



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:48 AM UTC

PDB ID : 5XDA / pdb_00005xda
Title : Structural basis for Ufm1 recognition by UfSP
Authors : Kim, K.H.; Ha, B.H.; Kim, E.E.
Deposited on : 2017-03-28
Resolution : 3.29 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

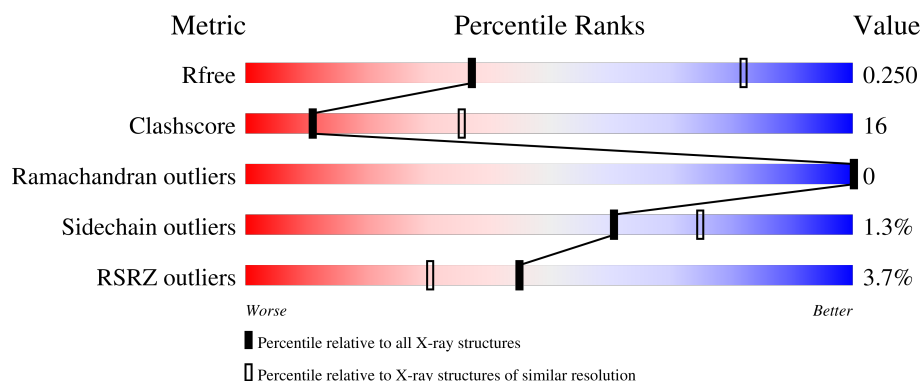
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	565	3% 72% 21% • 5%
1	B	565	3% 74% 20% • •
1	C	565	2% 74% 20% • •
1	D	565	5% 68% 25% • 5%
1	E	565	3% 69% 23% • 5%

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Mol	Chain	Length	Quality of chain
1	F	565	7% 68% 24% 5%
2	G	84	% 79% 21%
2	H	84	2% 88% 12%
2	I	84	4% 81% 14% 5%
2	J	84	2% 71% 23% 6%
2	K	84	2% 95% 5%
2	L	84	% 85% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29730 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 Ufm1-specific protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4306	2733	755	802	16			
1	B	542	Total	C	N	O	S	0	0	0
			4342	2754	762	810	16			
1	C	541	Total	C	N	O	S	0	0	0
			4332	2748	759	809	16			
1	D	538	Total	C	N	O	S	0	0	0
			4312	2736	756	804	16			
1	E	535	Total	C	N	O	S	0	0	0
			4289	2723	751	799	16			
1	F	535	Total	C	N	O	S	0	0	0
			4289	2723	752	798	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	SER	CYS	engineered mutation	UNP Q94218
B	407	SER	CYS	engineered mutation	UNP Q94218
C	407	SER	CYS	engineered mutation	UNP Q94218
D	407	SER	CYS	engineered mutation	UNP Q94218
E	407	SER	CYS	engineered mutation	UNP Q94218
F	407	SER	CYS	engineered mutation	UNP Q94218

- Molecule 2 is a protein called Ubiquitin-fold modifier 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	H	84	Total	C	N	O	0	0	0
			627	405	106	116			
2	I	84	Total	C	N	O	0	0	0
			627	405	106	116			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	84	Total 627	C 405	N 106	O 116	0	0	0
2	K	84	Total 627	C 405	N 106	O 116	0	0	0
2	L	84	Total 627	C 405	N 106	O 116	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	94	GLY	HIS	engineered mutation	UNP P34661
H	94	GLY	HIS	engineered mutation	UNP P34661
I	94	GLY	HIS	engineered mutation	UNP P34661
J	94	GLY	HIS	engineered mutation	UNP P34661
K	94	GLY	HIS	engineered mutation	UNP P34661
L	94	GLY	HIS	engineered mutation	UNP P34661

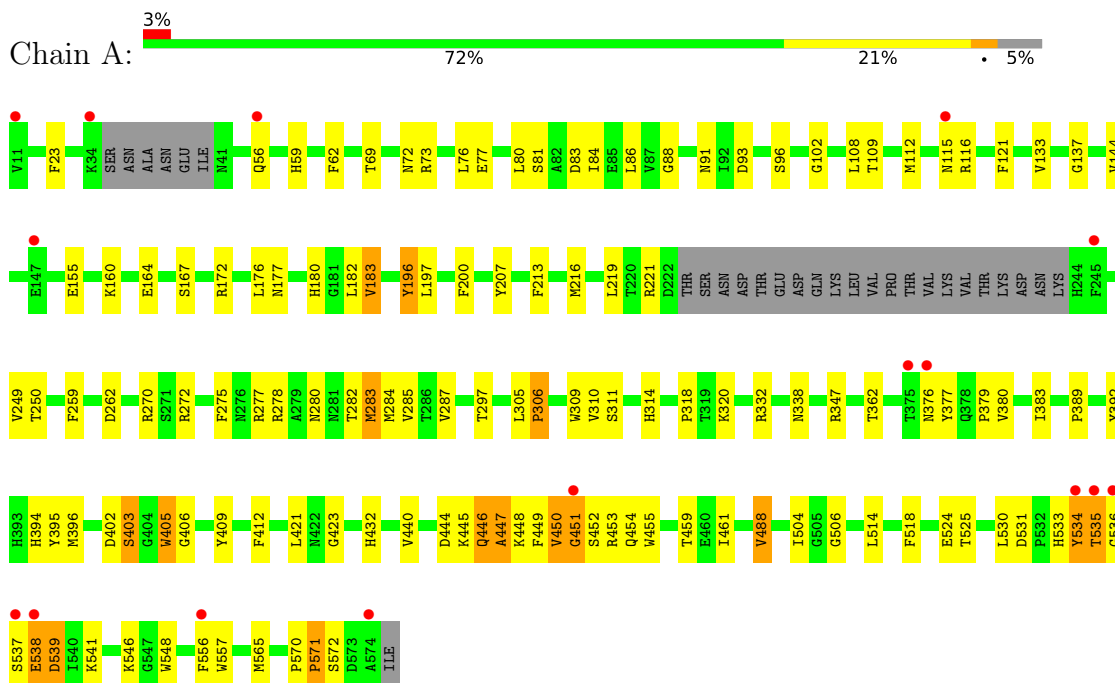
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	19	Total 19	O 19	0	0
3	C	27	Total 27	O 27	0	0
3	D	6	Total 6	O 6	0	0
3	E	11	Total 11	O 11	0	0
3	F	5	Total 5	O 5	0	0
3	G	4	Total 4	O 4	0	0
3	H	2	Total 2	O 2	0	0
3	I	4	Total 4	O 4	0	0
3	L	2	Total 2	O 2	0	0

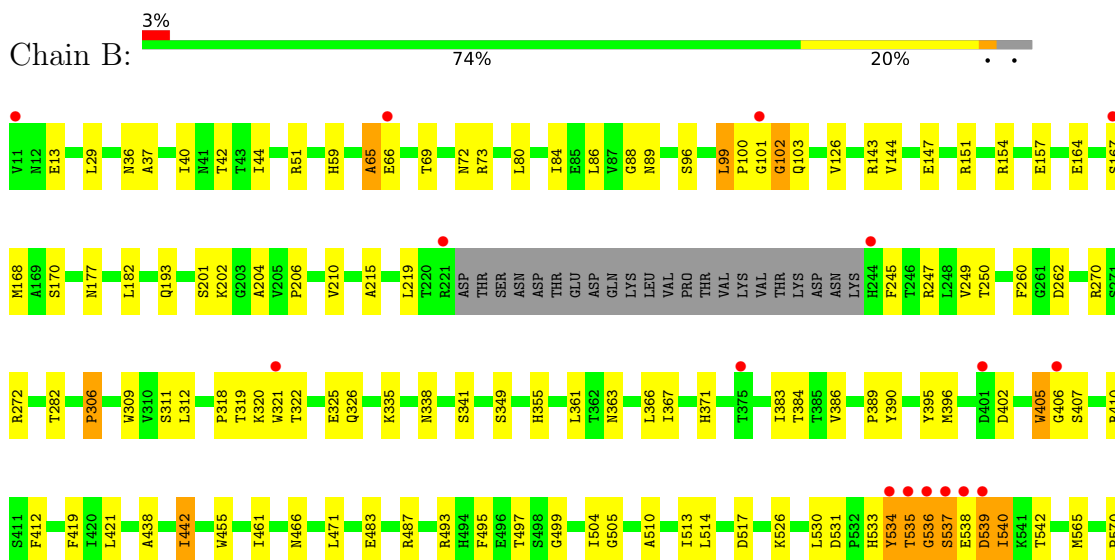
3 Residue-property plots [i](#)

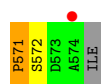
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ufm1-specific protease

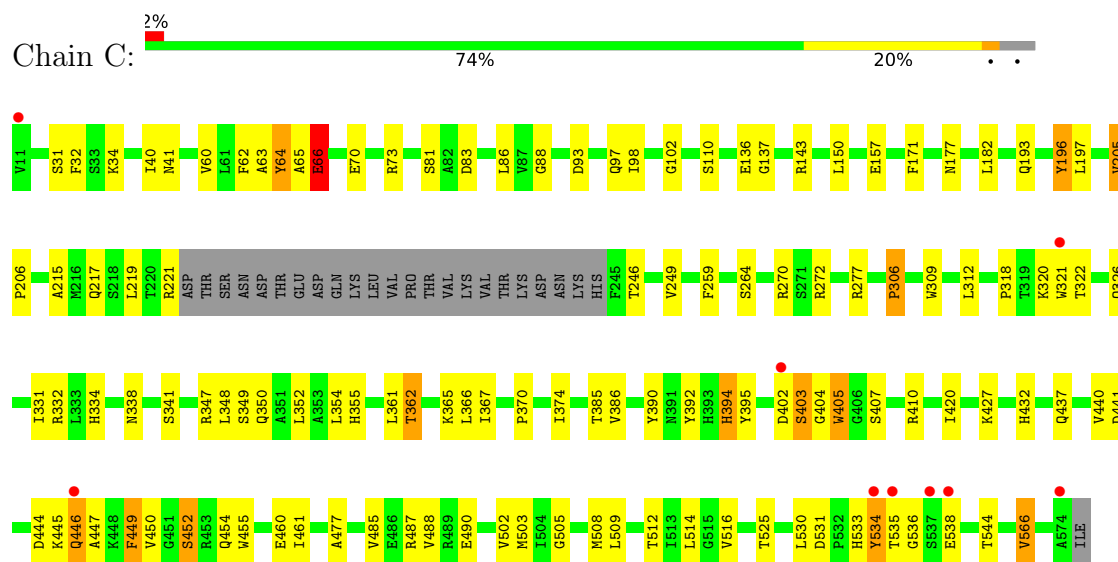


• Molecule 1: Ufm1-specific protease

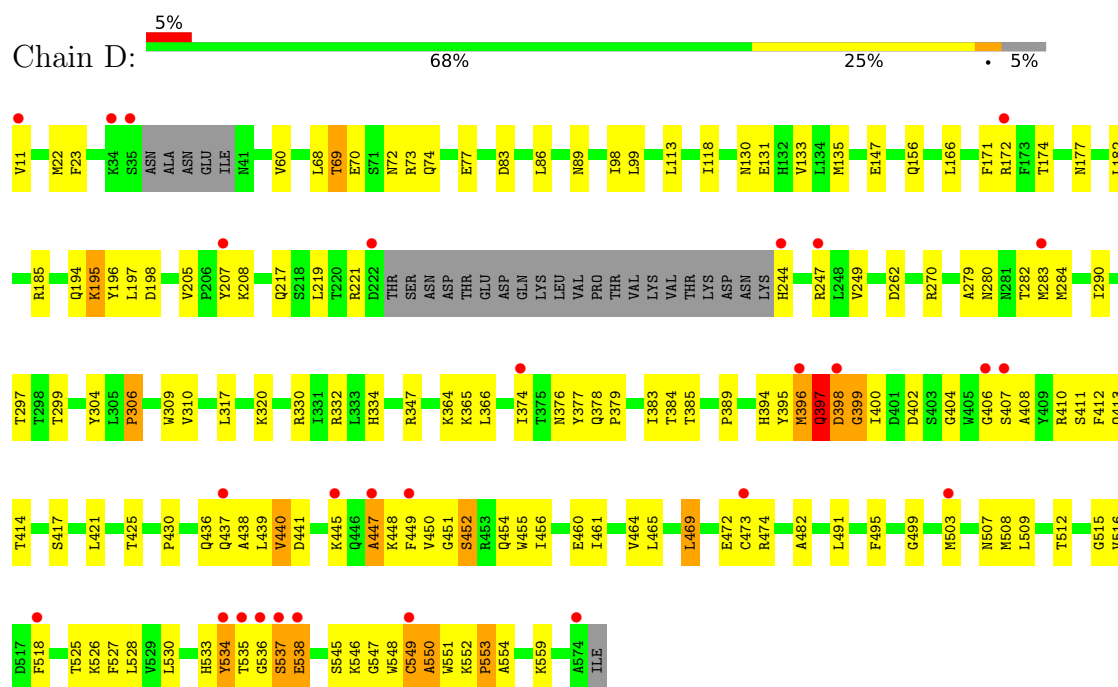




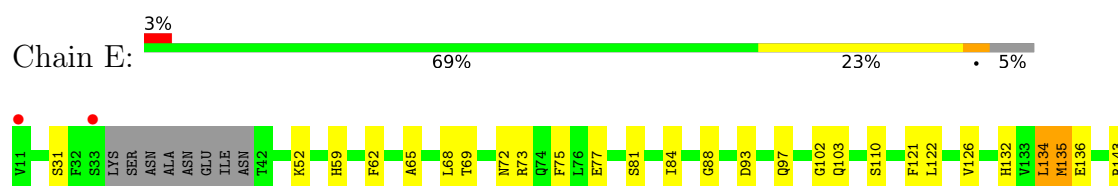
• Molecule 1: Ufm1-specific protease

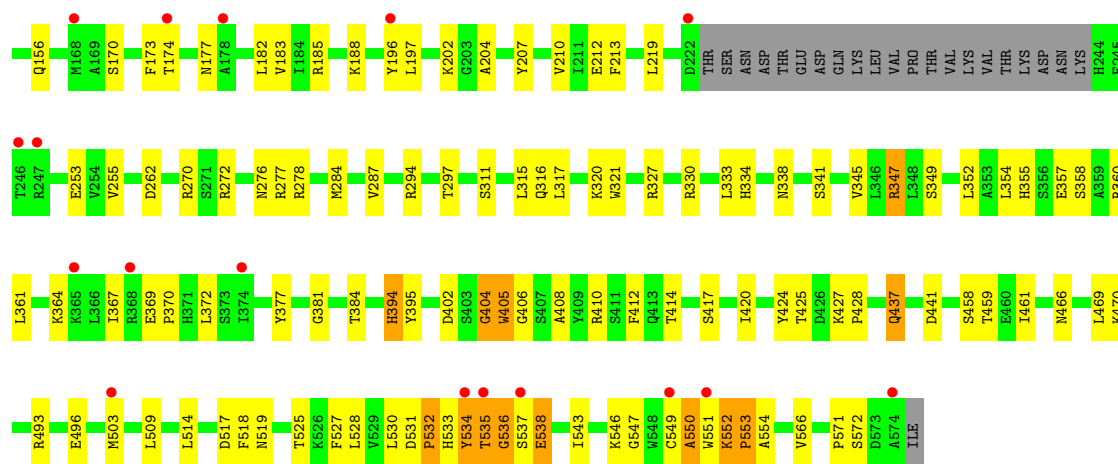


• Molecule 1: Ufm1-specific protease

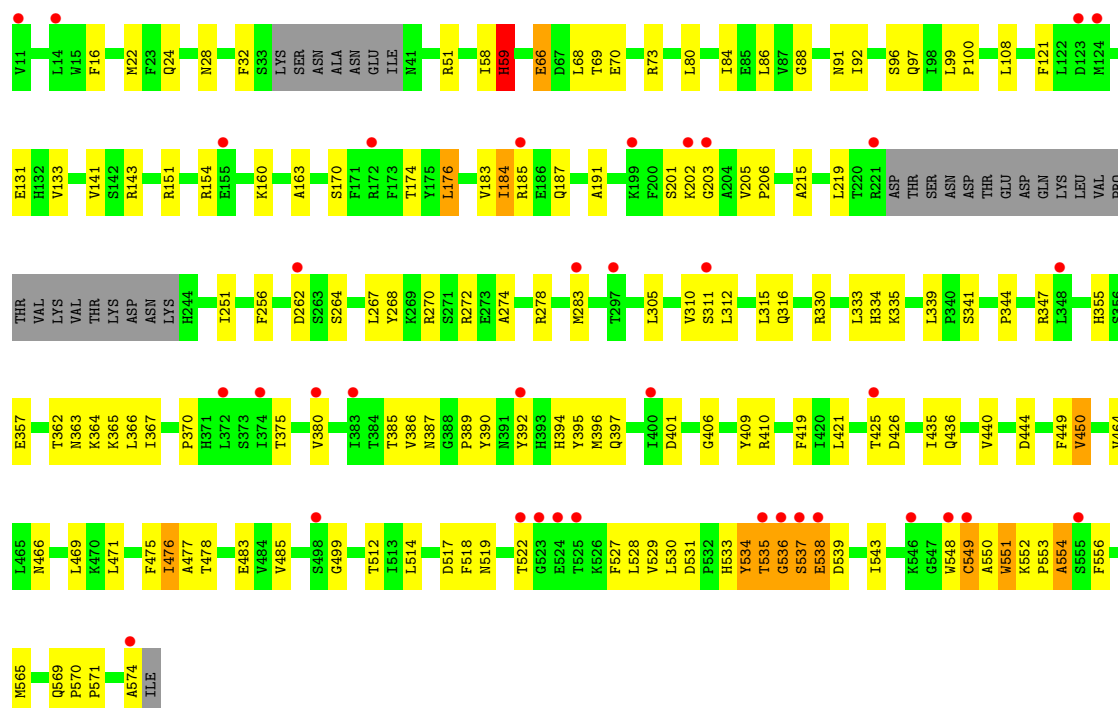


• Molecule 1: Ufm1-specific protease

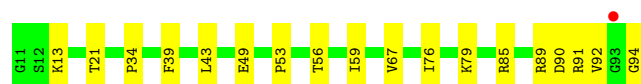
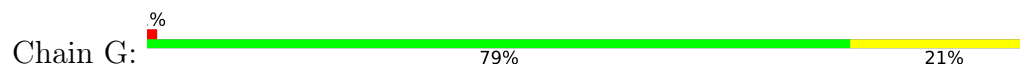




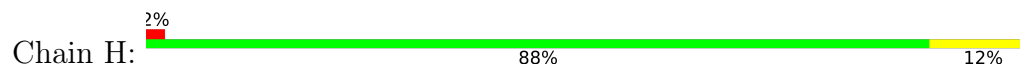
• Molecule 1: Ufm1-specific protease



• Molecule 2: Ubiquitin-fold modifier 1

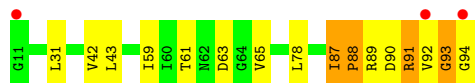
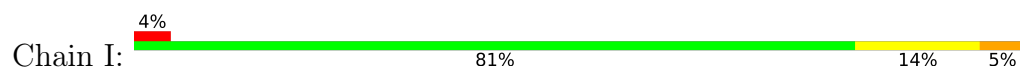


• Molecule 2: Ubiquitin-fold modifier 1

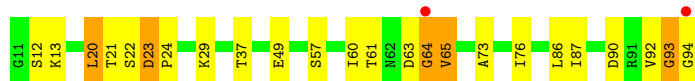




- Molecule 2: Ubiquitin-fold modifier 1



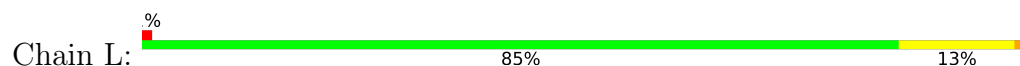
- Molecule 2: Ubiquitin-fold modifier 1



- Molecule 2: Ubiquitin-fold modifier 1



- Molecule 2: Ubiquitin-fold modifier 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	267.45Å 455.33Å 195.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 3.29 46.16 – 3.29	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.16-3.29) 95.9 (46.16-3.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.243 0.218 , 0.250	Depositor DCC
R_{free} test set	2018 reflections (1.12%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.045 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29730	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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	0.41	0/4407	0.93	20/5968 (0.3%)
1	B	0.42	1/4444 (0.0%)	1.15	27/6020 (0.4%)
1	C	0.55	8/4433 (0.2%)	0.94	19/6005 (0.3%)
1	D	0.48	6/4413 (0.1%)	1.02	32/5976 (0.5%)
1	E	0.46	4/4390 (0.1%)	1.05	37/5946 (0.6%)
1	F	0.39	3/4390 (0.1%)	1.08	23/5946 (0.4%)
2	G	0.65	0/641	0.77	0/870
2	H	0.30	0/641	0.80	1/870 (0.1%)
2	I	0.52	1/641 (0.2%)	1.16	6/870 (0.7%)
2	J	0.32	0/641	0.94	6/870 (0.7%)
2	K	0.31	0/641	0.77	0/870
2	L	0.30	0/641	0.86	2/870 (0.2%)
All	All	0.45	23/30323 (0.1%)	1.01	173/41081 (0.4%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	566	VAL	C-O	12.39	1.38	1.24
1	D	69	THR	CA-C	8.91	1.64	1.52
1	C	331	ILE	CB-CG1	8.53	1.70	1.53
2	I	88	PRO	N-CD	-8.37	1.36	1.47
1	C	331	ILE	CA-CB	-8.27	1.44	1.54

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	SER	N-CA-C	29.82	147.41	111.33
1	B	536	GLY	N-CA-C	-22.50	83.12	112.14
1	F	535	THR	N-CA-C	-22.31	74.84	109.65
1	C	403	SER	N-CA-C	21.20	133.75	111.07
1	E	404	GLY	N-CA-C	-20.52	79.58	111.18

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	4306	0	4218	153	0
1	B	4342	0	4254	122	0
1	C	4332	0	4247	156	0
1	D	4312	0	4223	211	0
1	E	4289	0	4199	132	0
1	F	4289	0	4201	152	0
2	G	627	0	652	15	0
2	H	627	0	652	7	0
2	I	627	0	652	41	0
2	J	627	0	652	31	0
2	K	627	0	652	3	0
2	L	627	0	652	8	0
3	A	18	0	0	0	0
3	B	19	0	0	0	0
3	C	27	0	0	1	0
3	D	6	0	0	1	0
3	E	11	0	0	1	0
3	F	5	0	0	0	0
3	G	4	0	0	0	0
3	H	2	0	0	0	0
3	I	4	0	0	0	0
3	L	2	0	0	0	0
All	All	29730	0	29254	968	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 16.

The worst 5 of 968 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:D:411:SER:HB3	1:D:503:MET:CE	1.32	1.59
1:D:411:SER:CB	1:D:503:MET:HE1	1.32	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:TRP:HE1	1:C:326:GLN:CB	1.15	1.52
1:A:394:HIS:CE1	1:A:535:THR:HB	1.45	1.50
1:C:321:TRP:NE1	1:C:326:GLN:HB2	1.21	1.44

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	531/565 (94%)	490 (92%)	41 (8%)	0	100	100
1	B	538/565 (95%)	509 (95%)	29 (5%)	0	100	100
1	C	537/565 (95%)	508 (95%)	29 (5%)	0	100	100
1	D	532/565 (94%)	495 (93%)	37 (7%)	0	100	100
1	E	529/565 (94%)	497 (94%)	32 (6%)	0	100	100
1	F	529/565 (94%)	471 (89%)	58 (11%)	0	100	100
2	G	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
2	H	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
2	I	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
2	J	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
2	K	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	L	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
All	All	3688/3894 (95%)	3442 (93%)	246 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	468/495 (94%)	462 (99%)	6 (1%)	61	75
1	B	472/495 (95%)	466 (99%)	6 (1%)	61	75
1	C	471/495 (95%)	465 (99%)	6 (1%)	61	75
1	D	469/495 (95%)	464 (99%)	5 (1%)	65	76
1	E	466/495 (94%)	463 (99%)	3 (1%)	78	82
1	F	466/495 (94%)	456 (98%)	10 (2%)	47	67
2	G	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	H	69/69 (100%)	69 (100%)	0	100	100
2	I	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	J	69/69 (100%)	67 (97%)	2 (3%)	37	62
2	K	69/69 (100%)	68 (99%)	1 (1%)	59	74
2	L	69/69 (100%)	68 (99%)	1 (1%)	59	74
All	All	3226/3384 (95%)	3184 (99%)	42 (1%)	61	75

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	141	VAL
1	F	518	PHE
1	F	176	LEU
1	F	305	LEU
2	I	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	324	ASN
1	F	437	GLN
1	F	561	HIS
1	F	466	ASN

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Mol	Chain	Res	Type
1	C	130	ASN

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 [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	537/565 (95%)	-0.11	16 (2%)	52	35	6, 35, 74, 110	0
1	B	542/565 (95%)	-0.25	17 (3%)	51	34	7, 27, 76, 117	0
1	C	541/565 (95%)	-0.26	9 (1%)	69	50	6, 31, 77, 120	0
1	D	538/565 (95%)	0.21	28 (5%)	33	22	19, 58, 105, 131	0
1	E	535/565 (94%)	0.14	19 (3%)	46	31	16, 53, 94, 128	0
1	F	535/565 (94%)	0.52	37 (6%)	23	16	31, 72, 111, 134	0
2	G	84/84 (100%)	-0.52	1 (1%)	76	58	10, 23, 50, 87	0
2	H	84/84 (100%)	-0.45	2 (2%)	59	40	15, 28, 49, 83	0
2	I	84/84 (100%)	-0.28	3 (3%)	46	31	5, 24, 48, 84	0
2	J	84/84 (100%)	0.04	2 (2%)	59	40	33, 62, 88, 131	0
2	K	84/84 (100%)	-0.56	2 (2%)	59	40	9, 27, 53, 91	0
2	L	84/84 (100%)	0.26	1 (1%)	76	58	24, 70, 90, 100	0
All	All	3732/3894 (95%)	0.00	137 (3%)	45	30	5, 45, 95, 134	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	574	ALA	7.3
2	I	94	GLY	7.3
1	A	538	GLU	7.1
1	A	536	GLY	7.0
1	D	549	CYS	5.8

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.