



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 4, 2016 – 04:52 AM EDT

PDB ID : 5JHC
Title : Crystal structure of the self-assembled propeptides from Ape1
Authors : Yamasaki, A.; Noda, N.N.
Deposited on : 2016-04-20
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

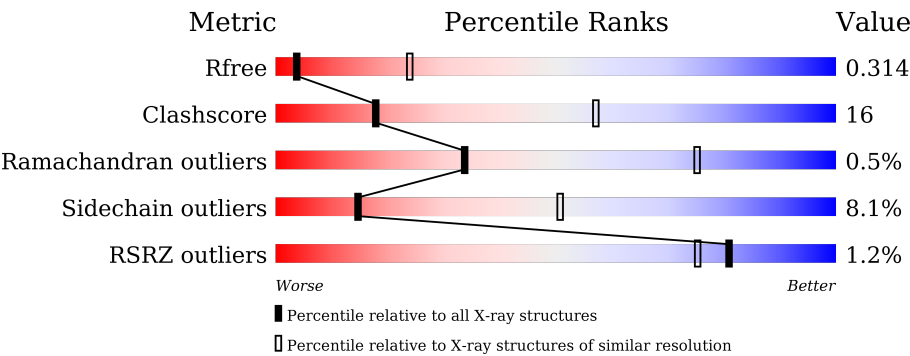
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	24	<div><div></div><div></div><div></div><div></div></div> <div>63%38%</div>
1	B	24	<div><div></div><div></div><div></div><div></div><div></div></div> <div>63%33%. .</div>
1	C	24	<div><div></div><div></div><div></div><div></div><div></div></div> <div>63%33%. .</div>
1	D	24	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>38%42%13%8%</div>
1	E	24	<div><div></div><div></div><div></div><div></div><div></div></div> <div>58%38%. .</div>
1	F	24	<div><div></div><div></div><div></div><div></div><div></div></div> <div>58%33%8%</div>

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Mol	Chain	Length	Quality of chain
1	G	24	
1	H	24	
1	I	24	
1	J	24	
1	K	24	
1	L	24	
1	M	24	
1	N	24	
1	O	24	
1	P	24	
1	Q	24	
1	R	24	
1	S	24	
1	T	24	
1	U	24	
1	V	24	
1	W	24	
1	X	24	
1	Y	24	
1	Z	24	
1	a	24	
1	b	24	
1	c	24	
1	d	24	
1	e	24	

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Mol	Chain	Length	Quality of chain
1	f	24	<div><div></div><div>92%</div><div>8%</div></div>
1	g	24	<div><div>4%</div><div></div><div>100%</div></div>
1	h	24	<div><div>8%</div><div></div><div>92%</div><div>8%</div></div>
1	i	24	<div><div>4%</div><div></div><div>88%</div><div>13%</div></div>
1	j	24	<div><div></div><div>96%</div><div>.</div></div>
1	k	24	<div><div></div><div>96%</div><div>.</div></div>
1	l	24	<div><div></div><div>96%</div><div>.</div></div>
1	m	24	<div><div></div><div>83%</div><div>.</div><div>.</div><div>8%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6607 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 Vacuolar aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	24	Total	C	N	O	S	0	0	0
			173	111	28	33	1			
1	C	24	Total	C	N	O	S	0	0	0
			158	100	25	32	1			
1	E	24	Total	C	N	O	S	0	0	0
			172	110	26	34	2			
1	G	24	Total	C	N	O	S	0	0	0
			179	111	28	38	2			
1	I	24	Total	C	N	O	S	0	0	0
			173	109	27	35	2			
1	K	24	Total	C	N	O	S	0	0	0
			189	118	29	40	2			
1	M	24	Total	C	N	O	S	0	0	0
			186	117	31	36	2			
1	O	24	Total	C	N	O	S	0	0	0
			170	106	26	37	1			
1	Q	24	Total	C	N	O	S	0	0	0
			185	116	28	40	1			
1	S	24	Total	C	N	O	S	0	0	0
			162	103	27	31	1			
1	U	24	Total	C	N	O	S	0	0	0
			186	117	31	36	2			
1	W	24	Total	C	N	O	S	0	0	0
			180	115	29	34	2			
1	Y	20	Total	C	N	O	S	0	0	0
			116	73	21	21	1			
1	B	24	Total	C	N	O	S	0	0	0
			167	104	27	35	1			
1	a	23	Total	C	N	O		0	0	0
			156	99	25	32				
1	b	23	Total	C	N	O	S	0	0	0
			151	95	24	31	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	22	Total	C	N	O	S	0	0	0
			152	97	27	27	1			
1	F	24	Total	C	N	O		0	0	0
			172	108	29	35				
1	c	24	Total	C	N	O	S	0	0	0
			166	105	26	34	1			
1	H	23	Total	C	N	O	S	0	0	0
			181	115	27	38	1			
1	d	24	Total	C	N	O	S	0	0	0
			172	111	28	31	2			
1	J	24	Total	C	N	O		0	0	0
			176	111	30	35				
1	e	24	Total	C	N	O	S	0	0	0
			179	112	30	35	2			
1	L	24	Total	C	N	O	S	0	0	0
			191	120	31	39	1			
1	f	24	Total	C	N	O	S	0	0	0
			173	110	29	32	2			
1	N	24	Total	C	N	O	S	0	0	0
			180	112	31	36	1			
1	g	24	Total	C	N	O	S	0	0	0
			164	105	25	32	2			
1	P	23	Total	C	N	O	S	0	0	0
			177	113	28	35	1			
1	h	24	Total	C	N	O	S	0	0	0
			177	112	30	34	1			
1	R	24	Total	C	N	O	S	0	0	0
			182	116	31	33	2			
1	i	24	Total	C	N	O	S	0	0	0
			173	109	26	37	1			
1	T	24	Total	C	N	O	S	0	0	0
			182	116	31	33	2			
1	j	24	Total	C	N	O	S	0	0	0
			186	117	31	36	2			
1	V	24	Total	C	N	O	S	0	0	0
			177	110	27	38	2			
1	k	24	Total	C	N	O	S	0	0	0
			176	112	28	34	2			
1	X	24	Total	C	N	O	S	0	0	0
			173	109	28	35	1			
1	l	24	Total	C	N	O	S	0	0	0
			184	116	28	38	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Z	14	Total	C	N	O	0	0	0
			89	55	16	18			
1	m	22	Total	C	N	O	0	0	0
			122	76	22	24			

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P14904
A	0	PRO	-	expression tag	UNP P14904
A	22	LEU	PRO	engineered mutation	UNP P14904
C	-1	GLY	-	expression tag	UNP P14904
C	0	PRO	-	expression tag	UNP P14904
C	22	LEU	PRO	engineered mutation	UNP P14904
E	-1	GLY	-	expression tag	UNP P14904
E	0	PRO	-	expression tag	UNP P14904
E	22	LEU	PRO	engineered mutation	UNP P14904
G	-1	GLY	-	expression tag	UNP P14904
G	0	PRO	-	expression tag	UNP P14904
G	22	LEU	PRO	engineered mutation	UNP P14904
I	-1	GLY	-	expression tag	UNP P14904
I	0	PRO	-	expression tag	UNP P14904
I	22	LEU	PRO	engineered mutation	UNP P14904
K	-1	GLY	-	expression tag	UNP P14904
K	0	PRO	-	expression tag	UNP P14904
K	22	LEU	PRO	engineered mutation	UNP P14904
M	-1	GLY	-	expression tag	UNP P14904
M	0	PRO	-	expression tag	UNP P14904
M	22	LEU	PRO	engineered mutation	UNP P14904
O	-1	GLY	-	expression tag	UNP P14904
O	0	PRO	-	expression tag	UNP P14904
O	22	LEU	PRO	engineered mutation	UNP P14904
Q	-1	GLY	-	expression tag	UNP P14904
Q	0	PRO	-	expression tag	UNP P14904
Q	22	LEU	PRO	engineered mutation	UNP P14904
S	-1	GLY	-	expression tag	UNP P14904
S	0	PRO	-	expression tag	UNP P14904
S	22	LEU	PRO	engineered mutation	UNP P14904
U	-1	GLY	-	expression tag	UNP P14904
U	0	PRO	-	expression tag	UNP P14904
U	22	LEU	PRO	engineered mutation	UNP P14904
W	-1	GLY	-	expression tag	UNP P14904

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Chain	Residue	Modelled	Actual	Comment	Reference
W	0	PRO	-	expression tag	UNP P14904
W	22	LEU	PRO	engineered mutation	UNP P14904
Y	-1	GLY	-	expression tag	UNP P14904
Y	0	PRO	-	expression tag	UNP P14904
Y	22	LEU	PRO	engineered mutation	UNP P14904
B	-1	GLY	-	expression tag	UNP P14904
B	0	PRO	-	expression tag	UNP P14904
B	22	LEU	PRO	engineered mutation	UNP P14904
a	-1	GLY	-	expression tag	UNP P14904
a	0	PRO	-	expression tag	UNP P14904
a	22	LEU	PRO	engineered mutation	UNP P14904
b	-1	GLY	-	expression tag	UNP P14904
b	0	PRO	-	expression tag	UNP P14904
b	22	LEU	PRO	engineered mutation	UNP P14904
D	-1	GLY	-	expression tag	UNP P14904
D	0	PRO	-	expression tag	UNP P14904
D	22	LEU	PRO	engineered mutation	UNP P14904
F	-1	GLY	-	expression tag	UNP P14904
F	0	PRO	-	expression tag	UNP P14904
F	22	LEU	PRO	engineered mutation	UNP P14904
c	-1	GLY	-	expression tag	UNP P14904
c	0	PRO	-	expression tag	UNP P14904
c	22	LEU	PRO	engineered mutation	UNP P14904
H	-1	GLY	-	expression tag	UNP P14904
H	0	PRO	-	expression tag	UNP P14904
H	22	LEU	PRO	engineered mutation	UNP P14904
d	-1	GLY	-	expression tag	UNP P14904
d	0	PRO	-	expression tag	UNP P14904
d	22	LEU	PRO	engineered mutation	UNP P14904
J	-1	GLY	-	expression tag	UNP P14904
J	0	PRO	-	expression tag	UNP P14904
J	22	LEU	PRO	engineered mutation	UNP P14904
e	-1	GLY	-	expression tag	UNP P14904
e	0	PRO	-	expression tag	UNP P14904
e	22	LEU	PRO	engineered mutation	UNP P14904
L	-1	GLY	-	expression tag	UNP P14904
L	0	PRO	-	expression tag	UNP P14904
L	22	LEU	PRO	engineered mutation	UNP P14904
f	-1	GLY	-	expression tag	UNP P14904
f	0	PRO	-	expression tag	UNP P14904
f	22	LEU	PRO	engineered mutation	UNP P14904
N	-1	GLY	-	expression tag	UNP P14904

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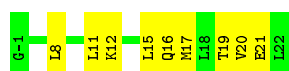
Chain	Residue	Modelled	Actual	Comment	Reference
N	0	PRO	-	expression tag	UNP P14904
N	22	LEU	PRO	engineered mutation	UNP P14904
g	-1	GLY	-	expression tag	UNP P14904
g	0	PRO	-	expression tag	UNP P14904
g	22	LEU	PRO	engineered mutation	UNP P14904
P	-1	GLY	-	expression tag	UNP P14904
P	0	PRO	-	expression tag	UNP P14904
P	22	LEU	PRO	engineered mutation	UNP P14904
h	-1	GLY	-	expression tag	UNP P14904
h	0	PRO	-	expression tag	UNP P14904
h	22	LEU	PRO	engineered mutation	UNP P14904
R	-1	GLY	-	expression tag	UNP P14904
R	0	PRO	-	expression tag	UNP P14904
R	22	LEU	PRO	engineered mutation	UNP P14904
i	-1	GLY	-	expression tag	UNP P14904
i	0	PRO	-	expression tag	UNP P14904
i	22	LEU	PRO	engineered mutation	UNP P14904
T	-1	GLY	-	expression tag	UNP P14904
T	0	PRO	-	expression tag	UNP P14904
T	22	LEU	PRO	engineered mutation	UNP P14904
j	-1	GLY	-	expression tag	UNP P14904
j	0	PRO	-	expression tag	UNP P14904
j	22	LEU	PRO	engineered mutation	UNP P14904
V	-1	GLY	-	expression tag	UNP P14904
V	0	PRO	-	expression tag	UNP P14904
V	22	LEU	PRO	engineered mutation	UNP P14904
k	-1	GLY	-	expression tag	UNP P14904
k	0	PRO	-	expression tag	UNP P14904
k	22	LEU	PRO	engineered mutation	UNP P14904
X	-1	GLY	-	expression tag	UNP P14904
X	0	PRO	-	expression tag	UNP P14904
X	22	LEU	PRO	engineered mutation	UNP P14904
l	-1	GLY	-	expression tag	UNP P14904
l	0	PRO	-	expression tag	UNP P14904
l	22	LEU	PRO	engineered mutation	UNP P14904
Z	-1	GLY	-	expression tag	UNP P14904
Z	0	PRO	-	expression tag	UNP P14904
Z	22	LEU	PRO	engineered mutation	UNP P14904
m	-1	GLY	-	expression tag	UNP P14904
m	0	PRO	-	expression tag	UNP P14904
m	22	LEU	PRO	engineered mutation	UNP P14904

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Vacuolar aminopeptidase 1

Chain A: 



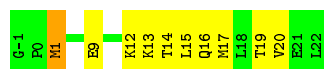
- Molecule 1: Vacuolar aminopeptidase 1

Chain C: 



- Molecule 1: Vacuolar aminopeptidase 1

Chain E: 



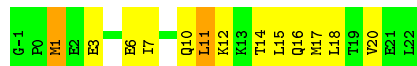
- Molecule 1: Vacuolar aminopeptidase 1

Chain G: 



- Molecule 1: Vacuolar aminopeptidase 1

Chain I: 

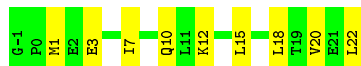


- Molecule 1: Vacuolar aminopeptidase 1

Chain K: 



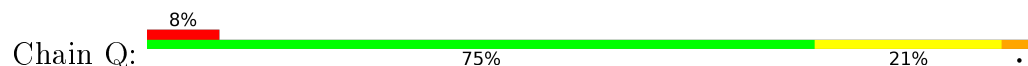
- Molecule 1: Vacuolar aminopeptidase 1



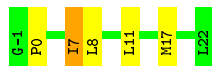
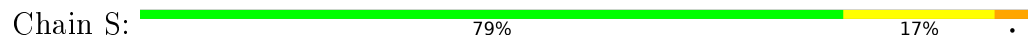
- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



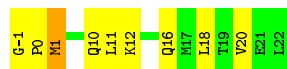
- Molecule 1: Vacuolar aminopeptidase 1



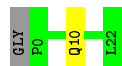
- Molecule 1: Vacuolar aminopeptidase 1



• Molecule 1: Vacuolar aminopeptidase 1

Chain B:  63% 33% .

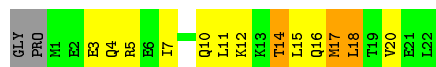
• Molecule 1: Vacuolar aminopeptidase 1

Chain a:  92% . .

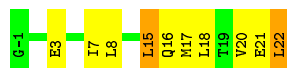
• Molecule 1: Vacuolar aminopeptidase 1

Chain b:  4% 96% .

• Molecule 1: Vacuolar aminopeptidase 1

Chain D:  38% 42% 13% 8%

• Molecule 1: Vacuolar aminopeptidase 1

Chain F:  58% 33% 8%

• Molecule 1: Vacuolar aminopeptidase 1

Chain c:  92% 8%

• Molecule 1: Vacuolar aminopeptidase 1

Chain H:  4% 33% 54% 8% .

• Molecule 1: Vacuolar aminopeptidase 1

Chain d:  92% 8%



- Molecule 1: Vacuolar aminopeptidase 1

Chain J:  42% 54% .



- Molecule 1: Vacuolar aminopeptidase 1

Chain e:  96% .




- Molecule 1: Vacuolar aminopeptidase 1

Chain L:  8% 29% 67% .




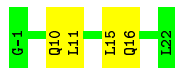
- Molecule 1: Vacuolar aminopeptidase 1

Chain f:  92% 8%



- Molecule 1: Vacuolar aminopeptidase 1

Chain N:  83% 17%



- Molecule 1: Vacuolar aminopeptidase 1

Chain g:  4% 100%

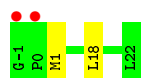


- Molecule 1: Vacuolar aminopeptidase 1

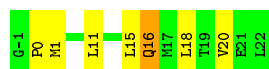
Chain P:  54% 42% .



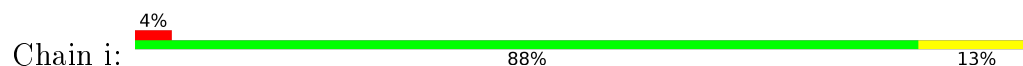
- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



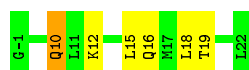
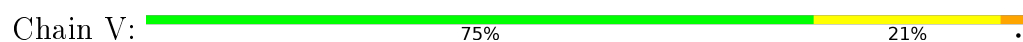
- Molecule 1: Vacuolar aminopeptidase 1



- Molecule 1: Vacuolar aminopeptidase 1



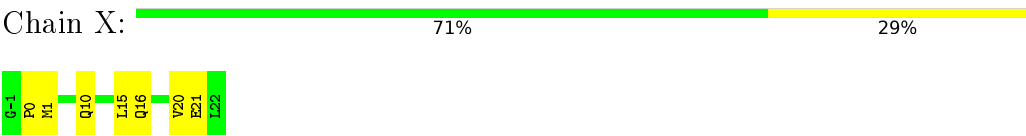
- Molecule 1: Vacuolar aminopeptidase 1



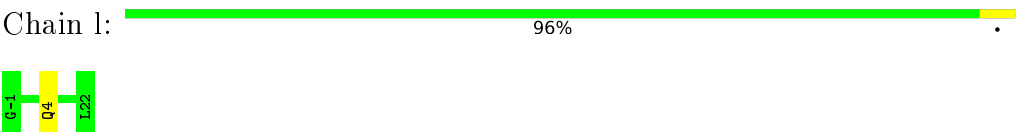
- Molecule 1: Vacuolar aminopeptidase 1



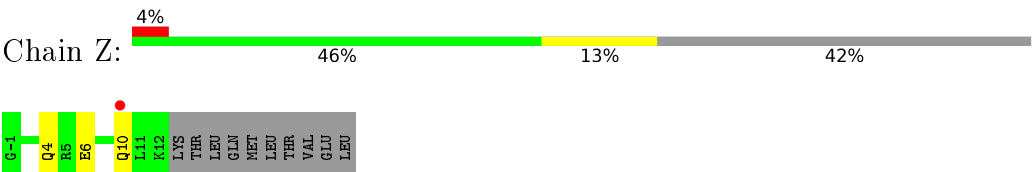
● Molecule 1: Vacuolar aminopeptidase 1



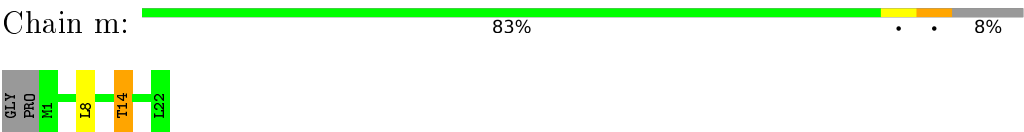
● Molecule 1: Vacuolar aminopeptidase 1



● Molecule 1: Vacuolar aminopeptidase 1



● Molecule 1: Vacuolar aminopeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	248.76 Å 248.76 Å 164.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.52 – 3.40 39.52 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.52-3.40) 99.7 (39.52-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.276 , 0.311 0.280 , 0.314	Depositor DCC
R_{free} test set	1320 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	107.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 101.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6607	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	0.51	0/173	0.66	0/232
1	B	0.40	0/167	0.48	0/225
1	C	0.39	0/158	0.54	0/215
1	D	0.43	0/151	0.56	0/204
1	E	0.47	0/172	0.65	0/231
1	F	0.34	0/172	0.54	0/233
1	G	0.46	0/179	0.62	0/239
1	H	0.64	0/181	0.74	0/241
1	I	0.44	0/173	0.68	0/232
1	J	0.41	0/176	0.66	0/237
1	K	0.48	0/189	0.67	0/251
1	L	0.60	0/191	0.79	0/254
1	M	0.52	0/186	0.65	0/248
1	N	0.41	0/180	0.47	0/241
1	O	0.40	0/170	0.61	0/230
1	P	0.61	0/177	0.83	0/236
1	Q	0.43	0/185	0.65	0/248
1	R	0.50	0/182	0.73	0/242
1	S	0.40	0/162	0.51	0/219
1	T	0.57	0/182	0.81	0/242
1	U	0.45	0/186	0.63	0/248
1	V	0.57	0/177	0.72	0/238
1	W	0.50	0/180	0.71	0/240
1	X	0.51	0/173	0.68	0/234
1	Y	0.36	0/116	0.55	0/158
1	Z	0.34	0/89	0.46	0/121
1	a	0.36	0/156	0.41	0/212
1	b	0.35	0/151	0.44	0/205
1	c	0.38	0/166	0.55	0/224
1	d	0.54	0/172	0.74	0/230
1	e	0.41	0/179	0.61	0/239
1	f	0.48	0/173	0.73	0/231
1	g	0.56	0/164	0.77	0/222
1	h	0.39	0/177	0.64	0/237

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.49	0/173	0.75	0/234
1	j	0.47	0/186	0.61	0/248
1	k	0.53	0/176	0.69	0/236
1	l	0.63	0/184	0.81	0/246
1	m	0.43	0/121	0.50	0/166
All	All	0.48	0/6605	0.65	0/8869

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 [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	173	0	176	13	0
1	B	167	0	151	7	0
1	C	158	0	139	9	0
1	D	152	0	147	19	0
1	E	172	0	170	12	0
1	F	172	0	162	12	0
1	G	179	0	170	14	0
1	H	181	0	185	23	0
1	I	173	0	167	16	0
1	J	176	0	173	14	0
1	K	189	0	192	12	0
1	L	191	0	199	18	0
1	M	186	0	193	8	0
1	N	180	0	177	5	0
1	O	170	0	153	12	0
1	P	177	0	183	12	0
1	Q	185	0	183	7	0
1	R	182	0	194	9	0
1	S	162	0	152	3	0
1	T	182	0	194	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	186	0	193	5	0
1	V	177	0	166	4	0
1	W	180	0	189	7	0
1	X	173	0	166	6	0
1	Y	116	0	89	4	0
1	Z	89	0	70	4	0
1	a	156	0	137	0	0
1	b	151	0	127	0	0
1	c	166	0	154	0	0
1	d	172	0	179	0	0
1	e	179	0	178	0	0
1	f	173	0	176	0	0
1	g	164	0	155	0	0
1	h	177	0	175	0	0
1	i	173	0	162	0	0
1	j	186	0	193	0	0
1	k	176	0	178	0	0
1	l	184	0	186	0	0
1	m	122	0	78	0	1
All	All	6607	0	6411	185	1

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 185 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:F:15:LEU:HD22	1:L:12:LYS:HD3	64.14	0.84
1:W:8:LEU:HD12	1:L:11:LEU:HG	23.00	0.75
1:G:4:GLN:NE2	1:D:4:GLN:OE1	37.23	0.75
1:O:21:GLU:HG3	1:J:5:ARG:HH12	26.32	0.74
1:E:1:MET:N	1:E:1:MET:SD	2.59	0.73

All (1) 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:m:14:THR:OG1	1:m:14:THR:OG1[12_555]	2.10	0.10

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	22/24 (92%)	22 (100%)	0	0	100	100
1	B	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
1	C	22/24 (92%)	21 (96%)	0	1 (4%)	3	27
1	D	20/24 (83%)	16 (80%)	4 (20%)	0	100	100
1	E	22/24 (92%)	22 (100%)	0	0	100	100
1	F	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	G	22/24 (92%)	22 (100%)	0	0	100	100
1	H	21/24 (88%)	21 (100%)	0	0	100	100
1	I	22/24 (92%)	22 (100%)	0	0	100	100
1	J	22/24 (92%)	22 (100%)	0	0	100	100
1	K	22/24 (92%)	22 (100%)	0	0	100	100
1	L	22/24 (92%)	22 (100%)	0	0	100	100
1	M	22/24 (92%)	22 (100%)	0	0	100	100
1	N	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
1	O	22/24 (92%)	22 (100%)	0	0	100	100
1	P	21/24 (88%)	21 (100%)	0	0	100	100
1	Q	22/24 (92%)	22 (100%)	0	0	100	100
1	R	22/24 (92%)	21 (96%)	0	1 (4%)	3	27
1	S	22/24 (92%)	20 (91%)	1 (4%)	1 (4%)	3	27
1	T	22/24 (92%)	22 (100%)	0	0	100	100
1	U	22/24 (92%)	21 (96%)	0	1 (4%)	3	27
1	V	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	W	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	X	22/24 (92%)	22 (100%)	0	0	100	100
1	Y	18/24 (75%)	18 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	12/24 (50%)	11 (92%)	1 (8%)	0	100	100
1	a	21/24 (88%)	21 (100%)	0	0	100	100
1	b	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
1	c	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	d	22/24 (92%)	22 (100%)	0	0	100	100
1	e	22/24 (92%)	22 (100%)	0	0	100	100
1	f	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
1	g	22/24 (92%)	22 (100%)	0	0	100	100
1	h	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	i	22/24 (92%)	22 (100%)	0	0	100	100
1	j	22/24 (92%)	22 (100%)	0	0	100	100
1	k	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
1	l	22/24 (92%)	22 (100%)	0	0	100	100
1	m	20/24 (83%)	20 (100%)	0	0	100	100
All	All	836/936 (89%)	813 (97%)	19 (2%)	4 (0%)	34	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	0	PRO
1	R	0	PRO
1	U	20	VAL
1	C	0	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	17/23 (74%)	17 (100%)	0	100	100
1	B	15/23 (65%)	14 (93%)	1 (7%)	20	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	13/23 (56%)	12 (92%)	1 (8%)	16	53
1	D	13/23 (56%)	10 (77%)	3 (23%)	1	4
1	E	17/23 (74%)	16 (94%)	1 (6%)	24	64
1	F	16/23 (70%)	14 (88%)	2 (12%)	6	27
1	G	18/23 (78%)	16 (89%)	2 (11%)	8	33
1	H	20/23 (87%)	18 (90%)	2 (10%)	9	38
1	I	17/23 (74%)	15 (88%)	2 (12%)	6	29
1	J	17/23 (74%)	16 (94%)	1 (6%)	24	64
1	K	21/23 (91%)	19 (90%)	2 (10%)	11	41
1	L	21/23 (91%)	18 (86%)	3 (14%)	4	22
1	M	20/23 (87%)	19 (95%)	1 (5%)	30	69
1	N	18/23 (78%)	18 (100%)	0	100	100
1	O	16/23 (70%)	14 (88%)	2 (12%)	6	27
1	P	19/23 (83%)	19 (100%)	0	100	100
1	Q	20/23 (87%)	19 (95%)	1 (5%)	30	69
1	R	19/23 (83%)	17 (90%)	2 (10%)	8	36
1	S	14/23 (61%)	12 (86%)	2 (14%)	4	22
1	T	19/23 (83%)	19 (100%)	0	100	100
1	U	20/23 (87%)	18 (90%)	2 (10%)	9	38
1	V	18/23 (78%)	17 (94%)	1 (6%)	26	66
1	W	19/23 (83%)	18 (95%)	1 (5%)	28	67
1	X	17/23 (74%)	16 (94%)	1 (6%)	24	64
1	Y	6/23 (26%)	5 (83%)	1 (17%)	3	14
1	Z	6/23 (26%)	6 (100%)	0	100	100
1	a	13/23 (56%)	12 (92%)	1 (8%)	16	53
1	b	12/23 (52%)	12 (100%)	0	100	100
1	c	15/23 (65%)	13 (87%)	2 (13%)	5	24
1	d	17/23 (74%)	15 (88%)	2 (12%)	6	29
1	e	18/23 (78%)	17 (94%)	1 (6%)	26	66
1	f	17/23 (74%)	15 (88%)	2 (12%)	6	29
1	g	15/23 (65%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	17/23 (74%)	15 (88%)	2 (12%)	6	29
1	i	17/23 (74%)	14 (82%)	3 (18%)	2	12
1	j	20/23 (87%)	19 (95%)	1 (5%)	30	69
1	k	18/23 (78%)	17 (94%)	1 (6%)	26	66
1	l	20/23 (87%)	19 (95%)	1 (5%)	30	69
1	m	4/23 (17%)	2 (50%)	2 (50%)	0	0
All	All	639/897 (71%)	587 (92%)	52 (8%)	15	51

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	15	LEU
1	d	1	MET
1	X	21	GLU
1	F	22	LEU
1	c	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	b	10	GLN
1	Z	10	GLN
1	f	16	GLN
1	M	10	GLN
1	P	4	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 carbohydrates 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	24/24 (100%)	-0.26	0 100 100	84, 112, 177, 187	0
1	B	24/24 (100%)	-0.36	0 100 100	104, 125, 168, 170	0
1	C	24/24 (100%)	-0.46	0 100 100	131, 182, 261, 271	0
1	D	22/24 (91%)	-0.55	0 100 100	83, 107, 129, 151	0
1	E	24/24 (100%)	-0.24	0 100 100	80, 128, 279, 312	0
1	F	24/24 (100%)	-0.30	0 100 100	93, 137, 176, 204	0
1	G	24/24 (100%)	-0.54	0 100 100	92, 126, 180, 223	0
1	H	23/24 (95%)	0.40	1 (4%) 39 34	67, 91, 128, 303	0
1	I	24/24 (100%)	-0.24	0 100 100	53, 121, 279, 301	0
1	J	24/24 (100%)	-0.38	0 100 100	81, 133, 170, 189	0
1	K	24/24 (100%)	-0.33	0 100 100	90, 117, 150, 202	0
1	L	24/24 (100%)	0.36	2 (8%) 14 13	67, 84, 130, 189	0
1	M	24/24 (100%)	-0.27	0 100 100	77, 97, 165, 201	0
1	N	24/24 (100%)	-0.03	0 100 100	72, 102, 145, 151	0
1	O	24/24 (100%)	-0.36	0 100 100	93, 123, 194, 261	0
1	P	23/24 (95%)	-0.06	0 100 100	72, 95, 120, 246	0
1	Q	24/24 (100%)	0.01	2 (8%) 14 13	90, 134, 282, 324	0
1	R	24/24 (100%)	-0.20	0 100 100	63, 119, 208, 251	0
1	S	24/24 (100%)	0.19	0 100 100	94, 133, 168, 183	0
1	T	24/24 (100%)	-0.14	0 100 100	64, 93, 203, 250	0
1	U	24/24 (100%)	-0.01	0 100 100	67, 91, 153, 161	0
1	V	24/24 (100%)	-0.56	0 100 100	85, 94, 127, 153	0
1	W	24/24 (100%)	-0.33	0 100 100	55, 81, 142, 180	0
1	X	24/24 (100%)	-0.35	0 100 100	59, 94, 181, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	20/24 (83%)	-0.04	0 100 100	142, 175, 252, 288	0
1	Z	14/24 (58%)	0.94	1 (7%) 19 18	179, 219, 271, 348	0
1	a	23/24 (95%)	-0.45	0 100 100	84, 134, 206, 318	0
1	b	23/24 (95%)	-0.53	1 (4%) 39 34	113, 160, 228, 234	0
1	c	24/24 (100%)	-0.38	0 100 100	85, 123, 301, 310	0
1	d	24/24 (100%)	-0.16	0 100 100	106, 124, 156, 266	0
1	e	24/24 (100%)	-0.24	0 100 100	82, 123, 202, 221	0
1	f	24/24 (100%)	-0.24	0 100 100	72, 108, 230, 242	0
1	g	24/24 (100%)	-0.60	1 (4%) 40 35	87, 104, 212, 259	0
1	h	24/24 (100%)	-0.19	2 (8%) 14 13	81, 123, 192, 261	0
1	i	24/24 (100%)	-0.19	1 (4%) 40 35	105, 128, 168, 184	0
1	j	24/24 (100%)	-0.02	0 100 100	70, 105, 186, 222	0
1	k	24/24 (100%)	-0.51	0 100 100	59, 79, 137, 218	0
1	l	24/24 (100%)	-0.37	0 100 100	63, 74, 98, 120	0
1	m	22/24 (91%)	-0.15	0 100 100	145, 207, 299, 311	0
All	All	914/936 (97%)	-0.22	11 (1%) 81 75	53, 120, 242, 348	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	-1	GLY	4.8
1	b	0	PRO	3.5
1	L	-1	GLY	3.5
1	g	-1	GLY	3.4
1	Q	-1	GLY	2.9

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 carbohydrates 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.