wwPDB X-ray Structure Validation Summary Report (i)

Apr 14, 2025 – 08:23 PM JST

PDB ID	:	8Z7A / pdb_00008z7a
Title	:	Open Barrel Structure of Translin from Trichoderma virens
Authors	:	Kumari, S.; Gupta, G.D.
Deposited on	:	2024-04-19
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

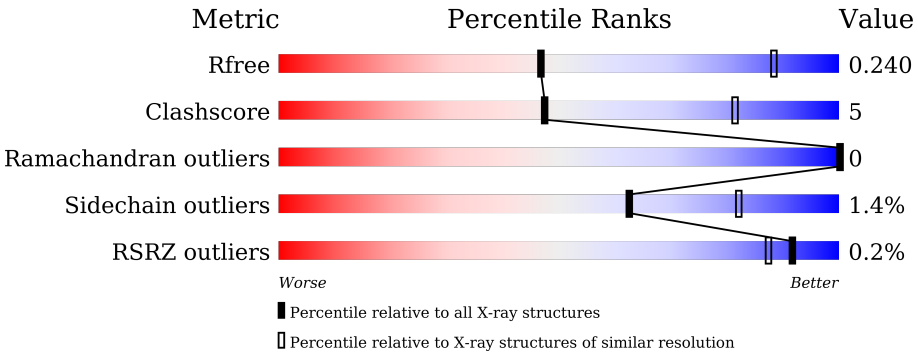
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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 <=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	276	69% 13% 18%
1	B	276	72% 9% 18%
1	C	276	65% 16% 19%
1	D	276	73% 9% • 17%
1	E	276	70% 12% 18%
1	F	276	64% 17% 18%

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Mol	Chain	Length	Quality of chain
1	G	276	
1	H	276	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14312 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 Translin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1792	1143	307	340	2			
1	B	226	Total	C	N	O	S	0	0	0
			1792	1143	306	341	2			
1	C	224	Total	C	N	O	S	0	0	0
			1778	1135	303	338	2			
1	D	228	Total	C	N	O	S	0	0	0
			1806	1152	309	343	2			
1	E	226	Total	C	N	O	S	0	0	0
			1794	1143	308	341	2			
1	F	225	Total	C	N	O	S	0	0	0
			1789	1141	306	340	2			
1	G	224	Total	C	N	O	S	0	0	0
			1771	1132	299	338	2			
1	H	224	Total	C	N	O	S	0	0	0
			1783	1138	305	338	2			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP G9MJL3
A	-18	GLY	-	expression tag	UNP G9MJL3
A	-17	SER	-	expression tag	UNP G9MJL3
A	-16	SER	-	expression tag	UNP G9MJL3
A	-15	HIS	-	expression tag	UNP G9MJL3
A	-14	HIS	-	expression tag	UNP G9MJL3
A	-13	HIS	-	expression tag	UNP G9MJL3
A	-12	HIS	-	expression tag	UNP G9MJL3
A	-11	HIS	-	expression tag	UNP G9MJL3
A	-10	HIS	-	expression tag	UNP G9MJL3
A	-9	SER	-	expression tag	UNP G9MJL3
A	-8	SER	-	expression tag	UNP G9MJL3
A	-7	GLY	-	expression tag	UNP G9MJL3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP G9MJL3
A	-5	VAL	-	expression tag	UNP G9MJL3
A	-4	PRO	-	expression tag	UNP G9MJL3
A	-3	ARG	-	expression tag	UNP G9MJL3
A	-2	GLY	-	expression tag	UNP G9MJL3
A	-1	SER	-	expression tag	UNP G9MJL3
A	0	HIS	-	expression tag	UNP G9MJL3
B	-19	MET	-	initiating methionine	UNP G9MJL3
B	-18	GLY	-	expression tag	UNP G9MJL3
B	-17	SER	-	expression tag	UNP G9MJL3
B	-16	SER	-	expression tag	UNP G9MJL3
B	-15	HIS	-	expression tag	UNP G9MJL3
B	-14	HIS	-	expression tag	UNP G9MJL3
B	-13	HIS	-	expression tag	UNP G9MJL3
B	-12	HIS	-	expression tag	UNP G9MJL3
B	-11	HIS	-	expression tag	UNP G9MJL3
B	-10	HIS	-	expression tag	UNP G9MJL3
B	-9	SER	-	expression tag	UNP G9MJL3
B	-8	SER	-	expression tag	UNP G9MJL3
B	-7	GLY	-	expression tag	UNP G9MJL3
B	-6	LEU	-	expression tag	UNP G9MJL3
B	-5	VAL	-	expression tag	UNP G9MJL3
B	-4	PRO	-	expression tag	UNP G9MJL3
B	-3	ARG	-	expression tag	UNP G9MJL3
B	-2	GLY	-	expression tag	UNP G9MJL3
B	-1	SER	-	expression tag	UNP G9MJL3
B	0	HIS	-	expression tag	UNP G9MJL3
C	-19	MET	-	initiating methionine	UNP G9MJL3
C	-18	GLY	-	expression tag	UNP G9MJL3
C	-17	SER	-	expression tag	UNP G9MJL3
C	-16	SER	-	expression tag	UNP G9MJL3
C	-15	HIS	-	expression tag	UNP G9MJL3
C	-14	HIS	-	expression tag	UNP G9MJL3
C	-13	HIS	-	expression tag	UNP G9MJL3
C	-12	HIS	-	expression tag	UNP G9MJL3
C	-11	HIS	-	expression tag	UNP G9MJL3
C	-10	HIS	-	expression tag	UNP G9MJL3
C	-9	SER	-	expression tag	UNP G9MJL3
C	-8	SER	-	expression tag	UNP G9MJL3
C	-7	GLY	-	expression tag	UNP G9MJL3
C	-6	LEU	-	expression tag	UNP G9MJL3
C	-5	VAL	-	expression tag	UNP G9MJL3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP G9MJL3
C	-3	ARG	-	expression tag	UNP G9MJL3
C	-2	GLY	-	expression tag	UNP G9MJL3
C	-1	SER	-	expression tag	UNP G9MJL3
C	0	HIS	-	expression tag	UNP G9MJL3
D	-19	MET	-	initiating methionine	UNP G9MJL3
D	-18	GLY	-	expression tag	UNP G9MJL3
D	-17	SER	-	expression tag	UNP G9MJL3
D	-16	SER	-	expression tag	UNP G9MJL3
D	-15	HIS	-	expression tag	UNP G9MJL3
D	-14	HIS	-	expression tag	UNP G9MJL3
D	-13	HIS	-	expression tag	UNP G9MJL3
D	-12	HIS	-	expression tag	UNP G9MJL3
D	-11	HIS	-	expression tag	UNP G9MJL3
D	-10	HIS	-	expression tag	UNP G9MJL3
D	-9	SER	-	expression tag	UNP G9MJL3
D	-8	SER	-	expression tag	UNP G9MJL3
D	-7	GLY	-	expression tag	UNP G9MJL3
D	-6	LEU	-	expression tag	UNP G9MJL3
D	-5	VAL	-	expression tag	UNP G9MJL3
D	-4	PRO	-	expression tag	UNP G9MJL3
D	-3	ARG	-	expression tag	UNP G9MJL3
D	-2	GLY	-	expression tag	UNP G9MJL3
D	-1	SER	-	expression tag	UNP G9MJL3
D	0	HIS	-	expression tag	UNP G9MJL3
E	-19	MET	-	initiating methionine	UNP G9MJL3
E	-18	GLY	-	expression tag	UNP G9MJL3
E	-17	SER	-	expression tag	UNP G9MJL3
E	-16	SER	-	expression tag	UNP G9MJL3
E	-15	HIS	-	expression tag	UNP G9MJL3
E	-14	HIS	-	expression tag	UNP G9MJL3
E	-13	HIS	-	expression tag	UNP G9MJL3
E	-12	HIS	-	expression tag	UNP G9MJL3
E	-11	HIS	-	expression tag	UNP G9MJL3
E	-10	HIS	-	expression tag	UNP G9MJL3
E	-9	SER	-	expression tag	UNP G9MJL3
E	-8	SER	-	expression tag	UNP G9MJL3
E	-7	GLY	-	expression tag	UNP G9MJL3
E	-6	LEU	-	expression tag	UNP G9MJL3
E	-5	VAL	-	expression tag	UNP G9MJL3
E	-4	PRO	-	expression tag	UNP G9MJL3
E	-3	ARG	-	expression tag	UNP G9MJL3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP G9MJL3
E	-1	SER	-	expression tag	UNP G9MJL3
E	0	HIS	-	expression tag	UNP G9MJL3
F	-19	MET	-	initiating methionine	UNP G9MJL3
F	-18	GLY	-	expression tag	UNP G9MJL3
F	-17	SER	-	expression tag	UNP G9MJL3
F	-16	SER	-	expression tag	UNP G9MJL3
F	-15	HIS	-	expression tag	UNP G9MJL3
F	-14	HIS	-	expression tag	UNP G9MJL3
F	-13	HIS	-	expression tag	UNP G9MJL3
F	-12	HIS	-	expression tag	UNP G9MJL3
F	-11	HIS	-	expression tag	UNP G9MJL3
F	-10	HIS	-	expression tag	UNP G9MJL3
F	-9	SER	-	expression tag	UNP G9MJL3
F	-8	SER	-	expression tag	UNP G9MJL3
F	-7	GLY	-	expression tag	UNP G9MJL3
F	-6	LEU	-	expression tag	UNP G9MJL3
F	-5	VAL	-	expression tag	UNP G9MJL3
F	-4	PRO	-	expression tag	UNP G9MJL3
F	-3	ARG	-	expression tag	UNP G9MJL3
F	-2	GLY	-	expression tag	UNP G9MJL3
F	-1	SER	-	expression tag	UNP G9MJL3
F	0	HIS	-	expression tag	UNP G9MJL3
G	-19	MET	-	initiating methionine	UNP G9MJL3
G	-18	GLY	-	expression tag	UNP G9MJL3
G	-17	SER	-	expression tag	UNP G9MJL3
G	-16	SER	-	expression tag	UNP G9MJL3
G	-15	HIS	-	expression tag	UNP G9MJL3
G	-14	HIS	-	expression tag	UNP G9MJL3
G	-13	HIS	-	expression tag	UNP G9MJL3
G	-12	HIS	-	expression tag	UNP G9MJL3
G	-11	HIS	-	expression tag	UNP G9MJL3
G	-10	HIS	-	expression tag	UNP G9MJL3
G	-9	SER	-	expression tag	UNP G9MJL3
G	-8	SER	-	expression tag	UNP G9MJL3
G	-7	GLY	-	expression tag	UNP G9MJL3
G	-6	LEU	-	expression tag	UNP G9MJL3
G	-5	VAL	-	expression tag	UNP G9MJL3
G	-4	PRO	-	expression tag	UNP G9MJL3
G	-3	ARG	-	expression tag	UNP G9MJL3
G	-2	GLY	-	expression tag	UNP G9MJL3
G	-1	SER	-	expression tag	UNP G9MJL3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP G9MJL3
H	-19	MET	-	initiating methionine	UNP G9MJL3
H	-18	GLY	-	expression tag	UNP G9MJL3
H	-17	SER	-	expression tag	UNP G9MJL3
H	-16	SER	-	expression tag	UNP G9MJL3
H	-15	HIS	-	expression tag	UNP G9MJL3
H	-14	HIS	-	expression tag	UNP G9MJL3
H	-13	HIS	-	expression tag	UNP G9MJL3
H	-12	HIS	-	expression tag	UNP G9MJL3
H	-11	HIS	-	expression tag	UNP G9MJL3
H	-10	HIS	-	expression tag	UNP G9MJL3
H	-9	SER	-	expression tag	UNP G9MJL3
H	-8	SER	-	expression tag	UNP G9MJL3
H	-7	GLY	-	expression tag	UNP G9MJL3
H	-6	LEU	-	expression tag	UNP G9MJL3
H	-5	VAL	-	expression tag	UNP G9MJL3
H	-4	PRO	-	expression tag	UNP G9MJL3
H	-3	ARG	-	expression tag	UNP G9MJL3
H	-2	GLY	-	expression tag	UNP G9MJL3
H	-1	SER	-	expression tag	UNP G9MJL3
H	0	HIS	-	expression tag	UNP G9MJL3

- Molecule 2 is water.

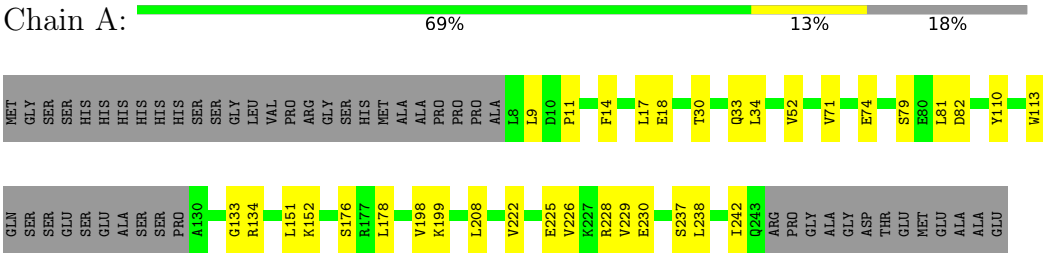
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0
2	G	1	Total O 1 1	0	0
2	H	1	Total O 1 1	0	0

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.

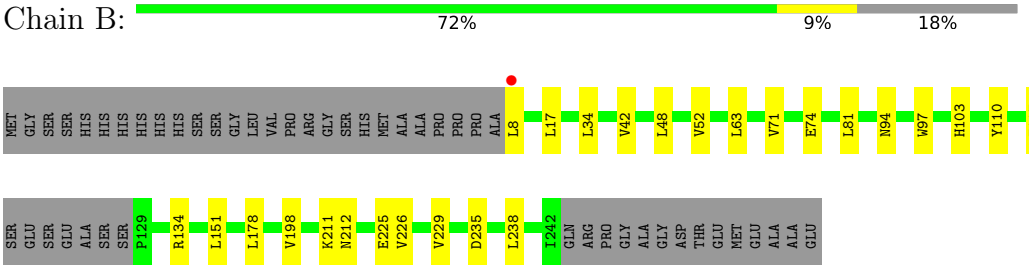
• Molecule 1: Translin

Chain A:



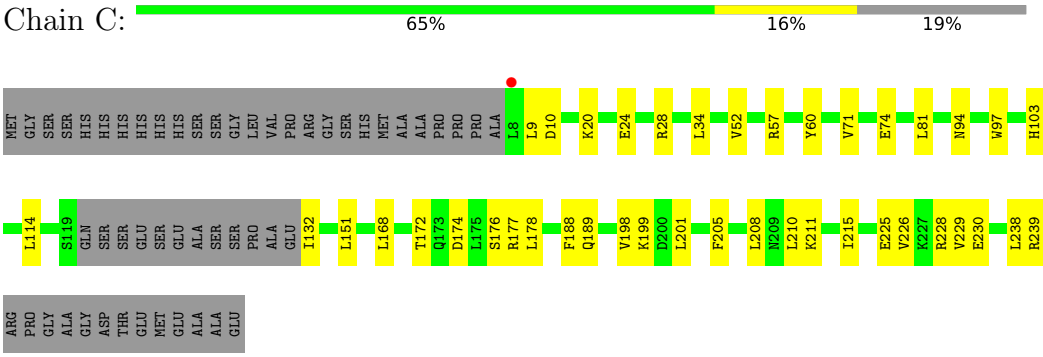
• Molecule 1: Translin

Chain B:



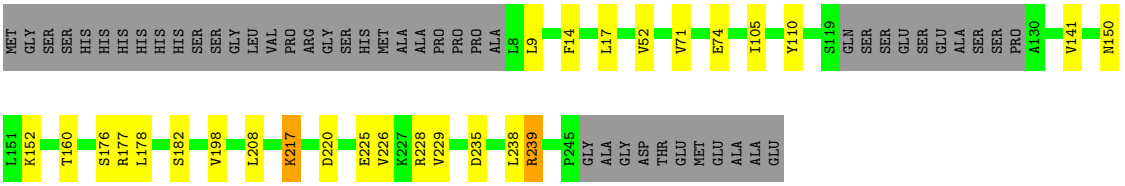
• Molecule 1: Translin

Chain C:



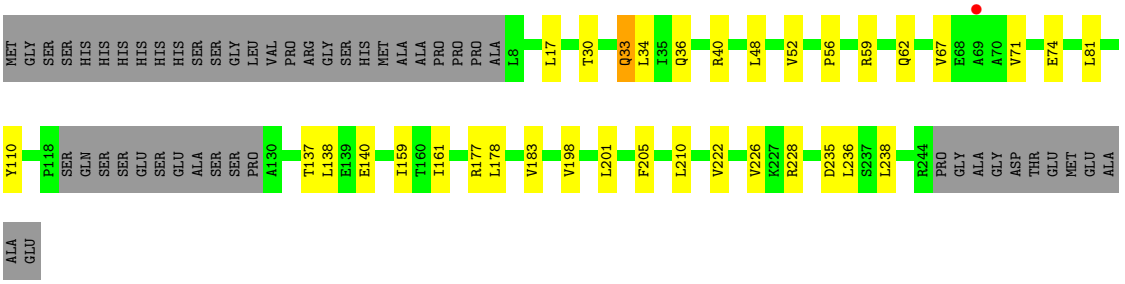
• Molecule 1: Translin

Chain D:



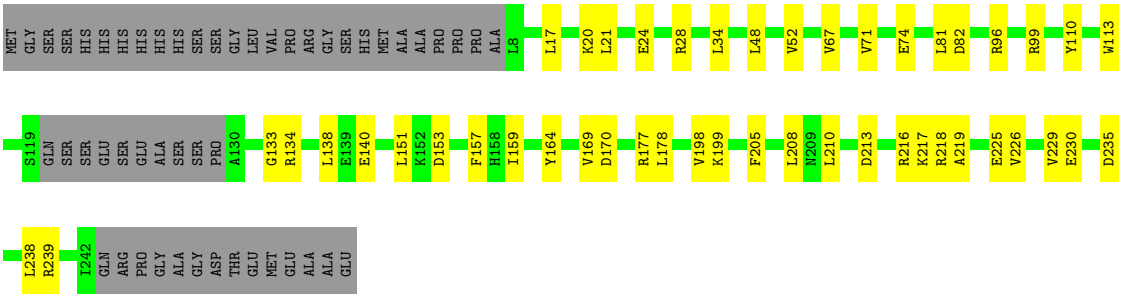
• Molecule 1: Translin

Chain E:



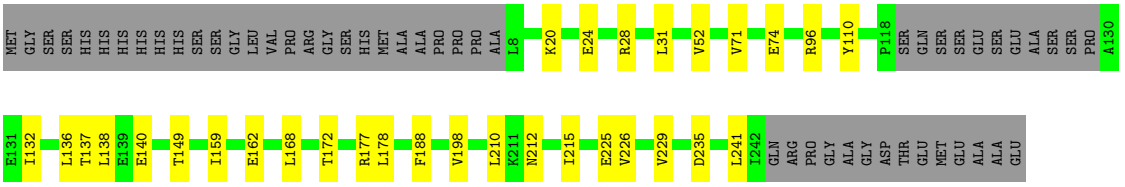
• Molecule 1: Translin

Chain F:



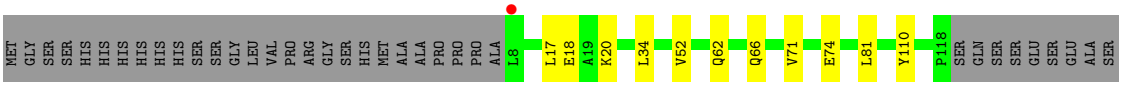
• Molecule 1: Translin

Chain G:



• Molecule 1: Translin

Chain H:




SER
PRO
A130
N150
L151
K152
H158
L178
V198
L201
L208
N209
L210
K211
N212
D213
I214
I215
R216
V222
E225
V226
V229
D235
R239
I242
GLN
ARG
PRO
GLY
ALA
GLY
ASP
THR
GLU
MET
GLU
ALA
ALA
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.55Å 153.22Å 103.95Å 90.00° 111.47° 90.00°	Depositor
Resolution (Å)	38.28 – 3.20 38.28 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.28-3.20) 99.8 (38.28-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.213 , 0.237 0.214 , 0.240	Depositor DCC
R_{free} test set	1787 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	80.4	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14312	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/1821	0.47	0/2469
1	B	0.26	0/1822	0.46	0/2472
1	C	0.25	0/1807	0.47	0/2451
1	D	0.26	0/1836	0.47	0/2491
1	E	0.25	0/1823	0.47	0/2472
1	F	0.25	0/1818	0.46	0/2465
1	G	0.26	0/1800	0.46	0/2443
1	H	0.26	0/1812	0.47	0/2457
All	All	0.26	0/14539	0.47	0/19720

There are no bond length outliers.

There are no bond angle outliers.

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	1792	0	1825	22	0
1	B	1792	0	1819	15	0
1	C	1778	0	1808	30	0
1	D	1806	0	1833	19	0
1	E	1794	0	1818	25	0
1	F	1789	0	1822	27	0
1	G	1771	0	1795	20	0
1	H	1783	0	1817	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	14312	0	14537	158	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 5.

The worst 5 of 158 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:9:LEU:HD11	1:E:201:LEU:HD12	1.58	0.84
1:C:211:LYS:HE2	1:G:28:ARG:HH22	1.51	0.76
1:C:176:SER:HB3	1:C:228:ARG:HD3	1.68	0.74
1:G:28:ARG:HG2	1:G:96:ARG:HH22	1.53	0.74
1:D:176:SER:HB3	1:D:228:ARG:HD3	1.70	0.73

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	221/276 (80%)	218 (99%)	3 (1%)	0	100	100
1	B	222/276 (80%)	221 (100%)	1 (0%)	0	100	100
1	C	220/276 (80%)	215 (98%)	5 (2%)	0	100	100
1	D	224/276 (81%)	221 (99%)	3 (1%)	0	100	100
1	E	222/276 (80%)	217 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	221/276 (80%)	215 (97%)	6 (3%)	0	100	100
1	G	220/276 (80%)	213 (97%)	7 (3%)	0	100	100
1	H	220/276 (80%)	220 (100%)	0	0	100	100
All	All	1770/2208 (80%)	1740 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	197/236 (84%)	196 (100%)	1 (0%)	86	93
1	B	197/236 (84%)	196 (100%)	1 (0%)	86	93
1	C	196/236 (83%)	195 (100%)	1 (0%)	86	93
1	D	198/236 (84%)	191 (96%)	7 (4%)	31	63
1	E	196/236 (83%)	193 (98%)	3 (2%)	60	81
1	F	197/236 (84%)	191 (97%)	6 (3%)	36	66
1	G	194/236 (82%)	192 (99%)	2 (1%)	73	87
1	H	196/236 (83%)	195 (100%)	1 (0%)	86	93
All	All	1571/1888 (83%)	1549 (99%)	22 (1%)	62	82

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	153	ASP
1	F	216	ARG
1	F	177	ARG
1	F	239	ARG
1	D	182	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	225/276 (81%)	-0.29	0 100 100	43, 64, 101, 110	0
1	B	226/276 (81%)	-0.45	1 (0%) 89 81	40, 58, 104, 124	0
1	C	224/276 (81%)	-0.21	1 (0%) 89 81	52, 82, 118, 139	0
1	D	228/276 (82%)	-0.20	0 100 100	44, 70, 108, 118	0
1	E	226/276 (81%)	-0.18	1 (0%) 89 81	45, 73, 113, 131	0
1	F	225/276 (81%)	-0.28	0 100 100	51, 75, 109, 122	0
1	G	224/276 (81%)	-0.19	0 100 100	55, 80, 117, 162	0
1	H	224/276 (81%)	-0.35	1 (0%) 89 81	38, 62, 103, 140	0
All	All	1802/2208 (81%)	-0.27	4 (0%) 92 87	38, 72, 111, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	8	LEU	4.0
1	B	8	LEU	2.5
1	H	8	LEU	2.3
1	E	69	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.