



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:00 AM UTC

PDB ID : 8RJ8 / pdb_00008rj8
Title : CytK nanopore mutant
Authors : Whittaker, J.J.; Sauciuc, A.; Guskov, A.
Deposited on : 2023-12-20
Resolution : 4.32 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	:	4-5-2 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

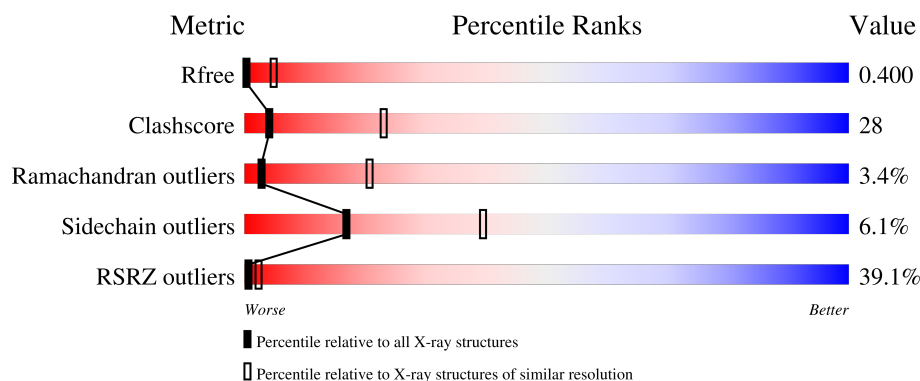
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.32 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	1056 (4.72-3.90)
Clashscore	190562	1101 (4.72-3.90)
Ramachandran outliers	187476	1003 (4.72-3.90)
Sidechain outliers	187428	1010 (4.76-3.88)
RSRZ outliers	180081	1053 (4.72-3.90)

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	310	35% 40% 45% 7% 6%
1	B	310	35% 45% 40% 12%
1	C	310	37% 49% 38% 5% 8%
1	D	310	45% 37% 43% 8% 10%
1	E	310	43% 49% 40% 6%

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Mol	Chain	Length	Quality of chain
1	F	310	27% 43% 49% . . .
1	G	310	32% 54% 38% . 6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 15699 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 Cytotoxin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2267	1419	381	460	7			
1	B	272	Total	C	N	O	S	0	0	0
			2119	1324	357	431	7			
1	C	284	Total	C	N	O	S	0	0	0
			2227	1396	376	448	7			
1	D	279	Total	C	N	O	S	0	0	0
			2184	1371	368	438	7			
1	E	292	Total	C	N	O	S	0	0	0
			2267	1420	380	460	7			
1	F	302	Total	C	N	O	S	0	0	0
			2351	1472	393	478	8			
1	G	292	Total	C	N	O	S	0	0	0
			2284	1432	382	463	7			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q09KJ1
A	130	ASP	LYS	conflict	UNP Q09KJ1
A	149	ASP	THR	conflict	UNP Q09KJ1
A	157	ASP	LYS	conflict	UNP Q09KJ1
A	308	GLY	-	expression tag	UNP Q09KJ1
A	309	SER	-	expression tag	UNP Q09KJ1
A	310	ALA	-	expression tag	UNP Q09KJ1
B	1	MET	-	initiating methionine	UNP Q09KJ1
B	130	ASP	LYS	conflict	UNP Q09KJ1
B	149	ASP	THR	conflict	UNP Q09KJ1
B	157	ASP	LYS	conflict	UNP Q09KJ1
B	308	GLY	-	expression tag	UNP Q09KJ1
B	309	SER	-	expression tag	UNP Q09KJ1
B	310	ALA	-	expression tag	UNP Q09KJ1
C	1	MET	-	initiating methionine	UNP Q09KJ1

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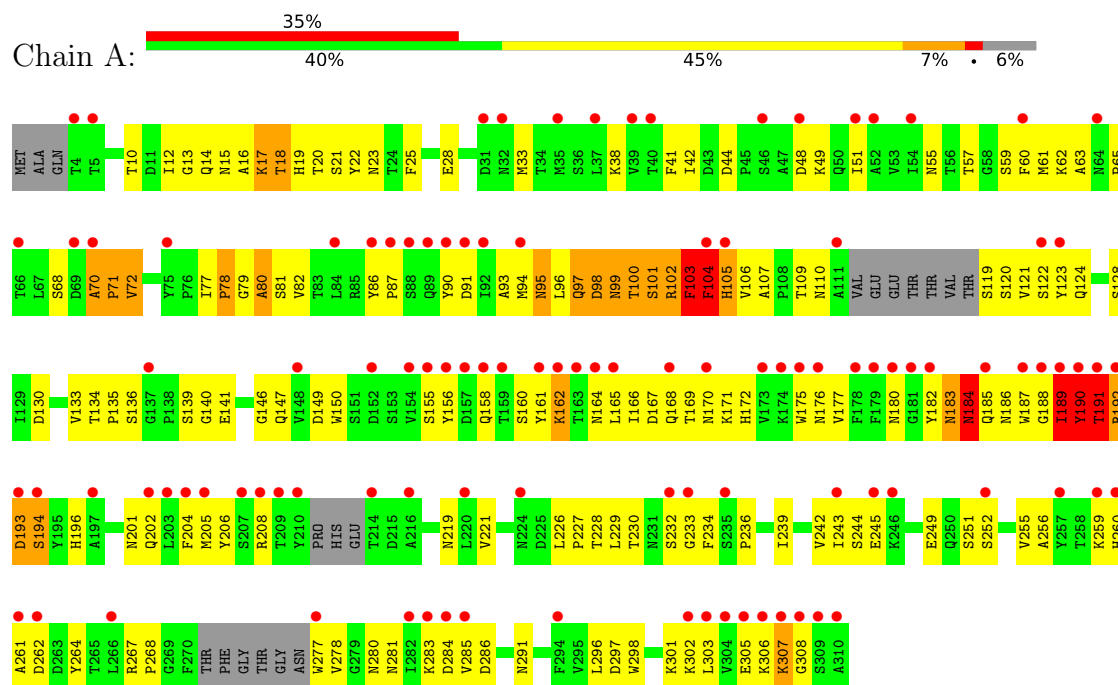
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Chain	Residue	Modelled	Actual	Comment	Reference
C	130	ASP	LYS	conflict	UNP Q09KJ1
C	149	ASP	THR	conflict	UNP Q09KJ1
C	157	ASP	LYS	conflict	UNP Q09KJ1
C	308	GLY	-	expression tag	UNP Q09KJ1
C	309	SER	-	expression tag	UNP Q09KJ1
C	310	ALA	-	expression tag	UNP Q09KJ1
D	1	MET	-	initiating methionine	UNP Q09KJ1
D	130	ASP	LYS	conflict	UNP Q09KJ1
D	149	ASP	THR	conflict	UNP Q09KJ1
D	157	ASP	LYS	conflict	UNP Q09KJ1
D	308	GLY	-	expression tag	UNP Q09KJ1
D	309	SER	-	expression tag	UNP Q09KJ1
D	310	ALA	-	expression tag	UNP Q09KJ1
E	1	MET	-	initiating methionine	UNP Q09KJ1
E	130	ASP	LYS	conflict	UNP Q09KJ1
E	149	ASP	THR	conflict	UNP Q09KJ1
E	157	ASP	LYS	conflict	UNP Q09KJ1
E	308	GLY	-	expression tag	UNP Q09KJ1
E	309	SER	-	expression tag	UNP Q09KJ1
E	310	ALA	-	expression tag	UNP Q09KJ1
F	1	MET	-	initiating methionine	UNP Q09KJ1
F	130	ASP	LYS	conflict	UNP Q09KJ1
F	149	ASP	THR	conflict	UNP Q09KJ1
F	157	ASP	LYS	conflict	UNP Q09KJ1
F	308	GLY	-	expression tag	UNP Q09KJ1
F	309	SER	-	expression tag	UNP Q09KJ1
F	310	ALA	-	expression tag	UNP Q09KJ1
G	1	MET	-	initiating methionine	UNP Q09KJ1
G	130	ASP	LYS	conflict	UNP Q09KJ1
G	149	ASP	THR	conflict	UNP Q09KJ1
G	157	ASP	LYS	conflict	UNP Q09KJ1
G	308	GLY	-	expression tag	UNP Q09KJ1
G	309	SER	-	expression tag	UNP Q09KJ1
G	310	ALA	-	expression tag	UNP Q09KJ1

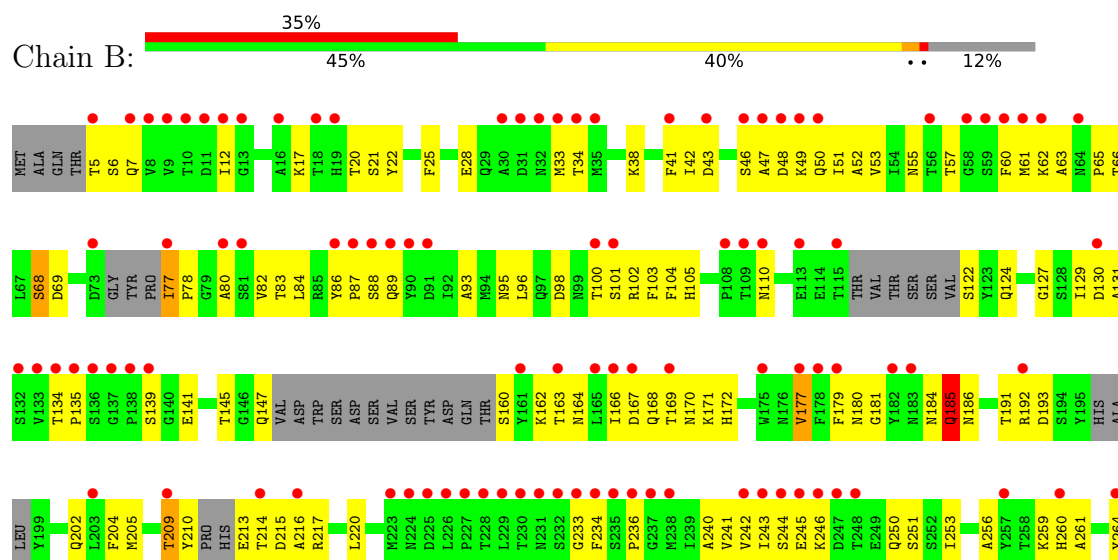
3 Residue-property plots

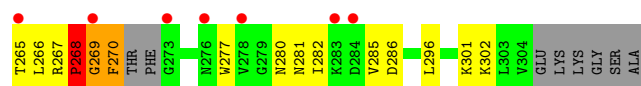
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytotoxin K

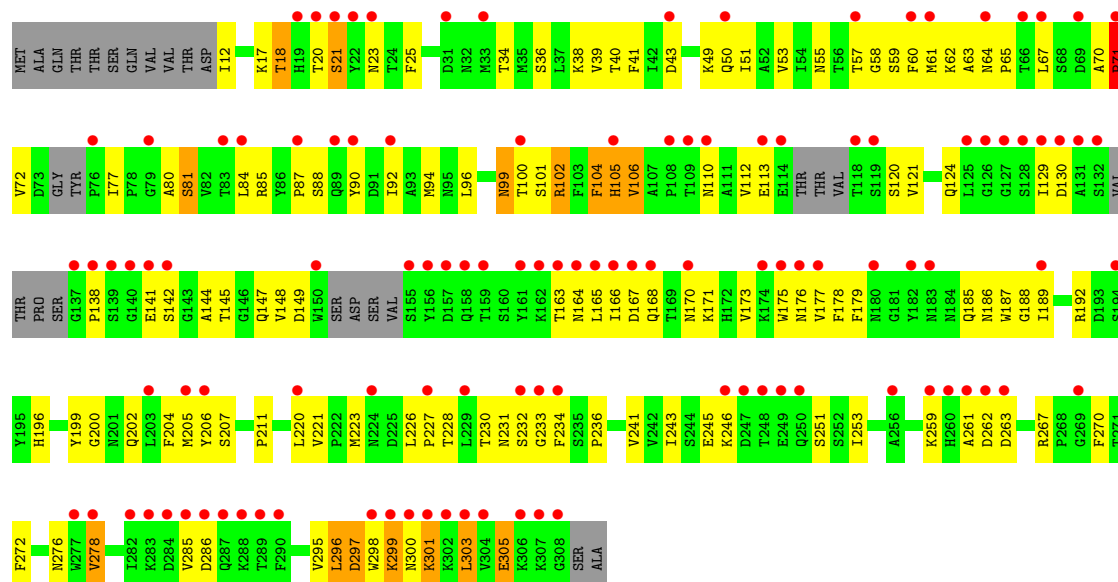


• Molecule 1: Cytotoxin K

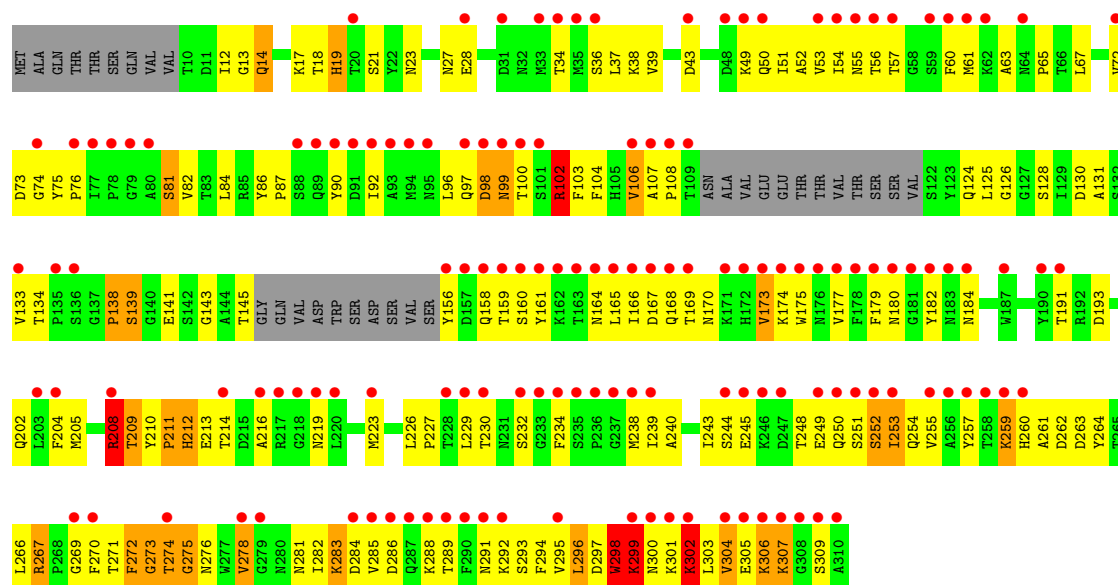




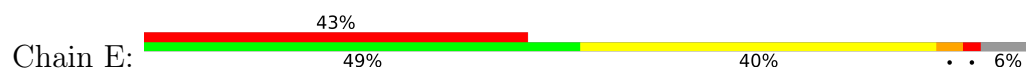
• Molecule 1: Cytotoxin K

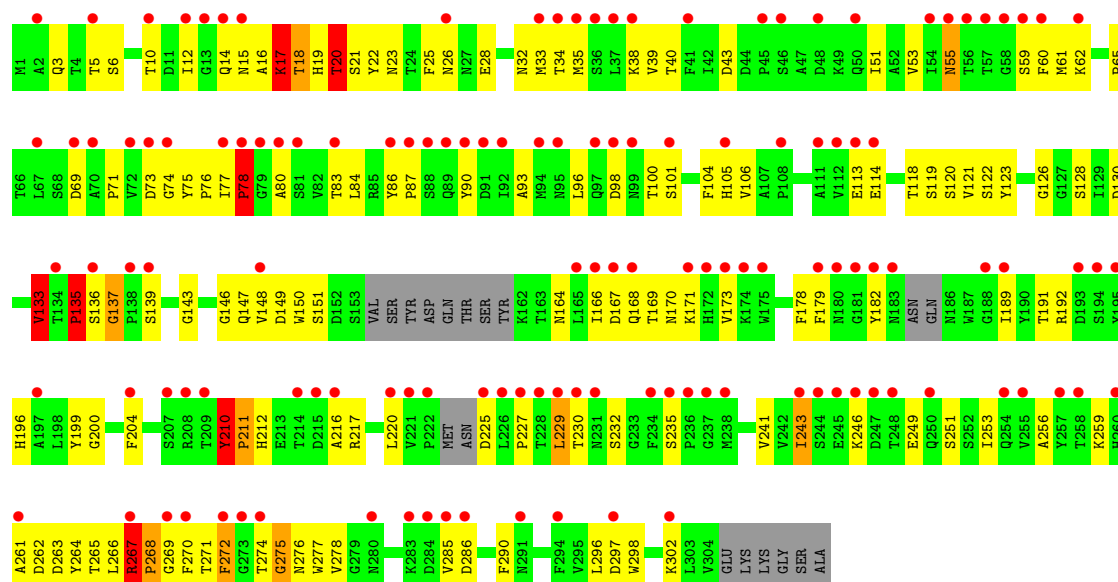


• Molecule 1: Cytotoxin K

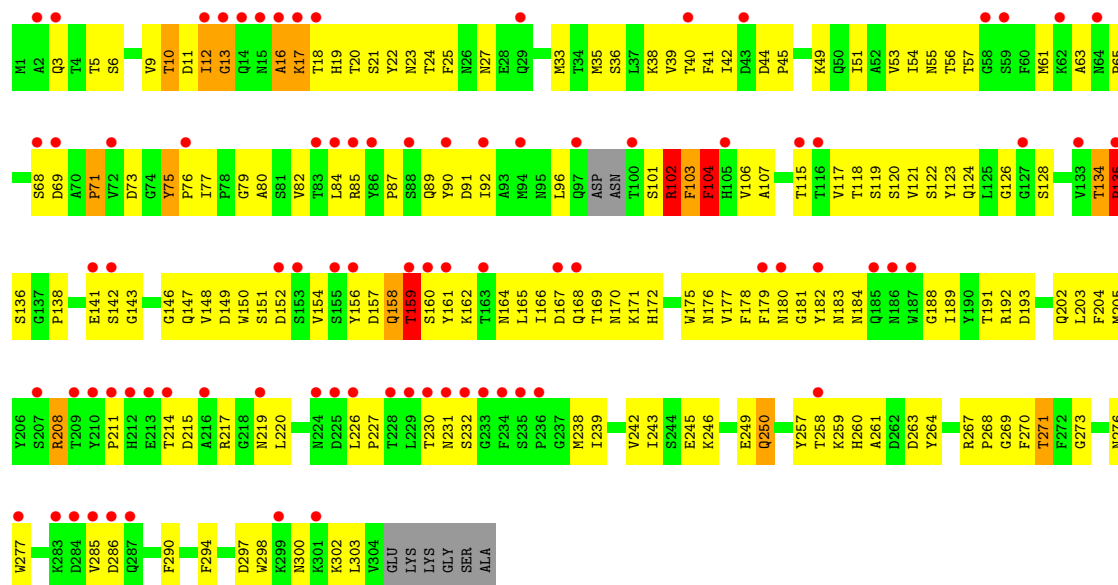


• Molecule 1: Cytotoxin K

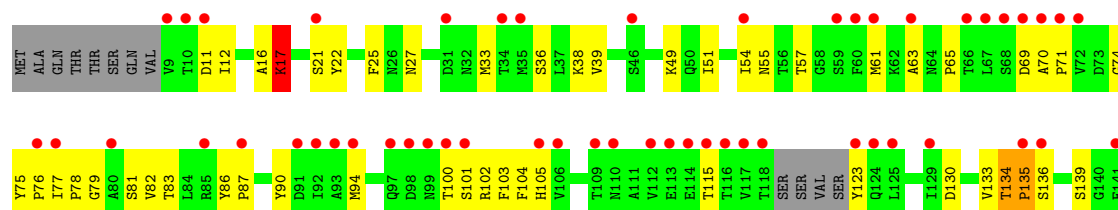


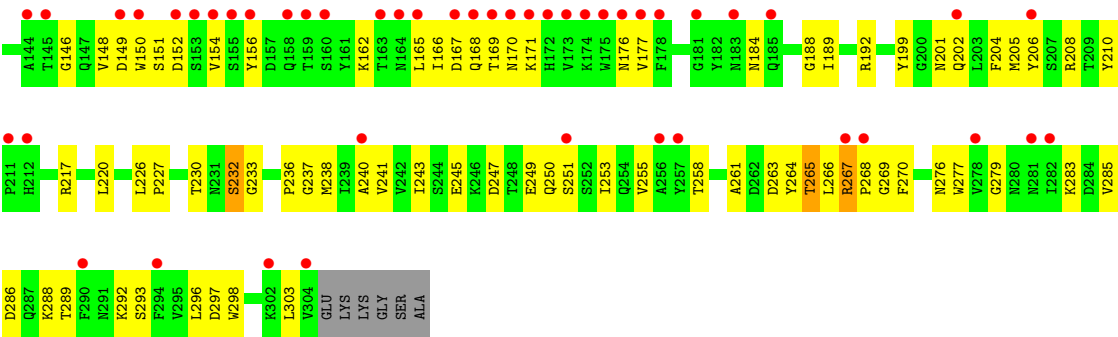


• Molecule 1: Cytotoxin K



• Molecule 1: Cytotoxin K





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.23Å 186.22Å 104.53Å 90.00° 115.85° 90.00°	Depositor
Resolution (Å)	94.07 – 4.32 94.07 – 4.32	Depositor EDS
% Data completeness (in resolution range)	95.5 (94.07-4.32) 97.0 (94.07-4.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.30Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.322 , 0.407 0.326 , 0.400	Depositor DCC
R_{free} test set	1277 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 178.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	15699	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

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	0.53	0/2318	0.82	8/3153 (0.3%)
1	B	0.32	0/2161	0.69	4/2933 (0.1%)
1	C	0.40	0/2278	0.72	4/3093 (0.1%)
1	D	0.60	0/2237	0.91	5/3042 (0.2%)
1	E	0.43	0/2319	0.76	3/3159 (0.1%)
1	F	0.32	0/2407	0.74	9/3282 (0.3%)
1	G	0.32	0/2340	0.65	0/3191
All	All	0.43	0/16060	0.76	33/21853 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	LYS	N-CA-C	10.09	121.86	111.07
1	B	209	THR	N-CA-C	10.08	121.96	110.97
1	F	250	GLN	N-CA-C	9.29	123.36	110.35
1	E	78	PRO	N-CA-CB	-8.76	94.05	103.25
1	E	135	PRO	N-CA-CB	-8.28	94.56	103.25

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	190	TYR	Mainchain
1	B	267	ARG	Sidechain
1	C	102	ARG	Sidechain
1	D	102	ARG	Sidechain

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	2267	0	2148	158	0
1	B	2119	0	2006	127	0
1	C	2227	0	2102	144	0
1	D	2184	0	2067	120	0
1	E	2267	0	2149	126	0
1	F	2351	0	2226	154	0
1	G	2284	0	2151	107	0
All	All	15699	0	14849	842	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 28.

The worst 5 of 842 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:C:296:LEU:HA	1:C:303:LEU:HD23	1.28	1.12
1:D:87:PRO:HA	1:D:261:ALA:HA	1.12	1.11
1:A:72:VAL:HA	1:A:79:GLY:HA2	1.12	1.11
1:A:96:LEU:HD21	1:A:101:SER:H	1.21	1.05
1:G:265:THR:OG1	1:G:267:ARG:HG2	1.58	1.01

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/310 (91%)	222 (78%)	42 (15%)	19 (7%)	1	12
1	B	258/310 (83%)	223 (86%)	31 (12%)	4 (2%)	7	36
1	C	274/310 (88%)	231 (84%)	37 (14%)	6 (2%)	5	29
1	D	273/310 (88%)	206 (76%)	52 (19%)	15 (6%)	1	15
1	E	284/310 (92%)	235 (83%)	38 (13%)	11 (4%)	2	19
1	F	298/310 (96%)	257 (86%)	34 (11%)	7 (2%)	5	28
1	G	288/310 (93%)	247 (86%)	36 (12%)	5 (2%)	7	35
All	All	1958/2170 (90%)	1621 (83%)	270 (14%)	67 (3%)	3	21

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	98	ASP
1	A	103	PHE
1	A	104	PHE
1	A	135	PRO

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	254/270 (94%)	234 (92%)	20 (8%)	11	32
1	B	237/270 (88%)	231 (98%)	6 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	247/270 (92%)	235 (95%)	12 (5%)	22	45
1	D	242/270 (90%)	204 (84%)	38 (16%)	2	13
1	E	254/270 (94%)	238 (94%)	16 (6%)	16	38
1	F	264/270 (98%)	255 (97%)	9 (3%)	32	54
1	G	255/270 (94%)	249 (98%)	6 (2%)	43	63
All	All	1753/1890 (93%)	1646 (94%)	107 (6%)	17	39

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	272	PHE
1	D	302	LYS
1	F	159	THR
1	D	281	ASN
1	D	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	32	ASN
1	G	15	ASN
1	D	276	ASN
1	F	180	ASN
1	D	219	ASN

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	291/310 (93%)	2.08	108 (37%) 1 3	30, 84, 154, 262	0
1	B	272/310 (87%)	2.26	107 (39%) 1 2	39, 89, 150, 256	0
1	C	284/310 (91%)	2.53	115 (40%) 0 2	30, 93, 166, 237	0
1	D	279/310 (90%)	3.10	141 (50%) 0 1	30, 82, 141, 167	0
1	E	292/310 (94%)	2.51	133 (45%) 0 1	30, 80, 134, 204	0
1	F	302/310 (97%)	1.65	84 (27%) 1 4	30, 85, 137, 197	0
1	G	292/310 (94%)	2.10	99 (33%) 1 3	43, 80, 137, 203	0
All	All	2012/2170 (92%)	2.31	787 (39%) 1 2	30, 85, 145, 262	0

The worst 5 of 787 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	SER	25.0
1	C	140	GLY	21.3
1	C	130	ASP	20.6
1	C	141	GLU	20.1
1	D	165	LEU	18.2

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.