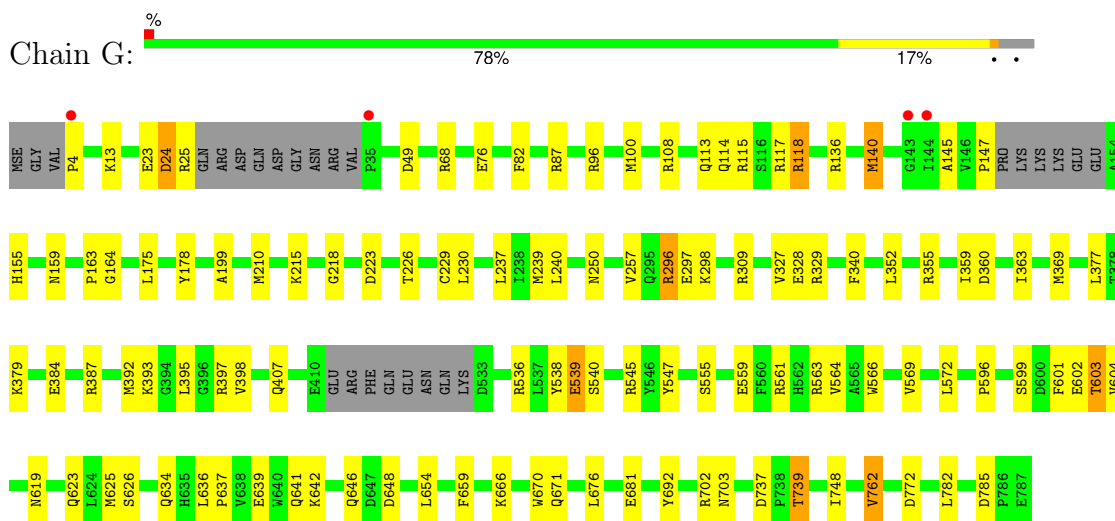




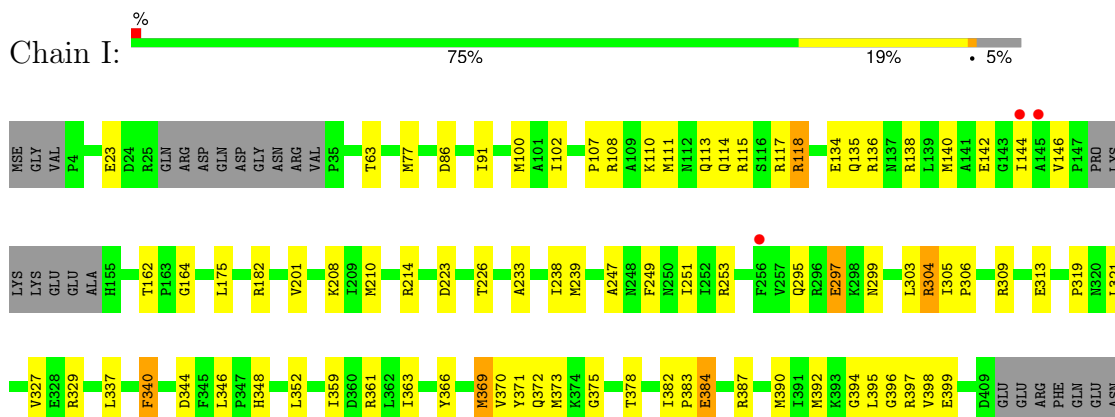
● Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

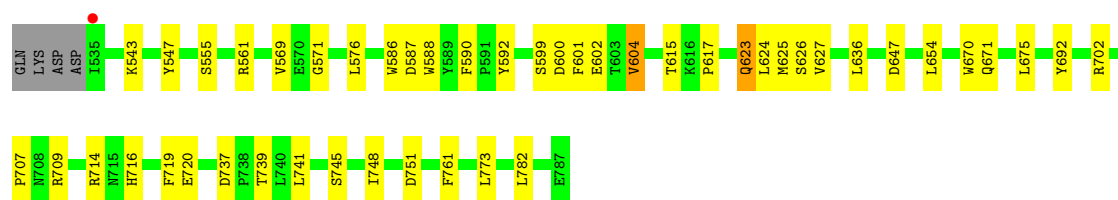


- Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

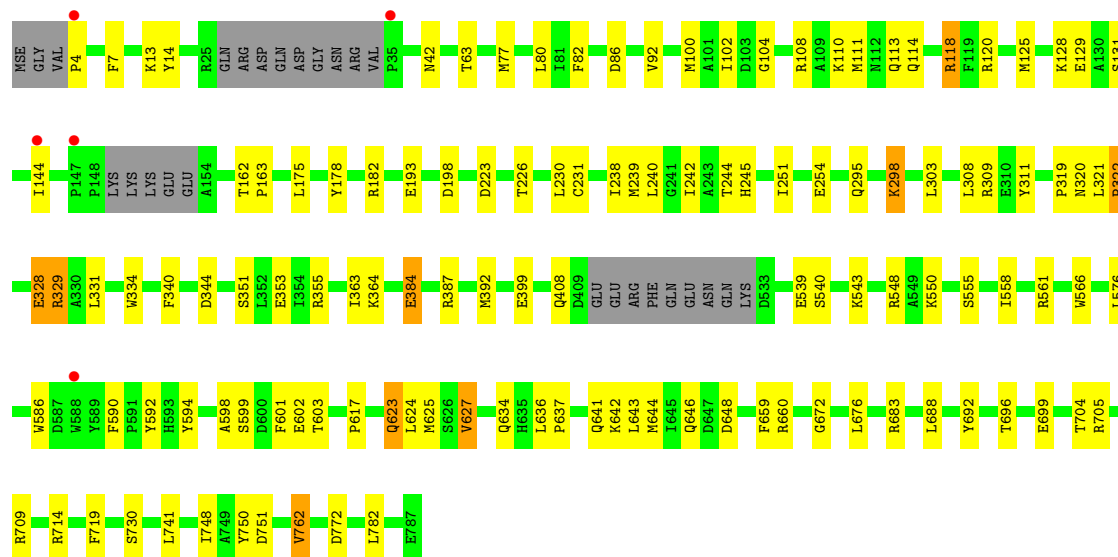
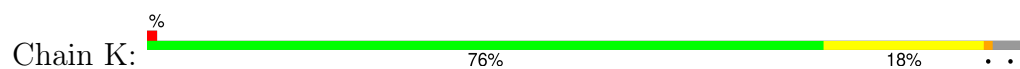


● Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG





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



• Molecule 2: PAXT-1



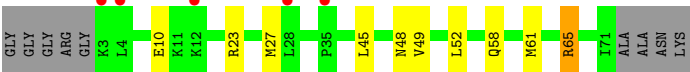
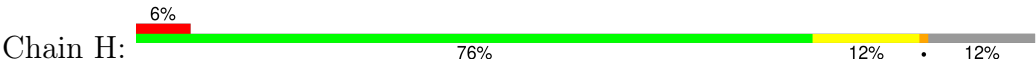
• Molecule 2: PAXT-1



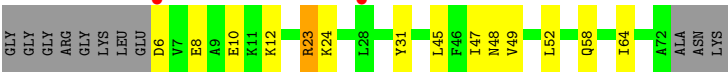
• Molecule 2: PAXT-1



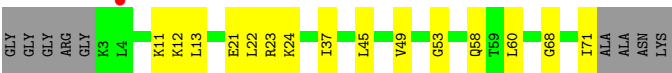
• Molecule 2: PAXT-1



• Molecule 2: PAXT-1



• Molecule 2: PAXT-1



4 Data and refinement statistics

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)	Xtriage
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	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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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.

All (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
1:A:87:ARG:HH12	1:A:298:LYS:HE3	1.37	0.90
1:A:376:TYR:O	1:A:387:ARG:NH1	2.06	0.88
1:K:709:ARG:NH1	1:K:751:ASP:OD2	2.08	0.87
1:I:100:MSE:HE1	1:I:175:LEU:HD22	1.57	0.86
1:A:136:ARG:NH1	1:A:147:PRO:O	2.11	0.83
1:G:296:ARG:HD2	1:G:297:GLU:H	1.43	0.83
1:C:545:ARG:HH11	1:C:545:ARG:HG3	1.44	0.82
1:K:566:TRP:HE1	1:K:603:THR:HG23	1.45	0.81
1:K:660:ARG:HD3	2:L:53:GLY:HA3	1.63	0.80
1:A:4:PRO:HD3	1:I:140:MSE:HB3	1.63	0.80
1:A:732:ASP:OD1	1:A:732:ASP:N	2.13	0.80
1:C:369:MSE:HG2	1:C:373:MSE:HG3	1.63	0.79
1:A:545:ARG:HG3	1:A:545:ARG:HH11	1.46	0.79
1:I:304:ARG:HH11	1:I:304:ARG:HG2	1.48	0.79
1:I:113:GLN:HE22	1:I:117:ARG:NH1	1.81	0.78
1:E:108:ARG:HA	1:E:111:MSE:HG3	1.67	0.76
1:E:100:MSE:HE1	1:E:175:LEU:HD22	1.67	0.76
2:J:8:GLU:OE1	2:J:24:LYS:NZ	2.17	0.76
1:G:100:MSE:HE1	1:G:175:LEU:HD22	1.65	0.76
1:K:118:ARG:NH1	1:K:162:THR:OG1	2.18	0.76
2:D:12:LYS:HB3	2:D:13:LEU:HA	1.69	0.75
1:A:100:MSE:HE1	1:A:175:LEU:HD22	1.69	0.74
1:E:543:LYS:NZ	1:E:599:SER:OG	2.21	0.73
1:E:115:ARG:NH2	1:E:654:LEU:O	2.21	0.73
1:A:625:MSE:SE	1:A:636:LEU:HD22	2.39	0.73
1:E:136:ARG:NH1	1:E:147:PRO:O	2.21	0.72
1:K:223:ASP:O	1:K:226:THR:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:HG3	1:A:545:ARG:NH1	2.03	0.72
1:A:569:VAL:HG11	1:A:604:VAL:HG11	1.72	0.71
1:C:100:MSE:HE1	1:C:175:LEU:HD22	1.73	0.70
1:I:625:MSE:SE	1:I:636:LEU:HD22	2.42	0.70
1:G:68:ARG:HH22	1:G:298:LYS:HE3	1.58	0.69
1:I:361:ARG:NH1	1:I:398:VAL:HG21	2.08	0.69
1:C:63:THR:HG22	1:C:77:MSE:HB3	1.75	0.69
1:G:24:ASP:N	1:G:24:ASP:OD1	2.27	0.68
1:I:394:GLY:HA2	1:I:397:ARG:HD3	1.74	0.68
1:C:545:ARG:HG3	1:C:545:ARG:NH1	2.08	0.68
1:E:223:ASP:O	1:E:226:THR:HG23	1.93	0.68
1:I:118:ARG:NH1	1:I:162:THR:OG1	2.27	0.68
1:C:601:PHE:O	1:C:604:VAL:HB	1.94	0.68
1:K:329:ARG:HH11	1:K:329:ARG:CG	2.06	0.68
1:I:113:GLN:HE22	1:I:117:ARG:HH12	1.41	0.67
1:I:543:LYS:NZ	1:I:600:ASP:OD1	2.27	0.67
2:D:11:LYS:HE2	2:D:12:LYS:HG3	1.77	0.66
1:I:369:MSE:HE2	1:I:390:MSE:HE2	1.78	0.66
1:A:407:GLN:HE21	1:A:538:TYR:HB2	1.62	0.65
1:E:23:GLU:HG3	1:E:91:ILE:HG12	1.78	0.65
2:B:1:ARG:HG2	2:B:2:GLY:H	1.60	0.64
1:A:115:ARG:NH2	1:A:654:LEU:O	2.31	0.63
1:E:558:ILE:HG22	1:E:561:ARG:HD2	1.80	0.63
1:C:4:PRO:HD3	1:G:140:MSE:HE3	1.80	0.63
1:E:407:GLN:O	1:E:407:GLN:HG3	1.97	0.63
1:C:140:MSE:HE3	1:G:4:PRO:HD3	1.80	0.62
1:K:245:HIS:CD2	1:K:328:GLU:OE1	2.53	0.62
1:E:359:ILE:O	1:E:363:ILE:HG12	2.00	0.62
1:A:223:ASP:HB3	1:A:226:THR:HG23	1.82	0.62
1:C:155:HIS:CD2	1:C:156:PHE:H	2.17	0.62
1:K:245:HIS:CG	1:K:328:GLU:OE1	2.53	0.61
1:A:545:ARG:HH11	1:A:545:ARG:CG	2.14	0.61
1:C:714:ARG:HA	1:C:719:PHE:CD1	2.35	0.61
1:I:223:ASP:O	1:I:226:THR:HG23	1.99	0.61
2:B:23:ARG:HG3	2:B:47:ILE:HD13	1.81	0.61
1:C:383:PRO:HD3	1:C:576:LEU:HD23	1.82	0.61
2:F:1:ARG:HH11	2:F:3:LYS:HB3	1.66	0.60
1:K:63:THR:HG22	1:K:77:MSE:HB3	1.83	0.60
1:A:4:PRO:HD3	1:I:140:MSE:HE3	1.83	0.60
1:G:230:LEU:HD21	1:G:237:LEU:HD22	1.83	0.60
1:E:369:MSE:HG2	1:E:373:MSE:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ASP:O	1:G:226:THR:HG23	2.01	0.60
1:E:118:ARG:NH2	3:E:1788:SO4:O4	2.34	0.60
1:C:137:ASN:HA	1:C:140:MSE:HG3	1.84	0.60
1:I:709:ARG:NH1	1:I:751:ASP:OD2	2.28	0.60
1:I:319:PRO:HD2	1:I:371:TYR:OH	2.02	0.59
1:C:348[A]:HIS:HD2	1:C:349:LEU:O	1.86	0.59
1:I:737:ASP:OD1	1:I:739:THR:HB	2.01	0.59
1:I:108:ARG:HD2	1:I:111:MSE:HE3	1.83	0.59
1:A:407:GLN:HG3	1:A:538:TYR:CG	2.37	0.59
1:C:4:PRO:HG2	1:C:8:ARG:HB2	1.85	0.59
1:A:392:MSE:HA	1:A:392:MSE:HE2	1.85	0.59
1:G:539:GLU:HG3	1:G:540:SER:H	1.67	0.59
1:G:646:GLN:HG3	1:G:648:ASP:OD1	2.03	0.59
1:C:155:HIS:CG	1:C:156:PHE:H	2.20	0.58
1:K:100:MSE:HE1	1:K:175:LEU:HD22	1.84	0.58
1:K:242:ILE:HD11	1:K:308:LEU:HD23	1.85	0.58
1:I:115:ARG:HB2	1:I:627:VAL:HA	1.84	0.58
1:A:667:LYS:N	1:A:671:GLN:OE1	2.36	0.58
1:K:110:LYS:O	1:K:114:GLN:HG3	2.04	0.58
1:A:399:GLU:OE2	1:A:598:ALA:N	2.35	0.58
1:I:383:PRO:HD3	1:I:576:LEU:HD23	1.86	0.58
1:A:373:MSE:CG	1:A:387:ARG:HE	2.17	0.58
1:E:118:ARG:NH1	1:E:162:THR:OG1	2.37	0.58
1:A:554:GLY:O	1:A:556:ASP:N	2.33	0.57
2:L:11:LYS:HG2	2:L:12:LYS:N	2.18	0.57
1:E:538:TYR:CD1	1:E:538:TYR:N	2.72	0.57
1:K:602:GLU:O	1:K:603:THR:HG22	2.04	0.57
1:E:392:MSE:HE2	1:E:392:MSE:HA	1.86	0.57
1:A:407:GLN:HG3	1:A:538:TYR:CD2	2.39	0.57
1:A:140:MSE:HE2	1:A:146:VAL:HG21	1.87	0.57
1:G:625:MSE:SE	1:G:636:LEU:HD22	2.55	0.57
1:K:238:ILE:HD11	1:K:303:LEU:HG	1.87	0.57
1:K:329:ARG:HG2	1:K:329:ARG:NH1	2.19	0.57
1:I:399:GLU:OE2	1:I:599:SER:OG	2.15	0.57
1:I:295:GLN:HG3	1:I:297:GLU:H	1.70	0.57
1:A:369:MSE:HE2	1:A:377:LEU:HD13	1.87	0.56
1:I:352:LEU:HD21	1:I:395:LEU:HD21	1.86	0.56
1:C:384:GLU:HG2	1:C:387:ARG:HD2	1.88	0.56
1:I:370:VAL:HG22	1:I:373:MSE:HE2	1.87	0.56
2:D:27:MSE:HE2	2:D:39:LEU:HD23	1.87	0.56
2:H:10:GLU:HG3	2:H:27:MSE:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:329:ARG:HH11	1:K:329:ARG:HG2	1.71	0.56
1:C:114:GLN:O	1:C:118:ARG:HG2	2.06	0.56
1:G:639:GLU:OE2	1:G:642:LYS:NZ	2.38	0.56
1:C:223:ASP:O	1:C:226:THR:HG23	2.06	0.56
1:C:637:PRO:O	1:C:641:GLN:HG3	2.06	0.56
1:G:49:ASP:HB3	1:G:96:ARG:HD2	1.88	0.56
1:G:113:GLN:OE1	1:G:117:ARG:NH2	2.33	0.56
1:I:370:VAL:HA	1:I:373:MSE:HG3	1.87	0.56
1:C:384:GLU:HG2	1:C:387:ARG:CD	2.36	0.55
1:E:228:HIS:NE2	1:E:246:GLU:OE1	2.38	0.55
1:I:321:LEU:HD11	1:I:370:VAL:HG12	1.88	0.55
1:K:636:LEU:HD12	1:K:644:MSE:SE	2.57	0.55
1:I:23:GLU:HG3	1:I:91:ILE:HG12	1.89	0.55
1:K:230:LEU:HD12	1:K:231:CYS:N	2.21	0.55
2:B:23:ARG:O	2:B:27:MSE:HG3	2.06	0.55
1:C:82:PHE:CE1	1:C:178:TYR:HB2	2.40	0.55
1:C:351:SER:HB3	1:C:399:GLU:HG2	1.87	0.55
1:I:86:ASP:OD2	1:I:182:ARG:NH1	2.38	0.55
1:G:536:ARG:O	1:G:545:ARG:NH2	2.38	0.55
1:K:108:ARG:HD2	1:K:111:MSE:HE3	1.89	0.54
1:A:228:HIS:NE2	1:A:246:GLU:OE1	2.40	0.54
1:A:670:TRP:CZ3	1:A:671:GLN:HG2	2.42	0.54
1:C:296:ARG:HH22	1:C:299:ASN:HD21	1.53	0.54
1:K:102:ILE:HD12	1:K:198:ASP:HA	1.89	0.54
1:C:408:GLN:HE21	1:C:408:GLN:N	2.06	0.54
1:E:670:TRP:CZ3	1:E:671:GLN:HG2	2.42	0.54
1:K:762:VAL:HG23	1:K:772:ASP:OD2	2.07	0.54
1:A:547:TYR:CZ	1:A:561:ARG:HG2	2.42	0.54
2:J:23:ARG:HG3	2:J:47:ILE:HD13	1.90	0.54
1:A:108:ARG:HG3	1:A:589:TYR:HB3	1.89	0.54
2:J:58:GLN:H	2:J:58:GLN:CD	2.16	0.54
1:C:115:ARG:NH2	1:C:654:LEU:O	2.41	0.53
1:C:24:ASP:O	1:C:25:ARG:HG3	2.08	0.53
1:G:215:LYS:HD3	1:G:785:ASP:HB3	1.90	0.53
1:I:251:ILE:HB	1:I:303:LEU:HB2	1.90	0.53
1:I:714:ARG:HA	1:I:719:PHE:CD1	2.44	0.53
1:A:366:TYR:O	1:A:370:VAL:HG23	2.08	0.53
1:I:586:TRP:CE2	1:I:617:PRO:HG3	2.43	0.53
1:K:642:LYS:O	1:K:646:GLN:HG2	2.08	0.53
2:B:63:LYS:O	2:B:67:MSE:HG3	2.08	0.53
1:G:359:ILE:O	1:G:363:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:670:TRP:CZ3	1:G:671:GLN:HG2	2.43	0.53
2:L:58:GLN:CD	2:L:58:GLN:H	2.16	0.53
1:A:747:LYS:HE2	1:K:364:LYS:HD3	1.91	0.53
1:I:63:THR:HG22	1:I:77:MSE:HB3	1.91	0.53
1:I:359:ILE:O	1:I:363:ILE:HG12	2.09	0.53
1:K:586:TRP:CE2	1:K:617:PRO:HG3	2.43	0.53
1:E:548:ARG:HH21	1:E:554:GLY:HA3	1.73	0.53
1:I:329:ARG:NH2	1:I:378:THR:O	2.31	0.53
1:K:321:LEU:HD12	1:K:322:PRO:HD2	1.90	0.53
1:K:125:MSE:O	1:K:129:GLU:HG3	2.09	0.52
1:E:642:LYS:O	1:E:646:GLN:HG2	2.09	0.52
1:A:223:ASP:O	1:A:226:THR:HG23	2.09	0.52
1:E:535:ILE:HD11	1:E:549:ALA:HB3	1.90	0.52
1:I:164:GLY:O	1:I:702:ARG:HD2	2.09	0.52
1:A:536:ARG:O	1:A:542:TRP:HB3	2.09	0.52
1:E:543:LYS:NZ	1:E:600:ASP:OD1	2.34	0.52
1:C:84:TYR:HE1	1:C:298:LYS:HE3	1.73	0.52
1:E:399:GLU:OE2	1:E:598:ALA:N	2.42	0.52
1:G:559:GLU:OE2	1:G:563:ARG:NH1	2.38	0.52
1:A:164:GLY:O	1:A:702:ARG:HD2	2.10	0.52
2:D:58:GLN:CD	2:D:58:GLN:H	2.17	0.52
1:G:355:ARG:NH2	1:G:666:LYS:NZ	2.57	0.52
1:A:223:ASP:HB3	1:A:226:THR:CG2	2.40	0.52
1:I:201:VAL:HG12	1:I:208:LYS:HE2	1.91	0.52
1:E:587:ASP:OD2	1:E:615:THR:HG22	2.10	0.51
1:G:114:GLN:HB3	1:G:118:ARG:HH21	1.75	0.51
1:I:601:PHE:O	1:I:604:VAL:HB	2.10	0.51
1:C:381:GLY:HA2	1:C:576:LEU:HG	1.92	0.51
1:E:61:PRO:HG3	1:K:144:ILE:HD12	1.92	0.51
1:G:114:GLN:O	1:G:118:ARG:HG2	2.10	0.51
1:A:359:ILE:O	1:A:363:ILE:HG12	2.09	0.51
1:C:309:ARG:HH11	1:C:309:ARG:HB3	1.76	0.51
1:E:125:MSE:HA	1:E:128:LYS:HE3	1.92	0.51
1:E:381:GLY:HA2	1:E:576:LEU:HG	1.91	0.51
1:K:625:MSE:HE2	1:K:688:LEU:HD21	1.91	0.51
1:A:201:VAL:HG12	1:A:208:LYS:HE2	1.93	0.51
1:K:114:GLN:O	1:K:118:ARG:HG2	2.11	0.51
1:K:384:GLU:HG2	1:K:387:ARG:HD2	1.93	0.51
1:A:118:ARG:NH2	3:A:1788:SO4:O1	2.44	0.50
1:G:737:ASP:OD1	1:G:739:THR:HB	2.11	0.50
2:B:27:MSE:HE2	2:B:39:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:GLY:HA2	1:E:588:TRP:CZ2	2.46	0.50
1:G:393:LYS:O	1:G:397:ARG:HG3	2.12	0.50
1:K:539:GLU:CD	1:K:540:SER:H	2.20	0.50
1:C:318:MSE:HB3	1:C:371:TYR:OH	2.12	0.50
2:L:12:LYS:HB3	2:L:13:LEU:HA	1.94	0.50
1:K:14:TYR:HB3	1:K:311:TYR:CD2	2.46	0.50
2:D:12:LYS:CB	2:D:13:LEU:HA	2.40	0.50
1:C:707:PRO:HG2	1:C:782:LEU:HD22	1.93	0.50
1:A:375:GLY:C	1:A:387:ARG:NH1	2.70	0.49
1:A:642:LYS:O	1:A:646:GLN:HG2	2.11	0.49
1:C:741:LEU:O	1:C:744:VAL:HG23	2.12	0.49
1:E:625:MSE:SE	1:E:636:LEU:CD2	3.10	0.49
1:A:721:PHE:CD2	1:K:319:PRO:HB2	2.47	0.49
1:C:230:LEU:HD12	1:C:231:CYS:N	2.26	0.49
1:C:564:VAL:HG12	1:C:592:TYR:CE2	2.47	0.49
1:E:384:GLU:HG2	1:E:387:ARG:HD2	1.95	0.49
1:E:748:ILE:HA	1:E:782:LEU:O	2.12	0.49
1:K:110:LYS:HE3	1:K:344:ASP:OD2	2.12	0.49
1:A:373:MSE:HG3	1:A:387:ARG:HE	1.76	0.49
1:A:408:GLN:O	1:A:409:ASP:OD1	2.29	0.49
2:B:1:ARG:O	2:F:38:GLN:HG2	2.13	0.49
1:E:295:GLN:HB2	1:E:297:GLU:O	2.12	0.49
1:G:164:GLY:O	1:G:702:ARG:HD2	2.12	0.49
1:G:637:PRO:O	1:G:641:GLN:HG3	2.12	0.49
2:F:72:ALA:O	4:F:2001:HOH:O	2.18	0.49
2:J:48:ASN:HA	2:J:52:LEU:HD12	1.94	0.49
1:K:408:GLN:OE1	1:K:408:GLN:N	2.46	0.49
1:A:114:GLN:O	1:A:118:ARG:HG2	2.12	0.49
1:C:108:ARG:HD2	1:C:111:MSE:HE2	1.95	0.49
1:E:384:GLU:HG2	1:E:387:ARG:CD	2.43	0.49
2:F:58:GLN:CD	2:F:58:GLN:H	2.20	0.49
1:A:602:GLU:HG3	1:A:603:THR:HG23	1.94	0.49
1:G:384:GLU:HG2	1:G:387:ARG:CD	2.43	0.49
1:E:100:MSE:CE	1:E:175:LEU:HD22	2.40	0.49
1:I:366:TYR:O	1:I:370:VAL:HG23	2.13	0.49
1:A:329:ARG:NH1	1:A:378:THR:O	2.46	0.49
2:B:45:LEU:O	2:B:49:VAL:HG23	2.12	0.48
1:G:395:LEU:O	1:G:398:VAL:HG12	2.12	0.48
1:G:369:MSE:HE2	1:G:377:LEU:HD13	1.95	0.48
1:K:309:ARG:HG2	1:K:331:LEU:HD11	1.95	0.48
1:C:4:PRO:HD3	1:G:140:MSE:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:MSE:SE	1:C:636:LEU:CD2	3.11	0.48
1:A:240:LEU:O	1:A:244:THR:HG23	2.14	0.48
2:B:34:TYR:CE1	2:B:67:MSE:HE1	2.49	0.48
1:G:547:TYR:CZ	1:G:561:ARG:HG2	2.48	0.48
1:C:541:GLY:C	1:C:545:ARG:HH12	2.21	0.48
1:I:337:LEU:O	1:I:340:PHE:HB2	2.14	0.48
1:C:602:GLU:HG3	1:C:603:THR:HG23	1.96	0.48
2:F:45:LEU:O	2:F:49:VAL:HG23	2.14	0.48
1:I:118:ARG:NH2	3:I:1788:SO4:O4	2.46	0.48
1:G:114:GLN:NE2	3:G:1788:SO4:O1	2.37	0.48
1:I:748:ILE:HA	1:I:782:LEU:O	2.12	0.48
2:B:10:GLU:HG3	2:B:27:MSE:HE1	1.96	0.48
1:G:564:VAL:HG23	1:G:596:PRO:HB3	1.96	0.48
1:K:254:GLU:CD	1:K:298:LYS:HD3	2.39	0.48
1:A:408:GLN:H	1:A:408:GLN:HG2	1.46	0.48
2:B:64:ILE:HA	2:B:64:ILE:HD13	1.66	0.48
1:C:128:LYS:O	1:C:132:ILE:HG12	2.14	0.48
1:C:729:LYS:HA	1:C:750:TYR:CG	2.49	0.48
2:D:12:LYS:HD3	2:D:13:LEU:HD12	1.95	0.48
2:H:48:ASN:HA	2:H:52:LEU:HD12	1.96	0.48
1:I:623:GLN:O	1:I:627:VAL:HG22	2.13	0.48
1:E:544:ASP:OD1	1:E:561:ARG:NH2	2.45	0.48
1:I:675:LEU:HD23	1:I:675:LEU:HA	1.71	0.48
1:K:295:GLN:NE2	1:K:298:LYS:HA	2.29	0.48
1:G:748:ILE:HA	1:G:782:LEU:O	2.14	0.47
2:D:63:LYS:O	2:D:67:MSE:HG3	2.14	0.47
1:E:329:ARG:NH1	1:E:378:THR:O	2.47	0.47
1:G:296:ARG:CD	1:G:297:GLU:H	2.21	0.47
1:I:373:MSE:HE3	1:I:375:GLY:O	2.14	0.47
1:E:245:HIS:CE1	1:E:328:GLU:HG3	2.49	0.47
1:G:392:MSE:HE2	1:G:392:MSE:HA	1.97	0.47
1:A:136:ARG:O	1:A:140:MSE:HG3	2.14	0.47
1:A:363:ILE:O	1:A:367:LYS:HG3	2.14	0.47
2:F:63:LYS:HE3	2:F:67:MSE:SE	2.65	0.47
2:H:58:GLN:H	2:H:58:GLN:CD	2.21	0.47
1:K:86:ASP:OD2	1:K:182:ARG:NH1	2.47	0.47
2:B:65:ARG:NH2	4:B:2002:HOH:O	2.47	0.47
1:G:659:PHE:CD2	1:G:676:LEU:HD21	2.49	0.47
1:A:110:LYS:O	1:A:114:GLN:HG3	2.15	0.47
1:C:164:GLY:O	1:C:702:ARG:HD2	2.15	0.47
1:C:547:TYR:CE1	1:C:561:ARG:HG2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:GLU:O	1:E:603:THR:OG1	2.26	0.47
2:F:10:GLU:HG3	2:F:27:MSE:HE1	1.96	0.47
1:G:309:ARG:NH1	1:G:309:ARG:HB3	2.30	0.47
1:I:547:TYR:OH	1:I:600:ASP:OD2	2.30	0.47
1:I:761:PHE:HB3	1:I:773:LEU:HB3	1.97	0.47
2:J:45:LEU:O	2:J:49:VAL:HG23	2.14	0.47
1:C:571:GLY:O	1:C:575:VAL:HG23	2.14	0.47
1:K:42:ASN:ND2	1:K:92:VAL:O	2.48	0.47
1:K:334:TRP:HD1	1:K:363:ILE:HD11	1.79	0.47
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.69	0.47
1:G:210:MSE:HB2	1:G:240:LEU:HD11	1.97	0.47
1:A:373:MSE:HG2	1:A:387:ARG:HE	1.80	0.47
2:B:58:GLN:CD	2:B:58:GLN:H	2.23	0.47
1:C:642:LYS:O	1:C:646:GLN:HG2	2.15	0.47
1:C:147:PRO:HA	1:G:257:VAL:CG2	2.46	0.46
1:E:309:ARG:HH11	1:E:309:ARG:HB3	1.80	0.46
1:E:365:LEU:HD23	1:E:365:LEU:HA	1.59	0.46
1:G:639:GLU:CD	1:G:642:LYS:HZ3	2.22	0.46
1:I:107:PRO:O	1:I:111:MSE:HG3	2.15	0.46
1:I:138:ARG:O	1:I:142:GLU:HG2	2.16	0.46
1:I:716:HIS:HE1	1:I:741:LEU:HD23	1.80	0.46
1:I:110:LYS:O	1:I:114:GLN:HG3	2.15	0.46
1:A:128:LYS:O	1:A:132:ILE:HG12	2.15	0.46
1:I:118:ARG:NH2	3:I:1788:SO4:S	2.89	0.46
1:K:730:SER:O	1:K:750:TYR:HB3	2.16	0.46
1:A:87:ARG:HH12	1:A:298:LYS:CE	2.19	0.46
1:I:384:GLU:HG3	1:I:387:ARG:H	1.79	0.46
2:J:8:GLU:CD	2:J:24:LYS:NZ	2.73	0.46
1:K:104:GLY:C	1:K:163:PRO:HG3	2.41	0.46
1:A:369:MSE:O	1:A:372:GLN:HB2	2.16	0.46
1:A:564:VAL:HG12	1:A:592:TYR:CZ	2.51	0.46
1:G:13:LYS:NZ	1:G:360:ASP:OD1	2.49	0.46
1:G:355:ARG:NH2	1:G:666:LYS:HZ3	2.14	0.46
1:K:586:TRP:CZ2	1:K:617:PRO:HG3	2.50	0.46
1:C:321:LEU:HD12	1:C:322:PRO:HD3	1.98	0.46
1:I:113:GLN:NE2	1:I:117:ARG:NH1	2.58	0.46
1:I:707:PRO:HG2	1:I:782:LEU:HD22	1.97	0.46
2:L:45:LEU:O	2:L:49:VAL:HG23	2.15	0.46
2:D:62:GLN:OE1	2:D:65:ARG:NH1	2.49	0.46
1:G:559:GLU:HG2	1:G:563:ARG:HH12	1.81	0.46
1:I:102:ILE:HD11	1:I:175:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:748:ILE:HA	1:K:782:LEU:O	2.16	0.46
1:I:108:ARG:HA	1:I:111:MSE:HE3	1.97	0.46
1:K:82:PHE:CE1	1:K:178:TYR:HB2	2.51	0.46
1:A:4:PRO:CD	1:I:140:MSE:HE3	2.46	0.46
1:A:60:HIS:HB2	1:A:61:PRO:HD3	1.96	0.46
2:B:57:SER:O	2:B:61:MSE:HG2	2.16	0.46
1:C:407:GLN:HG3	1:C:538:TYR:CD2	2.51	0.45
1:E:249:PHE:O	1:E:305:ILE:HB	2.17	0.45
1:G:68:ARG:NH2	3:G:1790:SO4:O3	2.44	0.45
1:I:392:MSE:HE2	1:I:392:MSE:HA	1.98	0.45
1:K:555:SER:HA	1:K:561:ARG:NH2	2.31	0.45
1:G:352:LEU:HD21	1:G:395:LEU:HD21	1.97	0.45
1:K:113:GLN:HG3	1:K:344:ASP:O	2.16	0.45
1:A:249:PHE:O	1:A:306:PRO:HD3	2.15	0.45
1:C:240:LEU:O	1:C:244:THR:HG23	2.17	0.45
1:G:369:MSE:SE	1:G:369:MSE:C	3.09	0.45
1:G:136:ARG:O	1:G:140:MSE:HB2	2.16	0.45
1:G:118:ARG:HB3	1:G:159:ASN:CG	2.42	0.45
1:G:566:TRP:HA	1:G:569:VAL:HG22	1.98	0.45
1:A:238:ILE:HD11	1:A:303:LEU:HG	1.99	0.45
1:A:668:TYR:CG	1:I:134:GLU:HG3	2.51	0.45
1:A:750:TYR:CZ	1:A:752:SER:HA	2.52	0.45
1:I:304:ARG:HH11	1:I:304:ARG:CG	2.22	0.45
1:G:136:ARG:HH12	1:G:147:PRO:HA	1.82	0.45
1:I:100:MSE:CE	1:I:175:LEU:HD22	2.37	0.45
1:K:550:LYS:HB3	1:K:594:TYR:CD2	2.52	0.45
1:I:115:ARG:HD2	1:I:626:SER:O	2.16	0.45
1:K:623:GLN:O	1:K:627:VAL:HB	2.17	0.45
1:A:347:PRO:HG2	1:A:595:ALA:HB2	1.99	0.45
1:C:359:ILE:O	1:C:363:ILE:HG12	2.16	0.45
1:C:571:GLY:HA2	1:C:588:TRP:CH2	2.51	0.45
1:C:714:ARG:HA	1:C:719:PHE:CE1	2.52	0.45
1:G:82:PHE:CE1	1:G:178:TYR:HB2	2.52	0.45
1:G:407:GLN:HG3	1:G:538:TYR:CG	2.52	0.45
1:G:559:GLU:HG2	1:G:563:ARG:NH1	2.32	0.45
1:I:115:ARG:NH2	1:I:654:LEU:O	2.50	0.45
1:I:135:GLN:HA	1:I:138:ARG:NH1	2.32	0.45
1:C:351:SER:CB	1:C:399:GLU:HG2	2.47	0.44
1:C:541:GLY:C	1:C:545:ARG:NH1	2.76	0.44
1:G:115:ARG:NH2	1:G:654:LEU:O	2.50	0.44
1:I:569:VAL:HG21	1:I:604:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:LYS:HE2	1:E:787:GLU:OE2	2.17	0.44
1:E:623:GLN:HG3	1:E:624:LEU:N	2.31	0.44
1:K:193:GLU:HG2	1:K:741:LEU:HD22	2.00	0.44
1:K:384:GLU:O	1:K:384:GLU:HG3	2.17	0.44
1:K:714:ARG:HA	1:K:719:PHE:CD1	2.53	0.44
1:A:251:ILE:HB	1:A:303:LEU:HB2	1.98	0.44
1:E:201:VAL:HG22	1:E:706:GLY:O	2.17	0.44
1:I:587:ASP:OD2	1:I:615:THR:HG22	2.18	0.44
1:I:136:ARG:O	1:I:140:MSE:HG3	2.17	0.44
1:K:683:ARG:HG3	2:L:37:ILE:HD11	1.98	0.44
1:A:113:GLN:CD	1:A:117:ARG:HH12	2.24	0.44
1:C:257:VAL:HA	1:G:145:ALA:O	2.17	0.44
1:E:624:LEU:HA	1:E:624:LEU:HD23	1.58	0.44
1:G:309:ARG:HB3	1:G:309:ARG:HH11	1.82	0.44
1:E:625:MSE:SE	1:E:636:LEU:HD22	2.67	0.44
1:I:543:LYS:HZ2	1:I:600:ASP:CG	2.23	0.44
1:K:351:SER:HB3	1:K:399:GLU:HG2	1.99	0.44
1:A:318:MSE:SE	1:A:370:VAL:HG11	2.68	0.44
1:A:623:GLN:O	1:A:627:VAL:HB	2.18	0.44
1:C:547:TYR:CZ	1:C:561:ARG:HG2	2.52	0.44
1:E:98:LEU:O	1:E:194:ILE:HA	2.17	0.44
1:E:548:ARG:HH21	1:E:554:GLY:CA	2.31	0.44
1:E:710:ILE:HG22	1:E:783:TYR:HB2	2.00	0.44
1:I:396:GLY:O	1:I:399:GLU:HG2	2.18	0.44
1:K:351:SER:CB	1:K:399:GLU:HG2	2.47	0.44
1:A:399:GLU:OE1	1:A:599:SER:OG	2.34	0.44
2:B:10:GLU:O	2:B:23:ARG:NH2	2.51	0.44
1:I:547:TYR:CZ	1:I:561:ARG:HG2	2.52	0.44
1:K:114:GLN:HB3	1:K:118:ARG:HH21	1.83	0.44
1:K:309:ARG:HG2	1:K:331:LEU:CD1	2.48	0.44
2:L:45:LEU:HD21	2:L:60:LEU:HD22	1.99	0.44
2:H:61:MSE:O	2:H:65:ARG:HB2	2.17	0.43
1:K:660:ARG:CD	2:L:53:GLY:HA3	2.43	0.43
1:E:707:PRO:HG2	1:E:782:LEU:HD22	1.99	0.43
1:G:601:PHE:O	1:G:604:VAL:HG22	2.18	0.43
1:C:542:TRP:CD1	1:C:542:TRP:H	2.35	0.43
2:D:7:VAL:O	2:D:10:GLU:HB2	2.18	0.43
1:E:251:ILE:HB	1:E:303:LEU:HB2	2.00	0.43
1:I:247:ALA:O	1:I:306:PRO:HG3	2.18	0.43
1:C:369:MSE:CG	1:C:373:MSE:HG3	2.43	0.43
1:C:699:GLU:HG2	1:C:702:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:233:ALA:O	1:I:253:ARG:NH1	2.51	0.43
1:C:625:MSE:SE	1:C:636:LEU:HD22	2.68	0.43
1:I:670:TRP:CZ3	1:I:671:GLN:HG2	2.53	0.43
1:G:379:LYS:NZ	3:G:1791:SO4:O2	2.50	0.43
1:I:571:GLY:HA2	1:I:588:TRP:CH2	2.54	0.43
1:I:346:LEU:HD21	1:I:571:GLY:HA3	2.01	0.43
2:J:64:ILE:HD13	2:J:64:ILE:HA	1.93	0.43
2:J:12:LYS:HA	2:J:12:LYS:HD3	1.86	0.43
1:I:249:PHE:O	1:I:305:ILE:HB	2.19	0.43
1:I:709:ARG:HD3	1:I:751:ASP:OD2	2.19	0.43
1:E:407:GLN:HB3	1:E:408:GLN:NE2	2.34	0.42
1:G:384:GLU:HG2	1:G:387:ARG:HD2	2.01	0.42
1:G:762:VAL:HG23	1:G:772:ASP:OD1	2.19	0.42
1:I:114:GLN:O	1:I:118:ARG:HG2	2.19	0.42
1:I:321:LEU:HD12	1:I:321:LEU:HA	1.80	0.42
1:K:251:ILE:HB	1:K:303:LEU:HB2	2.01	0.42
1:G:163:PRO:HB3	1:G:199:ALA:HB1	2.02	0.42
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.84	0.42
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.80	0.42
1:C:251:ILE:HB	1:C:303:LEU:HB2	2.00	0.42
1:C:321:LEU:HD12	1:C:322:PRO:CD	2.48	0.42
1:C:392:MSE:HA	1:C:392:MSE:HE2	2.01	0.42
1:E:140:MSE:HE3	1:K:4:PRO:HD3	2.00	0.42
1:E:383:PRO:HD3	1:E:576:LEU:HD23	2.01	0.42
1:G:108:ARG:HG2	1:G:681:GLU:OE2	2.19	0.42
1:G:619:ASN:HB3	1:G:703:ASN:OD1	2.19	0.42
1:K:240:LEU:O	1:K:244:THR:HG23	2.19	0.42
1:K:625:MSE:SE	1:K:636:LEU:HD13	2.69	0.42
1:K:637:PRO:O	1:K:641:GLN:HG3	2.19	0.42
1:A:13:LYS:NZ	1:A:360:ASP:OD1	2.45	0.42
1:A:390:MSE:HE2	1:A:390:MSE:HB3	1.91	0.42
1:E:536:ARG:HG2	1:E:538:TYR:OH	2.19	0.42
1:E:589:TYR:CE2	1:E:591:PRO:HB3	2.54	0.42
1:A:348:HIS:ND1	1:A:348:HIS:O	2.51	0.42
1:A:564:VAL:HG12	1:A:592:TYR:CE1	2.54	0.42
1:E:340:PHE:CZ	1:E:392:MSE:SE	3.22	0.42
1:A:157:ASP:OD1	1:A:159:ASN:HB2	2.20	0.42
1:A:348:HIS:HD1	1:A:348:HIS:C	2.27	0.42
1:A:373:MSE:HG3	1:A:373:MSE:O	2.19	0.42
1:A:714:ARG:HA	1:A:719:PHE:CD1	2.54	0.42
1:C:321:LEU:HA	1:C:322:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:GLN:O	1:E:118:ARG:HG2	2.20	0.42
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.84	0.42
2:B:14:TRP:CD1	2:B:14:TRP:H	2.38	0.42
1:E:111:MSE:HE1	1:E:618:PHE:CE2	2.55	0.42
1:G:602:GLU:C	1:G:603:THR:HG23	2.44	0.42
1:A:251:ILE:O	1:A:302:PHE:HA	2.19	0.42
1:C:729:LYS:HA	1:C:750:TYR:CD2	2.55	0.42
1:E:48:PHE:CD2	1:E:229:CYS:HB2	2.55	0.42
1:C:181:ASP:OD2	1:C:182:ARG:NH1	2.51	0.42
1:G:23:GLU:OE2	1:G:87:ARG:NE	2.42	0.42
2:H:45:LEU:O	2:H:49:VAL:HG23	2.20	0.42
1:C:228:HIS:NE2	1:C:246:GLU:OE1	2.50	0.42
1:C:602:GLU:C	1:C:604:VAL:H	2.28	0.42
1:I:295:GLN:HG2	1:I:299:ASN:ND2	2.35	0.42
1:K:624:LEU:HD23	1:K:624:LEU:HA	1.89	0.42
1:A:399:GLU:OE2	1:A:597:PHE:HB3	2.20	0.41
1:C:155:HIS:CG	1:C:156:PHE:N	2.85	0.41
1:E:230:LEU:HD21	1:E:237:LEU:HD22	2.02	0.41
1:I:142:GLU:HB2	1:I:144:ILE:HD13	2.02	0.41
1:A:6:PHE:CZ	1:A:239:MSE:HE1	2.54	0.41
1:A:373:MSE:HG2	1:A:387:ARG:CG	2.50	0.41
1:A:646:GLN:HG3	1:A:648:ASP:OD1	2.20	0.41
2:B:47:ILE:O	2:B:51:LEU:HB2	2.20	0.41
1:E:633:LYS:NZ	1:E:645:ILE:HD13	2.34	0.41
1:K:576:LEU:HD12	1:K:576:LEU:HA	1.91	0.41
1:K:590:PHE:CE2	1:K:592:TYR:HB2	2.55	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.67	0.41
1:C:7:PHE:HB3	1:C:256:PHE:CZ	2.55	0.41
1:C:545:ARG:HH11	1:C:545:ARG:CG	2.23	0.41
1:E:309:ARG:HB3	1:E:309:ARG:NH1	2.35	0.41
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.86	0.41
1:A:571:GLY:O	1:A:575:VAL:HG23	2.20	0.41
2:B:71:ILE:HG22	2:B:71:ILE:O	2.21	0.41
1:E:108:ARG:HD2	1:E:111:MSE:HE3	2.01	0.41
1:E:321:LEU:HA	1:E:322:PRO:HD3	1.90	0.41
1:E:709:ARG:NH1	1:E:751:ASP:OD2	2.44	0.41
1:A:668:TYR:CD1	1:I:134:GLU:HG3	2.56	0.41
1:E:618:PHE:HZ	1:E:681:GLU:HG3	1.85	0.41
2:F:1:ARG:HD3	2:F:3:LYS:H	1.84	0.41
1:I:238:ILE:HD11	1:I:303:LEU:HG	2.03	0.41
1:K:128:LYS:O	1:K:131:SER:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:353:GLU:OE1	1:K:355:ARG:NH2	2.54	0.41
1:A:329:ARG:NH2	3:A:1789:SO4:S	2.92	0.41
1:I:210:MSE:HE3	1:I:214:ARG:HB2	2.02	0.41
1:I:313:GLU:HG3	1:I:327:VAL:HG21	2.03	0.41
1:K:399:GLU:OE2	1:K:598:ALA:N	2.50	0.41
1:A:537:LEU:HA	1:A:542:TRP:HB2	2.03	0.41
1:A:733:LEU:O	1:K:364:LYS:HE3	2.21	0.41
1:C:329:ARG:NH1	1:C:378:THR:O	2.54	0.41
1:C:646:GLN:HG3	1:C:648:ASP:OD1	2.21	0.41
2:D:45:LEU:O	2:D:49:VAL:HG23	2.20	0.41
1:E:683:ARG:HH21	2:F:44:GLN:NE2	2.19	0.41
1:G:572:LEU:HD23	1:G:572:LEU:HA	1.83	0.41
1:I:372:GLN:HB2	1:I:390:MSE:HE1	2.03	0.41
1:K:7:PHE:HE1	1:K:303:LEU:HD21	1.86	0.41
2:L:11:LYS:HE2	2:L:12:LYS:HG2	2.03	0.41
1:A:63:THR:HG22	1:A:77:MSE:HB3	2.03	0.41
1:A:73:ASN:O	1:A:77:MSE:HG3	2.21	0.41
2:B:10:GLU:O	2:B:12:LYS:HE3	2.21	0.41
1:C:728:SER:HA	1:I:397:ARG:HG2	2.02	0.41
1:E:118:ARG:HB3	1:E:159:ASN:CG	2.46	0.41
1:E:407:GLN:NE2	1:E:538:TYR:CE1	2.89	0.41
1:K:13:LYS:HG2	1:K:14:TYR:CE1	2.56	0.41
1:A:571:GLY:HA2	1:A:588:TRP:CH2	2.55	0.40
1:G:327:VAL:HG13	1:G:328:GLU:H	1.86	0.40
1:K:392:MSE:HB3	1:K:601:PHE:HB2	2.02	0.40
1:C:7:PHE:HB3	1:C:256:PHE:CE1	2.56	0.40
1:E:245:HIS:ND1	1:E:328:GLU:HG3	2.36	0.40
1:I:309:ARG:O	1:I:313:GLU:HB2	2.22	0.40
1:A:736:LEU:O	1:A:738:PRO:HD3	2.21	0.40
1:C:108:ARG:HG3	1:C:589:TYR:HB3	2.03	0.40
1:I:590:PHE:CE2	1:I:592:TYR:HB2	2.56	0.40
1:I:602:GLU:C	1:I:604:VAL:H	2.29	0.40
1:I:623:GLN:HG3	1:I:624:LEU:N	2.36	0.40
1:K:623:GLN:HG3	1:K:624:LEU:N	2.36	0.40
1:K:659:PHE:CD1	1:K:676:LEU:HD21	2.57	0.40
1:K:696:THR:HG23	1:K:699:GLU:OE1	2.21	0.40
1:C:209:ILE:O	1:C:210:MSE:C	2.65	0.40
1:C:408:GLN:O	1:C:409:ASP:HB2	2.20	0.40
2:D:48:ASN:HA	2:D:52:LEU:HD12	2.04	0.40
1:G:625:MSE:SE	1:G:636:LEU:CD2	3.19	0.40
1:K:120:ARG:NH2	1:K:672:GLY:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HG2	1:A:623:GLN:OE1	2.21	0.40
1:C:323:PHE:HE2	1:C:374:LYS:C	2.30	0.40
1:G:229:CYS:HA	1:G:250:ASN:O	2.20	0.40
2:L:68:GLY:O	2:L:71:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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

All (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
1	K	322	PRO

5.3.2 Protein sidechains ⓘ

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

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

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

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	VAL
1	A	113	GLN
1	A	118	ARG
1	A	133	GLU
1	A	168	MSE

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Mol	Chain	Res	Type
1	A	239	MSE
1	A	298	LYS
1	A	329	ARG
1	A	348	HIS
1	A	365	LEU
1	A	382	ILE
1	A	406	ARG
1	A	407	GLN
1	A	408	GLN
1	A	545	ARG
1	A	558	ILE
1	A	599	SER
1	A	603	THR
1	A	623	GLN
1	A	627	VAL
1	A	634	GLN
1	A	692	TYR
1	A	720	GLU
1	A	732	ASP
1	A	745	SER
1	A	762	VAL
1	A	776	ASN
2	B	22	LEU
1	C	10	LEU
1	C	113	GLN
1	C	118	ARG
1	C	146	VAL
1	C	216	GLN
1	C	239	MSE
1	C	295	GLN
1	C	296	ARG
1	C	324	LYS
1	C	329	ARG
1	C	340	PHE
1	C	348[A]	HIS
1	C	348[B]	HIS
1	C	373	MSE
1	C	405	ARG
1	C	408	GLN
1	C	545	ARG
1	C	599	SER
1	C	604	VAL

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Mol	Chain	Res	Type
1	C	623	GLN
1	C	634	GLN
1	C	643	LEU
1	C	682	THR
1	C	692	TYR
1	C	762	VAL
2	D	5	GLU
2	D	59	THR
2	D	64	ILE
1	E	80	LEU
1	E	118	ARG
1	E	155	HIS
1	E	239	MSE
1	E	298	LYS
1	E	324	LYS
1	E	329	ARG
1	E	373	MSE
1	E	382	ILE
1	E	408	GLN
1	E	540	SER
1	E	623	GLN
1	E	626	SER
1	E	634	GLN
1	E	643	LEU
1	E	692	TYR
1	E	745	SER
1	E	762	VAL
2	F	15	GLU
2	F	22	LEU
2	F	23	ARG
1	G	24	ASP
1	G	25	ARG
1	G	118	ARG
1	G	140	MSE
1	G	155	HIS
1	G	239	MSE
1	G	296	ARG
1	G	329	ARG
1	G	340	PHE
1	G	599	SER
1	G	603	THR
1	G	623	GLN

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Mol	Chain	Res	Type
1	G	626	SER
1	G	634	GLN
1	G	692	TYR
1	G	739	THR
1	G	762	VAL
2	H	23	ARG
2	H	65	ARG
1	I	118	ARG
1	I	146	VAL
1	I	239	MSE
1	I	297	GLU
1	I	304	ARG
1	I	340	PHE
1	I	344	ASP
1	I	348	HIS
1	I	369	MSE
1	I	382	ILE
1	I	384	GLU
1	I	604	VAL
1	I	623	GLN
1	I	647	ASP
1	I	692	TYR
1	I	720	GLU
1	I	745	SER
2	J	10	GLU
2	J	23	ARG
1	K	80	LEU
1	K	118	ARG
1	K	239	MSE
1	K	298	LYS
1	K	320	ASN
1	K	328	GLU
1	K	329	ARG
1	K	340	PHE
1	K	384	GLU
1	K	548	ARG
1	K	558	ILE
1	K	623	GLN
1	K	627	VAL
1	K	634	GLN
1	K	643	LEU
1	K	648	ASP

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Mol	Chain	Res	Type
1	K	692	TYR
1	K	704	THR
1	K	705	ARG
1	K	762	VAL
2	L	22	LEU
2	L	23	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	114	GLN
1	A	137	ASN
1	A	200	ASN
1	A	207	HIS
1	A	250	ASN
1	A	407	GLN
1	A	581	GLN
1	A	635	HIS
1	A	689	GLN
2	B	40	GLN
2	B	44	GLN
1	C	113	GLN
1	C	135	GLN
1	C	137	ASN
1	C	155	HIS
1	C	250	ASN
1	C	299	ASN
1	C	408	GLN
1	C	689	GLN
1	E	20	ASN
1	E	114	GLN
1	E	191	ASN
1	E	207	HIS
1	E	407	GLN
1	E	408	GLN
1	E	581	GLN
1	E	619	ASN
2	F	30	HIS
2	F	40	GLN
1	G	56	ASN
1	G	250	ASN

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Mol	Chain	Res	Type
1	G	299	ASN
1	G	320	ASN
1	G	689	GLN
1	G	771	GLN
2	H	40	GLN
1	I	20	ASN
1	I	135	GLN
1	I	137	ASN
1	I	250	ASN
1	I	372	GLN
1	I	635	HIS
1	I	646	GLN
1	I	671	GLN
2	J	40	GLN
1	K	20	ASN
1	K	137	ASN
1	K	250	ASN
1	K	320	ASN
1	K	407	GLN
2	L	38	GLN
2	L	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

6.1 Protein, DNA and RNA chains

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

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

All (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
2	H	4	LEU	3.5
1	E	4	PRO	3.4
1	A	257	VAL	3.2
2	J	28	LEU	2.9
1	I	145	ALA	2.9
1	A	35	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	144	ILE	2.7
1	G	143	GLY	2.7
2	H	12	LYS	2.6
1	I	144	ILE	2.6
1	K	35	PRO	2.5
1	A	4	PRO	2.5
1	E	35	PRO	2.5
1	K	4	PRO	2.5
2	L	4	LEU	2.4
1	K	147	PRO	2.3
2	H	35	PRO	2.3
1	E	145	ALA	2.2
1	C	35	PRO	2.2
1	C	128	LYS	2.2
2	D	72	ALA	2.2
1	G	35	PRO	2.2
2	H	28	LEU	2.2
1	K	588	TRP	2.1
1	E	257	VAL	2.1
2	H	3	LYS	2.1
1	C	144	ILE	2.1
1	A	148	PRO	2.0
1	I	256	PHE	2.0
2	J	6	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	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.