



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 4, 2017 – 03:17 AM EST

PDB ID : 5TCR  
EMDB ID: : EMD-8400  
Title : Atomic model of the Salmonella SPI-1 type III secretion injectisome basal body proteins InvG, 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 : 6.30 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](mailto: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.

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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

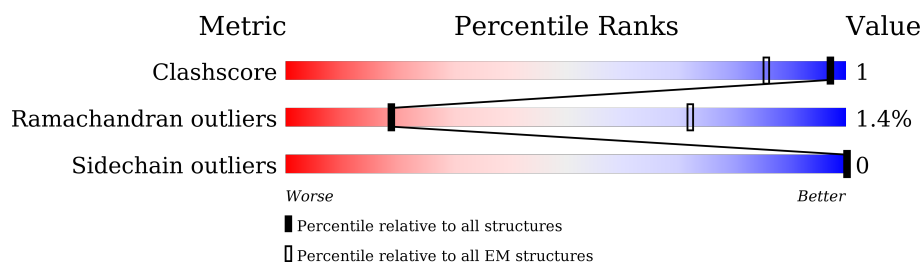
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.30 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  $\geq 3$ , 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	A	562	81% 16%
1	B	562	81% 16%
1	C	562	81% 16%
1	D	562	81% 16%
1	E	562	81% 16%
1	F	562	81% 16%
1	G	562	81% 16%
1	H	562	81% 16%
1	I	562	81% 16%


























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Mol	Chain	Length	Quality of chain
1	J	562	 81% 16%
1	K	562	 81% 16%
1	L	562	 81% 16%
1	M	562	 81% 16%
1	N	562	 81% 16%
1	O	562	 81% 16%
2	1	235	 76% 22%
2	3	235	 76% 22%
2	5	235	 76% 22%
2	7	235	 75% 22%
2	9	235	 75% 22%
2	P	235	 75% 22%
2	R	235	 76% 22%
2	T	235	 75% 22%
2	V	235	 75% 22%
2	X	235	 76% 22%
2	a	235	 77% 22%
2	c	235	 78% 22%
2	e	235	 78% 22%
2	g	235	 78% 22%
2	i	235	 78% 22%
2	k	235	 78% 22%
2	m	235	 78% 22%
2	o	235	 78% 22%
2	q	235	 78% 22%

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Mol	Chain	Length	Quality of chain	
2	s	235		78% 22%
2	u	235		78% 22%
2	w	235		78% 22%
2	y	235		78% 22%
2	z	235		78% 22%
3	0	263		72% 26%
3	10	263		72% 26%
3	2	263		72% 26%
3	4	263		72% 26%
3	6	263		72% 26%
3	8	263		72% 26%
3	Q	263		71% 26%
3	S	263		71% 26%
3	U	263		71% 26%
3	W	263		71% 26%
3	Y	263		71% 26%
3	Z	263		71% 26%
3	b	263		72% 26%
3	d	263		72% 26%
3	f	263		72% 26%
3	h	263		72% 26%
3	j	263		72% 26%
3	l	263		72% 26%
3	n	263		72% 26%
3	p	263		72% 26%

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Mol	Chain	Length	Quality of chain
3	r	263	<div><div></div><div>72%</div><div></div><div>•</div><div>26%</div></div>
3	t	263	<div><div></div><div>72%</div><div></div><div>•</div><div>26%</div></div>
3	v	263	<div><div></div><div>72%</div><div></div><div>•</div><div>26%</div></div>
3	x	263	<div><div></div><div>72%</div><div></div><div>•</div><div>26%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 128658 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 Protein InvG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	B	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	C	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	D	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	E	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	F	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	G	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	H	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	I	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	J	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	K	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	L	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	M	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	N	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		
1	O	474	Total	C	N	O	S	0	0
			3718	2357	645	704	12		

- Molecule 2 is a protein called Lipoprotein PrgK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	R	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	T	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	V	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	X	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	a	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	c	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	e	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	g	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	i	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	k	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	m	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	o	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	q	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	s	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	u	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	w	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	y	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	z	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	1	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	3	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	5	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		
2	9	184	Total	C	N	O	S	0	0
			1437	905	250	279	3		

- Molecule 3 is a protein called Protein PrgH.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	S	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	U	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	W	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	Y	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	Z	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	b	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	d	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	f	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	h	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	j	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	l	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	n	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	p	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	r	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	t	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		
3	v	194	Total	C	N	O	S	0	0
			1600	1011	288	297	4		

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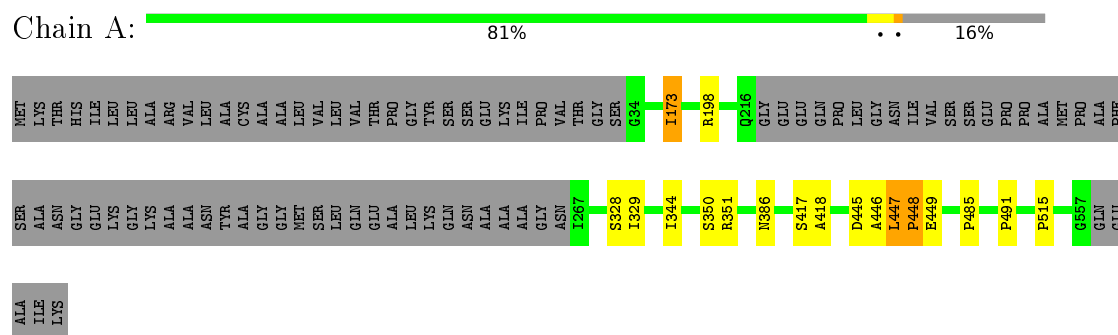
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	x	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	0	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	2	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	4	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	6	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	8	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	10	194	Total 1600	C 1011	N 288	O 297	S 4	0	0

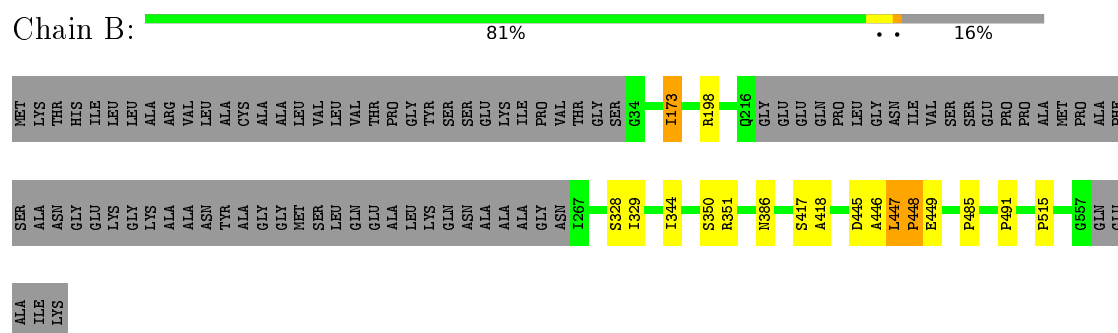
### 3 Residue-property plots [i](#)

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.

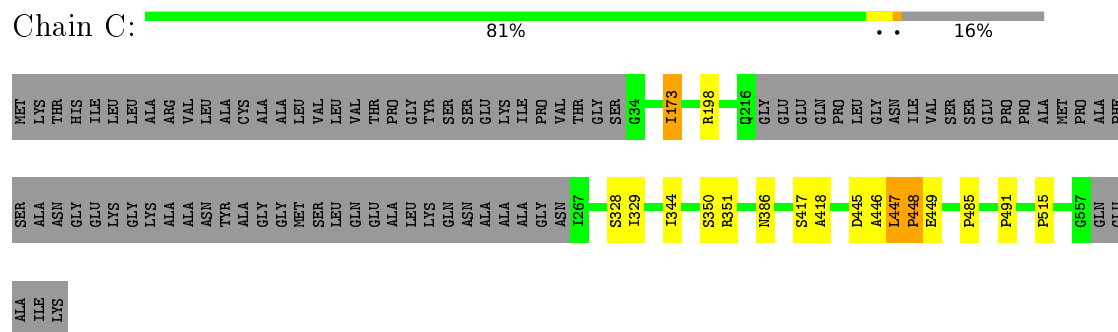
- Molecule 1: Protein InvG



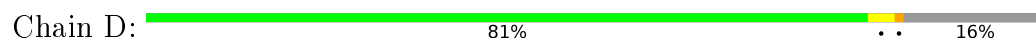
- Molecule 1: Protein InvG

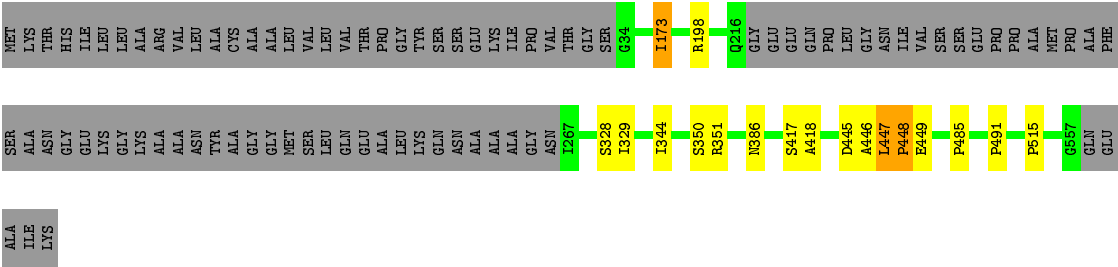


- Molecule 1: Protein InvG

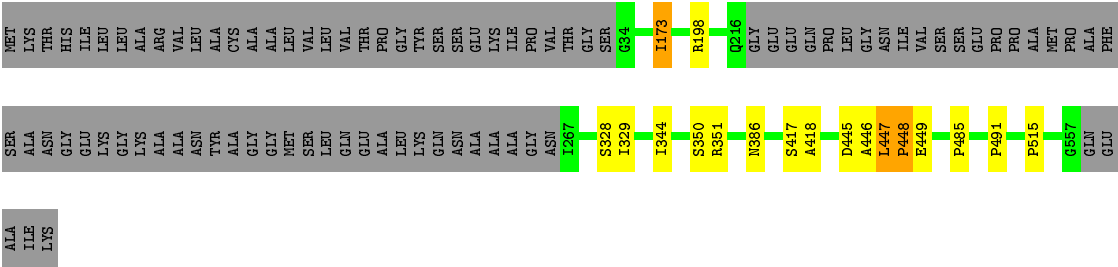
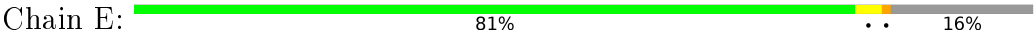


- Molecule 1: Protein InvG

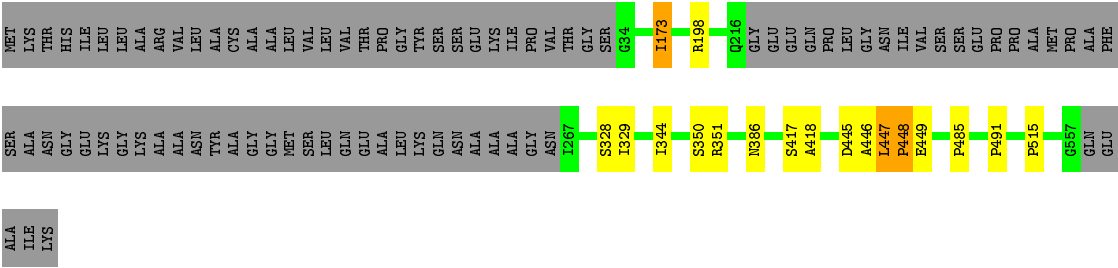
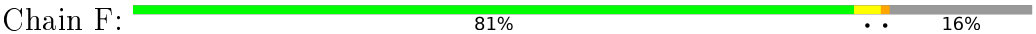




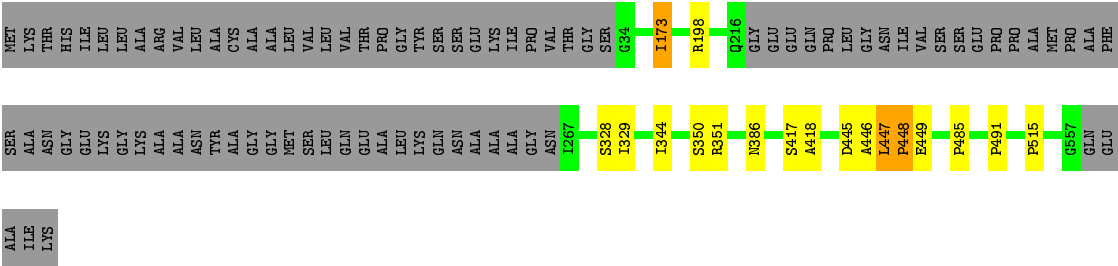
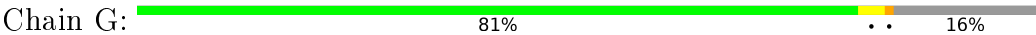
• Molecule 1: Protein InvG



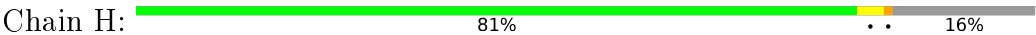
• Molecule 1: Protein InvG

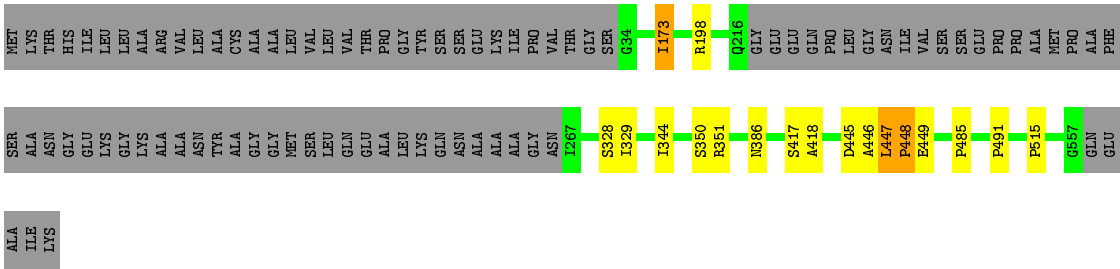


• Molecule 1: Protein InvG



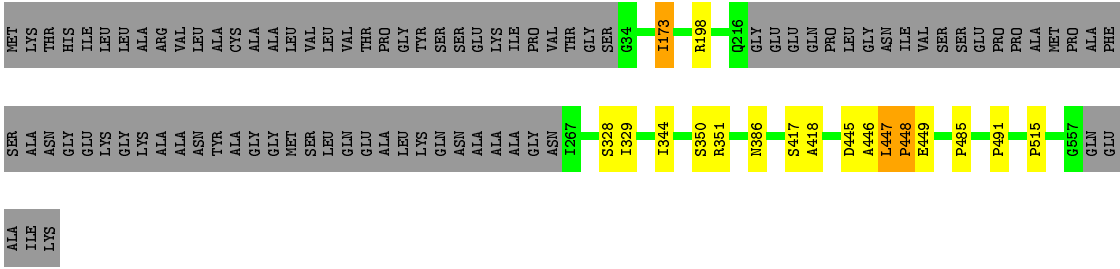
• Molecule 1: Protein InvG





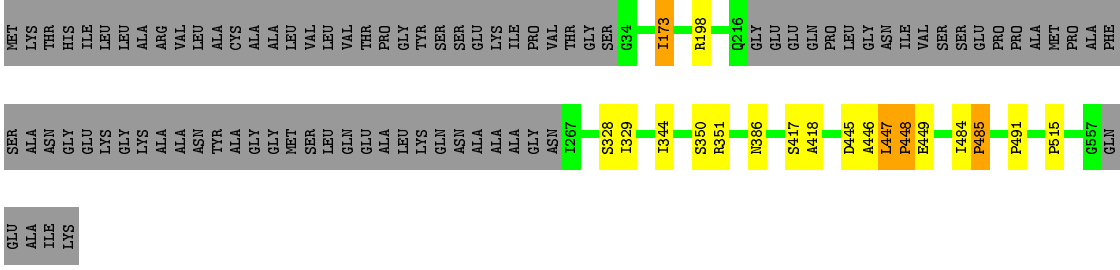
• Molecule 1: Protein InvG

Chain I: 81% 16%



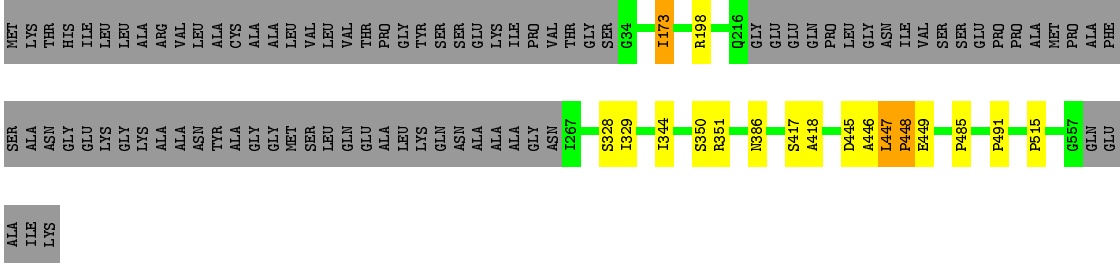
• Molecule 1: Protein InvG

Chain J: 81% 16%



• Molecule 1: Protein InvG

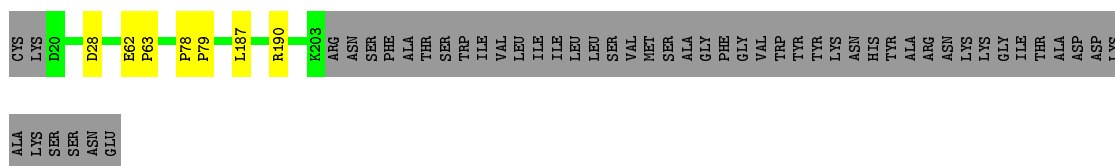
Chain K: 81% 16%



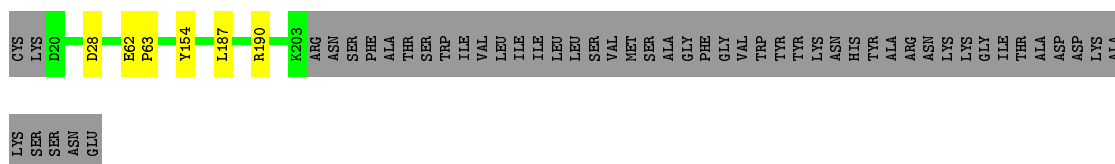
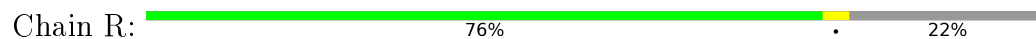
• Molecule 1: Protein InvG

Chain L: 81% 16%

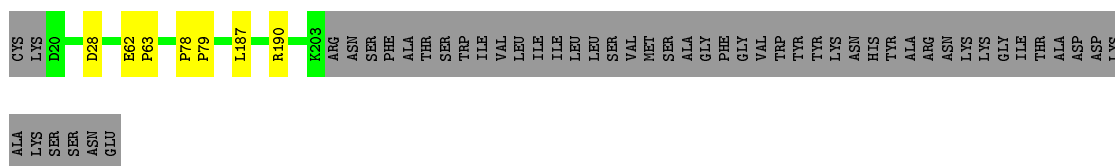
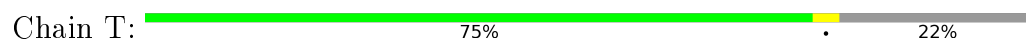




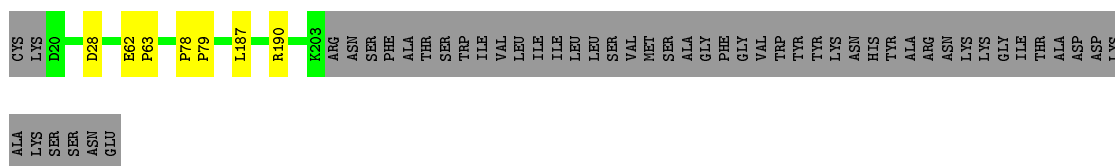
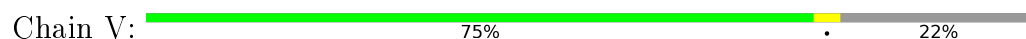
- Molecule 2: Lipoprotein PrgK



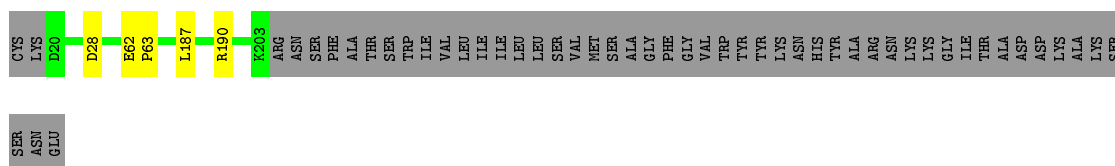
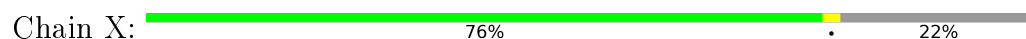
- Molecule 2: Lipoprotein PrgK



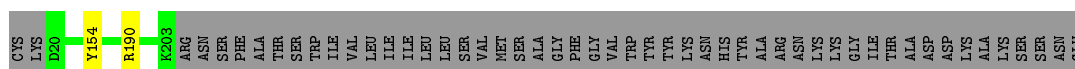
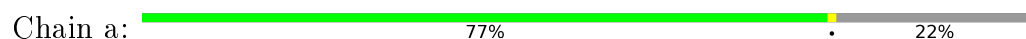
- Molecule 2: Lipoprotein PrgK




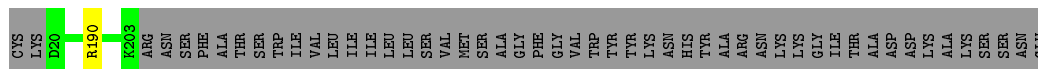
- Molecule 2: Lipoprotein PrgK




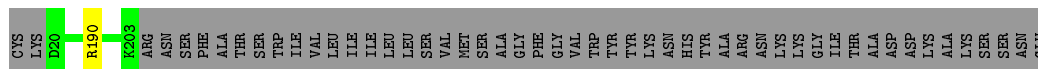
- Molecule 2: Lipoprotein PrgK




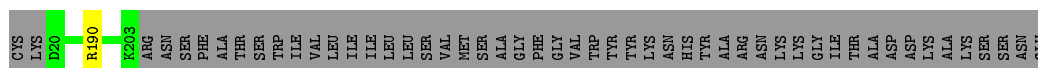
## ● Molecule 2: Lipoprotein PrgK

Chain c:  78% 22%


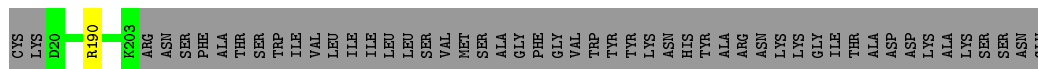
## ● Molecule 2: Lipoprotein PrgK

Chain e:  78% 22%


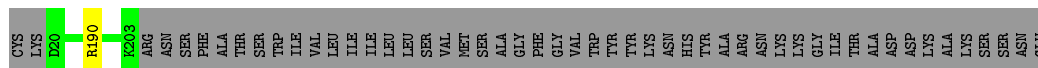
## ● Molecule 2: Lipoprotein PrgK

Chain g:  78% 22%


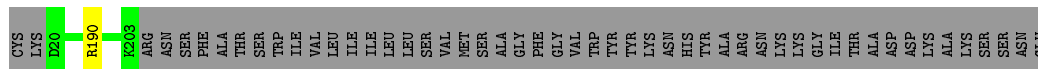
## ● Molecule 2: Lipoprotein PrgK

Chain i:  78% 22%


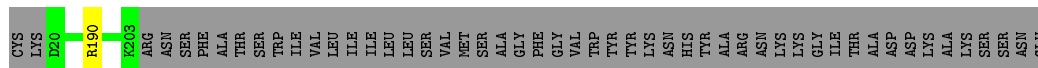
## ● Molecule 2: Lipoprotein PrgK

Chain k:  78% 22%


## ● Molecule 2: Lipoprotein PrgK

Chain m:  78% 22%

## ● Molecule 2: Lipoprotein PrgK


Chain o:  78% 22%

## ● Molecule 2: Lipoprotein PrgK

Chain q:  78% 22%


CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK

Chain s:  78% 22%


CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK

Chain u:  78% 22%


CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK

Chain w:  78% 22%


CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK

Chain y:  78% 22%


CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK

Chain z:  78% 22%

CYS LYS D20 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

- Molecule 2: Lipoprotein PrgK


Chain 1:  76% 22%

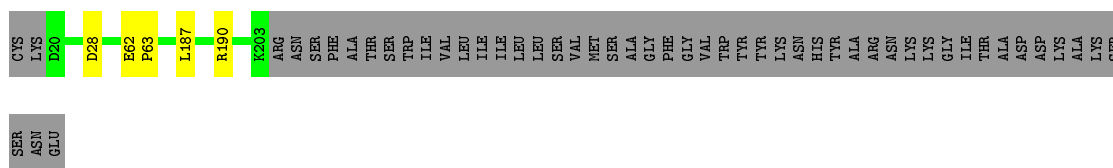
CYS LYS D20 D28 E82 P63 L187 R190 K203 ARG ASN SER SER PHE ALA THR SER TRP VAL LEU LEU ILE ILE LEU LEU SER SER VAL MET SER SER ALA ALA GLY PHE GLY VAL TRP TYR TYR LYS LYS ASN ASN HIS TYR ALA ARG ASN ASN LYS LYS ILE THR THR ASP ASP LYS ALA LYS SER SER ASN GLU

SER  
ASN  
GLU


- Molecule 2: Lipoprotein PrgK

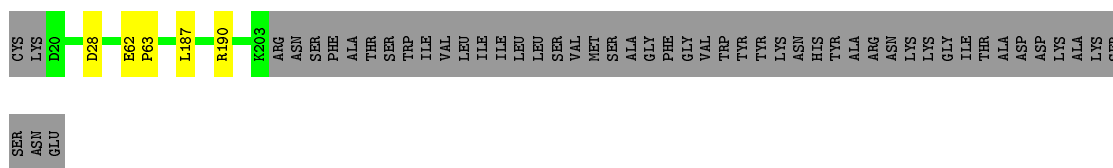


Chain 3:  76% 22%




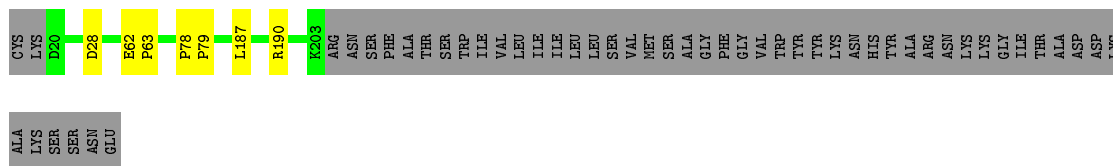
- Molecule 2: Lipoprotein PrgK

Chain 5:  76% 22%




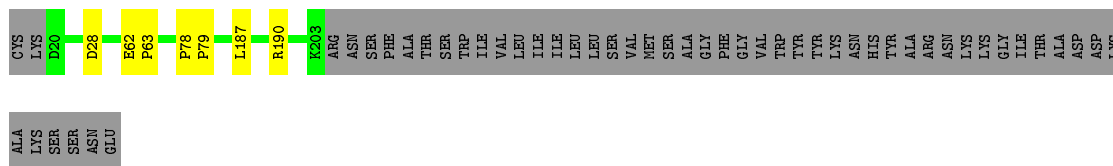
- Molecule 2: Lipoprotein PrgK

Chain 7:  75% 22%



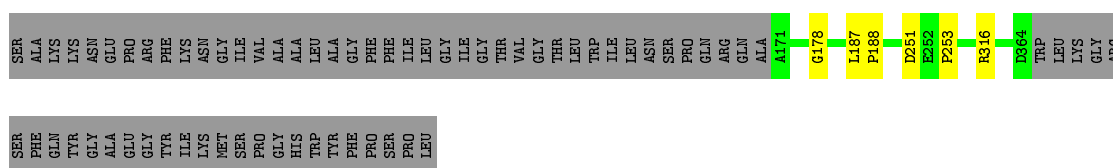
- Molecule 2: Lipoprotein PrgK

Chain 9:  75% 22%



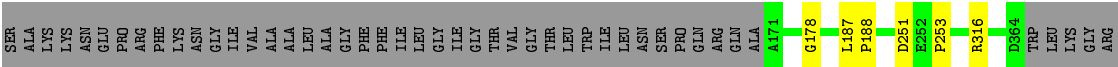
- Molecule 3: Protein PrgH

Chain Q:  71% 26%

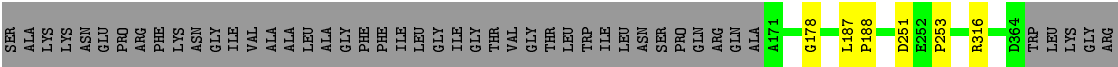


- Molecule 3: Protein PrgH

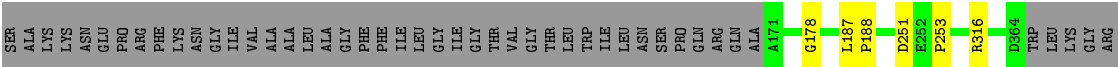
Chain S:  71% 26%



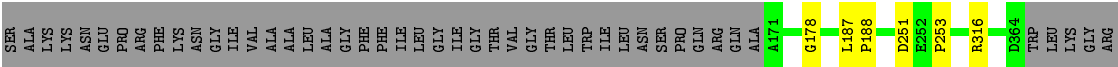
● Molecule 3: Protein PrgH



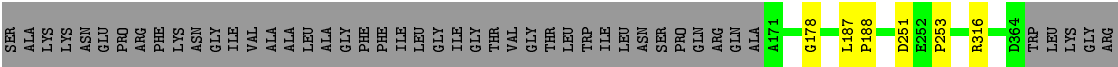
● Molecule 3: Protein PrgH



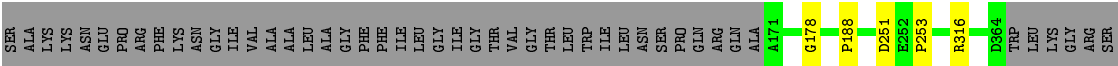
● Molecule 3: Protein PrgH



● Molecule 3: Protein PrgH



● Molecule 3: Protein PrgH



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• Molecule 3: Protein PrgH



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• Molecule 3: Protein PrgH



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• Molecule 3: Protein PrgH



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• Molecule 3: Protein PrgH



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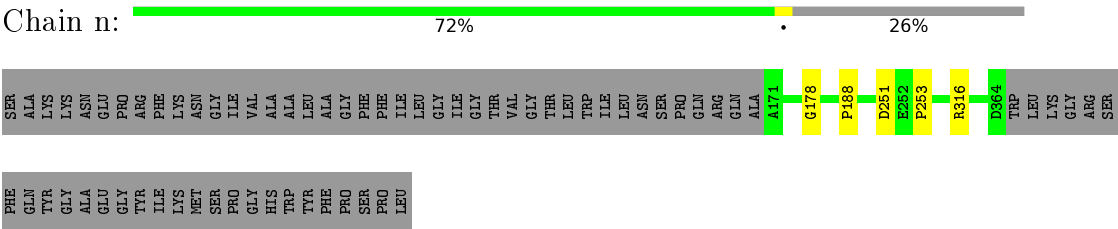
• Molecule 3: Protein PrgH



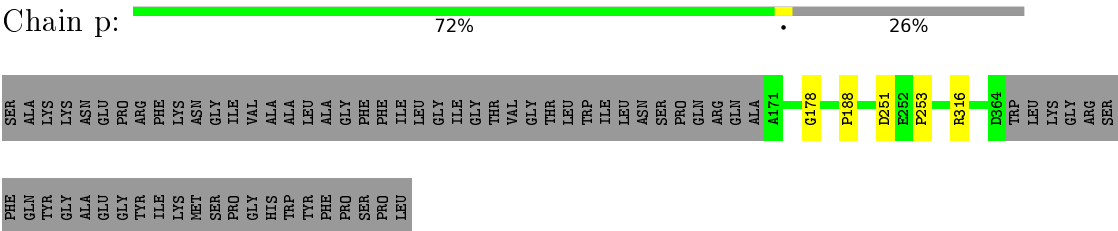
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VAL  
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GLN  
ALA  
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PRO  
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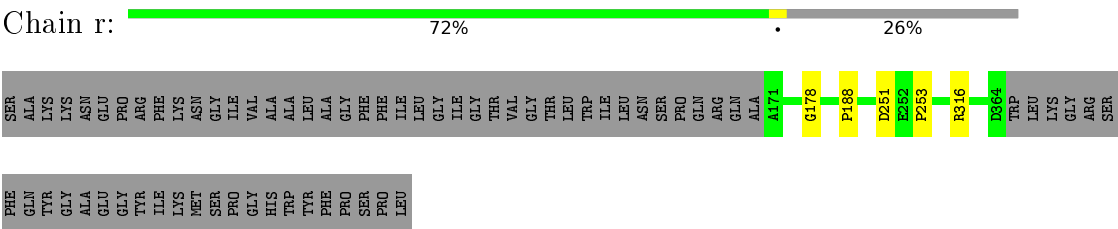
• Molecule 3: Protein PrgH



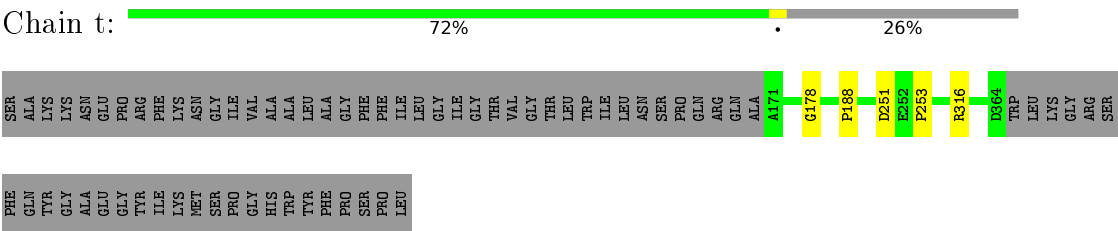
• Molecule 3: Protein PrgH



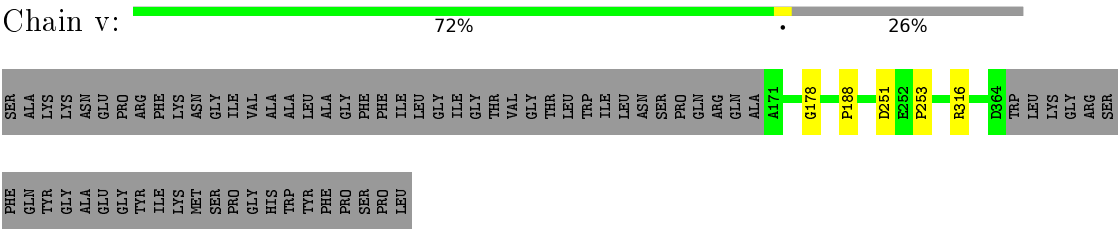
• Molecule 3: Protein PrgH




• Molecule 3: Protein PrgH



• Molecule 3: Protein PrgH



• Molecule 3: Protein PrgH

Chain x:  72% 26%

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

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

• Molecule 3: Protein PrgH

Chain 0:  72% 26%

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

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

• Molecule 3: Protein PrgH

Chain 2:  72% 26%

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

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

• Molecule 3: Protein PrgH

Chain 4:  72% 26%

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

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

• Molecule 3: Protein PrgH

Chain 6:  72% 26%

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

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

• Molecule 3: Protein PrgH

Chain 8:  72% 26%

SER	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ILE	VAL	ALA	LEU	ALA	GLY	PHE	PHE	ILE	LEU	GLY	ILE	GLY	THR	VAL	GLY	THR	LEU	TRP	ILE	LEU	ASN	SER	PRO	GLN	ARG	GLN	ALA	A171	G178	P188	D251	E252	P253	R316	D364	TRP	LEU	LYS	GLY	ARG	SER
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PHE	GLN	TYR	GLY	ALA	GLU	GLY	TYR	ILE	LYS	MET	ASN	SER	PRO	ILE	GLY	HIS	TRP	TYR	PHE	PRO	SER	PRO	LEU
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● Molecule 3: Protein PrgH



SER	ALA	LYS	ASN	GLU	PRO	ARG	PHE	LYS	ASN	GLY	ILE	VAL	ALA	LEU	ALA	GLY	PHE	PHE	ILE	LEU	GLY	ILE	GLY	THR	VAL	GLY	THR	LEU	TRP	ILE	LEU	ASN	SER	PRO	GLN	ARG	GLN	ALA	A171	G178	P188	D251	E252	P253	R316	D364	TRP	LEU	LYS	GLY	ARG	SER
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PHE	GLN	TYR	GLY	ALA	GLU	GLY	TYR	ILE	LYS	MET	ASN	SER	PRO	ILE	GLY	HIS	TRP	TYR	PHE	PRO	SER	PRO	LEU
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## 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	A	0.75	0/3780	0.69	0/5115
1	B	0.75	0/3780	0.69	0/5115
1	C	0.75	0/3780	0.69	0/5115
1	D	0.75	0/3780	0.69	0/5115
1	E	0.75	0/3780	0.69	0/5115
1	F	0.75	0/3780	0.69	0/5115
1	G	0.75	0/3780	0.69	0/5115
1	H	0.75	0/3780	0.69	0/5115
1	I	0.75	0/3780	0.69	0/5115
1	J	0.75	0/3780	0.69	0/5115
1	K	0.75	0/3780	0.69	0/5115
1	L	0.75	0/3780	0.69	0/5115
1	M	0.75	0/3780	0.69	0/5115
1	N	0.75	0/3780	0.69	0/5115
1	O	0.75	0/3780	0.69	0/5115
2	1	0.77	0/1465	0.68	1/1989 (0.1%)
2	3	0.77	0/1465	0.68	1/1989 (0.1%)
2	5	0.77	0/1465	0.68	1/1989 (0.1%)
2	7	0.77	0/1465	0.68	1/1989 (0.1%)
2	9	0.77	0/1465	0.68	1/1989 (0.1%)
2	P	0.77	0/1465	0.68	1/1989 (0.1%)
2	R	0.77	0/1465	0.68	2/1989 (0.1%)
2	T	0.77	0/1465	0.68	1/1989 (0.1%)
2	V	0.77	0/1465	0.68	1/1989 (0.1%)
2	X	0.77	0/1465	0.68	1/1989 (0.1%)
2	a	0.77	0/1465	0.68	2/1989 (0.1%)
2	c	0.77	0/1465	0.68	1/1989 (0.1%)
2	e	0.77	0/1465	0.68	1/1989 (0.1%)
2	g	0.77	0/1465	0.68	1/1989 (0.1%)
2	i	0.77	0/1465	0.68	1/1989 (0.1%)
2	k	0.77	0/1465	0.68	1/1989 (0.1%)
2	m	0.77	0/1465	0.68	1/1989 (0.1%)
2	o	0.77	0/1465	0.68	1/1989 (0.1%)
2	q	0.77	0/1465	0.68	1/1989 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	s	0.77	0/1465	0.68	1/1989 (0.1%)
2	u	0.77	0/1465	0.68	1/1989 (0.1%)
2	w	0.77	0/1465	0.68	1/1989 (0.1%)
2	y	0.77	0/1465	0.68	1/1989 (0.1%)
2	z	0.77	0/1465	0.68	1/1989 (0.1%)
3	0	0.77	0/1632	0.70	1/2204 (0.0%)
3	10	0.77	0/1632	0.70	1/2204 (0.0%)
3	2	0.77	0/1632	0.70	1/2204 (0.0%)
3	4	0.77	0/1632	0.70	1/2204 (0.0%)
3	6	0.77	0/1632	0.70	1/2204 (0.0%)
3	8	0.77	0/1632	0.70	1/2204 (0.0%)
3	Q	0.77	0/1632	0.70	1/2204 (0.0%)
3	S	0.77	0/1632	0.70	1/2204 (0.0%)
3	U	0.77	0/1632	0.71	1/2204 (0.0%)
3	W	0.77	0/1632	0.70	1/2204 (0.0%)
3	Y	0.77	0/1632	0.70	1/2204 (0.0%)
3	Z	0.77	0/1632	0.70	1/2204 (0.0%)
3	b	0.77	0/1632	0.70	1/2204 (0.0%)
3	d	0.77	0/1632	0.70	1/2204 (0.0%)
3	f	0.77	0/1632	0.71	1/2204 (0.0%)
3	h	0.77	0/1632	0.70	1/2204 (0.0%)
3	j	0.77	0/1632	0.70	1/2204 (0.0%)
3	l	0.77	0/1632	0.70	1/2204 (0.0%)
3	n	0.77	0/1632	0.70	1/2204 (0.0%)
3	p	0.77	0/1632	0.70	1/2204 (0.0%)
3	r	0.77	0/1632	0.70	1/2204 (0.0%)
3	t	0.77	0/1632	0.70	1/2204 (0.0%)
3	v	0.77	0/1632	0.70	1/2204 (0.0%)
3	x	0.77	0/1632	0.70	1/2204 (0.0%)
All	All	0.76	0/131028	0.69	50/177357 (0.0%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	y	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	T	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	m	190	ARG	NE-CZ-NH2	-5.78	117.41	120.30
2	o	190	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	3	190	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	c	190	ARG	NE-CZ-NH2	-5.73	117.43	120.30
2	w	190	ARG	NE-CZ-NH2	-5.73	117.44	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	s	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	u	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	z	190	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	R	190	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	1	190	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	q	190	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	5	190	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	V	190	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	g	190	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	e	190	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	k	190	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	a	190	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	i	190	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	7	190	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	P	190	ARG	NE-CZ-NH2	-5.59	117.51	120.30
2	X	190	ARG	NE-CZ-NH2	-5.58	117.51	120.30
3	Y	316	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	n	316	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	b	316	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	p	316	ARG	NE-CZ-NH2	-5.33	117.64	120.30
3	x	316	ARG	NE-CZ-NH2	-5.33	117.64	120.30
3	j	316	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	U	316	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	6	316	ARG	NE-CZ-NH2	-5.30	117.65	120.30
3	S	316	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	f	316	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	0	316	ARG	NE-CZ-NH2	-5.29	117.66	120.30
3	2	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	10	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	r	316	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	l	316	ARG	NE-CZ-NH2	-5.27	117.67	120.30
3	W	316	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	Z	316	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	4	316	ARG	NE-CZ-NH2	-5.24	117.68	120.30
3	t	316	ARG	NE-CZ-NH2	-5.23	117.68	120.30
3	8	316	ARG	NE-CZ-NH2	-5.23	117.68	120.30
3	v	316	ARG	NE-CZ-NH2	-5.22	117.69	120.30
3	d	316	ARG	NE-CZ-NH2	-5.21	117.69	120.30
3	Q	316	ARG	NE-CZ-NH2	-5.21	117.70	120.30
3	h	316	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	a	154	TYR	CB-CG-CD2	-5.03	117.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	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	A	3718	0	3777	8	0
1	B	3718	0	3777	8	0
1	C	3718	0	3777	8	0
1	D	3718	0	3777	8	0
1	E	3718	0	3777	8	0
1	F	3718	0	3777	8	0
1	G	3718	0	3777	8	0
1	H	3718	0	3777	8	0
1	I	3718	0	3777	8	0
1	J	3718	0	3777	9	0
1	K	3718	0	3777	8	0
1	L	3718	0	3777	8	0
1	M	3718	0	3777	8	0
1	N	3718	0	3777	9	0
1	O	3718	0	3777	8	0
2	1	1437	0	1434	4	0
2	3	1437	0	1434	4	0
2	5	1437	0	1434	4	0
2	7	1437	0	1434	5	0
2	9	1437	0	1434	5	0
2	P	1437	0	1434	5	0
2	R	1437	0	1434	4	0
2	T	1437	0	1434	5	0
2	V	1437	0	1434	5	0
2	X	1437	0	1434	4	0
2	a	1437	0	1434	0	0
2	c	1437	0	1434	0	0
2	e	1437	0	1434	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g	1437	0	1434	0	0
2	i	1437	0	1434	0	0
2	k	1437	0	1434	0	0
2	m	1437	0	1434	0	0
2	o	1437	0	1434	0	0
2	q	1437	0	1434	0	0
2	s	1437	0	1434	0	0
2	u	1437	0	1434	0	0
2	w	1437	0	1434	0	0
2	y	1437	0	1434	0	0
2	z	1437	0	1434	0	0
3	0	1600	0	1580	0	0
3	10	1600	0	1580	0	0
3	2	1600	0	1580	0	0
3	4	1600	0	1580	0	0
3	6	1600	0	1580	0	0
3	8	1600	0	1580	0	0
3	Q	1600	0	1580	2	0
3	S	1600	0	1580	2	0
3	U	1600	0	1580	2	0
3	W	1600	0	1580	2	0
3	Y	1600	0	1580	2	0
3	Z	1600	0	1580	2	0
3	b	1600	0	1580	0	0
3	d	1600	0	1580	0	0
3	f	1600	0	1580	0	0
3	h	1600	0	1580	0	0
3	j	1600	0	1580	0	0
3	l	1600	0	1580	0	0
3	n	1600	0	1580	0	0
3	p	1600	0	1580	0	0
3	r	1600	0	1580	0	0
3	t	1600	0	1580	0	0
3	v	1600	0	1580	0	0
3	x	1600	0	1580	0	0
All	All	128658	0	128991	179	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 (179) 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:E:173:ILE:HG22	1:E:173:ILE:O	1.92	0.70
1:H:173:ILE:HG22	1:H:173:ILE:O	1.92	0.70
1:I:173:ILE:HG22	1:I:173:ILE:O	1.92	0.70
1:D:173:ILE:O	1:D:173:ILE:HG22	1.92	0.70
1:F:173:ILE:HG22	1:F:173:ILE:O	1.92	0.69
1:G:173:ILE:HG22	1:G:173:ILE:O	1.91	0.69
1:A:173:ILE:HG22	1:A:173:ILE:O	1.91	0.69
1:B:173:ILE:O	1:B:173:ILE:HG22	1.91	0.69
1:L:173:ILE:HG22	1:L:173:ILE:O	1.92	0.69
1:O:173:ILE:O	1:O:173:ILE:HG22	1.91	0.69
1:J:173:ILE:HG22	1:J:173:ILE:O	1.92	0.69
1:M:173:ILE:HG22	1:M:173:ILE:O	1.92	0.69
1:K:173:ILE:O	1:K:173:ILE:HG22	1.92	0.69
1:N:173:ILE:O	1:N:173:ILE:HG22	1.92	0.69
1:C:173:ILE:O	1:C:173:ILE:HG22	1.92	0.68
2:X:28:ASP:OD1	2:X:28:ASP:C	2.48	0.52
2:5:28:ASP:C	2:5:28:ASP:OD1	2.48	0.52
2:3:28:ASP:OD1	2:3:28:ASP:C	2.48	0.52
2:9:187:LEU:HD12	2:9:187:LEU:C	2.31	0.52
2:R:187:LEU:HD12	2:R:187:LEU:C	2.31	0.52
3:Q:187:LEU:HD12	3:Q:187:LEU:C	4.98	0.51
3:Y:187:LEU:C	3:Y:187:LEU:HD12	4.98	0.51
2:T:187:LEU:HD12	2:T:187:LEU:C	2.31	0.51
2:3:187:LEU:C	2:3:187:LEU:HD12	2.31	0.51
2:5:187:LEU:C	2:5:187:LEU:HD12	2.31	0.51
2:P:187:LEU:HD12	2:P:187:LEU:C	2.31	0.51
3:S:187:LEU:C	3:S:187:LEU:HD12	4.99	0.51
2:V:187:LEU:HD12	2:V:187:LEU:C	2.31	0.51
2:X:187:LEU:C	2:X:187:LEU:HD12	2.31	0.51
2:7:187:LEU:C	2:7:187:LEU:HD12	2.31	0.51
3:U:187:LEU:C	3:U:187:LEU:HD12	4.98	0.51
3:W:187:LEU:C	3:W:187:LEU:HD12	4.98	0.51
3:Z:187:LEU:C	3:Z:187:LEU:HD12	4.98	0.51
2:1:187:LEU:C	2:1:187:LEU:HD12	2.31	0.51
2:7:28:ASP:C	2:7:28:ASP:OD1	2.48	0.51
2:P:28:ASP:OD1	2:P:28:ASP:C	2.48	0.51
2:R:28:ASP:OD1	2:R:28:ASP:C	2.48	0.51
2:T:28:ASP:OD1	2:T:28:ASP:C	2.48	0.51
2:1:28:ASP:C	2:1:28:ASP:OD1	2.48	0.51
2:V:28:ASP:C	2:V:28:ASP:OD1	2.48	0.51
2:9:28:ASP:OD1	2:9:28:ASP:C	2.48	0.50
1:A:328:SER:OG	1:A:329:ILE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:OG	1:B:329:ILE:N	2.45	0.49
1:O:328:SER:OG	1:O:329:ILE:N	2.45	0.49
1:C:328:SER:OG	1:C:329:ILE:N	2.46	0.49
1:J:328:SER:OG	1:J:329:ILE:N	2.45	0.49
1:K:328:SER:OG	1:K:329:ILE:N	2.45	0.49
1:N:328:SER:OG	1:N:329:ILE:N	2.45	0.49
1:L:386:ASN:C	1:L:386:ASN:OD1	2.51	0.49
1:F:328:SER:OG	1:F:329:ILE:N	2.45	0.49
1:J:386:ASN:OD1	1:J:386:ASN:C	2.51	0.49
1:N:386:ASN:C	1:N:386:ASN:OD1	2.51	0.49
1:I:328:SER:OG	1:I:329:ILE:N	2.45	0.49
1:L:328:SER:OG	1:L:329:ILE:N	2.45	0.49
1:A:386:ASN:OD1	1:A:386:ASN:C	2.51	0.48
1:M:328:SER:OG	1:M:329:ILE:N	2.45	0.48
1:D:328:SER:OG	1:D:329:ILE:N	2.45	0.48
1:E:328:SER:OG	1:E:329:ILE:N	2.45	0.48
1:O:386:ASN:C	1:O:386:ASN:OD1	2.51	0.48
1:M:386:ASN:C	1:M:386:ASN:OD1	2.51	0.48
1:B:386:ASN:C	1:B:386:ASN:OD1	2.51	0.48
1:K:386:ASN:C	1:K:386:ASN:OD1	2.51	0.48
1:H:328:SER:OG	1:H:329:ILE:N	2.45	0.47
1:I:386:ASN:OD1	1:I:386:ASN:C	2.51	0.47
1:G:328:SER:OG	1:G:329:ILE:N	2.45	0.47
1:D:386:ASN:C	1:D:386:ASN:OD1	2.52	0.47
1:C:386:ASN:C	1:C:386:ASN:OD1	2.51	0.47
1:G:386:ASN:OD1	1:G:386:ASN:C	2.52	0.47
1:F:386:ASN:OD1	1:F:386:ASN:C	2.51	0.47
1:E:386:ASN:C	1:E:386:ASN:OD1	2.51	0.46
1:H:386:ASN:OD1	1:H:386:ASN:C	2.51	0.46
2:T:187:LEU:HD12	2:T:187:LEU:O	2.17	0.45
2:V:187:LEU:HD12	2:V:187:LEU:O	2.17	0.45
2:P:187:LEU:HD12	2:P:187:LEU:O	2.17	0.45
2:X:187:LEU:O	2:X:187:LEU:HD12	2.17	0.45
2:9:187:LEU:HD12	2:9:187:LEU:O	2.17	0.45
2:R:187:LEU:O	2:R:187:LEU:HD12	2.17	0.45
1:A:447:LEU:N	1:A:448:PRO:CD	2.81	0.45
1:O:447:LEU:N	1:O:448:PRO:CD	2.80	0.45
3:Q:187:LEU:HD12	3:Q:187:LEU:O	5.22	0.45
3:U:187:LEU:HD12	3:U:187:LEU:O	5.22	0.45
1:B:447:LEU:N	1:B:448:PRO:CD	2.80	0.44
3:S:187:LEU:O	3:S:187:LEU:HD12	5.22	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:187:LEU:O	3:Z:187:LEU:HD12	5.22	0.44
2:5:187:LEU:O	2:5:187:LEU:HD12	2.17	0.44
1:N:447:LEU:N	1:N:448:PRO:CD	2.80	0.44
2:3:187:LEU:O	2:3:187:LEU:HD12	2.17	0.44
2:V:78:PRO:HA	2:V:79:PRO:HD3	1.83	0.44
1:K:447:LEU:N	1:K:448:PRO:CD	2.80	0.44
2:7:187:LEU:HD12	2:7:187:LEU:O	2.17	0.44
1:C:447:LEU:N	1:C:448:PRO:CD	2.80	0.44
1:J:447:LEU:N	1:J:448:PRO:CD	2.80	0.44
3:Y:187:LEU:O	3:Y:187:LEU:HD12	5.22	0.44
1:L:447:LEU:N	1:L:448:PRO:CD	2.80	0.44
1:M:447:LEU:N	1:M:448:PRO:CD	2.80	0.44
3:W:187:LEU:O	3:W:187:LEU:HD12	5.22	0.44
2:1:187:LEU:O	2:1:187:LEU:HD12	2.17	0.44
1:E:447:LEU:N	1:E:448:PRO:CD	2.80	0.44
1:F:447:LEU:N	1:F:448:PRO:CD	2.80	0.44
1:G:447:LEU:N	1:G:448:PRO:CD	2.81	0.43
1:I:447:LEU:N	1:I:448:PRO:CD	2.80	0.43
1:D:447:LEU:N	1:D:448:PRO:CD	2.80	0.43
1:F:350:SER:OG	1:F:351:ARG:N	2.52	0.43
1:G:350:SER:OG	1:G:351:ARG:N	2.52	0.43
2:7:62:GLU:HB3	2:7:63:PRO:HD3	2.01	0.43
1:A:350:SER:OG	1:A:351:ARG:N	2.52	0.43
1:H:447:LEU:N	1:H:448:PRO:CD	2.80	0.43
1:O:350:SER:OG	1:O:351:ARG:N	2.52	0.43
2:V:62:GLU:HB3	2:V:63:PRO:HD3	2.01	0.43
2:5:62:GLU:HB3	2:5:63:PRO:HD3	2.01	0.43
2:9:62:GLU:HB3	2:9:63:PRO:HD3	2.01	0.43
1:E:350:SER:OG	1:E:351:ARG:N	2.52	0.43
1:H:350:SER:OG	1:H:351:ARG:N	2.52	0.43
2:X:62:GLU:HB3	2:X:63:PRO:HD3	2.01	0.43
2:T:62:GLU:HB3	2:T:63:PRO:HD3	2.01	0.42
1:B:350:SER:OG	1:B:351:ARG:N	2.52	0.42
1:K:350:SER:OG	1:K:351:ARG:N	2.52	0.42
1:N:350:SER:OG	1:N:351:ARG:N	2.52	0.42
2:3:62:GLU:HB3	2:3:63:PRO:HD3	2.01	0.42
1:J:350:SER:OG	1:J:351:ARG:N	2.52	0.42
1:D:350:SER:OG	1:D:351:ARG:N	2.52	0.42
1:L:350:SER:OG	1:L:351:ARG:N	2.52	0.42
2:P:62:GLU:HB3	2:P:63:PRO:HD3	2.01	0.42
2:R:62:GLU:HB3	2:R:63:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:78:PRO:HA	2:7:79:PRO:HD3	1.83	0.42
1:F:417:SER:OG	1:F:418:ALA:N	2.53	0.42
1:E:417:SER:OG	1:E:418:ALA:N	2.53	0.42
1:G:417:SER:OG	1:G:418:ALA:N	2.53	0.42
1:I:417:SER:OG	1:I:418:ALA:N	2.53	0.42
2:1:62:GLU:HB3	2:1:63:PRO:HD3	2.01	0.41
1:A:445:ASP:O	1:A:447:LEU:N	2.53	0.41
1:B:445:ASP:O	1:B:447:LEU:N	2.53	0.41
1:C:350:SER:OG	1:C:351:ARG:N	2.52	0.41
1:H:417:SER:OG	1:H:418:ALA:N	2.53	0.41
1:I:445:ASP:O	1:I:447:LEU:N	2.53	0.41
1:J:417:SER:OG	1:J:418:ALA:N	2.53	0.41
1:J:445:ASP:O	1:J:447:LEU:N	2.53	0.41
2:P:78:PRO:HA	2:P:79:PRO:HD3	1.82	0.41
2:T:78:PRO:HA	2:T:79:PRO:HD3	1.82	0.41
1:D:417:SER:OG	1:D:418:ALA:N	2.53	0.41
1:I:350:SER:OG	1:I:351:ARG:N	2.52	0.41
1:K:417:SER:OG	1:K:418:ALA:N	2.53	0.41
1:K:445:ASP:O	1:K:447:LEU:N	2.53	0.41
1:F:445:ASP:O	1:F:447:LEU:N	2.53	0.41
1:M:350:SER:OG	1:M:351:ARG:N	2.52	0.41
1:C:417:SER:OG	1:C:418:ALA:N	2.53	0.41
1:E:445:ASP:O	1:E:447:LEU:N	2.53	0.41
1:L:445:ASP:O	1:L:447:LEU:N	2.53	0.41
1:H:445:ASP:O	1:H:447:LEU:N	2.53	0.41
1:L:417:SER:OG	1:L:418:ALA:N	2.53	0.41
1:L:447:LEU:O	1:L:449:GLU:N	2.54	0.41
1:O:445:ASP:O	1:O:447:LEU:N	2.53	0.41
1:M:447:LEU:O	1:M:449:GLU:N	2.54	0.41
1:B:417:SER:OG	1:B:418:ALA:N	2.53	0.41
1:D:447:LEU:O	1:D:449:GLU:N	2.54	0.41
1:K:447:LEU:O	1:K:449:GLU:N	2.54	0.41
1:A:417:SER:OG	1:A:418:ALA:N	2.53	0.41
1:C:445:ASP:O	1:C:447:LEU:N	2.53	0.41
1:C:447:LEU:O	1:C:449:GLU:N	2.54	0.41
1:E:447:LEU:O	1:E:449:GLU:N	2.54	0.41
1:F:447:LEU:O	1:F:449:GLU:N	2.54	0.41
1:M:417:SER:OG	1:M:418:ALA:N	2.53	0.41
1:N:447:LEU:O	1:N:449:GLU:N	2.54	0.41
1:N:490:LEU:HA	1:N:491:PRO:HD3	1.94	0.41
1:G:447:LEU:O	1:G:449:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:447:LEU:O	1:H:449:GLU:N	2.54	0.41
1:M:445:ASP:O	1:M:447:LEU:N	2.53	0.41
1:O:417:SER:OG	1:O:418:ALA:N	2.53	0.41
1:D:445:ASP:O	1:D:447:LEU:N	2.53	0.40
1:N:445:ASP:O	1:N:447:LEU:N	2.53	0.40
1:B:447:LEU:O	1:B:449:GLU:N	2.54	0.40
1:G:445:ASP:O	1:G:447:LEU:N	2.53	0.40
1:A:447:LEU:O	1:A:449:GLU:N	2.54	0.40
1:I:447:LEU:O	1:I:449:GLU:N	2.54	0.40
1:J:447:LEU:O	1:J:449:GLU:N	2.54	0.40
1:N:417:SER:OG	1:N:418:ALA:N	2.53	0.40
1:O:447:LEU:O	1:O:449:GLU:N	2.54	0.40
2:9:78:PRO:HA	2:9:79:PRO:HD3	1.82	0.40
1:J:484:ILE:HA	1:J:485:PRO:HD3	1.96	0.40

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	A	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	B	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	C	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	D	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	E	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	F	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	G	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	H	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	I	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	K	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	L	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	M	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	N	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
1	O	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	10	52
2	1	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	3	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	5	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	7	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	9	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	P	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	R	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	T	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	V	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	X	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	a	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	c	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	e	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	g	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	i	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	k	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	m	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	o	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	q	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	s	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	u	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	w	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	y	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
2	z	182/235 (77%)	175 (96%)	7 (4%)	0	100	100
3	0	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	10	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	2	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	4	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	6	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	8	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	Q	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	S	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	U	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	W	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	Y	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	Z	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	b	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	d	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	f	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	h	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	j	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	l	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	n	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	p	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	r	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	t	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	v	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
3	x	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	9	50
All	All	15996/20382 (78%)	15228 (95%)	537 (3%)	231 (1%)	19	58

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ALA
1	B	446	ALA
1	B	515	PRO
1	C	446	ALA
1	C	515	PRO
1	D	446	ALA

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Mol	Chain	Res	Type
1	D	515	PRO
1	E	446	ALA
1	E	515	PRO
1	F	446	ALA
1	F	515	PRO
1	G	446	ALA
1	G	515	PRO
1	H	446	ALA
1	H	515	PRO
1	I	446	ALA
1	I	515	PRO
1	J	446	ALA
1	K	446	ALA
1	K	515	PRO
1	L	446	ALA
1	L	515	PRO
1	M	446	ALA
1	M	515	PRO
1	N	446	ALA
1	O	446	ALA
3	Q	251	ASP
3	S	251	ASP
3	U	251	ASP
3	W	251	ASP
3	Y	251	ASP
3	Z	251	ASP
3	b	251	ASP
3	d	251	ASP
3	f	251	ASP
3	h	251	ASP
3	j	251	ASP
3	l	251	ASP
3	n	251	ASP
3	p	251	ASP
3	r	251	ASP
3	t	251	ASP
3	v	251	ASP
3	x	251	ASP
3	0	251	ASP
3	2	251	ASP
3	4	251	ASP
3	6	251	ASP

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Mol	Chain	Res	Type
3	8	251	ASP
3	10	251	ASP
1	A	448	PRO
1	A	515	PRO
1	B	448	PRO
1	C	448	PRO
1	D	448	PRO
1	E	448	PRO
1	F	448	PRO
1	G	448	PRO
1	H	448	PRO
1	I	448	PRO
1	J	448	PRO
1	J	515	PRO
1	K	448	PRO
1	L	448	PRO
1	M	448	PRO
1	N	448	PRO
1	N	515	PRO
1	O	448	PRO
1	O	515	PRO
3	Q	178	GLY
3	S	178	GLY
3	U	178	GLY
3	W	178	GLY
3	Y	178	GLY
3	Z	178	GLY
3	b	178	GLY
3	d	178	GLY
3	f	178	GLY
3	h	178	GLY
3	j	178	GLY
3	l	178	GLY
3	n	178	GLY
3	p	178	GLY
3	r	178	GLY
3	t	178	GLY
3	v	178	GLY
3	x	178	GLY
3	0	178	GLY
3	2	178	GLY
3	4	178	GLY

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Mol	Chain	Res	Type
3	6	178	GLY
3	8	178	GLY
3	10	178	GLY
1	A	198	ARG
1	B	198	ARG
1	C	198	ARG
1	D	198	ARG
1	E	198	ARG
1	F	198	ARG
1	G	198	ARG
1	H	198	ARG
1	I	198	ARG
1	J	198	ARG
1	K	198	ARG
1	L	198	ARG
1	M	198	ARG
1	N	198	ARG
1	O	198	ARG
3	Q	188	PRO
3	Q	253	PRO
3	S	188	PRO
3	S	253	PRO
3	U	188	PRO
3	U	253	PRO
3	W	188	PRO
3	W	253	PRO
3	Y	188	PRO
3	Y	253	PRO
3	Z	188	PRO
3	Z	253	PRO
3	b	188	PRO
3	b	253	PRO
3	d	188	PRO
3	d	253	PRO
3	f	188	PRO
3	f	253	PRO
3	h	188	PRO
3	h	253	PRO
3	j	188	PRO
3	j	253	PRO
3	l	188	PRO
3	l	253	PRO

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Mol	Chain	Res	Type
3	n	188	PRO
3	n	253	PRO
3	p	188	PRO
3	p	253	PRO
3	r	188	PRO
3	r	253	PRO
3	t	188	PRO
3	t	253	PRO
3	v	188	PRO
3	v	253	PRO
3	x	188	PRO
3	x	253	PRO
3	0	188	PRO
3	0	253	PRO
3	2	188	PRO
3	2	253	PRO
3	4	188	PRO
3	4	253	PRO
3	6	188	PRO
3	6	253	PRO
3	8	188	PRO
3	8	253	PRO
3	10	188	PRO
3	10	253	PRO
1	A	173	ILE
1	A	485	PRO
1	A	491	PRO
1	B	173	ILE
1	B	491	PRO
1	C	173	ILE
1	C	485	PRO
1	C	491	PRO
1	D	173	ILE
1	D	491	PRO
1	E	173	ILE
1	E	485	PRO
1	E	491	PRO
1	F	173	ILE
1	F	491	PRO
1	G	173	ILE
1	G	485	PRO
1	G	491	PRO

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Mol	Chain	Res	Type
1	H	173	ILE
1	H	485	PRO
1	H	491	PRO
1	I	173	ILE
1	I	491	PRO
1	J	173	ILE
1	J	491	PRO
1	K	173	ILE
1	K	485	PRO
1	K	491	PRO
1	L	173	ILE
1	L	491	PRO
1	M	173	ILE
1	M	491	PRO
1	N	173	ILE
1	N	485	PRO
1	N	491	PRO
1	O	173	ILE
1	O	491	PRO
1	B	485	PRO
1	D	485	PRO
1	F	485	PRO
1	I	485	PRO
1	J	485	PRO
1	L	485	PRO
1	M	485	PRO
1	O	485	PRO
1	K	344	ILE
1	A	344	ILE
1	A	447	LEU
1	B	344	ILE
1	B	447	LEU
1	C	344	ILE
1	C	447	LEU
1	D	344	ILE
1	D	447	LEU
1	E	344	ILE
1	E	447	LEU
1	F	344	ILE
1	F	447	LEU
1	G	344	ILE
1	G	447	LEU

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Mol	Chain	Res	Type
1	H	344	ILE
1	H	447	LEU
1	I	344	ILE
1	I	447	LEU
1	J	344	ILE
1	J	447	LEU
1	K	447	LEU
1	L	344	ILE
1	L	447	LEU
1	M	344	ILE
1	M	447	LEU
1	N	344	ILE
1	N	447	LEU
1	O	344	ILE
1	O	447	LEU

### 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	A	413/477 (87%)	413 (100%)	0	100	100
1	B	413/477 (87%)	413 (100%)	0	100	100
1	C	413/477 (87%)	413 (100%)	0	100	100
1	D	413/477 (87%)	413 (100%)	0	100	100
1	E	413/477 (87%)	413 (100%)	0	100	100
1	F	413/477 (87%)	413 (100%)	0	100	100
1	G	413/477 (87%)	413 (100%)	0	100	100
1	H	413/477 (87%)	413 (100%)	0	100	100
1	I	413/477 (87%)	413 (100%)	0	100	100
1	J	413/477 (87%)	413 (100%)	0	100	100
1	K	413/477 (87%)	413 (100%)	0	100	100
1	L	413/477 (87%)	413 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	413/477 (87%)	413 (100%)	0	100	100
1	N	413/477 (87%)	413 (100%)	0	100	100
1	O	413/477 (87%)	413 (100%)	0	100	100
2	1	157/200 (78%)	157 (100%)	0	100	100
2	3	157/200 (78%)	157 (100%)	0	100	100
2	5	157/200 (78%)	157 (100%)	0	100	100
2	7	157/200 (78%)	157 (100%)	0	100	100
2	9	157/200 (78%)	157 (100%)	0	100	100
2	P	157/200 (78%)	157 (100%)	0	100	100
2	R	157/200 (78%)	157 (100%)	0	100	100
2	T	157/200 (78%)	157 (100%)	0	100	100
2	V	157/200 (78%)	157 (100%)	0	100	100
2	X	157/200 (78%)	157 (100%)	0	100	100
2	a	157/200 (78%)	157 (100%)	0	100	100
2	c	157/200 (78%)	157 (100%)	0	100	100
2	e	157/200 (78%)	157 (100%)	0	100	100
2	g	157/200 (78%)	157 (100%)	0	100	100
2	i	157/200 (78%)	157 (100%)	0	100	100
2	k	157/200 (78%)	157 (100%)	0	100	100
2	m	157/200 (78%)	157 (100%)	0	100	100
2	o	157/200 (78%)	157 (100%)	0	100	100
2	q	157/200 (78%)	157 (100%)	0	100	100
2	s	157/200 (78%)	157 (100%)	0	100	100
2	u	157/200 (78%)	157 (100%)	0	100	100
2	w	157/200 (78%)	157 (100%)	0	100	100
2	y	157/200 (78%)	157 (100%)	0	100	100
2	z	157/200 (78%)	157 (100%)	0	100	100
3	0	167/221 (76%)	167 (100%)	0	100	100
3	10	167/221 (76%)	167 (100%)	0	100	100
3	2	167/221 (76%)	167 (100%)	0	100	100
3	4	167/221 (76%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	6	167/221 (76%)	167 (100%)	0	100	100
3	8	167/221 (76%)	167 (100%)	0	100	100
3	Q	167/221 (76%)	167 (100%)	0	100	100
3	S	167/221 (76%)	167 (100%)	0	100	100
3	U	167/221 (76%)	167 (100%)	0	100	100
3	W	167/221 (76%)	167 (100%)	0	100	100
3	Y	167/221 (76%)	167 (100%)	0	100	100
3	Z	167/221 (76%)	167 (100%)	0	100	100
3	b	167/221 (76%)	167 (100%)	0	100	100
3	d	167/221 (76%)	167 (100%)	0	100	100
3	f	167/221 (76%)	167 (100%)	0	100	100
3	h	167/221 (76%)	167 (100%)	0	100	100
3	j	167/221 (76%)	167 (100%)	0	100	100
3	l	167/221 (76%)	167 (100%)	0	100	100
3	n	167/221 (76%)	167 (100%)	0	100	100
3	p	167/221 (76%)	167 (100%)	0	100	100
3	r	167/221 (76%)	167 (100%)	0	100	100
3	t	167/221 (76%)	167 (100%)	0	100	100
3	v	167/221 (76%)	167 (100%)	0	100	100
3	x	167/221 (76%)	167 (100%)	0	100	100
All	All	13971/17259 (81%)	13971 (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 [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	J	1
1	D	1
1	K	1
1	E	1
1	H	1
1	B	1
1	I	1
1	C	1
1	A	1
1	N	1
1	O	1
1	L	1
1	F	1
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	171:ASP	C	172:GLY	N	24.97
1	L	171:ASP	C	172:GLY	N	24.97
1	M	171:ASP	C	172:GLY	N	24.97
1	J	171:ASP	C	172:GLY	N	24.95
1	N	171:ASP	C	172:GLY	N	24.95
1	O	171:ASP	C	172:GLY	N	24.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	171:ASP	C	172:GLY	N	24.92
1	A	171:ASP	C	172:GLY	N	24.90
1	H	171:ASP	C	172:GLY	N	24.89
1	B	171:ASP	C	172:GLY	N	24.87
1	G	171:ASP	C	172:GLY	N	24.86
1	C	171:ASP	C	172:GLY	N	24.84
1	F	171:ASP	C	172:GLY	N	24.84
1	D	171:ASP	C	172:GLY	N	24.83
1	E	171:ASP	C	172:GLY	N	24.83