



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 10:38 PM EDT

PDB ID : 6G7C
Title : Nt2-CTD domains of the TssA component from the type VI secretion system of *Aeromonas hydrophila*.
Authors : Dix, S.D.; Owen, H.J.; Sun, R.; Ahmad, A.; Shastri, S.; Spiewak, H.L.; Mosby, D.J.; Harris, M.J.; Batters, S.L.; Tzokov, S.B.; Sedelnikova, S.E.; Baker, P.J.; Bullough, P.A.; Rice, D.W.; Thomas, M.S.
Deposited on : 2018-04-05
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

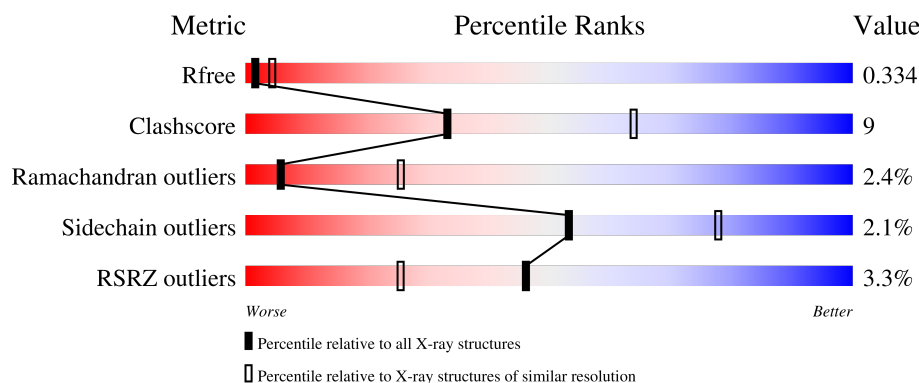
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	270	 63% 21% • 13%
1	B	270	 68% 18% •• 12%
1	C	270	 67% 20% • 11%
1	D	270	 67% 20% • 12%
1	E	270	 % 70% 16% • 12%

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Mol	Chain	Length	Quality of chain
1	F	270	<div><div></div><div>66%19%13%</div></div>
1	G	270	<div><div>2%</div><div></div><div>66%17%15%</div></div>
1	H	270	<div><div>%</div><div></div><div>71%15%14%</div></div>
1	I	270	<div><div>20%</div><div></div><div>69%15%15%</div></div>
1	J	270	<div><div>4%</div><div></div><div>65%20%15%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18363 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 ImpA-related domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1834	1157	336	335	6			
1	B	237	Total	C	N	O	S	0	0	0
			1858	1170	339	343	6			
1	G	230	Total	C	N	O	S	0	0	0
			1807	1143	331	327	6			
1	H	233	Total	C	N	O	S	0	0	0
			1831	1157	335	333	6			
1	C	239	Total	C	N	O	S	0	0	0
			1863	1175	341	341	6			
1	D	238	Total	C	N	O	S	0	0	0
			1863	1173	340	344	6			
1	I	230	Total	C	N	O	S	0	0	0
			1807	1143	331	327	6			
1	J	230	Total	C	N	O	S	0	0	0
			1807	1143	331	327	6			
1	E	237	Total	C	N	O	S	0	0	0
			1858	1170	339	343	6			
1	F	234	Total	C	N	O	S	0	0	0
			1835	1157	336	336	6			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	MET	-	initiating methionine	UNP A0KJC7
A	210	GLY	-	expression tag	UNP A0KJC7
A	211	SER	-	expression tag	UNP A0KJC7
A	212	SER	-	expression tag	UNP A0KJC7
A	213	HIS	-	expression tag	UNP A0KJC7
A	214	HIS	-	expression tag	UNP A0KJC7
A	215	HIS	-	expression tag	UNP A0KJC7
A	216	HIS	-	expression tag	UNP A0KJC7
A	217	HIS	-	expression tag	UNP A0KJC7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	218	HIS	-	expression tag	UNP A0KJC7
A	219	SER	-	expression tag	UNP A0KJC7
A	220	GLY	-	expression tag	UNP A0KJC7
A	221	ALA	-	expression tag	UNP A0KJC7
A	222	PRO	-	expression tag	UNP A0KJC7
B	209	MET	-	initiating methionine	UNP A0KJC7
B	210	GLY	-	expression tag	UNP A0KJC7
B	211	SER	-	expression tag	UNP A0KJC7
B	212	SER	-	expression tag	UNP A0KJC7
B	213	HIS	-	expression tag	UNP A0KJC7
B	214	HIS	-	expression tag	UNP A0KJC7
B	215	HIS	-	expression tag	UNP A0KJC7
B	216	HIS	-	expression tag	UNP A0KJC7
B	217	HIS	-	expression tag	UNP A0KJC7
B	218	HIS	-	expression tag	UNP A0KJC7
B	219	SER	-	expression tag	UNP A0KJC7
B	220	GLY	-	expression tag	UNP A0KJC7
B	221	ALA	-	expression tag	UNP A0KJC7
B	222	PRO	-	expression tag	UNP A0KJC7
G	209	MET	-	initiating methionine	UNP A0KJC7
G	210	GLY	-	expression tag	UNP A0KJC7
G	211	SER	-	expression tag	UNP A0KJC7
G	212	SER	-	expression tag	UNP A0KJC7
G	213	HIS	-	expression tag	UNP A0KJC7
G	214	HIS	-	expression tag	UNP A0KJC7
G	215	HIS	-	expression tag	UNP A0KJC7
G	216	HIS	-	expression tag	UNP A0KJC7
G	217	HIS	-	expression tag	UNP A0KJC7
G	218	HIS	-	expression tag	UNP A0KJC7
G	219	SER	-	expression tag	UNP A0KJC7
G	220	GLY	-	expression tag	UNP A0KJC7
G	221	ALA	-	expression tag	UNP A0KJC7
G	222	PRO	-	expression tag	UNP A0KJC7
H	209	MET	-	initiating methionine	UNP A0KJC7
H	210	GLY	-	expression tag	UNP A0KJC7
H	211	SER	-	expression tag	UNP A0KJC7
H	212	SER	-	expression tag	UNP A0KJC7
H	213	HIS	-	expression tag	UNP A0KJC7
H	214	HIS	-	expression tag	UNP A0KJC7
H	215	HIS	-	expression tag	UNP A0KJC7
H	216	HIS	-	expression tag	UNP A0KJC7
H	217	HIS	-	expression tag	UNP A0KJC7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	218	HIS	-	expression tag	UNP A0KJC7
H	219	SER	-	expression tag	UNP A0KJC7
H	220	GLY	-	expression tag	UNP A0KJC7
H	221	ALA	-	expression tag	UNP A0KJC7
H	222	PRO	-	expression tag	UNP A0KJC7
C	209	MET	-	initiating methionine	UNP A0KJC7
C	210	GLY	-	expression tag	UNP A0KJC7
C	211	SER	-	expression tag	UNP A0KJC7
C	212	SER	-	expression tag	UNP A0KJC7
C	213	HIS	-	expression tag	UNP A0KJC7
C	214	HIS	-	expression tag	UNP A0KJC7
C	215	HIS	-	expression tag	UNP A0KJC7
C	216	HIS	-	expression tag	UNP A0KJC7
C	217	HIS	-	expression tag	UNP A0KJC7
C	218	HIS	-	expression tag	UNP A0KJC7
C	219	SER	-	expression tag	UNP A0KJC7
C	220	GLY	-	expression tag	UNP A0KJC7
C	221	ALA	-	expression tag	UNP A0KJC7
C	222	PRO	-	expression tag	UNP A0KJC7
D	209	MET	-	initiating methionine	UNP A0KJC7
D	210	GLY	-	expression tag	UNP A0KJC7
D	211	SER	-	expression tag	UNP A0KJC7
D	212	SER	-	expression tag	UNP A0KJC7
D	213	HIS	-	expression tag	UNP A0KJC7
D	214	HIS	-	expression tag	UNP A0KJC7
D	215	HIS	-	expression tag	UNP A0KJC7
D	216	HIS	-	expression tag	UNP A0KJC7
D	217	HIS	-	expression tag	UNP A0KJC7
D	218	HIS	-	expression tag	UNP A0KJC7
D	219	SER	-	expression tag	UNP A0KJC7
D	220	GLY	-	expression tag	UNP A0KJC7
D	221	ALA	-	expression tag	UNP A0KJC7
D	222	PRO	-	expression tag	UNP A0KJC7
I	209	MET	-	initiating methionine	UNP A0KJC7
I	210	GLY	-	expression tag	UNP A0KJC7
I	211	SER	-	expression tag	UNP A0KJC7
I	212	SER	-	expression tag	UNP A0KJC7
I	213	HIS	-	expression tag	UNP A0KJC7
I	214	HIS	-	expression tag	UNP A0KJC7
I	215	HIS	-	expression tag	UNP A0KJC7
I	216	HIS	-	expression tag	UNP A0KJC7
I	217	HIS	-	expression tag	UNP A0KJC7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	218	HIS	-	expression tag	UNP A0KJC7
I	219	SER	-	expression tag	UNP A0KJC7
I	220	GLY	-	expression tag	UNP A0KJC7
I	221	ALA	-	expression tag	UNP A0KJC7
I	222	PRO	-	expression tag	UNP A0KJC7
J	209	MET	-	initiating methionine	UNP A0KJC7
J	210	GLY	-	expression tag	UNP A0KJC7
J	211	SER	-	expression tag	UNP A0KJC7
J	212	SER	-	expression tag	UNP A0KJC7
J	213	HIS	-	expression tag	UNP A0KJC7
J	214	HIS	-	expression tag	UNP A0KJC7
J	215	HIS	-	expression tag	UNP A0KJC7
J	216	HIS	-	expression tag	UNP A0KJC7
J	217	HIS	-	expression tag	UNP A0KJC7
J	218	HIS	-	expression tag	UNP A0KJC7
J	219	SER	-	expression tag	UNP A0KJC7
J	220	GLY	-	expression tag	UNP A0KJC7
J	221	ALA	-	expression tag	UNP A0KJC7
J	222	PRO	-	expression tag	UNP A0KJC7
E	209	MET	-	initiating methionine	UNP A0KJC7
E	210	GLY	-	expression tag	UNP A0KJC7
E	211	SER	-	expression tag	UNP A0KJC7
E	212	SER	-	expression tag	UNP A0KJC7
E	213	HIS	-	expression tag	UNP A0KJC7
E	214	HIS	-	expression tag	UNP A0KJC7
E	215	HIS	-	expression tag	UNP A0KJC7
E	216	HIS	-	expression tag	UNP A0KJC7
E	217	HIS	-	expression tag	UNP A0KJC7
E	218	HIS	-	expression tag	UNP A0KJC7
E	219	SER	-	expression tag	UNP A0KJC7
E	220	GLY	-	expression tag	UNP A0KJC7
E	221	ALA	-	expression tag	UNP A0KJC7
E	222	PRO	-	expression tag	UNP A0KJC7
F	209	MET	-	initiating methionine	UNP A0KJC7
F	210	GLY	-	expression tag	UNP A0KJC7
F	211	SER	-	expression tag	UNP A0KJC7
F	212	SER	-	expression tag	UNP A0KJC7
F	213	HIS	-	expression tag	UNP A0KJC7
F	214	HIS	-	expression tag	UNP A0KJC7
F	215	HIS	-	expression tag	UNP A0KJC7
F	216	HIS	-	expression tag	UNP A0KJC7
F	217	HIS	-	expression tag	UNP A0KJC7

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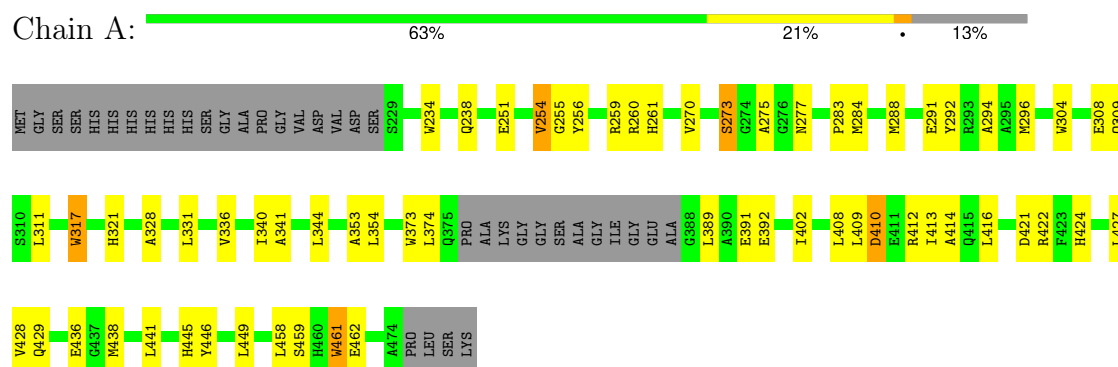
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Chain	Residue	Modelled	Actual	Comment	Reference
F	218	HIS	-	expression tag	UNP A0KJC7
F	219	SER	-	expression tag	UNP A0KJC7
F	220	GLY	-	expression tag	UNP A0KJC7
F	221	ALA	-	expression tag	UNP A0KJC7
F	222	PRO	-	expression tag	UNP A0KJC7

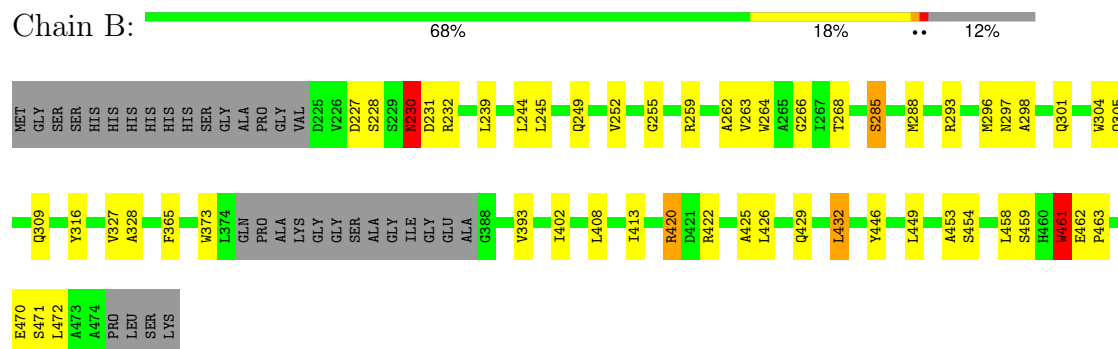
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

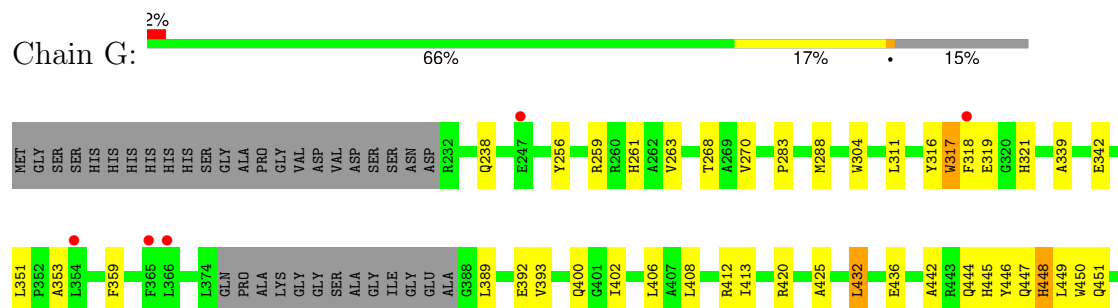
• Molecule 1: ImpA-related domain protein



• Molecule 1: ImpA-related domain protein

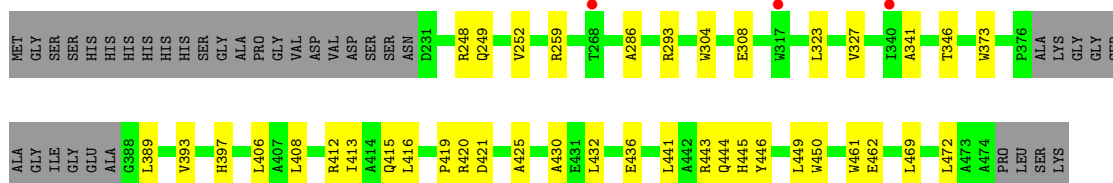


• Molecule 1: ImpA-related domain protein

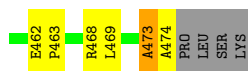
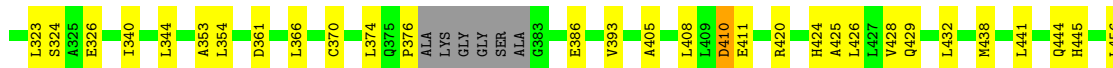
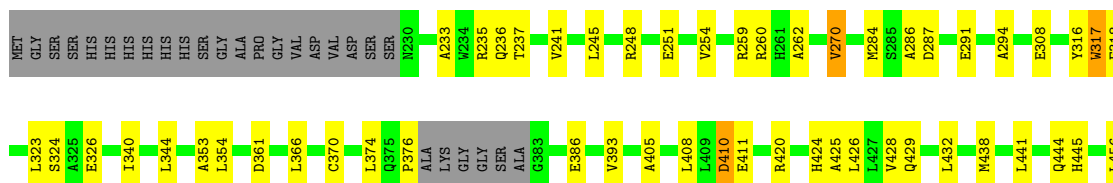




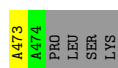
- Molecule 1: ImpA-related domain protein



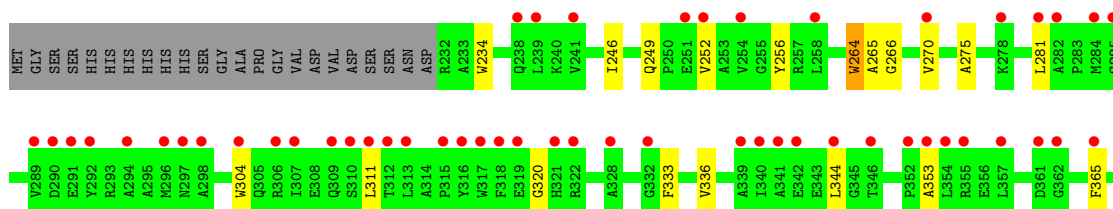
- Molecule 1: ImpA-related domain protein

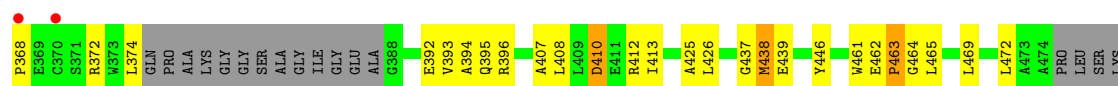


- Molecule 1: ImpA-related domain protein

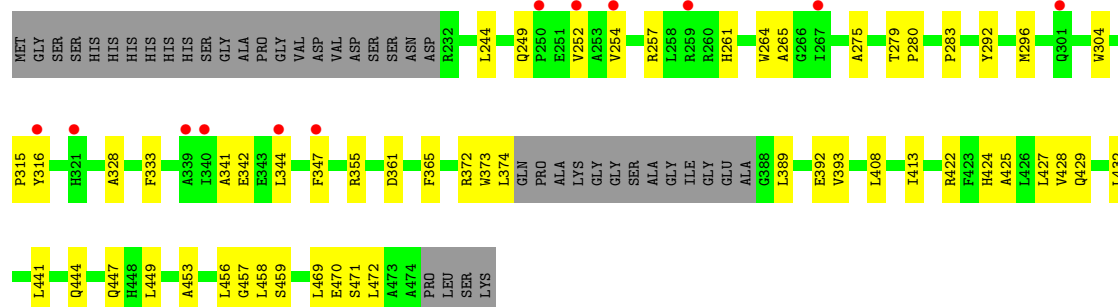


- Molecule 1: ImpA-related domain protein

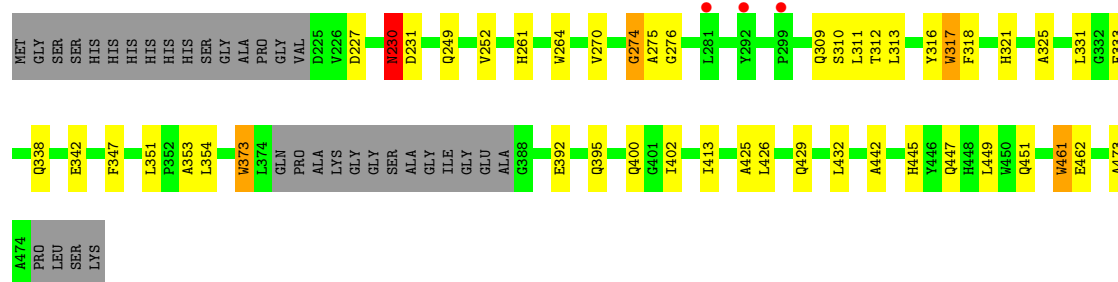




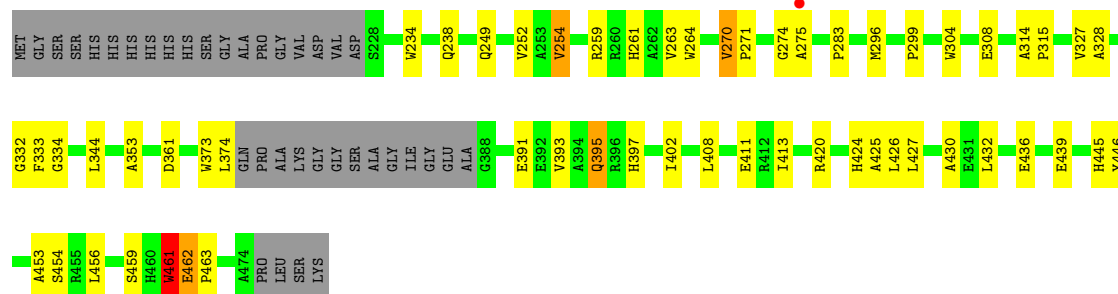
• Molecule 1: ImpA-related domain protein



• Molecule 1: ImpA-related domain protein



• Molecule 1: ImpA-related domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.03Å 202.08Å 139.01Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	202.08 – 3.13 139.00 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.8 (202.08-3.13) 98.8 (139.00-3.13)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.255 , 0.328 0.256 , 0.334	Depositor DCC
R_{free} test set	3343 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18363	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.62	0/1874	0.86	1/2541 (0.0%)
1	B	0.58	0/1898	0.81	2/2574 (0.1%)
1	C	0.62	0/1903	0.85	1/2580 (0.0%)
1	D	0.58	0/1903	0.84	2/2581 (0.1%)
1	E	0.60	0/1898	0.85	1/2574 (0.0%)
1	F	0.54	0/1875	0.76	0/2542
1	G	0.59	0/1847	0.78	1/2504 (0.0%)
1	H	0.52	0/1872	0.72	0/2539
1	I	0.56	0/1847	0.73	1/2504 (0.0%)
1	J	0.57	0/1847	0.77	0/2504
All	All	0.58	0/18764	0.80	9/25443 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	230	ASN	N-CA-C	-5.78	95.38	111.00
1	A	259	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	259	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	C	376	PRO	N-CA-CB	5.40	109.78	103.30
1	D	228	SER	N-CA-C	5.30	125.32	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1834	0	1804	46	0
1	B	1858	0	1824	32	0
1	C	1863	0	1828	42	0
1	D	1863	0	1826	38	0
1	E	1858	0	1824	33	0
1	F	1835	0	1807	36	0
1	G	1807	0	1787	36	0
1	H	1831	0	1806	30	0
1	I	1807	0	1787	30	0
1	J	1807	0	1787	31	0
All	All	18363	0	18080	315	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 9.

The worst 5 of 315 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:H:249:GLN:HE21	1:H:252:VAL:HG21	1.33	0.92
1:J:441:LEU:HD11	1:E:429:GLN:HE22	1.34	0.92
1:J:441:LEU:HD11	1:E:429:GLN:NE2	1.94	0.82
1:A:304:TRP:CZ2	1:A:328:ALA:HB2	2.17	0.79
1:E:270:VAL:HG11	1:E:353:ALA:HB3	1.65	0.78

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	230/270 (85%)	198 (86%)	25 (11%)	7 (3%)	4	21
1	B	233/270 (86%)	205 (88%)	23 (10%)	5 (2%)	7	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	235/270 (87%)	199 (85%)	32 (14%)	4 (2%)	9	34
1	D	234/270 (87%)	201 (86%)	29 (12%)	4 (2%)	9	34
1	E	233/270 (86%)	196 (84%)	28 (12%)	9 (4%)	3	16
1	F	230/270 (85%)	195 (85%)	26 (11%)	9 (4%)	3	16
1	G	226/270 (84%)	198 (88%)	25 (11%)	3 (1%)	12	41
1	H	229/270 (85%)	204 (89%)	24 (10%)	1 (0%)	34	67
1	I	226/270 (84%)	194 (86%)	24 (11%)	8 (4%)	3	18
1	J	226/270 (84%)	193 (85%)	27 (12%)	6 (3%)	5	23
All	All	2302/2700 (85%)	1983 (86%)	263 (11%)	56 (2%)	6	25

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASN
1	B	231	ASP
1	B	461	TRP
1	G	317	TRP
1	I	265	ALA

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	181/207 (87%)	175 (97%)	6 (3%)	38	68
1	B	185/207 (89%)	176 (95%)	9 (5%)	25	56
1	C	182/207 (88%)	178 (98%)	4 (2%)	52	77
1	D	185/207 (89%)	180 (97%)	5 (3%)	44	72
1	E	185/207 (89%)	184 (100%)	1 (0%)	88	95
1	F	182/207 (88%)	177 (97%)	5 (3%)	44	72
1	G	178/207 (86%)	176 (99%)	2 (1%)	73	88
1	H	181/207 (87%)	179 (99%)	2 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	178/207 (86%)	178 (100%)	0	100	100
1	J	178/207 (86%)	174 (98%)	4 (2%)	52	77
All	All	1815/2070 (88%)	1777 (98%)	38 (2%)	53	78

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	372	ARG
1	F	439	GLU
1	J	422	ARG
1	E	230	ASN
1	F	461	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	277	ASN
1	E	451	GLN
1	I	277	ASN
1	F	349	GLN
1	E	238	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/270 (86%)	0.02	0 100 100	47, 74, 106, 129	0
1	B	237/270 (87%)	0.11	0 100 100	52, 91, 124, 144	0
1	C	239/270 (88%)	0.11	0 100 100	48, 83, 122, 138	0
1	D	238/270 (88%)	0.10	0 100 100	47, 98, 140, 176	0
1	E	237/270 (87%)	0.17	3 (1%) 77 61	45, 88, 137, 160	0
1	F	234/270 (86%)	0.17	1 (0%) 92 86	53, 106, 143, 164	0
1	G	230/270 (85%)	0.24	5 (2%) 62 42	46, 100, 145, 159	0
1	H	233/270 (86%)	0.23	3 (1%) 77 61	57, 104, 138, 163	0
1	I	230/270 (85%)	1.22	54 (23%) 0 0	54, 154, 200, 236	0
1	J	230/270 (85%)	0.47	12 (5%) 27 12	52, 102, 163, 197	0
All	All	2342/2700 (86%)	0.28	78 (3%) 46 25	45, 94, 161, 236	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	352	PRO	6.9
1	I	297	ASN	6.1
1	I	355	ARG	6.1
1	I	346	THR	5.9
1	I	354	LEU	5.5

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.