W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 12, 2024 – 06:56 PM EST

PDB ID	:	3SDM
Title	:	Structure of oligomeric kinase/RNase Ire1 in complex with an oligonucleotide
Authors	:	Korennykh, A.; Korostelev, A.; Egea, P.; Finer-Moore, J.; Zhang, C.; Stroud, R.; Shokat, K.; Walter, P.
Deposited on	:	2011-06-09
Resolution	:	6.60 Å(reported)

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

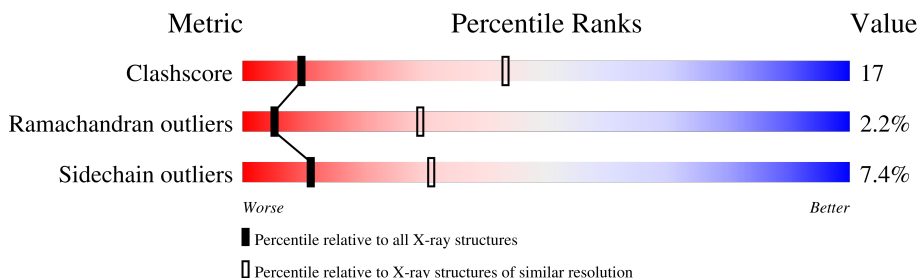|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 6.60 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		2.2%
Sidechain outliers		7.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1140 (9.00-4.00)
Ramachandran outliers	177936	1010 (9.00-4.00)
Sidechain outliers	177891	1032 (9.00-3.96)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	448	57% 31% 5% 7%
1	B	448	58% 30% 5% 7%
1	C	448	58% 29% 5% 7%
1	D	448	58% 29% 6% 7%
1	E	448	57% 31% 5% 7%
1	F	448	57% 31% 5% 7%
1	G	448	58% 31% • 7%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 23793 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	B	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	C	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	D	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	E	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	F	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	G	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			

There are 203 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	PRO	-	expression tag	UNP P32361
A	?	-	ASN	deletion	UNP P32361
A	?	-	ASN	deletion	UNP P32361
A	?	-	LEU	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	CYS	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
A	?	-	TYR	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	PRO	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
B	640	PRO	-	expression tag	UNP P32361
B	?	-	ASN	deletion	UNP P32361
B	?	-	ASN	deletion	UNP P32361
B	?	-	LEU	deletion	UNP P32361
B	?	-	GLN	deletion	UNP P32361
B	?	-	CYS	deletion	UNP P32361
B	?	-	GLN	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ARG	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361
B	?	-	TYR	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	PRO	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP P32361
C	640	PRO	-	expression tag	UNP P32361
C	?	-	ASN	deletion	UNP P32361
C	?	-	ASN	deletion	UNP P32361
C	?	-	LEU	deletion	UNP P32361
C	?	-	GLN	deletion	UNP P32361
C	?	-	CYS	deletion	UNP P32361
C	?	-	GLN	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	GLU	deletion	UNP P32361
C	?	-	THR	deletion	UNP P32361
C	?	-	GLU	deletion	UNP P32361
C	?	-	HIS	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	ARG	deletion	UNP P32361
C	?	-	HIS	deletion	UNP P32361
C	?	-	THR	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	VAL	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	ASP	deletion	UNP P32361
C	?	-	SER	deletion	UNP P32361
C	?	-	PHE	deletion	UNP P32361
C	?	-	TYR	deletion	UNP P32361
C	?	-	ASP	deletion	UNP P32361
C	?	-	PRO	deletion	UNP P32361
C	?	-	PHE	deletion	UNP P32361
D	640	PRO	-	expression tag	UNP P32361
D	?	-	ASN	deletion	UNP P32361
D	?	-	ASN	deletion	UNP P32361
D	?	-	LEU	deletion	UNP P32361
D	?	-	GLN	deletion	UNP P32361
D	?	-	CYS	deletion	UNP P32361
D	?	-	GLN	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	GLU	deletion	UNP P32361
D	?	-	THR	deletion	UNP P32361
D	?	-	GLU	deletion	UNP P32361
D	?	-	HIS	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	ARG	deletion	UNP P32361
D	?	-	HIS	deletion	UNP P32361
D	?	-	THR	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	VAL	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	ASP	deletion	UNP P32361
D	?	-	SER	deletion	UNP P32361
D	?	-	PHE	deletion	UNP P32361
D	?	-	TYR	deletion	UNP P32361
D	?	-	ASP	deletion	UNP P32361
D	?	-	PRO	deletion	UNP P32361
D	?	-	PHE	deletion	UNP P32361
E	640	PRO	-	expression tag	UNP P32361
E	?	-	ASN	deletion	UNP P32361
E	?	-	ASN	deletion	UNP P32361
E	?	-	LEU	deletion	UNP P32361
E	?	-	GLN	deletion	UNP P32361
E	?	-	CYS	deletion	UNP P32361
E	?	-	GLN	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
E	?	-	THR	deletion	UNP P32361
E	?	-	GLU	deletion	UNP P32361
E	?	-	HIS	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	ARG	deletion	UNP P32361
E	?	-	HIS	deletion	UNP P32361
E	?	-	THR	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	VAL	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	ASP	deletion	UNP P32361
E	?	-	SER	deletion	UNP P32361
E	?	-	PHE	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	TYR	deletion	UNP P32361
E	?	-	ASP	deletion	UNP P32361
E	?	-	PRO	deletion	UNP P32361
E	?	-	PHE	deletion	UNP P32361
F	640	PRO	-	expression tag	UNP P32361
F	?	-	ASN	deletion	UNP P32361
F	?	-	ASN	deletion	UNP P32361
F	?	-	LEU	deletion	UNP P32361
F	?	-	GLN	deletion	UNP P32361
F	?	-	CYS	deletion	UNP P32361
F	?	-	GLN	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	GLU	deletion	UNP P32361
F	?	-	THR	deletion	UNP P32361
F	?	-	GLU	deletion	UNP P32361
F	?	-	HIS	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	ARG	deletion	UNP P32361
F	?	-	HIS	deletion	UNP P32361
F	?	-	THR	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	VAL	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	ASP	deletion	UNP P32361
F	?	-	SER	deletion	UNP P32361
F	?	-	PHE	deletion	UNP P32361
F	?	-	TYR	deletion	UNP P32361
F	?	-	ASP	deletion	UNP P32361
F	?	-	PRO	deletion	UNP P32361
F	?	-	PHE	deletion	UNP P32361
G	640	PRO	-	expression tag	UNP P32361
G	?	-	ASN	deletion	UNP P32361
G	?	-	ASN	deletion	UNP P32361
G	?	-	LEU	deletion	UNP P32361
G	?	-	GLN	deletion	UNP P32361
G	?	-	CYS	deletion	UNP P32361
G	?	-	GLN	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	GLU	deletion	UNP P32361

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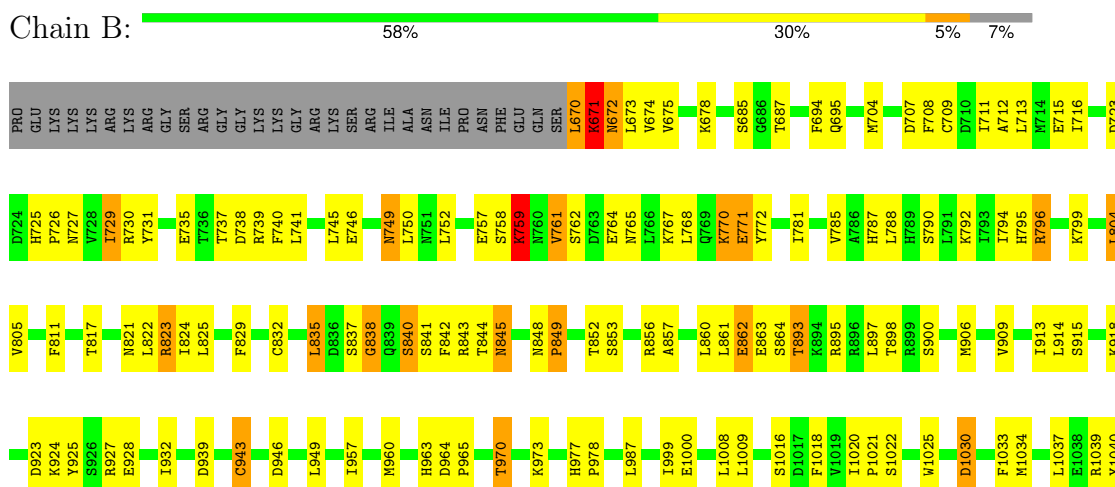| Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	THR	deletion	UNP P32361
G	?	-	GLU	deletion	UNP P32361
G	?	-	HIS	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	ARG	deletion	UNP P32361
G	?	-	HIS	deletion	UNP P32361
G	?	-	THR	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	VAL	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	ASP	deletion	UNP P32361
G	?	-	SER	deletion	UNP P32361
G	?	-	PHE	deletion	UNP P32361
G	?	-	TYR	deletion	UNP P32361
G	?	-	ASP	deletion	UNP P32361
G	?	-	PRO	deletion	UNP P32361
G	?	-	PHE	deletion	UNP P32361

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. 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. 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.

Note EDS failed to run properly.

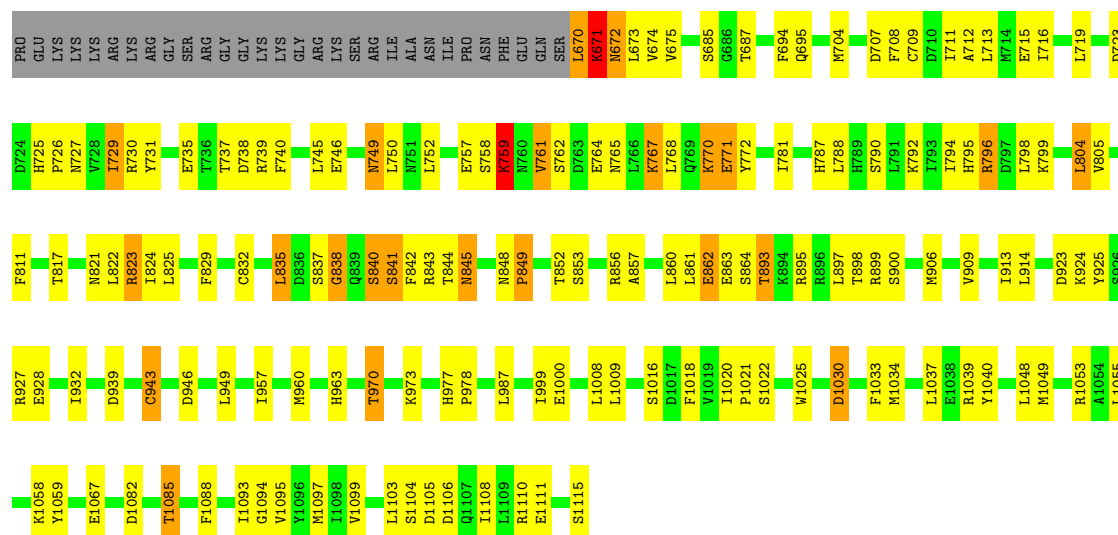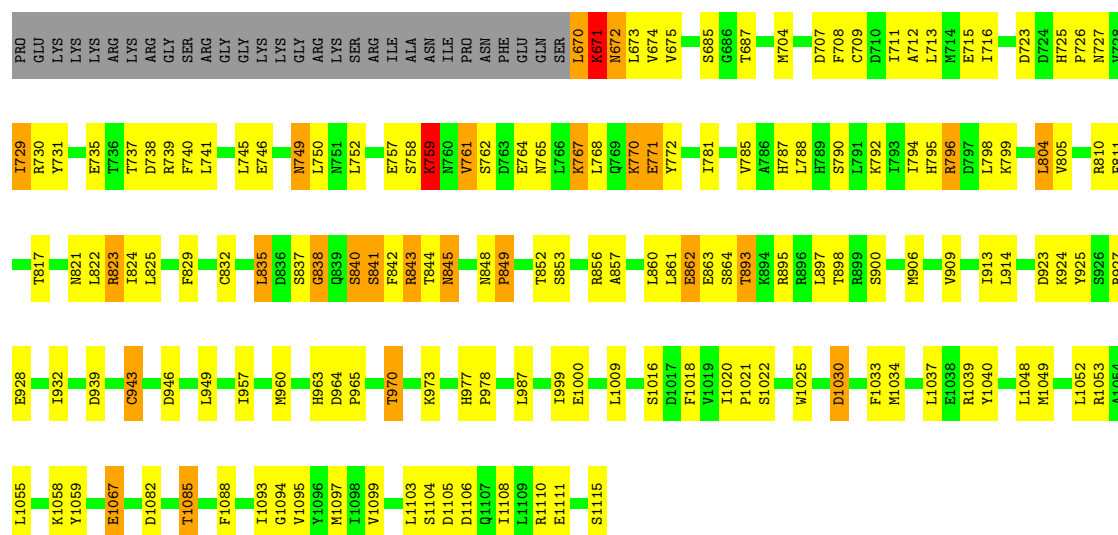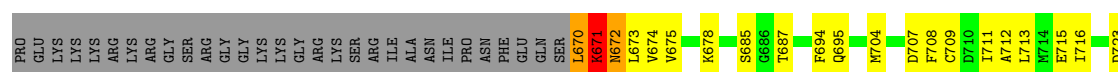• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain A:

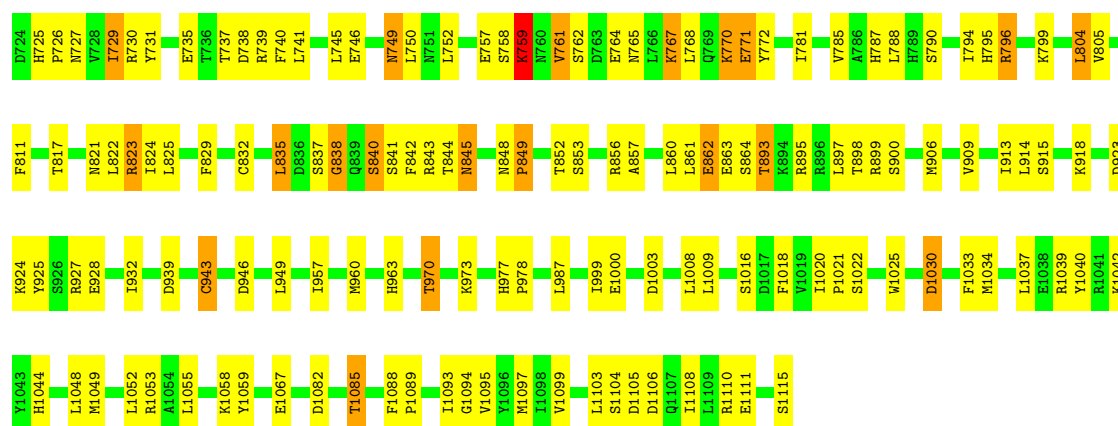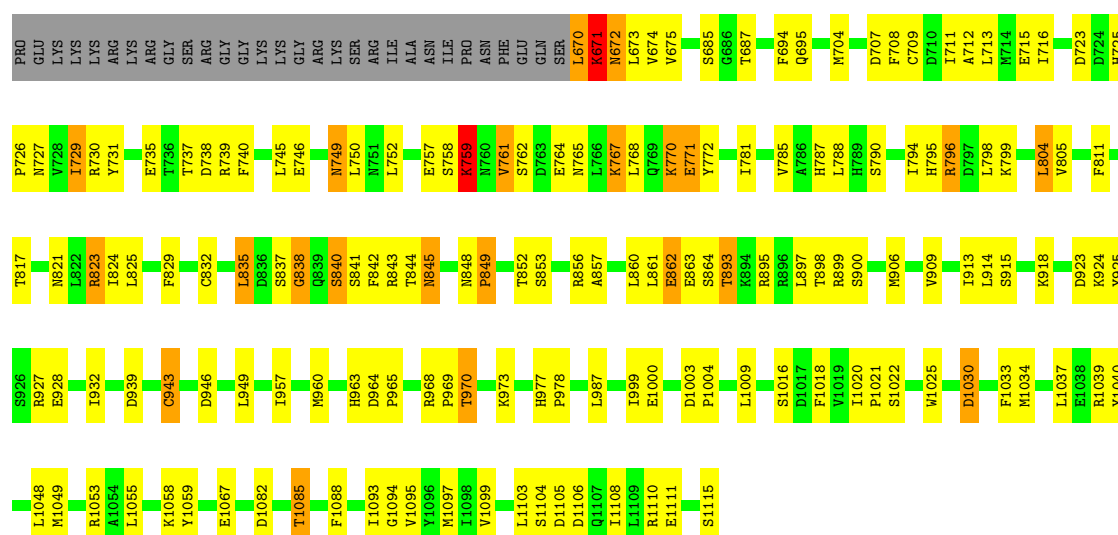• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain B:

L1048 M1049 R1053 A1054 L1055 K1058 E1067 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 R1110 E1111 S1115

• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain C:
58%   29%   5%   7%

PRO GLU LYS LYS LYS ARG ARG GLY LYS SER ARG GLY GLY LYS GLY ARG LYS SER ARG ILE ALA ASN ILE PRO ASN PHE GLU GLN SER L670 K671 N672 L673 V674 V675 S685 G686 T687 F694 Q695 M704 D707 F708 C709 D710 I711 A712 L713 M714 E715 I716 L719 D723

D724 H725 P726 N727 V728 I729 R730 Y731 E735 T736 T737 D738 R739 F740 L745 E746 N749 L750 N751 L752 E757 S758 K759 N760 V761 S762 D763 E764 N765 L766 K767 L768 Q769 K770 E771 Y772 I781 H787 L788 H789 S790 L791 K792 T793 I794 H795 R796 D797 L798 K799 L804 V805

F811 T817 N821 L822 R823 I824 L825 F829 C832 L835 D836 S837 G838 Q839 S840 S841 F842 R843 T844 N845 N848 P849 T852 S853 R856 A857 L860 L861 E862 E863 S864 T893 K894 R895 R896 L897 T898 H899 S900 M906 V909 I913 L914 D923 K924 Y925 S926

R927 E928 I932 D939 C943 D946 L949 I957 M960 H963 T970 K973 H977 P978 L987 I999 E1000 L1008 L1009 S1016 D1017 F1018 V1019 I1020 P1021 S1022 W1025 D1030 F1033 M1034 L1037 E1038 R1039 Y1040 L1048 M1049 R1053 A1054 L1055

K1058 Y1059 E1067 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 Q1107 I1108 L1109 R1110 E1111 S1115

• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain D:
58%   29%   6%   7%

PRO GLU LYS LYS LYS ARG LYS ARG GLY SER ARG GLY GLY LYS GLY ARG LYS SER ARG ILE ALA ASN ILE PRO ASN PHE GLU GLN SER L670 K671 N672 L673 V674 V675 S685 G686 T687 M704 D707 F708 C709 D710 I711 A712 L713 M714 E715 I716 D723 D724 H725 P726 N727 V728

I729 R730 Y731 E735 T736 T737 D738 R739 F740 L741 L745 E746 N749 L750 N751 L752 E757 S758 K759 N760 V761 S762 D763 E764 N765 L766 K767 L768 Q769 K770 E771 Y772 I781 V785 A786 H787 L788 H789 S790 L791 K792 T793 I794 H795 R796 D797 L798 K799 L804 V805 R810 F811

T817 N821 L822 R823 I824 L825 F829 C832 L835 D836 S837 G838 Q839 S840 S841 F842 R843 T844 N845 N848 P849 T852 S853 R856 A857 L860 L861 E862 E863 S864 T893 K894 R895 R896 L897 T898 H899 S900 M906 V909 I913 L914 D923 K924 Y925 S926 R927

E928 I932 D939 C943 D946 L949 I957 M960 H963 D964 P965 T970 K973 H977 P978 L987 I999 E1000 L1009 S1016 D1017 F1018 V1019 I1020 P1021 S1022 W1025 D1030 F1033 M1034 L1037 E1038 R1039 Y1040 L1048 M1049 L1052 R1053 A1054

L1055 K1058 Y1059 E1067 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 Q1107 I1108 L1109 R1110 E1111 S1115

• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain E:
57%   31%   5%   7%

PRO GLU LYS LYS LYS ARG ARG GLY SER ARG GLY GLY LYS GLY ARG LYS SER ARG ILE ALA ASN ILE PRO ASN PHE GLU GLN SER L670 K671 N672 L673 V674 V675 K678 S685 G686 T687 F694 Q695 M704 D707 F708 C709 D710 I711 A712 L713 M714 E715 I716 D723
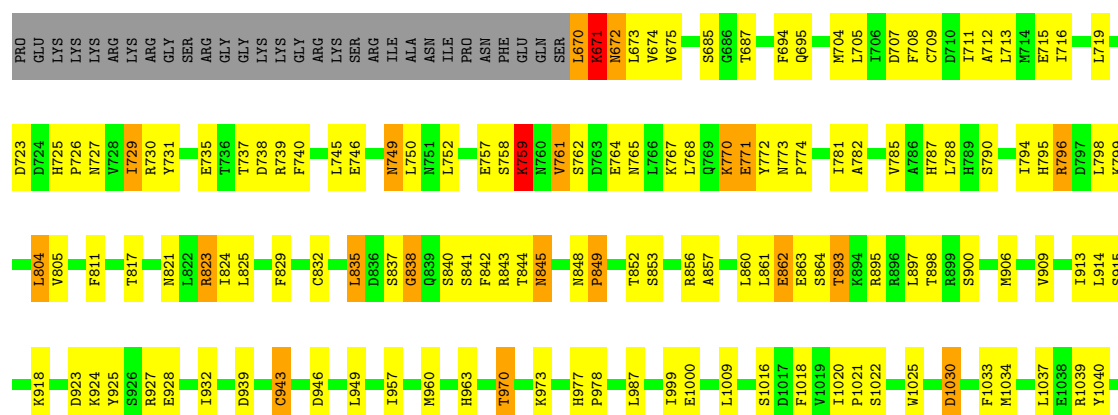
● Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain F:

● Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain G:

R1053 A1054 L1055 K1058 Y1059 E1067 E1071 D1082 T1085 F1088 I1093 G1094 V1095 Y1096 M1097 I1098 V1099 L1103 S1104 D1105 D1106 Q1107 I1108 L1109 R1110 E1111 S1115

4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	91.65Å 580.67Å 177.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.78 – 6.60	Depositor
% Data completeness (in resolution range)	99.8 (96.78-6.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.05 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.286 , 0.317	Depositor
Wilson B-factor (Å^2)	344.3	Xtriage
Anisotropy	0.407	Xtriage
L-test for twinning[2]	$<|L|> = 0.44$, $<L^2> = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23793	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.35	0/3437	0.49	0/4629
1	B	0.35	0/3437	0.49	0/4629
1	C	0.35	0/3437	0.49	0/4629
1	D	0.35	0/3437	0.49	0/4629
1	E	0.35	0/3437	0.49	0/4629
1	F	0.35	0/3437	0.49	0/4629
1	G	0.35	0/3437	0.49	0/4629
All	All	0.35	0/24059	0.49	0/32403

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	671	LYS	Peptide
1	B	671	LYS	Peptide
1	C	671	LYS	Peptide
1	D	671	LYS	Peptide
1	E	671	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3409	121	0
1	B	3399	0	3409	117	0
1	C	3399	0	3409	120	1
1	D	3399	0	3409	129	0
1	E	3399	0	3409	122	7
1	F	3399	0	3409	122	0
1	G	3399	0	3409	121	0
All	All	23793	0	23863	828	7

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 17.

The worst 5 of 828 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:D:840:SEP:O2P	1:E:761:VAL:HG11	1.35	1.23
1:A:848:ASN:HB3	1:A:849:PRO:HA	1.42	1.02
1:E:848:ASN:HB3	1:E:849:PRO:HA	1.42	1.01
1:D:848:ASN:HB3	1:D:849:PRO:HA	1.42	1.01
1:B:848:ASN:HB3	1:B:849:PRO:HA	1.42	1.00

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:ASP:O	1:E:1042:LYS:NZ[4_555]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:ASP:O	1:E:1042:LYS:CE[4_555]	1.50	0.70
1:E:1003:ASP:C	1:E:1042:LYS:NZ[4_555]	1.70	0.50
1:E:1003:ASP:OD2	1:E:1044:HIS:NE2[4_555]	1.73	0.47
1:C:761:VAL:CG1	1:E:840:SEP:O2P[2_555]	1.96	0.24

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	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	C	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	D	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	E	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
1	G	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	5	29
All	All	2891/3136 (92%)	2464 (85%)	364 (13%)	63 (2%)	5	29

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	LYS
1	A	770	LYS
1	A	771	GLU
1	A	862	GLU
1	B	759	LYS

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	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	B	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	C	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	D	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	E	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	F	380/405 (94%)	352 (93%)	28 (7%)	11	31
1	G	380/405 (94%)	352 (93%)	28 (7%)	11	31
All	All	2660/2835 (94%)	2464 (93%)	196 (7%)	11	31

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	707	ASP
1	F	707	ASP
1	E	750	LEU
1	E	845	ASN
1	F	767	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	725	HIS
1	G	725	HIS
1	E	691	GLN
1	G	691	GLN
1	G	845	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

21 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	TPO	C	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	C	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	C	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.74	0
1	SEP	A	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	TPO	B	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	B	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	TPO	G	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	E	844	1	8,10,11	3.11	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	G	840	1	8,9,10	1.65	1 (12%)	7,12,14	1.39	1 (14%)
1	TPO	F	844	1	8,10,11	3.12	5 (62%)	10,14,16	1.64	2 (20%)
1	SEP	D	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	F	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	A	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	SEP	B	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.42	1 (14%)
1	TPO	A	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.64	2 (20%)
1	TPO	D	844	1	8,10,11	3.10	5 (62%)	10,14,16	1.65	2 (20%)
1	SEP	E	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.40	1 (14%)
1	SEP	G	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.74	0
1	SEP	E	841	1	8,9,10	1.58	1 (12%)	7,12,14	0.73	0
1	SEP	D	841	1	8,9,10	1.57	1 (12%)	7,12,14	0.73	0
1	SEP	F	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.41	1 (14%)

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
1	TPO	C	844	1	-	4/9/11/13	-
1	SEP	C	840	1	-	4/6/8/10	-
1	SEP	C	841	1	-	1/6/8/10	-
1	SEP	A	841	1	-	1/6/8/10	-
1	TPO	B	844	1	-	4/9/11/13	-
1	SEP	B	841	1	-	1/6/8/10	-
1	TPO	G	844	1	-	4/9/11/13	-
1	TPO	E	844	1	-	4/9/11/13	-
1	SEP	G	840	1	-	4/6/8/10	-
1	TPO	F	844	1	-	4/9/11/13	-
1	SEP	D	840	1	-	4/6/8/10	-
1	SEP	F	841	1	-	1/6/8/10	-
1	SEP	A	840	1	-	4/6/8/10	-
1	SEP	B	840	1	-	4/6/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	TPO	D	844	1	-	4/9/11/13	-
1	SEP	E	840	1	-	4/6/8/10	-
1	SEP	G	841	1	-	1/6/8/10	-
1	SEP	E	841	1	-	1/6/8/10	-
1	SEP	D	841	1	-	1/6/8/10	-
1	SEP	F	840	1	-	4/6/8/10	-

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	844	TPO	O-C	5.56	1.41	1.20
1	D	844	TPO	O-C	5.56	1.41	1.20
1	G	844	TPO	O-C	5.56	1.41	1.20
1	C	844	TPO	O-C	5.55	1.41	1.20
1	F	844	TPO	O-C	5.55	1.41	1.20

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	844	TPO	O-C-CA	-4.04	114.39	124.77
1	D	844	TPO	O-C-CA	-4.04	114.39	124.77
1	E	844	TPO	O-C-CA	-4.02	114.43	124.77
1	C	844	TPO	O-C-CA	-4.02	114.43	124.77
1	F	844	TPO	O-C-CA	-4.01	114.45	124.77

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	840	SEP	N-CA-CB-OG
1	A	840	SEP	CB-OG-P-O2P
1	A	840	SEP	CB-OG-P-O3P
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	840	SEP	1	0
1	C	841	SEP	1	0
1	D	840	SEP	3	0
1	A	840	SEP	1	0
1	B	840	SEP	1	0
1	E	840	SEP	0	1
1	D	841	SEP	2	0
1	F	840	SEP	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.