Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:29 PM GMT

PDB ID	:	5FIR
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

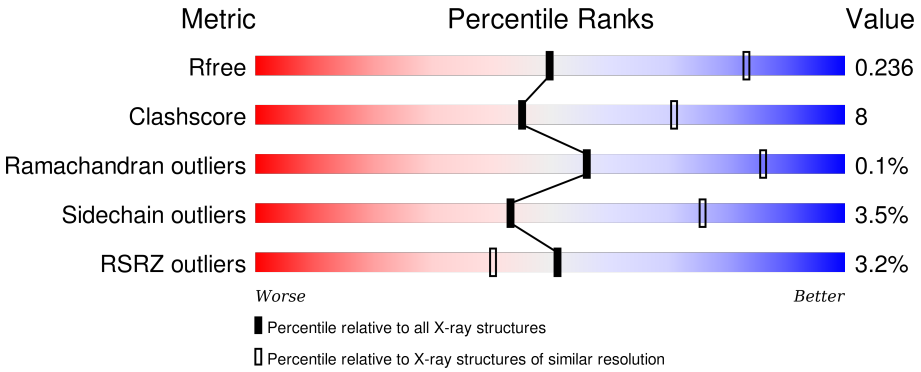
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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}	91344	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 76% 18%
1	C	636	2% 77% 17%
1	E	636	2% 77% 17%
1	G	636	2% 78% 17%
1	I	636	2% 75% 19% 5%

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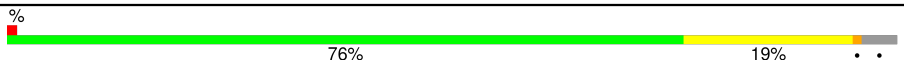
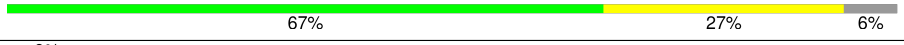
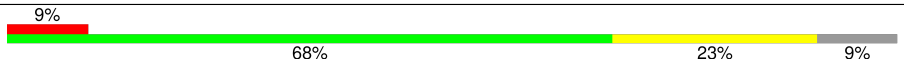
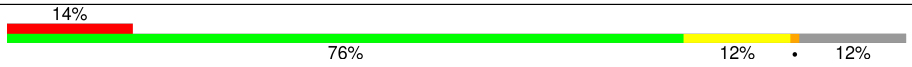
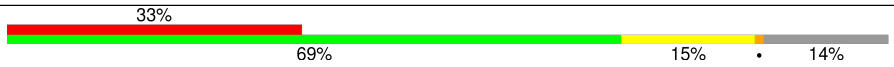
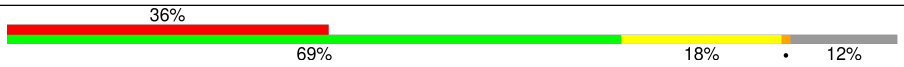
Mol	Chain	Length	Quality of chain
1	K	636	
2	B	78	
2	D	78	
2	F	78	
2	H	78	
2	J	78	
2	L	78	

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	C	1788	-	-	-	X
3	SO4	C	1790	-	-	-	X
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	.	-	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

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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	.	-	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	.	-	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	.	-	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	.	-	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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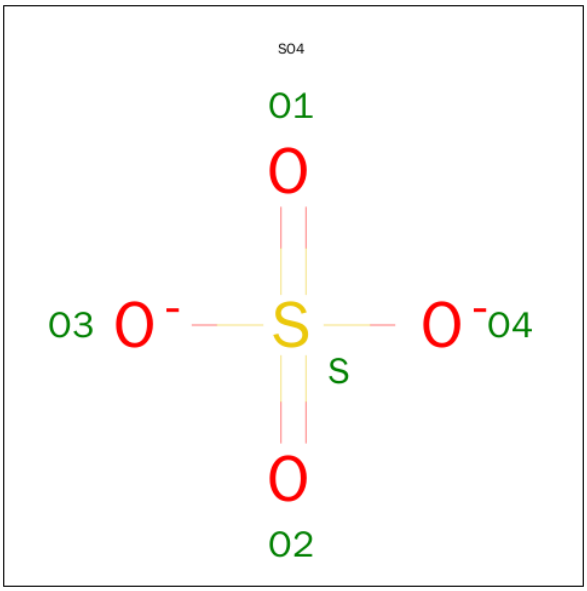
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	EXPRESSION TAG	UNP Q21738
F	0	GLY	-	EXPRESSION TAG	UNP Q21738
F	1	ARG	-	EXPRESSION TAG	UNP Q21738
H	-2	GLY	-	EXPRESSION TAG	UNP Q21738
H	-1	GLY	-	EXPRESSION TAG	UNP Q21738
H	0	GLY	-	EXPRESSION TAG	UNP Q21738
H	1	ARG	-	EXPRESSION TAG	UNP Q21738
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 (three-letter code: SO4) (formula: O_4S).



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

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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
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

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

- Molecule 4 is water.

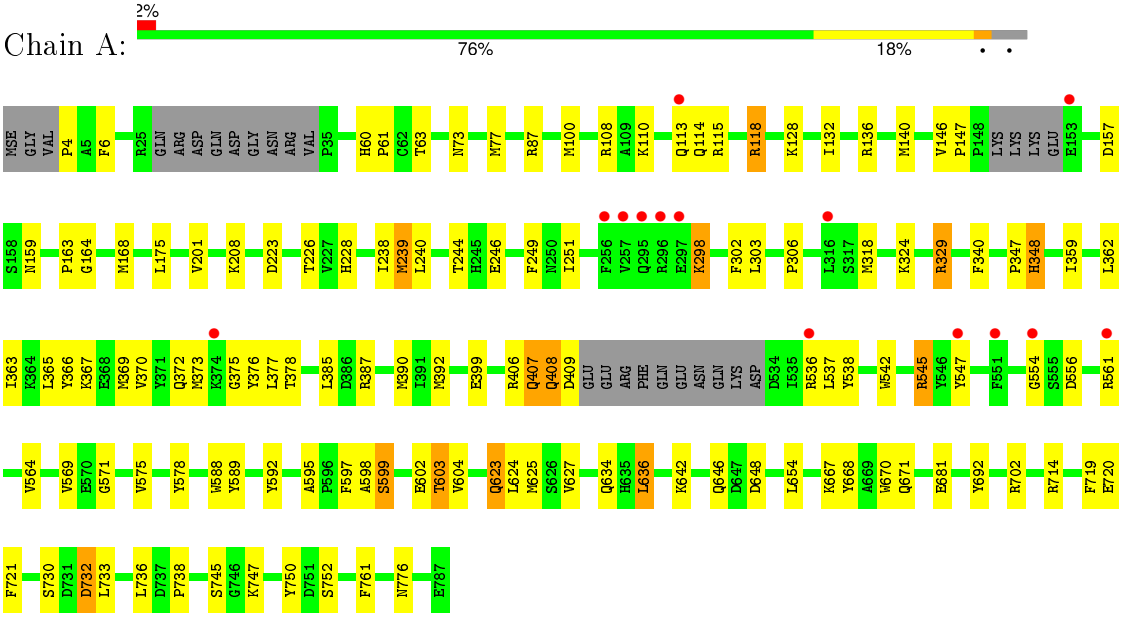
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	2	Total O 2 2	0	0
4	C	8	Total O 8 8	0	0
4	E	14	Total O 14 14	0	0
4	F	1	Total O 1 1	0	0
4	G	5	Total O 5 5	0	0
4	I	7	Total O 7 7	0	0
4	K	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

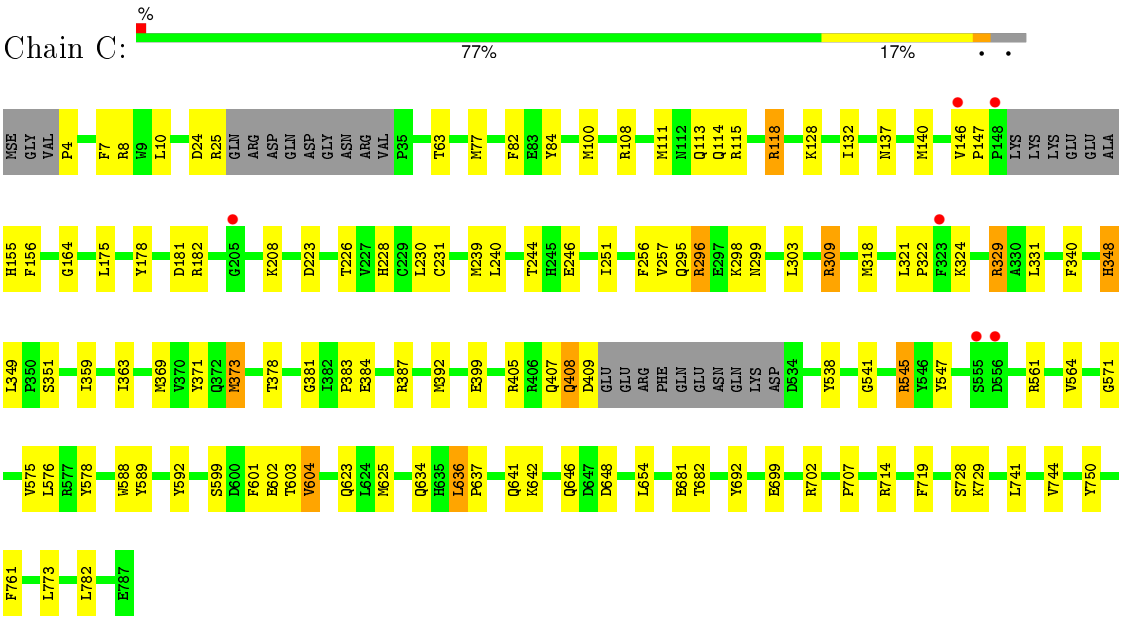
- Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

Chain A:



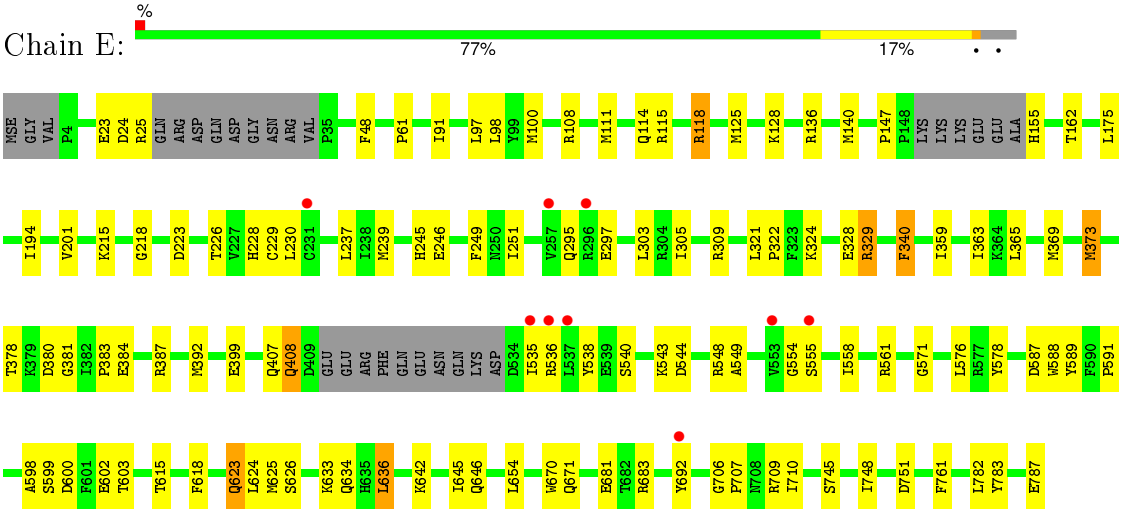
- Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

Chain C:



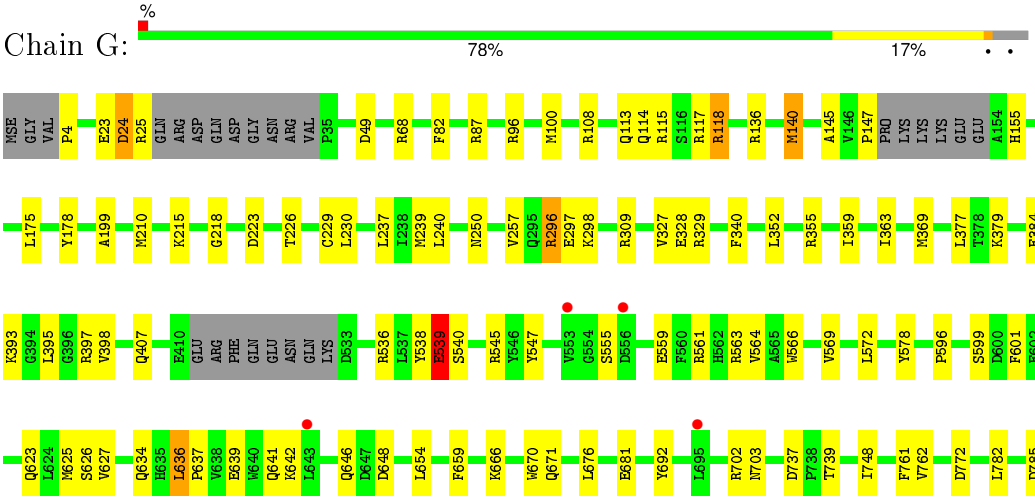
• Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

Chain E:



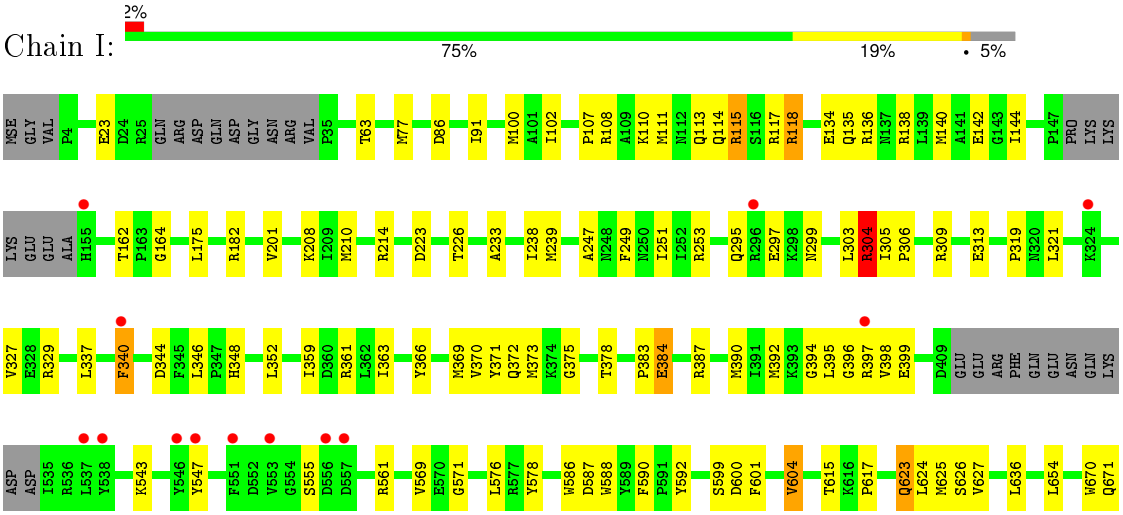
• Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

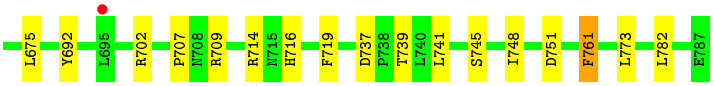
Chain G:



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

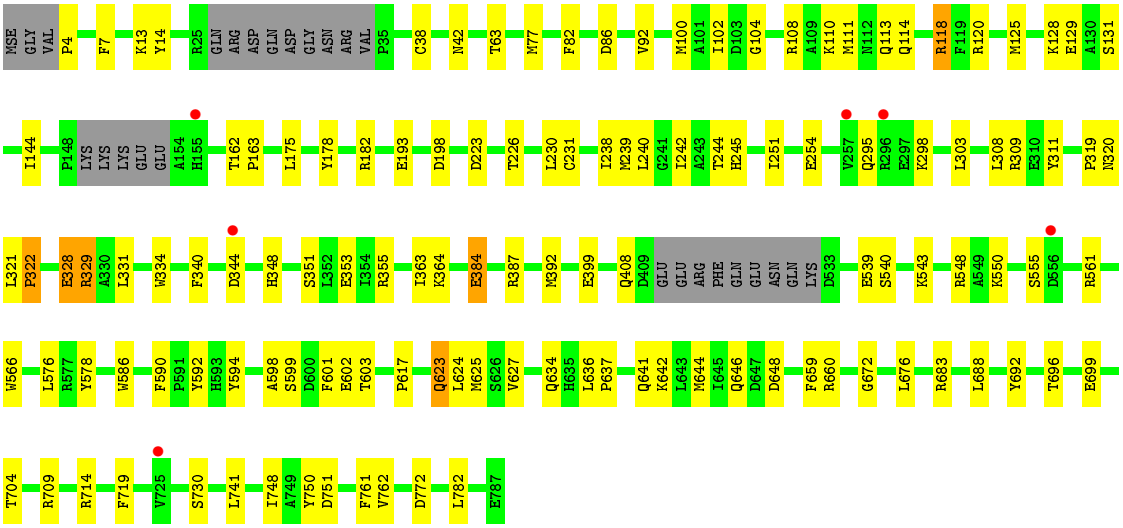
Chain I:





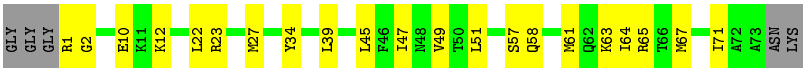
• Molecule 1: 5'-3' EXORIBONUCLEASE 2 HOMOLOG

Chain K:



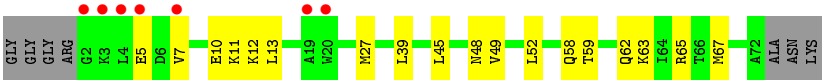
• Molecule 2: PAXT-1

Chain B:



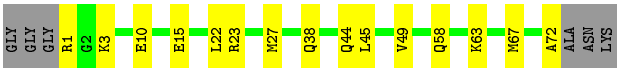
• Molecule 2: PAXT-1

Chain D:



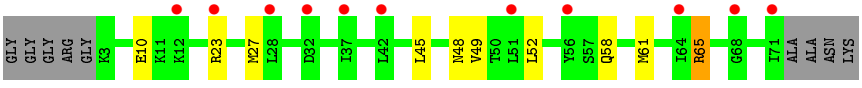
• Molecule 2: PAXT-1

Chain F:



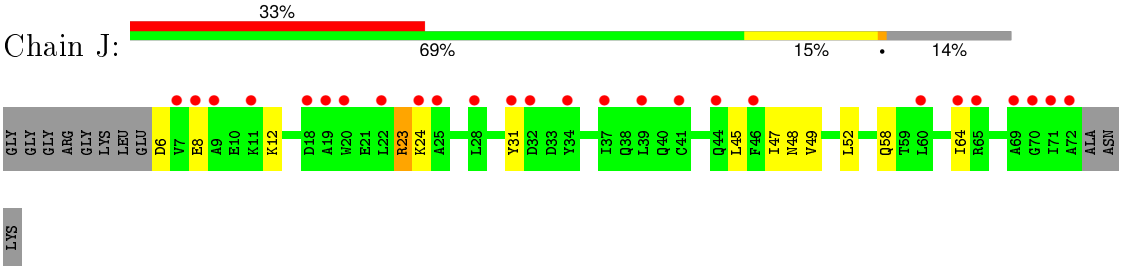
• Molecule 2: PAXT-1

Chain H:



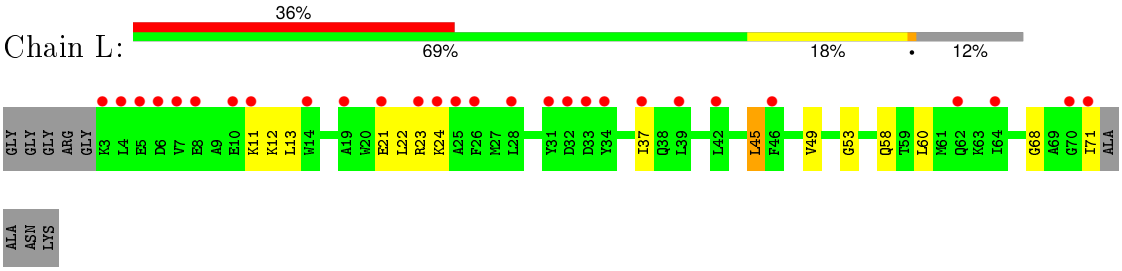
• Molecule 2: PAXT-1

Chain J:



• Molecule 2: PAXT-1

Chain L:



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) 94.6 (49.39-2.84)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.86Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.238 0.183 , 0.236	Depositor DCC
R_{free} test set	3902 reflections (2.51%)	DCC
Wilson B-factor (Å^2)	72.5	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.6	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 155519 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/5118	0.67	1/6916 (0.0%)
1	C	0.58	0/5115	0.70	3/6912 (0.0%)
1	E	0.59	1/5104 (0.0%)	0.69	2/6897 (0.0%)
1	G	0.61	2/5129 (0.0%)	0.69	2/6930 (0.0%)
1	I	0.52	0/5088	0.68	2/6874 (0.0%)
1	K	0.52	1/5117 (0.0%)	0.65	0/6915
2	B	0.51	0/596	0.70	0/796
2	D	0.48	0/580	0.67	0/775
2	F	0.43	0/591	0.63	0/789
2	H	0.36	0/571	0.56	0/763
2	J	0.41	0/550	0.56	0/736
2	L	0.36	0/571	0.57	1/763 (0.1%)
All	All	0.55	4/34130 (0.0%)	0.67	11/46066 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	218	GLY	C-N	-6.81	1.18	1.34
1	G	539	GLU	CB-CG	5.57	1.62	1.52
1	K	38	CYS	CB-SG	-5.50	1.72	1.81
1	E	218	GLY	C-N	-5.21	1.22	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	636	LEU	CA-CB-CG	-6.12	101.22	115.30
1	G	627	VAL	C-N-CA	-6.01	106.67	121.70
1	I	115	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	A	636	LEU	CA-CB-CG	-5.82	101.92	115.30
1	I	304	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	C	636	LEU	CA-CB-CG	-5.49	102.67	115.30
1	E	97	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	C	208	LYS	CD-CE-NZ	-5.16	99.83	111.70
1	C	773	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	G	636	LEU	CA-CB-CG	-5.08	103.61	115.30
2	L	45	LEU	CA-CB-CG	5.07	126.96	115.30

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	93	0
1	C	4993	0	4832	75	0
1	E	4983	0	4826	70	0
1	G	5008	0	4839	67	0
1	I	4968	0	4815	88	0
1	K	4996	0	4835	82	0
2	B	589	0	592	17	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	K	7	0	0	0	0
All	All	33550	0	32398	516	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 (516) 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
2:L:21:GLU:OE2	2:L:24:LYS:NZ	2.00	0.94
1:A:730:SER:OG	1:A:732:ASP:OD1	1.86	0.94
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:543:LYS:HZ3	1:K:599:SER:HB2	1.46	0.80
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:N	1:A:732:ASP:OD1	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:HG2	1:I:304:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:545:ARG:NH1	1:A:545:ARG:HG3	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:K:543:LYS:HZ1	1:K:599:SER:HB2	1.54	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:OD1	1:G:24:ASP:N	2.27	0.68
1:I:394:GLY:HA2	1:I:397:ARG:HD3	1.74	0.68
1:C:545:ARG:NH1	1:C:545:ARG:HG3	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:E:558:ILE:HG22	1:E:561:ARG:HD2	1.80	0.63
1:A:115:ARG:NH2	1:A:654:LEU:O	2.31	0.63
1:E:407:GLN:HG3	1:E:407:GLN:O	1.97	0.63
1:C:4:PRO:HD3	1:G:140:MSE:HE3	1.80	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:C:155:HIS:CD2	1:C:156:PHE:H	2.17	0.62
1:A:223:ASP:HB3	1:A:226:THR:HG23	1.82	0.62
1:K:245:HIS:CG	1:K:328:GLU:OE1	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:CG	1:A:545:ARG:HH11	2.14	0.61
1:I:223:ASP:O	1:I:226:THR:HG23	1.99	0.61
1:C:714:ARG:HA	1:C:719:PHE:CD1	2.35	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
1:K:63:THR:HG22	1:K:77:MSE:HB3	1.83	0.60
2:F:1:ARG:HH11	2:F:3:LYS:HB3	1.66	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:G:223:ASP:O	1:G:226:THR:HG23	2.01	0.60
1:E:369:MSE:HG2	1:E:373:MSE:HG3	1.84	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: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:A:392:MSE:HA	1:A:392:MSE:HE2	1.85	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:K:110:LYS:O	1:K:114:GLN:HG3	2.04	0.58
1:A:667:LYS:N	1:A:671:GLN:OE1	2.36	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:K:602:GLU:O	1:K:603:THR:HG22	2.04	0.57
1:E:538:TYR:N	1:E:538:TYR:CD1	2.72	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:K:329:ARG:HG2	1:K:329:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:370:VAL:HG22	1:I:373:MSE:HE2	1.87	0.56
1:C:384:GLU:HG2	1:C:387:ARG:HD2	1.88	0.56
1:K:329:ARG:HG2	1:K:329:ARG:HH11	1.71	0.56
2:H:10:GLU:HG3	2:H:27:MSE:HE1	1.87	0.56
2:D:27:MSE:HE2	2:D:39:LEU:HD23	1.87	0.56
1:G:639:GLU:OE2	1:G:642:LYS:NZ	2.38	0.56
1:C:114:GLN:O	1:C:118:ARG:HG2	2.06	0.56
1:I:370:VAL:HA	1:I:373:MSE:HG3	1.87	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:113:GLN:OE1	1:G:117:ARG:NH2	2.33	0.56
1:G:49:ASP:HB3	1:G:96:ARG:HD2	1.88	0.56
1:I:321:LEU:HD11	1:I:370:VAL:HG12	1.88	0.55
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: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:I:86:ASP:OD2	1:I:182:ARG:NH1	2.38	0.55
1:C:351:SER:HB3	1:C:399:GLU:HG2	1.87	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:670:TRP:CZ3	1:A:671:GLN:HG2	2.42	0.54
1:A:228:HIS:NE2	1:A:246:GLU:OE1	2.40	0.54
1:K:102:ILE:HD12	1:K:198:ASP:HA	1.89	0.54
1:C:296:ARG:HH22	1:C:299:ASN:HD21	1.53	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
1:C:115:ARG:NH2	1:C:654:LEU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:ILE:HB	1:I:303:LEU:HB2	1.90	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:714:ARG:HA	1:I:719:PHE:CD1	2.44	0.53
1:K:642:LYS:O	1:K:646:GLN:HG2	2.08	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:G:359:ILE:O	1:G:363:ILE:HG12	2.08	0.53
2:B:63:LYS:O	2:B:67:MSE:HG3	2.08	0.53
1:G:670:TRP:CZ3	1:G:671:GLN:HG2	2.43	0.53
1:I:359:ILE:O	1:I:363:ILE:HG12	2.09	0.53
1:I:63:THR:HG22	1:I:77:MSE:HB3	1.91	0.53
1:A:747:LYS:HE2	1:K:364:LYS:HD3	1.91	0.53
1:K:586:TRP:CE2	1:K:617:PRO:HG3	2.43	0.53
1:K:321:LEU:HD12	1:K:322:PRO:HD2	1.90	0.53
1:I:329:ARG:NH2	1:I:378:THR:O	2.31	0.53
1:E:548:ARG:HH21	1:E:554:GLY:HA3	1.73	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:I:164:GLY:O	1:I:702:ARG:HD2	2.09	0.52
1:E:535:ILE:HD11	1:E:549:ALA:HB3	1.90	0.52
1:A:536:ARG:O	1:A:542:TRP:HB3	2.09	0.52
1:G:559:GLU:OE2	1:G:563:ARG:NH1	2.38	0.52
1:E:399:GLU:OE2	1:E:598:ALA:N	2.42	0.52
1:C:84:TYR:HE1	1:C:298:LYS:HE3	1.73	0.52
1:A:164:GLY:O	1:A:702:ARG:HD2	2.10	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:I:601:PHE:O	1:I:604:VAL:HB	2.10	0.51
1:G:114:GLN:HB3	1:G:118:ARG:HH21	1.75	0.51
1:E:543:LYS:HZ2	1:E:599:SER:HG	1.57	0.51
1:C:381:GLY:HA2	1:C:576:LEU:HG	1.92	0.51
1:G:114:GLN:O	1:G:118:ARG:HG2	2.10	0.51
1:E:61:PRO:HG3	1:K:144:ILE:HD12	1.92	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:K:625:MSE:HE2	1:K:688:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:381:GLY:HA2	1:E:576:LEU:HG	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:G:737:ASP:OD1	1:G:739:THR:HB	2.11	0.50
1:A:118:ARG:NH2	3:A:1788:SO4:O1	2.44	0.50
2:B:27:MSE:HE2	2:B:39:LEU:HD23	1.93	0.50
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
2:L:12:LYS:HB3	2:L:13:LEU:HA	1.94	0.50
1:C:318:MSE:HB3	1:C:371:TYR:OH	2.12	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: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:K:110:LYS:HE3	1:K:344:ASP:OD2	2.12	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:C:230:LEU:HD12	1:C:231:CYS:N	2.26	0.49
1:A:721:PHE:CD2	1:K:319:PRO:HB2	2.47	0.49
1:C:564:VAL:HG12	1:C:592:TYR:CE2	2.47	0.49
1:A:373:MSE:HG3	1:A:387:ARG:HE	1.76	0.49
2:B:1:ARG:O	2:F:38:GLN:HG2	2.13	0.49
1:A:408:GLN:O	1:A:409:ASP:OD1	2.29	0.49
1:G:164:GLY:O	1:G:702:ARG:HD2	2.12	0.49
1:E:295:GLN:HB2	1:E:297:GLU:O	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
1:K:408:GLN:OE1	1:K:408:GLN:N	2.46	0.49
2:J:48:ASN:HA	2:J:52:LEU:HD12	1.94	0.49
1:A:114:GLN:O	1:A:118:ARG:HG2	2.12	0.49
1:E:384:GLU:HG2	1:E:387:ARG:CD	2.43	0.49
1:C:108:ARG:HD2	1:C:111:MSE:HE2	1.95	0.49
1:G:384:GLU:HG2	1:G:387:ARG:CD	2.43	0.49
2:J:58:GLN:H	2:J:58:GLN:CD	2.16	0.49
1:A:602:GLU:HG3	1:A:603:THR:HG23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:LEU:O	1:G:398:VAL:HG12	2.12	0.48
2:B:45:LEU:O	2:B:49:VAL:HG23	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
2:L:58:GLN:H	2:L:58:GLN:CD	2.16	0.48
1:C:4:PRO:HD3	1:G:140:MSE:CE	2.43	0.48
1:C:625:MSE:SE	1:C:636:LEU:CD2	3.11	0.48
2:B:34:TYR:CE1	2:B:67:MSE:HE1	2.49	0.48
1:A:240:LEU:O	1:A:244:THR:HG23	2.14	0.48
1:G:547:TYR:CZ	1:G:561:ARG:HG2	2.48	0.48
1:I:337:LEU:O	1:I:340:PHE:HB2	2.14	0.48
1:I:118:ARG:NH2	3:I:1788:SO4:O4	2.46	0.48
2:F:45:LEU:O	2:F:49:VAL:HG23	2.14	0.48
1:C:602:GLU:HG3	1:C:603:THR:HG23	1.96	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
2:D:58:GLN:H	2:D:58:GLN:CD	2.17	0.48
2:D:12:LYS:HD3	2:D:13:LEU:HD12	1.95	0.48
1:I:623:GLN:O	1:I:627:VAL:HG22	2.13	0.48
1:A:408:GLN:H	1:A:408:GLN:HG2	1.46	0.48
1:C:128:LYS:O	1:C:132:ILE:HG12	2.14	0.48
2:H:48:ASN:HA	2:H:52:LEU:HD12	1.96	0.48
1:C:729:LYS:HA	1:C:750:TYR:CG	2.49	0.48
2:B:64:ILE:HA	2:B:64:ILE:HD13	1.66	0.48
1:E:544:ASP:OD1	1:E:561:ARG:NH2	2.45	0.48
1:K:295:GLN:NE2	1:K:298:LYS:HA	2.29	0.48
1:I:675:LEU:HA	1:I:675:LEU:HD23	1.71	0.48
1:G:748:ILE:HA	1:G:782:LEU:O	2.14	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:329:ARG:NH1	1:E:378:THR:O	2.47	0.47
2:D:63:LYS:O	2:D:67:MSE:HG3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:659:PHE:CD2	1:G:676:LEU:HD21	2.49	0.47
1:I:547:TYR:OH	1:I:600:ASP:OD2	2.30	0.47
1:A:110:LYS:O	1:A:114:GLN:HG3	2.15	0.47
2:J:45:LEU:O	2:J:49:VAL:HG23	2.14	0.47
2:F:10:GLU:HG3	2:F:27:MSE:HE1	1.96	0.47
1:I:761:PHE:HB3	1:I:773:LEU:HB3	1.97	0.47
1:C:164:GLY:O	1:C:702:ARG:HD2	2.15	0.47
1:E:602:GLU:O	1:E:603:THR:OG1	2.26	0.47
1:G:309:ARG:NH1	1:G:309:ARG:HB3	2.30	0.47
1:C:547:TYR:CE1	1:C:561:ARG:HG2	2.50	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:571:GLY:O	1:C:575:VAL:HG23	2.14	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
1:C:642:LYS:O	1:C:646:GLN:HG2	2.15	0.47
1:I:107:PRO:O	1:I:111:MSE:HG3	2.15	0.46
1:C:147:PRO:HA	1:G:257:VAL:CG2	2.46	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:E:365:LEU:HD23	1:E:365:LEU:HA	1.59	0.46
1:E:309:ARG:HB3	1:E:309:ARG:HH11	1.80	0.46
1:I:110:LYS:O	1:I:114:GLN:HG3	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:128:LYS:O	1:A:132:ILE:HG12	2.15	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
1:A:369:MSE:O	1:A:372:GLN:HB2	2.16	0.46
1:K:586:TRP:CZ2	1:K:617:PRO:HG3	2.50	0.46
1:G:355:ARG:NH2	1:G:666:LYS:HZ3	2.14	0.46
1:A:564:VAL:HG12	1:A:592:TYR:CZ	2.51	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
1:C:321:LEU:HD12	1:C:322:PRO:HD3	1.98	0.46
1:I:102:ILE:HD11	1:I:175:LEU:HD12	1.96	0.46
1:G:559:GLU:HG2	1:G:563:ARG:HH12	1.81	0.46
2:D:62:GLN:OE1	2:D:65:ARG:NH1	2.49	0.46
1:K:748:ILE:HA	1:K:782:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:57:SER:O	2:B:61:MSE:HG2	2.16	0.46
1:A:60:HIS:HB2	1:A:61:PRO:HD3	1.96	0.46
1:G:68:ARG:NH2	3:G:1790:SO4:O3	2.44	0.45
1:K:555:SER:HA	1:K:561:ARG:NH2	2.31	0.45
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:I:392:MSE:HE2	1:I:392:MSE:HA	1.98	0.45
1:K:113:GLN:HG3	1:K:344:ASP:O	2.16	0.45
1:G:352:LEU:HD21	1:G:395:LEU:HD21	1.97	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:K:539:GLU:CD	1:K:540:SER:H	2.20	0.45
1:G:136:ARG:O	1:G:140:MSE:HB2	2.16	0.45
1:G:566:TRP:HA	1:G:569:VAL:HG22	1.98	0.45
1:I:304:ARG:HH11	1:I:304:ARG:CG	2.22	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:100:MSE:CE	1:I:175:LEU:HD22	2.37	0.45
1:G:136:ARG:HH12	1:G:147:PRO:HA	1.82	0.45
1:K:550:LYS:HB3	1:K:594:TYR:CD2	2.52	0.45
1:A:375:GLY:C	1:A:387:ARG:NH1	2.70	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:714:ARG:HA	1:C:719:PHE:CE1	2.52	0.45
1:I:115:ARG:NH2	1:I:654:LEU:O	2.50	0.45
1:G:559:GLU:HG2	1:G:563:ARG:NH1	2.32	0.45
1:C:571:GLY:HA2	1:C:588:TRP:CH2	2.51	0.45
1:I:135:GLN:HA	1:I:138:ARG:NH1	2.32	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:C:351:SER:CB	1:C:399:GLU:HG2	2.47	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
2:F:58:GLN:H	2:F:58:GLN:CD	2.20	0.44
1:K:384:GLU:O	1:K:384:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:193:GLU:HG2	1:K:741:LEU:HD22	2.00	0.44
1:E:215:LYS:HE2	1:E:787:GLU:OE2	2.17	0.44
1:K:714:ARG:HA	1:K:719:PHE:CD1	2.53	0.44
1:E:623:GLN:HG3	1:E:624:LEU:N	2.31	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:G:309:ARG:HB3	1:G:309:ARG:HH11	1.82	0.44
1:E:624:LEU:HA	1:E:624:LEU:HD23	1.58	0.44
1:C:257:VAL:HA	1:G:145:ALA:O	2.17	0.44
1:E:625:MSE:SE	1:E:636:LEU:HD22	2.67	0.44
1:K:351:SER:HB3	1:K:399:GLU:HG2	1.99	0.44
1:I:396:GLY:O	1:I:399:GLU:HG2	2.18	0.44
1:A:318:MSE:SE	1:A:370:VAL:HG11	2.68	0.44
1:E:548:ARG:HH21	1:E:554:GLY:CA	2.31	0.44
1:C:547:TYR:CZ	1:C:561:ARG:HG2	2.52	0.44
1:K:351:SER:CB	1:K:399:GLU:HG2	2.47	0.44
1:A:623:GLN:O	1:A:627:VAL:HB	2.18	0.44
1:E:710:ILE:HG22	1:E:783:TYR:HB2	2.00	0.44
1:E:98:LEU:O	1:E:194:ILE:HA	2.17	0.44
1:K:114:GLN:HB3	1:K:118:ARG:HH21	1.83	0.44
1:I:547:TYR:CZ	1:I:561:ARG:HG2	2.52	0.44
2:B:10:GLU:O	2:B:23:ARG:NH2	2.51	0.44
1:A:399:GLU:OE1	1:A:599:SER:OG	2.34	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
1:C:541:GLY:C	1:C:545:ARG:HH12	2.21	0.43
1:K:660:ARG:CD	2:L:53:GLY:HA3	2.43	0.43
2:H:61:MSE:O	2:H:65:ARG:HB2	2.17	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:I:247:ALA:O	1:I:306:PRO:HG3	2.18	0.43
1:E:251:ILE:HB	1:E:303:LEU:HB2	2.00	0.43
2:D:7:VAL:O	2:D:10:GLU:HB2	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
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:K:254:GLU:CD	1:K:298:LYS:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:670:TRP:CZ3	1:I:671:GLN:HG2	2.53	0.43
1:K:543:LYS:HZ1	1:K:599:SER:CB	2.28	0.43
1:I:571:GLY:HA2	1:I:588:TRP:CH2	2.54	0.43
1:G:379:LYS:NZ	3:G:1791:SO4:O2	2.50	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:HD3	2:J:12:LYS:HA	1.86	0.43
1:I:709:ARG:HD3	1:I:751:ASP:OD2	2.19	0.43
1:I:249:PHE:O	1:I:305:ILE:HB	2.19	0.43
1:I:114:GLN:O	1:I:118:ARG:HG2	2.19	0.42
1:E:407:GLN:HB3	1:E:408:GLN:NE2	2.34	0.42
1:K:251:ILE:HB	1:K:303:LEU:HB2	2.01	0.42
1:I:321:LEU:HD12	1:I:321:LEU:HA	1.80	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
2:H:58:GLN:CD	2:H:58:GLN:H	2.21	0.42
1:G:163:PRO:HB3	1:G:199:ALA:HB1	2.02	0.42
1:K:625:MSE:SE	1:K:636:LEU:HD13	2.69	0.42
1:E:383:PRO:HD3	1:E:576:LEU:HD23	2.01	0.42
1:C:321:LEU:HD12	1:C:322:PRO:CD	2.48	0.42
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.84	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:C:251:ILE:HB	1:C:303:LEU:HB2	2.00	0.42
1:E:140:MSE:HE3	1:K:4:PRO:HD3	2.00	0.42
1:K:240:LEU:O	1:K:244:THR:HG23	2.19	0.42
1:C:392:MSE:HA	1:C:392:MSE:HE2	2.01	0.42
1:A:624:LEU:HD23	1:A:624:LEU:HA	1.80	0.42
1:K:637:PRO:O	1:K:641:GLN:HG3	2.19	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:390:MSE:HE2	1:A:390:MSE:HB3	1.91	0.42
1:E:340:PHE:CZ	1:E:392:MSE:SE	3.22	0.42
1:A:564:VAL:HG12	1:A:592:TYR:CE1	2.54	0.42
1:A:348:HIS:ND1	1:A:348:HIS:O	2.51	0.42
1:A:373:MSE:HG3	1:A:373:MSE:O	2.19	0.42
1:C:155:HIS:CG	1:C:156:PHE:N	2.85	0.42
1:E:114:GLN:O	1:E:118:ARG:HG2	2.20	0.42
1:C:321:LEU:HA	1:C:322:PRO:HD3	1.88	0.42
1:A:157:ASP:OD1	1:A:159:ASN:HB2	2.20	0.42
1:A:714:ARG:HA	1:A:719:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:MSE:HE1	1:E:618:PHE:CE2	2.55	0.42
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.84	0.42
1:C:408:GLN:O	1:C:409:ASP:HB2	2.20	0.42
1:C:729:LYS:HA	1:C:750:TYR:CD2	2.55	0.42
1:A:251:ILE:O	1:A:302:PHE:HA	2.19	0.42
1:E:48:PHE:CD2	1:E:229:CYS:HB2	2.55	0.42
2:B:58:GLN:CD	2:B:58:GLN:H	2.23	0.42
1:E:543:LYS:NZ	1:E:600:ASP:OD1	2.34	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:181:ASP:OD2	1:C:182:ARG:NH1	2.51	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:C:228:HIS:NE2	1:C:246:GLU:OE1	2.50	0.42
1:A:399:GLU:OE2	1:A:597:PHE:HB3	2.20	0.41
1:I:142:GLU:HB2	1:I:144:ILE:HD13	2.02	0.41
1:E:230:LEU:HD21	1:E:237:LEU:HD22	2.02	0.41
1:A:373:MSE:HG2	1:A:387:ARG:CG	2.50	0.41
2:J:8:GLU:CD	2:J:24:LYS:NZ	2.73	0.41
2:B:47:ILE:O	2:B:51:LEU:HB2	2.20	0.41
1:A:646:GLN:HG3	1:A:648:ASP:OD1	2.20	0.41
1:E:633:LYS:NZ	1:E:645:ILE:HD13	2.34	0.41
1:K:104:GLY:C	1:K:163:PRO:HG3	2.41	0.41
1:K:590:PHE:CE2	1:K:592:TYR:HB2	2.55	0.41
1:K:576:LEU:HD12	1:K:576:LEU:HA	1.91	0.41
1:A:6:PHE:CZ	1:A:239:MSE:HE1	2.54	0.41
1:C:545:ARG:HH11	1:C:545:ARG:CG	2.23	0.41
1:C:7:PHE:HB3	1:C:256:PHE:CZ	2.55	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.67	0.41
1:E:309:ARG:NH1	1:E:309:ARG:HB3	2.35	0.41
1:E:108:ARG:HD2	1:E:111:MSE:HE3	2.01	0.41
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.86	0.41
1:E:709:ARG:NH1	1:E:751:ASP:OD2	2.44	0.41
1:E:321:LEU:HA	1:E:322:PRO:HD3	1.90	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: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:A:668:TYR:CD1	1:I:134:GLU:HG3	2.56	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:K:399:GLU:OE2	1:K:598:ALA:N	2.50	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:I:372:GLN:HB2	1:I:390:MSE:HE1	2.03	0.41
2:L:11:LYS:HE2	2:L:12:LYS:HG2	2.03	0.41
1:K:7:PHE:HE1	1:K:303:LEU:HD21	1.86	0.41
1:A:733:LEU:O	1:K:364:LYS:HE3	2.21	0.41
1:A:537:LEU:HA	1:A:542:TRP:HB2	2.03	0.41
1:C:646:GLN:HG3	1:C:648:ASP:OD1	2.21	0.41
1:C:329:ARG:NH1	1:C:378:THR:O	2.54	0.41
1:G:572:LEU:HD23	1:G:572:LEU:HA	1.83	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:C:728:SER:HA	1:I:397:ARG:HG2	2.02	0.41
1:E:407:GLN:NE2	1:E:538:TYR:CE1	2.89	0.41
2:B:10:GLU:O	2:B:12:LYS:HE3	2.21	0.41
1:K:13:LYS:HG2	1:K:14:TYR:CE1	2.56	0.41
1:G:369:MSE:C	1:G:369:MSE:SE	3.09	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
1:A:571:GLY:HA2	1:A:588:TRP:CH2	2.55	0.40
1:K:392:MSE:HB3	1:K:601:PHE:HB2	2.02	0.40
1:G:327:VAL:HG13	1:G:328:GLU:H	1.86	0.40
1:E:245:HIS:ND1	1:E:328:GLU:HG3	2.36	0.40
1:C:7:PHE:HB3	1:C:256:PHE:CE1	2.56	0.40
1:I:309:ARG:O	1:I:313:GLU:HB2	2.22	0.40
1:I:623:GLN:HG3	1:I:624:LEU:N	2.36	0.40
1:C:108:ARG:HG3	1:C:589:TYR:HB3	2.03	0.40
1:K:623:GLN:HG3	1:K:624:LEU:N	2.36	0.40
1:I:590:PHE:CE2	1:I:592:TYR:HB2	2.56	0.40
1:K:659:PHE:CD1	1:K:676:LEU:HD21	2.57	0.40
1:A:736:LEU:O	1:A:738:PRO:HD3	2.21	0.40
1:K:696:THR:HG23	1:K:699:GLU:OE1	2.21	0.40
1:G:625:MSE:SE	1:G:636:LEU:CD2	3.19	0.40
1:G:118:ARG:HB3	1:G:159:ASN:CG	2.42	0.40
1:K:120:ARG:NH2	1:K:672:GLY:O	2.55	0.40
2:D:48:ASN:HA	2:D:52:LEU:HD12	2.04	0.40
1:A:163:PRO:HG2	1:A:623:GLN:OE1	2.21	0.40
2:L:68:GLY:O	2:L:71:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:CYS:HA	1:G:250:ASN:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	602/636 (95%)	583 (97%)	18 (3%)	1 (0%)	52 83
1	C	601/636 (94%)	584 (97%)	17 (3%)	0	100 100
1	E	600/636 (94%)	583 (97%)	15 (2%)	2 (0%)	46 77
1	G	603/636 (95%)	586 (97%)	16 (3%)	1 (0%)	52 83
1	I	598/636 (94%)	580 (97%)	17 (3%)	1 (0%)	52 83
1	K	602/636 (95%)	584 (97%)	17 (3%)	1 (0%)	52 83
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%)	56 86

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	555	SER
1	E	555	SER
1	I	555	SER

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Mol	Chain	Res	Type
1	E	380	ASP
1	A	324	LYS
1	K	322	PRO

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%)	513 (95%)	25 (5%)	33	66
1	C	538/545 (99%)	512 (95%)	26 (5%)	31	64
1	E	537/545 (98%)	519 (97%)	18 (3%)	44	77
1	G	539/545 (99%)	522 (97%)	17 (3%)	46	79
1	I	535/545 (98%)	522 (98%)	13 (2%)	57	86
1	K	538/545 (99%)	522 (97%)	16 (3%)	48	80
2	B	62/61 (102%)	61 (98%)	1 (2%)	70	91
2	D	61/61 (100%)	59 (97%)	2 (3%)	45	77
2	F	62/61 (102%)	59 (95%)	3 (5%)	31	64
2	H	61/61 (100%)	59 (97%)	2 (3%)	45	77
2	J	58/61 (95%)	57 (98%)	1 (2%)	68	91
2	L	61/61 (100%)	59 (97%)	2 (3%)	45	77
All	All	3590/3636 (99%)	3464 (96%)	126 (4%)	43	76

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	118	ARG
1	A	168	MSE
1	A	239	MSE
1	A	298	LYS
1	A	329	ARG
1	A	340	PHE

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Mol	Chain	Res	Type
1	A	348	HIS
1	A	365	LEU
1	A	406	ARG
1	A	407	GLN
1	A	408	GLN
1	A	545	ARG
1	A	578	TYR
1	A	599	SER
1	A	603	THR
1	A	623	GLN
1	A	634	GLN
1	A	681	GLU
1	A	692	TYR
1	A	720	GLU
1	A	732	ASP
1	A	745	SER
1	A	761	PHE
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	239	MSE
1	C	295	GLN
1	C	296	ARG
1	C	309	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	578	TYR
1	C	599	SER
1	C	604	VAL
1	C	623	GLN
1	C	634	GLN
1	C	681	GLU

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Mol	Chain	Res	Type
1	C	682	THR
1	C	692	TYR
1	C	761	PHE
2	D	5	GLU
2	D	59	THR
1	E	24	ASP
1	E	25	ARG
1	E	118	ARG
1	E	155	HIS
1	E	239	MSE
1	E	324	LYS
1	E	329	ARG
1	E	340	PHE
1	E	373	MSE
1	E	408	GLN
1	E	540	SER
1	E	578	TYR
1	E	623	GLN
1	E	626	SER
1	E	634	GLN
1	E	692	TYR
1	E	745	SER
1	E	761	PHE
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	578	TYR
1	G	599	SER
1	G	603	THR
1	G	623	GLN
1	G	626	SER
1	G	634	GLN
1	G	692	TYR

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Mol	Chain	Res	Type
1	G	761	PHE
2	H	23	ARG
2	H	65	ARG
1	I	118	ARG
1	I	239	MSE
1	I	304	ARG
1	I	340	PHE
1	I	344	ASP
1	I	348	HIS
1	I	384	GLU
1	I	578	TYR
1	I	604	VAL
1	I	623	GLN
1	I	692	TYR
1	I	745	SER
1	I	761	PHE
2	J	23	ARG
1	K	118	ARG
1	K	239	MSE
1	K	320	ASN
1	K	328	GLU
1	K	329	ARG
1	K	340	PHE
1	K	348	HIS
1	K	384	GLU
1	K	548	ARG
1	K	578	TYR
1	K	623	GLN
1	K	634	GLN
1	K	648	ASP
1	K	692	TYR
1	K	704	THR
1	K	761	PHE
2	L	22	LEU
2	L	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	GLN
1	C	113	GLN
1	C	155	HIS

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Mol	Chain	Res	Type
1	C	299	ASN
1	C	408	GLN
1	C	623	GLN
1	E	408	GLN
1	E	581	GLN
2	F	44	GLN
1	G	299	ASN
2	J	40	GLN
1	K	348	HIS
1	K	407	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	1788	-	4,4,4	0.20	0	6,6,6	0.63	0
3	SO4	A	1789	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	A	1790	-	4,4,4	0.16	0	6,6,6	0.27	0
3	SO4	A	1791	-	4,4,4	0.21	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	A	1792	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	A	1793	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	1794	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	A	1795	-	4,4,4	0.15	0	6,6,6	0.26	0
3	SO4	C	1788	-	4,4,4	0.16	0	6,6,6	0.28	0
3	SO4	C	1789	-	4,4,4	0.18	0	6,6,6	0.57	0
3	SO4	C	1790	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	E	1788	-	4,4,4	0.56	0	6,6,6	0.26	0
3	SO4	E	1789	-	4,4,4	0.26	0	6,6,6	0.39	0
3	SO4	E	1790	-	4,4,4	0.23	0	6,6,6	0.36	0
3	SO4	E	1791	-	4,4,4	0.16	0	6,6,6	0.35	0
3	SO4	E	1792	-	4,4,4	0.21	0	6,6,6	0.15	0
3	SO4	G	1788	-	4,4,4	0.34	0	6,6,6	0.51	0
3	SO4	G	1789	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SO4	G	1790	-	4,4,4	0.21	0	6,6,6	0.20	0
3	SO4	G	1791	-	4,4,4	0.20	0	6,6,6	0.32	0
3	SO4	I	1788	-	4,4,4	0.31	0	6,6,6	0.32	0
3	SO4	I	1789	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	I	1790	-	4,4,4	0.19	0	6,6,6	0.16	0
3	SO4	K	1788	-	4,4,4	0.25	0	6,6,6	0.57	0
3	SO4	K	1789	-	4,4,4	0.21	0	6,6,6	0.38	0
3	SO4	K	1790	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	K	1791	-	4,4,4	0.22	0	6,6,6	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1789	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1791	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1792	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1793	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1794	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1795	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1789	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1789	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	E	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1791	-	-	0/0/0/0	0/0/0/0
3	SO4	E	1792	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1789	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	G	1791	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1789	-	-	0/0/0/0	0/0/0/0
3	SO4	I	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1788	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1789	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1790	-	-	0/0/0/0	0/0/0/0
3	SO4	K	1791	-	-	0/0/0/0	0/0/0/0

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	A	1788	SO4	1	0
3	A	1789	SO4	1	0
3	E	1788	SO4	1	0
3	G	1788	SO4	1	0
3	G	1790	SO4	1	0
3	G	1791	SO4	1	0
3	I	1788	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	594/636 (93%)	-0.02	14 (2%) 62 52	44, 75, 142, 177	0
1	C	592/636 (93%)	-0.13	6 (1%) 84 78	40, 66, 119, 197	0
1	E	592/636 (93%)	-0.09	9 (1%) 76 69	39, 67, 124, 154	0
1	G	594/636 (93%)	-0.01	4 (0%) 89 85	37, 71, 126, 170	0
1	I	590/636 (92%)	0.02	14 (2%) 62 52	40, 91, 152, 189	0
1	K	594/636 (93%)	-0.07	6 (1%) 84 78	40, 82, 143, 179	0
2	B	70/78 (89%)	-0.13	0 100 100	69, 89, 117, 134	0
2	D	68/78 (87%)	0.38	7 (10%) 9 4	69, 98, 144, 182	0
2	F	69/78 (88%)	0.02	0 100 100	80, 103, 130, 149	0
2	H	66/78 (84%)	1.21	11 (16%) 2 1	107, 151, 187, 203	0
2	J	64/78 (82%)	1.88	26 (40%) 0 0	114, 147, 185, 211	0
2	L	66/78 (84%)	1.85	28 (42%) 0 0	119, 154, 185, 197	0
All	All	3959/4284 (92%)	0.04	125 (3%) 51 40	37, 77, 148, 211	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	4	LEU	6.5
2	J	64	ILE	5.2
1	I	551	PHE	4.8
1	A	374	LYS	4.7
2	L	26	PHE	4.7
2	J	72	ALA	4.6
2	J	28	LEU	4.5
2	L	3	LYS	4.5
1	I	553	VAL	4.4
2	L	28	LEU	4.3
2	L	39	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	537	LEU	4.3
2	J	60	LEU	4.3
2	H	64	ILE	4.2
2	L	64	ILE	4.2
2	D	2	GLY	4.1
2	L	32	ASP	4.1
2	L	7	VAL	4.1
1	A	257	VAL	4.0
2	J	9	ALA	3.9
2	L	5	GLU	3.9
2	J	34	TYR	3.8
2	J	25	ALA	3.8
2	J	39	LEU	3.6
1	A	256	PHE	3.5
1	C	146	VAL	3.5
1	E	537	LEU	3.5
2	L	6	ASP	3.5
1	E	257	VAL	3.3
1	K	296	ARG	3.3
2	L	25	ALA	3.3
1	I	155	HIS	3.2
1	C	555	SER	3.2
2	D	3	LYS	3.2
2	J	32	ASP	3.2
2	L	31	TYR	3.1
2	J	20	TRP	3.1
1	E	296	ARG	3.0
2	J	7	VAL	3.0
2	J	70	GLY	3.0
2	D	4	LEU	2.9
2	H	28	LEU	2.9
1	A	153	GLU	2.9
2	J	71	ILE	2.9
2	H	51	LEU	2.9
1	C	556	ASP	2.8
1	I	556	ASP	2.8
2	J	37	ILE	2.8
2	J	46	PHE	2.8
2	J	44	GLN	2.8
2	L	33	ASP	2.8
2	J	8	GLU	2.8
1	G	643	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	538	TYR	2.7
2	J	31	TYR	2.7
2	L	23	ARG	2.7
1	I	546	TYR	2.7
2	J	24	LYS	2.7
1	A	554	GLY	2.7
1	I	296	ARG	2.7
2	L	14	TRP	2.7
2	J	69	ALA	2.7
2	J	41	CYS	2.7
1	G	556	ASP	2.6
2	H	71	ILE	2.6
2	H	56	TYR	2.6
2	L	37	ILE	2.6
1	C	205	GLY	2.5
1	K	155	HIS	2.5
1	E	555	SER	2.5
1	I	547	TYR	2.5
2	L	62	GLN	2.5
1	E	553	VAL	2.5
2	D	5	GLU	2.5
2	H	32	ASP	2.5
1	G	553	VAL	2.4
2	L	19	ALA	2.4
1	A	296	ARG	2.4
2	H	37	ILE	2.4
2	L	10	GLU	2.4
2	H	68	GLY	2.4
1	A	547	TYR	2.4
2	L	34	TYR	2.4
1	K	556	ASP	2.4
2	L	24	LYS	2.4
1	A	536	ARG	2.4
1	A	113	GLN	2.3
2	L	42	LEU	2.3
1	A	551	PHE	2.3
2	J	18	ASP	2.3
1	E	692	TYR	2.3
1	G	695	LEU	2.3
2	L	46	PHE	2.3
2	J	19	ALA	2.3
2	L	71	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	42	LEU	2.2
2	J	22	LEU	2.2
2	H	23	ARG	2.2
2	D	20	TRP	2.2
1	I	695	LEU	2.2
2	J	11	LYS	2.2
1	K	344	ASP	2.2
2	D	19	ALA	2.2
2	D	7	VAL	2.2
1	I	340	PHE	2.2
1	A	295	GLN	2.2
1	E	535	ILE	2.2
1	I	397	ARG	2.1
2	J	65	ARG	2.1
2	H	12	LYS	2.1
1	A	561	ARG	2.1
2	L	21	GLU	2.1
2	L	11	LYS	2.1
1	K	725	VAL	2.1
2	L	8	GLU	2.1
1	E	231	CYS	2.1
1	I	557	ASP	2.1
1	A	297	GLU	2.1
1	K	257	VAL	2.1
1	C	323	PHE	2.1
1	I	324	LYS	2.0
2	L	70	GLY	2.0
1	C	148	PRO	2.0
1	A	316	LEU	2.0
1	E	536	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	C	1790	5/5	0.89	0.24	3.39	153,154,155,156	0
3	SO4	C	1788	5/5	0.99	0.37	2.10	55,68,79,81	0
3	SO4	I	1788	5/5	0.98	0.29	1.98	83,85,88,91	0
3	SO4	E	1788	5/5	0.98	0.31	1.91	61,67,73,75	0
3	SO4	A	1788	5/5	0.99	0.31	1.49	71,72,74,76	0
3	SO4	G	1788	5/5	0.98	0.28	0.93	65,66,77,83	0
3	SO4	K	1788	5/5	0.97	0.26	0.57	78,80,84,96	0
3	SO4	I	1790	5/5	0.93	0.13	-0.88	140,143,144,144	0
3	SO4	E	1791	5/5	0.90	0.13	-1.48	107,119,122,122	0
3	SO4	G	1789	5/5	0.95	0.10	-4.46	110,115,118,120	0
3	SO4	A	1790	5/5	0.95	0.19	-	112,116,120,122	0
3	SO4	K	1791	5/5	0.96	0.18	-	138,139,139,140	0
3	SO4	C	1789	5/5	0.85	0.14	-	106,121,126,134	0
3	SO4	G	1790	5/5	0.90	0.11	-	132,133,135,136	0
3	SO4	A	1794	5/5	0.92	0.28	-	155,157,158,159	0
3	SO4	A	1795	5/5	0.89	0.25	-	119,131,132,135	0
3	SO4	E	1792	5/5	0.90	0.37	-	141,144,144,148	0
3	SO4	I	1789	5/5	0.91	0.15	-	156,156,158,159	0
3	SO4	A	1789	5/5	0.85	0.18	-	141,146,147,147	0
3	SO4	E	1790	5/5	0.84	0.24	-	126,134,136,144	0
3	SO4	K	1789	5/5	0.87	0.23	-	131,148,151,151	0
3	SO4	A	1791	5/5	0.89	0.19	-	146,146,150,151	0
3	SO4	G	1791	5/5	0.91	0.15	-	114,125,128,130	0
3	SO4	A	1792	5/5	0.91	0.14	-	143,147,147,149	0
3	SO4	A	1793	5/5	0.93	0.14	-	125,125,126,133	0
3	SO4	E	1789	5/5	0.92	0.18	-	117,120,126,127	0
3	SO4	K	1790	5/5	0.95	0.13	-	108,119,122,125	0

6.5 Other polymers

There are no such residues in this entry.