



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:02 PM UTC

PDB ID : 6G7C / pdb_00006g7c
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

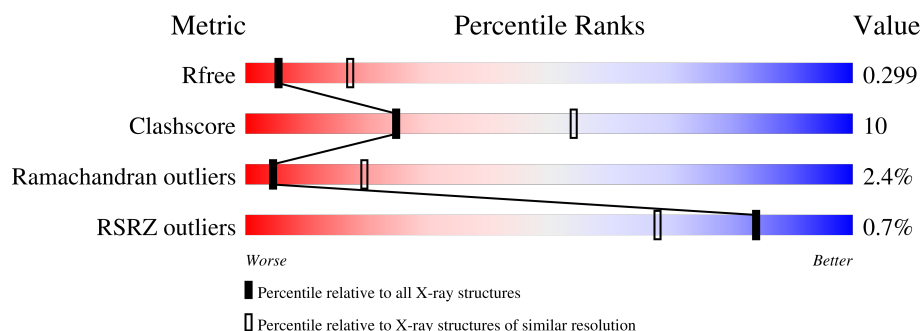
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (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	
1	B	270	
1	C	270	
1	D	270	
1	E	270	
1	F	270	

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Mol	Chain	Length	Quality of chain
1	G	270	% 62%22%15%
1	H	270	70%16%14%
1	I	270	% 66%17%15%
1	J	270	2% 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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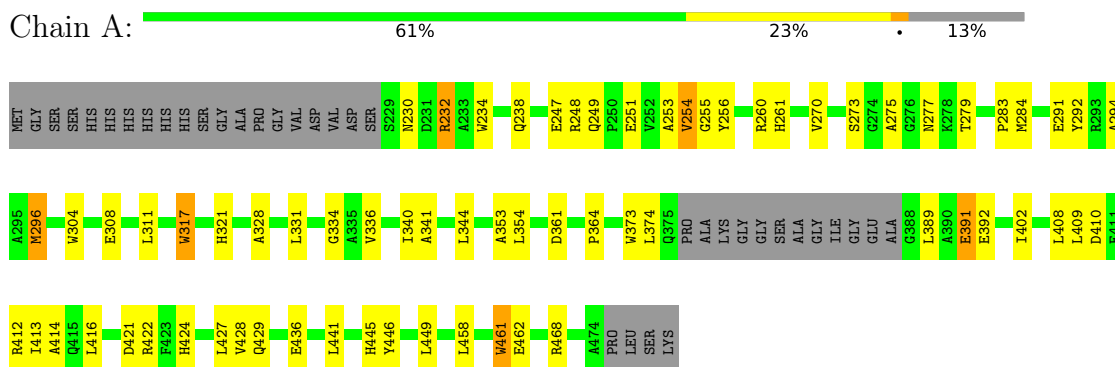
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Chain	Residue	Modelled	Actual	Comment	Reference
F	218	HIS	-	expression tag	UNP A0KJC7
F	219	SER	-	expression tag	UNP A0KJC7
F	220	GLY	-	expression tag	UNP A0KJC7
F	221	ALA	-	expression tag	UNP A0KJC7
F	222	PRO	-	expression tag	UNP A0KJC7

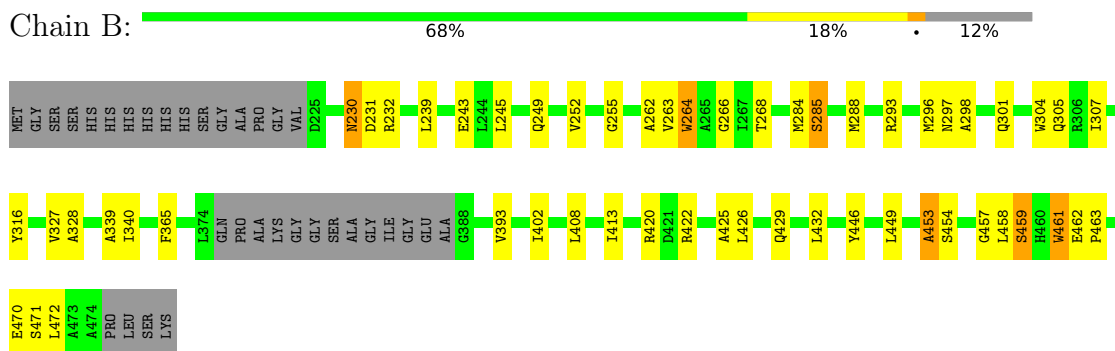
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

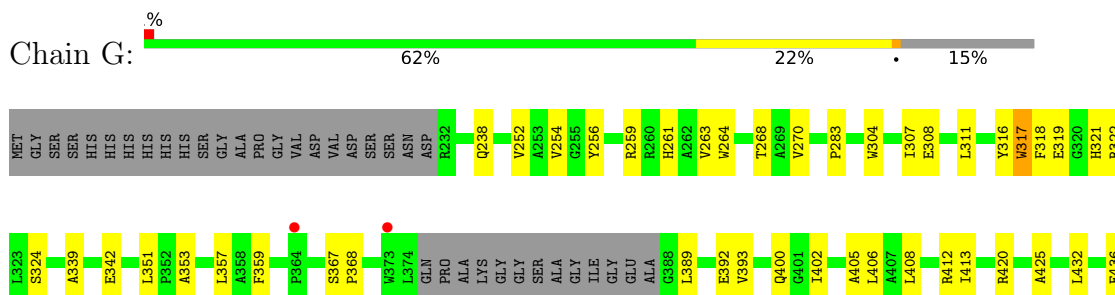
- Molecule 1: ImpA-related domain protein

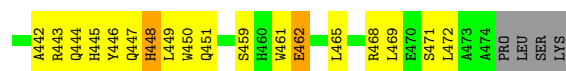


- Molecule 1: ImpA-related domain protein



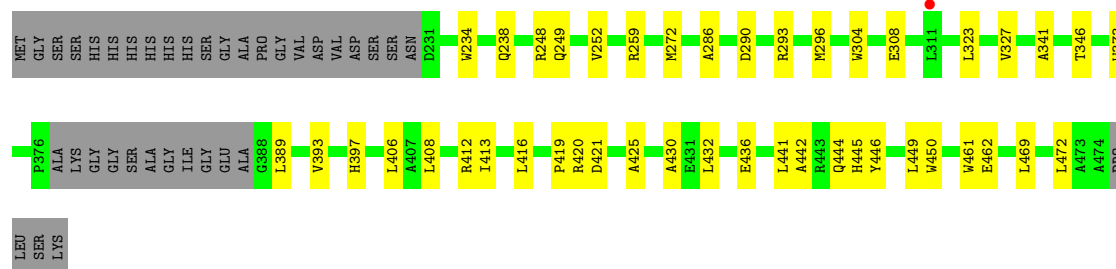
- Molecule 1: ImpA-related domain protein





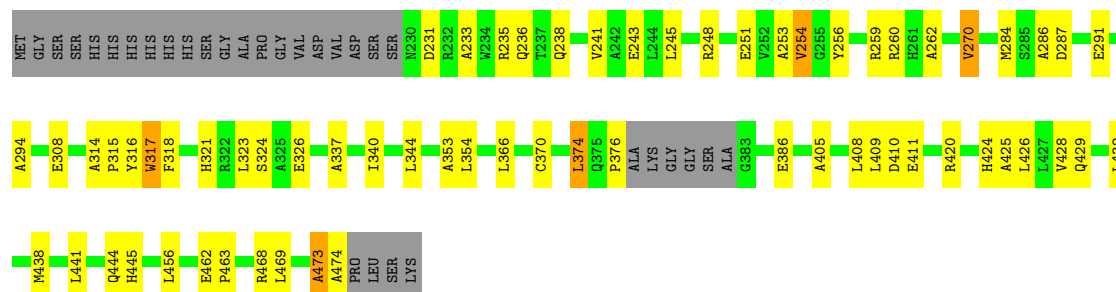
- Molecule 1: ImpA-related domain protein

Chain H: 70% 16% 14%



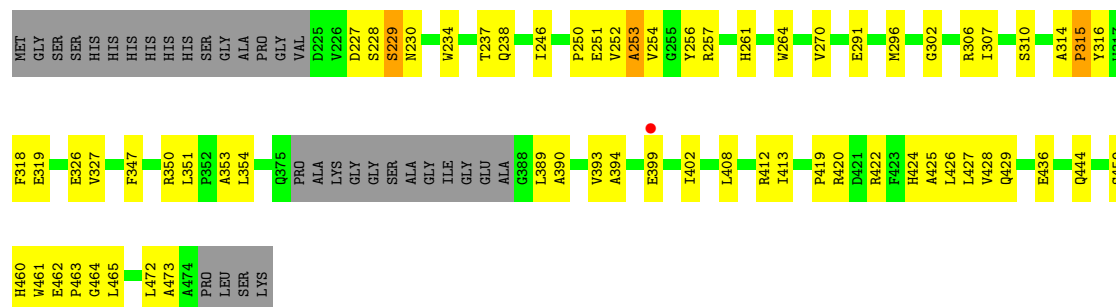
- Molecule 1: ImpA-related domain protein

Chain C: 64% 22% 11%



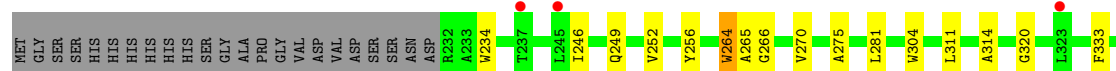
- Molecule 1: ImpA-related domain protein

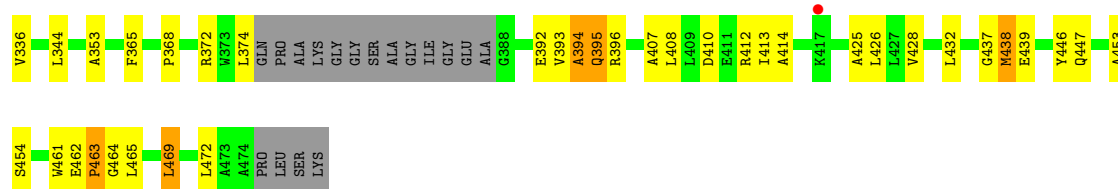
Chain D: 64% 23% 12%



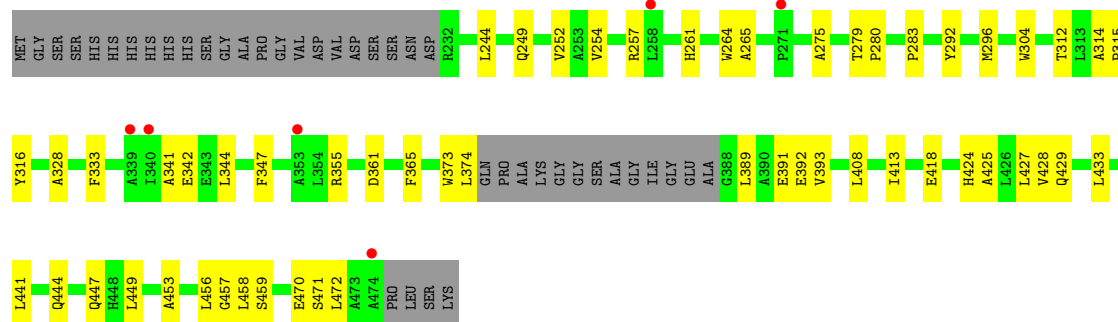
- Molecule 1: ImpA-related domain protein

Chain I: 66% 17% 15%

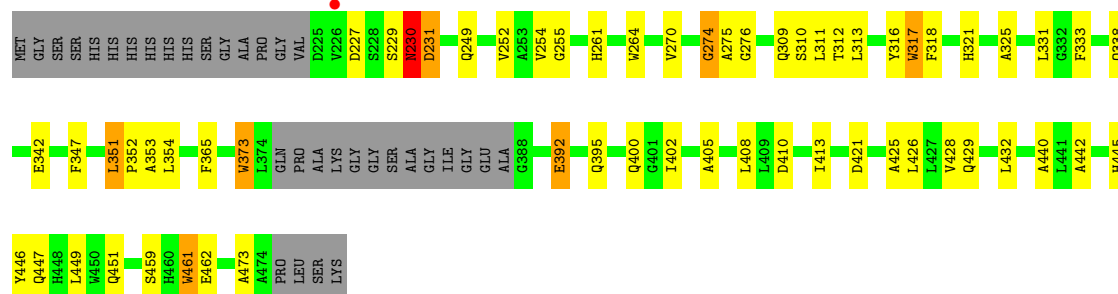




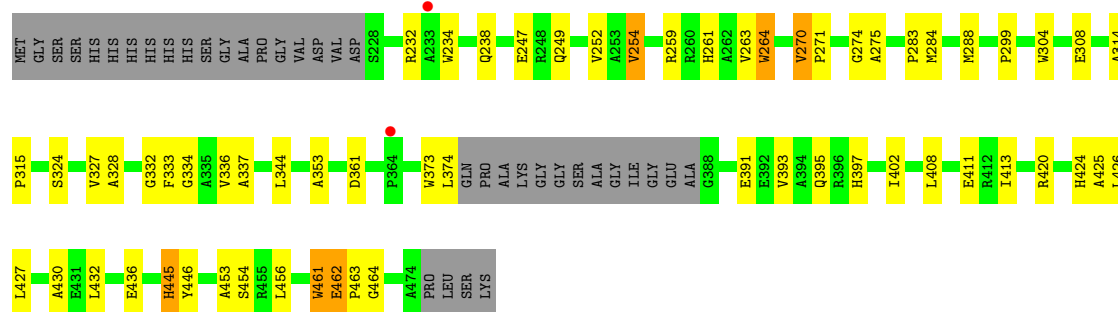
• Molecule 1: ImpA-related domain protein



• 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 – 3.13 202.08 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.8 (202.08-3.13) 89.2 (202.08-3.13)	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 (Not available) , 0.299	Depositor DCC
R_{free} test set	3386 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)	0.31 , 49.9	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	0.93	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	0.84	0/1874	1.17	8/2541 (0.3%)
1	B	0.82	0/1898	1.16	5/2574 (0.2%)
1	C	0.85	0/1903	1.18	10/2580 (0.4%)
1	D	0.80	0/1903	1.22	15/2581 (0.6%)
1	E	0.82	1/1898 (0.1%)	1.14	13/2574 (0.5%)
1	F	0.74	0/1875	1.13	5/2542 (0.2%)
1	G	0.81	0/1847	1.11	8/2504 (0.3%)
1	H	0.74	0/1872	1.02	1/2539 (0.0%)
1	I	0.82	0/1847	1.02	6/2504 (0.2%)
1	J	0.83	0/1847	1.14	7/2504 (0.3%)
All	All	0.81	1/18764 (0.0%)	1.13	78/25443 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	229	SER	CA-C	6.57	1.60	1.52

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	SER	N-CA-C	13.39	125.32	108.45
1	B	307	ILE	N-CA-C	-8.83	102.26	110.82
1	C	374	LEU	N-CA-C	7.96	119.96	111.28
1	D	253	ALA	N-CA-C	7.68	120.32	111.11
1	D	459	SER	N-CA-C	-7.53	104.12	113.38
1	D	296	MET	N-CA-C	7.49	119.08	111.07
1	D	254	VAL	N-CA-C	7.48	118.22	110.36
1	G	307	ILE	N-CA-C	-7.44	103.53	110.53
1	F	464	GLY	N-CA-C	-7.44	103.49	112.49
1	E	230	ASN	N-CA-C	-7.24	95.38	110.80
1	G	405	ALA	N-CA-C	-7.17	103.40	111.14
1	J	418	GLU	CA-C-N	7.16	127.77	119.47
1	J	418	GLU	C-N-CA	7.16	127.77	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	314	ALA	CA-C-N	7.15	128.77	119.84
1	J	314	ALA	C-N-CA	7.15	128.77	119.84
1	F	264	TRP	N-CA-C	6.93	121.83	113.23
1	G	357	LEU	N-CA-C	6.87	119.43	110.43
1	F	445	HIS	N-CA-C	-6.83	106.84	114.62
1	I	314	ALA	CA-C-N	6.76	126.27	119.24
1	I	314	ALA	C-N-CA	6.76	126.27	119.24
1	A	232	ARG	N-CA-C	-6.75	103.53	111.03
1	F	232	ARG	N-CA-C	-6.63	102.61	111.96
1	H	290	ASP	N-CA-C	6.63	118.50	111.28
1	G	322	ARG	N-CA-C	-6.59	103.36	111.40
1	I	469	LEU	N-CA-C	-6.59	104.18	111.82
1	J	391	GLU	N-CA-C	-6.57	104.05	111.14
1	G	252	VAL	N-CA-C	6.33	117.25	108.89
1	C	256	TYR	N-CA-C	-6.29	104.33	111.07
1	C	376	PRO	N-CA-CB	6.16	109.78	103.00
1	D	229	SER	CB-CA-C	-6.04	100.90	110.86
1	J	433	LEU	N-CA-C	-5.94	104.72	111.14
1	C	337	ALA	N-CA-C	-5.89	104.55	110.97
1	C	243	GLU	N-CA-C	-5.88	104.56	110.97
1	B	243	GLU	N-CA-C	-5.87	104.80	111.14
1	D	252	VAL	N-CA-C	5.86	116.87	107.73
1	A	247	GLU	N-CA-C	-5.84	104.82	111.07
1	A	468	ARG	N-CA-C	-5.83	104.56	111.03
1	B	459	SER	N-CA-C	-5.79	105.32	112.90
1	D	228	SER	CA-C-N	5.77	130.24	120.88
1	D	228	SER	C-N-CA	5.77	130.24	120.88
1	A	334	GLY	N-CA-C	5.76	119.64	112.73
1	E	440	ALA	N-CA-C	5.75	117.23	110.97
1	A	296	MET	N-CA-C	5.74	119.09	111.75
1	E	421	ASP	N-CA-C	-5.73	104.67	111.03
1	B	264	TRP	N-CA-C	5.69	120.07	113.18
1	D	251	GLU	CA-C-N	5.69	129.59	122.43
1	D	251	GLU	C-N-CA	5.69	129.59	122.43
1	I	395	GLN	N-CA-C	-5.66	104.75	111.03
1	E	459	SER	N-CA-C	-5.64	104.75	111.69
1	E	229	SER	CB-CA-C	5.61	119.47	109.65
1	E	365	PHE	N-CA-C	-5.46	105.24	111.14
1	I	428	VAL	CB-CA-C	-5.46	104.87	112.02
1	E	351	LEU	CA-C-N	5.46	125.54	119.32
1	E	351	LEU	C-N-CA	5.46	125.54	119.32
1	J	312	THR	N-CA-C	-5.43	107.20	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	GLU	N-CA-C	-5.42	105.28	111.07
1	D	307	ILE	N-CA-CB	5.41	117.49	110.57
1	C	238	GLN	N-CA-C	-5.41	105.28	111.07
1	G	254	VAL	N-CA-C	5.39	118.61	111.17
1	A	364	PRO	N-CA-C	5.39	119.65	111.19
1	B	453	ALA	N-CA-C	-5.37	104.31	111.24
1	C	253	ALA	N-CA-C	5.36	120.16	111.37
1	F	247	GLU	N-CA-C	-5.35	105.34	111.07
1	C	254	VAL	N-CA-C	5.32	120.40	109.34
1	D	327	VAL	CB-CA-C	-5.29	105.20	111.97
1	C	231	ASP	N-CA-C	-5.29	104.94	111.33
1	E	231	ASP	N-CA-C	5.24	121.97	110.80
1	A	391	GLU	N-CA-C	-5.20	105.26	111.03
1	G	264	TRP	N-CA-C	5.20	120.62	113.97
1	E	392	GLU	N-CA-C	5.13	117.78	111.82
1	C	321	HIS	N-CA-C	-5.12	106.54	112.89
1	D	426	LEU	N-CA-C	-5.08	106.93	113.23
1	E	405	ALA	N-CA-C	-5.08	105.65	111.14
1	A	279	THR	N-CA-C	-5.04	103.33	110.29
1	I	447	GLN	N-CA-C	-5.03	105.26	111.40
1	G	459	SER	N-CA-C	-5.02	105.89	111.36
1	E	229	SER	CA-C-N	5.00	131.09	121.54
1	E	229	SER	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

There are no planarity outliers.

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	1834	0	1804	51	0
1	B	1858	0	1824	37	0
1	C	1863	0	1828	46	0
1	D	1863	0	1826	40	0
1	E	1858	0	1824	38	0
1	F	1835	0	1807	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1807	0	1787	40	0
1	H	1831	0	1806	37	0
1	I	1807	0	1787	35	0
1	J	1807	0	1787	34	0
All	All	18363	0	18080	357	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 10.

All (357) 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:E:230:ASN:CG	1:E:230:ASN:O	2.34	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:N	1:C:251:GLU:OE1	2.27	0.67
1:I:413:ILE:HD11	1:I:425:ALA:HB3	1.76	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:457:GLY:C	1:J:459:SER:H	2.09	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: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:E:261:HIS:HE2	1:F:249:GLN:HE22	1.50	0.58
1:C:284:MET:HG3	1:C:317:TRP:CD2	2.39	0.57
1:B:284:MET:HE1	1:B:288:MET:HE3	1.85	0.56
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:283:PRO:HG3	1:J:361:ASP:OD2	2.06	0.56
1:A:410:ASP:C	1:A:410:ASP:OD1	2.49	0.56
1:H:234:TRP:NE1	1:H:238:GLN:HE21	2.04	0.56
1:C:456:LEU:HD21	1:D:460:HIS:CB	2.35	0.56
1:H:272:MET:HE2	1:H:272:MET:HA	1.88	0.55
1:C:405:ALA:HB1	1:C:432:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:428:VAL:O	1:J:429:GLN:C	2.50	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:C:286:ALA:O	1:C:287:ASP:C	2.50	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:420:ARG:HH22	1:G:462:GLU:CD	2.16	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:C:410:ASP:C	1:C:410:ASP:OD1	2.51	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:J:470:GLU:C	1:J:472:LEU:H	2.17	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:G:461:TRP:O	1:G:462:GLU:HB2	2.08	0.52
1:F:304:TRP:CZ2	1:F:328:ALA:HB2	2.43	0.52
1:G:319:GLU:OE1	1:G:319:GLU:HA	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:J:447:GLN:C	1:J:449:LEU:H	2.17	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:G:283:PRO:HB3	1:G:359:PHE:CD2	2.46	0.51
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:C:425:ALA:O	1:C:426:LEU:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:GLU:OE1	1:I:412:ARG:NH1	2.38	0.51
1:F:308:GLU:OE2	1:F:324:SER:OG	2.23	0.50
1:G:468:ARG:O	1:G:471:SER:OG	2.26	0.50
1:D:253:ALA:O	1:D:257:ARG:HG3	2.11	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:A:408:LEU:O	1:A:409:LEU:C	2.52	0.50
1:B:453:ALA:O	1:B:454:SER:C	2.55	0.50
1:H:249:GLN:HE21	1:H:252:VAL:CG2	2.15	0.50
1:H:430:ALA:HB1	1:H:446:TYR:CE2	2.47	0.50
1:E:311:LEU:HB2	1:E:321:HIS:CE1	2.46	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:468:ARG:O	1:C:469:LEU:C	2.54	0.49
1:A:311:LEU:HD13	1:A:321:HIS:CE1	2.48	0.49
1:G:444:GLN:CG	1:I:426:LEU:HD11	2.42	0.49
1:C:344:LEU:HD23	1:C:374:LEU:HD11	1.93	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: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:E:325:ALA:CB	1:E:373:TRP:CZ2	2.96	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:F:314:ALA:O	1:F:315:PRO:C	2.56	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:C:366:LEU:HD12	1:C:370:CYS:SG	2.53	0.48
1:I:461:TRP:O	1:I:462:GLU:CB	2.61	0.48
1:E:261:HIS:HE2	1:F:249:GLN:NE2	2.11	0.48
1:E:447:GLN:HE21	1:E:451:GLN:NE2	2.11	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:HIS:O	1:A:427:LEU:HB3	2.14	0.48
1:C:323:LEU:O	1:C:324:SER:C	2.56	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:A:261:HIS:NE2	1:B:249:GLN:OE1	2.48	0.47
1:H:461:TRP:O	1:H:462:GLU:CB	2.60	0.47
1:C:473:ALA:O	1:C:474:ALA:C	2.58	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:C:308:GLU:OE2	1:C:324:SER:OG	2.28	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:389:LEU:C	1:A:391:GLU:N	2.71	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:G:339:ALA:O	1:G:342:GLU:N	2.49	0.46
1:E:338:GLN:NE2	1:E:342:GLU:OE2	2.47	0.46
1:J:389:LEU:O	1:J:392:GLU:HB3	2.16	0.46
1:F:252:VAL:HG12	1:F:254:VAL:HG12	1.98	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:B:470:GLU:C	1:B:472:LEU:H	2.23	0.46
1:C:259:ARG:O	1:C:260:ARG:C	2.59	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:HG22	1:H:346:THR:O	2.16	0.45
1:D:318:PHE:O	1:D:319:GLU:C	2.59	0.45
1:D:291:GLU:C	1:D:291:GLU:CD	2.85	0.45
1:F:283:PRO:HG3	1:F:361:ASP:CG	2.42	0.45
1:F:402:ILE:HD12	1:F:436:GLU:CD	2.42	0.45
1:F:453:ALA:O	1:F:454:SER:C	2.60	0.45
1:F:461:TRP:O	1:F:462:GLU:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:CG1	1:B:432:LEU:HD21	2.47	0.45
1:B:413:ILE:HD11	1:B:425:ALA:CB	2.46	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:D:464:GLY:O	1:D:465:LEU:C	2.60	0.45
1:E:310:SER:C	1:E:312:THR:H	2.24	0.45
1:A:410:ASP:OD2	1:C:438:MET:HA	2.17	0.45
1:B:316:TYR:CD1	1:B:365:PHE:CE2	3.05	0.45
1:G:447:GLN:O	1:G:448:HIS:C	2.59	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:B:457:GLY:C	1:B:459:SER:H	2.24	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:F:336:VAL:O	1:F:337:ALA:C	2.60	0.45
1:J:304:TRP:CZ2	1:J:328:ALA:HB2	2.51	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:H:442:ALA:C	1:H:444:GLN:N	2.75	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:J:249:GLN:NE2	1:J:252:VAL:HG21	2.33	0.44
1:E:311:LEU:HD13	1:E:321:HIS:NE2	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:I:413:ILE:O	1:I:414:ALA:C	2.59	0.44
1:A:253:ALA:O	1:A:254:VAL:C	2.61	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:C:314:ALA:O	1:C:315:PRO:C	2.61	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:E:254:VAL:O	1:E:255:GLY:C	2.60	0.43
1:H:248:ARG:C	1:H:249:GLN:HG3	2.41	0.43
1:H:296:MET:HE1	1:H:327:VAL:HG23	1.99	0.43
1:A:311:LEU:HD22	1:A:321:HIS:CE1	2.53	0.43
1:G:256:TYR:OH	1:G:304:TRP:CH2	2.69	0.43
1:G:406:LEU:HB2	1:I:438:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:MET:HE1	1:H:327:VAL:CG2	2.49	0.43
1:E:392:GLU:O	1:E:395:GLN:HB3	2.18	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:B:230:ASN:ND2	1:B:230:ASN:C	2.74	0.43
1:C:270:VAL:HG11	1:C:353:ALA:HB3	2.00	0.43
1:J:447:GLN:C	1:J:449:LEU:N	2.77	0.43
1:H:341:ALA:HB2	1:H:373:TRP:CZ2	2.53	0.43
1:B:446:TYR:HA	1:B:449:LEU:HD12	1.99	0.43
1:D:314:ALA:O	1:D:315:PRO:C	2.62	0.43
1:E:325:ALA:HB3	1:E:373:TRP:CZ2	2.53	0.43
1:E:408:LEU:C	1:E:410:ASP:N	2.75	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:G:442:ALA:O	1:G:443:ARG:C	2.61	0.43
1:H:389:LEU:HD11	1:H:412:ARG:HG3	2.01	0.43
1:H:413:ILE:HG12	1:H:416:LEU:HD12	2.00	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:I:437:GLY:O	1:I:439:GLU:N	2.51	0.43
1:E:311:LEU:HD13	1:E:321:HIS:CE1	2.54	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:G:308:GLU:OE2	1:G:324:SER:OG	2.34	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:C:428:VAL:O	1:C:429:GLN:C	2.62	0.42
1:E:428:VAL:O	1:E:429:GLN:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:C	1:A:311:LEU:HD12	2.44	0.42
1:G:461:TRP:O	1:G:462:GLU:CB	2.66	0.42
1:H:445:HIS:O	1:H:449:LEU:N	2.52	0.42
1:H:446:TYR:CD1	1:H:472:LEU:HB3	2.54	0.42
1:I:446:TYR:CZ	1:I:472:LEU:HD13	2.55	0.42
1:A:361:ASP:OD1	1:A:361:ASP:C	2.62	0.42
1:G:400:GLN:OE1	1:G:400:GLN:N	2.52	0.42
1:D:390:ALA:O	1:D:394:ALA:HB3	2.19	0.42
1:I:311:LEU:HD11	1:I:320:GLY:HA3	2.01	0.42
1:I:252:VAL:HG11	1:J:261:HIS:CD2	2.54	0.42
1:I:432:LEU:C	1:I:432:LEU:HD23	2.44	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:E:316:TYR:O	1:E:318:PHE:N	2.53	0.42
1:G:316:TYR:O	1:G:318:PHE:N	2.52	0.42
1:I:393:VAL:O	1:I:394:ALA:C	2.61	0.42
1:F:408:LEU:O	1:F:411:GLU:HG2	2.19	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:C:408:LEU:O	1:C:409:LEU:C	2.62	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:A:248:ARG:C	1:A:249:GLN:HG3	2.45	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:J:453:ALA:O	1:J:456:LEU:N	2.52	0.42
1:F:344:LEU:HD23	1:F:374:LEU:HD11	2.01	0.42
1:F:430:ALA:HB1	1:F:446:TYR:CZ	2.55	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:C:432:LEU:C	1:C:432:LEU:HD23	2.45	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:B:339:ALA:O	1:B:340:ILE:C	2.62	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:I:453:ALA:O	1:I:454:SER:C	2.62	0.41
1:F:332:GLY:O	1:F:334:GLY:N	2.53	0.41
1:J:470:GLU:C	1:J:472:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:367:SER:O	1:G:368:PRO:C	2.63	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:B:461:TRP:O	1:B:462:GLU:C	2.63	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: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:E:352:PRO:O	1:E:353:ALA:C	2.63	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:G:402:ILE:HB	1:G:436:GLU:OE2	2.21	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:D:310:SER:O	1:D:314:ALA:N	2.54	0.41
1:D:424:HIS:HA	1:D:427:LEU:HB3	2.02	0.41
1:I:368:PRO:O	1:I:372:ARG:NH2	2.54	0.41
1:E:316:TYR:CE1	1:E:354:LEU:HD21	2.55	0.41
1:A:230:ASN:C	1:A:232:ARG:H	2.29	0.41
1:C:241:VAL:HG12	1:C:245:LEU:CD1	2.51	0.41
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:E:413:ILE:HD11	1:E:425:ALA:CB	2.51	0.40
1:E:446:TYR:O	1:E:447:GLN:C	2.64	0.40
1:H:419:PRO:O	1:H:420:ARG:C	2.63	0.40
1:D:270:VAL:HG12	1:D:354:LEU:CD2	2.51	0.40
1:J:252:VAL:CG1	1:J:254:VAL:HG12	2.51	0.40
1:F:284:MET:CE	1:F:288:MET:HE3	2.51	0.40
1:D:389:LEU:HD11	1:D:412:ARG:HG3	2.04	0.40
1:G:442:ALA:O	1:G:445:HIS:N	2.55	0.40
1:C:456:LEU:HD21	1:D:460:HIS:HB2	2.03	0.40
1:I:463:PRO:O	1:I:465:LEU:N	2.54	0.40
1:J:457:GLY:C	1:J:459:SER:N	2.74	0.40
1:B:301:GLN:O	1:B:305:GLN:HG3	2.21	0.40
1:G:447:GLN:NE2	1:G:451:GLN:HE21	2.20	0.40
1:D:246:ILE:HG12	1:D:256:TYR:CE2	2.56	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%)	3	16
1	B	233/270 (86%)	205 (88%)	23 (10%)	5 (2%)	5	22
1	C	235/270 (87%)	199 (85%)	32 (14%)	4 (2%)	7	27
1	D	234/270 (87%)	201 (86%)	29 (12%)	4 (2%)	7	27
1	E	233/270 (86%)	196 (84%)	28 (12%)	9 (4%)	2	12
1	F	230/270 (85%)	195 (85%)	26 (11%)	9 (4%)	2	12
1	G	226/270 (84%)	198 (88%)	25 (11%)	3 (1%)	9	32
1	H	229/270 (85%)	204 (89%)	24 (10%)	1 (0%)	30	59
1	I	226/270 (84%)	194 (86%)	24 (11%)	8 (4%)	3	14
1	J	226/270 (84%)	193 (85%)	27 (12%)	6 (3%)	4	18
All	All	2302/2700 (85%)	1983 (86%)	263 (11%)	56 (2%)	4	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	E	274	GLY
1	F	299	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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%)	-0.25	0 100 100	47, 74, 106, 129	0
1	B	237/270 (87%)	-0.08	0 100 100	52, 91, 124, 144	0
1	C	239/270 (88%)	-0.16	0 100 100	48, 83, 122, 138	0
1	D	238/270 (88%)	0.01	1 (0%) 88 76	47, 98, 140, 176	0
1	E	237/270 (87%)	-0.09	1 (0%) 88 76	45, 88, 137, 160	0
1	F	234/270 (86%)	0.03	2 (0%) 81 63	53, 106, 143, 164	0
1	G	230/270 (85%)	0.08	2 (0%) 81 63	46, 100, 145, 159	0
1	H	233/270 (86%)	-0.06	1 (0%) 88 76	57, 104, 138, 163	0
1	I	230/270 (85%)	0.34	4 (1%) 69 48	54, 154, 200, 236	0
1	J	230/270 (85%)	0.11	6 (2%) 57 35	52, 102, 163, 197	0
All	All	2342/2700 (86%)	-0.01	17 (0%) 84 68	45, 94, 161, 236	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	353	ALA	3.1
1	G	373	TRP	2.7
1	E	226	VAL	2.6
1	F	364	PRO	2.5
1	J	474	ALA	2.5
1	J	271	PRO	2.4
1	J	340	ILE	2.2
1	J	339	ALA	2.2
1	F	233	ALA	2.2
1	I	323	LEU	2.2
1	H	311	LEU	2.2
1	I	245	LEU	2.2
1	I	237	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	417	LYS	2.1
1	G	364	PRO	2.1
1	D	399	GLU	2.0
1	J	258	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.