



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 4, 2017 – 03:00 AM EST

PDB ID : 5TCP
EMDB ID: : EMD-8398
Title : Near-atomic resolution cryo-EM structure of the periplasmic domains of PrgH and PrgK
Authors : Worrall, L.J.; Hong, C.; Vuckovic, M.; Bergeron, J.R.C.; Huang, R.K.; Yu, Z.; Strynadka, N.C.J.
Deposited on : 2016-09-15
Resolution : 4.30 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

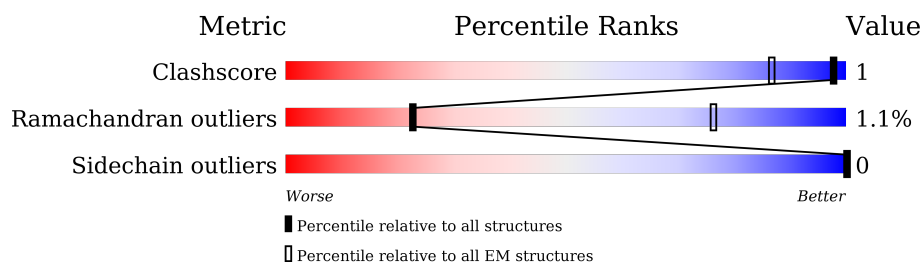
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.














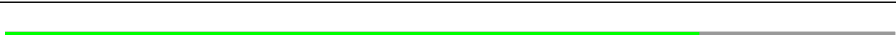

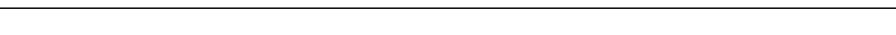
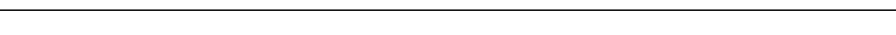
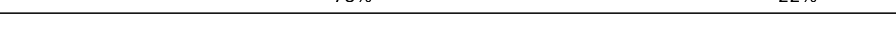

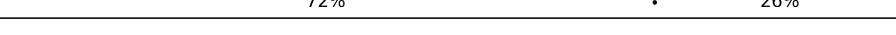







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	235	75% 22%
1	2	235	76% 22%
1	4	235	75% 22%
1	6	235	75% 22%
1	8	235	76% 22%
1	B	235	75% 22%
1	D	235	75% 22%
1	F	235	75% 22%
1	H	235	75% 22%

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Mol	Chain	Length	Quality of chain
1	J	235	 76% 22%
1	L	235	 76% 22%
1	N	235	 76% 22%
1	P	235	 76% 22%
1	R	235	 75% 22%
1	T	235	 76% 22%
1	V	235	 75% 22%
1	X	235	 76% 22%
1	Z	235	 76% 22%
1	a	235	 78% 22%
1	c	235	 78% 22%
1	e	235	 78% 22%
1	g	235	 78% 22%
1	i	235	 78% 22%
1	k	235	 78% 22%
2	1	263	 72% 26%
2	3	263	 72% 26%
2	5	263	 72% 26%
2	7	263	 72% 26%
2	9	263	 72% 26%
2	A	263	 71% 26%
2	C	263	 71% 26%
2	E	263	 71% 26%
2	G	263	 71% 26%
2	I	263	 71% 26%

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Mol	Chain	Length	Quality of chain
2	K	263	
2	M	263	
2	O	263	
2	Q	263	
2	S	263	
2	U	263	
2	W	263	
2	Y	263	
2	b	263	
2	d	263	
2	f	263	
2	h	263	
2	j	263	
2	l	263	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 72888 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	2	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	4	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	6	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	8	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	B	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	D	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	F	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	H	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	J	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	L	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	N	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	P	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	R	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	T	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	V	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	X	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	a	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	c	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	e	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	g	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	i	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
1	k	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		

- Molecule 2 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	3	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	5	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	7	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	9	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	A	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	C	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	E	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	G	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	I	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	K	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
2	M	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		

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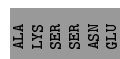
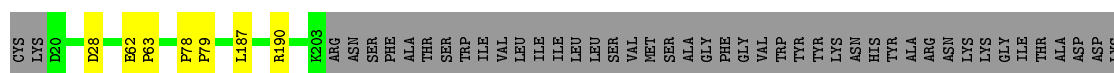
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	Q	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	S	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	U	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	W	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	Y	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	b	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	d	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	f	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	h	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	j	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
2	l	194	Total 1600	C 1011	N 288	O 297	S 4	0	0

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. 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. 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.

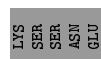
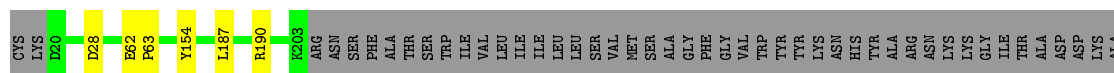
- Molecule 1: Lipoprotein PrgK

Chain 0:  75% 22%




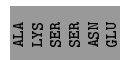
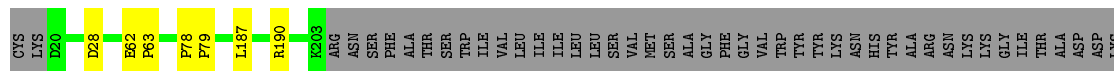
- Molecule 1: Lipoprotein PrgK

Chain 2:  76% 22%




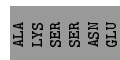
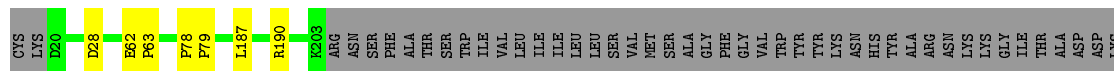
- Molecule 1: Lipoprotein PrgK

Chain 4:  75% 22%



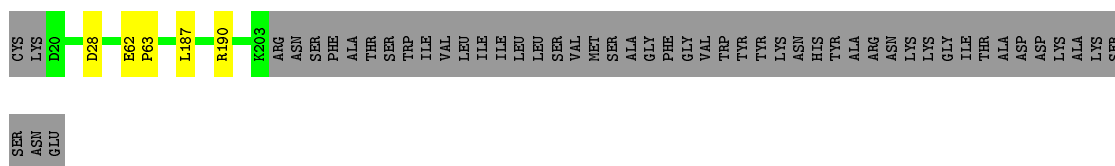
- Molecule 1: Lipoprotein PrgK

Chain 6:  75% 22%



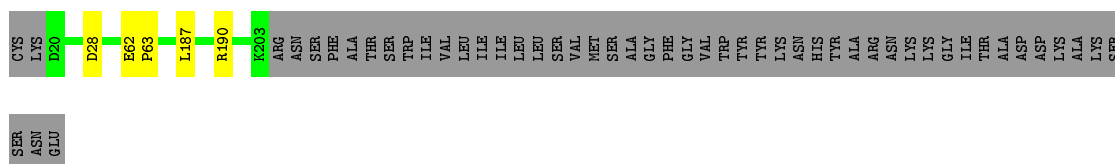
- Molecule 1: Lipoprotein PrgK





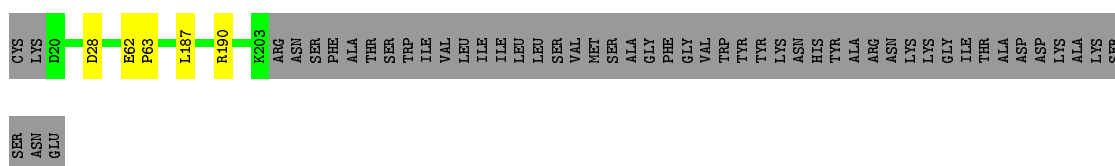
- Molecule 1: Lipoprotein PrgK

Chain L: 76% 22%



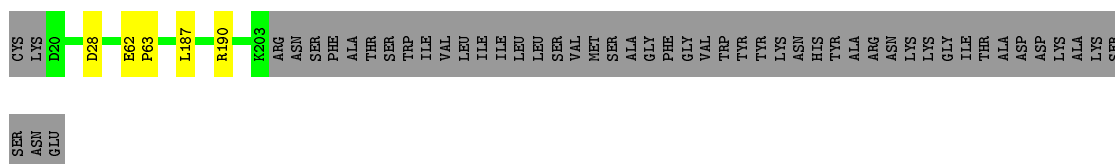
- Molecule 1: Lipoprotein PrgK

Chain N: 76% 22%



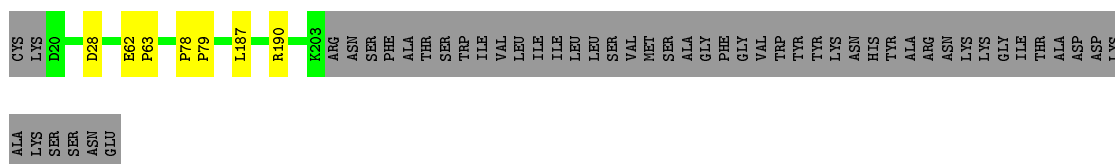
- Molecule 1: Lipoprotein PrgK

Chain P: 76% 22%



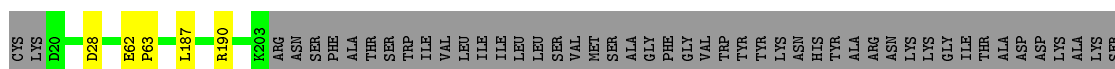
- Molecule 1: Lipoprotein PrgK

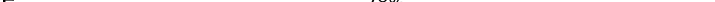
Chain R: 75% 22%

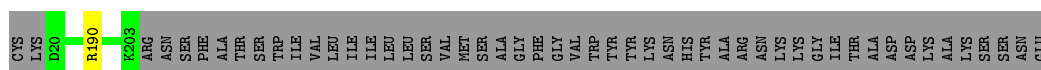


- Molecule 1: Lipoprotein PrgK

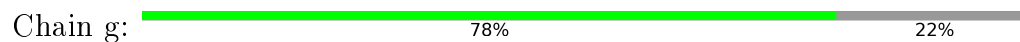
Chain T: 76% 22%



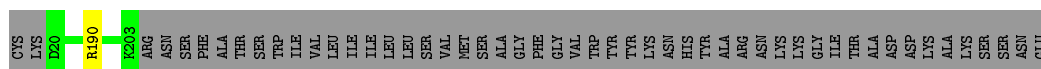
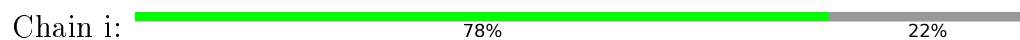
Chain e:  78% 22%



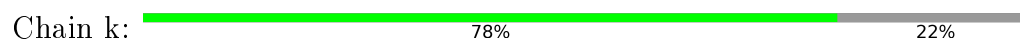
- Molecule 1: Lipoprotein PrgK



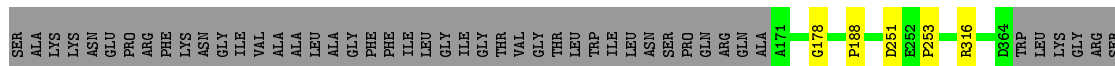
- Molecule 1: Lipoprotein PrgK



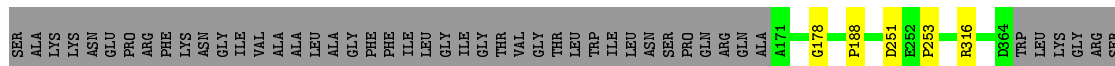
- Molecule 1: Lipoprotein PrgK



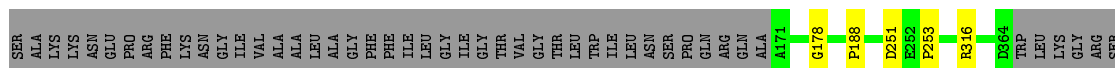
- Molecule 2: Protein PrgH



- Molecule 2: Protein PrgH



- Molecule 2: Protein PrgH



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• Molecule 2: Protein PrgH



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• Molecule 2: Protein PrgH



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• Molecule 2: Protein PrgH



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• Molecule 2: Protein PrgH



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• Molecule 2: Protein PrgH



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PRO
LEU

- Molecule 2: Protein PrgH

Chain G:  71% 26%

SER ALA LYS ASN GLU PRO ARG PHE LYS ASN GLY ILE MET ILE VAL ALA ALA LEU LEU GLY PHE PHE ILE ILE LEU LEU GLY ILE ILE GLY THR VAL GLY THR THR TRP ILE ILE LEU ASN SER PRO GLN ARG GLN GLN ALA A171 G178 L187 P188 D251 P252 P253 R316 D364 TRP LEU LYS GLY ARG

SER PHE GLN TYR GLY ALA GLU GLY TYR LYS LYS MET SER ILE PRO GLY HIS ALA TRP TYR PHE PRO SER PRO LEU

- Molecule 2: Protein PrgH

Chain I:  71% 26%

SER ALA LYS ASN GLU PRO ARG PHE LYS ASN GLY ILE MET ILE VAL ALA ALA LEU LEU GLY PHE PHE ILE ILE LEU LEU GLY ILE ILE GLY THR VAL GLY THR THR TRP ILE ILE LEU ASN SER PRO GLN ARG GLN GLN ALA A171 G178 L187 P188 D251 P252 P253 R316 D364 TRP LEU LYS GLY ARG

SER PHE GLN TYR GLY ALA GLU GLY TYR LYS LYS MET SER ILE PRO GLY HIS ALA TRP TYR PHE PRO SER PRO LEU

- Molecule 2: Protein PrgH

Chain K:  71% 26%

SER ALA LYS ASN GLU PRO ARG PHE LYS ASN GLY ILE MET ILE VAL ALA ALA LEU LEU GLY PHE PHE ILE ILE LEU LEU GLY ILE ILE GLY THR VAL GLY THR THR TRP ILE ILE LEU ASN SER PRO GLN ARG GLN GLN ALA A171 G178 L187 P188 D251 P252 P253 R316 D364 TRP LEU LYS GLY ARG

SER PHE GLN TYR GLY ALA GLU GLY TYR LYS LYS MET SER ILE PRO GLY HIS ALA TRP TYR PHE PRO SER PRO LEU

- Molecule 2: Protein PrgH

Chain M:  72% 26%

SER ALA LYS ASN GLU PRO ARG PHE LYS ASN GLY ILE MET ILE VAL ALA ALA LEU LEU GLY PHE PHE ILE ILE LEU LEU GLY ILE ILE GLY THR VAL GLY THR THR TRP ILE ILE LEU ASN SER PRO GLN ARG GLN GLN ALA A171 G178 P188 D251 E252 P253 R316 D364 TRP LEU LYS GLY ARG SER

PHE GLN TYR GLY ALA GLU GLY TYR LYS LYS MET SER PRO GLY HIS TRP TYR PHE PRO SER PRO LEU

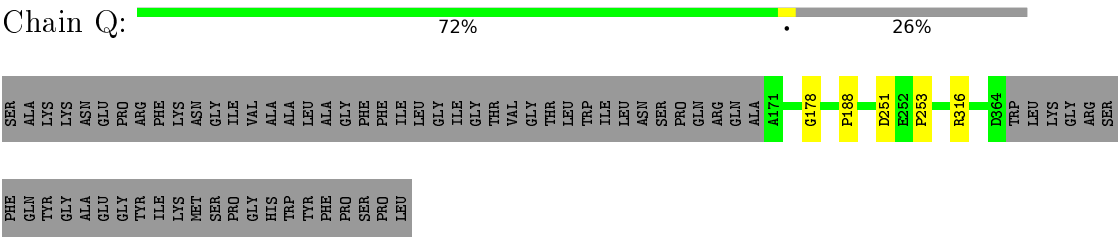
- Molecule 2: Protein PrgH

Chain O:  72% 26%

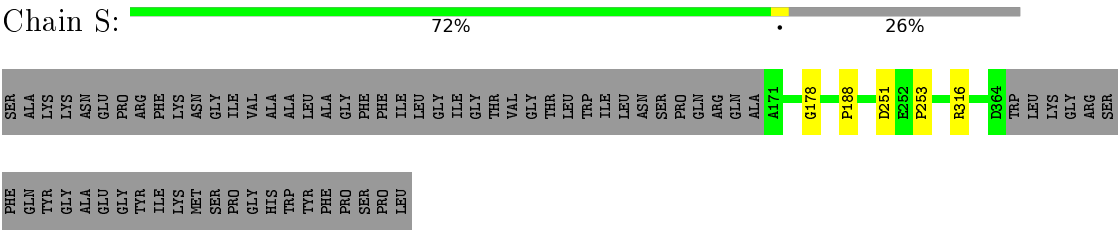
SER ALA LYS ASN GLU PRO ARG PHE LYS ASN GLY ILE MET ILE VAL ALA ALA LEU LEU GLY PHE PHE ILE ILE LEU LEU GLY ILE ILE GLY THR VAL GLY THR THR TRP ILE ILE LEU ASN SER PRO GLN ARG GLN GLN ALA A171 G178 P188 D251 E252 P253 R316 D364 TRP LEU LYS GLY ARG SER

PHE GLN TYR GLY ALA GLU GLY TYR LYS LYS MET SER PRO GLY HIS TRP TYR PHE PRO SER PRO LEU

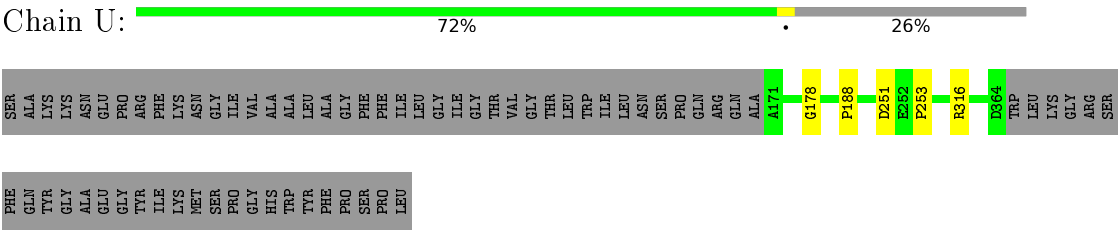
- Molecule 2: Protein PrgH



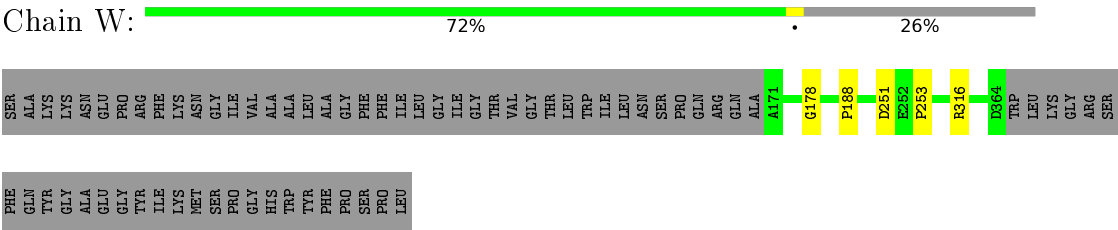
• Molecule 2: Protein PrgH



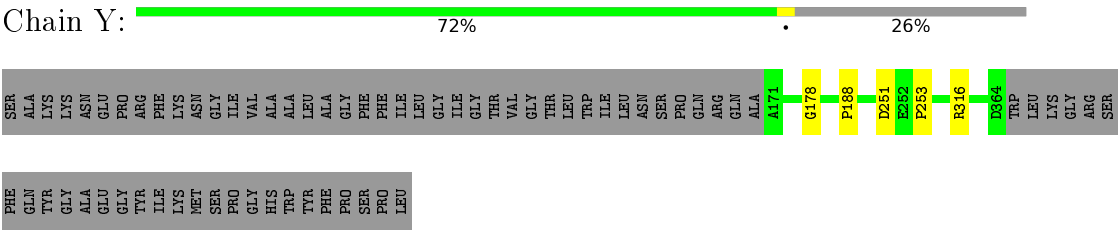
• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH

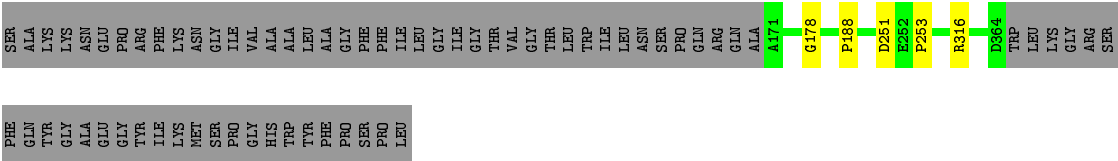


• Molecule 2: Protein PrgH

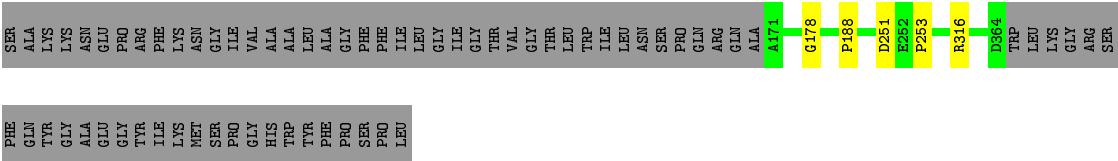


• Molecule 2: Protein PrgH

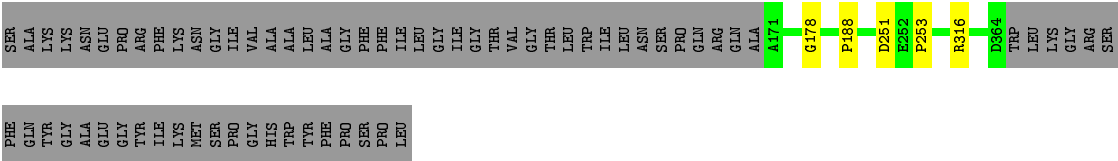




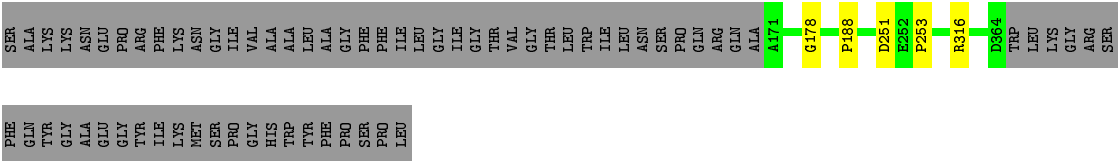
• Molecule 2: Protein PrgH



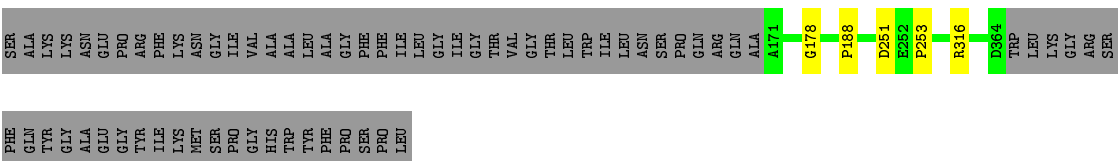
• Molecule 2: Protein PrgH



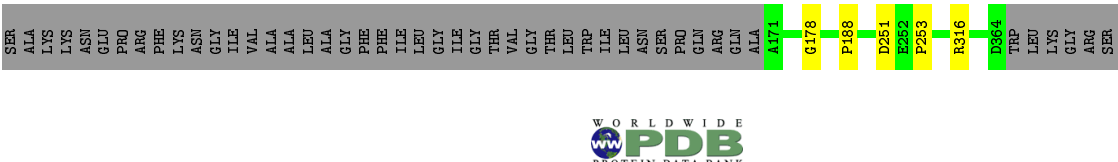
• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH



• Molecule 2: Protein PrgH



PHE
GLN
TYR
GLY
ALA
GLU
GLY
TYR
ILE
LYS
MET
SER
PRO
GLY
HIS
TRP
TYR
PHE
PRO
SER
PRO
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	67800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29240	Depositor
Image detector	Not provided	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	0	0.77	0/1465	0.68	1/1989 (0.1%)
1	2	0.77	0/1465	0.68	2/1989 (0.1%)
1	4	0.77	0/1465	0.68	1/1989 (0.1%)
1	6	0.77	0/1465	0.68	1/1989 (0.1%)
1	8	0.77	0/1465	0.68	1/1989 (0.1%)
1	B	0.77	0/1465	0.68	2/1989 (0.1%)
1	D	0.77	0/1465	0.68	1/1989 (0.1%)
1	F	0.77	0/1465	0.68	1/1989 (0.1%)
1	H	0.77	0/1465	0.68	1/1989 (0.1%)
1	J	0.77	0/1465	0.68	1/1989 (0.1%)
1	L	0.77	0/1465	0.68	1/1989 (0.1%)
1	N	0.77	0/1465	0.68	1/1989 (0.1%)
1	P	0.77	0/1465	0.68	1/1989 (0.1%)
1	R	0.77	0/1465	0.68	1/1989 (0.1%)
1	T	0.77	0/1465	0.68	1/1989 (0.1%)
1	V	0.77	0/1465	0.68	1/1989 (0.1%)
1	X	0.77	0/1465	0.68	1/1989 (0.1%)
1	Z	0.77	0/1465	0.68	1/1989 (0.1%)
1	a	0.77	0/1465	0.68	1/1989 (0.1%)
1	c	0.77	0/1465	0.68	1/1989 (0.1%)
1	e	0.77	0/1465	0.68	1/1989 (0.1%)
1	g	0.77	0/1465	0.68	1/1989 (0.1%)
1	i	0.77	0/1465	0.68	1/1989 (0.1%)
1	k	0.77	0/1465	0.68	1/1989 (0.1%)
2	1	0.77	0/1632	0.70	1/2204 (0.0%)
2	3	0.77	0/1632	0.70	1/2204 (0.0%)
2	5	0.77	0/1632	0.71	1/2204 (0.0%)
2	7	0.77	0/1632	0.70	1/2204 (0.0%)
2	9	0.77	0/1632	0.70	1/2204 (0.0%)
2	A	0.77	0/1632	0.70	1/2204 (0.0%)
2	C	0.77	0/1632	0.70	1/2204 (0.0%)
2	E	0.77	0/1632	0.70	1/2204 (0.0%)
2	G	0.77	0/1632	0.71	1/2204 (0.0%)
2	I	0.77	0/1632	0.70	1/2204 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	K	0.77	0/1632	0.70	1/2204 (0.0%)
2	M	0.77	0/1632	0.70	1/2204 (0.0%)
2	O	0.77	0/1632	0.70	1/2204 (0.0%)
2	Q	0.77	0/1632	0.70	1/2204 (0.0%)
2	S	0.77	0/1632	0.70	1/2204 (0.0%)
2	U	0.77	0/1632	0.70	1/2204 (0.0%)
2	W	0.76	0/1632	0.70	1/2204 (0.0%)
2	Y	0.77	0/1632	0.70	1/2204 (0.0%)
2	b	0.77	0/1632	0.70	1/2204 (0.0%)
2	d	0.77	0/1632	0.70	1/2204 (0.0%)
2	f	0.77	0/1632	0.70	1/2204 (0.0%)
2	h	0.77	0/1632	0.70	1/2204 (0.0%)
2	j	0.77	0/1632	0.70	1/2204 (0.0%)
2	l	0.77	0/1632	0.70	1/2204 (0.0%)
All	All	0.77	0/74328	0.69	50/100632 (0.0%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	4	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	N	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	P	190	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	e	190	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	190	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	X	190	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	k	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	T	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	V	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	a	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	2	190	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	c	190	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	R	190	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	g	190	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	6	190	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	H	190	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	F	190	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	L	190	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	190	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	J	190	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	i	190	ARG	NE-CZ-NH2	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	190	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	8	190	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	9	316	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	O	316	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	C	316	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	Q	316	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	Y	316	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	K	316	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	5	316	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	h	316	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	3	316	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	G	316	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	b	316	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	d	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	l	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	S	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	M	316	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	7	316	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	A	316	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	f	316	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	U	316	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	j	316	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	W	316	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	E	316	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	1	316	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	I	316	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	154	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	2	154	TYR	CB-CG-CD2	-5.01	118.00	121.00

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	0	1437	0	1434	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1437	0	1434	4	0
1	4	1437	0	1434	5	0
1	6	1437	0	1434	5	0
1	8	1437	0	1434	4	0
1	B	1437	0	1434	5	0
1	D	1437	0	1434	5	0
1	F	1437	0	1434	5	0
1	H	1437	0	1434	5	0
1	J	1437	0	1434	4	0
1	L	1437	0	1434	4	0
1	N	1437	0	1434	4	0
1	P	1437	0	1434	4	0
1	R	1437	0	1434	5	0
1	T	1437	0	1434	4	0
1	V	1437	0	1434	5	0
1	X	1437	0	1434	4	0
1	Z	1437	0	1434	4	0
1	a	1437	0	1434	0	0
1	c	1437	0	1434	0	0
1	e	1437	0	1434	0	0
1	g	1437	0	1434	0	0
1	i	1437	0	1434	0	0
1	k	1437	0	1434	0	0
2	1	1600	0	1580	0	0
2	3	1600	0	1580	0	0
2	5	1600	0	1580	0	0
2	7	1600	0	1580	0	0
2	9	1600	0	1580	0	0
2	A	1600	0	1580	2	0
2	C	1600	0	1580	2	0
2	E	1600	0	1580	2	0
2	G	1600	0	1580	2	0
2	I	1600	0	1580	2	0
2	K	1600	0	1580	2	0
2	M	1600	0	1580	0	0
2	O	1600	0	1580	0	0
2	Q	1600	0	1580	0	0
2	S	1600	0	1580	0	0
2	U	1600	0	1580	0	0
2	W	1600	0	1580	0	0
2	Y	1600	0	1580	0	0
2	b	1600	0	1580	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	1600	0	1580	0	0
2	f	1600	0	1580	0	0
2	h	1600	0	1580	0	0
2	j	1600	0	1580	0	0
2	l	1600	0	1580	0	0
All	All	72888	0	72336	93	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 1.

All (93) 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)
1:8:28:ASP:C	1:8:28:ASP:OD1	2.48	0.52
1:2:187:LEU:HD12	1:2:187:LEU:C	2.31	0.52
2:K:187:LEU:C	2:K:187:LEU:HD12	4.98	0.52
1:R:187:LEU:HD12	1:R:187:LEU:C	2.31	0.51
1:Z:187:LEU:HD12	1:Z:187:LEU:C	2.31	0.51
1:4:187:LEU:HD12	1:4:187:LEU:C	2.31	0.51
1:N:28:ASP:OD1	1:N:28:ASP:C	2.48	0.51
1:0:187:LEU:HD12	1:0:187:LEU:C	2.31	0.51
1:6:187:LEU:C	1:6:187:LEU:HD12	2.31	0.51
1:8:187:LEU:C	1:8:187:LEU:HD12	2.31	0.51
2:E:187:LEU:HD12	2:E:187:LEU:C	4.98	0.51
2:G:187:LEU:C	2:G:187:LEU:HD12	4.98	0.51
1:J:28:ASP:C	1:J:28:ASP:OD1	2.48	0.51
1:T:187:LEU:C	1:T:187:LEU:HD12	2.31	0.51
2:A:187:LEU:HD12	2:A:187:LEU:C	4.98	0.51
2:I:187:LEU:HD12	2:I:187:LEU:C	4.98	0.51
1:V:187:LEU:HD12	1:V:187:LEU:C	2.31	0.51
1:X:187:LEU:C	1:X:187:LEU:HD12	2.31	0.51
2:C:187:LEU:C	2:C:187:LEU:HD12	4.98	0.51
1:P:28:ASP:OD1	1:P:28:ASP:C	2.48	0.51
1:T:28:ASP:OD1	1:T:28:ASP:C	2.48	0.51
1:0:28:ASP:C	1:0:28:ASP:OD1	2.48	0.51
1:2:28:ASP:OD1	1:2:28:ASP:C	2.48	0.51
1:B:187:LEU:C	1:B:187:LEU:HD12	2.31	0.51
1:H:28:ASP:C	1:H:28:ASP:OD1	2.48	0.51
1:4:28:ASP:OD1	1:4:28:ASP:C	2.48	0.51
1:F:28:ASP:OD1	1:F:28:ASP:C	2.48	0.51
1:H:187:LEU:C	1:H:187:LEU:HD12	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:187:LEU:HD12	1:P:187:LEU:C	2.31	0.51
1:R:28:ASP:C	1:R:28:ASP:OD1	2.48	0.51
1:J:187:LEU:HD12	1:J:187:LEU:C	2.31	0.51
1:L:28:ASP:OD1	1:L:28:ASP:C	2.48	0.51
1:6:28:ASP:C	1:6:28:ASP:OD1	2.48	0.51
1:B:28:ASP:OD1	1:B:28:ASP:C	2.48	0.51
1:X:28:ASP:OD1	1:X:28:ASP:C	2.48	0.51
1:L:187:LEU:C	1:L:187:LEU:HD12	2.31	0.50
1:D:187:LEU:C	1:D:187:LEU:HD12	2.31	0.50
1:F:187:LEU:HD12	1:F:187:LEU:C	2.31	0.50
1:D:28:ASP:C	1:D:28:ASP:OD1	2.48	0.50
1:V:28:ASP:C	1:V:28:ASP:OD1	2.48	0.50
1:Z:28:ASP:C	1:Z:28:ASP:OD1	2.48	0.50
1:N:187:LEU:HD12	1:N:187:LEU:C	2.31	0.50
1:F:78:PRO:HA	1:F:79:PRO:HD3	1.83	0.46
1:F:187:LEU:HD12	1:F:187:LEU:O	2.17	0.45
1:L:187:LEU:O	1:L:187:LEU:HD12	2.17	0.45
1:4:187:LEU:HD12	1:4:187:LEU:O	2.17	0.45
1:6:187:LEU:O	1:6:187:LEU:HD12	2.17	0.45
1:0:187:LEU:HD12	1:0:187:LEU:O	2.17	0.45
1:8:187:LEU:O	1:8:187:LEU:HD12	2.17	0.45
1:D:187:LEU:O	1:D:187:LEU:HD12	2.17	0.45
2:K:187:LEU:HD12	2:K:187:LEU:O	5.22	0.45
1:2:187:LEU:O	1:2:187:LEU:HD12	2.17	0.45
1:J:187:LEU:HD12	1:J:187:LEU:O	2.17	0.45
1:R:187:LEU:HD12	1:R:187:LEU:O	2.17	0.45
1:V:187:LEU:HD12	1:V:187:LEU:O	2.17	0.45
2:A:187:LEU:HD12	2:A:187:LEU:O	5.22	0.44
1:T:187:LEU:O	1:T:187:LEU:HD12	2.17	0.44
1:B:187:LEU:O	1:B:187:LEU:HD12	2.17	0.44
2:G:187:LEU:O	2:G:187:LEU:HD12	5.22	0.44
1:H:187:LEU:O	1:H:187:LEU:HD12	2.17	0.44
1:N:187:LEU:HD12	1:N:187:LEU:O	2.17	0.44
1:6:78:PRO:HA	1:6:79:PRO:HD3	1.83	0.44
1:D:78:PRO:HA	1:D:79:PRO:HD3	1.83	0.44
2:E:187:LEU:HD12	2:E:187:LEU:O	5.22	0.44
2:I:187:LEU:HD12	2:I:187:LEU:O	5.22	0.44
1:Z:187:LEU:HD12	1:Z:187:LEU:O	2.17	0.44
1:X:187:LEU:O	1:X:187:LEU:HD12	2.17	0.44
1:P:187:LEU:O	1:P:187:LEU:HD12	2.17	0.44
2:C:187:LEU:O	2:C:187:LEU:HD12	5.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:PRO:HA	1:B:79:PRO:HD3	1.82	0.43
1:6:62:GLU:HB3	1:6:63:PRO:HD3	2.01	0.43
1:8:62:GLU:HB3	1:8:63:PRO:HD3	2.01	0.43
1:H:78:PRO:HA	1:H:79:PRO:HD3	1.83	0.43
1:4:62:GLU:HB3	1:4:63:PRO:HD3	2.01	0.42
1:R:62:GLU:HB3	1:R:63:PRO:HD3	2.01	0.42
1:P:62:GLU:HB3	1:P:63:PRO:HD3	2.01	0.42
1:N:62:GLU:HB3	1:N:63:PRO:HD3	2.01	0.42
1:R:78:PRO:HA	1:R:79:PRO:HD3	1.83	0.42
1:0:62:GLU:HB3	1:0:63:PRO:HD3	2.01	0.42
1:J:62:GLU:HB3	1:J:63:PRO:HD3	2.01	0.42
1:L:62:GLU:HB3	1:L:63:PRO:HD3	2.01	0.42
1:T:62:GLU:HB3	1:T:63:PRO:HD3	2.01	0.42
1:2:62:GLU:HB3	1:2:63:PRO:HD3	2.01	0.42
1:V:62:GLU:HB3	1:V:63:PRO:HD3	2.01	0.42
1:H:62:GLU:HB3	1:H:63:PRO:HD3	2.01	0.42
1:F:62:GLU:HB3	1:F:63:PRO:HD3	2.01	0.42
1:0:78:PRO:HA	1:0:79:PRO:HD3	1.82	0.41
1:4:78:PRO:HA	1:4:79:PRO:HD3	1.82	0.41
1:X:62:GLU:HB3	1:X:63:PRO:HD3	2.01	0.41
1:D:62:GLU:HB3	1:D:63:PRO:HD3	2.01	0.41
1:B:62:GLU:HB3	1:B:63:PRO:HD3	2.01	0.41
1:Z:62:GLU:HB3	1:Z:63:PRO:HD3	2.01	0.41
1:V:78:PRO:HA	1:V:79:PRO:HD3	1.82	0.41

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 PDB entries followed by that with respect to all EM entries.

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	0	182/235 (77%)	175 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	4	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	6	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	8	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	B	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	D	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	F	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	H	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	J	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	L	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	N	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	P	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	R	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	T	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	V	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	X	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	Z	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	a	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	c	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	e	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	g	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	i	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
1	k	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	1	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	3	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	5	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	7	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	9	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	A	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	C	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	E	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	I	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	K	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	M	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	O	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	Q	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	S	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	U	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	W	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	Y	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	b	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	d	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	f	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	h	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	j	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
2	l	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	52
All	All	8976/11952 (75%)	8568 (96%)	312 (4%)	96 (1%)	23	64

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	251	ASP
2	3	251	ASP
2	5	251	ASP
2	7	251	ASP
2	9	251	ASP
2	A	251	ASP
2	C	251	ASP
2	E	251	ASP
2	G	251	ASP
2	I	251	ASP
2	K	251	ASP
2	M	251	ASP
2	O	251	ASP
2	Q	251	ASP
2	S	251	ASP

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Mol	Chain	Res	Type
2	U	251	ASP
2	W	251	ASP
2	Y	251	ASP
2	b	251	ASP
2	d	251	ASP
2	f	251	ASP
2	h	251	ASP
2	j	251	ASP
2	l	251	ASP
2	1	178	GLY
2	3	178	GLY
2	5	178	GLY
2	7	178	GLY
2	9	178	GLY
2	A	178	GLY
2	C	178	GLY
2	E	178	GLY
2	G	178	GLY
2	I	178	GLY
2	K	178	GLY
2	M	178	GLY
2	O	178	GLY
2	Q	178	GLY
2	S	178	GLY
2	U	178	GLY
2	W	178	GLY
2	Y	178	GLY
2	b	178	GLY
2	d	178	GLY
2	f	178	GLY
2	h	178	GLY
2	j	178	GLY
2	l	178	GLY
2	1	188	PRO
2	1	253	PRO
2	3	188	PRO
2	3	253	PRO
2	5	188	PRO
2	5	253	PRO
2	7	188	PRO
2	7	253	PRO
2	9	188	PRO

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Mol	Chain	Res	Type
2	9	253	PRO
2	A	188	PRO
2	A	253	PRO
2	C	188	PRO
2	C	253	PRO
2	E	188	PRO
2	E	253	PRO
2	G	188	PRO
2	G	253	PRO
2	I	188	PRO
2	I	253	PRO
2	K	188	PRO
2	K	253	PRO
2	M	188	PRO
2	M	253	PRO
2	O	188	PRO
2	O	253	PRO
2	Q	188	PRO
2	Q	253	PRO
2	S	188	PRO
2	S	253	PRO
2	U	188	PRO
2	U	253	PRO
2	W	188	PRO
2	W	253	PRO
2	Y	188	PRO
2	Y	253	PRO
2	b	188	PRO
2	b	253	PRO
2	d	188	PRO
2	d	253	PRO
2	f	188	PRO
2	f	253	PRO
2	h	188	PRO
2	h	253	PRO
2	j	188	PRO
2	j	253	PRO
2	l	188	PRO
2	l	253	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 PDB entries followed by that with respect to all EM entries.

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	0	157/200 (78%)	157 (100%)	0	100	100
1	2	157/200 (78%)	157 (100%)	0	100	100
1	4	157/200 (78%)	157 (100%)	0	100	100
1	6	157/200 (78%)	157 (100%)	0	100	100
1	8	157/200 (78%)	157 (100%)	0	100	100
1	B	157/200 (78%)	157 (100%)	0	100	100
1	D	157/200 (78%)	157 (100%)	0	100	100
1	F	157/200 (78%)	157 (100%)	0	100	100
1	H	157/200 (78%)	157 (100%)	0	100	100
1	J	157/200 (78%)	157 (100%)	0	100	100
1	L	157/200 (78%)	157 (100%)	0	100	100
1	N	157/200 (78%)	157 (100%)	0	100	100
1	P	157/200 (78%)	157 (100%)	0	100	100
1	R	157/200 (78%)	157 (100%)	0	100	100
1	T	157/200 (78%)	157 (100%)	0	100	100
1	V	157/200 (78%)	157 (100%)	0	100	100
1	X	157/200 (78%)	157 (100%)	0	100	100
1	Z	157/200 (78%)	157 (100%)	0	100	100
1	a	157/200 (78%)	157 (100%)	0	100	100
1	c	157/200 (78%)	157 (100%)	0	100	100
1	e	157/200 (78%)	157 (100%)	0	100	100
1	g	157/200 (78%)	157 (100%)	0	100	100
1	i	157/200 (78%)	157 (100%)	0	100	100
1	k	157/200 (78%)	157 (100%)	0	100	100
2	1	167/221 (76%)	167 (100%)	0	100	100
2	3	167/221 (76%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	5	167/221 (76%)	167 (100%)	0	100	100
2	7	167/221 (76%)	167 (100%)	0	100	100
2	9	167/221 (76%)	167 (100%)	0	100	100
2	A	167/221 (76%)	167 (100%)	0	100	100
2	C	167/221 (76%)	167 (100%)	0	100	100
2	E	167/221 (76%)	167 (100%)	0	100	100
2	G	167/221 (76%)	167 (100%)	0	100	100
2	I	167/221 (76%)	167 (100%)	0	100	100
2	K	167/221 (76%)	167 (100%)	0	100	100
2	M	167/221 (76%)	167 (100%)	0	100	100
2	O	167/221 (76%)	167 (100%)	0	100	100
2	Q	167/221 (76%)	167 (100%)	0	100	100
2	S	167/221 (76%)	167 (100%)	0	100	100
2	U	167/221 (76%)	167 (100%)	0	100	100
2	W	167/221 (76%)	167 (100%)	0	100	100
2	Y	167/221 (76%)	167 (100%)	0	100	100
2	b	167/221 (76%)	167 (100%)	0	100	100
2	d	167/221 (76%)	167 (100%)	0	100	100
2	f	167/221 (76%)	167 (100%)	0	100	100
2	h	167/221 (76%)	167 (100%)	0	100	100
2	j	167/221 (76%)	167 (100%)	0	100	100
2	l	167/221 (76%)	167 (100%)	0	100	100
All	All	7776/10104 (77%)	7776 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 carbohydrates 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.