



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:10 AM UTC

PDB ID : 1QXP / pdb_00001qxp
Title : Crystal Structure of a mu-like calpain
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.
Deposited on : 2003-09-08
Resolution : 2.80 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

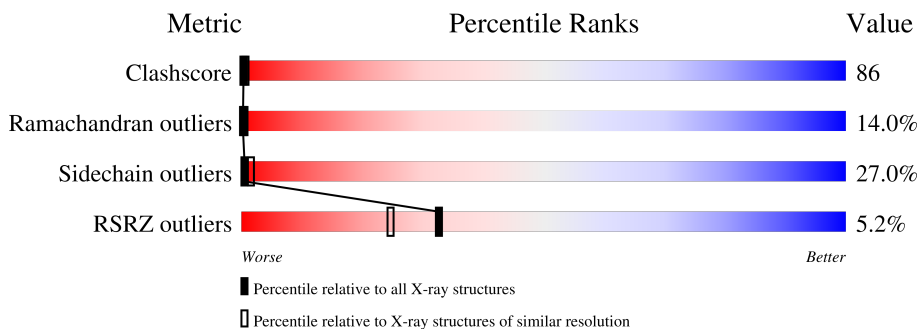
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	900	3% 21% 42% 22% 13%
1	B	900	6% 22% 42% 22% 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12368 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 mu-like calpain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6053	3846	1037	1143	27			
1	B	788	Total	C	N	O	S	0	0	0
			6003	3830	1015	1129	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	engineered mutation	UNP P97571
B	105	SER	CYS	engineered mutation	UNP P97571
A	702A	GLY	-	cloning artifact	UNP Q07009
A	702B	LYS	-	cloning artifact	UNP Q07009
A	702C	LEU	-	cloning artifact	UNP Q07009
A	702D	ALA	-	cloning artifact	UNP Q07009
A	702E	ALA	-	cloning artifact	UNP Q07009
A	702F	ALA	-	cloning artifact	UNP Q07009
A	702G	ILE	-	cloning artifact	UNP Q07009
A	702H	GLU	-	cloning artifact	UNP Q07009
A	702I	HIS	-	expression tag	UNP Q07009
A	702J	HIS	-	expression tag	UNP Q07009
A	702K	HIS	-	expression tag	UNP Q07009
A	702L	HIS	-	expression tag	UNP Q07009
A	702M	HIS	-	expression tag	UNP Q07009
A	702N	HIS	-	expression tag	UNP Q07009
B	702A	GLY	-	cloning artifact	UNP Q07009
B	702B	LYS	-	cloning artifact	UNP Q07009
B	702C	LEU	-	cloning artifact	UNP Q07009
B	702D	ALA	-	cloning artifact	UNP Q07009
B	702E	ALA	-	cloning artifact	UNP Q07009
B	702F	ALA	-	cloning artifact	UNP Q07009
B	702G	ILE	-	cloning artifact	UNP Q07009
B	702H	GLU	-	cloning artifact	UNP Q07009
B	702I	HIS	-	expression tag	UNP Q07009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	702J	HIS	-	expression tag	UNP Q07009
B	702K	HIS	-	expression tag	UNP Q07009
B	702L	HIS	-	expression tag	UNP Q07009
B	702M	HIS	-	expression tag	UNP Q07009
B	702N	HIS	-	expression tag	UNP Q07009

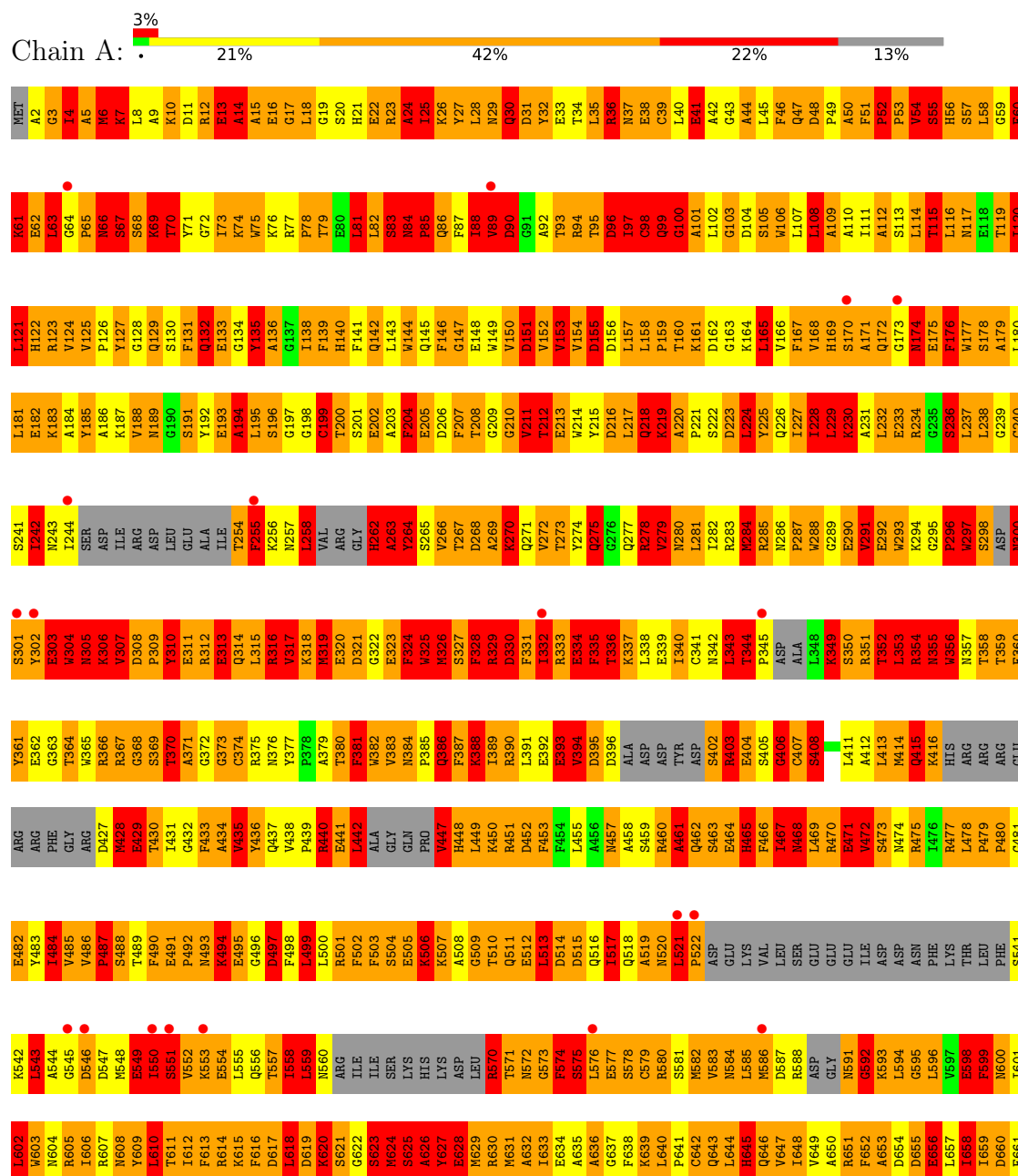
- Molecule 2 is water.

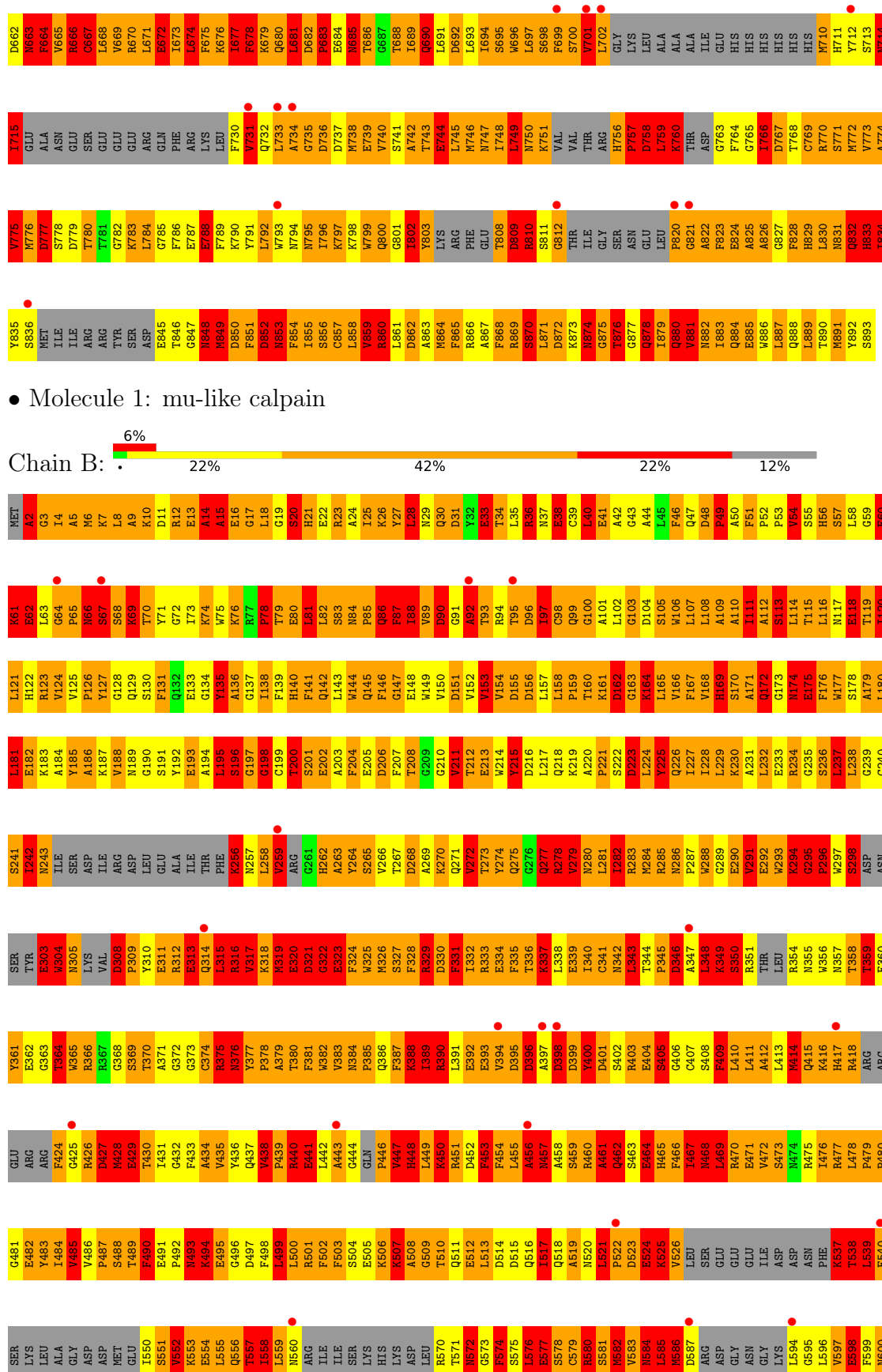
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	172	Total	O	0	0
			172	172		
2	B	140	Total	O	0	0
			140	140		

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: mu-like calpain





I601	F661	N714	I774	Y834	R637	I838	ARG	TYR	S843	D844	E845	T846	G847	M848	M849	D850	F851	D852	M853	F854	I855	S856	C857	L858	V859	R860	L861	D862	A863	M864	F865	R866	A867	F868	R869	S870	L871	D872	N874	G875	T876	G877	Q878	I879	Q880	V881	N882	I883	Q884	E885	W886	L887	Q888	L889	T890	M891	Y892	S893																																																																																																																																																																																																																																																																																																																																																																																																											
L602	D662	GLU	M776	S836	D777	D779	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
M603	N663	ALA	M776	S836	D777	D779	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
M604	N664	M718	D777	I838	D777	D779	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
R605	V665	N718	D777	I838	D777	D779	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
R606	R666	E719	R666	I839	D779	D779	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
N608	L668	E0	R667	I840	T780	T780	T780	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
Y609	V669	GLU	R669	ARG	T781	T781	T781	T781	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																										
L610	R670	E723	K783	S843	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																														
T611	L671	Q724	L671	D844	K783	L784	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																														
I612	E672	R725	Q725	E845	G785	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																
F613	L673	F726	R726	T846	F786	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																	
R614	L674	R727	R727	G847	E787	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																		
K615	F675	K728	F788	M848	F788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																			
F616	K676	L729	F789	M849	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																				
D617	L677	F730	K790	D850	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	R831	Q832	H833																																																																																																																																																																																																																																																																																																																																																																																																																				
L618	F678	F731	Y791	F851	D779	D779	T780	T780	F851	D779	D779	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780	T780

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	91.29 – 2.80 91.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 89.7 (91.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.311 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 106.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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	4.56	1459/6177 (23.6%)	3.06	804/8354 (9.6%)
1	B	4.50	1422/6128 (23.2%)	3.05	799/8288 (9.6%)
All	All	4.53	2881/12305 (23.4%)	3.05	1603/16642 (9.6%)

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	45
1	B	0	39
All	All	0	84

The worst 5 of 2881 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	869	ARG	CA-CB	26.29	1.92	1.53
1	B	67	SER	CA-CB	25.20	1.96	1.53
1	A	631	MET	SD-CE	24.79	2.41	1.79
1	A	789	PHE	CA-C	-23.95	1.32	1.52
1	B	316	ARG	CA-CB	23.69	1.93	1.53

The worst 5 of 1603 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	ALA	N-CA-C	-22.12	86.27	111.71
1	A	303	GLU	N-CA-C	17.00	132.20	108.74
1	B	858	LEU	N-CA-C	16.18	133.35	113.12
1	A	460	ARG	NE-CZ-NH1	-16.09	105.41	121.50
1	B	83	SER	CA-C-N	-15.83	104.00	123.15

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ILE	Mainchain
1	A	152	VAL	Mainchain
1	A	24	ALA	Mainchain
1	A	29	ASN	Mainchain
1	A	99	GLN	Mainchain,Peptide

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	6053	0	5616	996	3
1	B	6003	0	5477	1006	1
2	A	172	0	0	53	1
2	B	140	0	0	45	1
All	All	12368	0	11093	2002	3

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 86.

The worst 5 of 2002 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:A:583:VAL:CB	1:A:583:VAL:CA	1.74	1.65
1:B:0:GLU:CA	1:B:0:GLU:CB	1.75	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	1.64
1:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:B:8:LEU:CD2	1:B:8:LEU:CG	1.76	1.63

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ASN:OD1	2:B:1033:HOH:O[1_454]	1.56	0.64
1:A:442:LEU:CD2	2:A:922:HOH:O[1_455]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	1:B:303:GLU:N[2_656]	2.08	0.12

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	747/900 (83%)	500 (67%)	143 (19%)	104 (14%)	0	0
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0	0
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0	0

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	60	PHE
1	A	63	LEU
1	A	67	SER
1	A	83	SER

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	606/782 (78%)	450 (74%)	156 (26%)	0	2
1	B	584/782 (75%)	419 (72%)	165 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1190/1564 (76%)	869 (73%)	321 (27%)	0 1

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	359	THR
1	B	640	LEU
1	B	394	VAL
1	B	494	LYS
1	B	691	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	874	ASN
1	B	663	ASN
1	B	84	ASN
1	B	646	GLN
1	B	888	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	783/900 (87%)	0.22	31 (3%) 42 33	16, 49, 81, 98	0
1	B	788/900 (87%)	0.43	50 (6%) 26 19	17, 51, 84, 102	0
All	All	1571/1800 (87%)	0.32	81 (5%) 33 25	16, 50, 83, 102	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	843	SER	5.4
1	B	835	TYR	5.0
1	B	601	ILE	4.1
1	B	702	LEU	4.0
1	B	259	VAL	4.0

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.