



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:21 PM UTC

PDB ID : 5TCR / pdb_00005tcr
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 EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

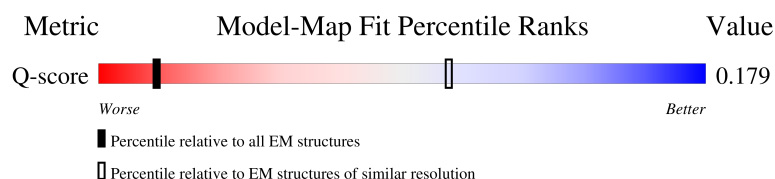
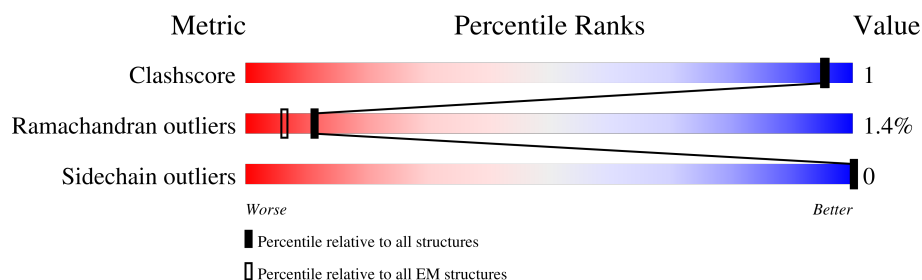
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

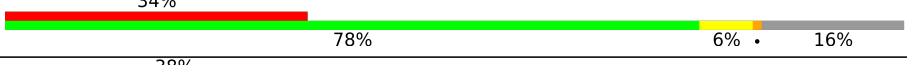
The reported resolution of this entry is 6.30 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	562	
1	B	562	
1	C	562	
1	D	562	

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Mol	Chain	Length	Quality of chain
1	E	562	36% 78% 6% 16%
1	F	562	36% 78% 6% 16%
1	G	562	34% 78% 6% 16%
1	H	562	36% 78% 6% 16%
1	I	562	37% 78% 6% 16%
1	J	562	36% 78% 6% 16%
1	K	562	36% 78% 6% 16%
1	L	562	40% 78% 6% 16%
1	M	562	38% 78% 6% 16%
1	N	562	35% 78% 6% 16%
1	O	562	34% 78% 6% 16%
2	1	235	73% 5% 22%
2	3	235	73% 5% 22%
2	5	235	73% 5% 22%
2	7	235	72% 5% 22%
2	9	235	72% 5% 22%
2	P	235	72% 5% 22%
2	R	235	73% 5% 22%
2	T	235	72% 5% 22%
2	V	235	5% 72% 5% 22%
2	X	235	73% 5% 22%
2	a	235	72% 5% 22%
2	c	235	5% 72% 5% 22%
2	e	235	7% 72% 5% 22%
2	g	235	5% 72% 5% 22%

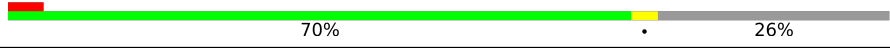
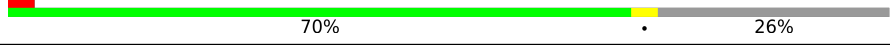
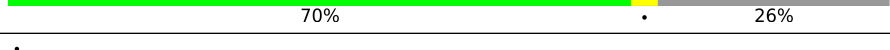
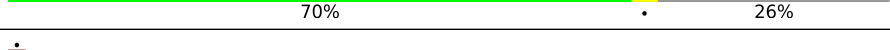
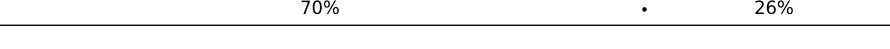
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Mol	Chain	Length	Quality of chain
2	i	235	
2	k	235	
2	m	235	
2	o	235	
2	q	235	
2	s	235	
2	u	235	
2	w	235	
2	y	235	
2	z	235	
3	0	263	
3	10	263	
3	2	263	
3	4	263	
3	6	263	
3	8	263	
3	Q	263	
3	S	263	
3	U	263	
3	W	263	
3	Y	263	
3	Z	263	
3	b	263	
3	d	263	
3	f	263	

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Mol	Chain	Length	Quality of chain
3	h	263	 70%26%
3	j	263	 70%26%
3	l	263	 70%26%
3	n	263	 70%26%
3	p	263	 70%26%
3	r	263	 70%26%
3	t	263	 70%26%
3	v	263	 70%26%
3	x	263	 70%26%

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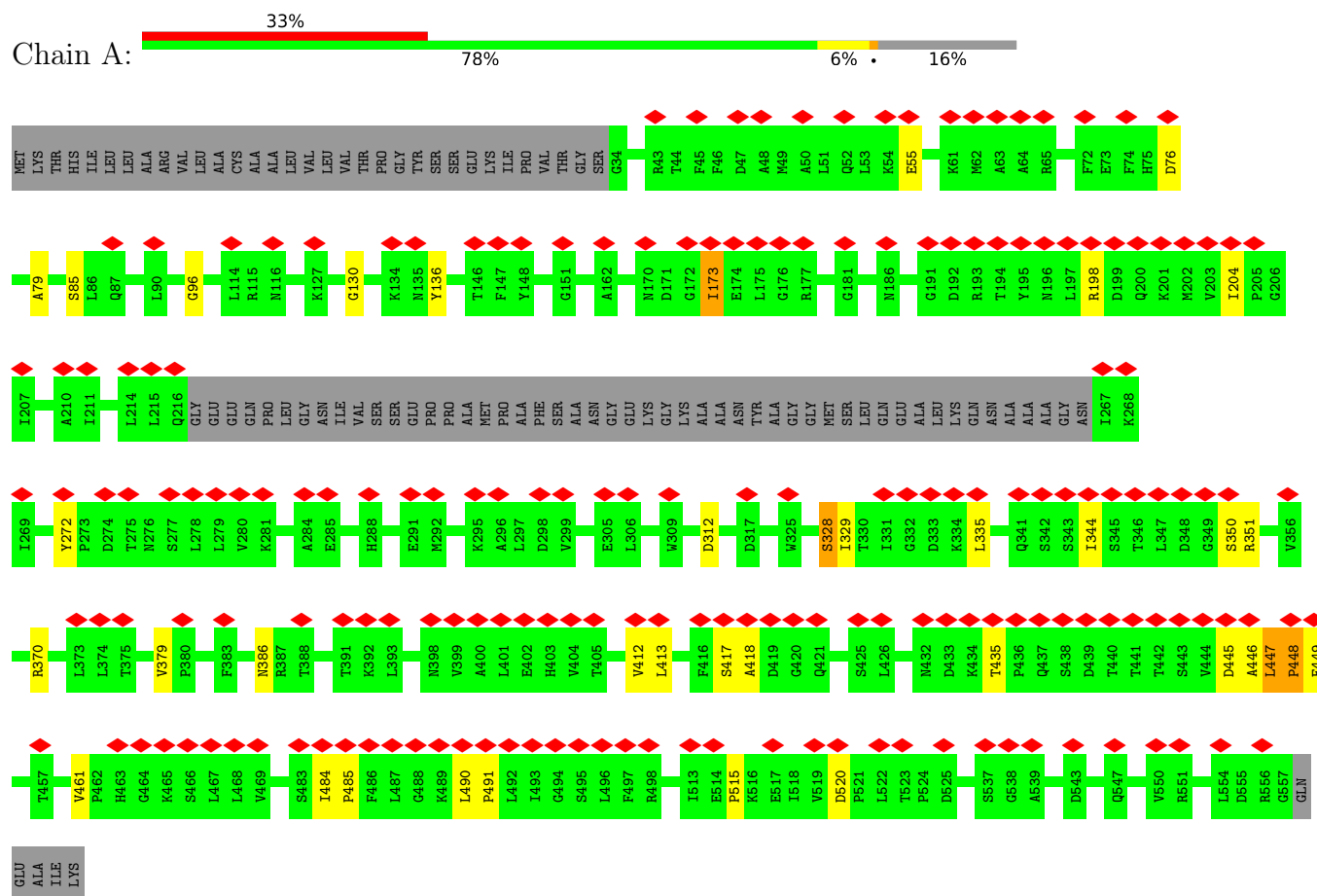
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	x	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	0	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	2	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	4	194	Total 1600	C 1011	N 288	O 297	S 4	0	0
3	6	194	Total 1600	C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

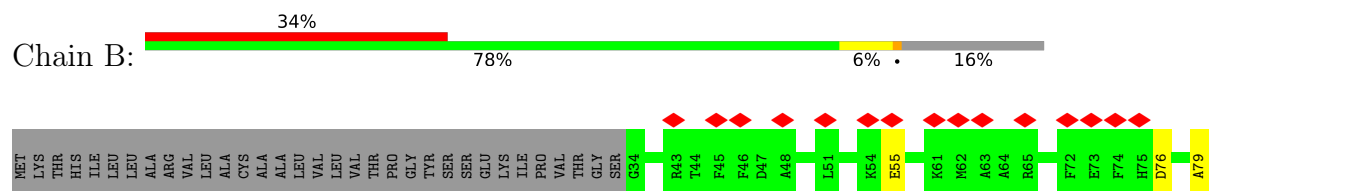
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

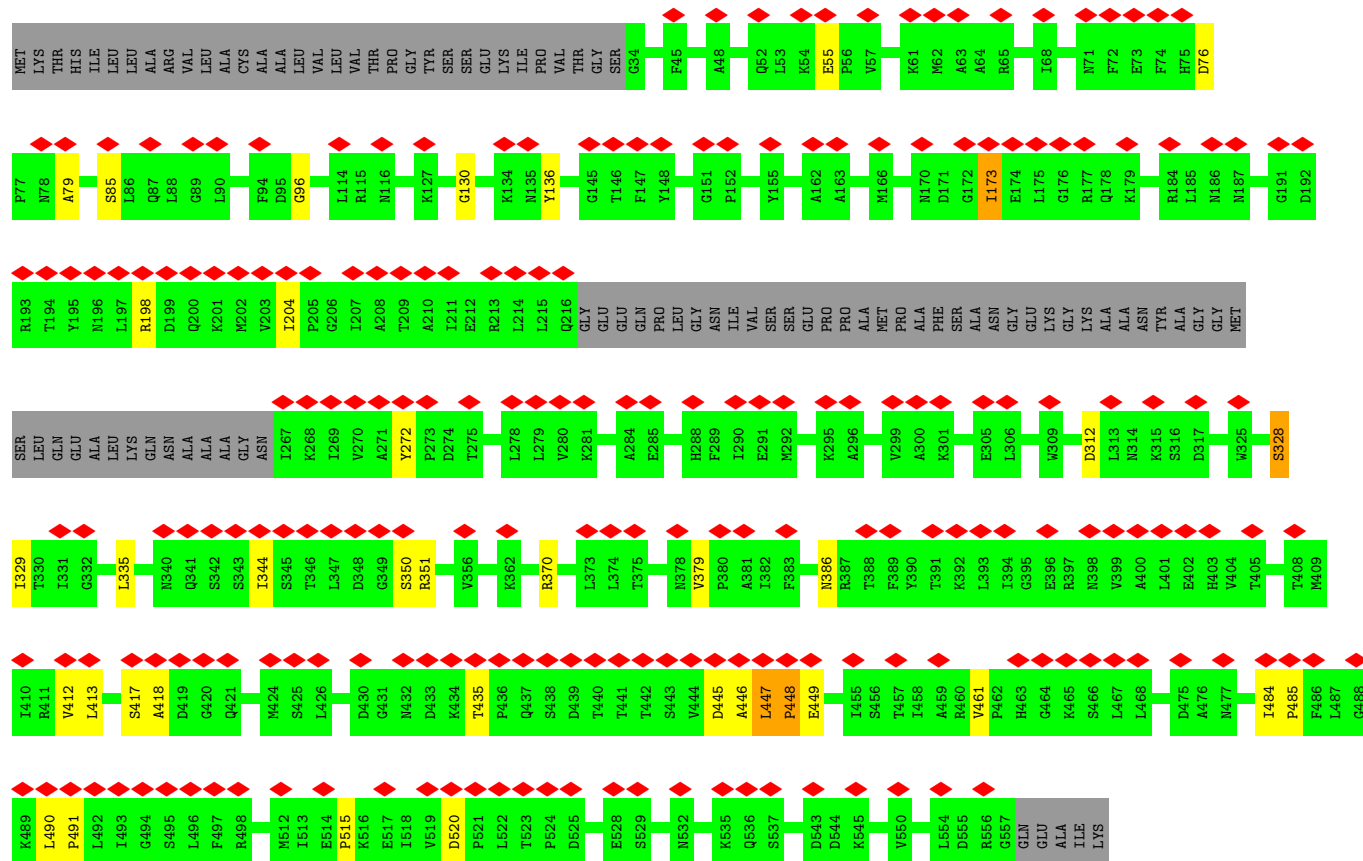
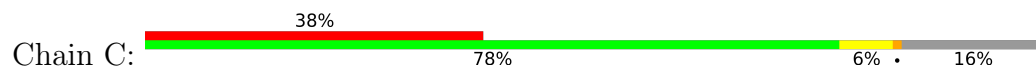


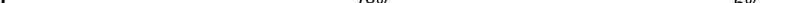
• Molecule 1: Protein InvG

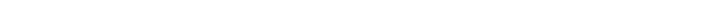


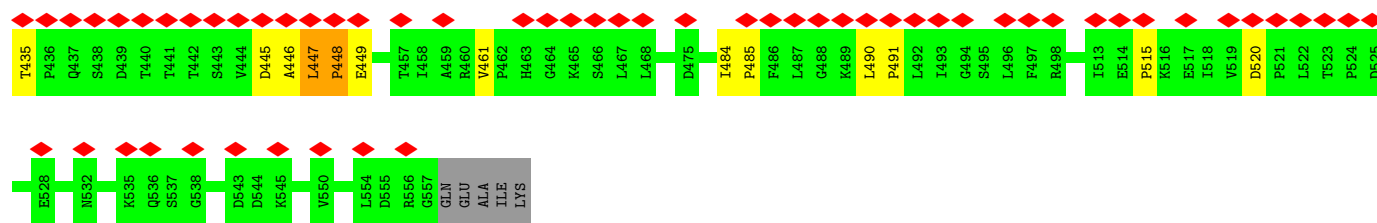


• Molecule 1: Protein InvG

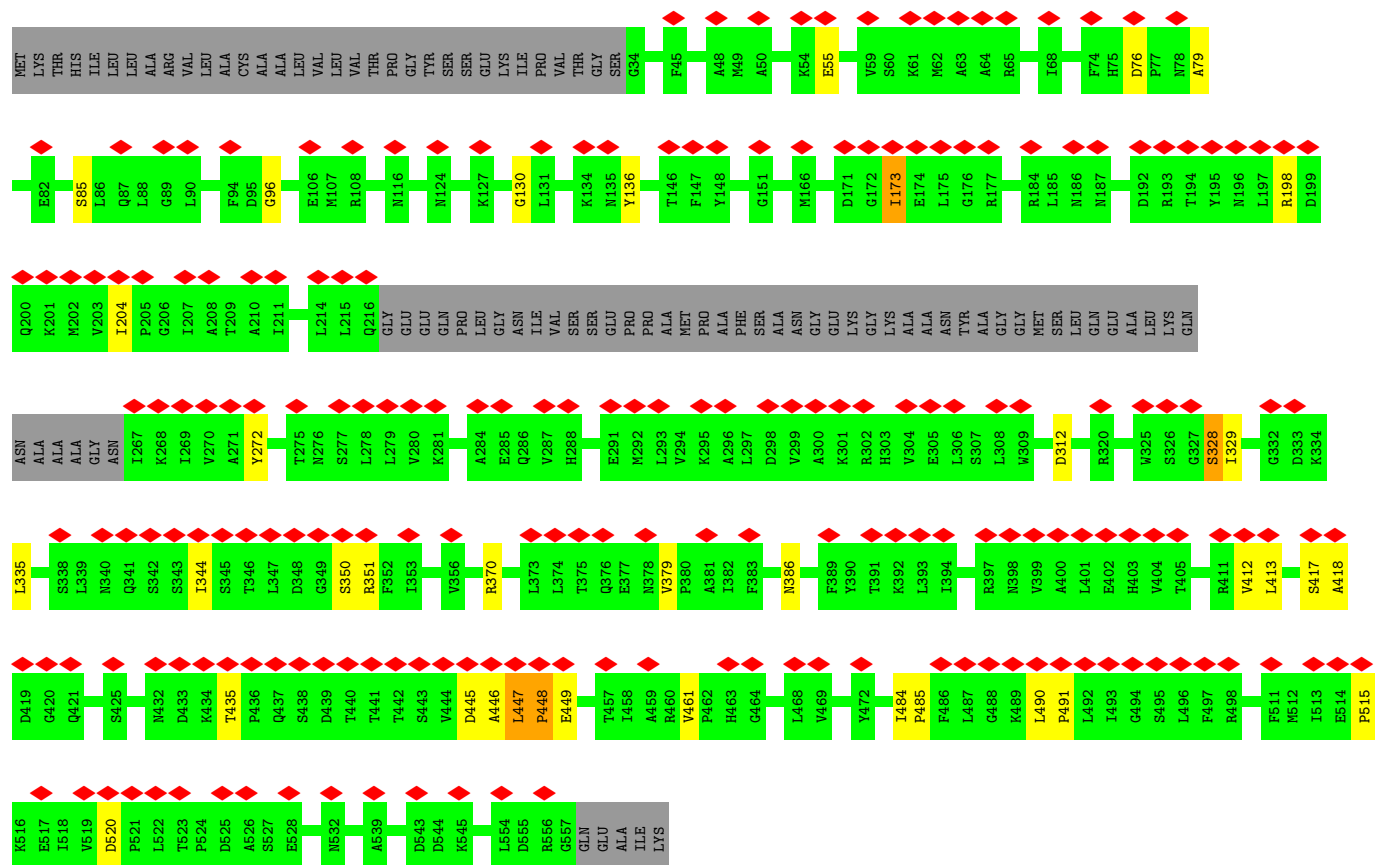
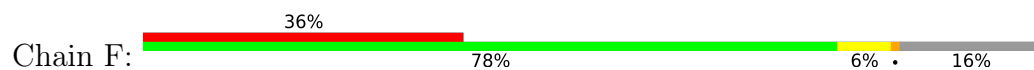


Chain D:  37% 78% 6% 16%

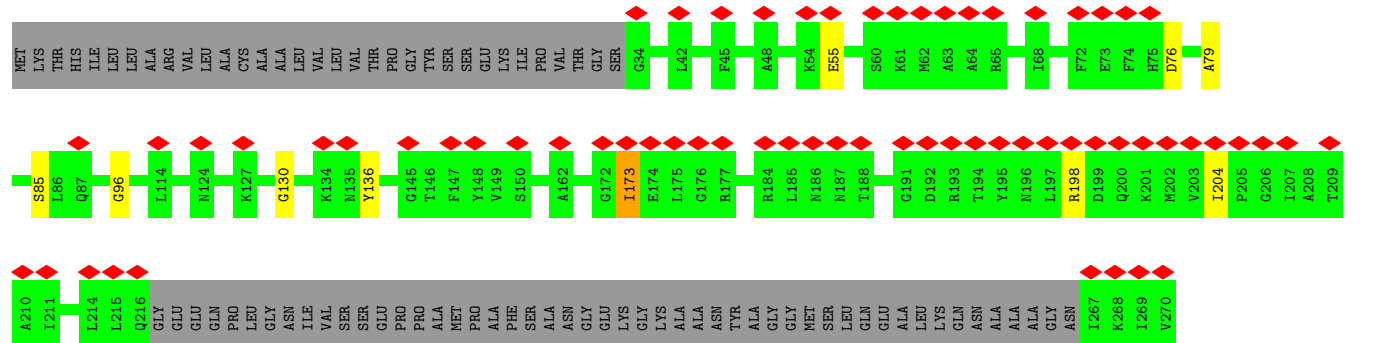
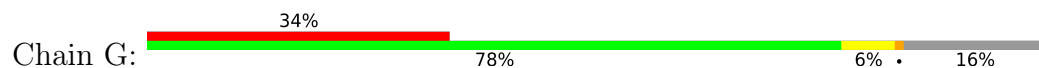
Chain E:  36% 78% 6% 16%

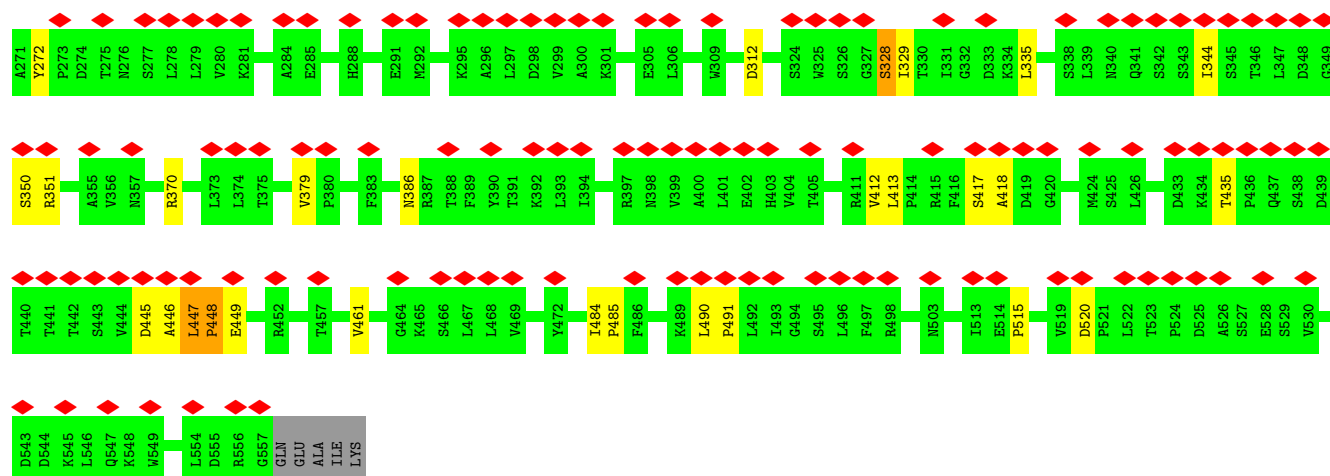


• Molecule 1: Protein InvG

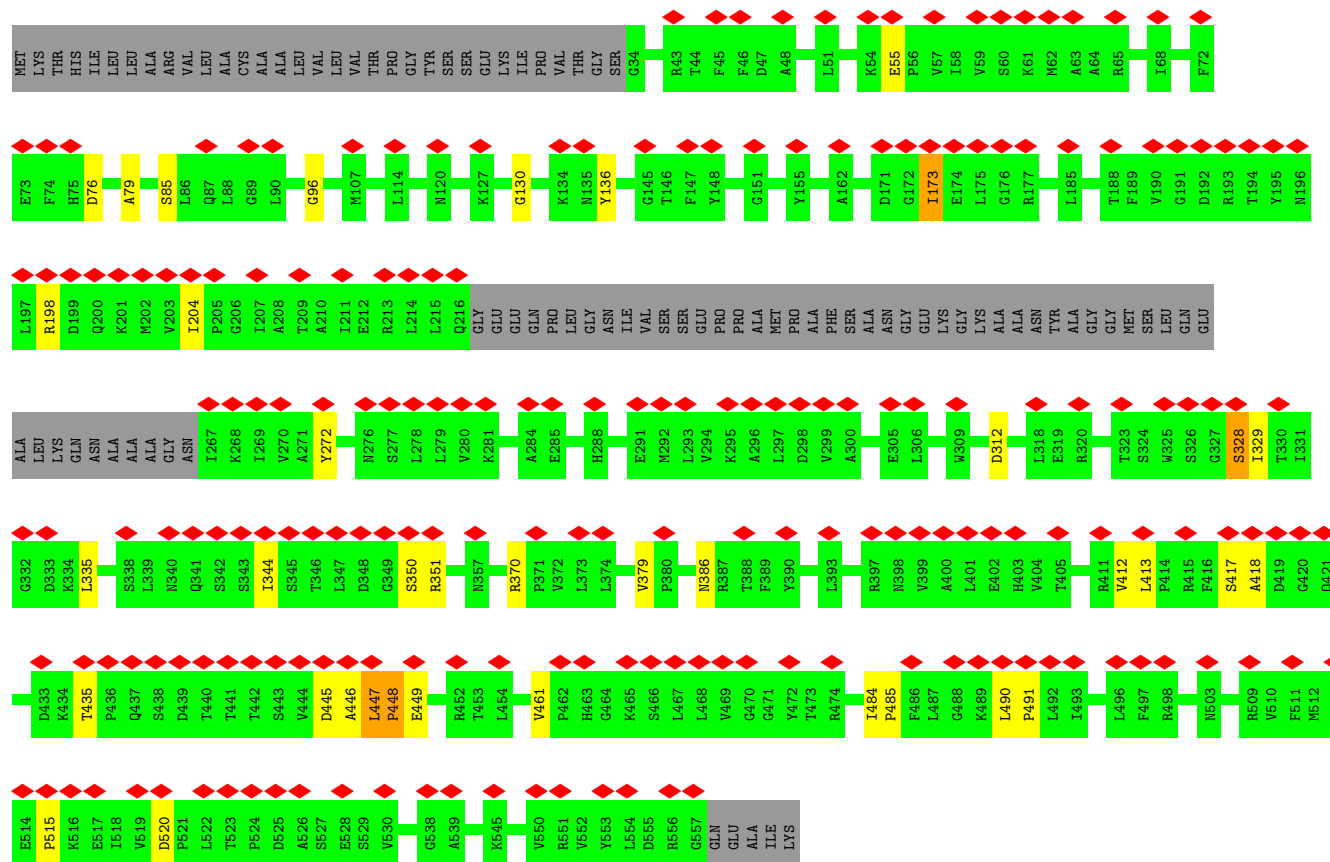
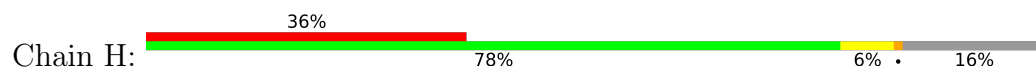


• Molecule 1: Protein InvG

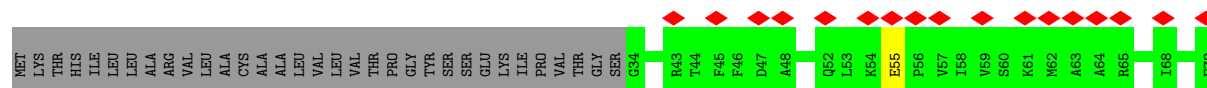
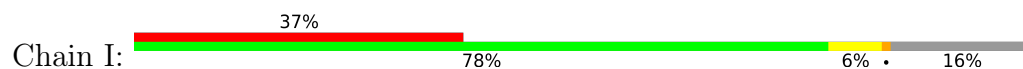


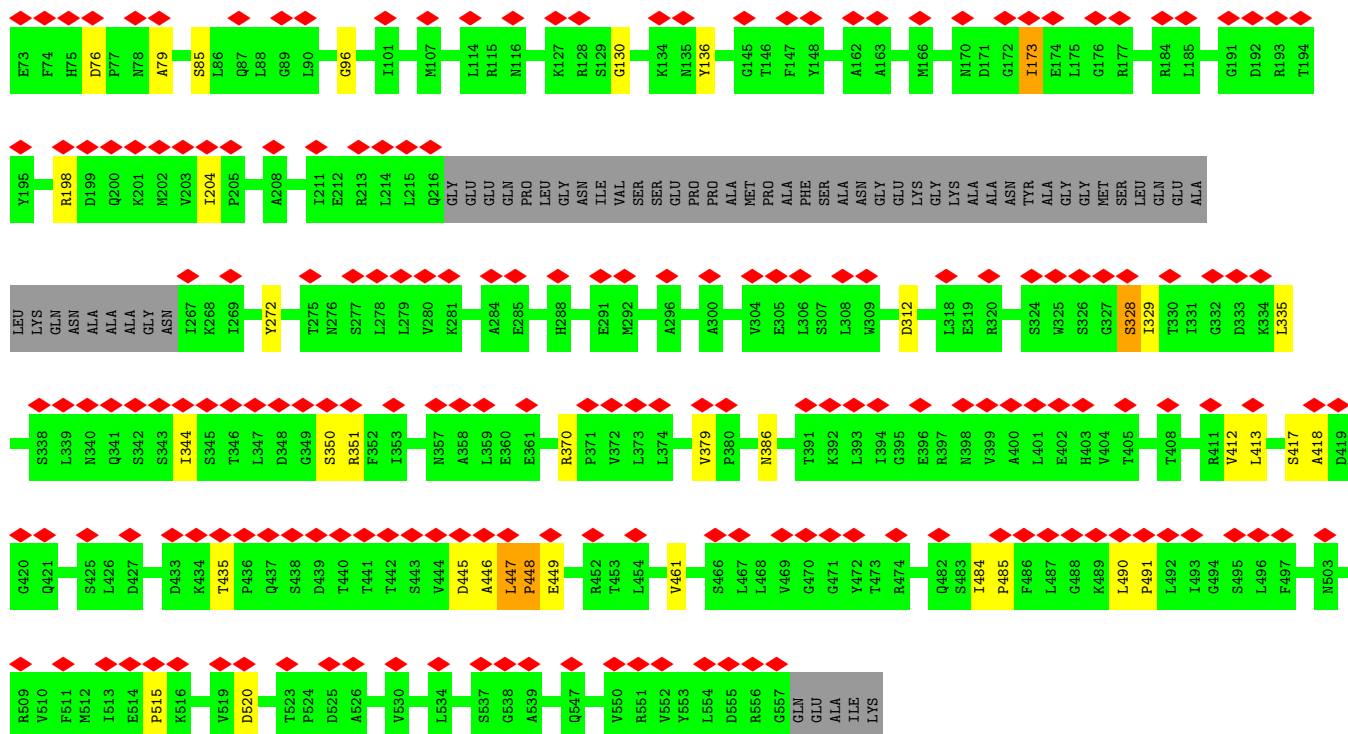


• Molecule 1: Protein InvG

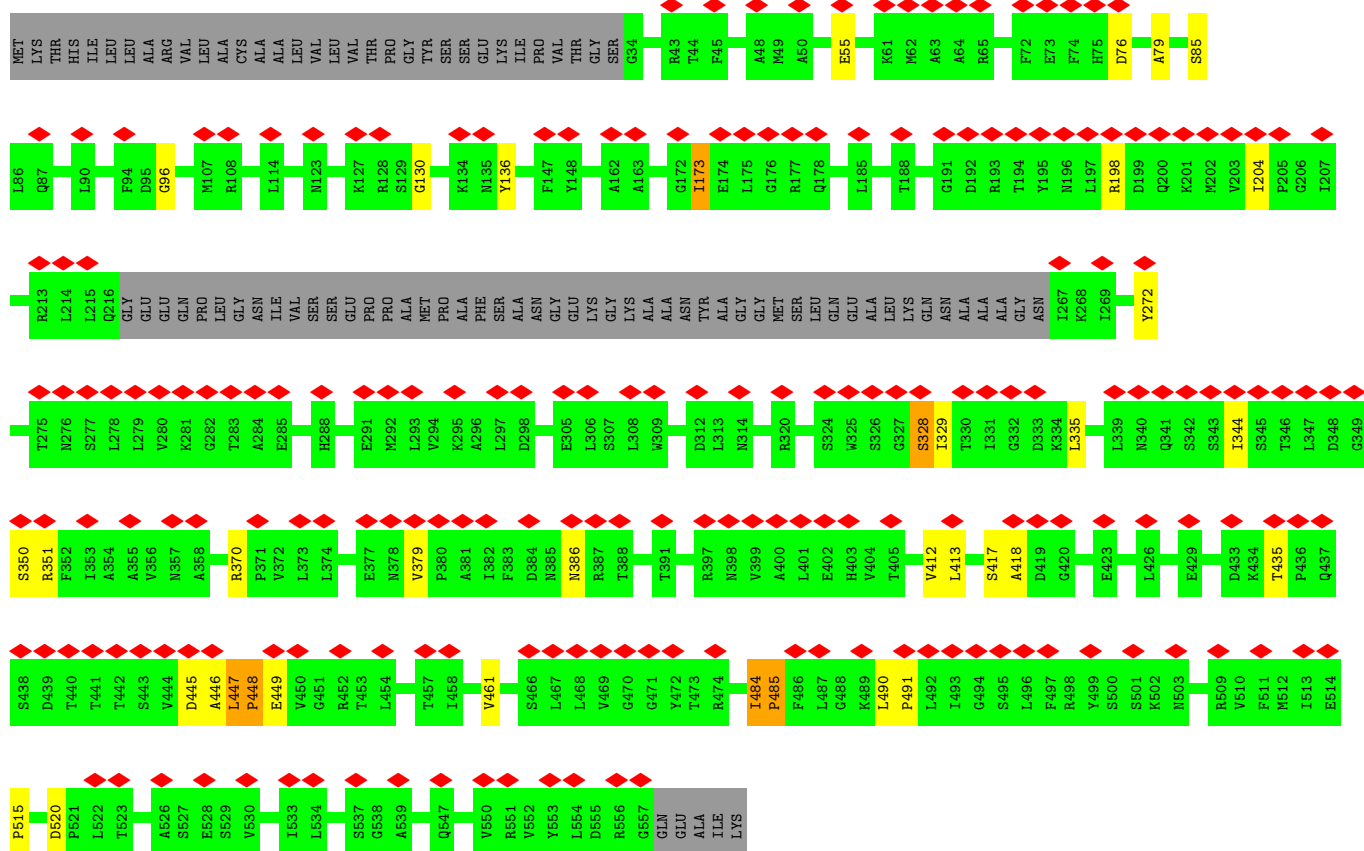
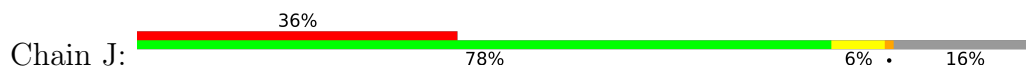


• Molecule 1: Protein InvG

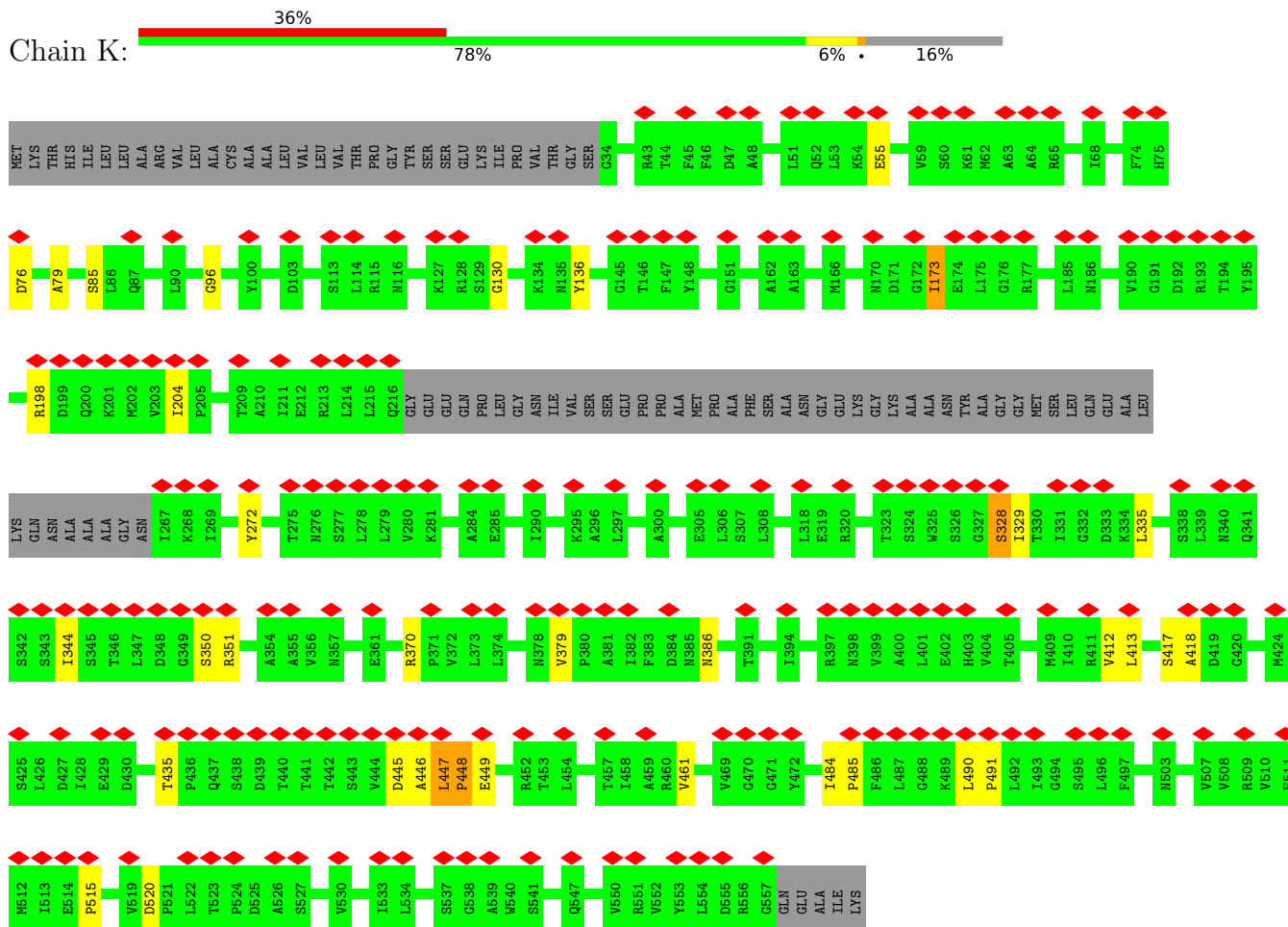




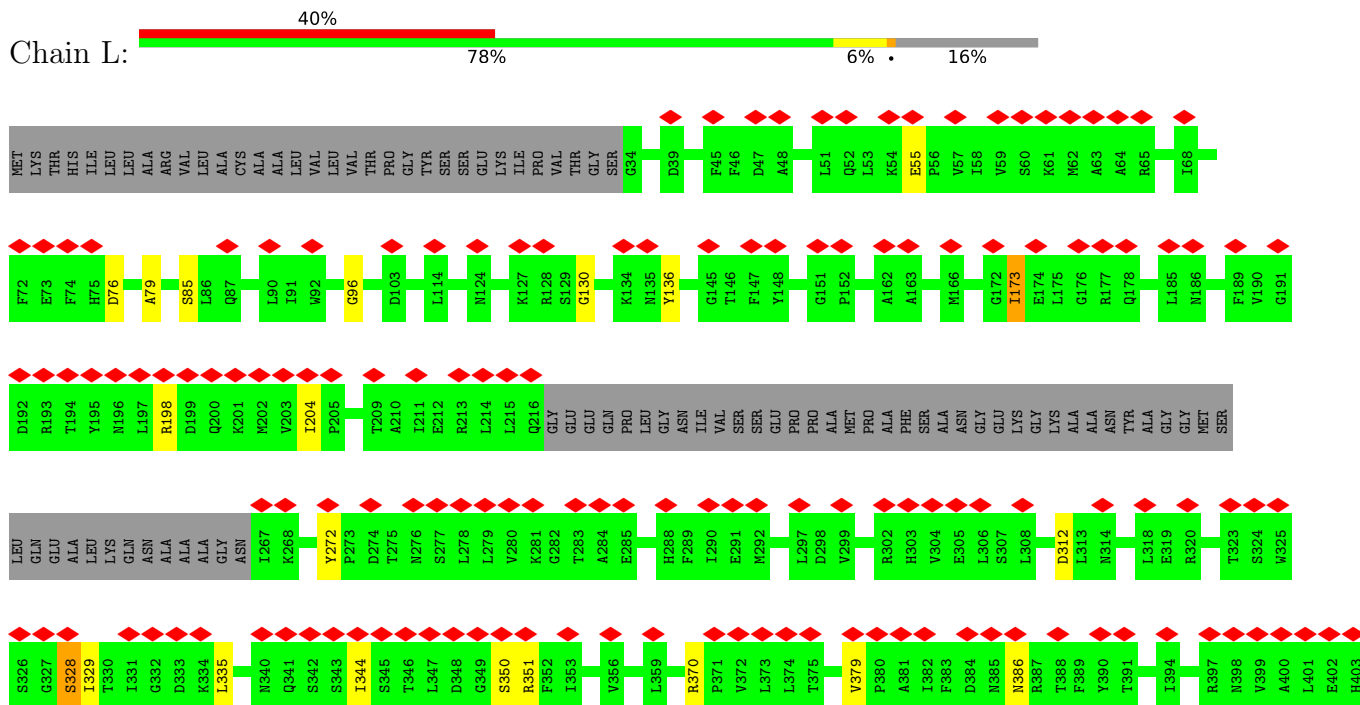
• Molecule 1: Protein InvG

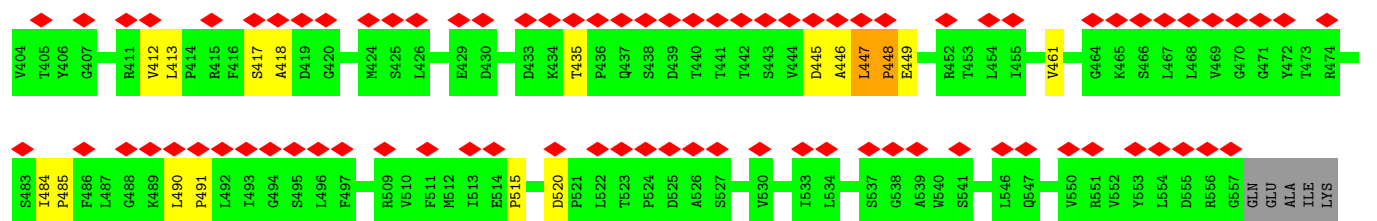


Chain K:

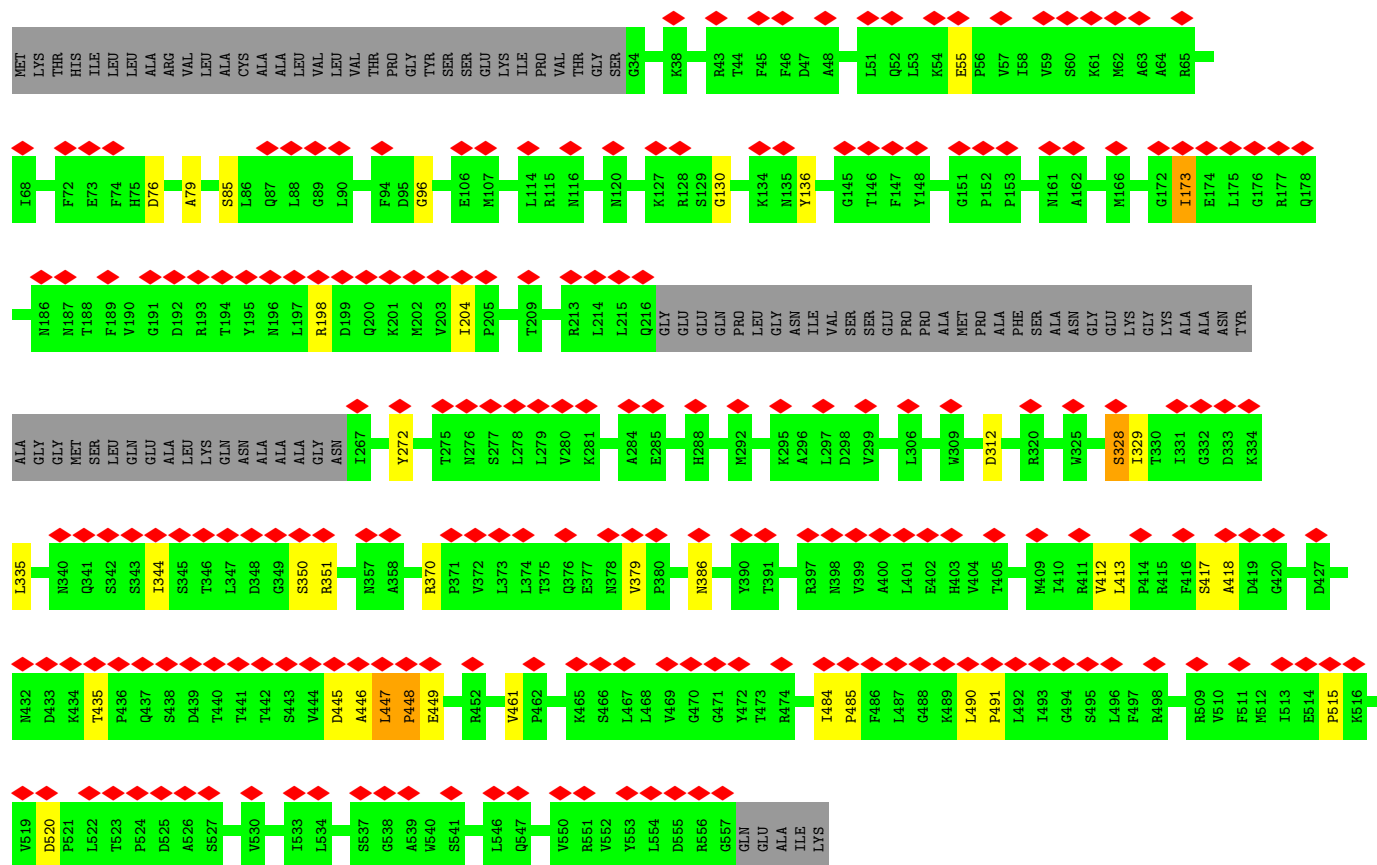
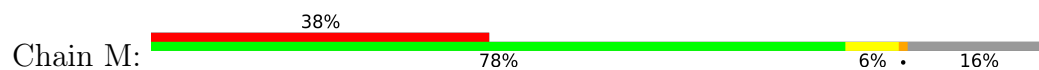


Chain L:

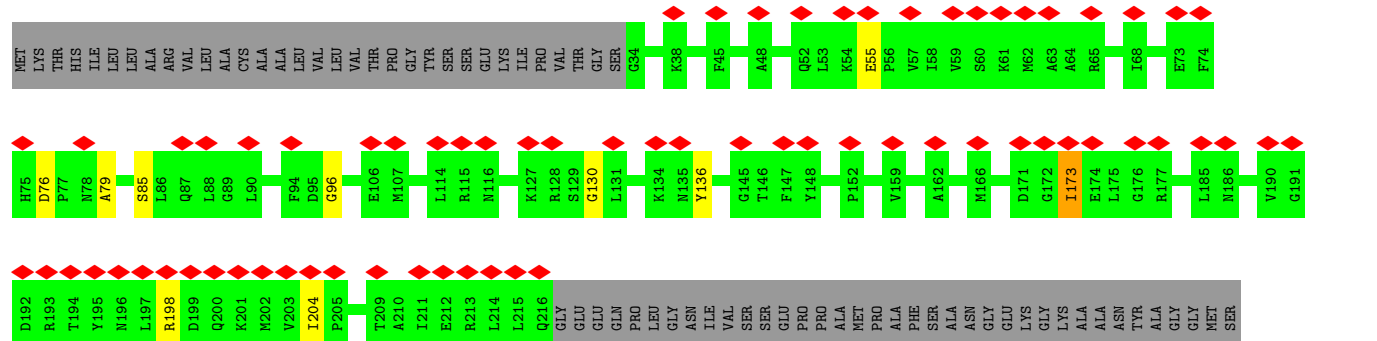
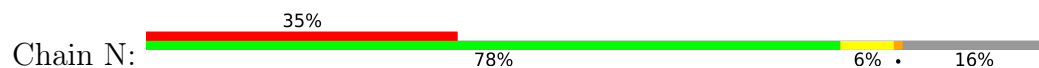




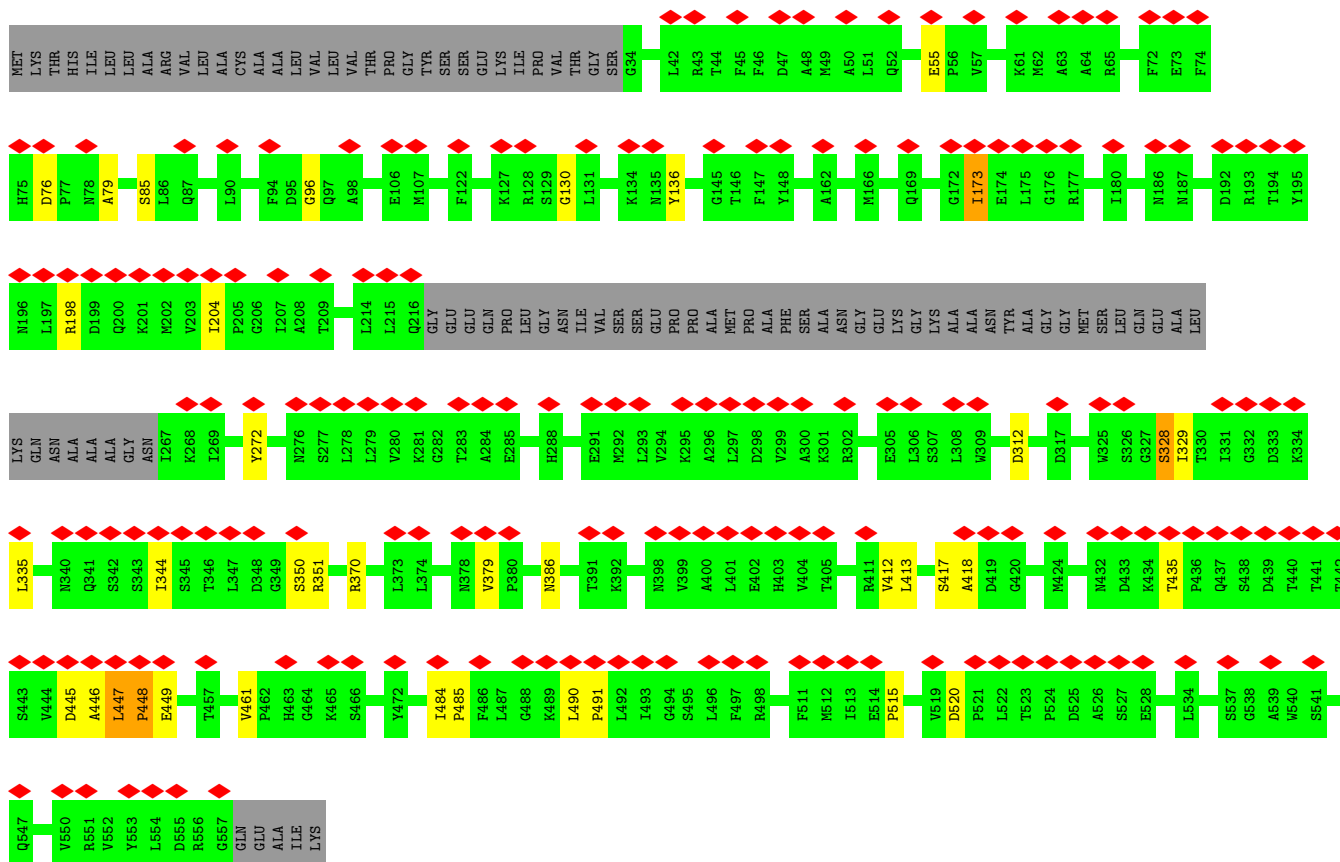
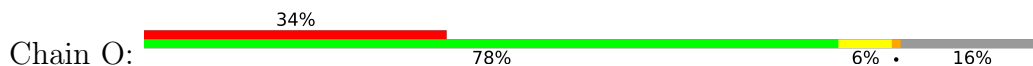
• Molecule 1: Protein InvG



• Molecule 1: Protein InvG

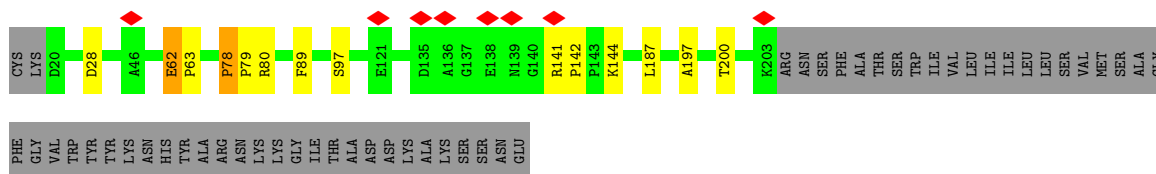


- Molecule 1: Protein InvG



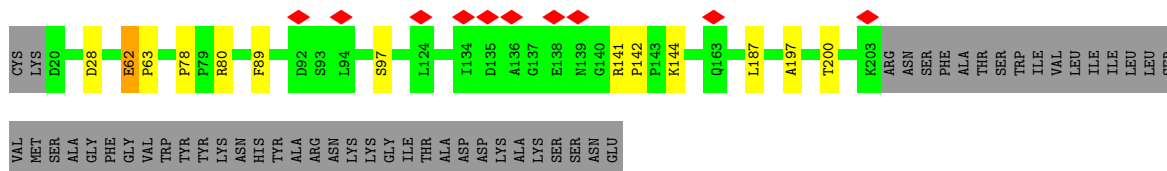
- Molecule 2: Lipoprotein PrgK





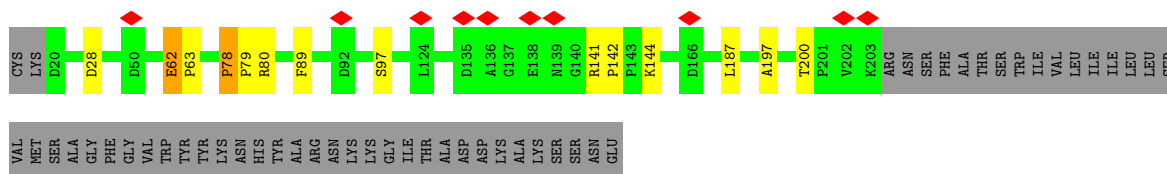
• Molecule 2: Lipoprotein PrgK

Chain R: 73% 5% 22%



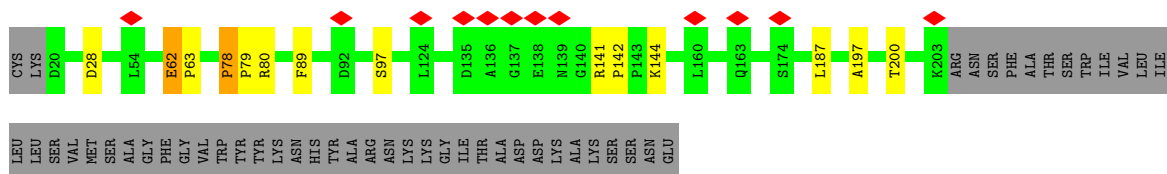
• Molecule 2: Lipoprotein PrgK

Chain T: 72% 5% 22%



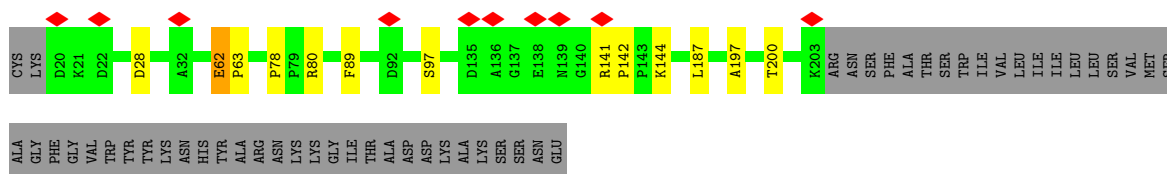
• Molecule 2: Lipoprotein PrgK

Chain V: 5% 72% 5% 22%



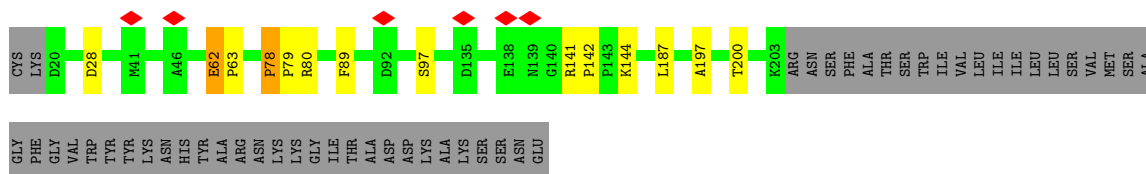
• Molecule 2: Lipoprotein PrgK

Chain X: 73% 5% 22%

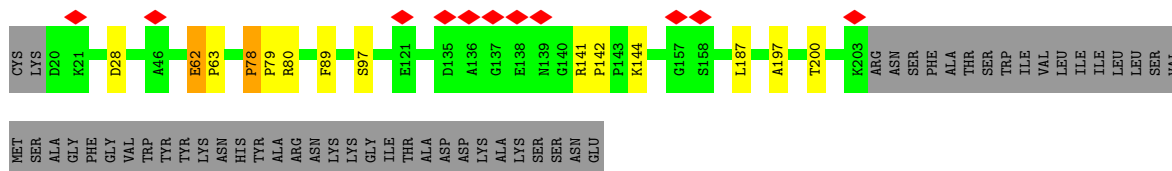


• Molecule 2: Lipoprotein PrgK

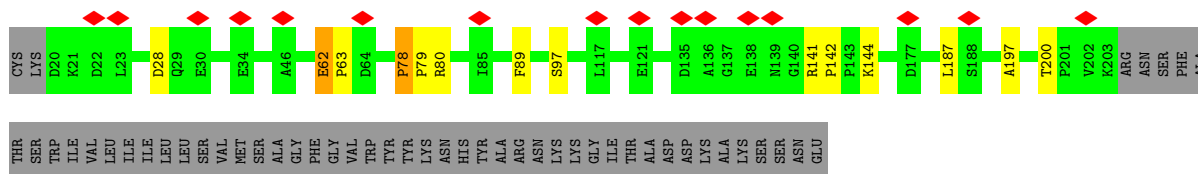
Chain a: 72% 5% 22%



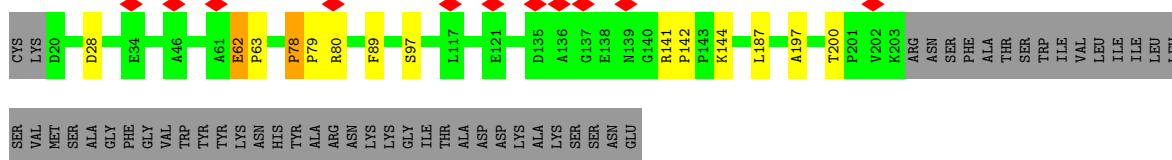
- Molecule 2: Lipoprotein PrgK



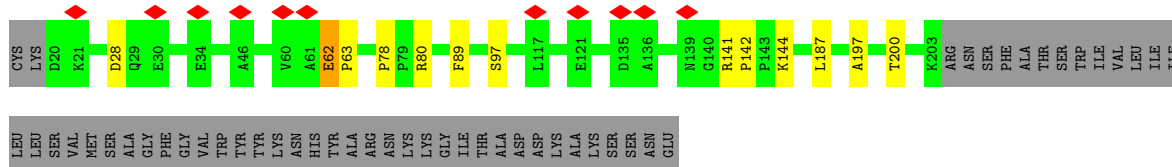
- Molecule 2: Lipoprotein PrgK



- Molecule 2: Lipoprotein PrgK

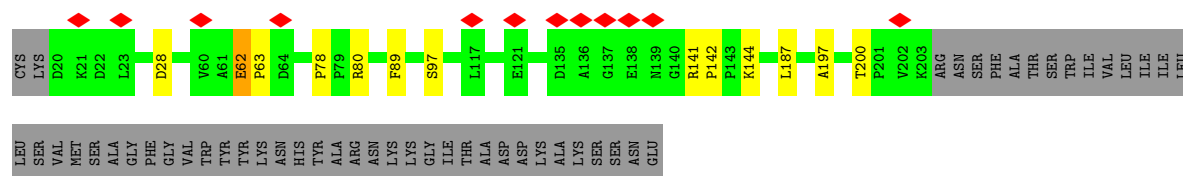


- Molecule 2: Lipoprotein PrgK

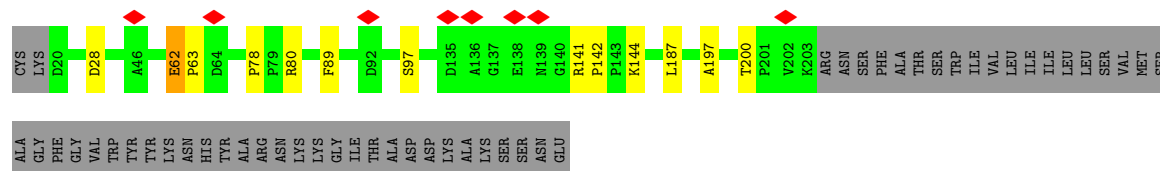


- Molecule 2: Lipoprotein PrgK

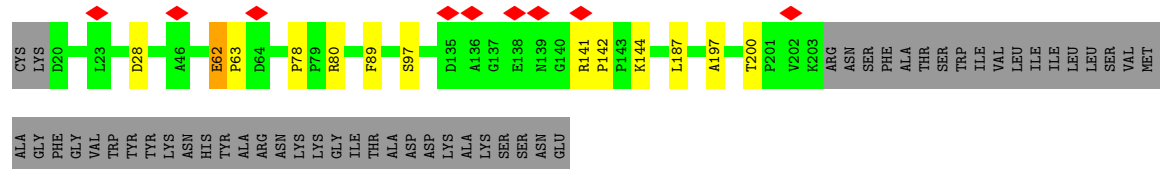




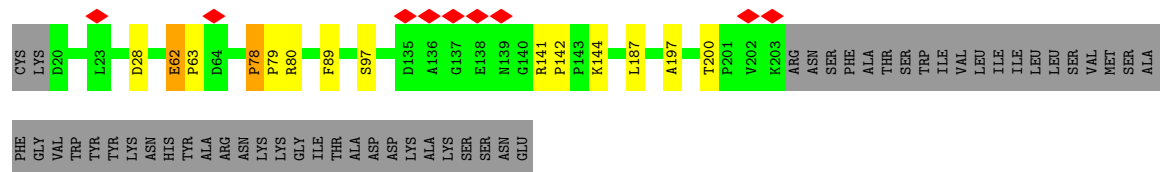
• Molecule 2: Lipoprotein PrgK



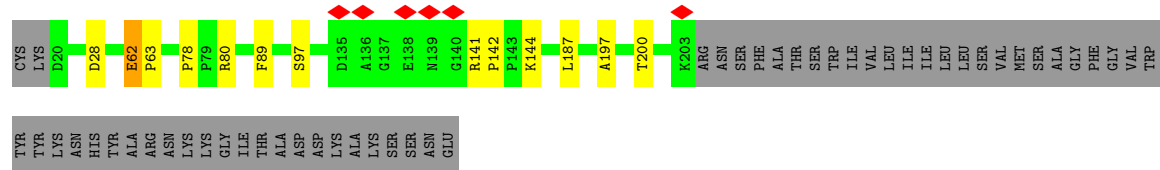
• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK

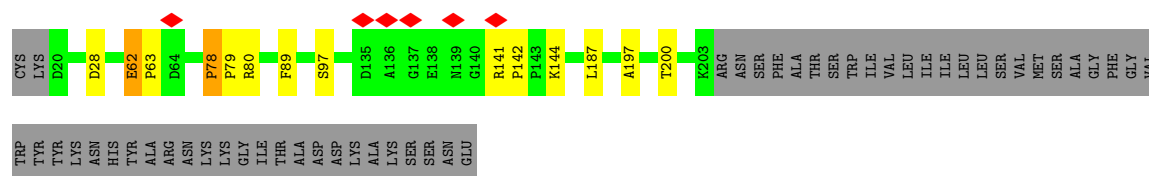


• Molecule 2: Lipoprotein PrgK

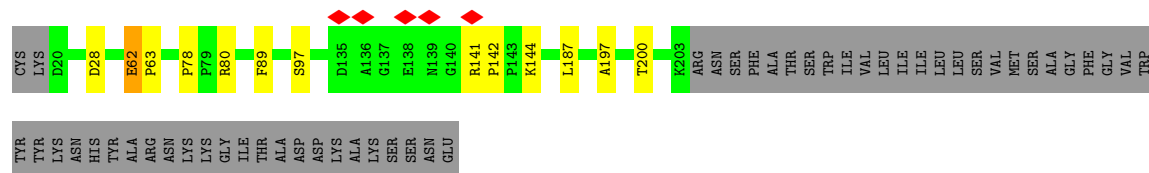


• Molecule 2: Lipoprotein PrgK

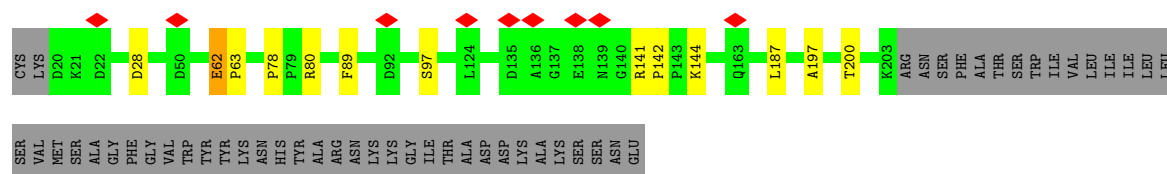




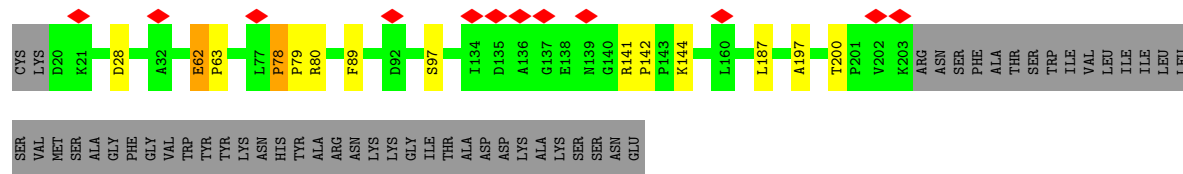
• Molecule 2: Lipoprotein PrgK



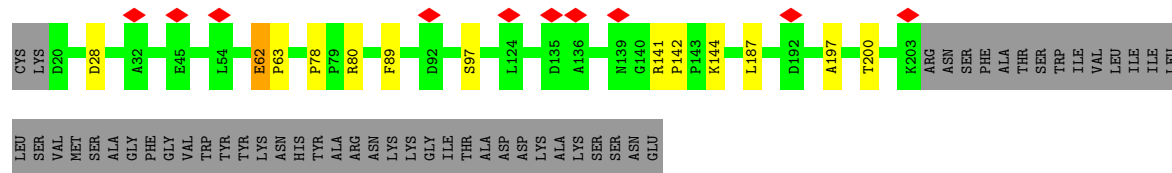
• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK

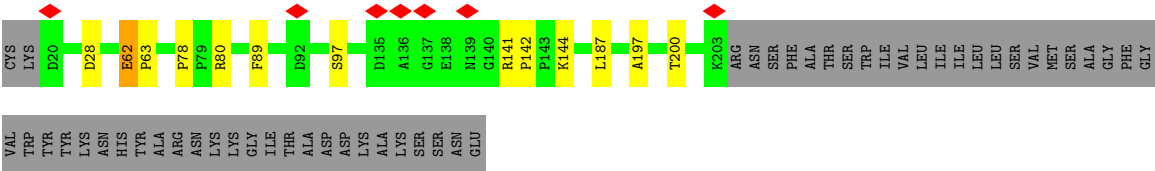


• Molecule 2: Lipoprotein PrgK

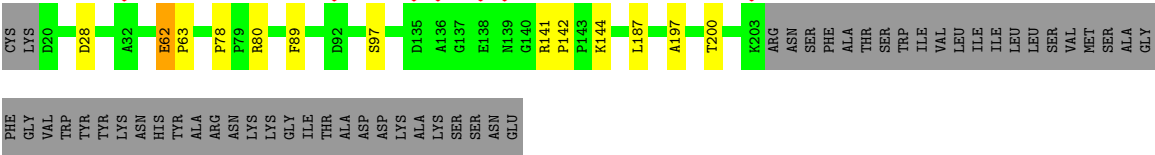


• Molecule 2: Lipoprotein PrgK

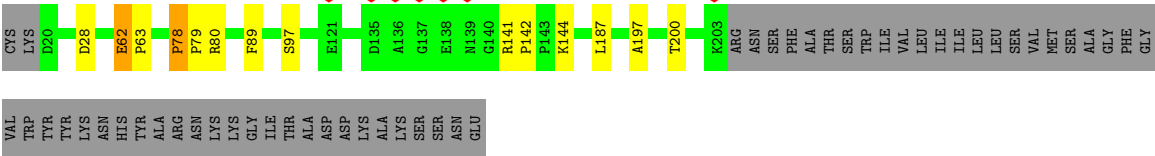




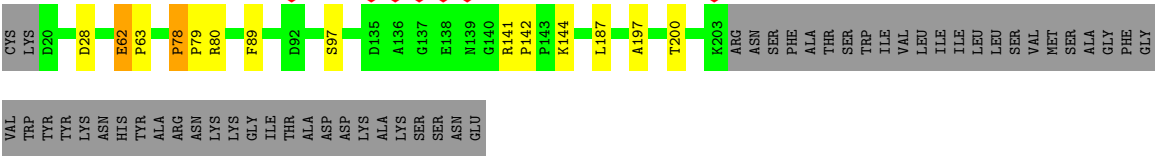
• Molecule 2: Lipoprotein PrgK



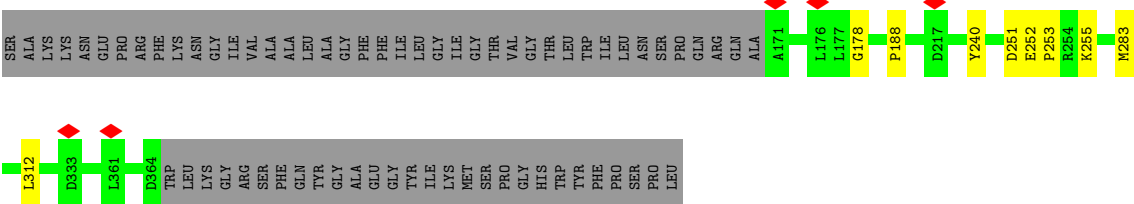
• Molecule 2: Lipoprotein PrgK



• Molecule 2: Lipoprotein PrgK

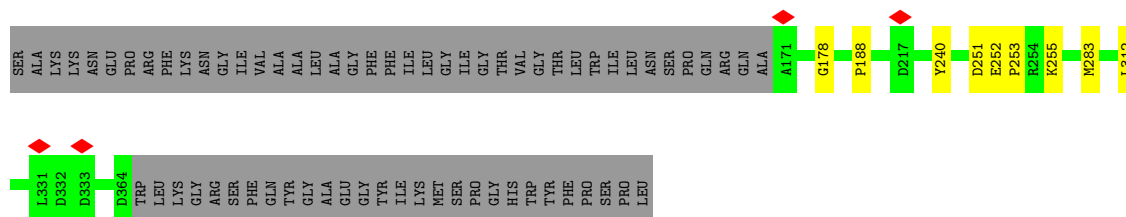


• Molecule 3: Protein PrgH



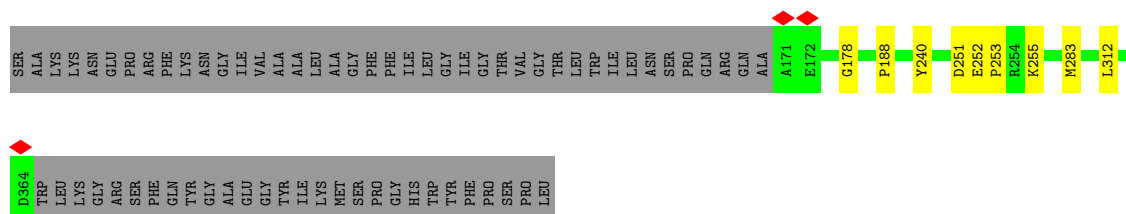
• Molecule 3: Protein PrgH

Chain S:  70% 26%



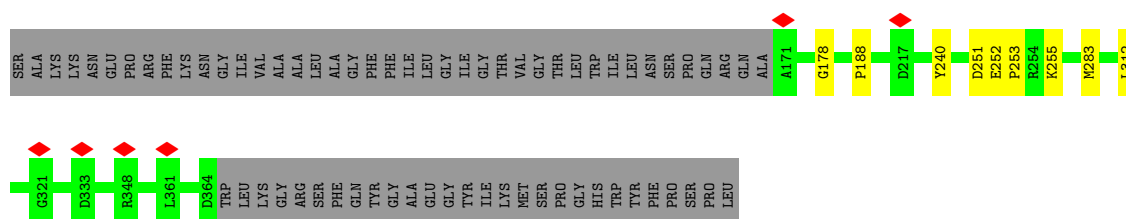
• Molecule 3: Protein PrgH

Chain U:  70% 26%



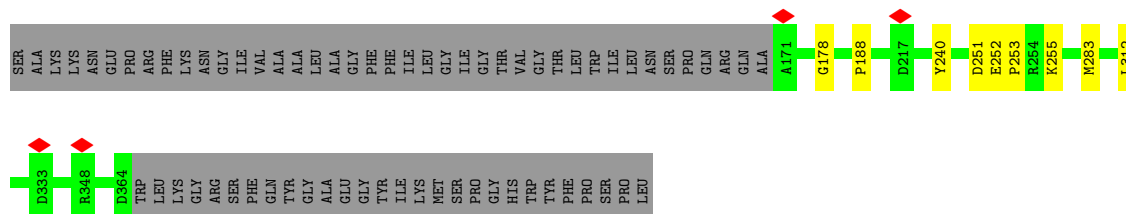
• Molecule 3: Protein PrgH

Chain W:  70% 26%



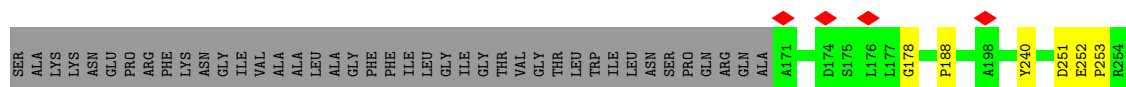
• Molecule 3: Protein PrgH

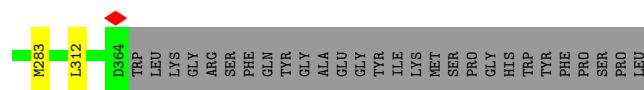
Chain Y:  70% 26%



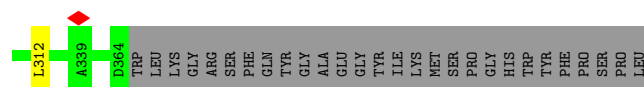
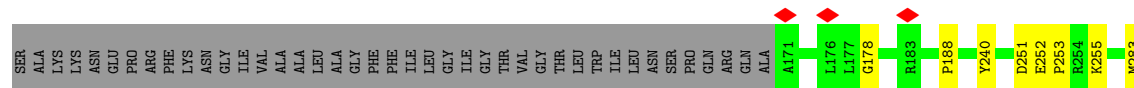
• Molecule 3: Protein PrgH

Chain Z:  70% 26%

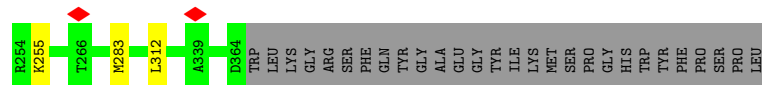
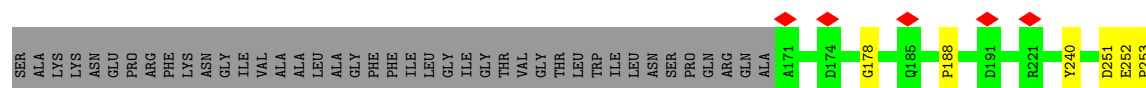




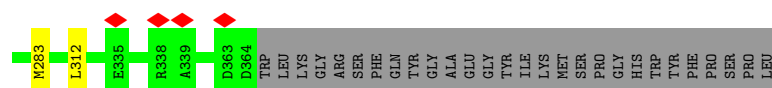
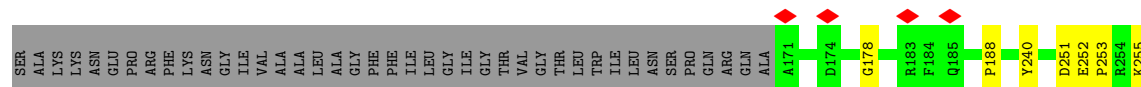
• Molecule 3: Protein PrgH



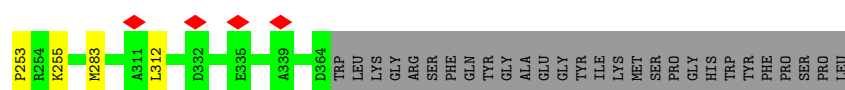
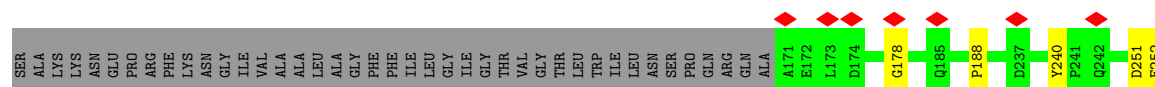
• Molecule 3: Protein PrgH



• Molecule 3: Protein PrgH

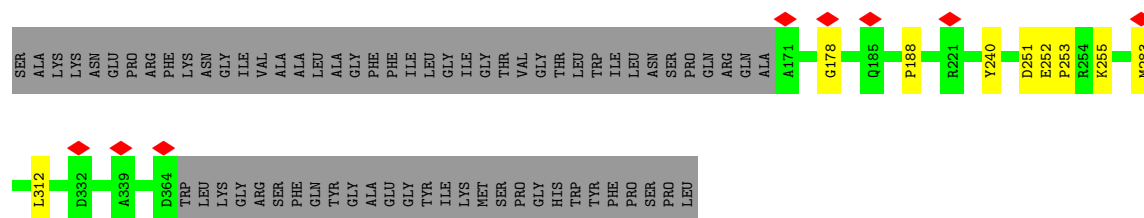


• Molecule 3: Protein PrgH



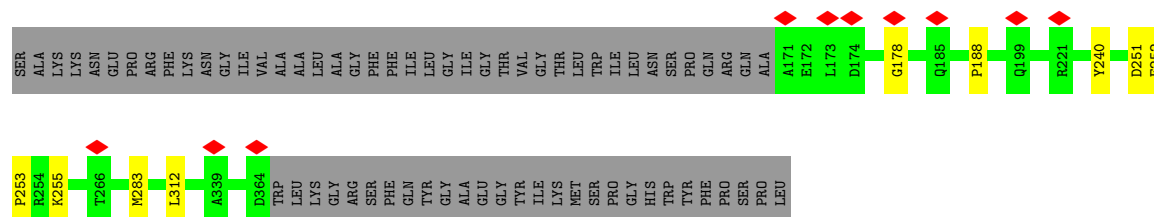
• Molecule 3: Protein PrgH

Chain j: 



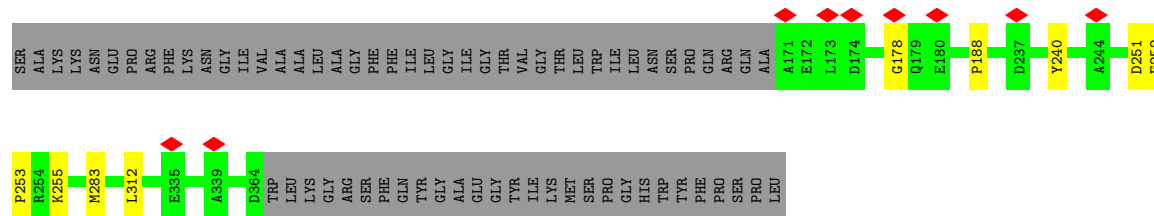
• Molecule 3: Protein PrgH

Chain l: 



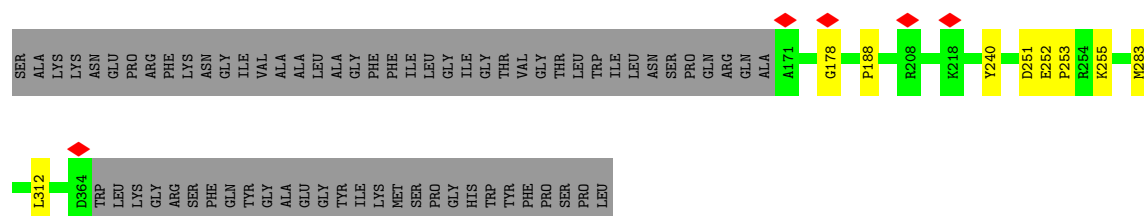
• Molecule 3: Protein PrgH

Chain n: 



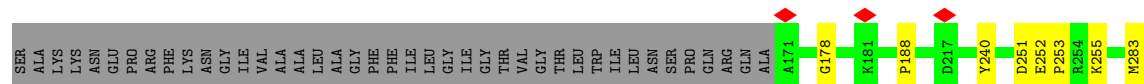
• Molecule 3: Protein PrgH

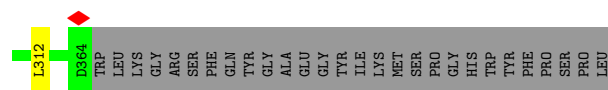
Chain p: 



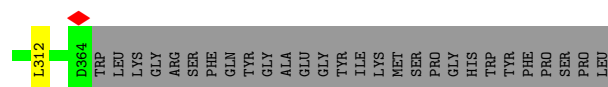
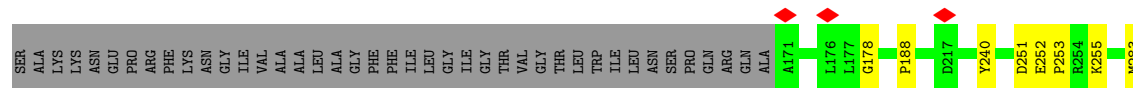
• Molecule 3: Protein PrgH

Chain r: 

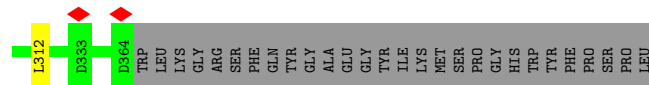
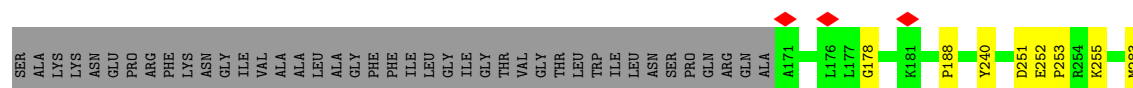




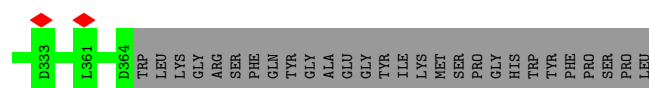
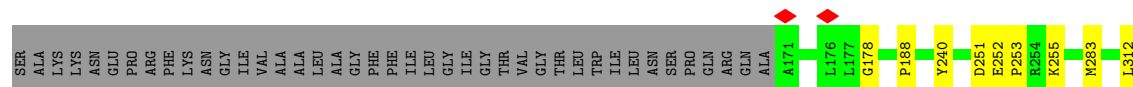
• Molecule 3: Protein PrgH



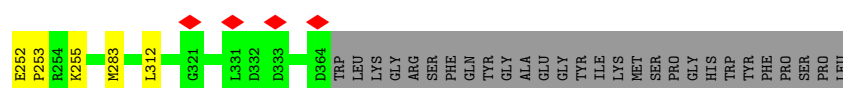
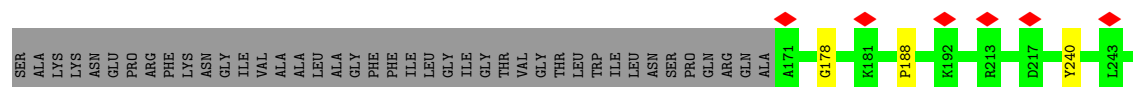
• Molecule 3: Protein PrgH



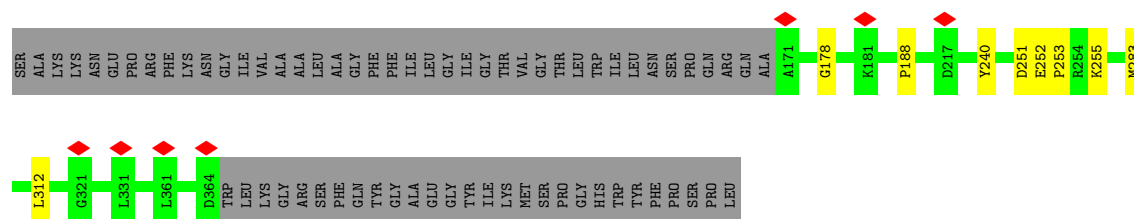
• Molecule 3: Protein PrgH



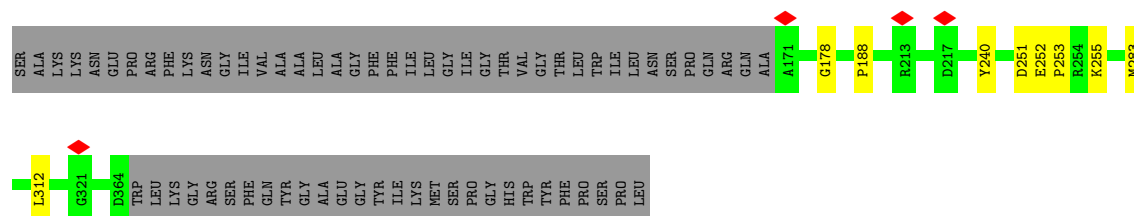
• Molecule 3: Protein PrgH



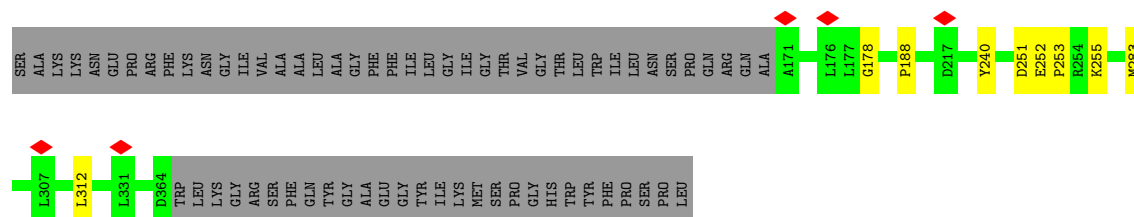
• Molecule 3: Protein PrgH



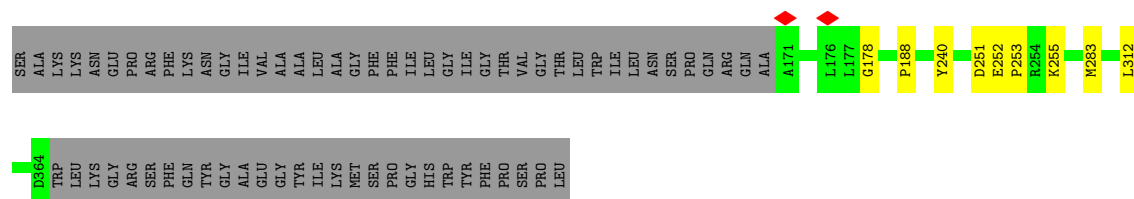
• Molecule 3: Protein PrgH



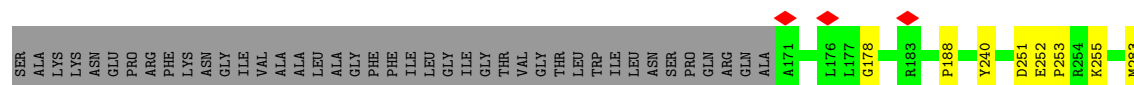
• Molecule 3: Protein PrgH

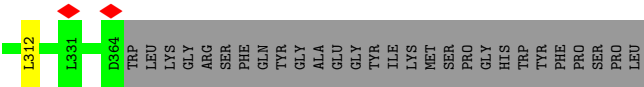


• Molecule 3: Protein PrgH



• Molecule 3: Protein PrgH





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.3	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	29240	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.71, 1.71, 1.71	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	B	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	C	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	D	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	E	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	F	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	G	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	H	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	I	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	J	0.85	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	K	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	L	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	M	0.85	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	N	0.86	1/3780 (0.0%)	1.11	30/5115 (0.6%)
1	O	0.85	1/3780 (0.0%)	1.11	30/5115 (0.6%)
2	1	0.77	0/1465	1.19	20/1989 (1.0%)
2	3	0.77	0/1465	1.19	20/1989 (1.0%)
2	5	0.77	0/1465	1.20	20/1989 (1.0%)
2	7	0.77	0/1465	1.19	20/1989 (1.0%)
2	9	0.77	0/1465	1.19	20/1989 (1.0%)
2	P	0.77	0/1465	1.19	20/1989 (1.0%)
2	R	0.77	0/1465	1.20	20/1989 (1.0%)
2	T	0.77	0/1465	1.19	20/1989 (1.0%)
2	V	0.77	0/1465	1.19	20/1989 (1.0%)
2	X	0.77	0/1465	1.19	20/1989 (1.0%)
2	a	0.77	0/1465	1.20	20/1989 (1.0%)
2	c	0.77	0/1465	1.19	20/1989 (1.0%)
2	e	0.77	0/1465	1.19	20/1989 (1.0%)
2	g	0.77	0/1465	1.19	20/1989 (1.0%)
2	i	0.77	0/1465	1.19	20/1989 (1.0%)
2	k	0.77	0/1465	1.19	20/1989 (1.0%)
2	m	0.77	0/1465	1.19	20/1989 (1.0%)
2	o	0.77	0/1465	1.19	20/1989 (1.0%)
2	q	0.77	0/1465	1.19	20/1989 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	s	0.77	0/1465	1.19	20/1989 (1.0%)
2	u	0.77	0/1465	1.19	20/1989 (1.0%)
2	w	0.77	0/1465	1.19	20/1989 (1.0%)
2	y	0.77	0/1465	1.19	20/1989 (1.0%)
2	z	0.77	0/1465	1.20	20/1989 (1.0%)
3	0	0.76	0/1632	0.99	10/2204 (0.5%)
3	10	0.76	0/1632	0.99	10/2204 (0.5%)
3	2	0.76	0/1632	0.99	10/2204 (0.5%)
3	4	0.76	0/1632	0.99	10/2204 (0.5%)
3	6	0.76	0/1632	0.99	10/2204 (0.5%)
3	8	0.76	0/1632	0.99	10/2204 (0.5%)
3	Q	0.76	0/1632	0.99	10/2204 (0.5%)
3	S	0.76	0/1632	0.99	10/2204 (0.5%)
3	U	0.76	0/1632	0.99	10/2204 (0.5%)
3	W	0.76	0/1632	0.99	10/2204 (0.5%)
3	Y	0.76	0/1632	0.99	10/2204 (0.5%)
3	Z	0.76	0/1632	0.99	10/2204 (0.5%)
3	b	0.76	0/1632	0.99	10/2204 (0.5%)
3	d	0.76	0/1632	0.99	10/2204 (0.5%)
3	f	0.76	0/1632	0.99	10/2204 (0.5%)
3	h	0.76	0/1632	0.99	10/2204 (0.5%)
3	j	0.76	0/1632	0.99	10/2204 (0.5%)
3	l	0.76	0/1632	0.99	10/2204 (0.5%)
3	n	0.76	0/1632	0.99	10/2204 (0.5%)
3	p	0.76	0/1632	0.99	10/2204 (0.5%)
3	r	0.76	0/1632	0.99	10/2204 (0.5%)
3	t	0.76	0/1632	0.99	10/2204 (0.5%)
3	v	0.76	0/1632	0.99	10/2204 (0.5%)
3	x	0.76	0/1632	0.99	10/2204 (0.5%)
All	All	0.80	15/131028 (0.0%)	1.10	1170/177357 (0.7%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	79	ALA	CA-CB	-5.11	1.44	1.53
1	K	79	ALA	CA-CB	-5.11	1.44	1.53
1	M	79	ALA	CA-CB	-5.10	1.44	1.53
1	G	79	ALA	CA-CB	-5.09	1.44	1.53
1	B	79	ALA	CA-CB	-5.09	1.44	1.53
1	I	79	ALA	CA-CB	-5.08	1.44	1.53
1	J	79	ALA	CA-CB	-5.08	1.44	1.53
1	E	79	ALA	CA-CB	-5.08	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	79	ALA	CA-CB	-5.08	1.44	1.53
1	A	79	ALA	CA-CB	-5.08	1.44	1.53
1	C	79	ALA	CA-CB	-5.07	1.44	1.53
1	H	79	ALA	CA-CB	-5.05	1.44	1.53
1	O	79	ALA	CA-CB	-5.05	1.45	1.53
1	F	79	ALA	CA-CB	-5.05	1.45	1.53
1	L	79	ALA	CA-CB	-5.04	1.45	1.53

All (1170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	141	ARG	CA-C-N	10.30	127.08	119.66
2	P	141	ARG	C-N-CA	10.30	127.08	119.66
2	e	141	ARG	CA-C-N	10.30	127.08	119.66
2	e	141	ARG	C-N-CA	10.30	127.08	119.66
2	R	141	ARG	CA-C-N	10.29	127.07	119.66
2	R	141	ARG	C-N-CA	10.29	127.07	119.66
2	m	141	ARG	CA-C-N	10.27	127.06	119.66
2	m	141	ARG	C-N-CA	10.27	127.06	119.66
2	a	141	ARG	CA-C-N	10.27	127.05	119.66
2	a	141	ARG	C-N-CA	10.27	127.05	119.66
2	y	141	ARG	CA-C-N	10.26	127.05	119.66
2	y	141	ARG	C-N-CA	10.26	127.05	119.66
2	X	141	ARG	CA-C-N	10.26	127.05	119.66
2	X	141	ARG	C-N-CA	10.26	127.05	119.66
2	3	141	ARG	CA-C-N	10.26	127.05	119.66
2	3	141	ARG	C-N-CA	10.26	127.05	119.66
2	s	141	ARG	CA-C-N	10.25	127.04	119.66
2	s	141	ARG	C-N-CA	10.25	127.04	119.66
2	g	141	ARG	CA-C-N	10.25	127.04	119.66
2	g	141	ARG	C-N-CA	10.25	127.04	119.66
2	u	141	ARG	CA-C-N	10.24	127.03	119.66
2	u	141	ARG	C-N-CA	10.24	127.03	119.66
2	o	141	ARG	CA-C-N	10.23	127.03	119.66
2	o	141	ARG	C-N-CA	10.23	127.03	119.66
2	5	141	ARG	CA-C-N	10.23	127.03	119.66
2	5	141	ARG	C-N-CA	10.23	127.03	119.66
2	k	141	ARG	CA-C-N	10.23	127.03	119.66
2	k	141	ARG	C-N-CA	10.23	127.03	119.66
2	i	141	ARG	CA-C-N	10.22	127.02	119.66
2	i	141	ARG	C-N-CA	10.22	127.02	119.66
2	9	141	ARG	CA-C-N	10.22	127.02	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	141	ARG	C-N-CA	10.22	127.02	119.66
2	c	141	ARG	CA-C-N	10.21	127.01	119.66
2	c	141	ARG	C-N-CA	10.21	127.01	119.66
2	V	141	ARG	CA-C-N	10.21	127.01	119.66
2	V	141	ARG	C-N-CA	10.21	127.01	119.66
2	z	141	ARG	CA-C-N	10.20	127.01	119.66
2	z	141	ARG	C-N-CA	10.20	127.01	119.66
2	q	141	ARG	CA-C-N	10.20	127.00	119.66
2	q	141	ARG	C-N-CA	10.20	127.00	119.66
2	7	141	ARG	CA-C-N	10.19	127.00	119.66
2	7	141	ARG	C-N-CA	10.19	127.00	119.66
2	w	141	ARG	CA-C-N	10.19	126.99	119.66
2	w	141	ARG	C-N-CA	10.19	126.99	119.66
2	1	141	ARG	CA-C-N	10.18	126.99	119.66
2	1	141	ARG	C-N-CA	10.18	126.99	119.66
2	T	141	ARG	CA-C-N	10.18	126.99	119.66
2	T	141	ARG	C-N-CA	10.18	126.99	119.66
1	L	272	TYR	CA-C-N	9.48	130.13	119.32
1	L	272	TYR	C-N-CA	9.48	130.13	119.32
1	H	272	TYR	CA-C-N	9.45	130.09	119.32
1	H	272	TYR	C-N-CA	9.45	130.09	119.32
1	I	272	TYR	CA-C-N	9.45	130.09	119.32
1	I	272	TYR	C-N-CA	9.45	130.09	119.32
1	E	272	TYR	CA-C-N	9.44	130.08	119.32
1	E	272	TYR	C-N-CA	9.44	130.08	119.32
1	G	272	TYR	CA-C-N	9.44	130.08	119.32
1	G	272	TYR	C-N-CA	9.44	130.08	119.32
1	M	272	TYR	CA-C-N	9.43	130.07	119.32
1	M	272	TYR	C-N-CA	9.43	130.07	119.32
1	K	272	TYR	CA-C-N	9.43	130.07	119.32
1	K	272	TYR	C-N-CA	9.43	130.07	119.32
1	B	272	TYR	CA-C-N	9.41	130.05	119.32
1	B	272	TYR	C-N-CA	9.41	130.05	119.32
1	C	272	TYR	CA-C-N	9.41	130.05	119.32
1	C	272	TYR	C-N-CA	9.41	130.05	119.32
1	F	272	TYR	CA-C-N	9.40	130.04	119.32
1	F	272	TYR	C-N-CA	9.40	130.04	119.32
1	N	272	TYR	CA-C-N	9.40	130.04	119.32
1	N	272	TYR	C-N-CA	9.40	130.04	119.32
1	D	272	TYR	CA-C-N	9.40	130.03	119.32
1	D	272	TYR	C-N-CA	9.40	130.03	119.32
1	A	272	TYR	CA-C-N	9.39	130.03	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	TYR	C-N-CA	9.39	130.03	119.32
1	J	272	TYR	CA-C-N	9.38	130.01	119.32
1	J	272	TYR	C-N-CA	9.38	130.01	119.32
1	O	272	TYR	CA-C-N	9.37	130.00	119.32
1	O	272	TYR	C-N-CA	9.37	130.00	119.32
3	6	283	MET	CA-C-N	9.21	130.15	119.47
3	6	283	MET	C-N-CA	9.21	130.15	119.47
3	x	283	MET	CA-C-N	9.20	130.15	119.47
3	x	283	MET	C-N-CA	9.20	130.15	119.47
3	8	283	MET	CA-C-N	9.19	130.14	119.47
3	8	283	MET	C-N-CA	9.19	130.14	119.47
3	n	283	MET	CA-C-N	9.19	130.13	119.47
3	n	283	MET	C-N-CA	9.19	130.13	119.47
3	t	283	MET	CA-C-N	9.19	130.13	119.47
3	t	283	MET	C-N-CA	9.19	130.13	119.47
3	Z	283	MET	CA-C-N	9.19	130.13	119.47
3	Z	283	MET	C-N-CA	9.19	130.13	119.47
3	b	283	MET	CA-C-N	9.19	130.13	119.47
3	b	283	MET	C-N-CA	9.19	130.13	119.47
3	l	283	MET	CA-C-N	9.19	130.12	119.47
3	l	283	MET	C-N-CA	9.19	130.12	119.47
3	0	283	MET	CA-C-N	9.19	130.13	119.47
3	0	283	MET	C-N-CA	9.19	130.13	119.47
3	2	283	MET	CA-C-N	9.18	130.12	119.47
3	2	283	MET	C-N-CA	9.18	130.12	119.47
3	j	283	MET	CA-C-N	9.18	130.12	119.47
3	j	283	MET	C-N-CA	9.18	130.12	119.47
3	p	283	MET	CA-C-N	9.18	130.12	119.47
3	p	283	MET	C-N-CA	9.18	130.12	119.47
3	10	283	MET	CA-C-N	9.18	130.11	119.47
3	10	283	MET	C-N-CA	9.18	130.11	119.47
3	v	283	MET	CA-C-N	9.17	130.11	119.47
3	v	283	MET	C-N-CA	9.17	130.11	119.47
3	U	283	MET	CA-C-N	9.17	130.10	119.47
3	U	283	MET	C-N-CA	9.17	130.10	119.47
3	Y	283	MET	CA-C-N	9.17	130.10	119.47
3	Y	283	MET	C-N-CA	9.17	130.10	119.47
3	S	283	MET	CA-C-N	9.16	130.10	119.47
3	S	283	MET	C-N-CA	9.16	130.10	119.47
3	W	283	MET	CA-C-N	9.16	130.10	119.47
3	W	283	MET	C-N-CA	9.16	130.10	119.47
3	4	283	MET	CA-C-N	9.16	130.10	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	283	MET	C-N-CA	9.16	130.10	119.47
3	f	283	MET	CA-C-N	9.16	130.09	119.47
3	f	283	MET	C-N-CA	9.16	130.09	119.47
3	h	283	MET	CA-C-N	9.15	130.09	119.47
3	h	283	MET	C-N-CA	9.15	130.09	119.47
3	d	283	MET	CA-C-N	9.15	130.08	119.47
3	d	283	MET	C-N-CA	9.15	130.08	119.47
1	K	76	ASP	CA-C-N	9.14	129.75	119.32
1	K	76	ASP	C-N-CA	9.14	129.75	119.32
3	r	283	MET	CA-C-N	9.14	130.08	119.47
3	r	283	MET	C-N-CA	9.14	130.08	119.47
3	Q	283	MET	CA-C-N	9.13	130.06	119.47
3	Q	283	MET	C-N-CA	9.13	130.06	119.47
1	O	76	ASP	CA-C-N	9.12	129.72	119.32
1	O	76	ASP	C-N-CA	9.12	129.72	119.32
1	B	76	ASP	CA-C-N	9.12	129.71	119.32
1	B	76	ASP	C-N-CA	9.12	129.71	119.32
1	G	76	ASP	CA-C-N	9.10	129.69	119.32
1	G	76	ASP	C-N-CA	9.10	129.69	119.32
1	A	76	ASP	CA-C-N	9.10	129.69	119.32
1	A	76	ASP	C-N-CA	9.10	129.69	119.32
1	F	76	ASP	CA-C-N	9.10	129.69	119.32
1	F	76	ASP	C-N-CA	9.10	129.69	119.32
1	I	76	ASP	CA-C-N	9.09	129.68	119.32
1	I	76	ASP	C-N-CA	9.09	129.68	119.32
1	E	76	ASP	CA-C-N	9.08	129.67	119.32
1	E	76	ASP	C-N-CA	9.08	129.67	119.32
1	L	76	ASP	CA-C-N	9.08	129.67	119.32
1	L	76	ASP	C-N-CA	9.08	129.67	119.32
1	D	76	ASP	CA-C-N	9.07	129.66	119.32
1	D	76	ASP	C-N-CA	9.07	129.66	119.32
1	H	76	ASP	CA-C-N	9.07	129.66	119.32
1	H	76	ASP	C-N-CA	9.07	129.66	119.32
1	J	76	ASP	CA-C-N	9.06	129.65	119.32
1	J	76	ASP	C-N-CA	9.06	129.65	119.32
1	C	76	ASP	CA-C-N	9.05	129.64	119.32
1	C	76	ASP	C-N-CA	9.05	129.64	119.32
1	N	76	ASP	CA-C-N	9.05	129.64	119.32
1	N	76	ASP	C-N-CA	9.05	129.64	119.32
1	M	76	ASP	CA-C-N	9.04	129.63	119.32
1	M	76	ASP	C-N-CA	9.04	129.63	119.32
2	5	78	PRO	CA-C-N	8.50	128.53	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	78	PRO	C-N-CA	8.50	128.53	119.78
2	k	78	PRO	CA-C-N	8.47	128.51	119.78
2	k	78	PRO	C-N-CA	8.47	128.51	119.78
2	c	78	PRO	CA-C-N	8.47	128.51	119.78
2	c	78	PRO	C-N-CA	8.47	128.51	119.78
2	u	78	PRO	CA-C-N	8.47	128.51	119.78
2	u	78	PRO	C-N-CA	8.47	128.51	119.78
2	7	78	PRO	CA-C-N	8.47	128.50	119.78
2	7	78	PRO	C-N-CA	8.47	128.50	119.78
2	e	78	PRO	CA-C-N	8.46	128.50	119.78
2	e	78	PRO	C-N-CA	8.46	128.50	119.78
2	i	78	PRO	CA-C-N	8.47	128.50	119.78
2	i	78	PRO	C-N-CA	8.47	128.50	119.78
2	o	78	PRO	CA-C-N	8.46	128.50	119.78
2	o	78	PRO	C-N-CA	8.46	128.50	119.78
2	1	78	PRO	CA-C-N	8.46	128.50	119.78
2	1	78	PRO	C-N-CA	8.46	128.50	119.78
2	a	78	PRO	CA-C-N	8.46	128.50	119.78
2	a	78	PRO	C-N-CA	8.46	128.50	119.78
2	R	78	PRO	CA-C-N	8.46	128.49	119.78
2	R	78	PRO	C-N-CA	8.46	128.49	119.78
2	g	78	PRO	CA-C-N	8.46	128.49	119.78
2	g	78	PRO	C-N-CA	8.46	128.49	119.78
2	9	78	PRO	CA-C-N	8.46	128.49	119.78
2	9	78	PRO	C-N-CA	8.46	128.49	119.78
2	m	78	PRO	CA-C-N	8.45	128.48	119.78
2	m	78	PRO	C-N-CA	8.45	128.48	119.78
2	z	78	PRO	CA-C-N	8.44	128.48	119.78
2	z	78	PRO	C-N-CA	8.44	128.48	119.78
2	P	78	PRO	CA-C-N	8.44	128.48	119.78
2	P	78	PRO	C-N-CA	8.44	128.48	119.78
2	V	78	PRO	CA-C-N	8.44	128.47	119.78
2	V	78	PRO	C-N-CA	8.44	128.47	119.78
2	T	78	PRO	CA-C-N	8.44	128.47	119.78
2	T	78	PRO	C-N-CA	8.44	128.47	119.78
2	X	78	PRO	CA-C-N	8.44	128.47	119.78
2	X	78	PRO	C-N-CA	8.44	128.47	119.78
2	3	78	PRO	CA-C-N	8.44	128.47	119.78
2	3	78	PRO	C-N-CA	8.44	128.47	119.78
2	s	78	PRO	CA-C-N	8.43	128.46	119.78
2	s	78	PRO	C-N-CA	8.43	128.46	119.78
2	w	78	PRO	CA-C-N	8.43	128.46	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	w	78	PRO	C-N-CA	8.43	128.46	119.78
2	q	78	PRO	CA-C-N	8.41	128.44	119.78
2	q	78	PRO	C-N-CA	8.41	128.44	119.78
2	y	78	PRO	CA-C-N	8.41	128.44	119.78
2	y	78	PRO	C-N-CA	8.41	128.44	119.78
2	y	89	PHE	CA-C-N	8.19	128.13	119.85
2	y	89	PHE	C-N-CA	8.19	128.13	119.85
2	g	89	PHE	CA-C-N	8.19	128.12	119.85
2	g	89	PHE	C-N-CA	8.19	128.12	119.85
2	1	89	PHE	CA-C-N	8.19	128.12	119.85
2	1	89	PHE	C-N-CA	8.19	128.12	119.85
2	V	89	PHE	CA-C-N	8.19	128.12	119.85
2	V	89	PHE	C-N-CA	8.19	128.12	119.85
2	P	89	PHE	CA-C-N	8.18	128.11	119.85
2	P	89	PHE	C-N-CA	8.18	128.11	119.85
2	a	89	PHE	CA-C-N	8.17	128.10	119.85
2	a	89	PHE	C-N-CA	8.17	128.10	119.85
2	3	89	PHE	CA-C-N	8.15	128.09	119.85
2	3	89	PHE	C-N-CA	8.15	128.09	119.85
2	s	89	PHE	CA-C-N	8.15	128.08	119.85
2	s	89	PHE	C-N-CA	8.15	128.08	119.85
2	z	89	PHE	CA-C-N	8.14	128.07	119.85
2	z	89	PHE	C-N-CA	8.14	128.07	119.85
2	5	89	PHE	CA-C-N	8.14	128.07	119.85
2	5	89	PHE	C-N-CA	8.14	128.07	119.85
2	X	89	PHE	CA-C-N	8.13	128.06	119.85
2	X	89	PHE	C-N-CA	8.13	128.06	119.85
2	7	89	PHE	CA-C-N	8.13	128.06	119.85
2	7	89	PHE	C-N-CA	8.13	128.06	119.85
2	T	89	PHE	CA-C-N	8.13	128.06	119.85
2	T	89	PHE	C-N-CA	8.13	128.06	119.85
2	m	89	PHE	CA-C-N	8.13	128.06	119.85
2	m	89	PHE	C-N-CA	8.13	128.06	119.85
2	i	89	PHE	CA-C-N	8.13	128.06	119.85
2	i	89	PHE	C-N-CA	8.13	128.06	119.85
2	w	89	PHE	CA-C-N	8.13	128.06	119.85
2	w	89	PHE	C-N-CA	8.13	128.06	119.85
2	e	89	PHE	CA-C-N	8.12	128.06	119.85
2	e	89	PHE	C-N-CA	8.12	128.06	119.85
2	c	89	PHE	CA-C-N	8.12	128.05	119.85
2	c	89	PHE	C-N-CA	8.12	128.05	119.85
2	o	89	PHE	CA-C-N	8.12	128.05	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	89	PHE	C-N-CA	8.12	128.05	119.85
2	u	89	PHE	CA-C-N	8.12	128.05	119.85
2	u	89	PHE	C-N-CA	8.12	128.05	119.85
2	R	89	PHE	CA-C-N	8.11	128.04	119.85
2	R	89	PHE	C-N-CA	8.11	128.04	119.85
2	9	89	PHE	CA-C-N	8.10	128.03	119.85
2	9	89	PHE	C-N-CA	8.10	128.03	119.85
2	k	89	PHE	CA-C-N	8.10	128.03	119.85
2	k	89	PHE	C-N-CA	8.10	128.03	119.85
2	q	89	PHE	CA-C-N	8.10	128.03	119.85
2	q	89	PHE	C-N-CA	8.10	128.03	119.85
1	L	520	ASP	CA-C-N	7.82	127.75	119.85
1	L	520	ASP	C-N-CA	7.82	127.75	119.85
1	I	520	ASP	CA-C-N	7.77	127.70	119.85
1	I	520	ASP	C-N-CA	7.77	127.70	119.85
1	O	520	ASP	CA-C-N	7.77	127.69	119.85
1	O	520	ASP	C-N-CA	7.77	127.69	119.85
1	M	520	ASP	CA-C-N	7.76	127.69	119.85
1	M	520	ASP	C-N-CA	7.76	127.69	119.85
1	E	520	ASP	CA-C-N	7.76	127.69	119.85
1	E	520	ASP	C-N-CA	7.76	127.69	119.85
1	K	520	ASP	CA-C-N	7.76	127.68	119.85
1	K	520	ASP	C-N-CA	7.76	127.68	119.85
1	J	520	ASP	CA-C-N	7.75	127.68	119.85
1	J	520	ASP	C-N-CA	7.75	127.68	119.85
2	a	142	PRO	CA-C-N	7.75	127.68	119.85
2	a	142	PRO	C-N-CA	7.75	127.68	119.85
1	D	520	ASP	CA-C-N	7.74	127.67	119.85
1	D	520	ASP	C-N-CA	7.74	127.67	119.85
1	F	520	ASP	CA-C-N	7.73	127.68	120.03
1	F	520	ASP	C-N-CA	7.73	127.68	120.03
1	H	520	ASP	CA-C-N	7.72	127.65	119.85
1	H	520	ASP	C-N-CA	7.72	127.65	119.85
1	B	520	ASP	CA-C-N	7.71	127.64	119.85
1	B	520	ASP	C-N-CA	7.71	127.64	119.85
1	G	520	ASP	CA-C-N	7.71	127.67	120.03
1	G	520	ASP	C-N-CA	7.71	127.67	120.03
2	T	142	PRO	CA-C-N	7.71	127.64	119.85
2	T	142	PRO	C-N-CA	7.71	127.64	119.85
2	q	142	PRO	CA-C-N	7.71	127.64	119.85
2	q	142	PRO	C-N-CA	7.71	127.64	119.85
1	C	520	ASP	CA-C-N	7.71	127.63	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	520	ASP	C-N-CA	7.71	127.63	119.85
2	V	142	PRO	CA-C-N	7.71	127.63	119.85
2	V	142	PRO	C-N-CA	7.71	127.63	119.85
2	z	142	PRO	CA-C-N	7.71	127.63	119.85
2	z	142	PRO	C-N-CA	7.71	127.63	119.85
2	c	142	PRO	CA-C-N	7.70	127.63	119.85
2	c	142	PRO	C-N-CA	7.70	127.63	119.85
2	w	142	PRO	CA-C-N	7.70	127.63	119.85
2	w	142	PRO	C-N-CA	7.70	127.63	119.85
2	o	142	PRO	CA-C-N	7.69	127.62	119.85
2	o	142	PRO	C-N-CA	7.69	127.62	119.85
2	9	142	PRO	CA-C-N	7.69	127.62	119.85
2	9	142	PRO	C-N-CA	7.69	127.62	119.85
1	N	520	ASP	CA-C-N	7.69	127.61	119.85
1	N	520	ASP	C-N-CA	7.69	127.61	119.85
2	R	142	PRO	CA-C-N	7.69	127.61	119.85
2	R	142	PRO	C-N-CA	7.69	127.61	119.85
2	l	142	PRO	CA-C-N	7.68	127.61	119.85
2	l	142	PRO	C-N-CA	7.68	127.61	119.85
2	e	142	PRO	CA-C-N	7.68	127.61	119.85
2	e	142	PRO	C-N-CA	7.68	127.61	119.85
2	X	142	PRO	CA-C-N	7.68	127.61	119.85
2	X	142	PRO	C-N-CA	7.68	127.61	119.85
2	s	142	PRO	CA-C-N	7.68	127.61	119.85
2	s	142	PRO	C-N-CA	7.68	127.61	119.85
2	u	142	PRO	CA-C-N	7.68	127.61	119.85
2	u	142	PRO	C-N-CA	7.68	127.61	119.85
2	y	142	PRO	CA-C-N	7.67	127.60	119.85
2	y	142	PRO	C-N-CA	7.67	127.60	119.85
2	g	142	PRO	CA-C-N	7.67	127.59	119.85
2	g	142	PRO	C-N-CA	7.67	127.59	119.85
2	P	142	PRO	CA-C-N	7.66	127.59	119.85
2	P	142	PRO	C-N-CA	7.66	127.59	119.85
1	A	520	ASP	CA-C-N	7.66	127.59	119.85
1	A	520	ASP	C-N-CA	7.66	127.59	119.85
2	k	142	PRO	CA-C-N	7.66	127.59	119.85
2	k	142	PRO	C-N-CA	7.66	127.59	119.85
2	5	142	PRO	CA-C-N	7.65	127.58	119.85
2	5	142	PRO	C-N-CA	7.65	127.58	119.85
2	7	142	PRO	CA-C-N	7.65	127.58	119.85
2	7	142	PRO	C-N-CA	7.65	127.58	119.85
2	3	142	PRO	CA-C-N	7.64	127.56	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	142	PRO	C-N-CA	7.64	127.56	119.85
2	m	142	PRO	CA-C-N	7.63	127.56	119.85
2	m	142	PRO	C-N-CA	7.63	127.56	119.85
2	i	142	PRO	CA-C-N	7.63	127.55	119.85
2	i	142	PRO	C-N-CA	7.63	127.55	119.85
2	u	197	ALA	CA-C-N	7.59	127.97	119.32
2	u	197	ALA	C-N-CA	7.59	127.97	119.32
2	T	197	ALA	CA-C-N	7.59	127.97	119.32
2	T	197	ALA	C-N-CA	7.59	127.97	119.32
2	s	197	ALA	CA-C-N	7.59	127.97	119.32
2	s	197	ALA	C-N-CA	7.59	127.97	119.32
1	K	413	LEU	CA-C-N	7.59	128.18	120.14
1	K	413	LEU	C-N-CA	7.59	128.18	120.14
2	z	197	ALA	CA-C-N	7.58	127.96	119.32
2	z	197	ALA	C-N-CA	7.58	127.96	119.32
2	5	197	ALA	CA-C-N	7.58	127.96	119.32
2	5	197	ALA	C-N-CA	7.58	127.96	119.32
2	1	197	ALA	CA-C-N	7.57	127.95	119.32
2	1	197	ALA	C-N-CA	7.57	127.95	119.32
2	9	197	ALA	CA-C-N	7.57	127.95	119.32
2	9	197	ALA	C-N-CA	7.57	127.95	119.32
1	M	413	LEU	CA-C-N	7.57	128.16	120.14
1	M	413	LEU	C-N-CA	7.57	128.16	120.14
2	R	197	ALA	CA-C-N	7.57	127.95	119.32
2	R	197	ALA	C-N-CA	7.57	127.95	119.32
2	c	197	ALA	CA-C-N	7.57	127.95	119.32
2	c	197	ALA	C-N-CA	7.57	127.95	119.32
1	I	435	THR	CA-C-N	7.57	129.08	120.98
1	I	435	THR	C-N-CA	7.57	129.08	120.98
2	X	197	ALA	CA-C-N	7.57	127.95	119.32
2	X	197	ALA	C-N-CA	7.57	127.95	119.32
2	e	197	ALA	CA-C-N	7.57	127.94	119.32
2	e	197	ALA	C-N-CA	7.57	127.94	119.32
2	3	197	ALA	CA-C-N	7.56	127.94	119.32
2	3	197	ALA	C-N-CA	7.56	127.94	119.32
2	o	197	ALA	CA-C-N	7.56	127.94	119.32
2	o	197	ALA	C-N-CA	7.56	127.94	119.32
2	y	197	ALA	CA-C-N	7.56	127.94	119.32
2	y	197	ALA	C-N-CA	7.56	127.94	119.32
2	7	197	ALA	CA-C-N	7.56	127.94	119.32
2	7	197	ALA	C-N-CA	7.56	127.94	119.32
2	V	197	ALA	CA-C-N	7.55	127.93	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	197	ALA	C-N-CA	7.55	127.93	119.32
2	m	197	ALA	CA-C-N	7.55	127.93	119.32
2	m	197	ALA	C-N-CA	7.55	127.93	119.32
2	P	197	ALA	CA-C-N	7.55	127.92	119.32
2	P	197	ALA	C-N-CA	7.55	127.92	119.32
2	i	197	ALA	CA-C-N	7.55	127.92	119.32
2	i	197	ALA	C-N-CA	7.55	127.92	119.32
2	g	197	ALA	CA-C-N	7.54	127.92	119.32
2	g	197	ALA	C-N-CA	7.54	127.92	119.32
2	q	197	ALA	CA-C-N	7.54	127.92	119.32
2	q	197	ALA	C-N-CA	7.54	127.92	119.32
1	E	413	LEU	CA-C-N	7.54	128.13	120.14
1	E	413	LEU	C-N-CA	7.54	128.13	120.14
1	J	413	LEU	CA-C-N	7.54	128.13	120.14
1	J	413	LEU	C-N-CA	7.54	128.13	120.14
1	J	435	THR	CA-C-N	7.54	129.05	120.98
1	J	435	THR	C-N-CA	7.54	129.05	120.98
1	L	413	LEU	CA-C-N	7.54	128.13	120.14
1	L	413	LEU	C-N-CA	7.54	128.13	120.14
2	a	197	ALA	CA-C-N	7.54	127.91	119.32
2	a	197	ALA	C-N-CA	7.54	127.91	119.32
1	C	413	LEU	CA-C-N	7.53	128.13	120.14
1	C	413	LEU	C-N-CA	7.53	128.13	120.14
2	w	197	ALA	CA-C-N	7.53	127.91	119.32
2	w	197	ALA	C-N-CA	7.53	127.91	119.32
1	A	435	THR	CA-C-N	7.53	129.04	120.98
1	A	435	THR	C-N-CA	7.53	129.04	120.98
2	k	197	ALA	CA-C-N	7.53	127.91	119.32
2	k	197	ALA	C-N-CA	7.53	127.91	119.32
1	B	435	THR	CA-C-N	7.52	129.02	120.98
1	B	435	THR	C-N-CA	7.52	129.02	120.98
1	F	435	THR	CA-C-N	7.51	129.02	120.98
1	F	435	THR	C-N-CA	7.51	129.02	120.98
1	A	413	LEU	CA-C-N	7.51	128.10	120.14
1	A	413	LEU	C-N-CA	7.51	128.10	120.14
1	O	413	LEU	CA-C-N	7.51	128.10	120.14
1	O	413	LEU	C-N-CA	7.51	128.10	120.14
1	F	413	LEU	CA-C-N	7.51	128.10	120.14
1	F	413	LEU	C-N-CA	7.51	128.10	120.14
1	E	435	THR	CA-C-N	7.51	129.01	120.98
1	E	435	THR	C-N-CA	7.51	129.01	120.98
1	G	413	LEU	CA-C-N	7.50	128.09	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	413	LEU	C-N-CA	7.50	128.09	120.14
1	D	413	LEU	CA-C-N	7.50	128.09	120.14
1	D	413	LEU	C-N-CA	7.50	128.09	120.14
1	B	413	LEU	CA-C-N	7.50	128.09	120.14
1	B	413	LEU	C-N-CA	7.50	128.09	120.14
1	I	413	LEU	CA-C-N	7.50	128.09	120.14
1	I	413	LEU	C-N-CA	7.50	128.09	120.14
1	N	413	LEU	CA-C-N	7.49	128.08	120.14
1	N	413	LEU	C-N-CA	7.49	128.08	120.14
1	H	413	LEU	CA-C-N	7.49	128.08	120.14
1	H	413	LEU	C-N-CA	7.49	128.08	120.14
1	G	435	THR	CA-C-N	7.49	128.99	120.98
1	G	435	THR	C-N-CA	7.49	128.99	120.98
1	L	435	THR	CA-C-N	7.49	128.99	120.98
1	L	435	THR	C-N-CA	7.49	128.99	120.98
1	O	435	THR	CA-C-N	7.49	128.99	120.98
1	O	435	THR	C-N-CA	7.49	128.99	120.98
1	D	435	THR	CA-C-N	7.49	128.99	120.98
1	D	435	THR	C-N-CA	7.49	128.99	120.98
1	H	435	THR	CA-C-N	7.48	128.98	120.98
1	H	435	THR	C-N-CA	7.48	128.98	120.98
1	M	435	THR	CA-C-N	7.47	128.97	120.98
1	M	435	THR	C-N-CA	7.47	128.97	120.98
1	K	435	THR	CA-C-N	7.47	128.97	120.98
1	K	435	THR	C-N-CA	7.47	128.97	120.98
1	N	435	THR	CA-C-N	7.46	128.96	120.98
1	N	435	THR	C-N-CA	7.46	128.96	120.98
1	C	435	THR	CA-C-N	7.46	128.96	120.98
1	C	435	THR	C-N-CA	7.46	128.96	120.98
2	w	144	LYS	CA-C-N	7.31	127.31	119.78
2	w	144	LYS	C-N-CA	7.31	127.31	119.78
2	R	144	LYS	CA-C-N	7.31	127.31	119.78
2	R	144	LYS	C-N-CA	7.31	127.31	119.78
2	z	144	LYS	CA-C-N	7.31	127.31	119.78
2	z	144	LYS	C-N-CA	7.31	127.31	119.78
2	3	144	LYS	CA-C-N	7.30	127.30	119.78
2	3	144	LYS	C-N-CA	7.30	127.30	119.78
2	5	144	LYS	CA-C-N	7.30	127.30	119.78
2	5	144	LYS	C-N-CA	7.30	127.30	119.78
2	s	144	LYS	CA-C-N	7.28	127.28	119.78
2	s	144	LYS	C-N-CA	7.28	127.28	119.78
2	1	144	LYS	CA-C-N	7.27	127.27	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	144	LYS	C-N-CA	7.27	127.27	119.78
2	c	144	LYS	CA-C-N	7.27	127.27	119.78
2	c	144	LYS	C-N-CA	7.27	127.27	119.78
2	V	144	LYS	CA-C-N	7.26	127.26	119.78
2	V	144	LYS	C-N-CA	7.26	127.26	119.78
2	m	144	LYS	CA-C-N	7.26	127.26	119.78
2	m	144	LYS	C-N-CA	7.26	127.26	119.78
2	y	144	LYS	CA-C-N	7.26	127.26	119.78
2	y	144	LYS	C-N-CA	7.26	127.26	119.78
2	i	144	LYS	CA-C-N	7.25	127.25	119.78
2	i	144	LYS	C-N-CA	7.25	127.25	119.78
2	o	144	LYS	CA-C-N	7.25	127.25	119.78
2	o	144	LYS	C-N-CA	7.25	127.25	119.78
2	P	144	LYS	CA-C-N	7.25	127.25	119.78
2	P	144	LYS	C-N-CA	7.25	127.25	119.78
2	T	144	LYS	CA-C-N	7.25	127.25	119.78
2	T	144	LYS	C-N-CA	7.25	127.25	119.78
2	q	144	LYS	CA-C-N	7.25	127.25	119.78
2	q	144	LYS	C-N-CA	7.25	127.25	119.78
2	a	144	LYS	CA-C-N	7.25	127.24	119.78
2	a	144	LYS	C-N-CA	7.25	127.24	119.78
2	9	144	LYS	CA-C-N	7.25	127.24	119.78
2	9	144	LYS	C-N-CA	7.25	127.24	119.78
2	u	144	LYS	CA-C-N	7.24	127.24	119.78
2	u	144	LYS	C-N-CA	7.24	127.24	119.78
2	g	144	LYS	CA-C-N	7.24	127.23	119.78
2	g	144	LYS	C-N-CA	7.24	127.23	119.78
2	X	144	LYS	CA-C-N	7.23	127.23	119.78
2	X	144	LYS	C-N-CA	7.23	127.23	119.78
2	k	144	LYS	CA-C-N	7.22	127.22	119.78
2	k	144	LYS	C-N-CA	7.22	127.22	119.78
2	c	200	THR	CA-C-N	7.22	127.14	119.85
2	c	200	THR	C-N-CA	7.22	127.14	119.85
2	V	200	THR	CA-C-N	7.21	127.14	119.85
2	V	200	THR	C-N-CA	7.21	127.14	119.85
2	e	144	LYS	CA-C-N	7.21	127.21	119.78
2	e	144	LYS	C-N-CA	7.21	127.21	119.78
2	R	200	THR	CA-C-N	7.21	127.13	119.85
2	R	200	THR	C-N-CA	7.21	127.13	119.85
2	m	200	THR	CA-C-N	7.21	127.13	119.85
2	m	200	THR	C-N-CA	7.21	127.13	119.85
2	z	200	THR	CA-C-N	7.21	127.13	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	z	200	THR	C-N-CA	7.21	127.13	119.85
2	T	200	THR	CA-C-N	7.20	127.12	119.85
2	T	200	THR	C-N-CA	7.20	127.12	119.85
2	7	144	LYS	CA-C-N	7.20	127.19	119.78
2	7	144	LYS	C-N-CA	7.20	127.19	119.78
2	k	200	THR	CA-C-N	7.19	127.11	119.85
2	k	200	THR	C-N-CA	7.19	127.11	119.85
2	o	200	THR	CA-C-N	7.19	127.11	119.85
2	o	200	THR	C-N-CA	7.19	127.11	119.85
2	9	200	THR	CA-C-N	7.19	127.11	119.85
2	9	200	THR	C-N-CA	7.19	127.11	119.85
2	X	200	THR	CA-C-N	7.18	127.11	119.85
2	X	200	THR	C-N-CA	7.18	127.11	119.85
2	q	200	THR	CA-C-N	7.18	127.10	119.85
2	q	200	THR	C-N-CA	7.18	127.10	119.85
2	g	200	THR	CA-C-N	7.17	127.10	119.85
2	g	200	THR	C-N-CA	7.17	127.10	119.85
2	7	200	THR	CA-C-N	7.17	127.09	119.85
2	7	200	THR	C-N-CA	7.17	127.09	119.85
2	i	200	THR	CA-C-N	7.17	127.09	119.85
2	i	200	THR	C-N-CA	7.17	127.09	119.85
2	u	200	THR	CA-C-N	7.17	127.09	119.85
2	u	200	THR	C-N-CA	7.17	127.09	119.85
2	e	200	THR	CA-C-N	7.17	127.09	119.85
2	e	200	THR	C-N-CA	7.17	127.09	119.85
2	3	200	THR	CA-C-N	7.17	127.09	119.85
2	3	200	THR	C-N-CA	7.17	127.09	119.85
2	w	200	THR	CA-C-N	7.16	127.09	119.85
2	w	200	THR	C-N-CA	7.16	127.09	119.85
2	P	200	THR	CA-C-N	7.16	127.08	119.85
2	P	200	THR	C-N-CA	7.16	127.08	119.85
2	1	200	THR	CA-C-N	7.15	127.07	119.85
2	1	200	THR	C-N-CA	7.15	127.07	119.85
2	5	200	THR	CA-C-N	7.15	127.07	119.85
2	5	200	THR	C-N-CA	7.15	127.07	119.85
2	y	200	THR	CA-C-N	7.15	127.07	119.85
2	y	200	THR	C-N-CA	7.15	127.07	119.85
2	s	200	THR	CA-C-N	7.13	127.05	119.85
2	s	200	THR	C-N-CA	7.13	127.05	119.85
2	a	200	THR	CA-C-N	7.12	127.05	119.85
2	a	200	THR	C-N-CA	7.12	127.05	119.85
2	9	97	SER	CA-C-N	7.02	127.33	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	97	SER	C-N-CA	7.02	127.33	119.32
2	T	97	SER	CA-C-N	7.01	127.32	119.32
2	T	97	SER	C-N-CA	7.01	127.32	119.32
2	m	97	SER	CA-C-N	7.01	127.32	119.32
2	m	97	SER	C-N-CA	7.01	127.32	119.32
2	s	97	SER	CA-C-N	7.01	127.31	119.32
2	s	97	SER	C-N-CA	7.01	127.31	119.32
2	q	97	SER	CA-C-N	7.01	127.31	119.32
2	q	97	SER	C-N-CA	7.01	127.31	119.32
2	e	97	SER	CA-C-N	7.00	127.30	119.32
2	e	97	SER	C-N-CA	7.00	127.30	119.32
2	R	97	SER	CA-C-N	7.00	127.30	119.32
2	R	97	SER	C-N-CA	7.00	127.30	119.32
2	c	97	SER	CA-C-N	7.00	127.30	119.32
2	c	97	SER	C-N-CA	7.00	127.30	119.32
2	u	97	SER	CA-C-N	7.00	127.30	119.32
2	u	97	SER	C-N-CA	7.00	127.30	119.32
2	y	97	SER	CA-C-N	7.00	127.30	119.32
2	y	97	SER	C-N-CA	7.00	127.30	119.32
2	z	97	SER	CA-C-N	7.00	127.29	119.32
2	z	97	SER	C-N-CA	7.00	127.29	119.32
2	X	97	SER	CA-C-N	6.99	127.29	119.32
2	X	97	SER	C-N-CA	6.99	127.29	119.32
2	g	97	SER	CA-C-N	6.99	127.29	119.32
2	g	97	SER	C-N-CA	6.99	127.29	119.32
2	5	97	SER	CA-C-N	6.99	127.29	119.32
2	5	97	SER	C-N-CA	6.99	127.29	119.32
2	i	97	SER	CA-C-N	6.98	127.28	119.32
2	i	97	SER	C-N-CA	6.98	127.28	119.32
2	w	97	SER	CA-C-N	6.98	127.28	119.32
2	w	97	SER	C-N-CA	6.98	127.28	119.32
2	3	97	SER	CA-C-N	6.98	127.28	119.32
2	3	97	SER	C-N-CA	6.98	127.28	119.32
2	k	97	SER	CA-C-N	6.98	127.28	119.32
2	k	97	SER	C-N-CA	6.98	127.28	119.32
2	7	97	SER	CA-C-N	6.98	127.28	119.32
2	7	97	SER	C-N-CA	6.98	127.28	119.32
2	P	97	SER	CA-C-N	6.97	127.27	119.32
2	P	97	SER	C-N-CA	6.97	127.27	119.32
2	V	97	SER	CA-C-N	6.97	127.26	119.32
2	V	97	SER	C-N-CA	6.97	127.26	119.32
2	o	97	SER	CA-C-N	6.96	127.26	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	97	SER	C-N-CA	6.96	127.26	119.32
2	a	97	SER	CA-C-N	6.96	127.25	119.32
2	a	97	SER	C-N-CA	6.96	127.25	119.32
2	1	97	SER	CA-C-N	6.95	127.24	119.32
2	1	97	SER	C-N-CA	6.95	127.24	119.32
3	Q	255	LYS	CA-C-N	6.79	126.71	119.85
3	Q	255	LYS	C-N-CA	6.79	126.71	119.85
3	10	255	LYS	CA-C-N	6.78	126.70	119.85
3	10	255	LYS	C-N-CA	6.78	126.70	119.85
3	h	255	LYS	CA-C-N	6.78	126.69	119.85
3	h	255	LYS	C-N-CA	6.78	126.69	119.85
3	S	255	LYS	CA-C-N	6.77	126.69	119.85
3	S	255	LYS	C-N-CA	6.77	126.69	119.85
3	b	255	LYS	CA-C-N	6.77	126.69	119.85
3	b	255	LYS	C-N-CA	6.77	126.69	119.85
3	l	255	LYS	CA-C-N	6.76	126.68	119.85
3	l	255	LYS	C-N-CA	6.76	126.68	119.85
3	j	255	LYS	CA-C-N	6.76	126.68	119.85
3	j	255	LYS	C-N-CA	6.76	126.68	119.85
3	4	255	LYS	CA-C-N	6.76	126.68	119.85
3	4	255	LYS	C-N-CA	6.76	126.68	119.85
3	0	255	LYS	CA-C-N	6.75	126.67	119.85
3	0	255	LYS	C-N-CA	6.75	126.67	119.85
3	2	255	LYS	CA-C-N	6.75	126.67	119.85
3	2	255	LYS	C-N-CA	6.75	126.67	119.85
3	x	255	LYS	CA-C-N	6.75	126.67	119.85
3	x	255	LYS	C-N-CA	6.75	126.67	119.85
3	n	255	LYS	CA-C-N	6.74	126.65	119.85
3	n	255	LYS	C-N-CA	6.74	126.65	119.85
3	U	255	LYS	CA-C-N	6.74	126.65	119.85
3	U	255	LYS	C-N-CA	6.74	126.65	119.85
3	r	255	LYS	CA-C-N	6.74	126.65	119.85
3	r	255	LYS	C-N-CA	6.74	126.65	119.85
3	W	255	LYS	CA-C-N	6.73	126.65	119.85
3	W	255	LYS	C-N-CA	6.73	126.65	119.85
3	f	255	LYS	CA-C-N	6.73	126.65	119.85
3	f	255	LYS	C-N-CA	6.73	126.65	119.85
3	v	255	LYS	CA-C-N	6.73	126.65	119.85
3	v	255	LYS	C-N-CA	6.73	126.65	119.85
3	d	255	LYS	CA-C-N	6.73	126.64	119.85
3	d	255	LYS	C-N-CA	6.73	126.64	119.85
3	t	255	LYS	CA-C-N	6.73	126.64	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	t	255	LYS	C-N-CA	6.73	126.64	119.85
3	Y	255	LYS	CA-C-N	6.72	126.64	119.85
3	Y	255	LYS	C-N-CA	6.72	126.64	119.85
3	8	255	LYS	CA-C-N	6.72	126.64	119.85
3	8	255	LYS	C-N-CA	6.72	126.64	119.85
3	Z	255	LYS	CA-C-N	6.71	126.63	119.85
3	Z	255	LYS	C-N-CA	6.71	126.63	119.85
3	p	255	LYS	CA-C-N	6.71	126.63	119.85
3	p	255	LYS	C-N-CA	6.71	126.63	119.85
3	6	255	LYS	CA-C-N	6.70	126.61	119.85
3	6	255	LYS	C-N-CA	6.70	126.61	119.85
3	h	312	LEU	CA-C-N	6.67	127.19	119.99
3	h	312	LEU	C-N-CA	6.67	127.19	119.99
3	4	312	LEU	CA-C-N	6.66	127.18	119.99
3	4	312	LEU	C-N-CA	6.66	127.18	119.99
3	r	312	LEU	CA-C-N	6.64	127.16	119.99
3	r	312	LEU	C-N-CA	6.64	127.16	119.99
3	2	312	LEU	CA-C-N	6.64	127.16	119.99
3	2	312	LEU	C-N-CA	6.64	127.16	119.99
3	p	312	LEU	CA-C-N	6.63	127.16	119.99
3	p	312	LEU	C-N-CA	6.63	127.16	119.99
3	Z	312	LEU	CA-C-N	6.63	127.15	119.99
3	Z	312	LEU	C-N-CA	6.63	127.15	119.99
3	l	312	LEU	CA-C-N	6.63	127.15	119.99
3	l	312	LEU	C-N-CA	6.63	127.15	119.99
3	Y	312	LEU	CA-C-N	6.63	127.15	119.99
3	Y	312	LEU	C-N-CA	6.63	127.15	119.99
3	n	312	LEU	CA-C-N	6.62	127.14	119.99
3	n	312	LEU	C-N-CA	6.62	127.14	119.99
3	U	312	LEU	CA-C-N	6.61	127.13	119.99
3	U	312	LEU	C-N-CA	6.61	127.13	119.99
3	0	312	LEU	CA-C-N	6.61	127.13	119.99
3	0	312	LEU	C-N-CA	6.61	127.13	119.99
3	S	312	LEU	CA-C-N	6.61	127.13	119.99
3	S	312	LEU	C-N-CA	6.61	127.13	119.99
3	d	312	LEU	CA-C-N	6.61	127.13	119.99
3	d	312	LEU	C-N-CA	6.61	127.13	119.99
3	t	312	LEU	CA-C-N	6.61	127.12	119.99
3	t	312	LEU	C-N-CA	6.61	127.12	119.99
3	Q	312	LEU	CA-C-N	6.61	127.12	119.99
3	Q	312	LEU	C-N-CA	6.61	127.12	119.99
3	x	312	LEU	CA-C-N	6.61	127.12	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	x	312	LEU	C-N-CA	6.61	127.12	119.99
3	6	312	LEU	CA-C-N	6.60	127.12	119.99
3	6	312	LEU	C-N-CA	6.60	127.12	119.99
3	b	312	LEU	CA-C-N	6.60	127.12	119.99
3	b	312	LEU	C-N-CA	6.60	127.12	119.99
3	f	312	LEU	CA-C-N	6.60	127.11	119.99
3	f	312	LEU	C-N-CA	6.60	127.11	119.99
3	v	312	LEU	CA-C-N	6.60	127.11	119.99
3	v	312	LEU	C-N-CA	6.60	127.11	119.99
3	W	312	LEU	CA-C-N	6.59	127.11	119.99
3	W	312	LEU	C-N-CA	6.59	127.11	119.99
3	8	312	LEU	CA-C-N	6.58	127.10	119.99
3	8	312	LEU	C-N-CA	6.58	127.10	119.99
3	10	312	LEU	CA-C-N	6.58	127.10	119.99
3	10	312	LEU	C-N-CA	6.58	127.10	119.99
1	L	379	VAL	CA-C-N	6.56	128.04	119.84
1	L	379	VAL	C-N-CA	6.56	128.04	119.84
3	j	312	LEU	CA-C-N	6.55	127.07	119.99
3	j	312	LEU	C-N-CA	6.55	127.07	119.99
1	J	379	VAL	CA-C-N	6.54	128.02	119.84
1	J	379	VAL	C-N-CA	6.54	128.02	119.84
1	F	461	VAL	CA-C-N	6.54	126.49	119.76
1	F	461	VAL	C-N-CA	6.54	126.49	119.76
1	C	490	LEU	CA-C-N	6.53	128.00	119.84
1	C	490	LEU	C-N-CA	6.53	128.00	119.84
1	I	490	LEU	CA-C-N	6.53	128.00	119.84
1	I	490	LEU	C-N-CA	6.53	128.00	119.84
1	M	461	VAL	CA-C-N	6.53	126.48	119.76
1	M	461	VAL	C-N-CA	6.53	126.48	119.76
1	A	379	VAL	CA-C-N	6.52	127.99	119.84
1	A	379	VAL	C-N-CA	6.52	127.99	119.84
1	B	379	VAL	CA-C-N	6.51	127.98	119.84
1	B	379	VAL	C-N-CA	6.51	127.98	119.84
1	I	461	VAL	CA-C-N	6.51	126.47	119.76
1	I	461	VAL	C-N-CA	6.51	126.47	119.76
1	A	490	LEU	CA-C-N	6.50	127.97	119.84
1	A	490	LEU	C-N-CA	6.50	127.97	119.84
1	F	379	VAL	CA-C-N	6.50	127.97	119.84
1	F	379	VAL	C-N-CA	6.50	127.97	119.84
1	F	490	LEU	CA-C-N	6.50	127.97	119.84
1	F	490	LEU	C-N-CA	6.50	127.97	119.84
1	E	379	VAL	CA-C-N	6.50	127.97	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	379	VAL	C-N-CA	6.50	127.97	119.84
1	L	490	LEU	CA-C-N	6.50	127.97	119.84
1	L	490	LEU	C-N-CA	6.50	127.97	119.84
1	D	379	VAL	CA-C-N	6.50	127.96	119.84
1	D	379	VAL	C-N-CA	6.50	127.96	119.84
1	O	490	LEU	CA-C-N	6.50	127.96	119.84
1	O	490	LEU	C-N-CA	6.50	127.96	119.84
1	D	461	VAL	CA-C-N	6.49	126.45	119.76
1	D	461	VAL	C-N-CA	6.49	126.45	119.76
1	I	379	VAL	CA-C-N	6.49	127.96	119.84
1	I	379	VAL	C-N-CA	6.49	127.96	119.84
1	N	490	LEU	CA-C-N	6.49	127.96	119.84
1	N	490	LEU	C-N-CA	6.49	127.96	119.84
1	H	461	VAL	CA-C-N	6.49	126.45	119.76
1	H	461	VAL	C-N-CA	6.49	126.45	119.76
1	M	379	VAL	CA-C-N	6.49	127.95	119.84
1	M	379	VAL	C-N-CA	6.49	127.95	119.84
1	G	490	LEU	CA-C-N	6.49	127.95	119.84
1	G	490	LEU	C-N-CA	6.49	127.95	119.84
1	O	461	VAL	CA-C-N	6.49	126.44	119.76
1	O	461	VAL	C-N-CA	6.49	126.44	119.76
1	C	379	VAL	CA-C-N	6.48	127.94	119.84
1	C	379	VAL	C-N-CA	6.48	127.94	119.84
1	D	490	LEU	CA-C-N	6.48	127.94	119.84
1	D	490	LEU	C-N-CA	6.48	127.94	119.84
1	N	379	VAL	CA-C-N	6.48	127.94	119.84
1	N	379	VAL	C-N-CA	6.48	127.94	119.84
1	J	461	VAL	CA-C-N	6.47	126.43	119.76
1	J	461	VAL	C-N-CA	6.47	126.43	119.76
1	K	490	LEU	CA-C-N	6.47	127.93	119.84
1	K	490	LEU	C-N-CA	6.47	127.93	119.84
1	H	379	VAL	CA-C-N	6.47	127.92	119.84
1	H	379	VAL	C-N-CA	6.47	127.92	119.84
1	N	461	VAL	CA-C-N	6.47	126.42	119.76
1	N	461	VAL	C-N-CA	6.47	126.42	119.76
1	H	490	LEU	CA-C-N	6.46	127.92	119.84
1	H	490	LEU	C-N-CA	6.46	127.92	119.84
1	L	461	VAL	CA-C-N	6.46	126.41	119.76
1	L	461	VAL	C-N-CA	6.46	126.41	119.76
1	M	490	LEU	CA-C-N	6.46	127.91	119.84
1	M	490	LEU	C-N-CA	6.46	127.91	119.84
1	E	490	LEU	CA-C-N	6.46	127.91	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	490	LEU	C-N-CA	6.46	127.91	119.84
1	B	490	LEU	CA-C-N	6.46	127.91	119.84
1	B	490	LEU	C-N-CA	6.46	127.91	119.84
1	K	379	VAL	CA-C-N	6.45	127.91	119.84
1	K	379	VAL	C-N-CA	6.45	127.91	119.84
1	K	461	VAL	CA-C-N	6.45	126.41	119.76
1	K	461	VAL	C-N-CA	6.45	126.41	119.76
1	O	379	VAL	CA-C-N	6.45	127.91	119.84
1	O	379	VAL	C-N-CA	6.45	127.91	119.84
1	G	379	VAL	CA-C-N	6.45	127.90	119.84
1	G	379	VAL	C-N-CA	6.45	127.90	119.84
1	A	461	VAL	CA-C-N	6.44	126.40	119.76
1	A	461	VAL	C-N-CA	6.44	126.40	119.76
1	G	461	VAL	CA-C-N	6.44	126.39	119.76
1	G	461	VAL	C-N-CA	6.44	126.39	119.76
1	E	461	VAL	CA-C-N	6.44	126.39	119.76
1	E	461	VAL	C-N-CA	6.44	126.39	119.76
1	J	490	LEU	CA-C-N	6.43	127.88	119.84
1	J	490	LEU	C-N-CA	6.43	127.88	119.84
1	C	461	VAL	CA-C-N	6.42	126.37	119.76
1	C	461	VAL	C-N-CA	6.42	126.37	119.76
1	B	461	VAL	CA-C-N	6.40	126.35	119.76
1	B	461	VAL	C-N-CA	6.40	126.35	119.76
1	J	370	ARG	CA-C-N	6.32	126.08	119.76
1	J	370	ARG	C-N-CA	6.32	126.08	119.76
1	H	484	ILE	CA-C-N	6.32	127.74	119.84
1	H	484	ILE	C-N-CA	6.32	127.74	119.84
1	I	370	ARG	CA-C-N	6.32	126.08	119.76
1	I	370	ARG	C-N-CA	6.32	126.08	119.76
1	O	484	ILE	CA-C-N	6.30	127.72	119.84
1	O	484	ILE	C-N-CA	6.30	127.72	119.84
2	w	80	ARG	CA-C-N	6.30	126.21	119.85
2	w	80	ARG	C-N-CA	6.30	126.21	119.85
1	F	370	ARG	CA-C-N	6.29	126.06	119.76
1	F	370	ARG	C-N-CA	6.29	126.06	119.76
2	P	80	ARG	CA-C-N	6.29	126.20	119.85
2	P	80	ARG	C-N-CA	6.29	126.20	119.85
1	L	370	ARG	CA-C-N	6.29	126.05	119.76
1	L	370	ARG	C-N-CA	6.29	126.05	119.76
1	J	204	ILE	CA-C-N	6.29	126.05	119.76
1	J	204	ILE	C-N-CA	6.29	126.05	119.76
1	C	370	ARG	CA-C-N	6.28	126.04	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	370	ARG	C-N-CA	6.28	126.04	119.76
1	G	370	ARG	CA-C-N	6.28	126.04	119.76
1	G	370	ARG	C-N-CA	6.28	126.04	119.76
1	J	484	ILE	CA-C-N	6.28	127.69	119.84
1	J	484	ILE	C-N-CA	6.28	127.69	119.84
2	k	80	ARG	CA-C-N	6.28	126.19	119.85
2	k	80	ARG	C-N-CA	6.28	126.19	119.85
1	N	370	ARG	CA-C-N	6.28	126.04	119.76
1	N	370	ARG	C-N-CA	6.28	126.04	119.76
1	D	370	ARG	CA-C-N	6.27	126.03	119.76
1	D	370	ARG	C-N-CA	6.27	126.03	119.76
1	M	370	ARG	CA-C-N	6.27	126.03	119.76
1	M	370	ARG	C-N-CA	6.27	126.03	119.76
2	i	80	ARG	CA-C-N	6.27	126.19	119.85
2	i	80	ARG	C-N-CA	6.27	126.19	119.85
2	o	80	ARG	CA-C-N	6.27	126.18	119.85
2	o	80	ARG	C-N-CA	6.27	126.18	119.85
1	M	484	ILE	CA-C-N	6.27	127.68	119.84
1	M	484	ILE	C-N-CA	6.27	127.68	119.84
2	5	80	ARG	CA-C-N	6.26	126.17	119.85
2	5	80	ARG	C-N-CA	6.26	126.17	119.85
2	9	80	ARG	CA-C-N	6.26	126.17	119.85
2	9	80	ARG	C-N-CA	6.26	126.17	119.85
1	E	370	ARG	CA-C-N	6.26	126.02	119.76
1	E	370	ARG	C-N-CA	6.26	126.02	119.76
1	D	484	ILE	CA-C-N	6.26	127.66	119.84
1	D	484	ILE	C-N-CA	6.26	127.66	119.84
1	E	484	ILE	CA-C-N	6.25	127.66	119.84
1	E	484	ILE	C-N-CA	6.25	127.66	119.84
2	u	80	ARG	CA-C-N	6.25	126.17	119.85
2	u	80	ARG	C-N-CA	6.25	126.17	119.85
1	L	484	ILE	CA-C-N	6.25	127.65	119.84
1	L	484	ILE	C-N-CA	6.25	127.65	119.84
1	N	484	ILE	CA-C-N	6.25	127.65	119.84
1	N	484	ILE	C-N-CA	6.25	127.65	119.84
2	s	80	ARG	CA-C-N	6.25	126.16	119.85
2	s	80	ARG	C-N-CA	6.25	126.16	119.85
2	g	80	ARG	CA-C-N	6.25	126.16	119.85
2	g	80	ARG	C-N-CA	6.25	126.16	119.85
1	I	204	ILE	CA-C-N	6.25	126.01	119.76
1	I	204	ILE	C-N-CA	6.25	126.01	119.76
1	I	484	ILE	CA-C-N	6.25	127.65	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	484	ILE	C-N-CA	6.25	127.65	119.84
1	B	484	ILE	CA-C-N	6.25	127.65	119.84
1	B	484	ILE	C-N-CA	6.25	127.65	119.84
2	c	80	ARG	CA-C-N	6.25	126.16	119.85
2	c	80	ARG	C-N-CA	6.25	126.16	119.85
1	F	484	ILE	CA-C-N	6.24	127.64	119.84
1	F	484	ILE	C-N-CA	6.24	127.64	119.84
1	G	484	ILE	CA-C-N	6.24	127.64	119.84
1	G	484	ILE	C-N-CA	6.24	127.64	119.84
2	z	80	ARG	CA-C-N	6.24	126.16	119.85
2	z	80	ARG	C-N-CA	6.24	126.16	119.85
1	A	370	ARG	CA-C-N	6.24	126.00	119.76
1	A	370	ARG	C-N-CA	6.24	126.00	119.76
2	a	80	ARG	CA-C-N	6.24	126.15	119.85
2	a	80	ARG	C-N-CA	6.24	126.15	119.85
2	y	80	ARG	CA-C-N	6.24	126.15	119.85
2	y	80	ARG	C-N-CA	6.24	126.15	119.85
2	3	80	ARG	CA-C-N	6.24	126.15	119.85
2	3	80	ARG	C-N-CA	6.24	126.15	119.85
1	E	204	ILE	CA-C-N	6.24	126.00	119.76
1	E	204	ILE	C-N-CA	6.24	126.00	119.76
2	q	80	ARG	CA-C-N	6.24	126.15	119.85
2	q	80	ARG	C-N-CA	6.24	126.15	119.85
2	1	80	ARG	CA-C-N	6.24	126.15	119.85
2	1	80	ARG	C-N-CA	6.24	126.15	119.85
2	7	80	ARG	CA-C-N	6.23	126.15	119.85
2	7	80	ARG	C-N-CA	6.23	126.15	119.85
1	A	484	ILE	CA-C-N	6.23	127.63	119.84
1	A	484	ILE	C-N-CA	6.23	127.63	119.84
1	K	370	ARG	CA-C-N	6.23	125.99	119.76
1	K	370	ARG	C-N-CA	6.23	125.99	119.76
1	L	204	ILE	CA-C-N	6.23	125.99	119.76
1	L	204	ILE	C-N-CA	6.23	125.99	119.76
1	F	204	ILE	CA-C-N	6.23	125.99	119.76
1	F	204	ILE	C-N-CA	6.23	125.99	119.76
2	X	80	ARG	CA-C-N	6.23	126.14	119.85
2	X	80	ARG	C-N-CA	6.23	126.14	119.85
2	m	80	ARG	CA-C-N	6.23	126.14	119.85
2	m	80	ARG	C-N-CA	6.23	126.14	119.85
1	K	484	ILE	CA-C-N	6.23	127.62	119.84
1	K	484	ILE	C-N-CA	6.23	127.62	119.84
1	H	370	ARG	CA-C-N	6.22	125.98	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	370	ARG	C-N-CA	6.22	125.98	119.76
2	T	80	ARG	CA-C-N	6.22	126.14	119.85
2	T	80	ARG	C-N-CA	6.22	126.14	119.85
2	R	80	ARG	CA-C-N	6.22	126.13	119.85
2	R	80	ARG	C-N-CA	6.22	126.13	119.85
2	e	80	ARG	CA-C-N	6.22	126.13	119.85
2	e	80	ARG	C-N-CA	6.22	126.13	119.85
1	B	370	ARG	CA-C-N	6.21	125.97	119.76
1	B	370	ARG	C-N-CA	6.21	125.97	119.76
1	O	370	ARG	CA-C-N	6.21	125.97	119.76
1	O	370	ARG	C-N-CA	6.21	125.97	119.76
1	C	484	ILE	CA-C-N	6.21	127.60	119.84
1	C	484	ILE	C-N-CA	6.21	127.60	119.84
1	M	204	ILE	CA-C-N	6.21	125.97	119.76
1	M	204	ILE	C-N-CA	6.21	125.97	119.76
2	V	80	ARG	CA-C-N	6.20	126.11	119.85
2	V	80	ARG	C-N-CA	6.20	126.11	119.85
1	C	204	ILE	CA-C-N	6.19	125.95	119.76
1	C	204	ILE	C-N-CA	6.19	125.95	119.76
1	O	204	ILE	CA-C-N	6.19	125.95	119.76
1	O	204	ILE	C-N-CA	6.19	125.95	119.76
1	N	204	ILE	CA-C-N	6.19	125.95	119.76
1	N	204	ILE	C-N-CA	6.19	125.95	119.76
1	G	204	ILE	CA-C-N	6.17	125.94	119.76
1	G	204	ILE	C-N-CA	6.17	125.94	119.76
1	H	204	ILE	CA-C-N	6.15	125.91	119.76
1	H	204	ILE	C-N-CA	6.15	125.91	119.76
1	B	204	ILE	CA-C-N	6.15	125.91	119.76
1	B	204	ILE	C-N-CA	6.15	125.91	119.76
1	D	204	ILE	CA-C-N	6.15	125.91	119.76
1	D	204	ILE	C-N-CA	6.15	125.91	119.76
1	A	204	ILE	CA-C-N	6.14	125.90	119.76
1	A	204	ILE	C-N-CA	6.14	125.90	119.76
1	K	204	ILE	CA-C-N	6.12	125.88	119.76
1	K	204	ILE	C-N-CA	6.12	125.88	119.76
1	B	328	SER	N-CA-C	6.10	116.61	108.38
1	H	328	SER	N-CA-C	6.10	116.61	108.38
1	N	328	SER	N-CA-C	6.09	116.60	108.38
1	I	328	SER	N-CA-C	6.08	116.59	108.38
1	F	328	SER	N-CA-C	6.08	116.58	108.38
1	J	328	SER	N-CA-C	6.08	116.58	108.38
1	K	328	SER	N-CA-C	6.07	116.57	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	SER	N-CA-C	6.06	116.57	108.38
1	D	328	SER	N-CA-C	6.06	116.56	108.38
1	G	328	SER	N-CA-C	6.06	116.56	108.38
1	L	328	SER	N-CA-C	6.05	116.55	108.38
1	E	328	SER	N-CA-C	6.04	116.54	108.38
1	O	328	SER	N-CA-C	6.04	116.53	108.38
1	A	328	SER	N-CA-C	6.03	116.52	108.38
3	2	240	TYR	CA-C-N	6.02	125.93	119.85
3	2	240	TYR	C-N-CA	6.02	125.93	119.85
1	M	328	SER	N-CA-C	6.02	116.51	108.38
3	p	240	TYR	CA-C-N	6.00	125.91	119.85
3	p	240	TYR	C-N-CA	6.00	125.91	119.85
3	h	240	TYR	CA-C-N	5.99	125.90	119.85
3	h	240	TYR	C-N-CA	5.99	125.90	119.85
3	f	240	TYR	CA-C-N	5.99	125.90	119.85
3	f	240	TYR	C-N-CA	5.99	125.90	119.85
3	j	240	TYR	CA-C-N	5.98	125.89	119.85
3	j	240	TYR	C-N-CA	5.98	125.89	119.85
3	n	240	TYR	CA-C-N	5.98	125.89	119.85
3	n	240	TYR	C-N-CA	5.98	125.89	119.85
3	Q	240	TYR	CA-C-N	5.97	125.88	119.85
3	Q	240	TYR	C-N-CA	5.97	125.88	119.85
3	x	240	TYR	CA-C-N	5.97	125.88	119.85
3	x	240	TYR	C-N-CA	5.97	125.88	119.85
3	0	240	TYR	CA-C-N	5.97	125.88	119.85
3	0	240	TYR	C-N-CA	5.97	125.88	119.85
3	r	240	TYR	CA-C-N	5.96	125.87	119.85
3	r	240	TYR	C-N-CA	5.96	125.87	119.85
3	S	240	TYR	CA-C-N	5.96	125.87	119.85
3	S	240	TYR	C-N-CA	5.96	125.87	119.85
3	v	240	TYR	CA-C-N	5.96	125.87	119.85
3	v	240	TYR	C-N-CA	5.96	125.87	119.85
3	d	240	TYR	CA-C-N	5.96	125.86	119.85
3	d	240	TYR	C-N-CA	5.96	125.86	119.85
3	4	240	TYR	CA-C-N	5.95	125.86	119.85
3	4	240	TYR	C-N-CA	5.95	125.86	119.85
3	U	240	TYR	CA-C-N	5.93	125.84	119.85
3	U	240	TYR	C-N-CA	5.93	125.84	119.85
3	Z	240	TYR	CA-C-N	5.93	125.84	119.85
3	Z	240	TYR	C-N-CA	5.93	125.84	119.85
3	8	240	TYR	CA-C-N	5.93	125.84	119.85
3	8	240	TYR	C-N-CA	5.93	125.84	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10	240	TYR	CA-C-N	5.93	125.84	119.85
3	10	240	TYR	C-N-CA	5.93	125.84	119.85
3	6	240	TYR	CA-C-N	5.93	125.84	119.85
3	6	240	TYR	C-N-CA	5.93	125.84	119.85
3	W	240	TYR	CA-C-N	5.93	125.84	119.85
3	W	240	TYR	C-N-CA	5.93	125.84	119.85
3	b	240	TYR	CA-C-N	5.92	125.83	119.85
3	b	240	TYR	C-N-CA	5.92	125.83	119.85
3	Y	240	TYR	CA-C-N	5.92	125.83	119.85
3	Y	240	TYR	C-N-CA	5.92	125.83	119.85
3	l	240	TYR	CA-C-N	5.91	125.82	119.85
3	l	240	TYR	C-N-CA	5.91	125.82	119.85
3	t	240	TYR	CA-C-N	5.91	125.82	119.85
3	t	240	TYR	C-N-CA	5.91	125.82	119.85
1	I	96	GLY	N-CA-C	-5.71	107.18	114.37
1	M	96	GLY	N-CA-C	-5.70	107.19	114.37
1	N	96	GLY	N-CA-C	-5.70	107.19	114.37
1	A	96	GLY	N-CA-C	-5.70	107.19	114.37
1	D	96	GLY	N-CA-C	-5.70	107.19	114.37
1	B	96	GLY	N-CA-C	-5.70	107.19	114.37
1	J	96	GLY	N-CA-C	-5.69	107.20	114.37
1	E	96	GLY	N-CA-C	-5.69	107.21	114.37
1	L	96	GLY	N-CA-C	-5.69	107.21	114.37
1	O	96	GLY	N-CA-C	-5.68	107.21	114.37
1	G	96	GLY	N-CA-C	-5.68	107.21	114.37
1	C	96	GLY	N-CA-C	-5.67	107.23	114.37
1	K	96	GLY	N-CA-C	-5.66	107.23	114.37
1	H	96	GLY	N-CA-C	-5.66	107.24	114.37
1	F	96	GLY	N-CA-C	-5.65	107.25	114.37
1	N	55	GLU	N-CA-C	5.59	116.74	109.64
1	G	55	GLU	N-CA-C	5.58	116.73	109.64
1	K	55	GLU	N-CA-C	5.58	116.73	109.64
3	10	252	GLU	CA-C-N	5.58	126.82	119.84
3	10	252	GLU	C-N-CA	5.58	126.82	119.84
1	H	55	GLU	N-CA-C	5.58	116.72	109.64
1	M	85	SER	N-CA-C	-5.58	105.98	112.89
3	l	252	GLU	CA-C-N	5.58	126.81	119.84
3	l	252	GLU	C-N-CA	5.58	126.81	119.84
1	O	55	GLU	N-CA-C	5.57	116.72	109.64
3	Z	252	GLU	CA-C-N	5.57	126.81	119.84
3	Z	252	GLU	C-N-CA	5.57	126.81	119.84
1	G	85	SER	N-CA-C	-5.57	105.98	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	252	GLU	CA-C-N	5.57	126.80	119.84
3	6	252	GLU	C-N-CA	5.57	126.80	119.84
3	p	252	GLU	CA-C-N	5.57	126.80	119.84
3	p	252	GLU	C-N-CA	5.57	126.80	119.84
1	J	55	GLU	N-CA-C	5.57	116.71	109.64
1	A	55	GLU	N-CA-C	5.56	116.70	109.64
1	M	55	GLU	N-CA-C	5.56	116.70	109.64
3	j	252	GLU	CA-C-N	5.56	126.79	119.84
3	j	252	GLU	C-N-CA	5.56	126.79	119.84
3	d	252	GLU	CA-C-N	5.56	126.79	119.84
3	d	252	GLU	C-N-CA	5.56	126.79	119.84
1	E	55	GLU	N-CA-C	5.56	116.70	109.64
1	B	85	SER	N-CA-C	-5.55	106.00	112.89
1	F	55	GLU	N-CA-C	5.55	116.69	109.64
1	I	55	GLU	N-CA-C	5.55	116.69	109.64
1	O	85	SER	N-CA-C	-5.55	106.01	112.89
3	0	252	GLU	CA-C-N	5.55	126.78	119.84
3	0	252	GLU	C-N-CA	5.55	126.78	119.84
1	B	55	GLU	N-CA-C	5.55	116.68	109.64
3	t	252	GLU	CA-C-N	5.55	126.77	119.84
3	t	252	GLU	C-N-CA	5.55	126.77	119.84
1	D	55	GLU	N-CA-C	5.54	116.68	109.64
3	r	252	GLU	CA-C-N	5.54	126.77	119.84
3	r	252	GLU	C-N-CA	5.54	126.77	119.84
3	f	252	GLU	CA-C-N	5.54	126.76	119.84
3	f	252	GLU	C-N-CA	5.54	126.76	119.84
1	C	85	SER	N-CA-C	-5.54	106.02	112.89
3	8	252	GLU	CA-C-N	5.54	126.76	119.84
3	8	252	GLU	C-N-CA	5.54	126.76	119.84
1	C	55	GLU	N-CA-C	5.53	116.67	109.64
3	h	252	GLU	CA-C-N	5.53	126.76	119.84
3	h	252	GLU	C-N-CA	5.53	126.76	119.84
1	H	85	SER	N-CA-C	-5.53	106.03	112.89
1	D	85	SER	N-CA-C	-5.53	106.03	112.89
3	2	252	GLU	CA-C-N	5.53	126.75	119.84
3	2	252	GLU	C-N-CA	5.53	126.75	119.84
3	4	252	GLU	CA-C-N	5.53	126.75	119.84
3	4	252	GLU	C-N-CA	5.53	126.75	119.84
1	E	85	SER	N-CA-C	-5.53	106.03	112.89
3	Q	252	GLU	CA-C-N	5.52	126.74	119.84
3	Q	252	GLU	C-N-CA	5.52	126.74	119.84
1	L	55	GLU	N-CA-C	5.52	116.65	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	252	GLU	CA-C-N	5.52	126.74	119.84
3	S	252	GLU	C-N-CA	5.52	126.74	119.84
1	L	85	SER	N-CA-C	-5.52	106.05	112.89
3	U	252	GLU	CA-C-N	5.52	126.74	119.84
3	U	252	GLU	C-N-CA	5.52	126.74	119.84
1	K	85	SER	N-CA-C	-5.52	106.05	112.89
3	n	252	GLU	CA-C-N	5.52	126.74	119.84
3	n	252	GLU	C-N-CA	5.52	126.74	119.84
3	x	252	GLU	CA-C-N	5.52	126.74	119.84
3	x	252	GLU	C-N-CA	5.52	126.74	119.84
1	F	85	SER	N-CA-C	-5.51	106.05	112.89
3	v	252	GLU	CA-C-N	5.51	126.73	119.84
3	v	252	GLU	C-N-CA	5.51	126.73	119.84
1	J	85	SER	N-CA-C	-5.51	106.06	112.89
3	Y	252	GLU	CA-C-N	5.51	126.72	119.84
3	Y	252	GLU	C-N-CA	5.51	126.72	119.84
1	I	85	SER	N-CA-C	-5.51	106.06	112.89
3	b	252	GLU	CA-C-N	5.51	126.72	119.84
3	b	252	GLU	C-N-CA	5.51	126.72	119.84
1	A	85	SER	N-CA-C	-5.50	106.06	112.89
2	T	62	GLU	CA-C-N	5.50	125.33	119.28
2	T	62	GLU	C-N-CA	5.50	125.33	119.28
3	W	252	GLU	CA-C-N	5.50	126.71	119.84
3	W	252	GLU	C-N-CA	5.50	126.71	119.84
2	R	62	GLU	CA-C-N	5.48	125.31	119.28
2	R	62	GLU	C-N-CA	5.48	125.31	119.28
2	3	62	GLU	CA-C-N	5.48	125.31	119.28
2	3	62	GLU	C-N-CA	5.48	125.31	119.28
1	N	85	SER	N-CA-C	-5.48	106.09	112.89
2	7	62	GLU	CA-C-N	5.48	125.31	119.28
2	7	62	GLU	C-N-CA	5.48	125.31	119.28
2	m	62	GLU	CA-C-N	5.48	125.31	119.28
2	m	62	GLU	C-N-CA	5.48	125.31	119.28
2	s	62	GLU	CA-C-N	5.47	125.30	119.28
2	s	62	GLU	C-N-CA	5.47	125.30	119.28
2	P	62	GLU	CA-C-N	5.47	125.30	119.28
2	P	62	GLU	C-N-CA	5.47	125.30	119.28
2	9	62	GLU	CA-C-N	5.47	125.30	119.28
2	9	62	GLU	C-N-CA	5.47	125.30	119.28
2	k	62	GLU	CA-C-N	5.47	125.30	119.28
2	k	62	GLU	C-N-CA	5.47	125.30	119.28
2	1	62	GLU	CA-C-N	5.47	125.30	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	62	GLU	C-N-CA	5.47	125.30	119.28
2	V	62	GLU	CA-C-N	5.47	125.30	119.28
2	V	62	GLU	C-N-CA	5.47	125.30	119.28
2	i	62	GLU	CA-C-N	5.47	125.30	119.28
2	i	62	GLU	C-N-CA	5.47	125.30	119.28
2	q	62	GLU	CA-C-N	5.47	125.29	119.28
2	q	62	GLU	C-N-CA	5.47	125.29	119.28
2	a	62	GLU	CA-C-N	5.46	125.29	119.28
2	a	62	GLU	C-N-CA	5.46	125.29	119.28
2	z	62	GLU	CA-C-N	5.46	125.29	119.28
2	z	62	GLU	C-N-CA	5.46	125.29	119.28
2	y	62	GLU	CA-C-N	5.45	125.28	119.28
2	y	62	GLU	C-N-CA	5.45	125.28	119.28
2	o	62	GLU	CA-C-N	5.45	125.27	119.28
2	o	62	GLU	C-N-CA	5.45	125.27	119.28
2	u	62	GLU	CA-C-N	5.45	125.27	119.28
2	u	62	GLU	C-N-CA	5.45	125.27	119.28
2	X	62	GLU	CA-C-N	5.44	125.27	119.28
2	X	62	GLU	C-N-CA	5.44	125.27	119.28
2	5	62	GLU	CA-C-N	5.44	125.26	119.28
2	5	62	GLU	C-N-CA	5.44	125.26	119.28
2	e	62	GLU	CA-C-N	5.44	125.26	119.28
2	e	62	GLU	C-N-CA	5.44	125.26	119.28
2	g	62	GLU	CA-C-N	5.44	125.26	119.28
2	g	62	GLU	C-N-CA	5.44	125.26	119.28
2	c	62	GLU	CA-C-N	5.43	125.26	119.28
2	c	62	GLU	C-N-CA	5.43	125.26	119.28
1	F	136	TYR	CA-C-N	5.42	125.34	119.76
1	F	136	TYR	C-N-CA	5.42	125.34	119.76
1	I	136	TYR	CA-C-N	5.41	125.33	119.76
1	I	136	TYR	C-N-CA	5.41	125.33	119.76
1	H	130	GLY	N-CA-C	-5.40	106.23	115.08
1	J	136	TYR	CA-C-N	5.39	125.31	119.76
1	J	136	TYR	C-N-CA	5.39	125.31	119.76
2	w	62	GLU	CA-C-N	5.39	125.21	119.28
2	w	62	GLU	C-N-CA	5.39	125.21	119.28
1	K	136	TYR	CA-C-N	5.39	125.31	119.76
1	K	136	TYR	C-N-CA	5.39	125.31	119.76
1	M	130	GLY	N-CA-C	-5.39	106.24	115.08
1	K	130	GLY	N-CA-C	-5.39	106.25	115.08
1	J	130	GLY	N-CA-C	-5.38	106.27	115.08
1	D	136	TYR	CA-C-N	5.37	125.30	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	TYR	C-N-CA	5.37	125.30	119.76
1	L	130	GLY	N-CA-C	-5.37	106.27	115.08
1	E	130	GLY	N-CA-C	-5.37	106.28	115.08
1	B	130	GLY	N-CA-C	-5.37	106.28	115.08
1	C	130	GLY	N-CA-C	-5.37	106.28	115.08
1	D	130	GLY	N-CA-C	-5.37	106.28	115.08
1	G	136	TYR	CA-C-N	5.37	125.29	119.76
1	G	136	TYR	C-N-CA	5.37	125.29	119.76
1	I	130	GLY	N-CA-C	-5.37	106.28	115.08
1	L	136	TYR	CA-C-N	5.36	125.28	119.76
1	L	136	TYR	C-N-CA	5.36	125.28	119.76
1	F	130	GLY	N-CA-C	-5.36	106.29	115.08
1	A	130	GLY	N-CA-C	-5.36	106.29	115.08
1	N	130	GLY	N-CA-C	-5.36	106.29	115.08
1	N	136	TYR	CA-C-N	5.36	125.28	119.76
1	N	136	TYR	C-N-CA	5.36	125.28	119.76
1	G	130	GLY	N-CA-C	-5.36	106.29	115.08
1	H	136	TYR	CA-C-N	5.36	125.28	119.76
1	H	136	TYR	C-N-CA	5.36	125.28	119.76
1	A	136	TYR	CA-C-N	5.35	125.27	119.76
1	A	136	TYR	C-N-CA	5.35	125.27	119.76
1	O	130	GLY	N-CA-C	-5.35	106.31	115.08
1	O	136	TYR	CA-C-N	5.34	125.27	119.76
1	O	136	TYR	C-N-CA	5.34	125.27	119.76
1	E	136	TYR	CA-C-N	5.33	125.25	119.76
1	E	136	TYR	C-N-CA	5.33	125.25	119.76
1	C	136	TYR	CA-C-N	5.33	125.25	119.76
1	C	136	TYR	C-N-CA	5.33	125.25	119.76
1	B	136	TYR	CA-C-N	5.31	125.23	119.76
1	B	136	TYR	C-N-CA	5.31	125.23	119.76
1	M	136	TYR	CA-C-N	5.31	125.23	119.76
1	M	136	TYR	C-N-CA	5.31	125.23	119.76
1	L	412	VAL	N-CA-C	5.18	116.11	108.45
1	G	412	VAL	N-CA-C	5.17	116.10	108.45
1	H	412	VAL	N-CA-C	5.17	116.11	108.45
1	C	412	VAL	N-CA-C	5.16	116.08	108.45
1	D	412	VAL	N-CA-C	5.14	116.06	108.45
1	J	412	VAL	N-CA-C	5.14	116.06	108.45
1	A	412	VAL	N-CA-C	5.14	116.05	108.45
1	E	412	VAL	N-CA-C	5.13	116.04	108.45
1	M	412	VAL	N-CA-C	5.13	116.04	108.45
1	I	412	VAL	N-CA-C	5.12	116.03	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	412	VAL	N-CA-C	5.12	116.03	108.45
1	O	412	VAL	N-CA-C	5.12	116.02	108.45
1	F	412	VAL	N-CA-C	5.10	116.00	108.45
1	B	412	VAL	N-CA-C	5.09	115.98	108.45
1	N	412	VAL	N-CA-C	5.08	115.97	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3718	0	3777	10	0
1	B	3718	0	3777	10	0
1	C	3718	0	3777	10	0
1	D	3718	0	3777	9	0
1	E	3718	0	3777	9	0
1	F	3718	0	3777	10	0
1	G	3718	0	3777	10	0
1	H	3718	0	3777	10	0
1	I	3718	0	3777	10	0
1	J	3718	0	3777	10	0
1	K	3718	0	3777	9	0
1	L	3718	0	3777	10	0
1	M	3718	0	3777	10	0
1	N	3718	0	3777	11	0
1	O	3718	0	3777	10	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	1437	0	1434	4	0
2	a	1437	0	1434	5	0
2	c	1437	0	1434	5	0
2	e	1437	0	1434	5	0
2	g	1437	0	1434	5	0
2	i	1437	0	1434	4	0
2	k	1437	0	1434	4	0
2	m	1437	0	1434	4	0
2	o	1437	0	1434	4	0
2	q	1437	0	1434	5	0
2	s	1437	0	1434	4	0
2	u	1437	0	1434	5	0
2	w	1437	0	1434	4	0
2	y	1437	0	1434	4	0
2	z	1437	0	1434	5	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	0	0
3	S	1600	0	1580	0	0
3	U	1600	0	1580	0	0
3	W	1600	0	1580	0	0
3	Y	1600	0	1580	0	0
3	Z	1600	0	1580	0	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	256	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 (256) 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:O	1:H:173:ILE:HG22	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:G:173:ILE:HG22	1:G:173:ILE:O	1.91	0.69
1:F:173:ILE:O	1:F:173:ILE:HG22	1.92	0.69
1:A:173:ILE:O	1:A:173:ILE:HG22	1.91	0.69
1:B:173:ILE:HG22	1:B:173:ILE:O	1.91	0.69
1:L:173:ILE:HG22	1:L:173:ILE:O	1.92	0.69
1:J:173:ILE:HG22	1:J:173:ILE:O	1.92	0.69
1:M:173:ILE:O	1:M:173:ILE:HG22	1.92	0.69
1:O:173:ILE:HG22	1:O:173:ILE:O	1.91	0.69
1:K:173:ILE:O	1:K:173:ILE:HG22	1.92	0.69
1:N:173:ILE:HG22	1:N:173:ILE:O	1.92	0.69
1:C:173:ILE:O	1:C:173:ILE:HG22	1.92	0.68
2:z:28:ASP:OD1	2:z:28:ASP:C	2.48	0.57
2:X:28:ASP:OD1	2:X:28:ASP:C	2.48	0.57
2:3:28:ASP:OD1	2:3:28:ASP:C	2.48	0.56
2:R:187:LEU:C	2:R:187:LEU:HD12	2.31	0.56
2:9:187:LEU:HD12	2:9:187:LEU:C	2.31	0.56
2:q:187:LEU:HD12	2:q:187:LEU:C	2.31	0.56
2:y:187:LEU:C	2:y:187:LEU:HD12	2.31	0.56
2:T:187:LEU:C	2:T:187:LEU:HD12	2.31	0.56
2:m:28:ASP:OD1	2:m:28:ASP:C	2.48	0.56
2:3:187:LEU:C	2:3:187:LEU:HD12	2.31	0.56
2:5:187:LEU:C	2:5:187:LEU:HD12	2.31	0.56
2:P:187:LEU:C	2:P:187:LEU:HD12	2.31	0.56
2:X:187:LEU:HD12	2:X:187:LEU:C	2.31	0.56
2:i:28:ASP:OD1	2:i:28:ASP:C	2.48	0.56
2:s:187:LEU:HD12	2:s:187:LEU:C	2.31	0.56
2:V:187:LEU:HD12	2:V:187:LEU:C	2.31	0.56
2:u:187:LEU:C	2:u:187:LEU:HD12	2.31	0.56
2:w:187:LEU:C	2:w:187:LEU:HD12	2.31	0.56
2:z:187:LEU:HD12	2:z:187:LEU:C	2.31	0.56
2:7:187:LEU:C	2:7:187:LEU:HD12	2.31	0.56
2:o:28:ASP:C	2:o:28:ASP:OD1	2.48	0.56
2:s:28:ASP:C	2:s:28:ASP:OD1	2.48	0.56
2:1:187:LEU:HD12	2:1:187:LEU:C	2.31	0.56
2:a:187:LEU:C	2:a:187:LEU:HD12	2.31	0.56
2:R:28:ASP:OD1	2:R:28:ASP:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:28:ASP:OD1	2:P:28:ASP:C	2.48	0.55
2:T:28:ASP:C	2:T:28:ASP:OD1	2.48	0.55
2:e:28:ASP:C	2:e:28:ASP:OD1	2.48	0.55
2:q:28:ASP:C	2:q:28:ASP:OD1	2.48	0.55
2:g:187:LEU:HD12	2:g:187:LEU:C	2.31	0.55
2:k:28:ASP:OD1	2:k:28:ASP:C	2.48	0.55
2:o:187:LEU:C	2:o:187:LEU:HD12	2.31	0.55
2:V:28:ASP:C	2:V:28:ASP:OD1	2.48	0.55
2:i:187:LEU:HD12	2:i:187:LEU:C	2.31	0.55
2:w:28:ASP:OD1	2:w:28:ASP:C	2.48	0.55
2:a:28:ASP:OD1	2:a:28:ASP:C	2.48	0.55
2:g:28:ASP:C	2:g:28:ASP:OD1	2.48	0.55
2:k:187:LEU:C	2:k:187:LEU:HD12	2.31	0.55
2:c:187:LEU:C	2:c:187:LEU:HD12	2.31	0.55
2:u:28:ASP:OD1	2:u:28:ASP:C	2.48	0.55
2:c:28:ASP:C	2:c:28:ASP:OD1	2.48	0.55
2:e:187:LEU:C	2:e:187:LEU:HD12	2.31	0.55
2:9:28:ASP:C	2:9:28:ASP:OD1	2.48	0.54
2:m:187:LEU:C	2:m:187:LEU:HD12	2.31	0.54
2:y:28:ASP:OD1	2:y:28:ASP:C	2.48	0.54
2:1:28:ASP:OD1	2:1:28:ASP:C	2.48	0.54
1:J:386:ASN:C	1:J:386:ASN:OD1	2.51	0.54
1:L:386:ASN:OD1	1:L:386:ASN:C	2.51	0.54
1:N:386:ASN:OD1	1:N:386:ASN:C	2.51	0.53
1:A:386:ASN:OD1	1:A:386:ASN:C	2.51	0.53
1:O:386:ASN:C	1:O:386:ASN:OD1	2.51	0.53
1:M:386:ASN:C	1:M:386:ASN:OD1	2.51	0.53
2:5:28:ASP:OD1	2:5:28:ASP:C	2.48	0.53
2:7:28:ASP:C	2:7:28:ASP:OD1	2.48	0.53
1:B:386:ASN:OD1	1:B:386:ASN:C	2.51	0.53
1:K:386:ASN:OD1	1:K:386:ASN:C	2.51	0.53
1:I:386:ASN:OD1	1:I:386:ASN:C	2.51	0.52
1:D:386:ASN:OD1	1:D:386:ASN:C	2.52	0.52
1:C:386:ASN:C	1:C:386:ASN:OD1	2.51	0.52
1:G:386:ASN:OD1	1:G:386:ASN:C	2.52	0.52
1:F:386:ASN:OD1	1:F:386:ASN:C	2.51	0.52
1:E:386:ASN:C	1:E:386:ASN:OD1	2.51	0.51
1:H:386:ASN:C	1:H:386:ASN:OD1	2.51	0.51
1:A:328:SER:OG	1:A:329:ILE:N	2.45	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:SER:OG	1:C:329:ILE:N	2.46	0.49
1:N:328:SER:OG	1:N:329:ILE:N	2.45	0.49
1:I:328:SER:OG	1:I:329:ILE:N	2.45	0.49
1:M:328:SER:OG	1:M:329:ILE:N	2.45	0.48
1:E:328:SER:OG	1:E:329:ILE:N	2.45	0.48
1:L:328:SER:OG	1:L:329:ILE:N	2.45	0.48
1:D:328:SER:OG	1:D:329:ILE:N	2.45	0.47
1:H:328:SER:OG	1:H:329:ILE:N	2.45	0.47
1:F:328:SER:OG	1:F:329:ILE:N	2.45	0.47
1:G:328:SER:OG	1:G:329:ILE:N	2.45	0.47
1:K:328:SER:OG	1:K:329:ILE:N	2.45	0.47
1:J:328:SER:OG	1:J:329:ILE:N	2.45	0.46
2:e:78:PRO:HA	2:e:79:PRO:HD3	1.83	0.46
2:e:187:LEU:HD12	2:e:187:LEU:O	2.17	0.45
2:k:187:LEU:HD12	2:k:187:LEU:O	2.17	0.45
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:HD12	2:X:187:LEU:O	2.17	0.45
2:c:187:LEU:HD12	2:c:187:LEU:O	2.17	0.45
2:9:187:LEU:HD12	2:9:187:LEU:O	2.17	0.45
2:R:187:LEU:HD12	2:R:187:LEU:O	2.17	0.45
2:i:187:LEU:HD12	2:i:187:LEU:O	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
2:q:187:LEU:HD12	2:q:187:LEU:O	2.17	0.45
2:u:187:LEU:HD12	2:u:187:LEU:O	2.17	0.45
1:B:447:LEU:N	1:B:448:PRO:CD	2.80	0.44
2:s:187:LEU:HD12	2:s:187:LEU:O	2.17	0.44
2:z:187:LEU:HD12	2:z:187:LEU:O	2.17	0.44
1:N:447:LEU:N	1:N:448:PRO:CD	2.80	0.44
2:a:187:LEU:HD12	2:a:187:LEU:O	2.17	0.44
2:g:187:LEU:HD12	2:g:187:LEU:O	2.17	0.44
2:m:187:LEU:HD12	2:m:187:LEU:O	2.17	0.44
2:5:187:LEU:HD12	2:5:187:LEU:O	2.17	0.44
2:V:78:PRO:HA	2:V:79:PRO:HD3	1.83	0.44
2:c:78:PRO:HA	2:c:79:PRO:HD3	1.83	0.44
2:3:187:LEU:HD12	2:3:187:LEU:O	2.17	0.44
1:K:447:LEU:N	1:K:448:PRO:CD	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:187:LEU:HD12	2:y:187:LEU:O	2.17	0.44
2:7:187:LEU:HD12	2:7:187:LEU:O	2.17	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
2:w:187:LEU:HD12	2:w:187:LEU:O	2.17	0.44
2:o:187:LEU:HD12	2:o:187:LEU:O	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
2:1:187:LEU:HD12	2:1:187:LEU:O	2.17	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:a:78:PRO:HA	2:a:79:PRO:HD3	1.82	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
2:7:62:GLU:HB3	2:7:63:PRO:HD3	2.01	0.43
2:5:62:GLU:HB3	2:5:63:PRO:HD3	2.01	0.43
1:E:335:LEU:HD12	1:E:335:LEU:C	2.44	0.43
1:E:350:SER:OG	1:E:351:ARG:N	2.52	0.43
1:F:335:LEU:C	1:F:335:LEU:HD12	2.44	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:g:78:PRO:HA	2:g:79:PRO:HD3	1.83	0.43
2:9:62:GLU:HB3	2:9:63:PRO:HD3	2.01	0.43
1:G:335:LEU:C	1:G:335:LEU:HD12	2.44	0.42
1:H:335:LEU:HD12	1:H:335:LEU:C	2.44	0.42
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:C:335:LEU:HD12	1:C:335:LEU:C	2.44	0.42
1:K:350:SER:OG	1:K:351:ARG:N	2.52	0.42
1:D:335:LEU:C	1:D:335:LEU:HD12	2.44	0.42
1:N:350:SER:OG	1:N:351:ARG:N	2.52	0.42
2:q:62:GLU:HB3	2:q:63:PRO:HD3	2.01	0.42
1:J:350:SER:OG	1:J:351:ARG:N	2.52	0.42
2:o:62:GLU:HB3	2:o:63:PRO:HD3	2.01	0.42
2:3:62:GLU:HB3	2:3:63:PRO:HD3	2.01	0.42
1:D:350:SER:OG	1:D:351:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:350:SER:OG	1:L:351:ARG:N	2.52	0.42
2:m:62:GLU:HB3	2:m:63:PRO:HD3	2.01	0.42
2:q:78:PRO:HA	2:q:79:PRO:HD3	1.83	0.42
1:J:335:LEU:HD12	1:J:335:LEU:C	2.44	0.42
2:P:62:GLU:HB3	2:P:63:PRO:HD3	2.01	0.42
2:i:62:GLU:HB3	2:i:63:PRO:HD3	2.01	0.42
2:k:62:GLU:HB3	2:k:63:PRO:HD3	2.01	0.42
2:s:62:GLU:HB3	2:s:63:PRO:HD3	2.01	0.42
2:z:62:GLU:HB3	2:z:63:PRO:HD3	2.01	0.42
1:A:335:LEU:HD12	1:A:335:LEU:C	2.44	0.42
2:R:62:GLU:HB3	2:R:63:PRO:HD3	2.01	0.42
2:u:62:GLU:HB3	2:u:63:PRO:HD3	2.01	0.42
1:M:335:LEU:HD12	1:M:335:LEU:C	2.44	0.42
1:N:335:LEU:C	1:N:335:LEU:HD12	2.44	0.42
2:g:62:GLU:HB3	2:g:63:PRO:HD3	2.01	0.42
1:F:417:SER:OG	1:F:418:ALA:N	2.53	0.42
1:I:335:LEU:C	1:I:335:LEU:HD12	2.44	0.42
1:O:335:LEU:HD12	1:O:335:LEU:C	2.44	0.42
2:e:62:GLU:HB3	2:e:63:PRO:HD3	2.01	0.42
2:7:78:PRO:HA	2:7:79:PRO:HD3	1.83	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
1:L:335:LEU:C	1:L:335:LEU:HD12	2.44	0.42
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
2:w:62:GLU:HB3	2:w:63:PRO:HD3	2.01	0.41
2:1:62:GLU:HB3	2:1:63:PRO:HD3	2.01	0.41
1:B:335:LEU:C	1:B:335:LEU:HD12	2.44	0.41
1:K:335:LEU:C	1:K:335:LEU:HD12	2.44	0.41
2:c:62:GLU:HB3	2:c:63:PRO:HD3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:312:ASP:OD1	1:M:312:ASP:C	2.64	0.41
1:O:445:ASP:O	1:O:447:LEU:N	2.53	0.41
2:a:62:GLU:HB3	2:a:63:PRO:HD3	2.01	0.41
2:y:62:GLU:HB3	2:y:63:PRO:HD3	2.01	0.41
1:M:447:LEU:O	1:M:449:GLU:N	2.54	0.41
1:A:312:ASP:OD1	1:A:312:ASP:C	2.64	0.41
1:B:312:ASP:OD1	1:B:312:ASP:C	2.64	0.41
1:B:417:SER:OG	1:B:418:ALA:N	2.53	0.41
1:L:312:ASP:OD1	1:L:312:ASP:C	2.64	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:D:447:LEU:O	1:D: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:K:447:LEU:O	1:K: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
2:u:78:PRO:HA	2:u:79:PRO:HD3	1.82	0.41
1:G:447:LEU:O	1:G:449:GLU:N	2.54	0.41
1:H:312:ASP:OD1	1:H:312:ASP:C	2.64	0.41
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:312:ASP:OD1	1:N:312:ASP:C	2.64	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:C:312:ASP:OD1	1:C:312:ASP:C	2.64	0.40
1:G:445:ASP:O	1:G:447:LEU:N	2.53	0.40
1:I:312:ASP:OD1	1:I:312:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:78:PRO:HA	2:z:79:PRO:HD3	1.82	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:312:ASP:C	1:O:312:ASP:OD1	2.64	0.40
1:G:312:ASP:OD1	1:G:312:ASP:C	2.64	0.40
1:O:447:LEU:O	1:O:449:GLU:N	2.54	0.40
1:F:312:ASP:C	1:F:312:ASP:OD1	2.64	0.40
1:J:484:ILE:HA	1:J:485:PRO:HD3	1.96	0.40
2:9:78:PRO:HA	2:9:79:PRO:HD3	1.82	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%)	6	32
1	B	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	C	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	D	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	E	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	F	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	G	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	H	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	I	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	J	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	K	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	M	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	N	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
1	O	468/562 (83%)	444 (95%)	15 (3%)	9 (2%)	6	32
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%)	5	29
3	10	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	2	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	6	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	8	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	Q	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	S	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	U	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	W	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	Y	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	Z	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	b	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	d	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	f	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	h	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	j	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	l	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	n	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	p	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	r	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	t	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	v	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
3	x	192/263 (73%)	182 (95%)	6 (3%)	4 (2%)	5	29
All	All	15996/20382 (78%)	15228 (95%)	537 (3%)	231 (1%)	11	40

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
1	D	515	PRO
1	E	446	ALA
1	E	515	PRO

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Mol	Chain	Res	Type
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
3	8	251	ASP
3	10	251	ASP
1	A	448	PRO

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Mol	Chain	Res	Type
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
3	6	178	GLY
3	8	178	GLY
3	10	178	GLY

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Mol	Chain	Res	Type
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
3	n	188	PRO
3	n	253	PRO
3	p	188	PRO

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Mol	Chain	Res	Type
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
1	H	173	ILE
1	H	485	PRO
1	H	491	PRO

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Mol	Chain	Res	Type
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
1	H	344	ILE
1	H	447	LEU
1	I	344	ILE

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Mol	Chain	Res	Type
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
1	M	413/477 (87%)	413 (100%)	0	100	100
1	N	413/477 (87%)	413 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
3	6	167/221 (76%)	167 (100%)	0	100	100
3	8	167/221 (76%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	357	ASN
1	B	196	ASN
1	B	357	ASN
1	C	97	GLN
1	C	196	ASN
1	D	196	ASN
1	D	357	ASN
1	E	196	ASN
1	F	196	ASN

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Mol	Chain	Res	Type
1	G	196	ASN
1	H	196	ASN
1	H	357	ASN
1	I	196	ASN
1	I	357	ASN
1	J	196	ASN
1	J	357	ASN
1	K	196	ASN
1	L	196	ASN
1	M	196	ASN
1	N	196	ASN
1	O	196	ASN
1	O	357	ASN
2	T	47	ASN
2	X	47	ASN
2	a	47	ASN
2	c	47	ASN
2	e	47	ASN
2	q	47	ASN
2	s	47	ASN
2	u	47	ASN
2	w	47	ASN
2	z	47	ASN
2	1	47	ASN
2	3	47	ASN
2	7	47	ASN
2	9	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	K	1
1	L	1
1	M	1
1	J	1
1	N	1
1	O	1
1	I	1
1	A	1
1	H	1
1	B	1
1	G	1
1	C	1
1	F	1
1	D	1
1	E	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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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

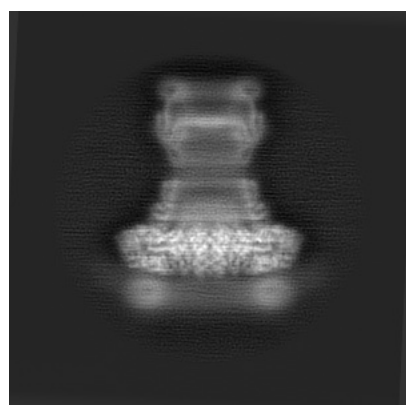
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8400. These allow visual inspection of the internal detail of the map and identification of artifacts.

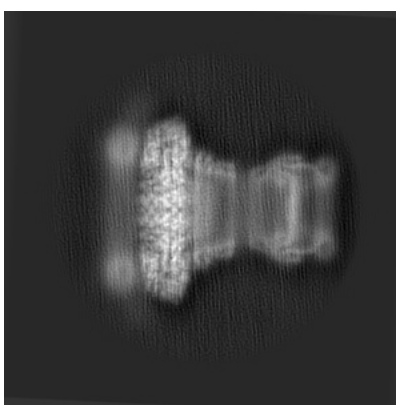
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

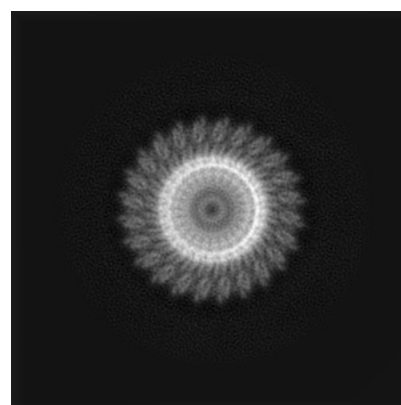
6.1.1 Primary map



X



Y

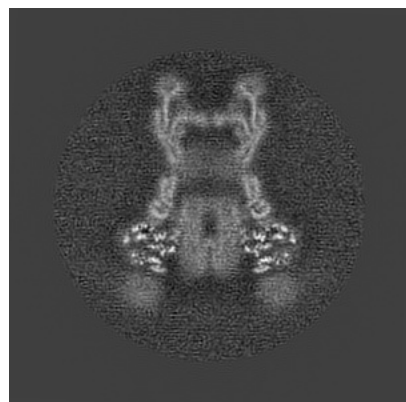


Z

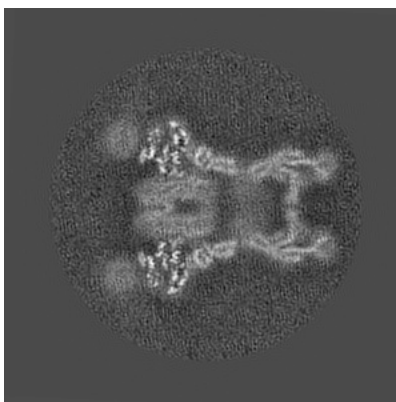
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

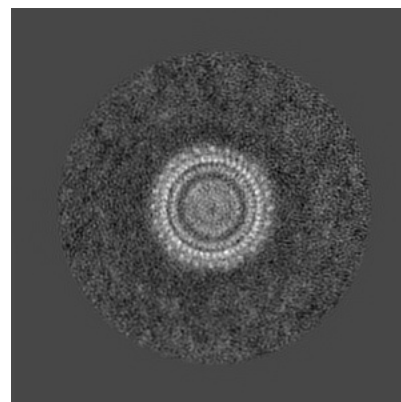
6.2.1 Primary map



X Index: 150



Y Index: 150

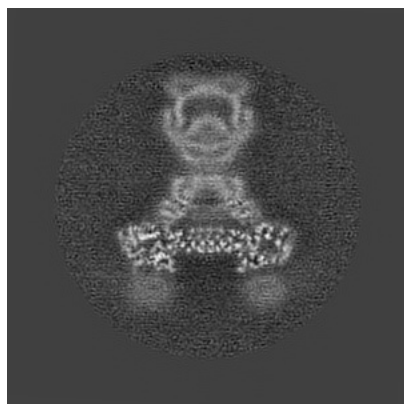


Z Index: 150

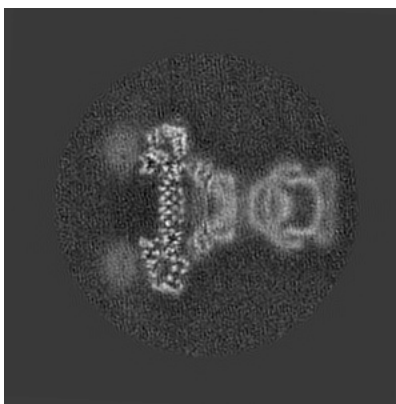
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

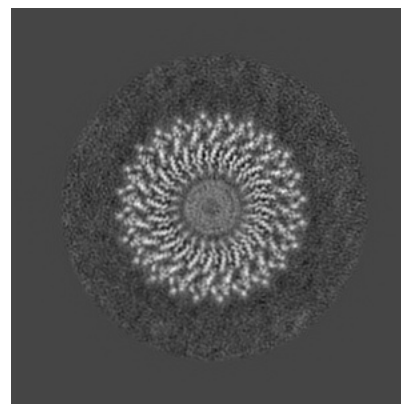
6.3.1 Primary map



X Index: 176



Y Index: 177

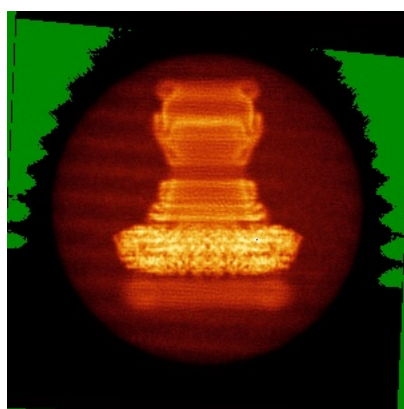


Z Index: 127

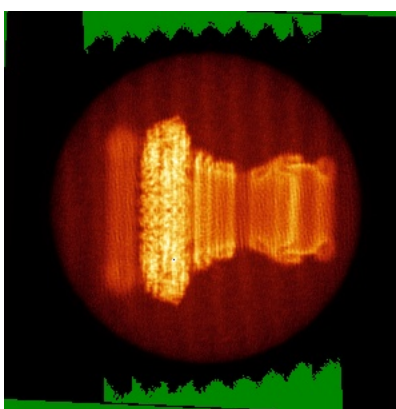
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

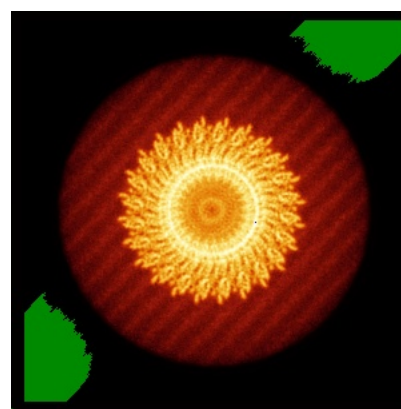
6.4.1 Primary map



X



Y



Z

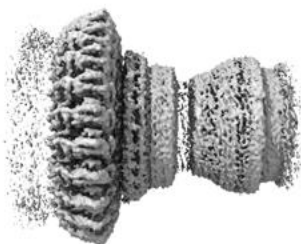
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

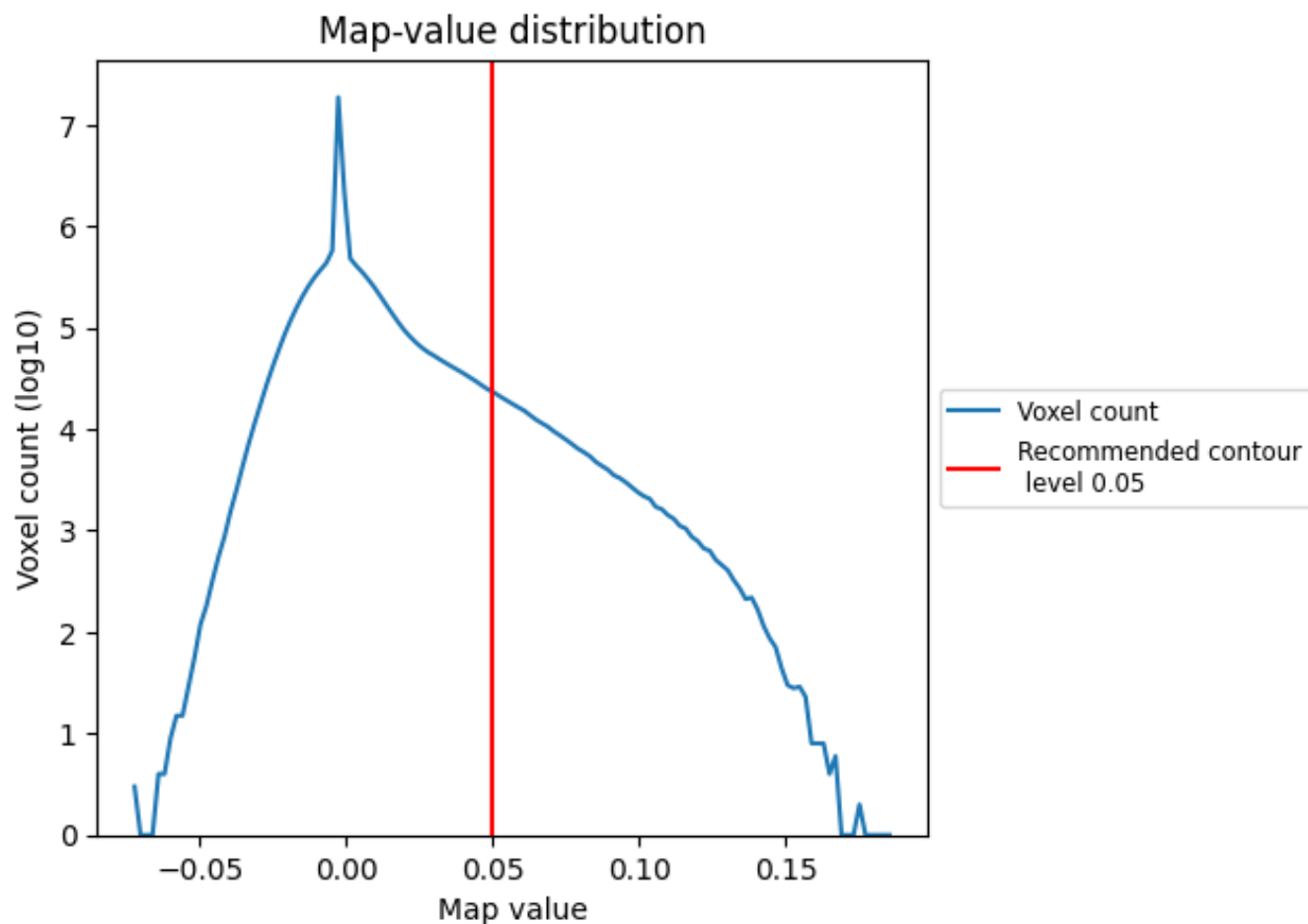
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

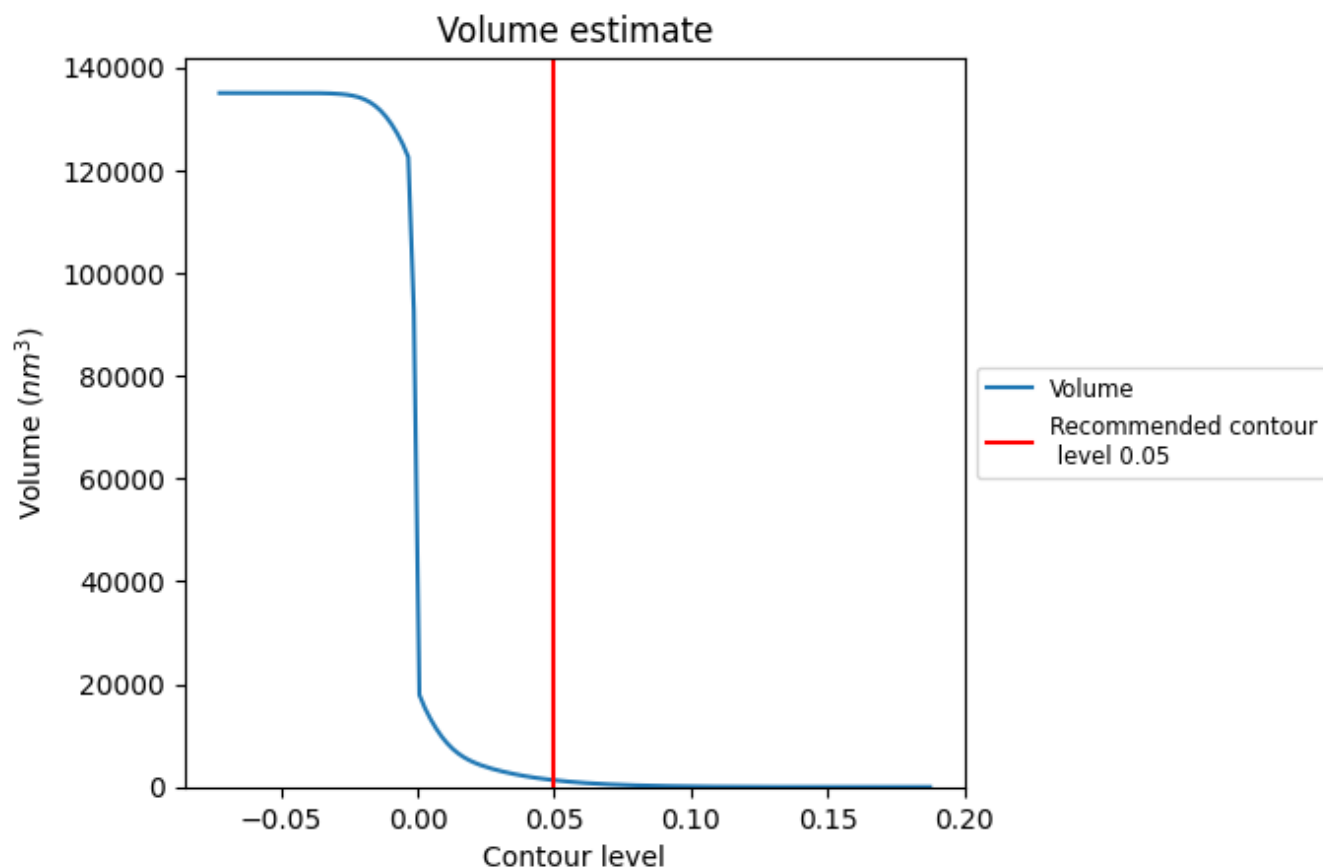
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

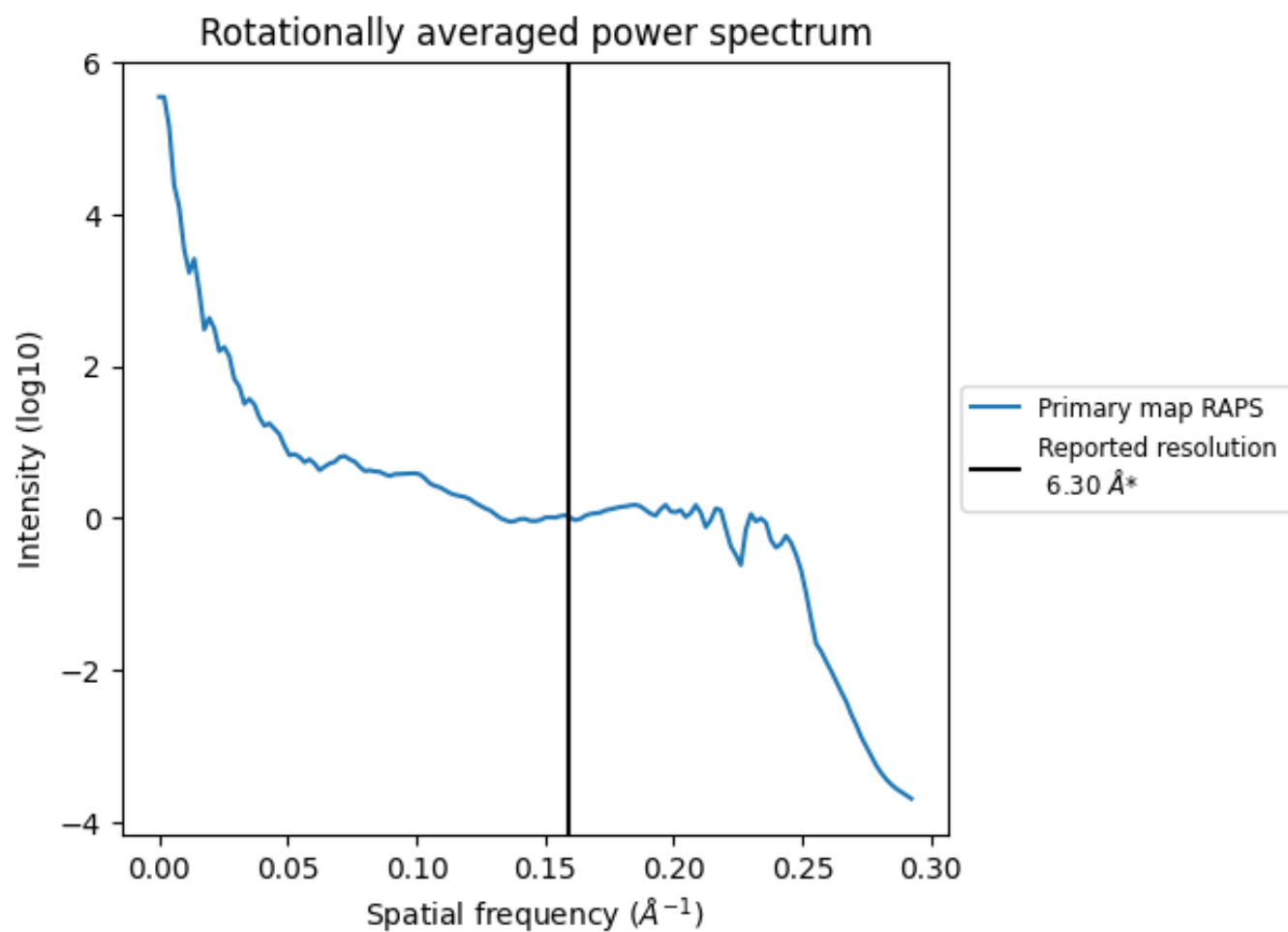
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1316 nm^3 ; this corresponds to an approximate mass of 1189 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

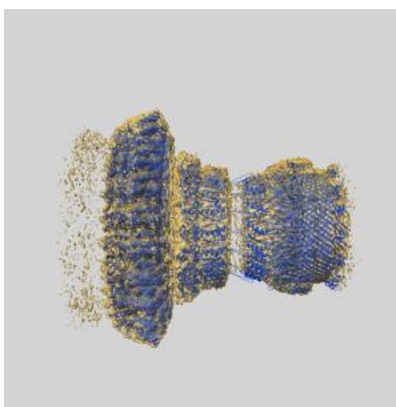
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8400 and PDB model 5TCR. Per-residue inclusion information can be found in section 3 on page 10.

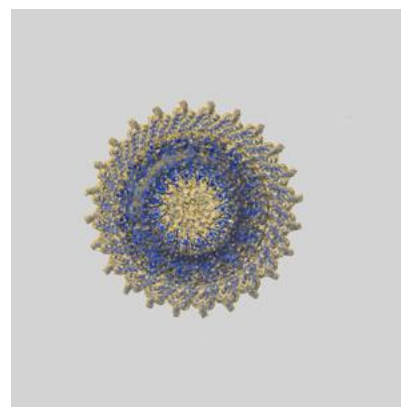
9.1 Map-model overlay [i](#)



X



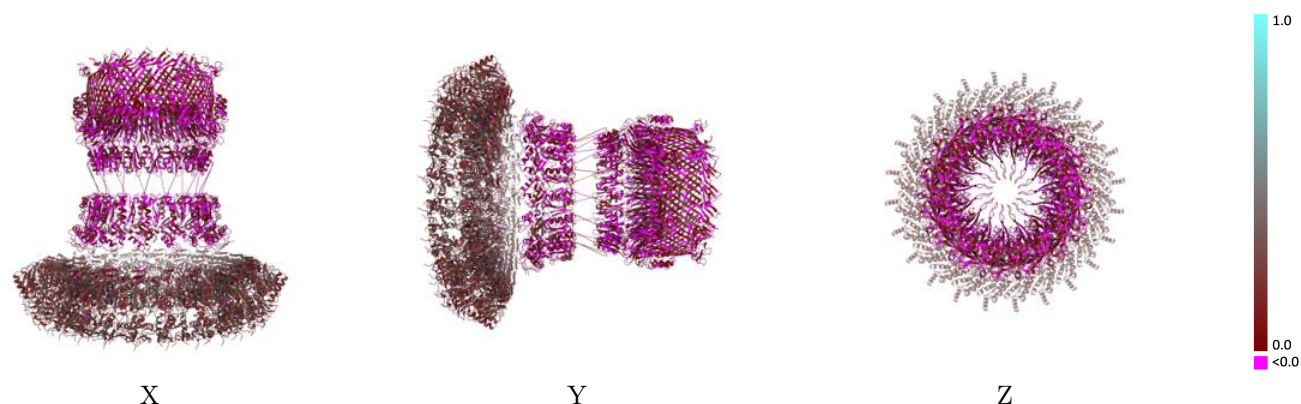
Y



Z

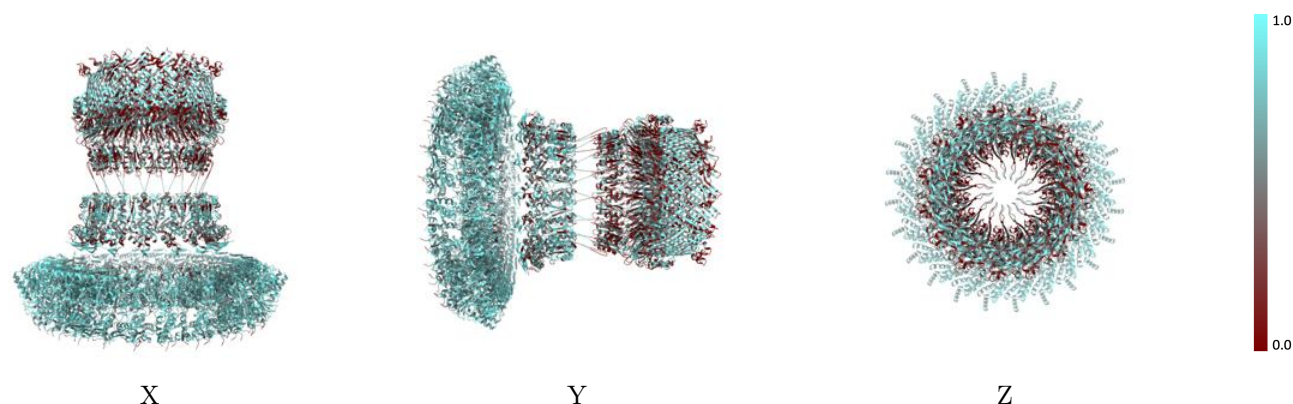
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



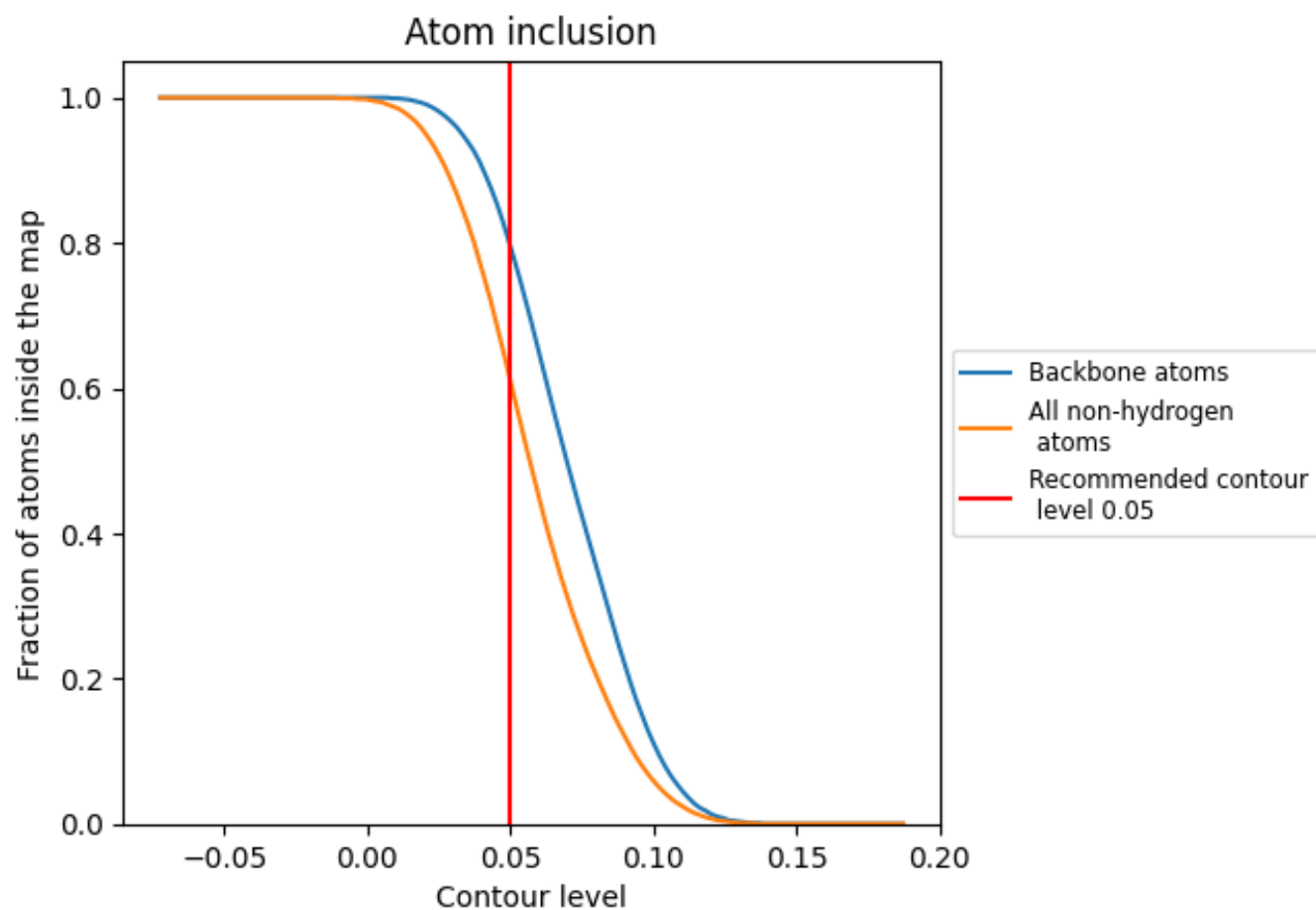
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.1790
0	 0.7240	 0.2520
1	 0.7030	 0.2960
10	 0.7410	 0.2850
2	 0.7410	 0.2650
3	 0.7030	 0.3050
4	 0.7460	 0.2830
5	 0.7170	 0.3110
6	 0.7420	 0.2740
7	 0.7080	 0.3070
8	 0.7510	 0.2980
9	 0.7070	 0.3060
A	 0.4940	 0.0620
B	 0.4970	 0.0670
C	 0.4650	 0.0480
D	 0.4580	 0.0340
E	 0.4620	 0.0460
F	 0.4720	 0.0480
G	 0.4760	 0.0680
H	 0.4750	 0.0570
I	 0.4720	 0.0450
J	 0.4770	 0.0480
K	 0.4680	 0.0420
L	 0.4580	 0.0340
M	 0.4600	 0.0430
N	 0.4730	 0.0410
O	 0.4760	 0.0480
P	 0.7010	 0.2960
Q	 0.7550	 0.2670
R	 0.7160	 0.3040
S	 0.7370	 0.2600
T	 0.7180	 0.3010
U	 0.7260	 0.2480
V	 0.7070	 0.2960
W	 0.7400	 0.2620



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Chain	Atom inclusion	Q-score
X	 0.7130	 0.2990
Y	 0.7270	 0.2470
Z	 0.7350	 0.2750
a	 0.6980	 0.2930
b	 0.7280	 0.2670
c	 0.6880	 0.2960
d	 0.7230	 0.2530
e	 0.6810	 0.2740
f	 0.7130	 0.2510
g	 0.6980	 0.2800
h	 0.7000	 0.2370
i	 0.6810	 0.2720
j	 0.7090	 0.2340
k	 0.6890	 0.2830
l	 0.7000	 0.2350
m	 0.6910	 0.2820
n	 0.7050	 0.2460
o	 0.6950	 0.2940
p	 0.7240	 0.2530
q	 0.7080	 0.2990
r	 0.7440	 0.2740
s	 0.7130	 0.3050
t	 0.7410	 0.2690
u	 0.7180	 0.3020
v	 0.7510	 0.2800
w	 0.7260	 0.3070
x	 0.7550	 0.2790
y	 0.7160	 0.3100
z	 0.7090	 0.2970