Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 01:04 pm BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

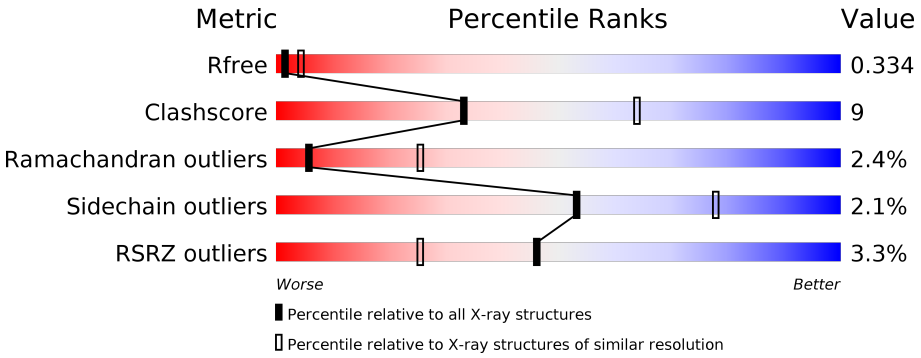
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 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 on 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% 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%
1	F	270	66% 19% • 13%

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Mol	Chain	Length	Quality of chain
1	G	270	2% 66% 17% 15%
1	H	270	% 71% 15% 14%
1	I	270	20% 69% 15% 15%
1	J	270	4% 65% 20% 15%

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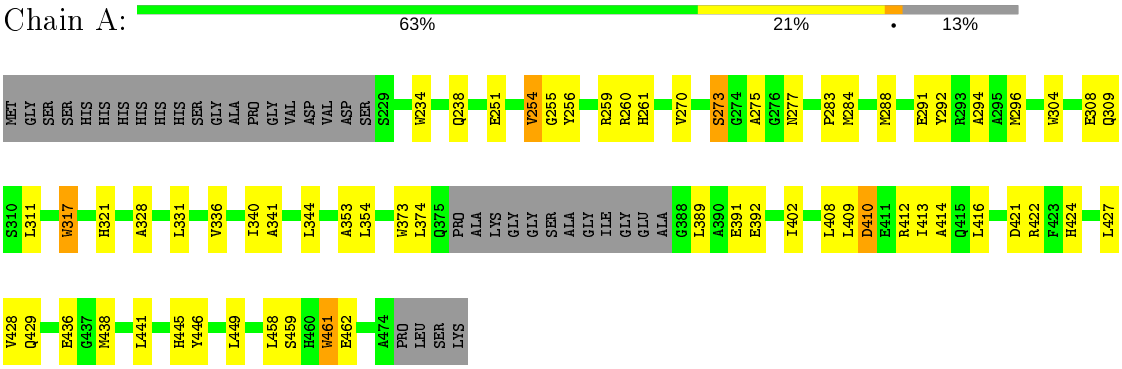
Chain	Residue	Modelled	Actual	Comment	Reference
F	218	HIS	-	expression tag	UNP A0KJC7
F	219	SER	-	expression tag	UNP A0KJC7
F	220	GLY	-	expression tag	UNP A0KJC7
F	221	ALA	-	expression tag	UNP A0KJC7
F	222	PRO	-	expression tag	UNP A0KJC7

3 Residue-property plots (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 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.

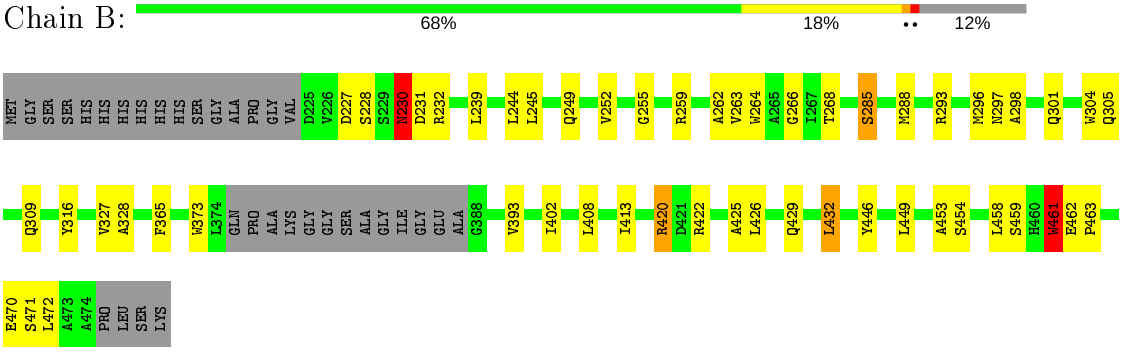
- Molecule 1: ImpA-related domain protein

Chain A:



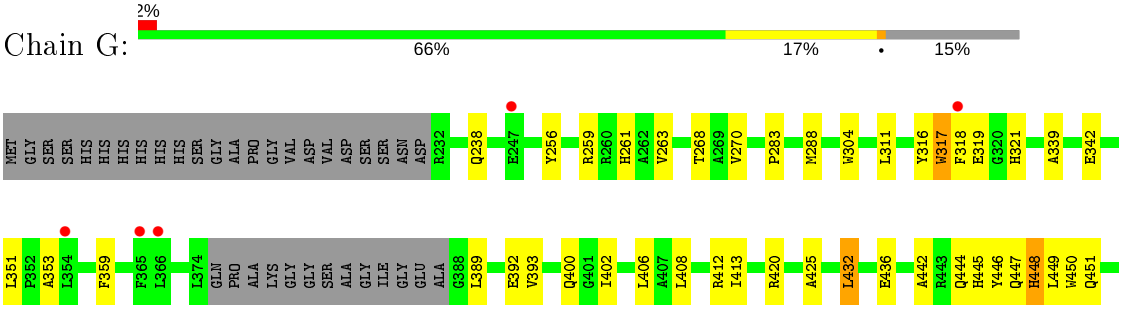
- Molecule 1: ImpA-related domain protein

Chain B:



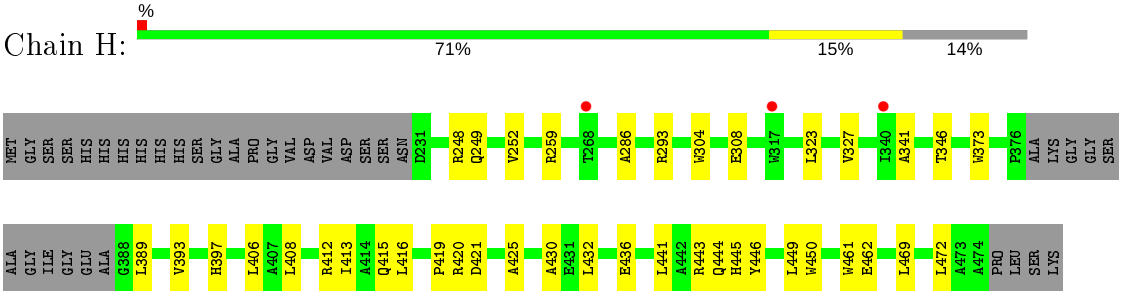
- Molecule 1: ImpA-related domain protein

Chain G:



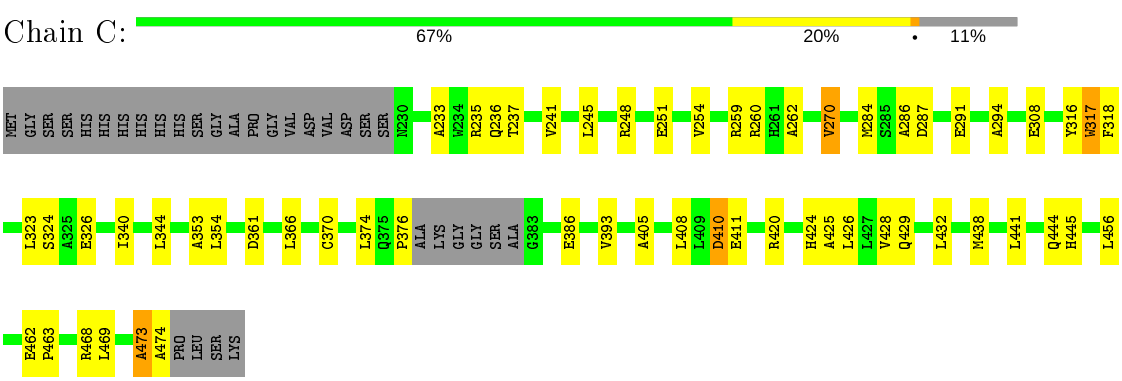
• Molecule 1: ImpA-related domain protein

Chain H:



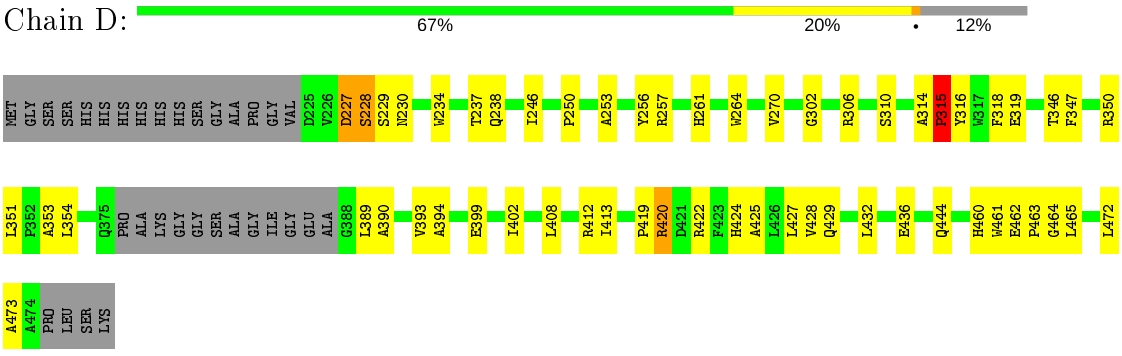
• Molecule 1: ImpA-related domain protein

Chain C:



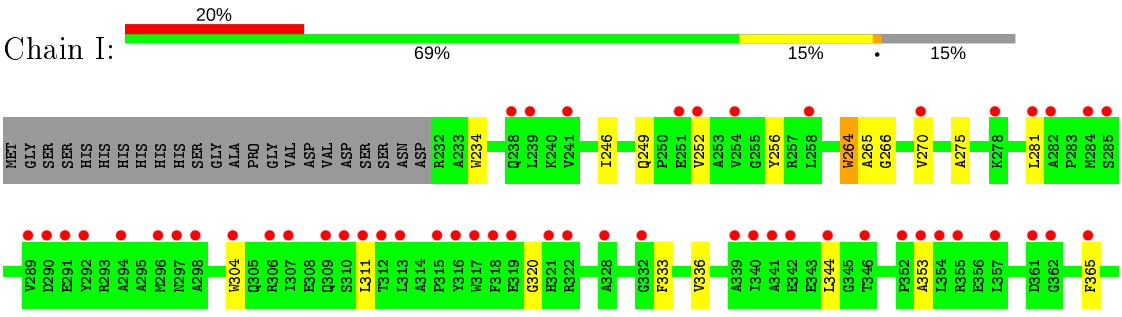
• Molecule 1: ImpA-related domain protein

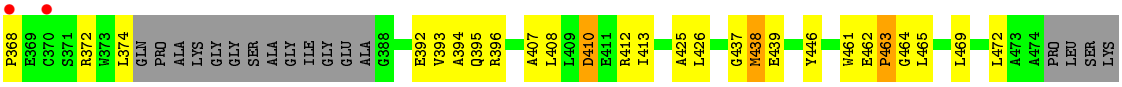
Chain D:



• Molecule 1: ImpA-related domain protein

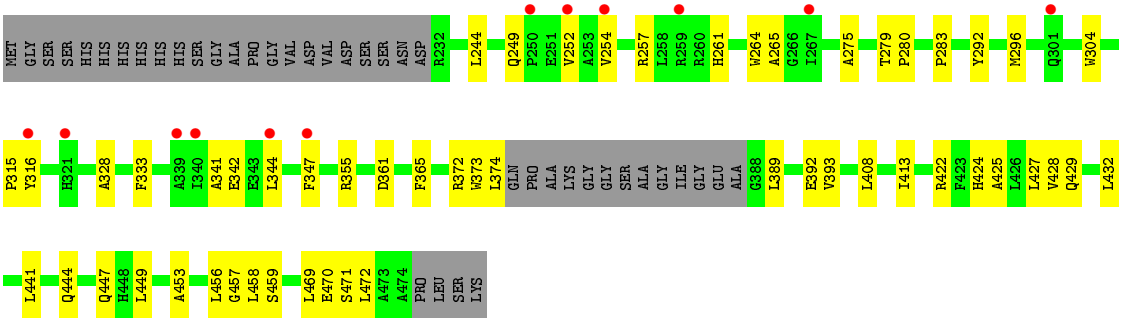
Chain I:





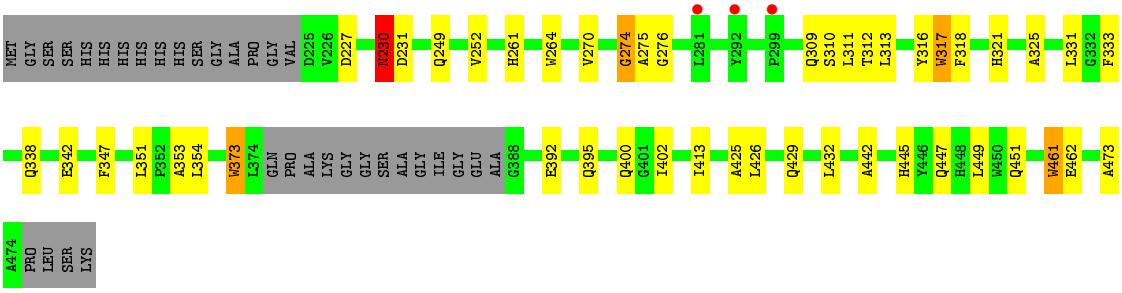
• Molecule 1: ImpA-related domain protein

Chain J:



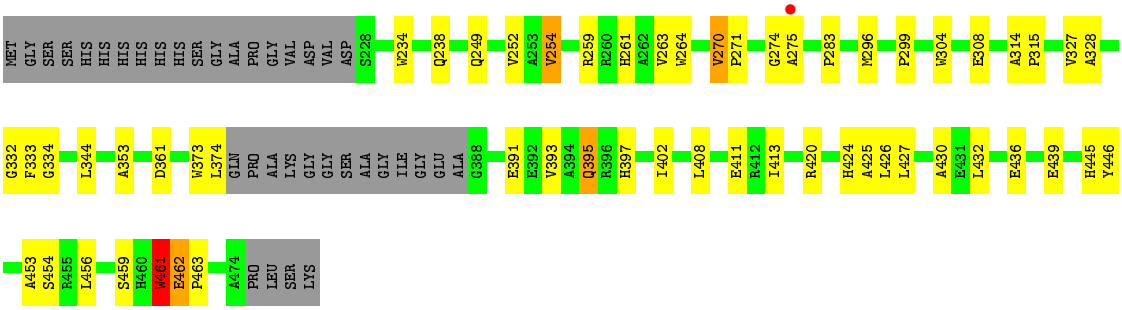
• Molecule 1: ImpA-related domain protein

Chain E:



• Molecule 1: ImpA-related domain protein

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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

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.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	I	410	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	432	LEU	CA-CB-CG	5.24	127.34	115.30
1	G	432	LEU	CA-CB-CG	5.03	126.86	115.30
1	B	432	LEU	CA-CB-CG	5.00	126.80	115.30

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.

All (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
1:G:393:VAL:HG22	1:G:408:LEU:HD23	1.67	0.76
1:G:446:TYR:CE1	1:G:472:LEU:HD13	2.23	0.73
1:D:413:ILE:HD11	1:D:425:ALA:HB1	1.69	0.72
1:H:248:ARG:O	1:H:249:GLN:HG3	1.90	0.72
1:F:270:VAL:HG11	1:F:353:ALA:HB3	1.71	0.71
1:D:229:SER:OG	1:D:230:ASN:N	2.24	0.70
1:B:413:ILE:HD11	1:B:425:ALA:HB1	1.75	0.69
1:I:264:TRP:O	1:I:266:GLY:N	2.25	0.68
1:A:429:GLN:NE2	1:C:441:LEU:HD11	2.09	0.67
1:A:389:LEU:HD23	1:A:428:VAL:HG21	1.75	0.67
1:C:251:GLU:OE1	1:C:251:GLU:N	2.27	0.67
1:I:413:ILE:HD11	1:I:425:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:TRP:CZ3	1:H:420:ARG:HA	2.30	0.67
1:E:351:LEU:HB2	1:E:354:LEU:HD12	1.76	0.67
1:E:230:ASN:O	1:E:230:ASN:CG	2.34	0.65
1:D:462:GLU:N	1:D:463:PRO:HD3	2.12	0.64
1:C:260:ARG:HH21	1:C:340:ILE:HG23	1.63	0.64
1:H:249:GLN:NE2	1:H:252:VAL:HG21	2.10	0.64
1:G:270:VAL:HG11	1:G:353:ALA:HB3	1.80	0.64
1:D:270:VAL:HG11	1:D:353:ALA:HB3	1.80	0.64
1:J:444:GLN:HG2	1:E:426:LEU:HD21	1.79	0.63
1:B:230:ASN:O	1:B:232:ARG:N	2.31	0.63
1:D:393:VAL:HG22	1:D:408:LEU:HD23	1.79	0.63
1:I:446:TYR:CE1	1:I:472:LEU:HD13	2.34	0.62
1:B:245:LEU:HD12	1:B:255:GLY:HA2	1.80	0.62
1:B:304:TRP:CZ2	1:B:328:ALA:HB2	2.33	0.62
1:B:429:GLN:NE2	1:H:441:LEU:HD11	2.15	0.62
1:A:441:LEU:HD11	1:C:429:GLN:NE2	2.15	0.62
1:A:422:ARG:NH2	1:C:444:GLN:OE1	2.33	0.61
1:G:444:GLN:HG3	1:I:426:LEU:HD11	1.83	0.61
1:H:393:VAL:HG22	1:H:408:LEU:HD23	1.82	0.61
1:B:393:VAL:HG22	1:B:408:LEU:HD23	1.83	0.61
1:D:227:ASP:OD1	1:D:227:ASP:N	2.34	0.61
1:A:251:GLU:OE1	1:A:251:GLU:N	2.27	0.60
1:F:413:ILE:HD11	1:F:425:ALA:HB1	1.82	0.60
1:C:270:VAL:HG12	1:C:354:LEU:CD2	2.32	0.60
1:I:413:ILE:HD11	1:I:425:ALA:CB	2.32	0.60
1:E:249:GLN:HE22	1:F:261:HIS:CE1	2.20	0.60
1:B:239:LEU:HD21	1:B:262:ALA:HB3	1.84	0.59
1:A:270:VAL:HG11	1:A:353:ALA:HB3	1.83	0.59
1:F:234:TRP:NE1	1:F:238:GLN:NE2	2.51	0.59
1:A:308:GLU:HA	1:A:311:LEU:HG	1.85	0.59
1:E:442:ALA:O	1:E:445:HIS:N	2.35	0.59
1:J:344:LEU:HD23	1:J:374:LEU:HD11	1.85	0.59
1:A:311:LEU:HD22	1:A:321:HIS:ND1	2.18	0.58
1:A:402:ILE:HB	1:A:436:GLU:OE2	2.02	0.58
1:I:461:TRP:O	1:I:462:GLU:HB3	2.02	0.58
1:F:453:ALA:O	1:F:456:LEU:N	2.37	0.58
1:A:270:VAL:HG12	1:A:354:LEU:CD2	2.33	0.58
1:E:261:HIS:HE2	1:F:249:GLN:HE22	1.50	0.58
1:G:461:TRP:CH2	1:H:420:ARG:HA	2.39	0.58
1:J:413:ILE:HD11	1:J:425:ALA:CB	2.32	0.58
1:C:284:MET:HG3	1:C:317:TRP:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:VAL:HG12	1:B:264:TRP:CD1	2.40	0.56
1:H:416:LEU:HD22	1:H:421:ASP:HB3	1.87	0.56
1:B:422:ARG:NH2	1:H:444:GLN:OE1	2.39	0.56
1:A:234:TRP:HZ2	1:B:245:LEU:HD23	1.71	0.56
1:J:457:GLY:C	1:J:459:SER:H	2.09	0.56
1:J:283:PRO:HG3	1:J:361:ASP:OD2	2.06	0.56
1:C:456:LEU:HD21	1:D:460:HIS:CB	2.35	0.56
1:C:405:ALA:HB1	1:C:432:LEU:HD11	1.87	0.55
1:A:341:ALA:HB2	1:A:373:TRP:CZ2	2.41	0.55
1:F:259:ARG:NH1	1:F:308:GLU:HB3	2.22	0.55
1:H:304:TRP:HB2	1:H:327:VAL:HG11	1.89	0.54
1:A:238:GLN:OE1	1:A:261:HIS:ND1	2.35	0.54
1:B:402:ILE:HG13	1:B:432:LEU:HD21	1.90	0.54
1:B:420:ARG:NH1	1:B:462:GLU:OE1	2.41	0.54
1:G:461:TRP:HA	1:H:419:PRO:HG2	1.90	0.54
1:I:393:VAL:HG22	1:I:408:LEU:HD23	1.90	0.54
1:I:249:GLN:HE22	1:J:261:HIS:CE1	2.25	0.54
1:E:274:GLY:O	1:E:276:GLY:N	2.39	0.54
1:C:233:ALA:O	1:C:236:GLN:HB2	2.08	0.53
1:G:319:GLU:HA	1:G:319:GLU:OE1	2.08	0.53
1:H:461:TRP:O	1:H:462:GLU:HB3	2.08	0.53
1:G:402:ILE:HG13	1:G:432:LEU:HD21	1.90	0.53
1:J:393:VAL:HG22	1:J:408:LEU:HD23	1.91	0.53
1:D:350:ARG:HG2	1:D:351:LEU:HG	1.90	0.53
1:B:249:GLN:HB3	1:B:252:VAL:HG23	1.91	0.53
1:F:304:TRP:HB2	1:F:327:VAL:HG11	1.91	0.53
1:D:264:TRP:HB3	1:D:347:PHE:CE1	2.44	0.53
1:D:419:PRO:HA	1:D:422:ARG:HD2	1.91	0.53
1:C:291:GLU:O	1:C:294:ALA:HB3	2.08	0.52
1:I:465:LEU:O	1:I:469:LEU:HB2	2.09	0.52
1:F:304:TRP:CZ2	1:F:328:ALA:HB2	2.43	0.52
1:G:461:TRP:O	1:G:462:GLU:HB2	2.08	0.52
1:G:392:GLU:OE1	1:G:412:ARG:NH1	2.38	0.52
1:G:406:LEU:HB3	1:I:438:MET:SD	2.50	0.52
1:H:397:HIS:NE2	1:H:436:GLU:OE2	2.42	0.52
1:D:246:ILE:HG23	1:D:256:TYR:OH	2.10	0.51
1:J:279:THR:HB	1:J:280:PRO:HD2	1.92	0.51
1:B:462:GLU:N	1:B:463:PRO:HD3	2.25	0.51
1:F:249:GLN:HE21	1:F:252:VAL:HG21	1.74	0.51
1:A:410:ASP:C	1:A:410:ASP:OD1	2.49	0.51
1:G:283:PRO:HB3	1:G:359:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:413:ILE:HD11	1:G:425:ALA:HB1	1.93	0.51
1:J:413:ILE:HD11	1:J:425:ALA:HB1	1.93	0.51
1:I:392:GLU:OE1	1:I:412:ARG:NH1	2.38	0.51
1:D:253:ALA:O	1:D:257:ARG:HG3	2.11	0.50
1:G:468:ARG:O	1:G:471:SER:OG	2.26	0.50
1:E:461:TRP:CZ2	1:F:420:ARG:HG3	2.47	0.50
1:D:444:GLN:HG2	1:F:426:LEU:HD21	1.93	0.50
1:H:249:GLN:HE21	1:H:252:VAL:CG2	2.15	0.50
1:E:311:LEU:HB2	1:E:321:HIS:CE1	2.46	0.50
1:H:430:ALA:HB1	1:H:446:TYR:CE2	2.47	0.50
1:J:428:VAL:O	1:J:429:GLN:C	2.50	0.50
1:F:270:VAL:HB	1:F:271:PRO:CD	2.42	0.50
1:C:425:ALA:O	1:C:428:VAL:N	2.45	0.49
1:J:424:HIS:O	1:J:427:LEU:HB3	2.12	0.49
1:A:413:ILE:HD12	1:C:441:LEU:CD1	2.42	0.49
1:G:311:LEU:HD13	1:G:321:HIS:CE1	2.48	0.49
1:H:446:TYR:CE1	1:H:472:LEU:HD13	2.47	0.49
1:A:402:ILE:HD12	1:A:436:GLU:HG2	1.94	0.49
1:C:286:ALA:O	1:C:287:ASP:C	2.50	0.49
1:A:311:LEU:HD13	1:A:321:HIS:CE1	2.48	0.49
1:C:344:LEU:HD23	1:C:374:LEU:HD11	1.93	0.49
1:G:444:GLN:CG	1:I:426:LEU:HD11	2.42	0.49
1:C:410:ASP:C	1:C:410:ASP:OD1	2.51	0.49
1:G:268:THR:O	1:G:351:LEU:HD21	2.12	0.49
1:G:238:GLN:HE22	1:G:261:HIS:HD1	1.61	0.49
1:A:413:ILE:HD12	1:C:441:LEU:HD12	1.93	0.49
1:E:325:ALA:CB	1:E:373:TRP:CZ2	2.96	0.49
1:G:317:TRP:NE1	1:G:319:GLU:HB3	2.27	0.49
1:I:270:VAL:HG11	1:I:353:ALA:HB3	1.93	0.49
1:A:234:TRP:O	1:A:238:GLN:HG3	2.13	0.48
1:G:465:LEU:HG	1:G:469:LEU:HD12	1.95	0.48
1:J:413:ILE:HD11	1:J:425:ALA:HB3	1.94	0.48
1:G:420:ARG:HH22	1:G:462:GLU:CD	2.16	0.48
1:G:259:ARG:O	1:G:263:VAL:HG23	2.12	0.48
1:G:447:GLN:O	1:G:449:LEU:N	2.46	0.48
1:I:393:VAL:O	1:I:395:GLN:N	2.46	0.48
1:J:447:GLN:C	1:J:449:LEU:H	2.17	0.48
1:C:366:LEU:HD12	1:C:370:CYS:SG	2.53	0.48
1:E:447:GLN:HE21	1:E:451:GLN:NE2	2.11	0.48
1:E:261:HIS:HE2	1:F:249:GLN:NE2	2.11	0.48
1:I:461:TRP:O	1:I:462:GLU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ARG:NH2	1:C:462:GLU:OE1	2.47	0.48
1:F:462:GLU:N	1:F:463:PRO:CD	2.76	0.48
1:A:424:HIS:O	1:A:427:LEU:HB3	2.14	0.48
1:B:293:ARG:HA	1:B:296:MET:HG2	1.95	0.48
1:C:316:TYR:O	1:C:318:PHE:N	2.46	0.48
1:E:402:ILE:HG13	1:E:432:LEU:HD21	1.96	0.48
1:H:406:LEU:HD21	1:H:432:LEU:HD22	1.95	0.47
1:C:456:LEU:HD21	1:D:460:HIS:HB3	1.95	0.47
1:A:284:MET:HG3	1:A:317:TRP:CD2	2.49	0.47
1:J:316:TYR:HB3	1:J:365:PHE:CD2	2.49	0.47
1:J:470:GLU:C	1:J:472:LEU:H	2.17	0.47
1:H:461:TRP:O	1:H:462:GLU:CB	2.60	0.47
1:A:261:HIS:NE2	1:B:249:GLN:OE1	2.48	0.47
1:E:445:HIS:O	1:E:449:LEU:HG	2.14	0.47
1:J:393:VAL:CG2	1:J:408:LEU:HD23	2.45	0.47
1:B:426:LEU:HD11	1:H:444:GLN:HG3	1.97	0.47
1:F:393:VAL:HG12	1:F:432:LEU:HD12	1.97	0.46
1:F:393:VAL:HA	1:F:408:LEU:HD23	1.97	0.46
1:A:445:HIS:CE1	1:C:445:HIS:CE1	3.03	0.46
1:B:266:GLY:O	1:B:268:THR:HG23	2.15	0.46
1:H:450:TRP:HB2	1:H:469:LEU:HB3	1.96	0.46
1:I:446:TYR:CD2	1:I:472:LEU:HB3	2.50	0.46
1:E:338:GLN:NE2	1:E:342:GLU:OE2	2.47	0.46
1:G:339:ALA:O	1:G:342:GLU:N	2.49	0.46
1:C:425:ALA:O	1:C:426:LEU:C	2.53	0.46
1:F:252:VAL:HG12	1:F:254:VAL:HG12	1.98	0.46
1:J:389:LEU:O	1:J:392:GLU:HB3	2.16	0.46
1:F:259:ARG:NH1	1:F:308:GLU:OE1	2.45	0.46
1:H:416:LEU:HD22	1:H:421:ASP:CB	2.45	0.46
1:E:309:GLN:HE21	1:E:313:LEU:HD12	1.81	0.46
1:J:257:ARG:NH1	1:J:342:GLU:OE1	2.49	0.46
1:A:344:LEU:HD23	1:A:374:LEU:HD11	1.98	0.45
1:H:346:THR:O	1:H:346:THR:HG22	2.16	0.45
1:A:408:LEU:O	1:A:409:LEU:C	2.52	0.45
1:B:453:ALA:O	1:B:454:SER:C	2.55	0.45
1:F:461:TRP:O	1:F:462:GLU:HB3	2.15	0.45
1:B:413:ILE:HD11	1:B:425:ALA:CB	2.46	0.45
1:B:402:ILE:CG1	1:B:432:LEU:HD21	2.47	0.45
1:G:389:LEU:HD11	1:G:412:ARG:HG3	1.98	0.45
1:G:446:TYR:CG	1:G:472:LEU:HB3	2.52	0.45
1:A:410:ASP:OD2	1:C:438:MET:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TYR:CD1	1:B:365:PHE:CE2	3.05	0.45
1:D:238:GLN:OE1	1:D:261:HIS:ND1	2.49	0.45
1:I:393:VAL:O	1:I:396:ARG:N	2.50	0.45
1:A:416:LEU:HD22	1:A:421:ASP:HB3	1.98	0.45
1:C:248:ARG:NH1	1:D:234:TRP:HE1	2.15	0.45
1:J:304:TRP:CZ2	1:J:328:ALA:HB2	2.51	0.44
1:C:468:ARG:O	1:C:469:LEU:C	2.54	0.44
1:E:227:ASP:N	1:E:227:ASP:OD1	2.50	0.44
1:F:270:VAL:HB	1:F:271:PRO:HD2	2.00	0.44
1:D:227:ASP:HB3	1:D:237:THR:HG23	1.99	0.44
1:B:285:SER:O	1:B:288:MET:N	2.51	0.44
1:F:424:HIS:O	1:F:427:LEU:HB3	2.17	0.44
1:D:227:ASP:HB3	1:D:237:THR:CG2	2.48	0.44
1:E:311:LEU:HD13	1:E:321:HIS:NE2	2.33	0.44
1:J:249:GLN:NE2	1:J:252:VAL:HG21	2.33	0.44
1:A:445:HIS:HE1	1:C:445:HIS:CE1	2.36	0.44
1:I:281:LEU:HD12	1:I:365:PHE:HZ	1.81	0.44
1:F:314:ALA:O	1:F:315:PRO:C	2.56	0.44
1:J:264:TRP:HB3	1:J:347:PHE:CE1	2.53	0.44
1:J:292:TYR:O	1:J:296:MET:HG2	2.18	0.44
1:B:297:ASN:OD1	1:B:298:ALA:N	2.51	0.44
1:D:246:ILE:O	1:D:250:PRO:HG3	2.17	0.44
1:D:444:GLN:CG	1:F:426:LEU:HD21	2.47	0.43
1:A:311:LEU:HD22	1:A:321:HIS:CE1	2.53	0.43
1:E:392:GLU:O	1:E:395:GLN:HB3	2.18	0.43
1:G:256:TYR:OH	1:G:304:TRP:CH2	2.69	0.43
1:A:292:TYR:O	1:A:296:MET:HG2	2.19	0.43
1:A:389:LEU:O	1:A:392:GLU:N	2.51	0.43
1:C:323:LEU:O	1:C:324:SER:C	2.56	0.43
1:C:270:VAL:HG11	1:C:353:ALA:HB3	2.00	0.43
1:H:341:ALA:HB2	1:H:373:TRP:CZ2	2.53	0.43
1:A:389:LEU:C	1:A:391:GLU:N	2.71	0.43
1:B:446:TYR:HA	1:B:449:LEU:HD12	1.99	0.43
1:E:325:ALA:HB3	1:E:373:TRP:CZ2	2.53	0.43
1:F:263:VAL:HG12	1:F:264:TRP:CD1	2.54	0.43
1:E:317:TRP:CG	1:E:317:TRP:O	2.71	0.43
1:C:408:LEU:HA	1:C:411:GLU:HG2	2.01	0.43
1:D:424:HIS:O	1:D:428:VAL:N	2.49	0.43
1:D:429:GLN:HE22	1:F:445:HIS:CE1	2.37	0.43
1:E:311:LEU:HD13	1:E:321:HIS:CE1	2.54	0.43
1:H:389:LEU:HD11	1:H:412:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:413:ILE:HG12	1:H:416:LEU:HD12	2.00	0.43
1:I:437:GLY:O	1:I:439:GLU:N	2.51	0.43
1:A:291:GLU:O	1:A:294:ALA:HB3	2.18	0.43
1:A:461:TRP:CH2	1:B:458:LEU:HD11	2.54	0.43
1:D:402:ILE:HD12	1:D:436:GLU:OE2	2.19	0.43
1:E:249:GLN:OE1	1:E:252:VAL:HG21	2.19	0.43
1:E:331:LEU:HB3	1:E:333:PHE:CE2	2.53	0.43
1:A:260:ARG:HH21	1:A:340:ILE:HG23	1.84	0.42
1:A:461:TRP:CD1	1:A:462:GLU:HG3	2.54	0.42
1:D:302:GLY:O	1:D:306:ARG:HG3	2.19	0.42
1:D:472:LEU:O	1:D:472:LEU:HD23	2.19	0.42
1:E:264:TRP:CD2	1:E:347:PHE:CD2	3.07	0.42
1:F:461:TRP:O	1:F:462:GLU:CB	2.65	0.42
1:A:389:LEU:HD11	1:A:412:ARG:HG3	2.00	0.42
1:F:397:HIS:CD2	1:F:436:GLU:OE2	2.72	0.42
1:A:256:TYR:CD2	1:A:336:VAL:HG13	2.54	0.42
1:D:420:ARG:NH1	1:D:462:GLU:OE1	2.51	0.42
1:A:260:ARG:NH2	1:A:340:ILE:HG23	2.34	0.42
1:C:473:ALA:O	1:C:474:ALA:C	2.58	0.42
1:G:461:TRP:O	1:G:462:GLU:CB	2.66	0.42
1:H:446:TYR:CD1	1:H:472:LEU:HB3	2.54	0.42
1:H:445:HIS:O	1:H:449:LEU:N	2.52	0.42
1:I:446:TYR:CZ	1:I:472:LEU:HD13	2.55	0.42
1:C:308:GLU:OE2	1:C:324:SER:OG	2.28	0.42
1:D:390:ALA:O	1:D:394:ALA:HB3	2.19	0.42
1:G:400:GLN:OE1	1:G:400:GLN:N	2.52	0.42
1:I:311:LEU:HD11	1:I:320:GLY:HA3	2.01	0.42
1:E:316:TYR:O	1:E:318:PHE:N	2.53	0.42
1:I:252:VAL:HG11	1:J:261:HIS:CD2	2.54	0.42
1:J:261:HIS:CD2	1:J:265:ALA:HB2	2.54	0.42
1:J:341:ALA:HB2	1:J:373:TRP:CZ3	2.55	0.42
1:F:408:LEU:O	1:F:411:GLU:HG2	2.19	0.42
1:G:316:TYR:O	1:G:318:PHE:N	2.52	0.42
1:A:273:SER:HB2	1:A:277:ASN:HA	2.01	0.42
1:C:323:LEU:O	1:C:326:GLU:N	2.53	0.42
1:I:281:LEU:HD12	1:I:365:PHE:CZ	2.54	0.42
1:I:344:LEU:HD23	1:I:374:LEU:HD11	2.02	0.42
1:J:393:VAL:HA	1:J:408:LEU:HD23	2.01	0.42
1:B:249:GLN:HB3	1:B:252:VAL:CG2	2.49	0.42
1:F:391:GLU:O	1:F:395:GLN:HB2	2.20	0.42
1:F:344:LEU:HD23	1:F:374:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:ALA:HB1	1:F:446:TYR:CZ	2.55	0.42
1:J:453:ALA:O	1:J:456:LEU:N	2.52	0.42
1:A:402:ILE:HD12	1:A:436:GLU:CG	2.50	0.41
1:C:235:ARG:NE	1:C:262:ALA:O	2.51	0.41
1:D:315:PRO:HB2	1:D:316:TYR:CD2	2.55	0.41
1:D:390:ALA:O	1:D:394:ALA:CB	2.67	0.41
1:A:446:TYR:HA	1:A:449:LEU:HD12	2.02	0.41
1:F:332:GLY:O	1:F:334:GLY:N	2.53	0.41
1:I:246:ILE:HG23	1:I:256:TYR:CZ	2.54	0.41
1:I:304:TRP:HZ2	1:I:336:VAL:HG11	1.84	0.41
1:A:458:LEU:HD11	1:B:461:TRP:CH2	2.56	0.41
1:D:246:ILE:HG23	1:D:256:TYR:CZ	2.55	0.41
1:I:234:TRP:CH2	1:J:244:LEU:HB2	2.56	0.41
1:I:407:ALA:O	1:I:410:ASP:HB3	2.20	0.41
1:E:461:TRP:O	1:E:462:GLU:HB3	2.20	0.41
1:B:304:TRP:HB2	1:B:327:VAL:HG11	2.01	0.41
1:C:270:VAL:HG12	1:C:354:LEU:HD21	2.01	0.41
1:C:344:LEU:CD2	1:C:374:LEU:HD11	2.49	0.41
1:C:462:GLU:N	1:C:463:PRO:CD	2.83	0.41
1:B:470:GLU:C	1:B:472:LEU:H	2.23	0.41
1:C:259:ARG:O	1:C:260:ARG:C	2.59	0.41
1:H:413:ILE:HD11	1:H:425:ALA:HB1	2.03	0.41
1:H:259:ARG:NH1	1:H:308:GLU:HB3	2.36	0.41
1:A:254:VAL:HG13	1:A:255:GLY:N	2.36	0.41
1:A:461:TRP:CZ2	1:B:458:LEU:HD11	2.56	0.41
1:C:260:ARG:NH2	1:C:340:ILE:HG23	2.32	0.41
1:C:386:GLU:HB2	1:C:424:HIS:CE1	2.56	0.41
1:G:402:ILE:HB	1:G:436:GLU:OE2	2.21	0.41
1:I:368:PRO:O	1:I:372:ARG:NH2	2.54	0.41
1:D:310:SER:O	1:D:314:ALA:N	2.54	0.41
1:D:318:PHE:O	1:D:319:GLU:C	2.59	0.41
1:D:424:HIS:HA	1:D:427:LEU:HB3	2.02	0.41
1:E:316:TYR:CE1	1:E:354:LEU:HD21	2.55	0.41
1:C:241:VAL:HG12	1:C:245:LEU:CD1	2.51	0.41
1:E:413:ILE:HD11	1:E:425:ALA:CB	2.51	0.40
1:F:283:PRO:HG3	1:F:361:ASP:CG	2.42	0.40
1:G:447:GLN:O	1:G:450:TRP:N	2.54	0.40
1:H:293:ARG:HD3	1:H:323:LEU:HD11	2.03	0.40
1:D:270:VAL:HG12	1:D:354:LEU:CD2	2.51	0.40
1:F:402:ILE:HD12	1:F:436:GLU:CD	2.42	0.40
1:F:453:ALA:O	1:F:454:SER:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:VAL:CG1	1:J:254:VAL:HG12	2.51	0.40
1:D:389:LEU:HD11	1:D:412:ARG:HG3	2.04	0.40
1:E:310:SER:C	1:E:312:THR:H	2.24	0.40
1:C:456:LEU:HD21	1:D:460:HIS:HB2	2.03	0.40
1:G:442:ALA:O	1:G:445:HIS:N	2.55	0.40
1:G:447:GLN:O	1:G:448:HIS:C	2.59	0.40
1:I:463:PRO:O	1:I:465:LEU:N	2.54	0.40
1:B:301:GLN:O	1:B:305:GLN:HG3	2.21	0.40
1:D:246:ILE:HG12	1:D:256:TYR:CE2	2.56	0.40
1:D:464:GLY:O	1:D:465:LEU:C	2.60	0.40
1:G:447:GLN:NE2	1:G:451:GLN:HE21	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	230/270 (85%)	198 (86%)	25 (11%)	7 (3%)	4 21
1	B	233/270 (86%)	205 (88%)	23 (10%)	5 (2%)	7 28
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

All (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
1	I	438	MET
1	E	230	ASN
1	E	231	ASP
1	E	275	ALA
1	E	461	TRP
1	F	461	TRP
1	A	275	ALA
1	B	285	SER
1	D	399	GLU
1	I	264	TRP
1	I	394	ALA
1	I	464	GLY
1	J	333	PHE
1	J	471	SER
1	E	317	TRP
1	E	373	TRP
1	E	400	GLN
1	F	270	VAL
1	F	274	GLY
1	F	275	ALA
1	A	317	TRP
1	A	331	LEU
1	B	471	SER
1	G	448	HIS
1	H	286	ALA
1	C	254	VAL
1	C	317	TRP
1	C	473	ALA
1	D	473	ALA
1	J	275	ALA
1	J	458	LEU
1	F	333	PHE
1	A	283	PRO
1	A	414	ALA
1	C	270	VAL
1	I	275	ALA
1	J	355	ARG

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Mol	Chain	Res	Type
1	E	473	ALA
1	A	461	TRP
1	D	315	PRO
1	I	333	PHE
1	J	315	PRO
1	F	373	TRP
1	D	461	TRP
1	F	254	VAL
1	A	254	VAL
1	G	462	GLU
1	I	463	PRO
1	F	462	GLU
1	E	274	GLY
1	F	299	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	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
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

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	SER
1	A	288	MET
1	A	309	GLN
1	A	410	ASP
1	A	438	MET
1	A	459	SER
1	B	227	ASP
1	B	228	SER
1	B	230	ASN
1	B	244	LEU
1	B	309	GLN
1	B	373	TRP
1	B	420	ARG
1	B	459	SER
1	B	461	TRP
1	G	288	MET
1	G	467	ASN
1	H	415	GLN
1	H	443	ARG
1	C	237	THR
1	C	361	ASP
1	C	393	VAL
1	C	410	ASP
1	D	227	ASP
1	D	228	SER
1	D	315	PRO
1	D	346	THR
1	D	420	ARG
1	J	372	ARG
1	J	422	ARG
1	J	432	LEU
1	J	469	LEU
1	E	230	ASN
1	F	296	MET
1	F	395	GLN
1	F	439	GLU
1	F	459	SER
1	F	461	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN

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Mol	Chain	Res	Type
1	A	429	GLN
1	B	230	ASN
1	G	238	GLN
1	G	277	ASN
1	G	305	GLN
1	G	447	GLN
1	H	249	GLN
1	H	349	GLN
1	H	415	GLN
1	H	429	GLN
1	C	277	ASN
1	C	415	GLN
1	C	429	GLN
1	D	277	ASN
1	D	349	GLN
1	I	249	GLN
1	I	277	ASN
1	I	349	GLN
1	I	429	GLN
1	J	238	GLN
1	J	249	GLN
1	J	349	GLN
1	J	429	GLN
1	E	238	GLN
1	E	309	GLN
1	E	429	GLN
1	E	451	GLN
1	F	249	GLN
1	F	349	GLN
1	F	395	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

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

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	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

All (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	5.8
1	I	354	LEU	5.5
1	I	317	TRP	5.5
1	I	357	LEU	4.8
1	I	292	TYR	4.8
1	I	321	HIS	4.8
1	I	281	LEU	4.7
1	I	361	ASP	4.3
1	I	290	ASP	4.1
1	J	339	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	294	ALA	4.0
1	J	340	ILE	3.9
1	J	344	LEU	3.9
1	I	344	LEU	3.8
1	I	238	GLN	3.7
1	I	311	LEU	3.7
1	J	321	HIS	3.7
1	I	328	ALA	3.6
1	I	289	VAL	3.6
1	I	258	LEU	3.6
1	I	304	TRP	3.5
1	I	316	TYR	3.5
1	I	285	SER	3.4
1	J	254	VAL	3.4
1	I	282	ALA	3.3
1	I	296	MET	3.3
1	I	312	THR	3.3
1	I	315	PRO	3.3
1	G	354	LEU	3.3
1	I	278	LYS	3.2
1	I	291	GLU	3.2
1	I	353	ALA	3.2
1	G	318	PHE	3.1
1	I	239	LEU	3.1
1	I	306	ARG	3.1
1	I	270	VAL	2.9
1	E	292	TYR	2.9
1	I	318	PHE	2.8
1	I	332	GLY	2.8
1	J	259	ARG	2.8
1	F	275	ALA	2.8
1	I	322	ARG	2.7
1	I	362	GLY	2.7
1	J	347	PHE	2.7
1	H	340	ILE	2.6
1	E	299	PRO	2.6
1	I	340	ILE	2.6
1	G	365	PHE	2.5
1	I	298	ALA	2.5
1	I	313	LEU	2.5
1	I	284	MET	2.5
1	I	310	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	342	GLU	2.5
1	I	365	PHE	2.5
1	I	241	VAL	2.4
1	J	301	GLN	2.4
1	G	247	GLU	2.4
1	I	252	VAL	2.3
1	G	366	LEU	2.3
1	I	251	GLU	2.3
1	I	319	GLU	2.3
1	H	268	THR	2.3
1	I	368	PRO	2.3
1	H	317	TRP	2.2
1	I	309	GLN	2.2
1	I	307	ILE	2.2
1	J	250	PRO	2.2
1	I	370	CYS	2.2
1	E	281	LEU	2.1
1	J	267	ILE	2.1
1	J	252	VAL	2.1
1	J	316	TYR	2.1
1	I	254	VAL	2.1
1	I	341	ALA	2.1
1	I	339	ALA	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.