



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Oct 16, 2019 – 12:01 AM EDT

PDB ID : 2Y9J
EMDB ID: : EMD-1874
Title : THREE-DIMENSIONAL MODEL OF SALMONELLA'S NEEDLE COM-
PLEX AT SUBNANOMETER RESOLUTION
Authors : Schraidt, O.; Marlovits, T.C.
Deposited on : 2011-02-15
Resolution : 6.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

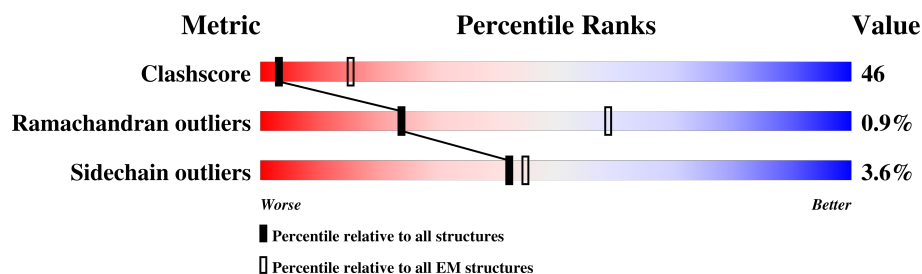
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



















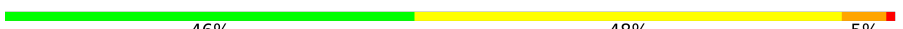





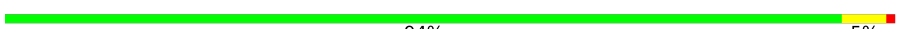


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	A	186	79% 20% .
1	B	186	79% 20% .
1	C	186	80% 20% .
1	D	186	78% 21% .
1	E	186	80% 19% .
1	F	186	80% 20% .
1	G	186	80% 20% .
1	H	186	80% 20% .
1	I	186	79% 20% .


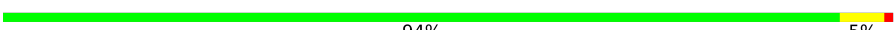



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Mol	Chain	Length	Quality of chain
1	J	186	 80% 20% .
1	K	186	 78% 21% .
1	L	186	 78% 21% .
1	M	186	 79% 20% .
1	N	186	 79% 20% .
1	O	186	 80% 20% .
1	P	186	 79% 20% .
1	Q	186	 79% 20% .
1	R	186	 78% 22% .
1	S	186	 80% 19% .
1	T	186	 80% 19% .
1	U	186	 79% 20% .
1	V	186	 80% 20% .
1	W	186	 78% 21% .
1	X	186	 79% 20% .
2	Y	170	 46% 48% 5% .
2	Z	170	 46% 48% 5% .
2	a	170	 94% 5% .
2	b	170	 94% 5% .
2	c	170	 94% 5% .
2	d	170	 94% 5% .
2	e	170	 94% 5% .
2	f	170	 94% 5% .
2	g	170	 94% 5% .
2	h	170	 94% 5% .

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Mol	Chain	Length	Quality of chain
2	i	170	 94% 5% .
2	j	170	 94% 5% .
2	k	170	 94% 5% .
2	l	170	 94% 5% .
2	m	170	 94% 5% .
2	n	170	 94% 5% .
2	o	170	 94% 5% .
2	p	170	 94% 5% .
2	q	170	 94% 5% .
2	r	170	 94% 5% .
2	s	170	 94% 5% .
2	t	170	 94% 5% .
2	u	170	 94% 5% .
2	v	170	 94% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 70704 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 PRGH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	B	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	C	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	D	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	E	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	F	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	G	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	H	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	I	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	J	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	K	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	L	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	M	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	N	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	O	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	P	186	Total 1541	C 976	N 280	O 281	S 4	0	0
1	Q	186	Total 1541	C 976	N 280	O 281	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	S	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	T	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	U	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	V	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	W	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		
1	X	186	Total	C	N	O	S	0	0
			1541	976	280	281	4		

- Molecule 2 is a protein called LIPOPROTEIN PRGK.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	Z	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	a	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	b	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	c	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	d	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	e	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	f	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	g	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	h	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	i	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	j	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	l	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	m	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	n	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	o	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	p	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	q	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	r	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	s	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	t	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	u	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		
2	v	170	Total	C	N	O	S	0	0
			1339	845	233	258	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	66	Total	O	0
			66	66	
3	B	66	Total	O	0
			66	66	
3	C	66	Total	O	0
			66	66	
3	D	66	Total	O	0
			66	66	
3	E	66	Total	O	0
			66	66	
3	F	66	Total	O	0
			66	66	
3	G	66	Total	O	0
			66	66	

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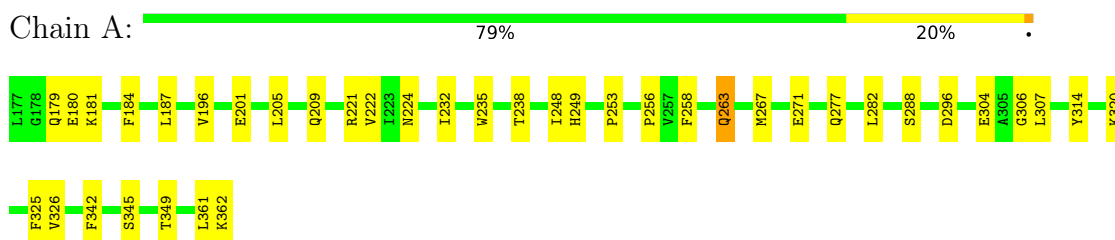
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Mol	Chain	Residues	Atoms		AltConf
3	H	66	Total 66	O 66	0
3	I	66	Total 66	O 66	0
3	J	66	Total 66	O 66	0
3	K	66	Total 66	O 66	0
3	L	66	Total 66	O 66	0
3	M	66	Total 66	O 66	0
3	N	66	Total 66	O 66	0
3	O	66	Total 66	O 66	0
3	P	66	Total 66	O 66	0
3	Q	66	Total 66	O 66	0
3	R	66	Total 66	O 66	0
3	S	66	Total 66	O 66	0
3	T	66	Total 66	O 66	0
3	U	66	Total 66	O 66	0
3	V	66	Total 66	O 66	0
3	W	66	Total 66	O 66	0
3	X	66	Total 66	O 66	0

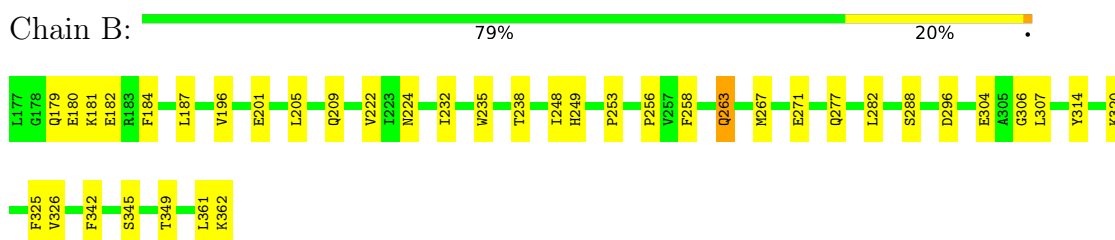
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

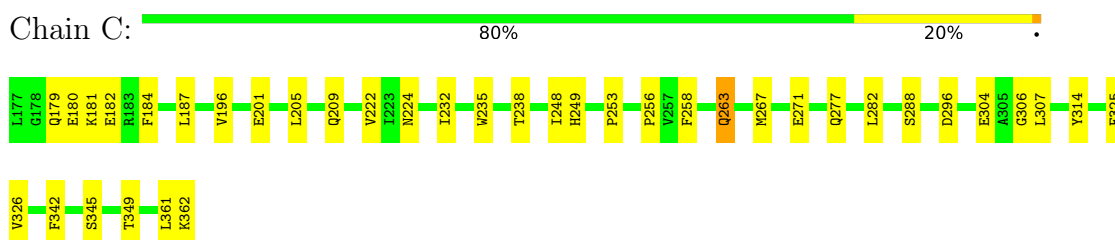
- Molecule 1: PROTEIN PRGH



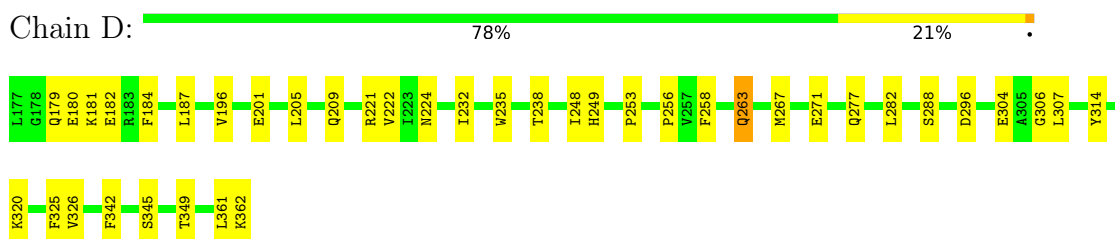
- Molecule 1: PROTEIN PRGH



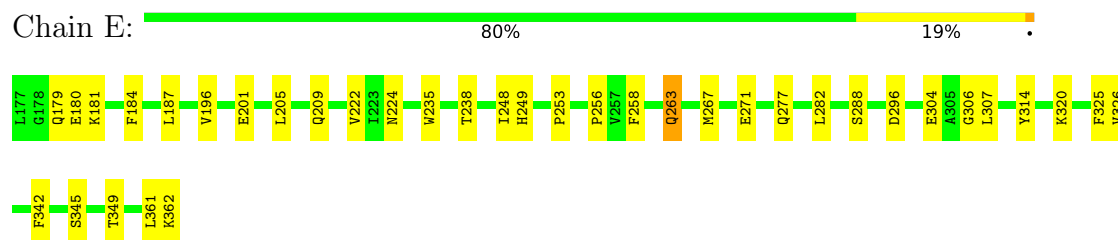
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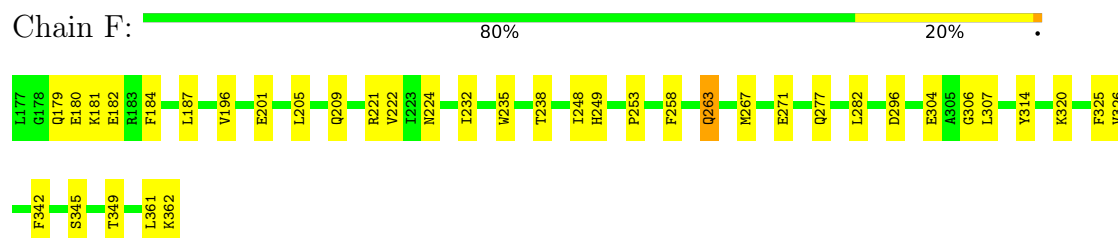
- Molecule 1: PROTEIN PRGH



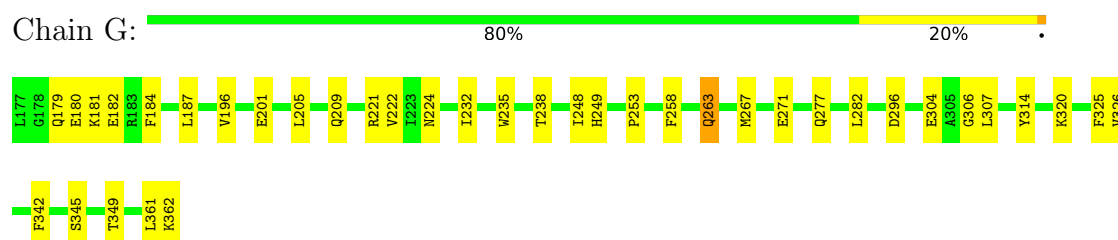
- Molecule 1: PROTEIN PRGH



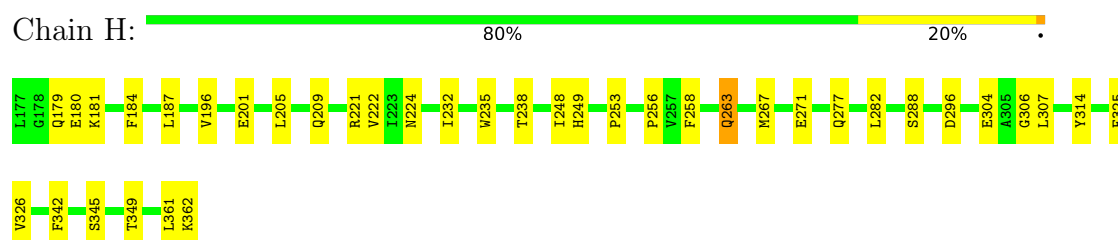
- Molecule 1: PROTEIN PRGH



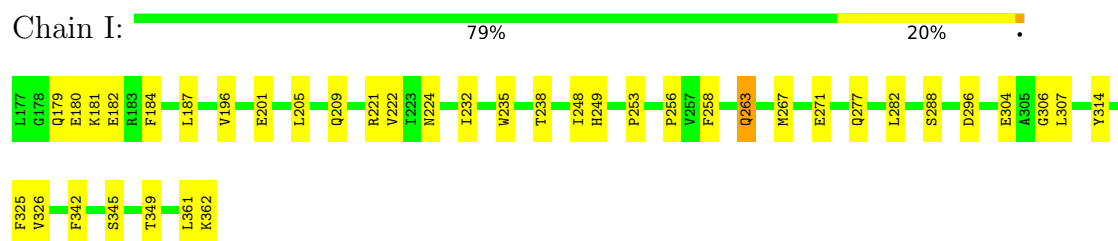
- Molecule 1: PROTEIN PRGH



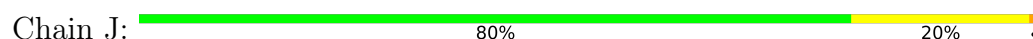
- Molecule 1: PROTEIN PRGH



- Molecule 1: PROTEIN PRGH



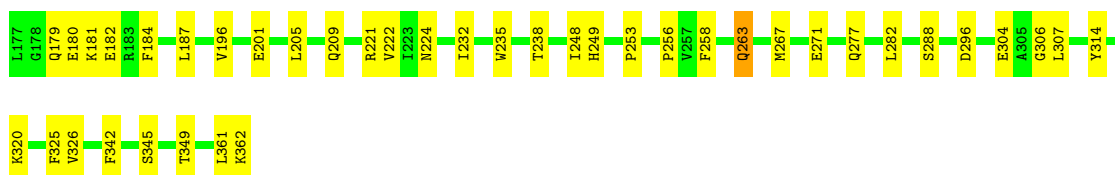
- Molecule 1: PROTEIN PRGH





- Molecule 1: PROTEIN PRGH

Chain K: 78% 21%



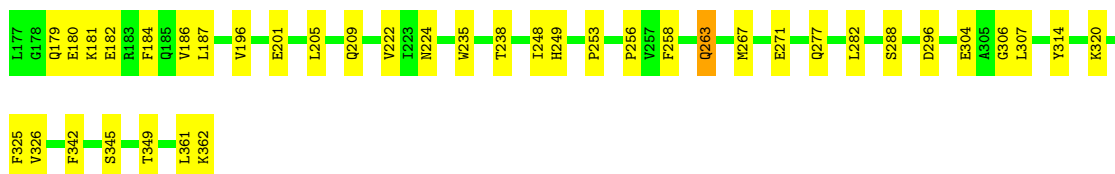
- Molecule 1: PROTEIN PRGH

Chain L: 78% 21%



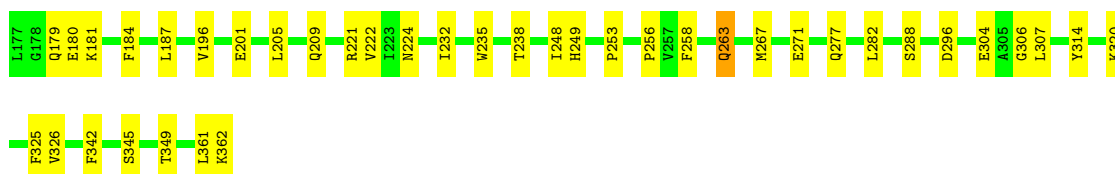
- Molecule 1: PROTEIN PRGH

Chain M: 79% 20%



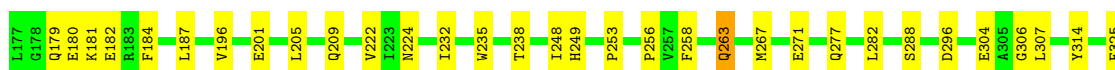
- Molecule 1: PROTEIN PRGH

Chain N: 79% 20%



- Molecule 1: PROTEIN PRGH

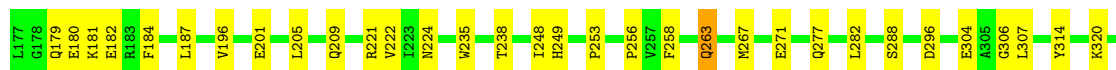
Chain O: 80% 20%





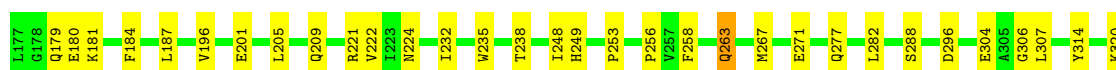
• Molecule 1: PROTEIN PRGH

Chain P: 79% 20%



• Molecule 1: PROTEIN PRGH

Chain Q: 79% 20%



• Molecule 1: PROTEIN PRGH

Chain R: 78% 22%



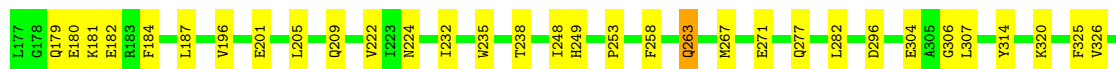
• Molecule 1: PROTEIN PRGH

Chain S: 80% 19%

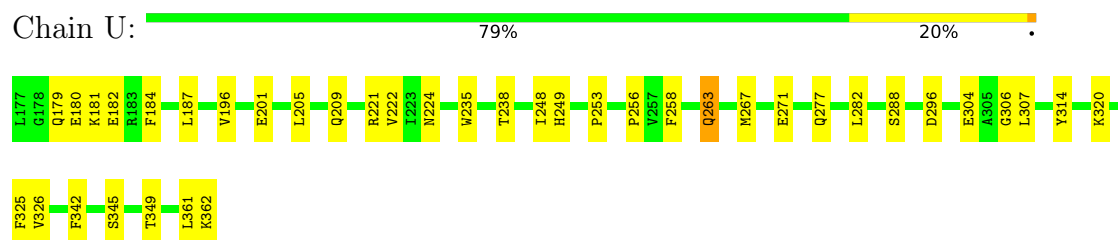


• Molecule 1: PROTEIN PRGH

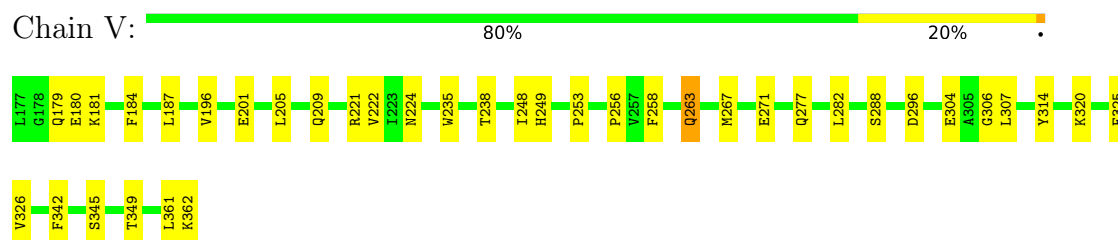
Chain T: 80% 19%



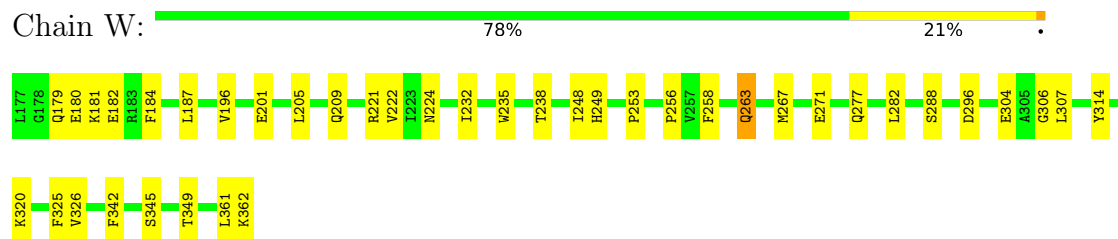
- Molecule 1: PROTEIN PRGH



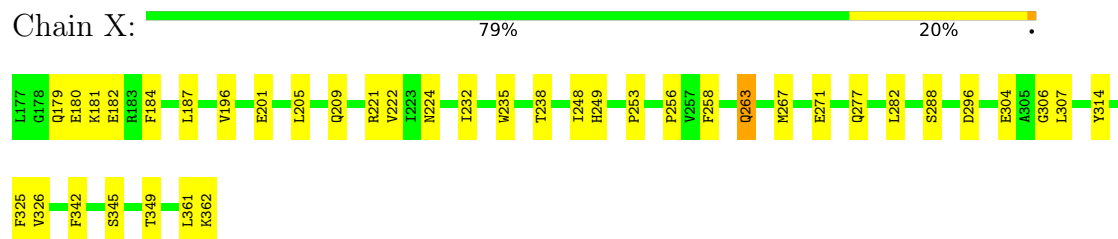
- Molecule 1: PROTEIN PRGH



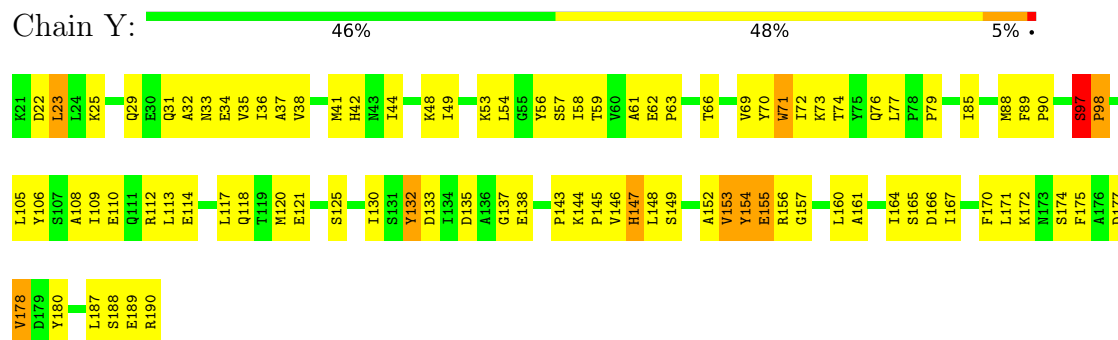
- Molecule 1: PROTEIN PRGH



- Molecule 1: PROTEIN PRGH



- Molecule 2: LIPOPROTEIN PRGK



- Molecule 2: LIPOPROTEIN PRGK

Chain Z:  46% 48% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain a:  94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain b:  94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain c:  94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain d:  94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain e:  94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain f:  94% 5% •



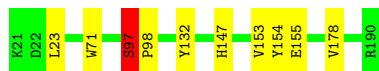
- Molecule 2: LIPOPROTEIN PRGK

Chain g: 94% 5% •



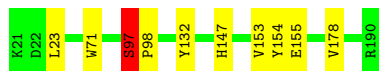
- Molecule 2: LIPOPROTEIN PRGK

Chain h: 94% 5% •



- Molecule 2: LIPOPROTEIN PRGK

Chain i: 94% 5% •



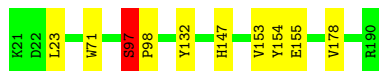
- Molecule 2: LIPOPROTEIN PRGK

Chain j: 94% 5% •



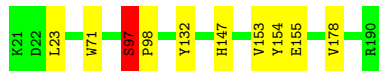
- Molecule 2: LIPOPROTEIN PRGK

Chain k: 94% 5% •



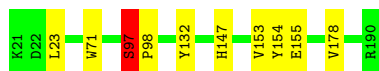
- Molecule 2: LIPOPROTEIN PRGK

Chain l: 94% 5% •

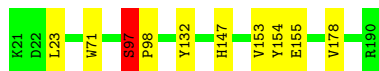


- Molecule 2: LIPOPROTEIN PRGK

Chain m: 94% 5% •



• Molecule 2: LIPOPROTEIN PRGK

Chain n:  94% 5%

• Molecule 2: LIPOPROTEIN PRGK

Chain o:  94% 5%

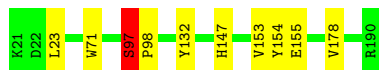
• Molecule 2: LIPOPROTEIN PRGK

Chain p:  94% 5%

• Molecule 2: LIPOPROTEIN PRGK

Chain q:  94% 5%

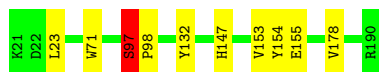
• Molecule 2: LIPOPROTEIN PRGK

Chain r:  94% 5%

• Molecule 2: LIPOPROTEIN PRGK

Chain s:  94% 5%

• Molecule 2: LIPOPROTEIN PRGK

Chain t:  94% 5%

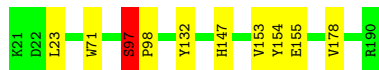
• Molecule 2: LIPOPROTEIN PRGK

Chain u:  94% 5%



● Molecule 2: LIPOPROTEIN PRGK

Chain v: 94% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C24	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	93000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	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	0.67	0/1573	0.70	0/2122
1	B	0.67	0/1573	0.70	0/2122
1	C	0.67	0/1573	0.70	0/2122
1	D	0.67	0/1573	0.70	0/2122
1	E	0.67	0/1573	0.70	0/2122
1	F	0.67	0/1573	0.70	0/2122
1	G	0.67	0/1573	0.70	0/2122
1	H	0.66	0/1573	0.70	0/2122
1	I	0.66	0/1573	0.70	0/2122
1	J	0.67	0/1573	0.70	0/2122
1	K	0.67	0/1573	0.70	0/2122
1	L	0.67	0/1573	0.70	0/2122
1	M	0.67	0/1573	0.70	0/2122
1	N	0.66	0/1573	0.70	0/2122
1	O	0.67	0/1573	0.70	0/2122
1	P	0.66	0/1573	0.70	0/2122
1	Q	0.67	0/1573	0.70	0/2122
1	R	0.66	0/1573	0.70	0/2122
1	S	0.66	0/1573	0.70	0/2122
1	T	0.66	0/1573	0.70	0/2122
1	U	0.67	0/1573	0.70	0/2122
1	V	0.67	0/1573	0.70	0/2122
1	W	0.67	0/1573	0.70	0/2122
1	X	0.67	0/1573	0.70	0/2122
2	Y	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	Z	0.86	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	a	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	b	0.86	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	c	0.86	3/1365 (0.2%)	1.08	7/1850 (0.4%)
2	d	0.86	3/1365 (0.2%)	1.08	6/1850 (0.3%)
2	e	0.87	3/1365 (0.2%)	1.08	7/1850 (0.4%)
2	f	0.86	3/1365 (0.2%)	1.08	7/1850 (0.4%)
2	g	0.87	3/1365 (0.2%)	1.09	6/1850 (0.3%)
2	h	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	i	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	j	0.86	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	k	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	l	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	m	0.87	3/1365 (0.2%)	1.08	7/1850 (0.4%)
2	n	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	o	0.86	3/1365 (0.2%)	1.08	7/1850 (0.4%)
2	p	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	q	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	r	0.86	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	s	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	t	0.87	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	u	0.86	3/1365 (0.2%)	1.09	7/1850 (0.4%)
2	v	0.86	3/1365 (0.2%)	1.08	7/1850 (0.4%)
All	All	0.76	72/70512 (0.1%)	0.90	166/95328 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Y	0	3
2	Z	0	3
2	a	0	3
2	b	0	3
2	c	0	3
2	d	0	3
2	e	0	3
2	f	0	3
2	g	0	3
2	h	0	3
2	i	0	3
2	j	0	3
2	k	0	3
2	l	0	3
2	m	0	3
2	n	0	3
2	o	0	3
2	p	0	3
2	q	0	3
2	r	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	s	0	3
2	t	0	3
2	u	0	3
2	v	0	3
All	All	0	72

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	q	154	TYR	CE2-CZ	8.95	1.50	1.38
2	l	154	TYR	CE2-CZ	8.91	1.50	1.38
2	k	154	TYR	CE2-CZ	8.90	1.50	1.38
2	i	154	TYR	CE2-CZ	8.90	1.50	1.38
2	Z	154	TYR	CE2-CZ	8.88	1.50	1.38

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	132	TYR	CB-CG-CD2	-10.52	114.69	121.00
2	e	132	TYR	CB-CG-CD2	-10.49	114.71	121.00
2	k	132	TYR	CB-CG-CD2	-10.47	114.72	121.00
2	v	132	TYR	CB-CG-CD2	-10.47	114.72	121.00
2	i	132	TYR	CB-CG-CD2	-10.44	114.73	121.00

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	155	GLU	Mainchain
2	Y	71	TRP	Mainchain
2	Y	97	SER	Peptide
2	Z	71	TRP	Mainchain
2	Z	97	SER	Peptide

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	1541	0	1530	24	0
1	B	1541	0	1530	25	0
1	C	1541	0	1530	23	0
1	D	1541	0	1530	26	0
1	E	1541	0	1530	23	0
1	F	1541	0	1530	25	0
1	G	1541	0	1530	24	0
1	H	1541	0	1530	24	0
1	I	1541	0	1530	25	0
1	J	1541	0	1530	24	0
1	K	1541	0	1530	26	0
1	L	1541	0	1530	27	0
1	M	1541	0	1530	38	0
1	N	1541	0	1530	25	0
1	O	1541	0	1530	23	0
1	P	1541	0	1530	24	0
1	Q	1541	0	1530	25	0
1	R	1541	0	1530	39	0
1	S	1541	0	1530	24	0
1	T	1541	0	1530	24	0
1	U	1541	0	1530	24	0
1	V	1541	0	1530	23	0
1	W	1541	0	1530	26	0
1	X	1541	0	1530	24	0
2	Y	1339	0	1331	114	0
2	Z	1339	0	1332	110	0
2	a	1339	0	1331	0	0
2	b	1339	0	1331	0	0
2	c	1339	0	1331	0	0
2	d	1339	0	1331	0	0
2	e	1339	0	1331	0	0
2	f	1339	0	1331	0	0
2	g	1339	0	1331	0	0
2	h	1339	0	1331	0	0
2	i	1339	0	1331	0	0
2	j	1339	0	1331	0	0
2	k	1339	0	1331	0	0
2	l	1339	0	1331	0	0
2	m	1339	0	1331	0	0
2	n	1339	0	1331	0	0
2	o	1339	0	1331	0	0
2	p	1339	0	1331	0	0
2	q	1339	0	1331	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	r	1339	0	1331	0	0
2	s	1339	0	1332	0	0
2	t	1339	0	1331	0	0
2	u	1339	0	1331	0	0
2	v	1339	0	1332	0	0
3	A	66	0	0	0	0
3	B	66	0	0	0	0
3	C	66	0	0	0	0
3	D	66	0	0	0	0
3	E	66	0	0	0	0
3	F	66	0	0	0	0
3	G	66	0	0	0	0
3	H	66	0	0	0	0
3	I	66	0	0	0	0
3	J	66	0	0	0	0
3	K	66	0	0	0	0
3	L	66	0	0	0	0
3	M	66	0	0	0	0
3	N	66	0	0	0	0
3	O	66	0	0	0	0
3	P	66	0	0	0	0
3	Q	66	0	0	0	0
3	R	66	0	0	0	0
3	S	66	0	0	0	0
3	T	66	0	0	0	0
3	U	66	0	0	0	0
3	V	66	0	0	0	0
3	W	66	0	0	0	0
3	X	66	0	0	0	0
All	All	70704	0	68667	794	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 46.

The worst 5 of 794 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:M:186:VAL:HG21	2:Z:170:PHE:CE1	123.92	1.62
1:R:186:VAL:HG21	2:Y:170:PHE:CE1	78.25	1.58
1:R:186:VAL:HG11	2:Y:170:PHE:CZ	77.51	1.50
1:R:186:VAL:HG21	2:Y:170:PHE:CZ	77.47	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:186:VAL:HG11	2:Z:170:PHE:CZ	126.67	1.48

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	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	B	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	C	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	D	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	E	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	F	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	G	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	H	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	I	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	J	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	K	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	L	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	M	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	N	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	O	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	P	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	Q	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	R	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	S	184/186 (99%)	180 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	U	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	V	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	W	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
1	X	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
2	Y	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	Z	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	a	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	b	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	c	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	d	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	e	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	f	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	g	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	h	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	i	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	j	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	k	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	l	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	m	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	n	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	o	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	p	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	q	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	r	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	s	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	t	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	u	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
2	v	168/170 (99%)	157 (94%)	8 (5%)	3 (2%)	9	47
All	All	8448/8544 (99%)	8088 (96%)	288 (3%)	72 (1%)	24	61

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	97	SER
2	Z	97	SER
2	a	97	SER
2	b	97	SER
2	c	97	SER

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	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	B	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	C	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	D	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	E	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	F	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	G	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	H	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	I	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	J	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	K	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	L	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	M	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	N	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	O	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	P	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	Q	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	R	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	S	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	T	160/160 (100%)	150 (94%)	10 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	V	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	W	160/160 (100%)	150 (94%)	10 (6%)	20	50
1	X	160/160 (100%)	150 (94%)	10 (6%)	20	50
2	Y	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	Z	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	a	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	b	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	c	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	d	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	e	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	f	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	g	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	h	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	i	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	j	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	k	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	l	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	m	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	n	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	o	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	p	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	q	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	r	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	s	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	t	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	u	146/146 (100%)	145 (99%)	1 (1%)	85	93
2	v	146/146 (100%)	145 (99%)	1 (1%)	85	93
All	All	7344/7344 (100%)	7080 (96%)	264 (4%)	42	65

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	362	LYS
1	O	345	SER
2	b	23	LEU
1	M	209	GLN
1	N	263	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 236 such sidechains are listed below:

Mol	Chain	Res	Type
2	Z	147	HIS
2	e	31	GLN
2	s	173	ASN
2	a	76	GLN
2	b	173	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.