



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:15 AM UTC

PDB ID : 8YMJ / pdb_00008ymj
EMDB ID : EMD-39395
Title : Cryo-EM structure of Hepatitis B virus surface antigen subviral particle with D2 symmetry
Authors : Wang, T.; Cao, L.; Mu, A.; Wang, Q.; Rao, Z.H.
Deposited on : 2024-03-09
Resolution : 6.60 Å(reported)
Based on initial model : .

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:

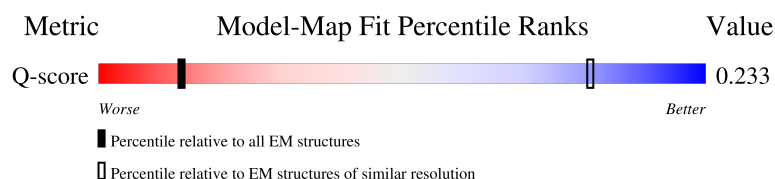
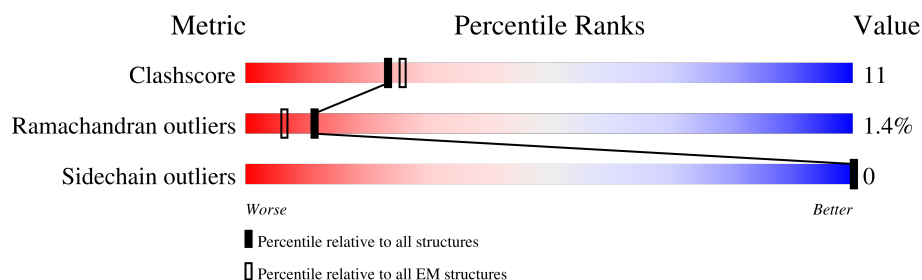
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.60 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	531 (6.10 - 7.10)

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	0	226	24% 85% 14% .
1	1	226	23% 87% 12% .
1	2	226	21% 82% 17% .
1	3	226	18% 86% 12% .

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Mol	Chain	Length	Quality of chain
1	4	226	
1	5	226	
1	6	226	
1	7	226	
1	8	226	
1	9	226	
1	A	226	
1	AA	226	
1	AB	226	
1	AC	226	
1	AD	226	
1	AE	226	
1	AF	226	
1	AG	226	
1	AH	226	
1	AI	226	
1	AJ	226	
1	AK	226	
1	AL	226	
1	AM	226	
1	AN	226	
1	AO	226	
1	AP	226	
1	AQ	226	
1	AR	226	

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Mol	Chain	Length	Quality of chain
1	B	226	15% 86% 13%
1	C	226	20% 84% 15%
1	D	226	21% 80% 19%
1	E	226	18% 88% 12%
1	F	226	17% 84% 15%
1	G	226	25% 87% 12%
1	H	226	23% 83% 16%
1	I	226	25% 87% 12%
1	J	226	28% 86% 13%
1	K	226	27% 91% 8%
1	L	226	28% 89% 9%
1	M	226	23% 87% 12%
1	N	226	21% 82% 16%
1	O	226	18% 86% 12%
1	P	226	21% 81% 17%
1	Q	226	23% 89% 11%
1	R	226	19% 85% 14%
1	S	226	19% 91% 9%
1	T	226	20% 88% 12%
1	U	226	19% 90% 9%
1	V	226	24% 86% 13%
1	W	226	18% 85% 13%
1	X	226	15% 86% 13%
1	Y	226	20% 84% 15%
1	Z	226	21% 79% 19%

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Mol	Chain	Length	Quality of chain
1	a	226	
1	b	226	
1	c	226	
1	d	226	
1	e	226	
1	f	226	
1	g	226	
1	h	226	
1	i	226	
1	j	226	
1	k	226	
1	l	226	
1	m	226	
1	n	226	
1	o	226	
1	p	226	
1	q	226	
1	r	226	
1	s	226	
1	t	226	
1	u	226	
1	v	226	
1	w	226	
1	x	226	
1	y	226	

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Mol	Chain	Length	Quality of chain
1	z	226	28% 89% 9%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 97912 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 Isoform S of Large envelope protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	B	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	C	226	Total	C	N	O	S	0	0
			1199	727	234	228	10		
1	D	226	Total	C	N	O	S	0	0
			1228	750	238	230	10		
1	E	226	Total	C	N	O	S	0	0
			1222	747	235	230	10		
1	F	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	G	226	Total	C	N	O	S	0	0
			1225	751	234	230	10		
1	H	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	I	226	Total	C	N	O	S	0	0
			1232	759	235	228	10		
1	J	226	Total	C	N	O	S	0	0
			1210	737	233	230	10		
1	K	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	L	226	Total	C	N	O	S	0	0
			1181	711	232	228	10		
1	M	226	Total	C	N	O	S	0	0
			1213	739	234	230	10		
1	N	226	Total	C	N	O	S	0	0
			1206	733	234	229	10		
1	O	226	Total	C	N	O	S	0	0
			1239	760	240	229	10		
1	P	226	Total	C	N	O	S	0	0
			1237	758	239	230	10		
1	Q	226	Total	C	N	O	S	0	0
			1216	743	233	230	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	226	Total	C	N	O	S	0	0
			1252	775	237	230	10		
1	S	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	T	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	U	226	Total	C	N	O	S	0	0
			1229	753	235	231	10		
1	V	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	W	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	X	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	Y	226	Total	C	N	O	S	0	0
			1199	727	234	228	10		
1	Z	226	Total	C	N	O	S	0	0
			1228	750	238	230	10		
1	a	226	Total	C	N	O	S	0	0
			1222	747	235	230	10		
1	b	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	c	226	Total	C	N	O	S	0	0
			1225	751	234	230	10		
1	d	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	e	226	Total	C	N	O	S	0	0
			1232	759	235	228	10		
1	f	226	Total	C	N	O	S	0	0
			1210	737	233	230	10		
1	g	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	h	226	Total	C	N	O	S	0	0
			1181	711	232	228	10		
1	i	226	Total	C	N	O	S	0	0
			1213	739	234	230	10		
1	j	226	Total	C	N	O	S	0	0
			1206	733	234	229	10		
1	k	226	Total	C	N	O	S	0	0
			1239	760	240	229	10		
1	l	226	Total	C	N	O	S	0	0
			1237	758	239	230	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	226	Total	C	N	O	S	0	0
			1216	743	233	230	10		
1	n	226	Total	C	N	O	S	0	0
			1252	775	237	230	10		
1	o	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	p	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	q	226	Total	C	N	O	S	0	0
			1229	753	235	231	10		
1	r	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	s	226	Total	C	N	O	S	0	0
			1199	727	234	228	10		
1	t	226	Total	C	N	O	S	0	0
			1228	750	238	230	10		
1	u	226	Total	C	N	O	S	0	0
			1222	747	235	230	10		
1	v	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	w	226	Total	C	N	O	S	0	0
			1232	759	235	228	10		
1	x	226	Total	C	N	O	S	0	0
			1210	737	233	230	10		
1	y	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	z	226	Total	C	N	O	S	0	0
			1181	711	232	228	10		
1	1	226	Total	C	N	O	S	0	0
			1213	739	234	230	10		
1	2	226	Total	C	N	O	S	0	0
			1206	733	234	229	10		
1	3	226	Total	C	N	O	S	0	0
			1239	760	240	229	10		
1	4	226	Total	C	N	O	S	0	0
			1237	758	239	230	10		
1	5	226	Total	C	N	O	S	0	0
			1216	743	233	230	10		
1	6	226	Total	C	N	O	S	0	0
			1252	775	237	230	10		
1	7	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		

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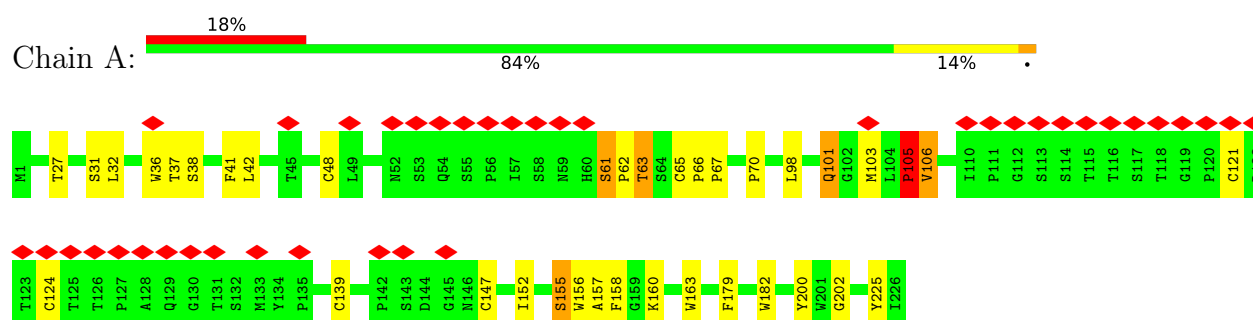
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Mol	Chain	Residues	Atoms					AltConf	Trace
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			1231	755	236	230	10		
1	9	226	Total	C	N	O	S	0	0
			1229	753	235	231	10		
1	0	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	AA	226	Total	C	N	O	S	0	0
			1199	727	234	228	10		
1	AB	226	Total	C	N	O	S	0	0
			1228	750	238	230	10		
1	AC	226	Total	C	N	O	S	0	0
			1222	747	235	230	10		
1	AD	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	AE	226	Total	C	N	O	S	0	0
			1232	759	235	228	10		
1	AF	226	Total	C	N	O	S	0	0
			1210	737	233	230	10		
1	AG	226	Total	C	N	O	S	0	0
			1219	745	234	230	10		
1	AH	226	Total	C	N	O	S	0	0
			1181	711	232	228	10		
1	AI	226	Total	C	N	O	S	0	0
			1213	739	234	230	10		
1	AJ	226	Total	C	N	O	S	0	0
			1206	733	234	229	10		
1	AK	226	Total	C	N	O	S	0	0
			1239	760	240	229	10		
1	AL	226	Total	C	N	O	S	0	0
			1237	758	239	230	10		
1	AM	226	Total	C	N	O	S	0	0
			1216	743	233	230	10		
1	AN	226	Total	C	N	O	S	0	0
			1252	775	237	230	10		
1	AO	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		
1	AP	226	Total	C	N	O	S	0	0
			1231	755	236	230	10		
1	AQ	226	Total	C	N	O	S	0	0
			1229	753	235	231	10		
1	AR	226	Total	C	N	O	S	0	0
			1240	763	237	230	10		

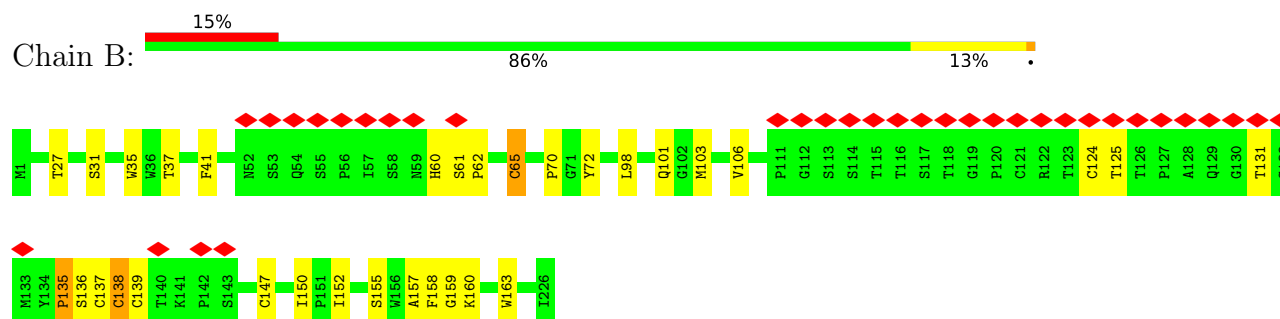
3 Residue-property plots

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.

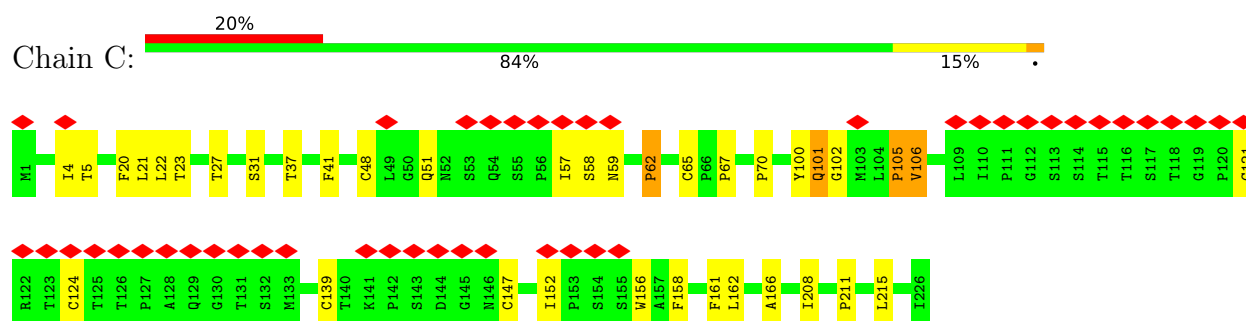
- Molecule 1: Isoform S of Large envelope protein



- Molecule 1: Isoform S of Large envelope protein

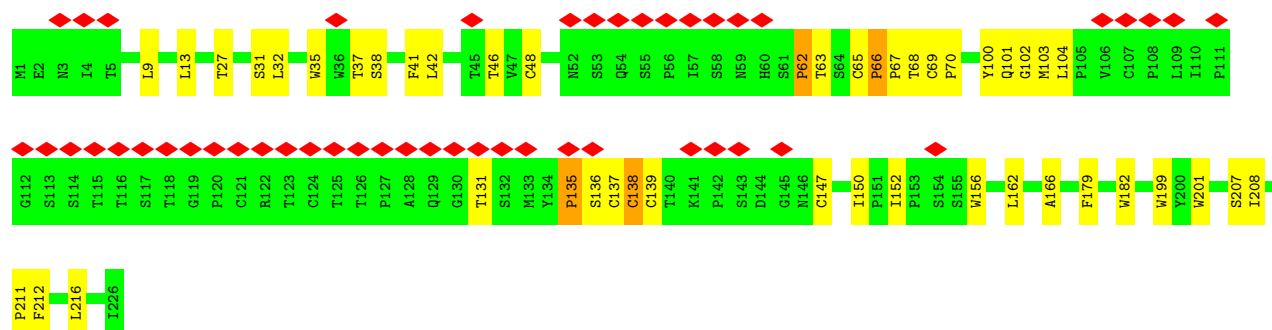


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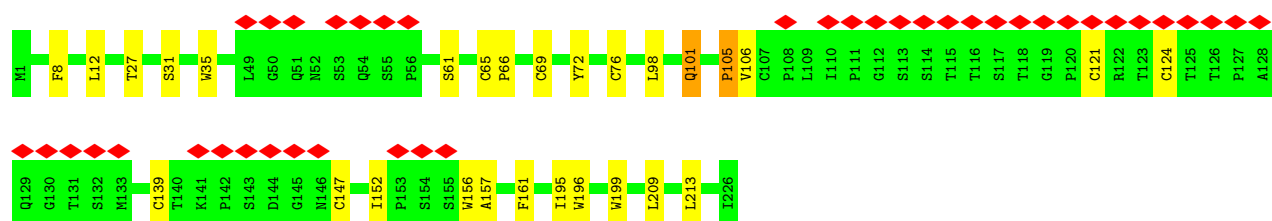
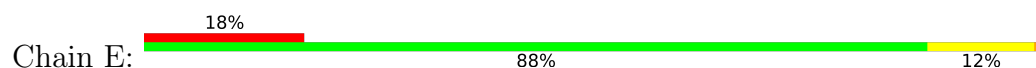


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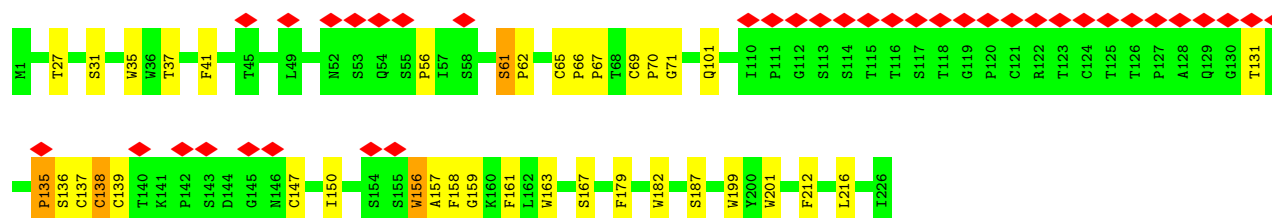
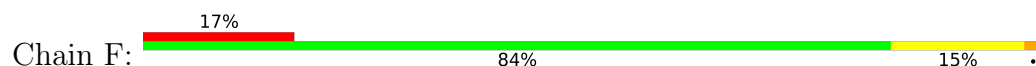




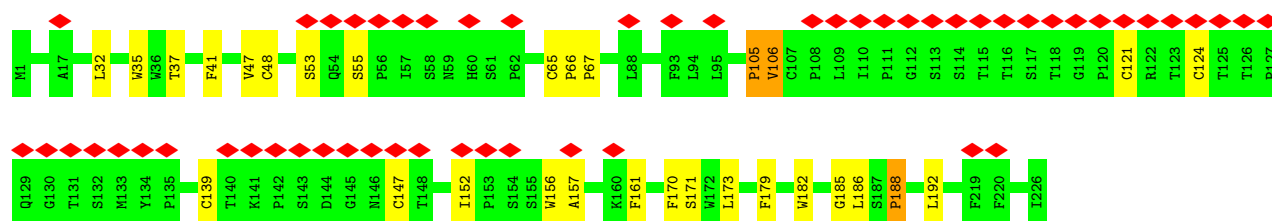
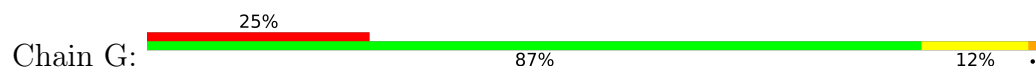
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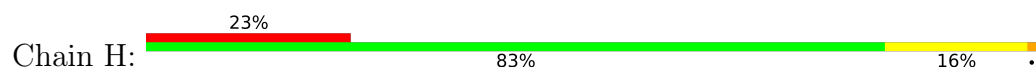
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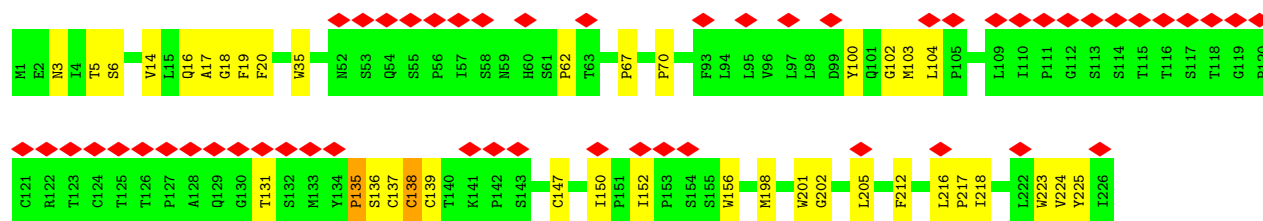


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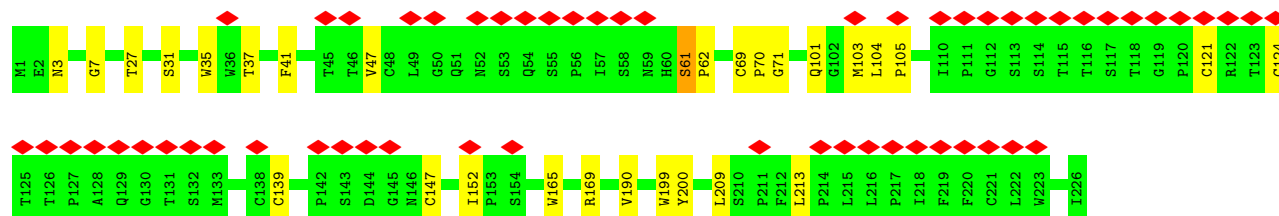
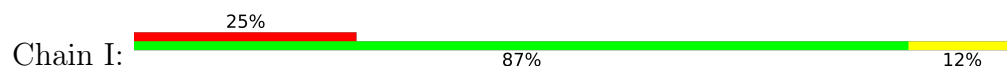


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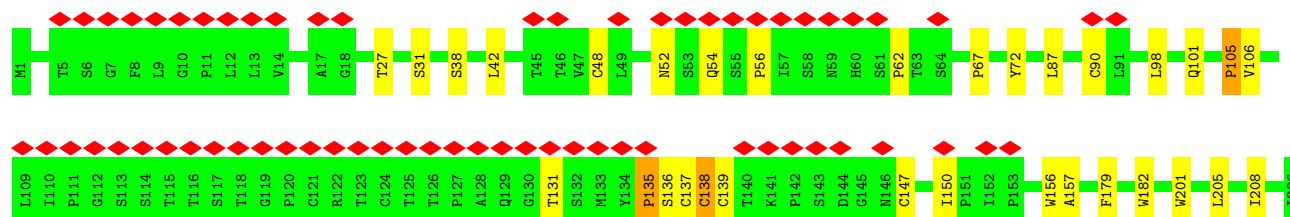
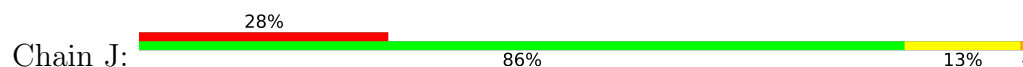




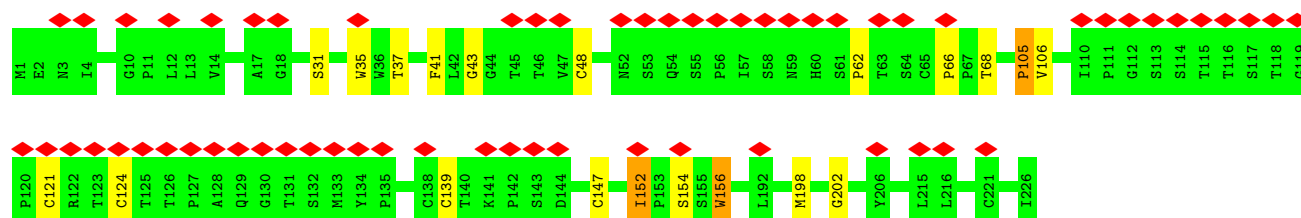
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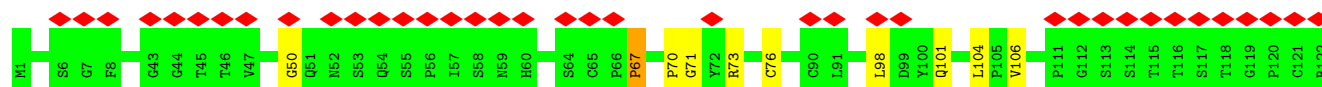
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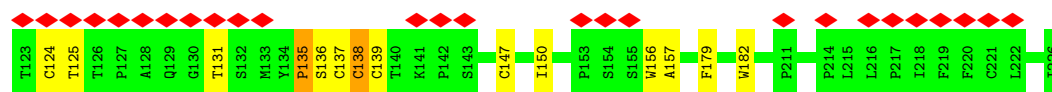


- Molecule 1: Isoform S of Large envelope protein

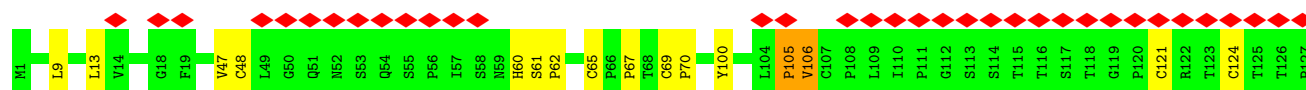
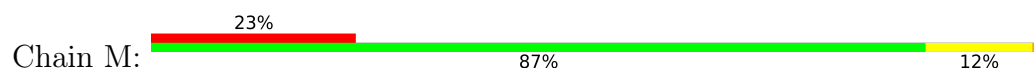


- Molecule 1: Isoform S of Large envelope protein

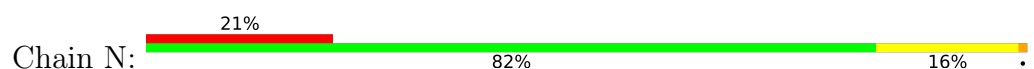




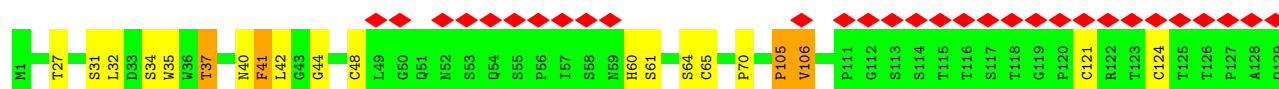
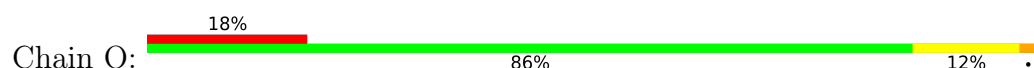
- Molecule 1: Isoform S of Large envelope protein



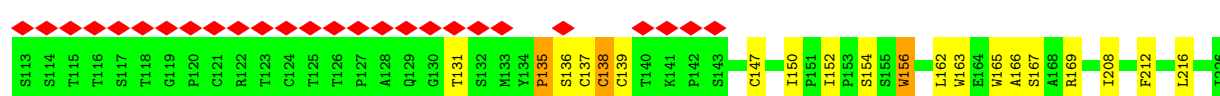
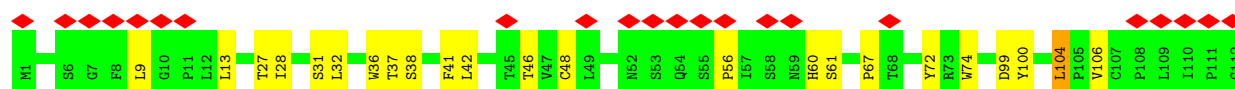
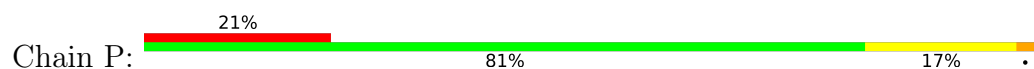
- Molecule 1: Isoform S of Large envelope protein



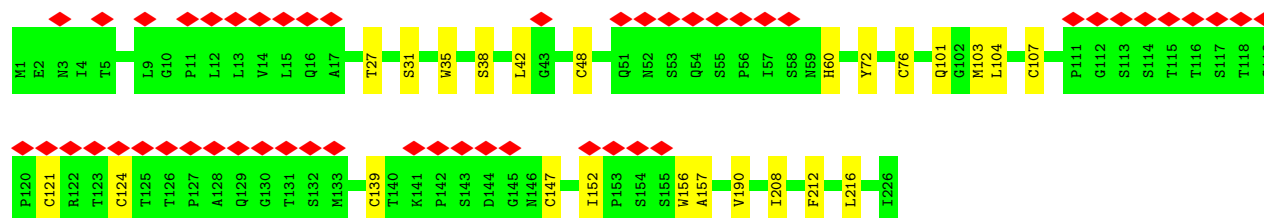
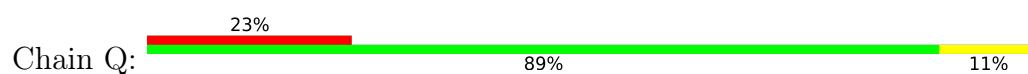
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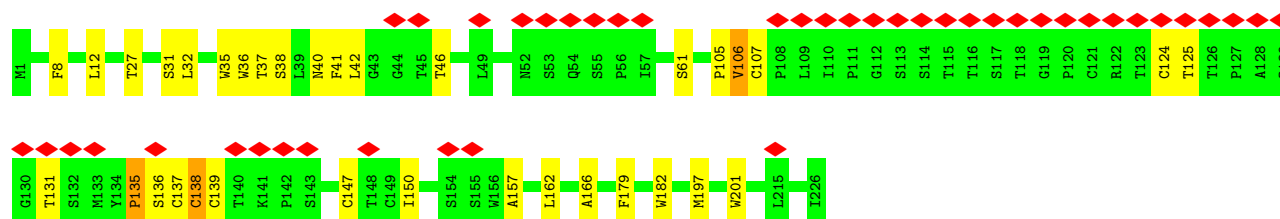
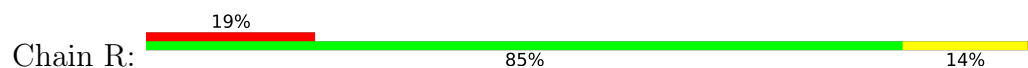
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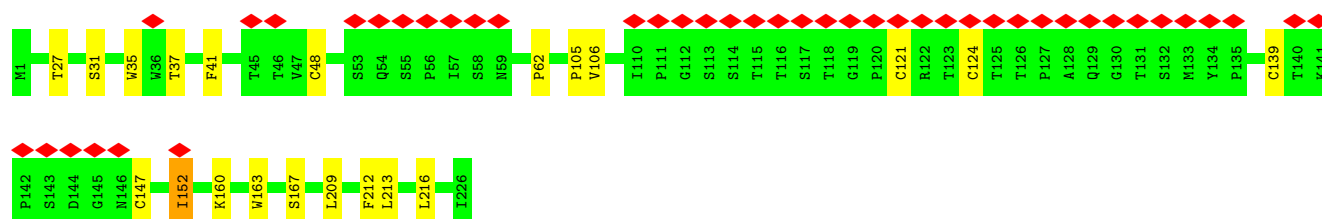
- Molecule 1: Isoform S of Large envelope protein



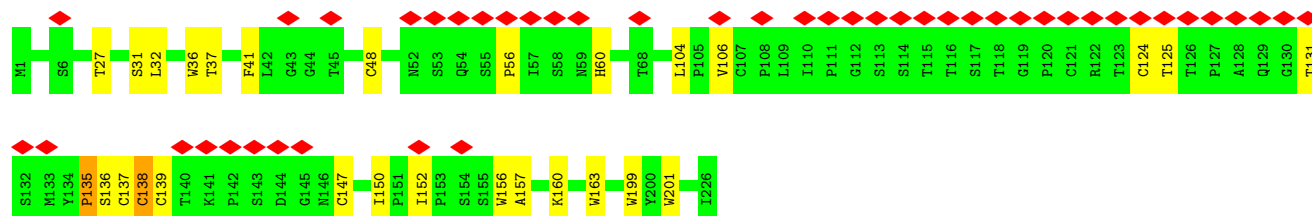
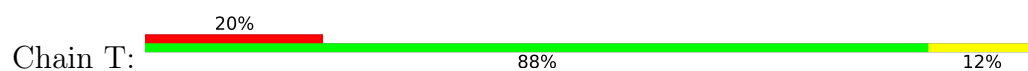
- Molecule 1: Isoform S of Large envelope protein



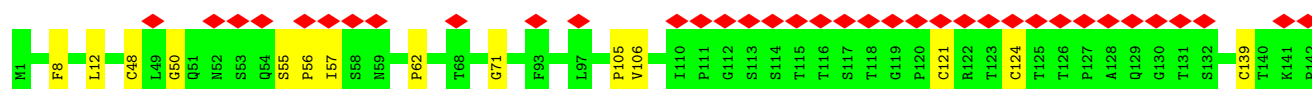
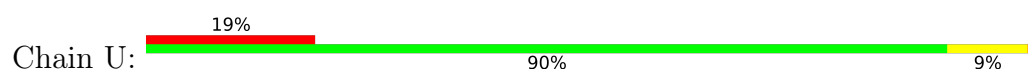
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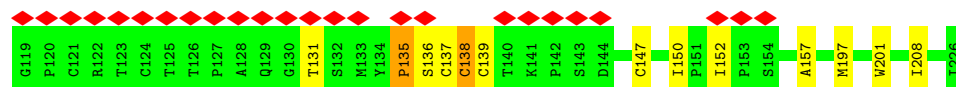
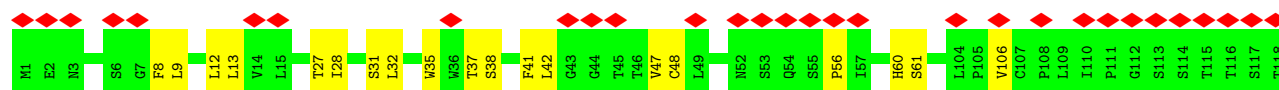
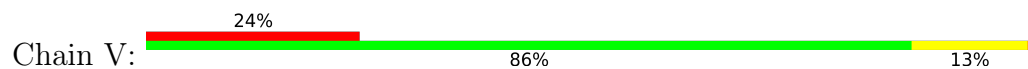


- Molecule 1: Isoform S of Large envelope protein

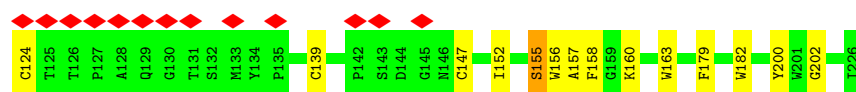
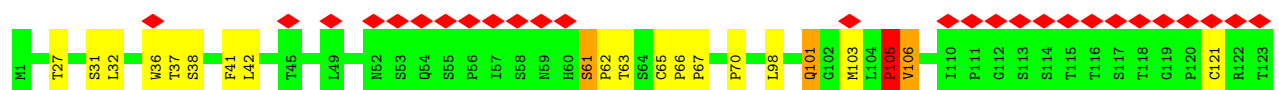
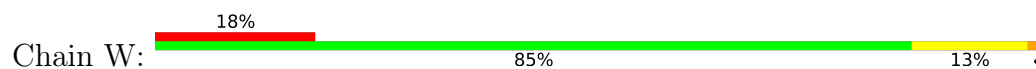




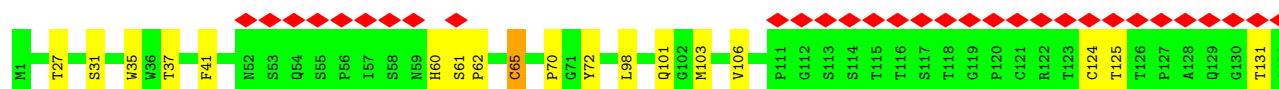
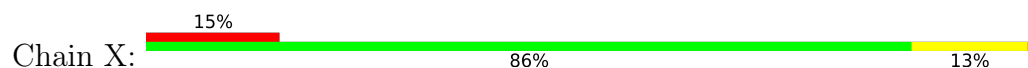
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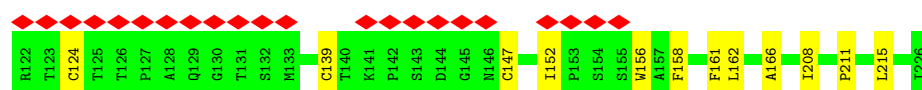
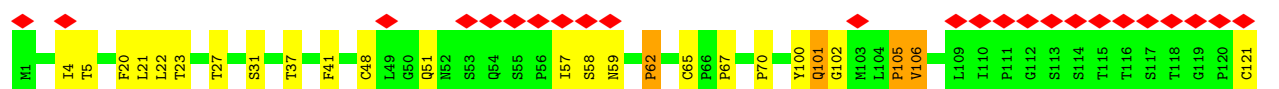
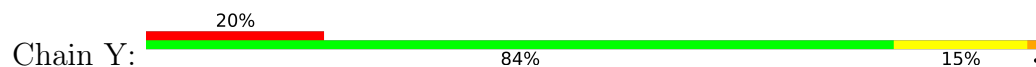
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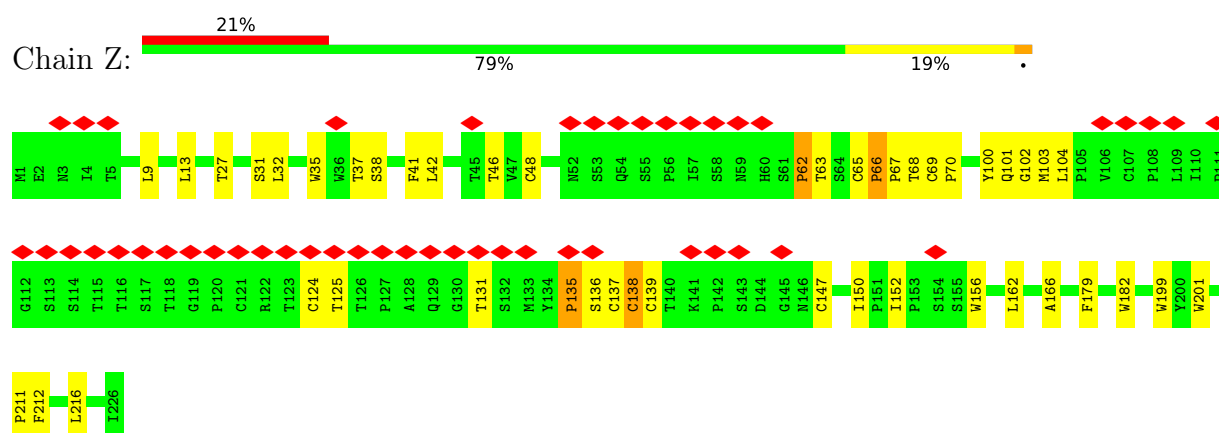
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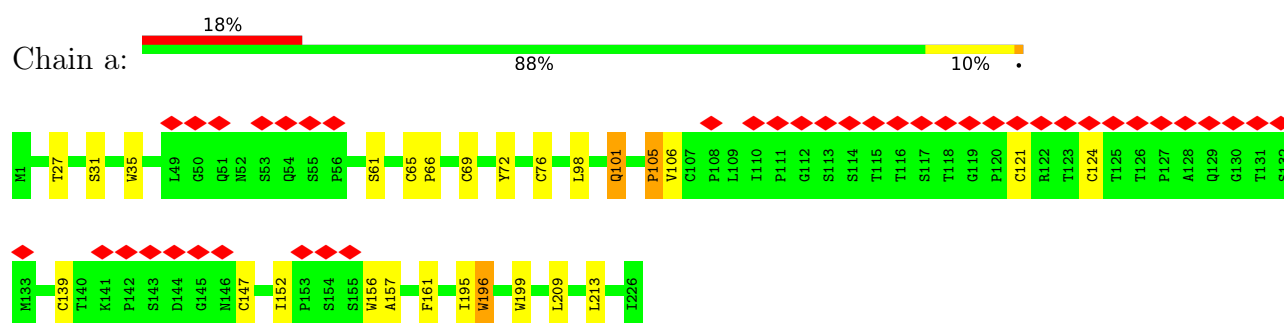
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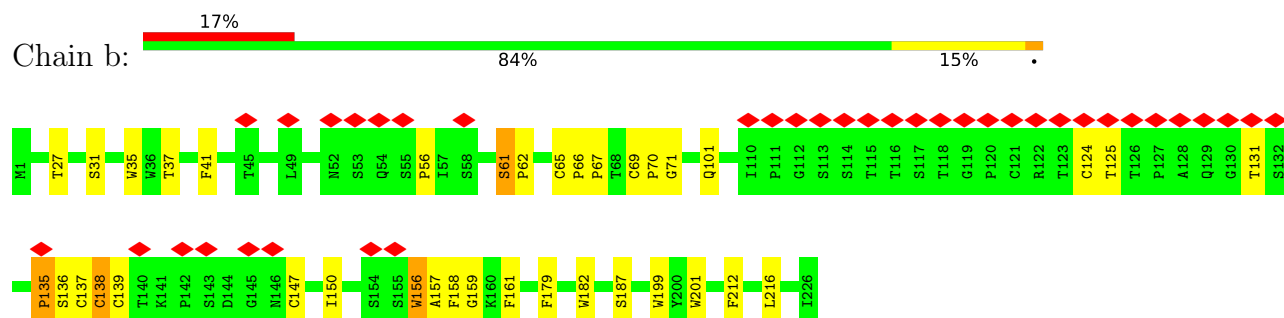
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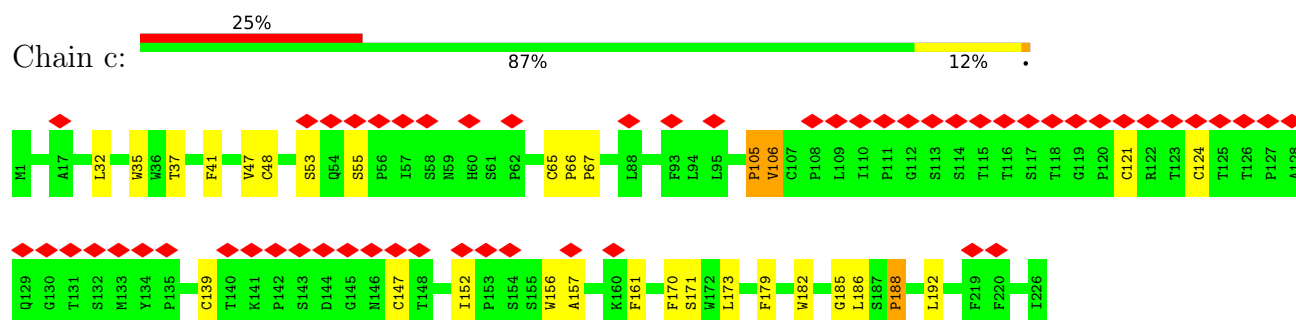
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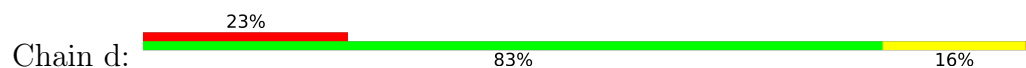
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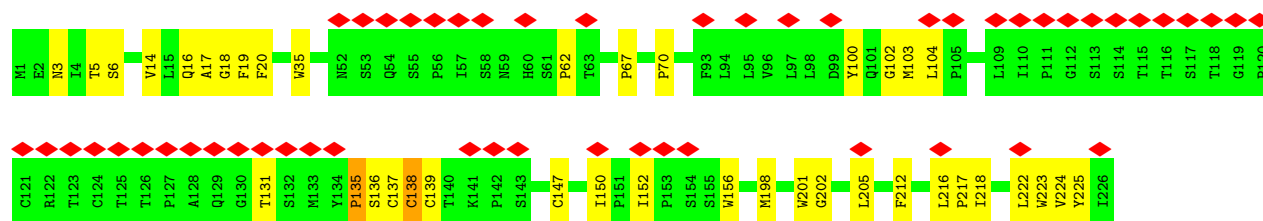


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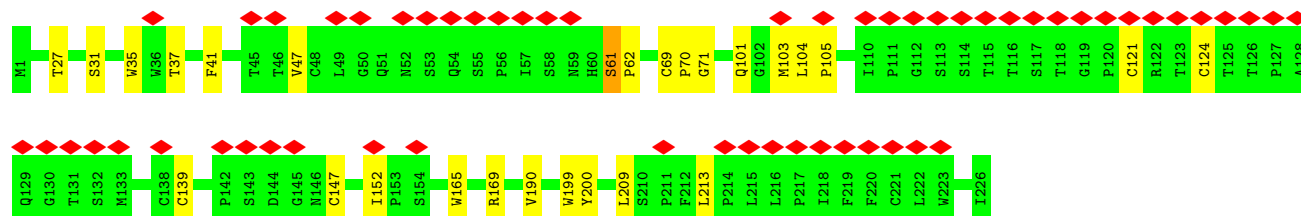
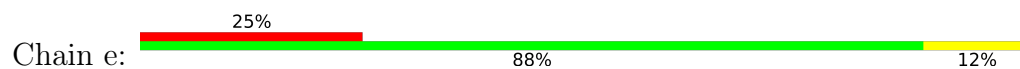


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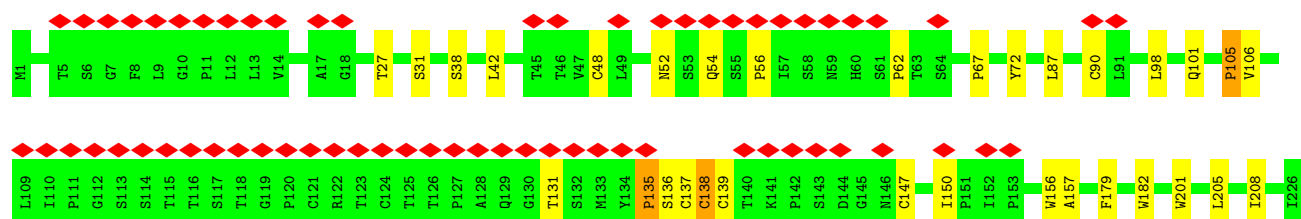
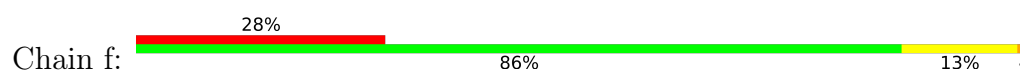




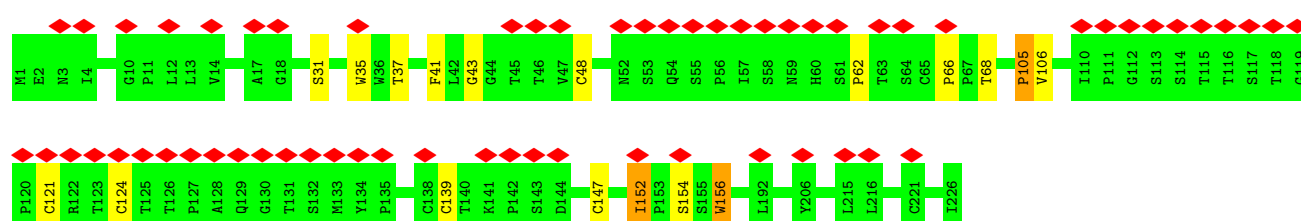
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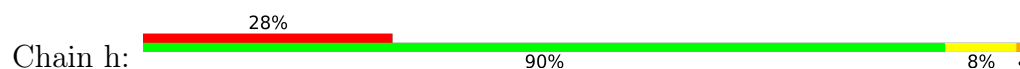
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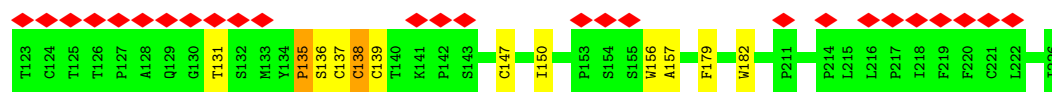


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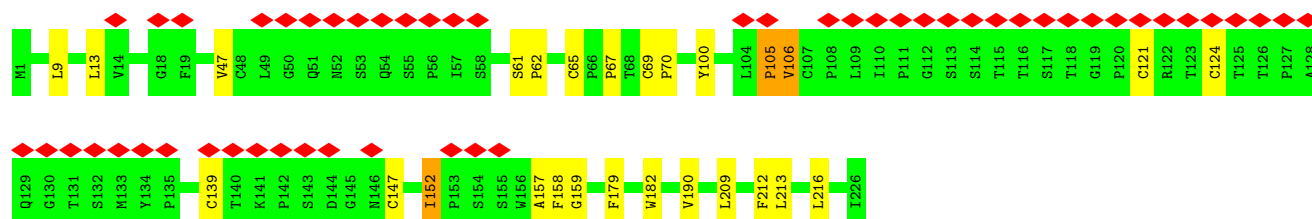
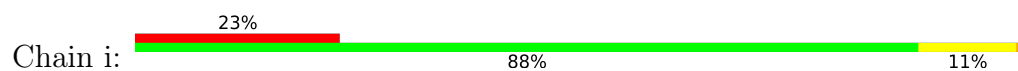


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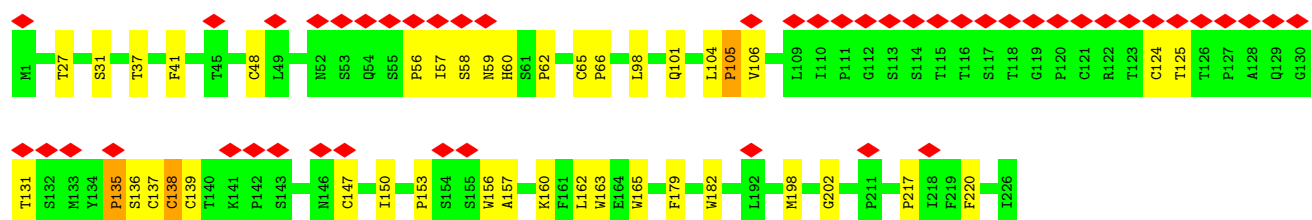
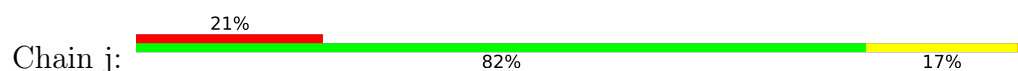




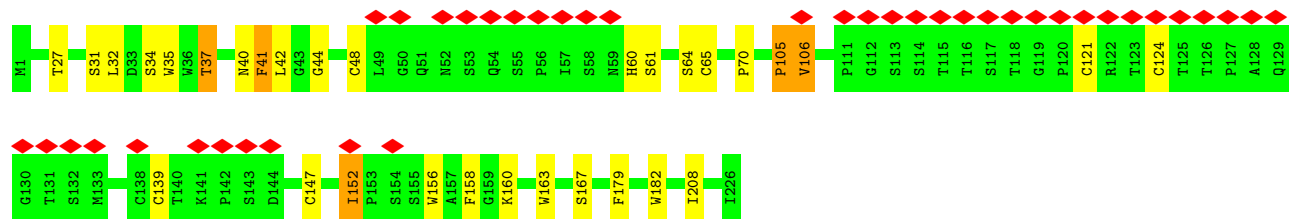
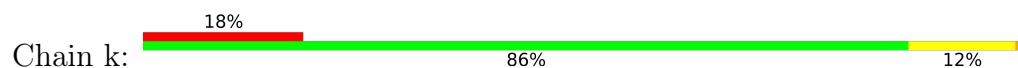
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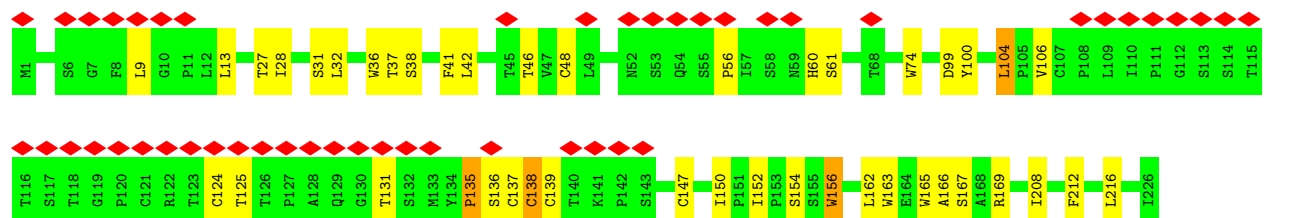
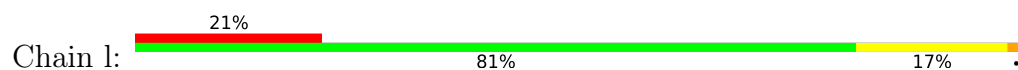
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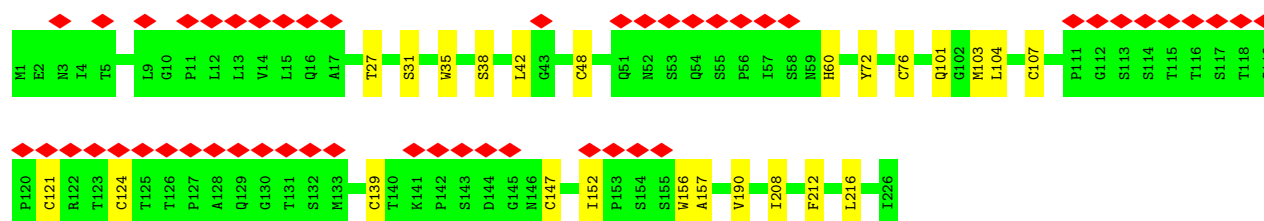
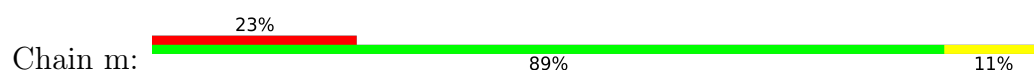
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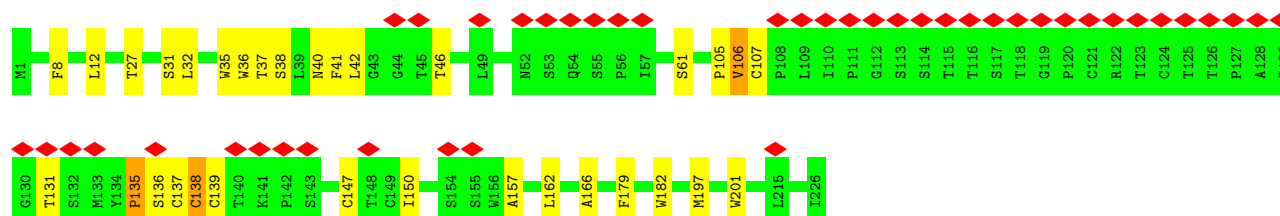
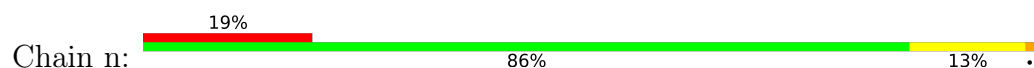
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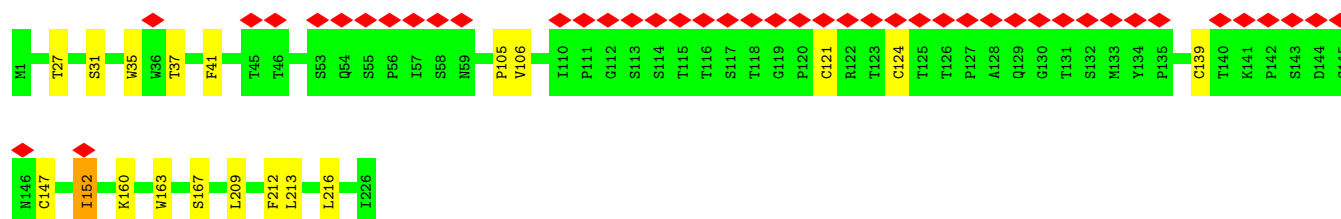
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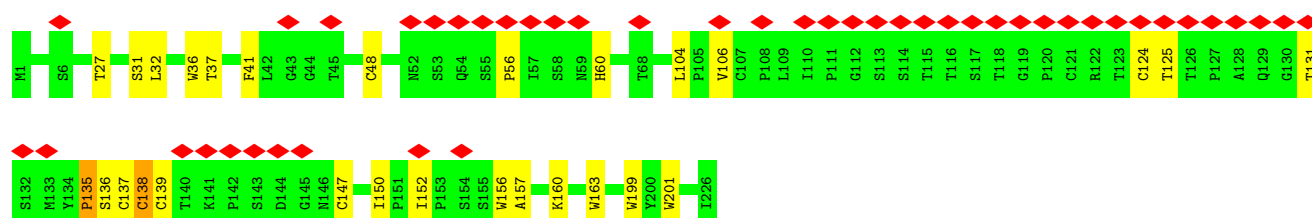
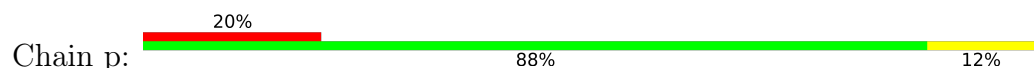
• Molecule 1: Isoform S of Large envelope protein



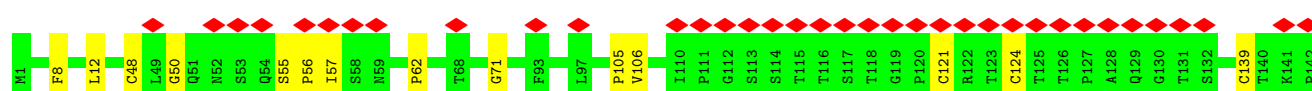
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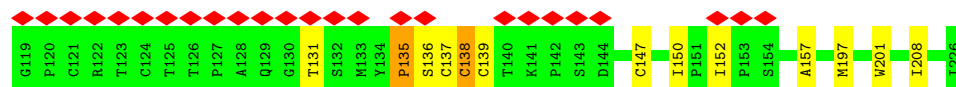
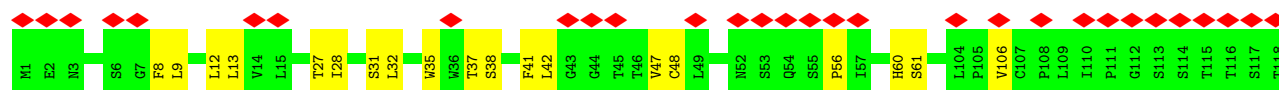
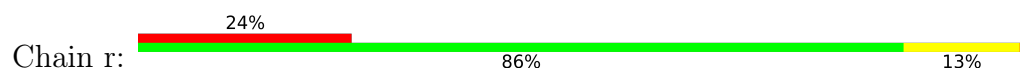


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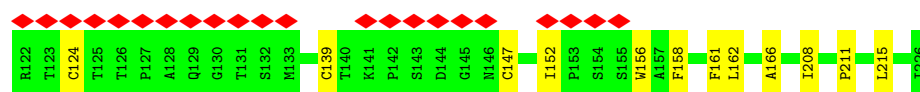
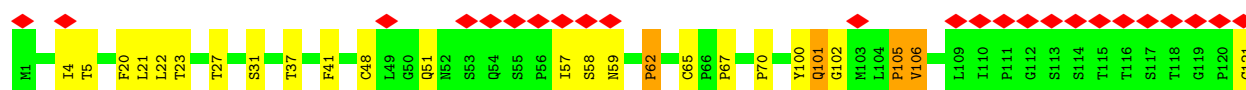
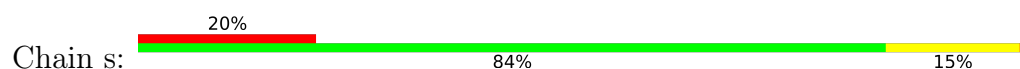




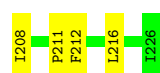
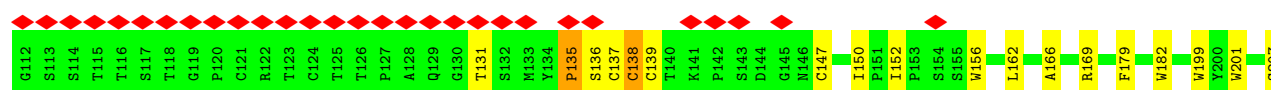
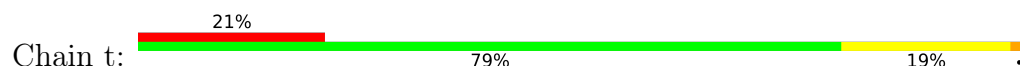
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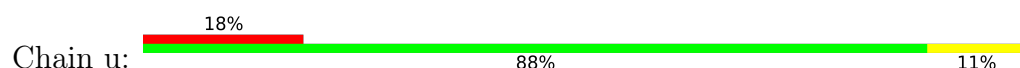
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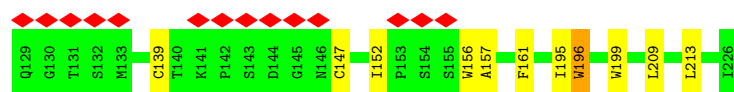


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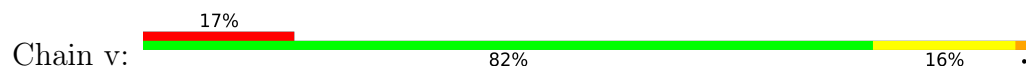


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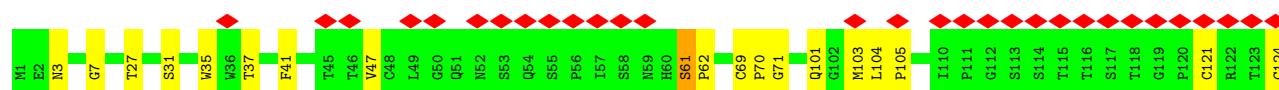
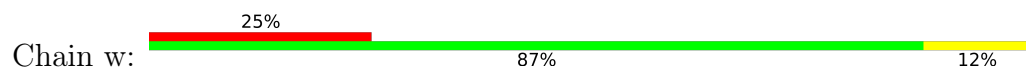




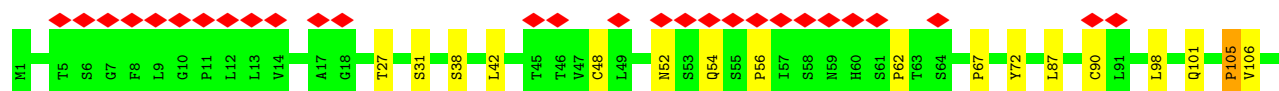
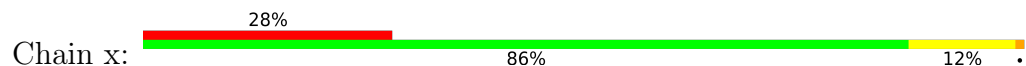
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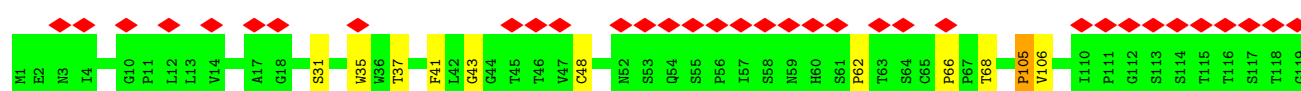
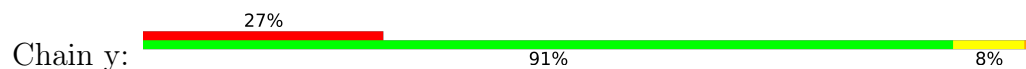
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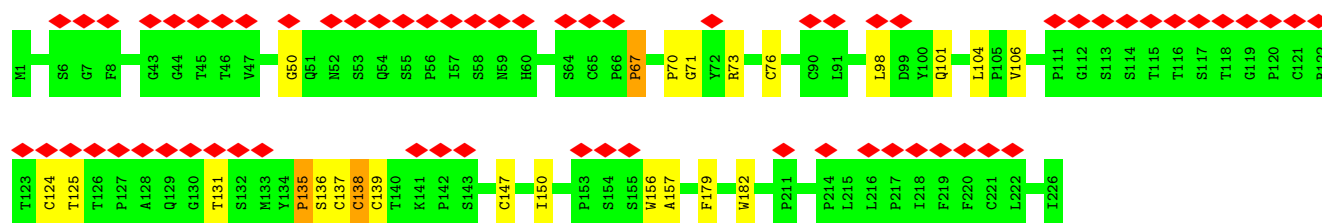
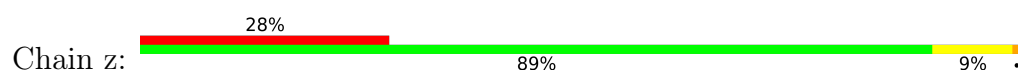


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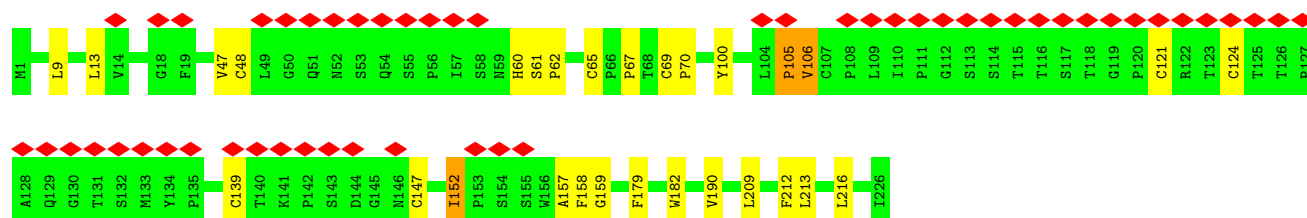
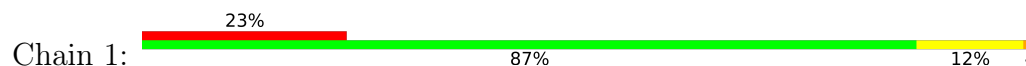


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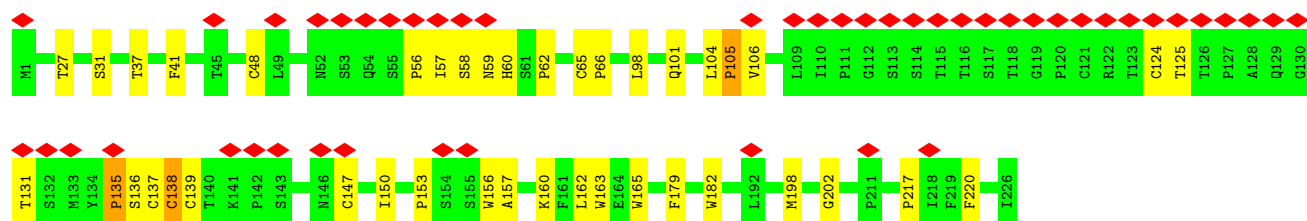
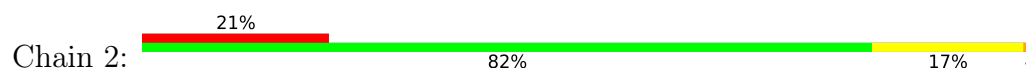




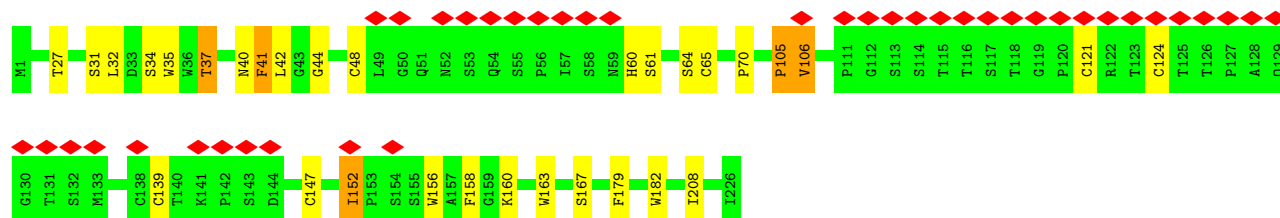
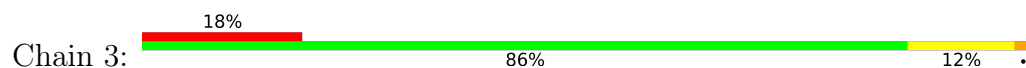
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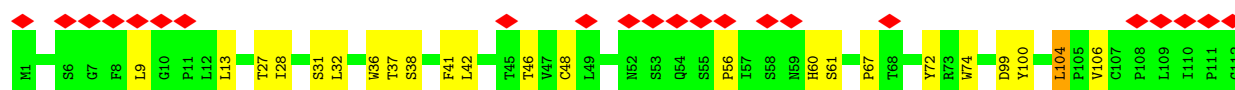
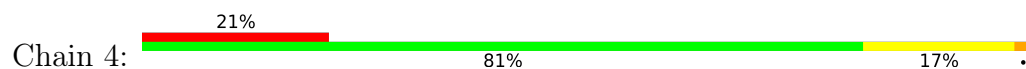
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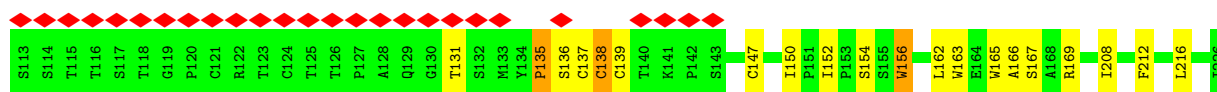


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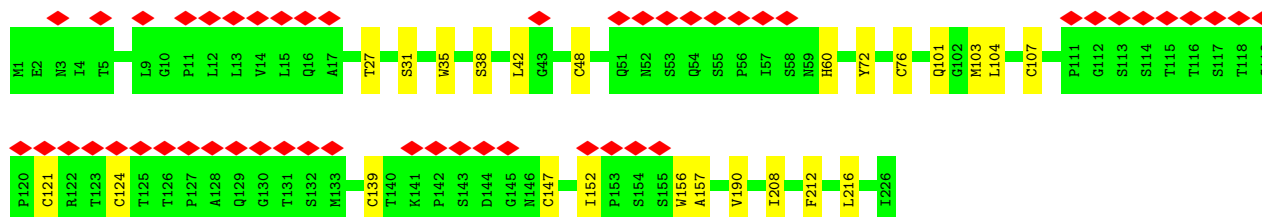
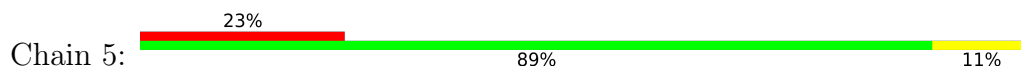


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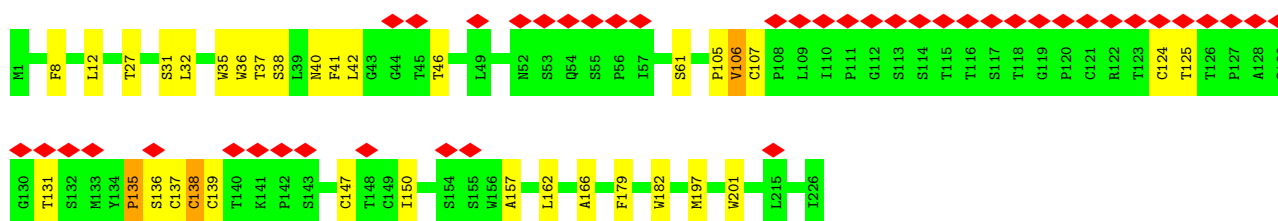
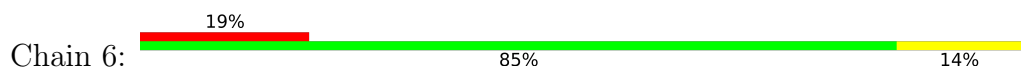




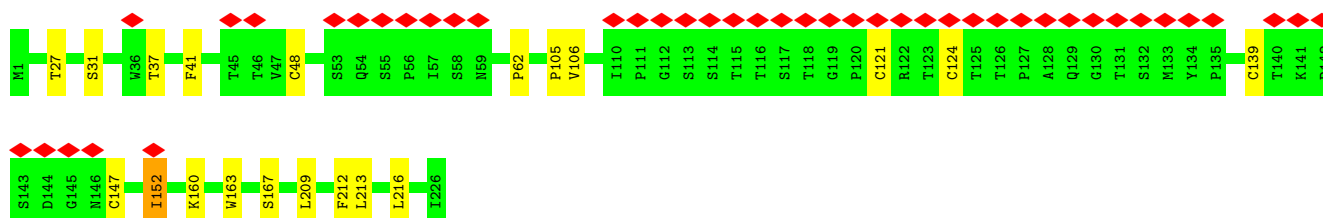
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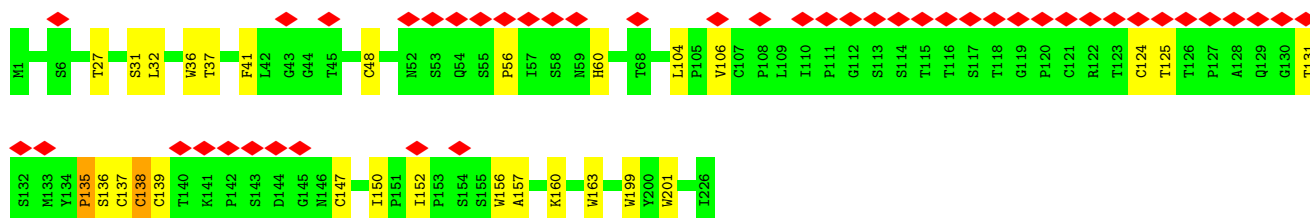
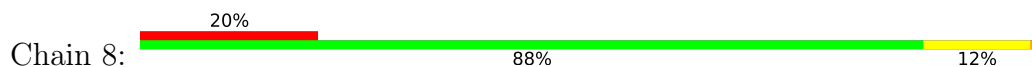
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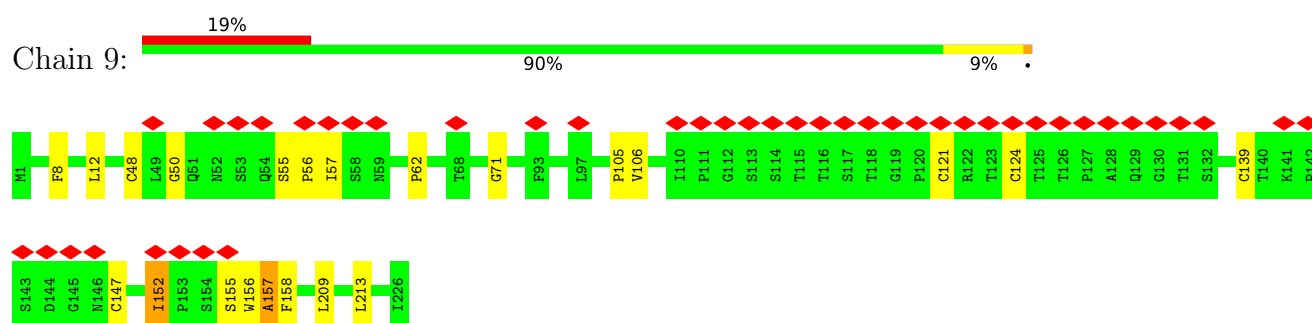
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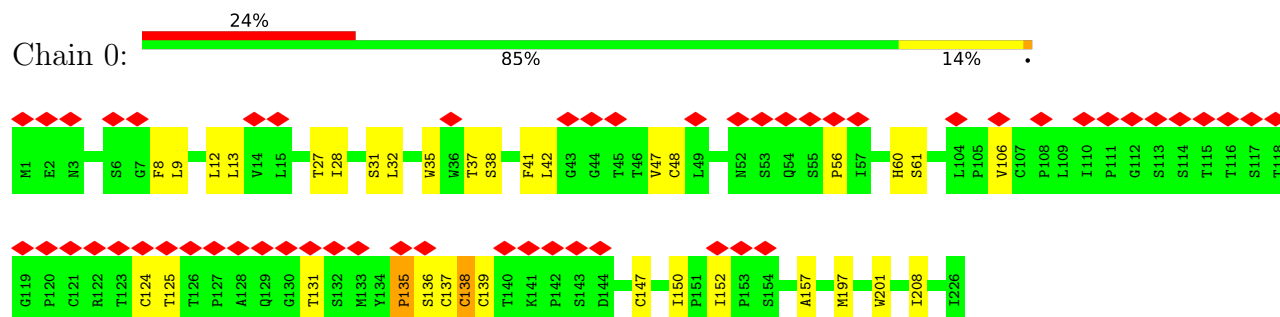
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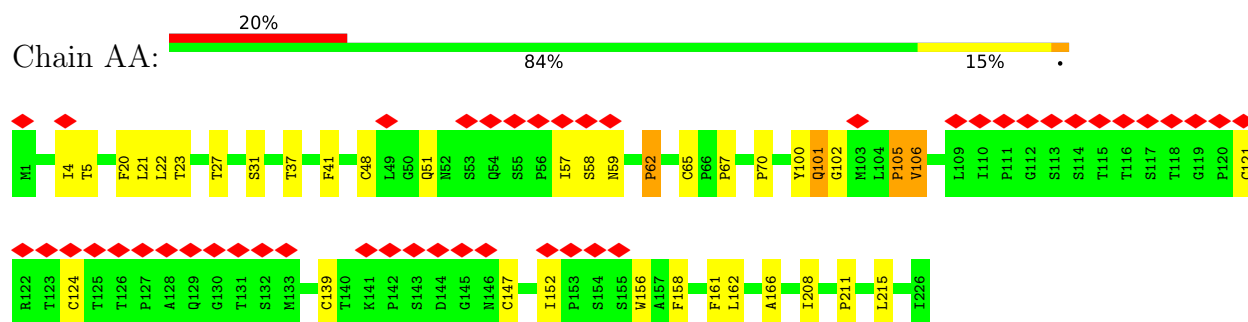
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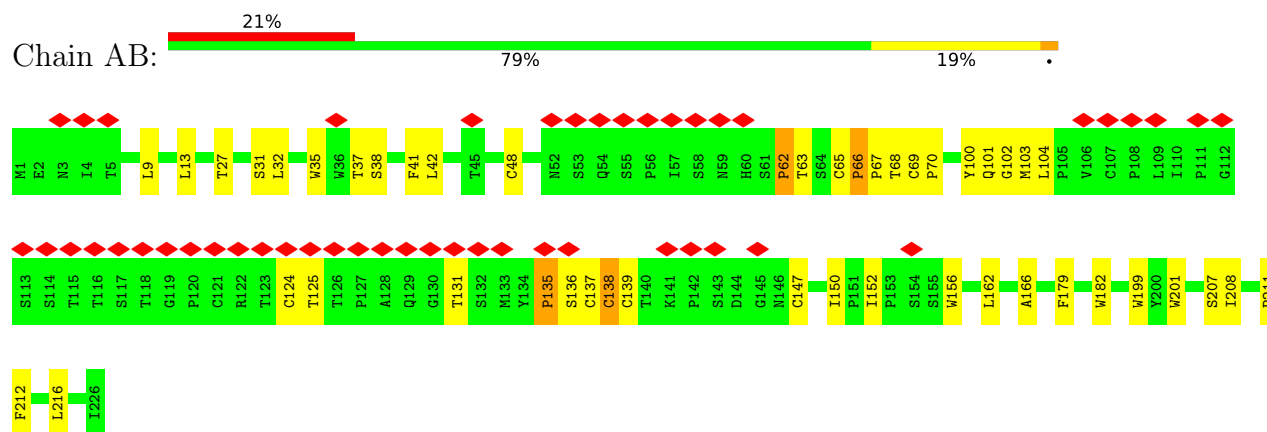
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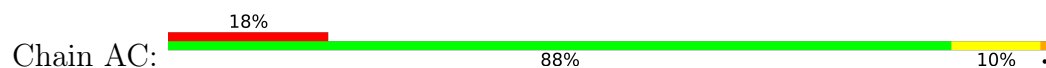
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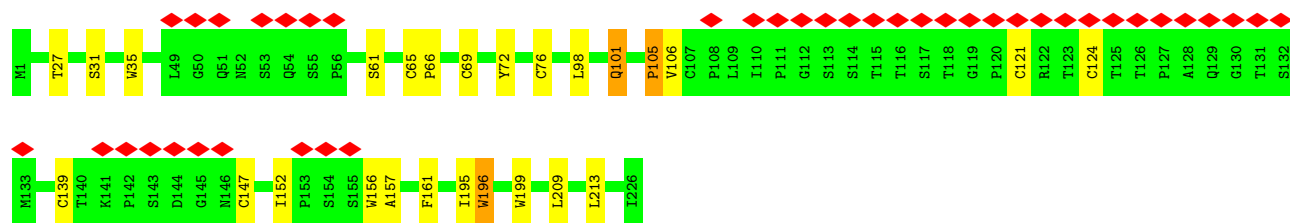


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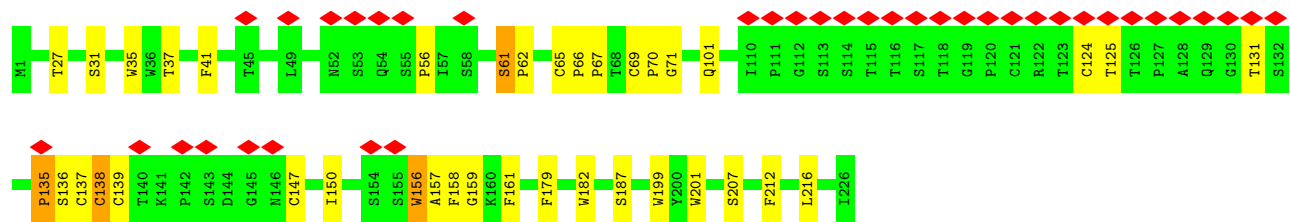
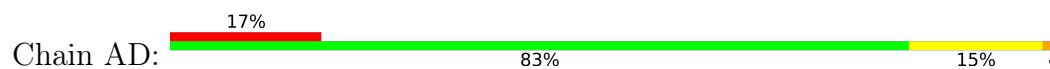


- Molecule 1: Isoform S of Large envelope protein

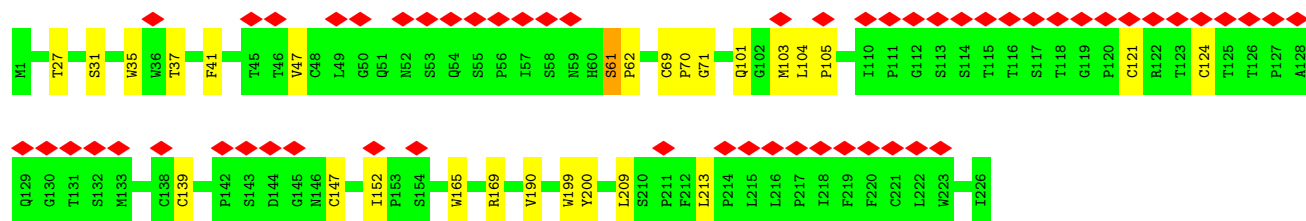
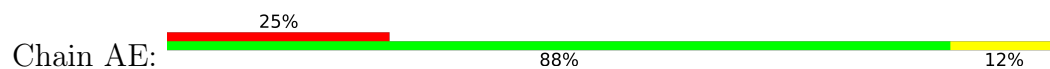




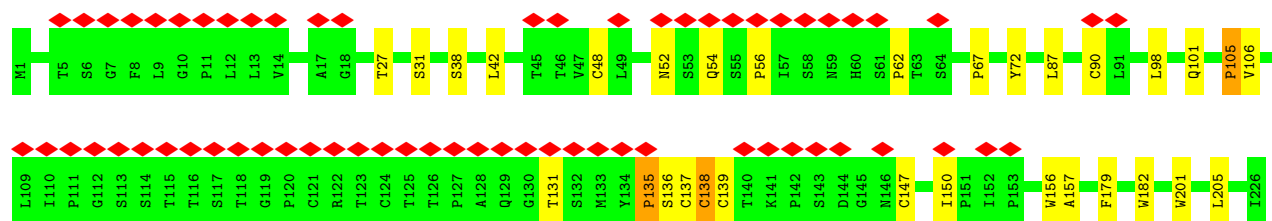
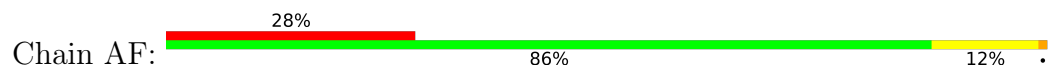
- Molecule 1: Isoform S of Large envelope protein



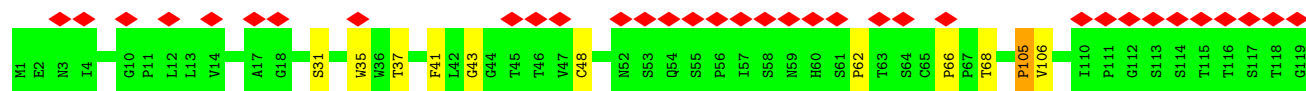
- Molecule 1: Isoform S of Large envelope protein

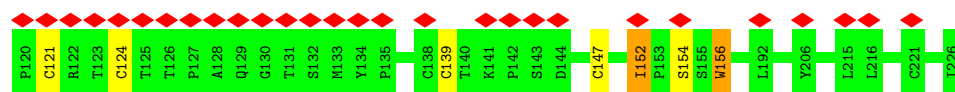


- Molecule 1: Isoform S of Large envelope protein

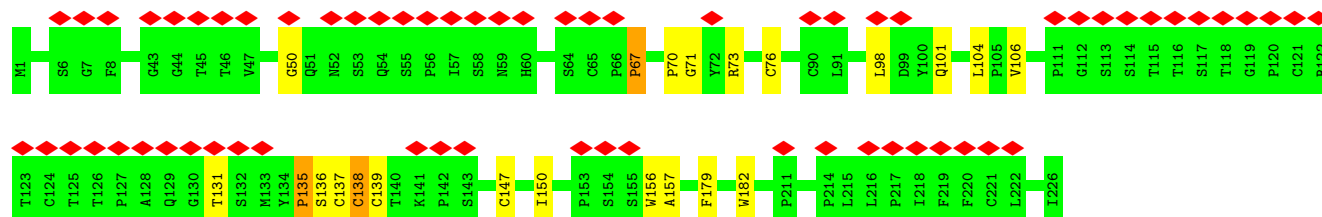


- Molecule 1: Isoform S of Large envelope protein

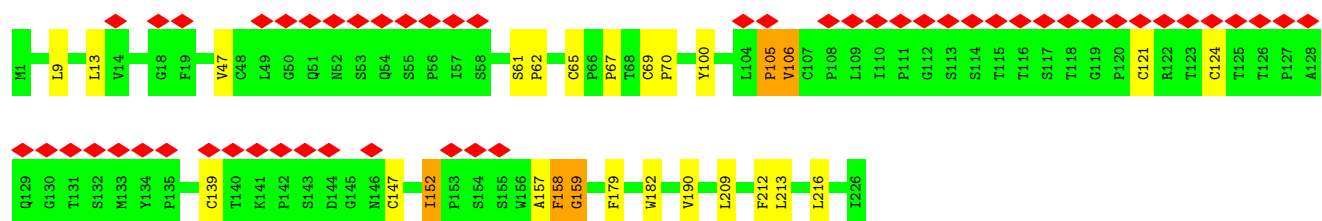
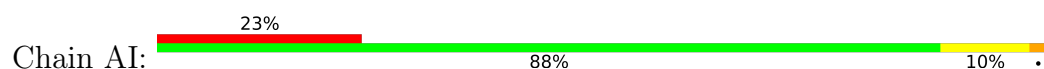




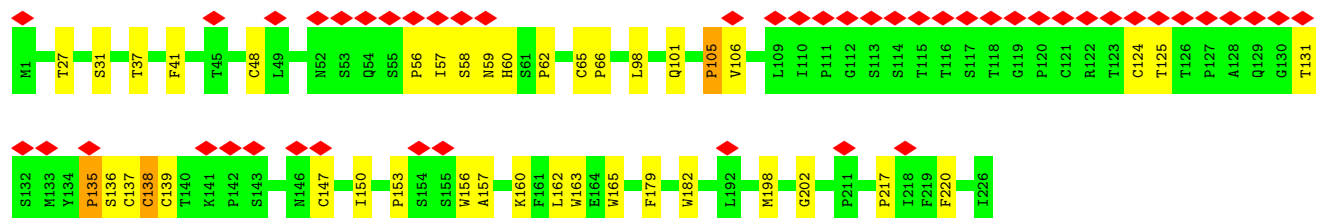
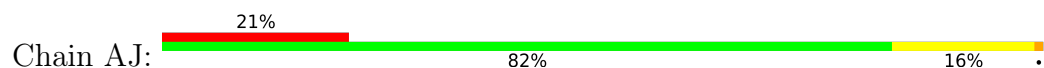
- Molecule 1: Isoform S of Large envelope protein



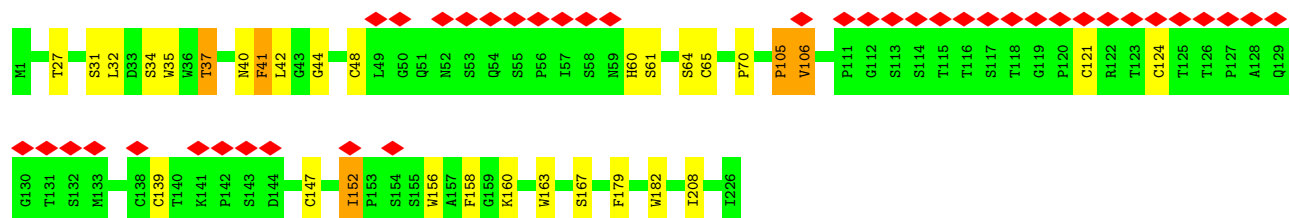
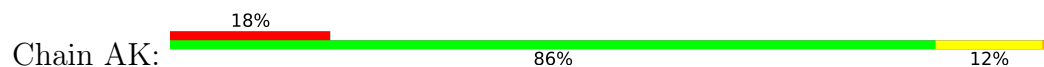
- Molecule 1: Isoform S of Large envelope protein



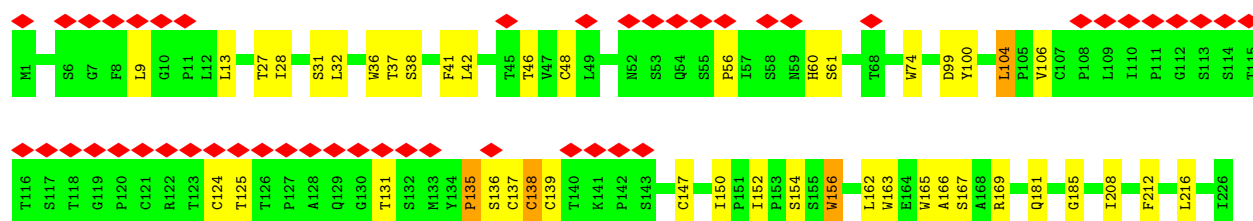
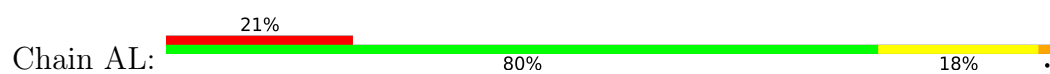
- Molecule 1: Isoform S of Large envelope protein



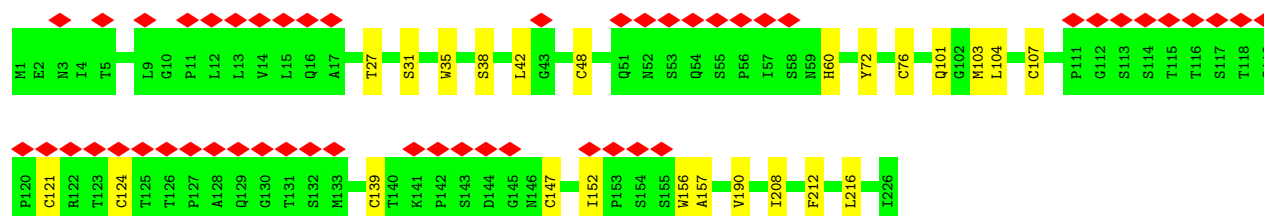
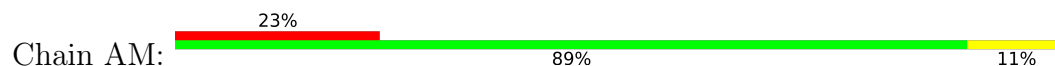
- Molecule 1: Isoform S of Large envelope protein



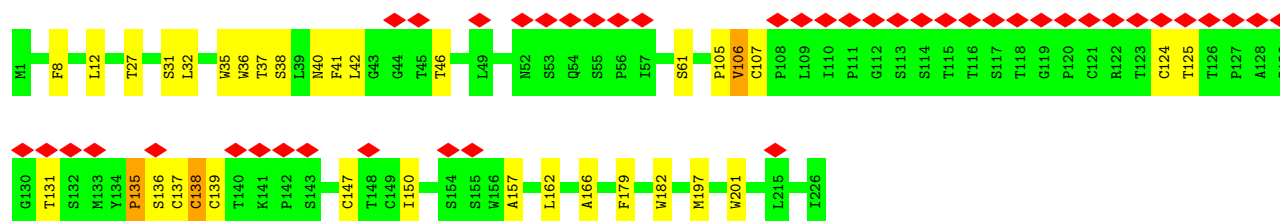
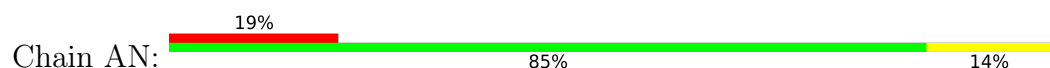
- Molecule 1: Isoform S of Large envelope protein



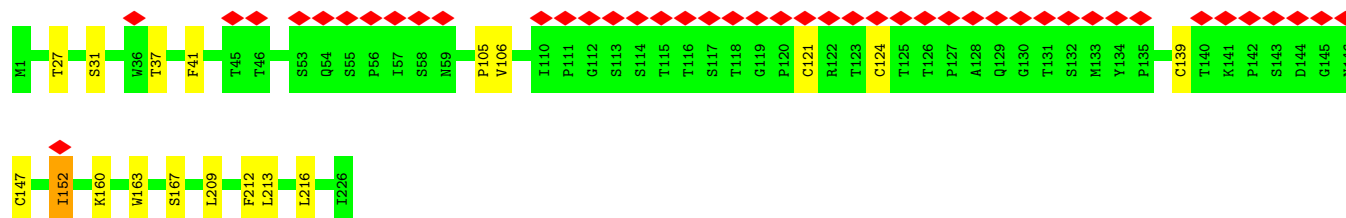
- Molecule 1: Isoform S of Large envelope protein



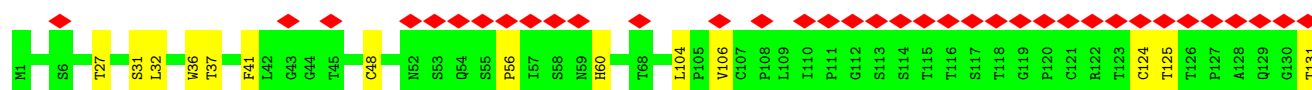
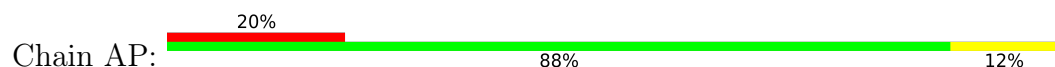
- Molecule 1: Isoform S of Large envelope protein

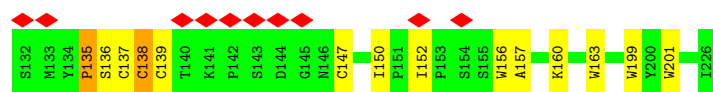


- Molecule 1: Isoform S of Large envelope protein

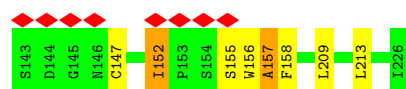
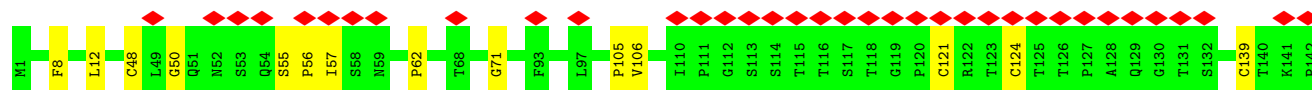


- Molecule 1: Isoform S of Large envelope protein

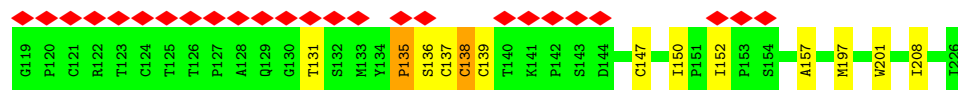
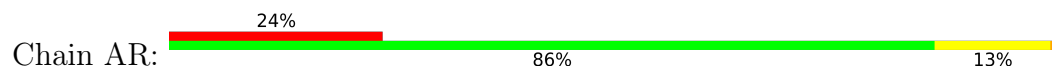




- Molecule 1: Isoform S of Large envelope protein



- Molecule 1: Isoform S of Large envelope protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	113208	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.079	Depositor
Minimum map value	-0.429	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.26	0/1262	0.87	8/1757 (0.5%)
1	1	0.25	0/1229	0.97	5/1709 (0.3%)
1	2	0.42	0/1221	0.96	8/1698 (0.5%)
1	3	0.32	0/1260	0.92	7/1753 (0.4%)
1	4	0.26	0/1257	0.93	11/1748 (0.6%)
1	5	0.20	0/1232	0.73	7/1711 (0.4%)
1	6	0.31	0/1276	0.80	6/1775 (0.3%)
1	7	0.17	0/1262	0.53	3/1757 (0.2%)
1	8	0.38	0/1251	0.98	10/1741 (0.6%)
1	9	0.17	0/1248	0.52	3/1736 (0.2%)
1	A	0.23	0/1251	0.66	3/1741 (0.2%)
1	AA	0.37	0/1213	0.82	5/1687 (0.3%)
1	AB	0.29	0/1246	0.98	12/1732 (0.7%)
1	AC	0.22	0/1240	0.67	4/1725 (0.2%)
1	AD	0.26	0/1251	0.85	8/1741 (0.5%)
1	AE	0.21	0/1252	0.73	7/1739 (0.4%)
1	AF	0.25	0/1225	0.81	7/1702 (0.4%)
1	AG	0.18	0/1236	0.78	7/1718 (0.4%)
1	AH	0.25	0/1191	0.85	8/1655 (0.5%)
1	AI	0.25	0/1229	0.99	7/1709 (0.4%)
1	AJ	0.42	0/1221	0.95	8/1698 (0.5%)
1	AK	0.32	0/1260	0.93	7/1753 (0.4%)
1	AL	0.26	0/1257	0.93	11/1748 (0.6%)
1	AM	0.20	0/1232	0.72	7/1711 (0.4%)
1	AN	0.31	0/1276	0.80	6/1775 (0.3%)
1	AO	0.17	0/1262	0.53	3/1757 (0.2%)
1	AP	0.38	0/1251	0.98	10/1741 (0.6%)
1	AQ	0.17	0/1248	0.52	3/1736 (0.2%)
1	AR	0.26	0/1262	0.87	8/1757 (0.5%)
1	B	0.26	0/1251	0.93	10/1741 (0.6%)
1	C	0.37	0/1213	0.83	5/1687 (0.3%)
1	D	0.29	0/1246	0.98	12/1732 (0.7%)
1	E	0.22	0/1240	0.64	3/1725 (0.2%)
1	F	0.26	0/1251	0.85	8/1741 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.25	0/1243	0.89	2/1727 (0.1%)
1	H	0.48	0/1236	1.19	16/1718 (0.9%)
1	I	0.21	0/1252	0.69	7/1739 (0.4%)
1	J	0.25	0/1225	0.82	7/1702 (0.4%)
1	K	0.18	0/1236	0.85	7/1718 (0.4%)
1	L	0.25	0/1191	0.85	8/1655 (0.5%)
1	M	0.25	0/1229	0.91	5/1709 (0.3%)
1	N	0.42	0/1221	0.95	8/1698 (0.5%)
1	O	0.32	0/1260	0.95	8/1753 (0.5%)
1	P	0.26	0/1257	0.93	11/1748 (0.6%)
1	Q	0.20	0/1232	0.72	7/1711 (0.4%)
1	R	0.31	0/1276	0.80	6/1775 (0.3%)
1	S	0.17	0/1262	0.51	3/1757 (0.2%)
1	T	0.40	0/1251	0.98	10/1741 (0.6%)
1	U	0.17	0/1248	0.51	3/1736 (0.2%)
1	V	0.26	0/1262	0.87	8/1757 (0.5%)
1	W	0.23	0/1251	0.66	3/1741 (0.2%)
1	X	0.26	0/1251	0.93	10/1741 (0.6%)
1	Y	0.37	0/1213	0.88	5/1687 (0.3%)
1	Z	0.29	0/1246	0.98	12/1732 (0.7%)
1	a	0.22	0/1240	0.65	4/1725 (0.2%)
1	b	0.26	0/1251	0.85	8/1741 (0.5%)
1	c	0.25	0/1243	0.89	2/1727 (0.1%)
1	d	0.48	0/1236	1.19	16/1718 (0.9%)
1	e	0.21	0/1252	0.73	7/1739 (0.4%)
1	f	0.25	0/1225	0.81	7/1702 (0.4%)
1	g	0.18	0/1236	0.83	7/1718 (0.4%)
1	h	0.25	0/1191	0.85	8/1655 (0.5%)
1	i	0.25	0/1229	0.97	5/1709 (0.3%)
1	j	0.42	0/1221	0.96	8/1698 (0.5%)
1	k	0.32	0/1260	0.74	7/1753 (0.4%)
1	l	0.26	0/1257	0.93	11/1748 (0.6%)
1	m	0.20	0/1232	0.74	7/1711 (0.4%)
1	n	0.31	0/1276	0.80	6/1775 (0.3%)
1	o	0.17	0/1262	0.52	3/1757 (0.2%)
1	p	0.38	0/1251	0.98	10/1741 (0.6%)
1	q	0.17	0/1248	0.52	3/1736 (0.2%)
1	r	0.26	0/1262	0.87	8/1757 (0.5%)
1	s	0.37	0/1213	0.83	6/1687 (0.4%)
1	t	0.29	0/1246	0.98	12/1732 (0.7%)
1	u	0.22	0/1240	0.65	5/1725 (0.3%)
1	v	0.26	0/1251	0.85	8/1741 (0.5%)
1	w	0.21	0/1252	0.69	7/1739 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	x	0.25	0/1225	0.82	7/1702 (0.4%)
1	y	0.18	0/1236	0.87	7/1718 (0.4%)
1	z	0.25	0/1191	0.85	8/1655 (0.5%)
All	All	0.28	0/99370	0.84	570/138190 (0.4%)

There are no bond length outliers.

All (570) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	106	VAL	N-CA-C	-23.60	92.30	112.12
1	c	106	VAL	N-CA-C	-23.60	92.30	112.12
1	O	106	VAL	N-CA-C	-23.34	92.51	112.12
1	i	106	VAL	N-CA-C	-22.65	93.56	111.90
1	l	106	VAL	N-CA-C	-22.65	93.56	111.90
1	AI	106	VAL	N-CA-C	-22.65	93.56	111.90
1	y	106	VAL	N-CA-C	-22.58	93.15	112.12
1	AK	106	VAL	N-CA-C	-22.54	93.19	112.12
1	K	106	VAL	N-CA-C	-22.23	93.89	111.90
1	3	106	VAL	N-CA-C	-22.20	93.92	111.90
1	g	106	VAL	N-CA-C	-21.32	94.63	111.90
1	M	106	VAL	N-CA-C	-18.62	94.34	112.96
1	AG	106	VAL	N-CA-C	-17.63	95.33	112.96
1	Y	106	VAL	N-CA-C	-15.07	99.46	112.12
1	O	105	PRO	CB-CA-C	14.32	131.11	110.20
1	i	152	ILE	CA-C-N	13.90	134.80	119.92
1	i	152	ILE	C-N-CA	13.90	134.80	119.92
1	l	152	ILE	CA-C-N	13.90	134.80	119.92
1	l	152	ILE	C-N-CA	13.90	134.80	119.92
1	M	152	ILE	CA-C-N	13.88	134.77	119.92
1	M	152	ILE	C-N-CA	13.88	134.77	119.92
1	AI	152	ILE	CA-C-N	13.86	134.75	119.92
1	AI	152	ILE	C-N-CA	13.86	134.75	119.92
1	s	105	PRO	CB-CA-C	13.71	134.18	111.56
1	AK	105	PRO	CB-CA-C	13.66	130.14	110.20
1	y	105	PRO	CB-CA-C	13.58	130.03	110.20
1	3	105	PRO	CB-CA-C	12.99	129.17	110.20
1	K	105	PRO	CB-CA-C	12.91	129.05	110.20
1	AA	105	PRO	CB-CA-C	12.52	132.22	111.56
1	C	106	VAL	N-CA-C	-12.29	101.95	111.90
1	g	105	PRO	CB-CA-C	12.22	128.04	110.20
1	m	157	ALA	N-CA-C	-11.99	98.63	113.38
1	Y	105	PRO	CB-CA-C	11.92	131.22	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	ILE	CA-C-N	11.85	131.60	119.76
1	B	152	ILE	C-N-CA	11.85	131.60	119.76
1	X	152	ILE	CA-C-N	11.85	131.60	119.76
1	X	152	ILE	C-N-CA	11.85	131.60	119.76
1	G	105	PRO	CB-CA-C	11.84	131.09	111.56
1	c	105	PRO	CB-CA-C	11.84	131.09	111.56
1	p	152	ILE	CA-C-N	11.81	131.57	119.76
1	p	152	ILE	C-N-CA	11.81	131.57	119.76
1	8	152	ILE	CA-C-N	11.81	131.57	119.76
1	8	152	ILE	C-N-CA	11.81	131.57	119.76
1	AP	152	ILE	CA-C-N	11.81	131.57	119.76
1	AP	152	ILE	C-N-CA	11.81	131.57	119.76
1	e	104	LEU	CA-C-N	11.70	133.49	120.85
1	e	104	LEU	C-N-CA	11.70	133.49	120.85
1	AE	104	LEU	CA-C-N	11.70	133.49	120.85
1	AE	104	LEU	C-N-CA	11.70	133.49	120.85
1	H	152	ILE	CA-C-N	11.67	131.64	119.85
1	H	152	ILE	C-N-CA	11.67	131.64	119.85
1	d	152	ILE	CA-C-N	11.67	131.64	119.85
1	d	152	ILE	C-N-CA	11.67	131.64	119.85
1	AG	105	PRO	CB-CA-C	11.65	127.06	110.17
1	D	152	ILE	CA-C-N	11.61	131.57	119.85
1	D	152	ILE	C-N-CA	11.61	131.57	119.85
1	Z	152	ILE	CA-C-N	11.61	131.57	119.85
1	Z	152	ILE	C-N-CA	11.61	131.57	119.85
1	t	152	ILE	CA-C-N	11.61	131.57	119.85
1	t	152	ILE	C-N-CA	11.61	131.57	119.85
1	AB	152	ILE	CA-C-N	11.61	131.57	119.85
1	AB	152	ILE	C-N-CA	11.61	131.57	119.85
1	T	152	ILE	CA-C-N	11.60	131.57	119.85
1	T	152	ILE	C-N-CA	11.60	131.57	119.85
1	P	152	ILE	CA-C-N	11.57	131.53	119.85
1	P	152	ILE	C-N-CA	11.57	131.53	119.85
1	l	152	ILE	CA-C-N	11.57	131.53	119.85
1	l	152	ILE	C-N-CA	11.57	131.53	119.85
1	4	152	ILE	CA-C-N	11.57	131.53	119.85
1	4	152	ILE	C-N-CA	11.57	131.53	119.85
1	AL	152	ILE	CA-C-N	11.57	131.53	119.85
1	AL	152	ILE	C-N-CA	11.57	131.53	119.85
1	5	157	ALA	N-CA-C	-11.39	99.37	113.38
1	B	150	ILE	CA-C-N	11.10	131.06	119.85
1	B	150	ILE	C-N-CA	11.10	131.06	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	150	ILE	CA-C-N	11.10	131.06	119.85
1	X	150	ILE	C-N-CA	11.10	131.06	119.85
1	L	150	ILE	CA-C-N	11.10	131.06	119.85
1	L	150	ILE	C-N-CA	11.10	131.06	119.85
1	h	150	ILE	CA-C-N	11.10	131.06	119.85
1	h	150	ILE	C-N-CA	11.10	131.06	119.85
1	z	150	ILE	CA-C-N	11.10	131.06	119.85
1	z	150	ILE	C-N-CA	11.10	131.06	119.85
1	AH	150	ILE	CA-C-N	11.10	131.06	119.85
1	AH	150	ILE	C-N-CA	11.10	131.06	119.85
1	F	150	ILE	CA-C-N	11.09	131.05	119.85
1	F	150	ILE	C-N-CA	11.09	131.05	119.85
1	b	150	ILE	CA-C-N	11.09	131.05	119.85
1	b	150	ILE	C-N-CA	11.09	131.05	119.85
1	v	150	ILE	CA-C-N	11.09	131.05	119.85
1	v	150	ILE	C-N-CA	11.09	131.05	119.85
1	AD	150	ILE	CA-C-N	11.09	131.05	119.85
1	AD	150	ILE	C-N-CA	11.09	131.05	119.85
1	H	150	ILE	CA-C-N	11.08	131.04	119.85
1	H	150	ILE	C-N-CA	11.08	131.04	119.85
1	d	150	ILE	CA-C-N	11.08	131.04	119.85
1	d	150	ILE	C-N-CA	11.08	131.04	119.85
1	V	150	ILE	CA-C-N	11.08	131.04	119.85
1	V	150	ILE	C-N-CA	11.08	131.04	119.85
1	r	150	ILE	CA-C-N	11.08	131.04	119.85
1	r	150	ILE	C-N-CA	11.08	131.04	119.85
1	0	150	ILE	CA-C-N	11.08	131.04	119.85
1	0	150	ILE	C-N-CA	11.08	131.04	119.85
1	AR	150	ILE	CA-C-N	11.08	131.04	119.85
1	AR	150	ILE	C-N-CA	11.08	131.04	119.85
1	R	150	ILE	CA-C-N	11.06	131.02	119.85
1	R	150	ILE	C-N-CA	11.06	131.02	119.85
1	n	150	ILE	CA-C-N	11.06	131.02	119.85
1	n	150	ILE	C-N-CA	11.06	131.02	119.85
1	6	150	ILE	CA-C-N	11.06	131.02	119.85
1	6	150	ILE	C-N-CA	11.06	131.02	119.85
1	AN	150	ILE	CA-C-N	11.06	131.02	119.85
1	AN	150	ILE	C-N-CA	11.06	131.02	119.85
1	N	150	ILE	CA-C-N	11.05	131.01	119.85
1	N	150	ILE	C-N-CA	11.05	131.01	119.85
1	j	150	ILE	CA-C-N	11.05	131.01	119.85
1	j	150	ILE	C-N-CA	11.05	131.01	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	150	ILE	CA-C-N	11.05	131.01	119.85
1	2	150	ILE	C-N-CA	11.05	131.01	119.85
1	AJ	150	ILE	CA-C-N	11.05	131.01	119.85
1	AJ	150	ILE	C-N-CA	11.05	131.01	119.85
1	T	150	ILE	CA-C-N	11.05	131.01	119.85
1	T	150	ILE	C-N-CA	11.05	131.01	119.85
1	p	150	ILE	CA-C-N	11.05	131.01	119.85
1	p	150	ILE	C-N-CA	11.05	131.01	119.85
1	8	150	ILE	CA-C-N	11.05	131.01	119.85
1	8	150	ILE	C-N-CA	11.05	131.01	119.85
1	AP	150	ILE	CA-C-N	11.05	131.01	119.85
1	AP	150	ILE	C-N-CA	11.05	131.01	119.85
1	D	150	ILE	CA-C-N	11.04	131.00	119.85
1	D	150	ILE	C-N-CA	11.04	131.00	119.85
1	Z	150	ILE	CA-C-N	11.04	131.00	119.85
1	Z	150	ILE	C-N-CA	11.04	131.00	119.85
1	t	150	ILE	CA-C-N	11.04	131.00	119.85
1	t	150	ILE	C-N-CA	11.04	131.00	119.85
1	AB	150	ILE	CA-C-N	11.04	131.00	119.85
1	AB	150	ILE	C-N-CA	11.04	131.00	119.85
1	J	150	ILE	CA-C-N	11.04	131.00	119.85
1	J	150	ILE	C-N-CA	11.04	131.00	119.85
1	f	150	ILE	CA-C-N	11.04	131.00	119.85
1	f	150	ILE	C-N-CA	11.04	131.00	119.85
1	x	150	ILE	CA-C-N	11.04	131.00	119.85
1	x	150	ILE	C-N-CA	11.04	131.00	119.85
1	AF	150	ILE	CA-C-N	11.04	131.00	119.85
1	AF	150	ILE	C-N-CA	11.04	131.00	119.85
1	P	150	ILE	CA-C-N	11.03	130.99	119.85
1	P	150	ILE	C-N-CA	11.03	130.99	119.85
1	l	150	ILE	CA-C-N	11.03	130.99	119.85
1	l	150	ILE	C-N-CA	11.03	130.99	119.85
1	4	150	ILE	CA-C-N	11.03	130.99	119.85
1	4	150	ILE	C-N-CA	11.03	130.99	119.85
1	AL	150	ILE	CA-C-N	11.03	130.99	119.85
1	AL	150	ILE	C-N-CA	11.03	130.99	119.85
1	k	105	PRO	CB-CA-C	11.01	126.13	110.17
1	I	104	LEU	CA-C-N	10.92	133.49	119.84
1	I	104	LEU	C-N-CA	10.92	133.49	119.84
1	w	104	LEU	CA-C-N	10.92	133.49	119.84
1	w	104	LEU	C-N-CA	10.92	133.49	119.84
1	Q	157	ALA	N-CA-C	-10.76	100.15	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AM	157	ALA	N-CA-C	-10.76	100.15	113.38
1	i	105	PRO	CB-CA-C	10.63	129.11	111.56
1	l	105	PRO	CB-CA-C	10.63	129.11	111.56
1	AI	105	PRO	CB-CA-C	10.63	129.11	111.56
1	e	105	PRO	CB-CA-C	10.49	125.52	110.20
1	M	105	PRO	CB-CA-C	10.09	128.21	111.56
1	AE	105	PRO	CB-CA-C	9.81	124.53	110.20
1	T	104	LEU	CA-C-N	9.79	129.84	119.76
1	T	104	LEU	C-N-CA	9.79	129.84	119.76
1	p	104	LEU	CA-C-N	9.79	129.84	119.76
1	p	104	LEU	C-N-CA	9.79	129.84	119.76
1	8	104	LEU	CA-C-N	9.79	129.84	119.76
1	8	104	LEU	C-N-CA	9.79	129.84	119.76
1	AP	104	LEU	CA-C-N	9.79	129.84	119.76
1	AP	104	LEU	C-N-CA	9.79	129.84	119.76
1	T	138	CYS	N-CA-C	-9.73	100.63	111.14
1	p	138	CYS	N-CA-C	-9.73	100.63	111.14
1	8	138	CYS	N-CA-C	-9.73	100.63	111.14
1	AP	138	CYS	N-CA-C	-9.73	100.63	111.14
1	R	138	CYS	N-CA-C	-9.71	100.65	111.14
1	n	138	CYS	N-CA-C	-9.71	100.65	111.14
1	6	138	CYS	N-CA-C	-9.71	100.65	111.14
1	AN	138	CYS	N-CA-C	-9.71	100.65	111.14
1	N	138	CYS	N-CA-C	-9.71	100.66	111.14
1	j	138	CYS	N-CA-C	-9.71	100.66	111.14
1	2	138	CYS	N-CA-C	-9.71	100.66	111.14
1	AJ	138	CYS	N-CA-C	-9.71	100.66	111.14
1	D	138	CYS	N-CA-C	-9.71	100.66	111.14
1	F	138	CYS	N-CA-C	-9.71	100.66	111.14
1	Z	138	CYS	N-CA-C	-9.71	100.66	111.14
1	b	138	CYS	N-CA-C	-9.71	100.66	111.14
1	t	138	CYS	N-CA-C	-9.71	100.66	111.14
1	v	138	CYS	N-CA-C	-9.71	100.66	111.14
1	AB	138	CYS	N-CA-C	-9.71	100.66	111.14
1	AD	138	CYS	N-CA-C	-9.71	100.66	111.14
1	B	138	CYS	N-CA-C	-9.70	100.67	111.14
1	X	138	CYS	N-CA-C	-9.70	100.67	111.14
1	H	138	CYS	N-CA-C	-9.69	100.68	111.14
1	d	138	CYS	N-CA-C	-9.69	100.68	111.14
1	P	138	CYS	N-CA-C	-9.69	100.68	111.14
1	l	138	CYS	N-CA-C	-9.69	100.68	111.14
1	4	138	CYS	N-CA-C	-9.69	100.68	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AL	138	CYS	N-CA-C	-9.69	100.68	111.14
1	J	138	CYS	N-CA-C	-9.68	100.69	111.14
1	f	138	CYS	N-CA-C	-9.68	100.69	111.14
1	x	138	CYS	N-CA-C	-9.68	100.69	111.14
1	AF	138	CYS	N-CA-C	-9.68	100.69	111.14
1	L	138	CYS	N-CA-C	-9.67	100.69	111.14
1	V	152	ILE	CA-C-N	9.67	129.75	119.89
1	V	152	ILE	C-N-CA	9.67	129.75	119.89
1	h	138	CYS	N-CA-C	-9.67	100.69	111.14
1	r	152	ILE	CA-C-N	9.67	129.75	119.89
1	r	152	ILE	C-N-CA	9.67	129.75	119.89
1	z	138	CYS	N-CA-C	-9.67	100.69	111.14
1	0	152	ILE	CA-C-N	9.67	129.75	119.89
1	0	152	ILE	C-N-CA	9.67	129.75	119.89
1	AH	138	CYS	N-CA-C	-9.67	100.69	111.14
1	AR	152	ILE	CA-C-N	9.67	129.75	119.89
1	AR	152	ILE	C-N-CA	9.67	129.75	119.89
1	V	138	CYS	N-CA-C	-9.66	100.71	111.14
1	r	138	CYS	N-CA-C	-9.66	100.71	111.14
1	0	138	CYS	N-CA-C	-9.66	100.71	111.14
1	AR	138	CYS	N-CA-C	-9.66	100.71	111.14
1	Q	104	LEU	CA-C-N	9.46	133.02	120.25
1	Q	104	LEU	C-N-CA	9.46	133.02	120.25
1	m	104	LEU	CA-C-N	9.46	133.02	120.25
1	m	104	LEU	C-N-CA	9.46	133.02	120.25
1	5	104	LEU	CA-C-N	9.46	133.02	120.25
1	5	104	LEU	C-N-CA	9.46	133.02	120.25
1	AM	104	LEU	CA-C-N	9.46	133.02	120.25
1	AM	104	LEU	C-N-CA	9.46	133.02	120.25
1	a	105	PRO	CB-CA-C	9.31	126.93	111.56
1	C	105	PRO	CB-CA-C	9.31	126.92	111.56
1	AC	106	VAL	N-CA-C	-9.11	99.50	112.35
1	D	104	LEU	CA-C-N	-9.11	110.15	119.99
1	D	104	LEU	C-N-CA	-9.11	110.15	119.99
1	Z	104	LEU	CA-C-N	-9.11	110.15	119.99
1	Z	104	LEU	C-N-CA	-9.11	110.15	119.99
1	t	104	LEU	CA-C-N	-9.11	110.15	119.99
1	t	104	LEU	C-N-CA	-9.11	110.15	119.99
1	AB	104	LEU	CA-C-N	-9.11	110.15	119.99
1	AB	104	LEU	C-N-CA	-9.11	110.15	119.99
1	m	156	TRP	N-CA-C	-8.57	93.61	108.52
1	A	156	TRP	N-CA-C	-8.56	101.86	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	156	TRP	N-CA-C	-8.56	101.86	111.71
1	u	156	TRP	N-CA-C	-8.54	97.49	110.30
1	P	104	LEU	CA-C-N	8.47	128.41	119.85
1	P	104	LEU	C-N-CA	8.47	128.41	119.85
1	l	104	LEU	CA-C-N	8.47	128.41	119.85
1	l	104	LEU	C-N-CA	8.47	128.41	119.85
1	4	104	LEU	CA-C-N	8.47	128.41	119.85
1	4	104	LEU	C-N-CA	8.47	128.41	119.85
1	AL	104	LEU	CA-C-N	8.47	128.41	119.85
1	AL	104	LEU	C-N-CA	8.47	128.41	119.85
1	E	105	PRO	CB-CA-C	8.42	125.45	111.56
1	u	105	PRO	CB-CA-C	8.42	125.45	111.56
1	E	156	TRP	N-CA-C	-8.23	97.95	110.30
1	a	156	TRP	N-CA-C	-8.23	97.95	110.30
1	AC	156	TRP	N-CA-C	-8.23	97.95	110.30
1	5	156	TRP	N-CA-C	-7.98	94.64	108.52
1	O	37	THR	N-CA-C	-7.62	103.06	111.36
1	k	37	THR	N-CA-C	-7.62	103.06	111.36
1	3	37	THR	N-CA-C	-7.62	103.06	111.36
1	AK	37	THR	N-CA-C	-7.62	103.06	111.36
1	AC	105	PRO	CB-CA-C	7.41	123.78	111.56
1	Q	156	TRP	N-CA-C	-7.39	95.67	108.52
1	AM	156	TRP	N-CA-C	-7.39	95.67	108.52
1	7	106	VAL	N-CA-C	-7.37	101.56	111.44
1	j	105	PRO	N-CA-C	-7.37	97.30	112.47
1	H	217	PRO	CA-C-N	-7.24	115.63	122.66
1	H	217	PRO	C-N-CA	-7.24	115.63	122.66
1	d	217	PRO	CA-C-N	-7.24	115.63	122.66
1	d	217	PRO	C-N-CA	-7.24	115.63	122.66
1	I	105	PRO	CB-CA-C	7.20	123.44	111.56
1	w	105	PRO	CB-CA-C	7.20	123.44	111.56
1	K	152	ILE	CA-C-N	7.19	126.95	119.76
1	K	152	ILE	C-N-CA	7.19	126.95	119.76
1	g	152	ILE	CA-C-N	7.19	126.95	119.76
1	g	152	ILE	C-N-CA	7.19	126.95	119.76
1	y	152	ILE	CA-C-N	7.19	126.95	119.76
1	y	152	ILE	C-N-CA	7.19	126.95	119.76
1	AG	152	ILE	CA-C-N	7.19	126.95	119.76
1	AG	152	ILE	C-N-CA	7.19	126.95	119.76
1	Q	152	ILE	CA-C-N	7.19	126.95	119.76
1	Q	152	ILE	C-N-CA	7.19	126.95	119.76
1	m	152	ILE	CA-C-N	7.19	126.95	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	152	ILE	C-N-CA	7.19	126.95	119.76
1	5	152	ILE	CA-C-N	7.19	126.95	119.76
1	5	152	ILE	C-N-CA	7.19	126.95	119.76
1	AM	152	ILE	CA-C-N	7.19	126.95	119.76
1	AM	152	ILE	C-N-CA	7.19	126.95	119.76
1	A	105	PRO	CB-CA-C	7.17	123.40	111.56
1	W	105	PRO	CB-CA-C	7.17	123.40	111.56
1	C	152	ILE	CA-C-N	7.14	126.90	119.76
1	C	152	ILE	C-N-CA	7.14	126.90	119.76
1	Y	152	ILE	CA-C-N	7.14	126.90	119.76
1	Y	152	ILE	C-N-CA	7.14	126.90	119.76
1	s	152	ILE	CA-C-N	7.14	126.90	119.76
1	s	152	ILE	C-N-CA	7.14	126.90	119.76
1	AA	152	ILE	CA-C-N	7.14	126.90	119.76
1	AA	152	ILE	C-N-CA	7.14	126.90	119.76
1	j	106	VAL	N-CA-CB	7.11	122.96	111.23
1	H	18	GLY	N-CA-C	-7.04	104.24	112.83
1	d	18	GLY	N-CA-C	-7.04	104.24	112.83
1	O	152	ILE	CA-C-N	7.03	126.95	119.85
1	O	152	ILE	C-N-CA	7.03	126.95	119.85
1	k	152	ILE	CA-C-N	7.03	126.95	119.85
1	k	152	ILE	C-N-CA	7.03	126.95	119.85
1	3	152	ILE	CA-C-N	7.03	126.95	119.85
1	3	152	ILE	C-N-CA	7.03	126.95	119.85
1	AK	152	ILE	CA-C-N	7.03	126.95	119.85
1	AK	152	ILE	C-N-CA	7.03	126.95	119.85
1	U	152	ILE	CA-C-N	7.03	126.95	119.85
1	U	152	ILE	C-N-CA	7.03	126.95	119.85
1	q	152	ILE	CA-C-N	7.03	126.95	119.85
1	q	152	ILE	C-N-CA	7.03	126.95	119.85
1	9	152	ILE	CA-C-N	7.03	126.95	119.85
1	9	152	ILE	C-N-CA	7.03	126.95	119.85
1	AQ	152	ILE	CA-C-N	7.03	126.95	119.85
1	AQ	152	ILE	C-N-CA	7.03	126.95	119.85
1	S	152	ILE	CA-C-N	6.99	126.91	119.85
1	S	152	ILE	C-N-CA	6.99	126.91	119.85
1	o	152	ILE	CA-C-N	6.99	126.91	119.85
1	o	152	ILE	C-N-CA	6.99	126.91	119.85
1	7	152	ILE	CA-C-N	6.99	126.91	119.85
1	7	152	ILE	C-N-CA	6.99	126.91	119.85
1	AO	152	ILE	CA-C-N	6.99	126.91	119.85
1	AO	152	ILE	C-N-CA	6.99	126.91	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	105	PRO	N-CA-C	-6.95	98.15	112.47
1	D	156	TRP	N-CA-C	6.95	120.27	108.67
1	Z	156	TRP	N-CA-C	6.95	120.27	108.67
1	t	156	TRP	N-CA-C	6.95	120.27	108.67
1	AB	156	TRP	N-CA-C	6.95	120.27	108.67
1	H	150	ILE	N-CA-C	6.92	115.84	107.61
1	d	150	ILE	N-CA-C	6.92	115.84	107.61
1	B	150	ILE	N-CA-C	6.90	115.82	107.61
1	X	150	ILE	N-CA-C	6.90	115.82	107.61
1	D	150	ILE	N-CA-C	6.90	115.82	107.61
1	Z	150	ILE	N-CA-C	6.90	115.82	107.61
1	t	150	ILE	N-CA-C	6.90	115.82	107.61
1	AB	150	ILE	N-CA-C	6.90	115.82	107.61
1	P	150	ILE	N-CA-C	6.89	115.81	107.61
1	T	150	ILE	N-CA-C	6.89	115.81	107.61
1	l	150	ILE	N-CA-C	6.89	115.81	107.61
1	p	150	ILE	N-CA-C	6.89	115.81	107.61
1	4	150	ILE	N-CA-C	6.89	115.81	107.61
1	8	150	ILE	N-CA-C	6.89	115.81	107.61
1	AL	150	ILE	N-CA-C	6.89	115.81	107.61
1	AP	150	ILE	N-CA-C	6.89	115.81	107.61
1	J	150	ILE	N-CA-C	6.89	115.81	107.61
1	f	150	ILE	N-CA-C	6.89	115.81	107.61
1	x	150	ILE	N-CA-C	6.89	115.81	107.61
1	AF	150	ILE	N-CA-C	6.89	115.81	107.61
1	L	150	ILE	N-CA-C	6.89	115.80	107.61
1	h	150	ILE	N-CA-C	6.89	115.80	107.61
1	z	150	ILE	N-CA-C	6.89	115.80	107.61
1	AH	150	ILE	N-CA-C	6.89	115.80	107.61
1	L	104	LEU	CA-C-N	6.88	128.44	119.84
1	L	104	LEU	C-N-CA	6.88	128.44	119.84
1	h	104	LEU	CA-C-N	6.88	128.44	119.84
1	h	104	LEU	C-N-CA	6.88	128.44	119.84
1	z	104	LEU	CA-C-N	6.88	128.44	119.84
1	z	104	LEU	C-N-CA	6.88	128.44	119.84
1	AH	104	LEU	CA-C-N	6.88	128.44	119.84
1	AH	104	LEU	C-N-CA	6.88	128.44	119.84
1	H	5	THR	N-CA-C	-6.88	103.78	111.28
1	d	5	THR	N-CA-C	-6.88	103.78	111.28
1	V	150	ILE	N-CA-C	6.87	115.78	107.61
1	r	150	ILE	N-CA-C	6.87	115.78	107.61
1	0	150	ILE	N-CA-C	6.87	115.78	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	150	ILE	N-CA-C	6.87	115.78	107.61
1	R	150	ILE	N-CA-C	6.87	115.78	107.61
1	n	150	ILE	N-CA-C	6.87	115.78	107.61
1	6	150	ILE	N-CA-C	6.87	115.78	107.61
1	AN	150	ILE	N-CA-C	6.87	115.78	107.61
1	N	150	ILE	N-CA-C	6.86	115.77	107.61
1	j	150	ILE	N-CA-C	6.86	115.77	107.61
1	2	150	ILE	N-CA-C	6.86	115.77	107.61
1	AJ	150	ILE	N-CA-C	6.86	115.77	107.61
1	F	150	ILE	N-CA-C	6.85	115.77	107.61
1	b	150	ILE	N-CA-C	6.85	115.77	107.61
1	v	150	ILE	N-CA-C	6.85	115.77	107.61
1	AD	150	ILE	N-CA-C	6.85	115.77	107.61
1	J	105	PRO	CB-CA-C	-6.85	100.26	111.56
1	x	105	PRO	CB-CA-C	-6.85	100.26	111.56
1	AO	106	VAL	N-CA-C	-6.82	102.31	111.44
1	2	106	VAL	N-CA-CB	6.64	122.19	111.23
1	N	105	PRO	N-CA-C	-6.53	99.02	112.47
1	AJ	105	PRO	N-CA-C	-6.53	99.02	112.47
1	AG	105	PRO	N-CA-C	-6.40	101.08	111.77
1	K	154	SER	N-CA-C	6.34	119.90	108.17
1	g	154	SER	N-CA-C	6.34	119.90	108.17
1	k	106	VAL	N-CA-C	-6.34	96.15	109.34
1	y	154	SER	N-CA-C	6.34	119.90	108.17
1	AG	154	SER	N-CA-C	6.34	119.90	108.17
1	A	106	VAL	N-CA-C	-6.33	96.17	109.34
1	W	106	VAL	N-CA-C	-6.33	96.17	109.34
1	AC	196	TRP	N-CA-C	-6.28	105.77	113.50
1	AI	158	PHE	CB-CA-C	-6.24	102.58	111.95
1	o	106	VAL	N-CA-C	-6.24	103.08	111.44
1	H	103	MET	N-CA-C	6.22	118.06	111.28
1	d	103	MET	N-CA-C	6.22	118.06	111.28
1	f	105	PRO	CB-CA-C	-6.21	101.32	111.56
1	K	156	TRP	N-CA-C	-6.20	99.53	109.39
1	g	156	TRP	N-CA-C	-6.20	99.53	109.39
1	y	156	TRP	N-CA-C	-6.20	99.53	109.39
1	AG	156	TRP	N-CA-C	-6.20	99.53	109.39
1	N	106	VAL	N-CA-CB	6.17	121.41	111.23
1	AJ	106	VAL	N-CA-CB	6.17	121.41	111.23
1	q	106	VAL	N-CA-C	-6.16	103.19	111.44
1	9	106	VAL	N-CA-C	-6.16	103.19	111.44
1	AQ	106	VAL	N-CA-C	-6.16	103.19	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	106	VAL	N-CA-C	-6.06	96.74	109.34
1	y	105	PRO	N-CA-C	-5.94	100.45	111.03
1	I	103	MET	CB-CA-C	-5.92	109.76	116.63
1	e	103	MET	CB-CA-C	-5.92	109.76	116.63
1	w	103	MET	CB-CA-C	-5.92	109.76	116.63
1	AE	103	MET	CB-CA-C	-5.92	109.76	116.63
1	AI	159	GLY	N-CA-C	-5.88	99.25	113.18
1	k	105	PRO	N-CA-C	-5.87	101.97	111.77
1	H	104	LEU	CA-C-N	-5.85	113.67	119.99
1	H	104	LEU	C-N-CA	-5.85	113.67	119.99
1	d	104	LEU	CA-C-N	-5.85	113.67	119.99
1	d	104	LEU	C-N-CA	-5.85	113.67	119.99
1	K	105	PRO	N-CA-C	-5.84	100.64	111.03
1	C	101	GLN	N-CA-C	5.81	118.49	109.60
1	Y	101	GLN	N-CA-C	5.81	118.49	109.60
1	s	101	GLN	N-CA-C	5.81	118.49	109.60
1	AA	101	GLN	N-CA-C	5.81	118.49	109.60
1	B	72	TYR	N-CA-C	-5.79	108.02	114.62
1	S	106	VAL	N-CA-C	-5.79	103.85	111.09
1	X	72	TYR	N-CA-C	-5.79	108.02	114.62
1	g	105	PRO	N-CA-C	-5.72	100.85	111.03
1	F	156	TRP	CA-C-N	5.70	132.43	121.54
1	F	156	TRP	C-N-CA	5.70	132.43	121.54
1	b	156	TRP	CA-C-N	5.70	132.43	121.54
1	b	156	TRP	C-N-CA	5.70	132.43	121.54
1	v	156	TRP	CA-C-N	5.70	132.43	121.54
1	v	156	TRP	C-N-CA	5.70	132.43	121.54
1	AD	156	TRP	CA-C-N	5.70	132.43	121.54
1	AD	156	TRP	C-N-CA	5.70	132.43	121.54
1	H	14	VAL	N-CA-C	-5.68	105.19	110.53
1	d	14	VAL	N-CA-C	-5.68	105.19	110.53
1	P	154	SER	N-CA-C	-5.65	105.20	111.36
1	l	154	SER	N-CA-C	-5.65	105.20	111.36
1	4	154	SER	N-CA-C	-5.65	105.20	111.36
1	AL	154	SER	N-CA-C	-5.65	105.20	111.36
1	O	105	PRO	N-CA-C	-5.64	100.99	111.03
1	D	156	TRP	CB-CA-C	-5.59	109.63	117.23
1	Z	156	TRP	CB-CA-C	-5.59	109.63	117.23
1	t	156	TRP	CB-CA-C	-5.59	109.63	117.23
1	AB	156	TRP	CB-CA-C	-5.59	109.63	117.23
1	AK	105	PRO	N-CA-C	-5.58	101.10	111.03
1	AF	105	PRO	CB-CA-C	-5.58	102.36	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	106	VAL	N-CA-C	-5.56	97.78	109.34
1	F	131	THR	CB-CA-C	-5.51	110.24	116.63
1	b	131	THR	CB-CA-C	-5.51	110.24	116.63
1	v	131	THR	CB-CA-C	-5.51	110.24	116.63
1	AD	131	THR	CB-CA-C	-5.51	110.24	116.63
1	D	131	THR	CB-CA-C	-5.51	110.24	116.63
1	Z	131	THR	CB-CA-C	-5.51	110.24	116.63
1	t	131	THR	CB-CA-C	-5.51	110.24	116.63
1	AB	131	THR	CB-CA-C	-5.51	110.24	116.63
1	N	131	THR	CB-CA-C	-5.50	110.25	116.63
1	j	131	THR	CB-CA-C	-5.50	110.25	116.63
1	2	131	THR	CB-CA-C	-5.50	110.25	116.63
1	AJ	131	THR	CB-CA-C	-5.50	110.25	116.63
1	3	105	PRO	N-CA-C	-5.50	101.24	111.03
1	R	131	THR	CB-CA-C	-5.49	110.27	116.63
1	n	131	THR	CB-CA-C	-5.49	110.27	116.63
1	6	131	THR	CB-CA-C	-5.49	110.27	116.63
1	AN	131	THR	CB-CA-C	-5.49	110.27	116.63
1	P	131	THR	CB-CA-C	-5.49	110.27	116.63
1	V	131	THR	CB-CA-C	-5.49	110.27	116.63
1	l	131	THR	CB-CA-C	-5.49	110.27	116.63
1	r	131	THR	CB-CA-C	-5.49	110.27	116.63
1	4	131	THR	CB-CA-C	-5.49	110.27	116.63
1	0	131	THR	CB-CA-C	-5.49	110.27	116.63
1	AL	131	THR	CB-CA-C	-5.49	110.27	116.63
1	AR	131	THR	CB-CA-C	-5.49	110.27	116.63
1	H	131	THR	CB-CA-C	-5.48	110.27	116.63
1	d	131	THR	CB-CA-C	-5.48	110.27	116.63
1	L	131	THR	CB-CA-C	-5.48	110.28	116.63
1	h	131	THR	CB-CA-C	-5.48	110.28	116.63
1	z	131	THR	CB-CA-C	-5.48	110.28	116.63
1	AH	131	THR	CB-CA-C	-5.48	110.28	116.63
1	J	131	THR	CB-CA-C	-5.47	110.28	116.63
1	f	131	THR	CB-CA-C	-5.47	110.28	116.63
1	x	131	THR	CB-CA-C	-5.47	110.28	116.63
1	AF	131	THR	CB-CA-C	-5.47	110.28	116.63
1	s	106	VAL	N-CA-CB	5.47	120.25	111.23
1	T	131	THR	CB-CA-C	-5.46	110.29	116.63
1	p	131	THR	CB-CA-C	-5.46	110.29	116.63
1	8	131	THR	CB-CA-C	-5.46	110.29	116.63
1	AP	131	THR	CB-CA-C	-5.46	110.29	116.63
1	B	131	THR	CB-CA-C	-5.44	110.32	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	131	THR	CB-CA-C	-5.44	110.32	116.63
1	E	106	VAL	N-CA-C	-5.39	98.13	109.34
1	u	106	VAL	N-CA-C	-5.39	98.13	109.34
1	a	196	TRP	N-CA-C	-5.38	106.56	113.23
1	u	196	TRP	N-CA-C	-5.38	106.56	113.23
1	I	152	ILE	CA-C-N	5.34	125.34	119.89
1	I	152	ILE	C-N-CA	5.34	125.34	119.89
1	e	152	ILE	CA-C-N	5.34	125.34	119.89
1	e	152	ILE	C-N-CA	5.34	125.34	119.89
1	w	152	ILE	CA-C-N	5.34	125.34	119.89
1	w	152	ILE	C-N-CA	5.34	125.34	119.89
1	AE	152	ILE	CA-C-N	5.34	125.34	119.89
1	AE	152	ILE	C-N-CA	5.34	125.34	119.89
1	U	106	VAL	N-CA-C	-5.32	105.35	110.72
1	Q	190	VAL	N-CA-C	-5.28	107.69	112.12
1	m	190	VAL	N-CA-C	-5.28	107.69	112.12
1	5	190	VAL	N-CA-C	-5.28	107.69	112.12
1	AM	190	VAL	N-CA-C	-5.28	107.69	112.12
1	B	155	SER	N-CA-C	-5.24	102.30	110.10
1	X	155	SER	N-CA-C	-5.24	102.30	110.10
1	I	190	VAL	N-CA-C	-5.20	107.76	112.12
1	e	190	VAL	N-CA-C	-5.20	107.76	112.12
1	w	190	VAL	N-CA-C	-5.20	107.76	112.12
1	AE	190	VAL	N-CA-C	-5.20	107.76	112.12
1	J	135	PRO	CB-CA-C	-5.15	103.06	111.56
1	f	135	PRO	CB-CA-C	-5.15	103.06	111.56
1	x	135	PRO	CB-CA-C	-5.15	103.06	111.56
1	AF	135	PRO	CB-CA-C	-5.15	103.06	111.56
1	H	135	PRO	CB-CA-C	-5.14	103.08	111.56
1	d	135	PRO	CB-CA-C	-5.14	103.08	111.56
1	R	135	PRO	CB-CA-C	-5.13	103.09	111.56
1	n	135	PRO	CB-CA-C	-5.13	103.09	111.56
1	u	156	TRP	CB-CA-C	5.13	117.19	110.06
1	6	135	PRO	CB-CA-C	-5.13	103.09	111.56
1	AN	135	PRO	CB-CA-C	-5.13	103.09	111.56
1	T	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	p	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	8	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	AP	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	B	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	F	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	X	135	PRO	CB-CA-C	-5.13	103.10	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	v	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	AD	135	PRO	CB-CA-C	-5.13	103.10	111.56
1	P	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	l	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	4	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	AL	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	D	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	N	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	Z	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	j	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	t	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	2	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	AB	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	AJ	135	PRO	CB-CA-C	-5.12	103.11	111.56
1	L	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	V	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	h	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	r	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	z	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	0	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	AH	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	AR	135	PRO	CB-CA-C	-5.10	103.14	111.56
1	O	32	LEU	N-CA-C	-5.10	105.85	111.71
1	k	32	LEU	N-CA-C	-5.10	105.85	111.71
1	3	32	LEU	N-CA-C	-5.10	105.85	111.71
1	AK	32	LEU	N-CA-C	-5.10	105.85	111.71
1	M	190	VAL	N-CA-C	-5.03	107.64	111.62
1	i	190	VAL	N-CA-C	-5.03	107.64	111.62
1	1	190	VAL	N-CA-C	-5.03	107.64	111.62
1	AI	190	VAL	N-CA-C	-5.03	107.64	111.62
1	O	106	VAL	N-CA-CB	5.02	118.78	111.90
1	AA	106	VAL	N-CA-C	-5.02	98.90	109.34

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	0	1240	0	592	25	0
1	1	1213	0	566	17	0
1	2	1206	0	561	28	0
1	3	1239	0	594	34	0
1	4	1237	0	595	26	0
1	5	1216	0	572	11	0
1	6	1252	0	606	30	0
1	7	1240	0	590	10	0
1	8	1231	0	584	15	0
1	9	1229	0	581	12	0
1	A	1231	0	582	23	0
1	AA	1199	0	552	21	0
1	AB	1228	0	587	48	0
1	AC	1222	0	574	13	0
1	AD	1231	0	584	26	0
1	AE	1232	0	588	13	0
1	AF	1210	0	567	23	0
1	AG	1219	0	573	9	0
1	AH	1181	0	538	19	0
1	AI	1213	0	566	14	0
1	AJ	1206	0	561	27	0
1	AK	1239	0	594	34	0
1	AL	1237	0	595	27	0
1	AM	1216	0	572	11	0
1	AN	1252	0	606	30	0
1	AO	1240	0	590	9	0
1	AP	1231	0	584	15	0
1	AQ	1229	0	581	12	0
1	AR	1240	0	592	24	0
1	B	1231	0	584	18	0
1	C	1199	0	552	21	0
1	D	1228	0	587	48	0
1	E	1222	0	574	14	0
1	F	1231	0	584	21	0
1	G	1225	0	580	14	0
1	H	1219	0	575	28	0
1	I	1232	0	588	14	0
1	J	1210	0	567	24	0
1	K	1219	0	573	10	0
1	L	1181	0	538	20	0
1	M	1213	0	566	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1206	0	561	27	0
1	O	1239	0	594	34	0
1	P	1237	0	595	26	0
1	Q	1216	0	572	11	0
1	R	1252	0	606	30	0
1	S	1240	0	590	12	0
1	T	1231	0	584	16	0
1	U	1229	0	581	12	0
1	V	1240	0	592	24	0
1	W	1231	0	582	22	0
1	X	1231	0	584	18	0
1	Y	1199	0	552	21	0
1	Z	1228	0	587	49	0
1	a	1222	0	574	13	0
1	b	1231	0	584	21	0
1	c	1225	0	580	14	0
1	d	1219	0	575	27	0
1	e	1232	0	588	13	0
1	f	1210	0	567	24	0
1	g	1219	0	573	9	0
1	h	1181	0	538	19	0
1	i	1213	0	566	16	0
1	j	1206	0	561	28	0
1	k	1239	0	594	34	0
1	l	1237	0	595	26	0
1	m	1216	0	572	11	0
1	n	1252	0	606	29	0
1	o	1240	0	590	10	0
1	p	1231	0	584	15	0
1	q	1229	0	581	12	0
1	r	1240	0	592	24	0
1	s	1199	0	552	21	0
1	t	1228	0	587	49	0
1	u	1222	0	574	14	0
1	v	1231	0	584	27	0
1	w	1232	0	588	14	0
1	x	1210	0	567	23	0
1	y	1219	0	573	10	0
1	z	1181	0	538	20	0
All	All	97912	0	46258	1551	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 11.

All (1551) 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:AN:106:VAL:CB	1:AN:157:ALA:HB1	1.18	1.59
1:R:106:VAL:CB	1:R:157:ALA:HB1	1.18	1.58
1:n:106:VAL:CB	1:n:157:ALA:HB1	1.18	1.58
1:6:106:VAL:CB	1:6:157:ALA:HB1	1.18	1.58
1:n:106:VAL:CB	1:n:157:ALA:CB	1.91	1.48
1:AN:106:VAL:CB	1:AN:157:ALA:CB	1.91	1.48
1:6:106:VAL:CB	1:6:157:ALA:CB	1.91	1.48
1:R:106:VAL:CB	1:R:157:ALA:CB	1.91	1.48
1:c:106:VAL:CB	1:c:161:PHE:CB	1.95	1.45
1:u:105:PRO:CB	1:u:152:ILE:CB	1.95	1.44
1:E:105:PRO:CB	1:E:152:ILE:CB	1.95	1.44
1:a:105:PRO:CB	1:a:152:ILE:CB	1.95	1.43
1:AC:105:PRO:CB	1:AC:152:ILE:CB	1.95	1.43
1:G:106:VAL:CB	1:G:161:PHE:CB	1.95	1.43
1:z:98:LEU:O	1:z:101:GLN:HG2	1.22	1.34
1:L:98:LEU:O	1:L:101:GLN:HG2	1.22	1.33
1:AF:106:VAL:CB	1:AF:157:ALA:CB	2.08	1.31
1:f:106:VAL:CB	1:f:157:ALA:CB	2.08	1.31
1:M:106:VAL:O	1:N:105:PRO:CB	1.77	1.30
1:i:106:VAL:O	1:j:105:PRO:CB	1.77	1.30
1:1:106:VAL:O	1:2:105:PRO:CB	1.77	1.30
1:AI:106:VAL:O	1:AJ:105:PRO:CB	1.77	1.30
1:x:106:VAL:CB	1:x:157:ALA:CB	2.08	1.29
1:J:106:VAL:CB	1:J:157:ALA:CB	2.08	1.29
1:h:98:LEU:O	1:h:101:GLN:HG2	1.22	1.28
1:AH:98:LEU:O	1:AH:101:GLN:HG2	1.22	1.27
1:H:35:TRP:CH2	1:AD:207:SER:O	1.91	1.24
1:d:35:TRP:CH2	1:v:207:SER:O	1.91	1.23
1:D:211:PRO:CB	1:AK:35:TRP:NE1	2.03	1.22
1:k:35:TRP:NE1	1:t:211:PRO:CB	2.03	1.22
1:Z:211:PRO:CB	1:3:35:TRP:NE1	2.03	1.21
1:O:35:TRP:NE1	1:AB:211:PRO:CB	2.03	1.21
1:f:106:VAL:CB	1:f:157:ALA:HB3	1.72	1.17
1:h:98:LEU:O	1:h:101:GLN:CG	1.92	1.17
1:z:98:LEU:O	1:z:101:GLN:CG	1.92	1.17
1:AH:98:LEU:O	1:AH:101:GLN:CG	1.92	1.17
1:L:98:LEU:O	1:L:101:GLN:CG	1.92	1.16
1:AF:106:VAL:CB	1:AF:157:ALA:HB3	1.72	1.16
1:f:106:VAL:CB	1:f:157:ALA:HB1	1.74	1.15
1:AF:106:VAL:CB	1:AF:157:ALA:HB1	1.74	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:VAL:CB	1:J:157:ALA:HB3	1.72	1.14
1:O:106:VAL:CB	1:O:157:ALA:HB3	1.77	1.14
1:V:106:VAL:CB	1:V:157:ALA:HB3	1.77	1.14
1:AR:106:VAL:CB	1:AR:157:ALA:HB3	1.77	1.14
1:r:106:VAL:CB	1:r:157:ALA:HB3	1.77	1.14
1:x:106:VAL:CB	1:x:157:ALA:HB3	1.72	1.14
1:x:106:VAL:CB	1:x:157:ALA:HB1	1.74	1.13
1:J:106:VAL:CB	1:J:157:ALA:HB1	1.74	1.13
1:Y:101:GLN:HG2	1:Y:102:GLY:H	1.15	1.12
1:AA:101:GLN:HG2	1:AA:102:GLY:H	1.15	1.12
1:s:101:GLN:HG2	1:s:102:GLY:H	1.15	1.10
1:C:101:GLN:HG2	1:C:102:GLY:H	1.15	1.10
1:D:207:SER:O	1:AK:35:TRP:CH2	2.06	1.09
1:k:35:TRP:CH2	1:t:207:SER:O	2.06	1.09
1:Z:207:SER:O	1:3:35:TRP:CH2	2.06	1.09
1:O:35:TRP:CH2	1:AB:207:SER:O	2.06	1.08
1:O:35:TRP:HH2	1:AB:207:SER:O	1.33	1.08
1:Z:207:SER:O	1:3:35:TRP:HH2	1.33	1.07
1:D:207:SER:O	1:AK:35:TRP:HH2	1.33	1.07
1:k:35:TRP:HH2	1:t:207:SER:O	1.33	1.06
1:O:35:TRP:HE1	1:AB:211:PRO:CA	1.71	1.04
1:P:139:CYS:HA	1:P:147:CYS:SG	1.98	1.04
1:Z:211:PRO:CA	1:3:35:TRP:HE1	1.71	1.04
1:4:139:CYS:HA	1:4:147:CYS:SG	1.98	1.04
1:H:139:CYS:HA	1:H:147:CYS:SG	1.98	1.03
1:Z:211:PRO:CB	1:3:35:TRP:HE1	1.71	1.03
1:h:139:CYS:HA	1:h:147:CYS:SG	1.98	1.03
1:AH:139:CYS:HA	1:AH:147:CYS:SG	1.98	1.03
1:O:35:TRP:HE1	1:AB:211:PRO:CB	1.71	1.03
1:l:139:CYS:HA	1:l:147:CYS:SG	1.98	1.03
1:AB:139:CYS:HA	1:AB:147:CYS:SG	1.98	1.03
1:AL:139:CYS:HA	1:AL:147:CYS:SG	1.98	1.03
1:B:139:CYS:HA	1:B:147:CYS:SG	1.98	1.03
1:J:139:CYS:HA	1:J:147:CYS:SG	1.98	1.03
1:L:139:CYS:HA	1:L:147:CYS:SG	1.98	1.03
1:N:139:CYS:HA	1:N:147:CYS:SG	1.98	1.03
1:j:139:CYS:HA	1:j:147:CYS:SG	1.98	1.03
1:2:139:CYS:HA	1:2:147:CYS:SG	1.98	1.03
1:AF:139:CYS:HA	1:AF:147:CYS:SG	1.98	1.03
1:AJ:139:CYS:HA	1:AJ:147:CYS:SG	1.98	1.03
1:f:139:CYS:HA	1:f:147:CYS:SG	1.98	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:x:139:CYS:HA	1:x:147:CYS:SG	1.98	1.03
1:z:139:CYS:HA	1:z:147:CYS:SG	1.98	1.03
1:Z:139:CYS:HA	1:Z:147:CYS:SG	1.98	1.03
1:b:139:CYS:HA	1:b:147:CYS:SG	1.98	1.03
1:0:139:CYS:HA	1:0:147:CYS:SG	1.98	1.03
1:AN:139:CYS:HA	1:AN:147:CYS:SG	1.98	1.03
1:V:139:CYS:HA	1:V:147:CYS:SG	1.98	1.02
1:n:139:CYS:HA	1:n:147:CYS:SG	1.98	1.02
1:AD:139:CYS:HA	1:AD:147:CYS:SG	1.98	1.02
1:AP:139:CYS:HA	1:AP:147:CYS:SG	1.98	1.02
1:D:139:CYS:HA	1:D:147:CYS:SG	1.98	1.02
1:p:139:CYS:HA	1:p:147:CYS:SG	1.98	1.02
1:8:139:CYS:HA	1:8:147:CYS:SG	1.98	1.02
1:T:139:CYS:HA	1:T:147:CYS:SG	1.98	1.02
1:X:139:CYS:HA	1:X:147:CYS:SG	1.98	1.02
1:t:139:CYS:HA	1:t:147:CYS:SG	1.98	1.02
1:v:139:CYS:HA	1:v:147:CYS:SG	1.98	1.02
1:D:211:PRO:CA	1:AK:35:TRP:HE1	1.71	1.02
1:R:139:CYS:HA	1:R:147:CYS:SG	1.98	1.02
1:r:139:CYS:HA	1:r:147:CYS:SG	1.98	1.02
1:6:139:CYS:HA	1:6:147:CYS:SG	1.98	1.02
1:F:139:CYS:HA	1:F:147:CYS:SG	1.98	1.02
1:k:35:TRP:HE1	1:t:211:PRO:CA	1.71	1.02
1:AR:139:CYS:HA	1:AR:147:CYS:SG	1.98	1.02
1:d:139:CYS:HA	1:d:147:CYS:SG	1.98	1.01
1:d:35:TRP:HH2	1:v:207:SER:O	1.32	0.99
1:O:35:TRP:CE2	1:AB:211:PRO:CB	2.46	0.98
1:Z:211:PRO:CB	1:3:35:TRP:CE2	2.46	0.98
1:H:35:TRP:HH2	1:AD:207:SER:O	1.32	0.98
1:k:35:TRP:CE2	1:t:211:PRO:CB	2.46	0.97
1:D:211:PRO:CB	1:AK:35:TRP:CE2	2.46	0.97
1:n:106:VAL:CB	1:n:157:ALA:C	2.38	0.97
1:AN:106:VAL:CB	1:AN:157:ALA:C	2.38	0.97
1:R:106:VAL:CB	1:R:157:ALA:C	2.38	0.97
1:6:106:VAL:CB	1:6:157:ALA:C	2.38	0.97
1:C:101:GLN:CG	1:C:102:GLY:H	1.79	0.95
1:O:35:TRP:HH2	1:AB:207:SER:C	1.74	0.95
1:Z:207:SER:C	1:3:35:TRP:HH2	1.74	0.95
1:A:106:VAL:CB	1:A:158:PHE:HA	1.98	0.94
1:D:207:SER:C	1:AK:35:TRP:HH2	1.74	0.94
1:k:35:TRP:HH2	1:t:207:SER:C	1.74	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:106:VAL:CB	1:W:158:PHE:HA	1.98	0.93
1:Y:101:GLN:CG	1:Y:102:GLY:H	1.79	0.93
1:AA:101:GLN:CG	1:AA:102:GLY:H	1.79	0.93
1:H:35:TRP:HH2	1:AD:207:SER:C	1.78	0.92
1:D:211:PRO:CB	1:AK:35:TRP:HE1	1.71	0.92
1:k:35:TRP:HE1	1:t:211:PRO:CB	1.71	0.92
1:s:101:GLN:CG	1:s:102:GLY:H	1.79	0.91
1:Y:101:GLN:HG2	1:Y:102:GLY:N	1.85	0.91
1:k:35:TRP:HZ2	1:t:211:PRO:N	1.69	0.91
1:D:211:PRO:N	1:AK:35:TRP:HZ2	1.69	0.91
1:O:35:TRP:HZ2	1:AB:211:PRO:N	1.69	0.90
1:Z:211:PRO:N	1:3:35:TRP:HZ2	1.69	0.90
1:AA:101:GLN:HG2	1:AA:102:GLY:N	1.85	0.90
1:d:35:TRP:HH2	1:v:207:SER:C	1.78	0.90
1:l:139:CYS:CB	1:l:147:CYS:SG	2.60	0.90
1:AL:139:CYS:CB	1:AL:147:CYS:SG	2.60	0.90
1:T:139:CYS:CB	1:T:147:CYS:SG	2.60	0.90
1:V:139:CYS:CB	1:V:147:CYS:SG	2.60	0.90
1:r:139:CYS:CB	1:r:147:CYS:SG	2.60	0.90
1:6:139:CYS:CB	1:6:147:CYS:SG	2.60	0.90
1:0:139:CYS:CB	1:0:147:CYS:SG	2.60	0.90
1:AR:139:CYS:CB	1:AR:147:CYS:SG	2.60	0.90
1:M:105:PRO:CB	1:M:152:ILE:CB	2.50	0.90
1:R:139:CYS:CB	1:R:147:CYS:SG	2.60	0.90
1:8:139:CYS:CB	1:8:147:CYS:SG	2.60	0.90
1:N:139:CYS:CB	1:N:147:CYS:SG	2.60	0.90
1:x:139:CYS:CB	1:x:147:CYS:SG	2.60	0.90
1:2:139:CYS:CB	1:2:147:CYS:SG	2.60	0.90
1:1:105:PRO:CB	1:1:152:ILE:CB	2.50	0.90
1:B:139:CYS:CB	1:B:147:CYS:SG	2.60	0.89
1:J:139:CYS:CB	1:J:147:CYS:SG	2.60	0.89
1:AN:139:CYS:CB	1:AN:147:CYS:SG	2.60	0.89
1:D:139:CYS:CB	1:D:147:CYS:SG	2.60	0.89
1:n:139:CYS:CB	1:n:147:CYS:SG	2.60	0.89
1:t:139:CYS:CB	1:t:147:CYS:SG	2.60	0.89
1:n:106:VAL:CB	1:n:157:ALA:CA	2.51	0.89
1:AN:106:VAL:CB	1:AN:157:ALA:CA	2.51	0.89
1:F:139:CYS:CB	1:F:147:CYS:SG	2.60	0.89
1:h:139:CYS:CB	1:h:147:CYS:SG	2.60	0.89
1:j:139:CYS:CB	1:j:147:CYS:SG	2.60	0.89
1:v:139:CYS:CB	1:v:147:CYS:SG	2.60	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:139:CYS:CB	1:AH:147:CYS:SG	2.60	0.89
1:AI:105:PRO:CB	1:AI:152:ILE:CB	2.50	0.89
1:H:139:CYS:CB	1:H:147:CYS:SG	2.60	0.89
1:i:105:PRO:CB	1:i:152:ILE:CB	2.50	0.89
1:AJ:139:CYS:CB	1:AJ:147:CYS:SG	2.60	0.89
1:L:139:CYS:CB	1:L:147:CYS:SG	2.60	0.89
1:AF:139:CYS:CB	1:AF:147:CYS:SG	2.60	0.89
1:P:139:CYS:CB	1:P:147:CYS:SG	2.60	0.89
1:f:139:CYS:CB	1:f:147:CYS:SG	2.60	0.89
1:4:139:CYS:CB	1:4:147:CYS:SG	2.60	0.89
1:p:139:CYS:CB	1:p:147:CYS:SG	2.60	0.89
1:z:139:CYS:CB	1:z:147:CYS:SG	2.60	0.89
1:AP:139:CYS:CB	1:AP:147:CYS:SG	2.60	0.89
1:d:139:CYS:CB	1:d:147:CYS:SG	2.60	0.88
1:X:139:CYS:CB	1:X:147:CYS:SG	2.60	0.88
1:AD:139:CYS:CB	1:AD:147:CYS:SG	2.60	0.88
1:Z:139:CYS:CB	1:Z:147:CYS:SG	2.60	0.88
1:b:139:CYS:CB	1:b:147:CYS:SG	2.60	0.88
1:AB:139:CYS:CB	1:AB:147:CYS:SG	2.60	0.88
1:C:101:GLN:HG2	1:C:102:GLY:N	1.85	0.88
1:6:106:VAL:CB	1:6:157:ALA:CA	2.51	0.88
1:R:106:VAL:CB	1:R:157:ALA:CA	2.51	0.88
1:s:101:GLN:HG2	1:s:102:GLY:N	1.85	0.88
1:c:105:PRO:CB	1:c:152:ILE:CB	2.55	0.84
1:r:106:VAL:CB	1:r:157:ALA:CB	2.56	0.83
1:AR:106:VAL:CB	1:AR:157:ALA:CB	2.56	0.83
1:D:211:PRO:HA	1:AK:35:TRP:HE1	1.43	0.83
1:Z:211:PRO:HA	1:3:35:TRP:HE1	1.43	0.83
1:O:35:TRP:HE1	1:AB:211:PRO:HA	1.43	0.83
1:k:35:TRP:HE1	1:t:211:PRO:HA	1.43	0.83
1:G:105:PRO:CB	1:G:152:ILE:CB	2.55	0.83
1:b:37:THR:O	1:b:41:PHE:N	2.12	0.83
1:0:106:VAL:CB	1:0:157:ALA:CB	2.56	0.83
1:AD:37:THR:O	1:AD:41:PHE:N	2.12	0.83
1:V:106:VAL:CB	1:V:157:ALA:CB	2.56	0.82
1:H:35:TRP:CZ2	1:AD:207:SER:O	2.32	0.82
1:d:35:TRP:CZ2	1:v:207:SER:O	2.32	0.82
1:l:37:THR:O	1:l:41:PHE:N	2.13	0.82
1:AL:37:THR:O	1:AL:41:PHE:N	2.13	0.82
1:v:37:THR:O	1:v:41:PHE:N	2.12	0.81
1:W:105:PRO:CB	1:W:152:ILE:CB	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:THR:O	1:F:41:PHE:N	2.12	0.81
1:F:138:CYS:O	1:F:139:CYS:SG	2.40	0.80
1:j:138:CYS:O	1:j:139:CYS:SG	2.40	0.80
1:V:138:CYS:O	1:V:139:CYS:SG	2.40	0.80
1:v:138:CYS:O	1:v:139:CYS:SG	2.40	0.80
1:O:138:CYS:O	1:O:139:CYS:SG	2.40	0.80
1:AJ:138:CYS:O	1:AJ:139:CYS:SG	2.40	0.80
1:L:138:CYS:O	1:L:139:CYS:SG	2.40	0.80
1:f:138:CYS:O	1:f:139:CYS:SG	2.40	0.80
1:z:138:CYS:O	1:z:139:CYS:SG	2.40	0.80
1:4:37:THR:O	1:4:41:PHE:N	2.13	0.80
1:AF:138:CYS:O	1:AF:139:CYS:SG	2.40	0.80
1:A:105:PRO:CB	1:A:152:ILE:CB	2.59	0.79
1:D:211:PRO:N	1:AK:35:TRP:CZ2	2.49	0.79
1:O:35:TRP:CZ2	1:AB:211:PRO:N	2.49	0.79
1:k:35:TRP:CZ2	1:t:211:PRO:N	2.49	0.79
1:D:138:CYS:O	1:D:139:CYS:SG	2.40	0.79
1:H:138:CYS:O	1:H:139:CYS:SG	2.40	0.79
1:P:37:THR:O	1:P:41:PHE:N	2.13	0.79
1:AB:138:CYS:O	1:AB:139:CYS:SG	2.40	0.79
1:Z:138:CYS:O	1:Z:139:CYS:SG	2.40	0.79
1:Z:211:PRO:N	1:3:35:TRP:CZ2	2.49	0.79
1:d:138:CYS:O	1:d:139:CYS:SG	2.40	0.79
1:p:138:CYS:O	1:p:139:CYS:SG	2.40	0.79
1:t:138:CYS:O	1:t:139:CYS:SG	2.40	0.79
1:6:138:CYS:O	1:6:139:CYS:SG	2.40	0.79
1:AP:138:CYS:O	1:AP:139:CYS:SG	2.40	0.79
1:B:138:CYS:O	1:B:139:CYS:SG	2.40	0.79
1:N:138:CYS:O	1:N:139:CYS:SG	2.40	0.79
1:X:138:CYS:O	1:X:139:CYS:SG	2.40	0.79
1:h:138:CYS:O	1:h:139:CYS:SG	2.40	0.79
1:r:138:CYS:O	1:r:139:CYS:SG	2.40	0.79
1:x:138:CYS:O	1:x:139:CYS:SG	2.40	0.79
1:2:138:CYS:O	1:2:139:CYS:SG	2.40	0.79
1:AH:138:CYS:O	1:AH:139:CYS:SG	2.40	0.79
1:J:138:CYS:O	1:J:139:CYS:SG	2.40	0.79
1:P:138:CYS:O	1:P:139:CYS:SG	2.40	0.79
1:R:138:CYS:O	1:R:139:CYS:SG	2.40	0.79
1:n:138:CYS:O	1:n:139:CYS:SG	2.40	0.79
1:4:138:CYS:O	1:4:139:CYS:SG	2.40	0.79
1:AN:138:CYS:O	1:AN:139:CYS:SG	2.40	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:138:CYS:O	1:AR:139:CYS:SG	2.40	0.79
1:R:37:THR:O	1:R:41:PHE:N	2.16	0.79
1:6:37:THR:O	1:6:41:PHE:N	2.16	0.79
1:T:138:CYS:O	1:T:139:CYS:SG	2.40	0.78
1:8:138:CYS:O	1:8:139:CYS:SG	2.40	0.78
1:l:138:CYS:O	1:l:139:CYS:SG	2.40	0.78
1:b:138:CYS:O	1:b:139:CYS:SG	2.40	0.78
1:AD:138:CYS:O	1:AD:139:CYS:SG	2.40	0.78
1:AL:138:CYS:O	1:AL:139:CYS:SG	2.40	0.78
1:AR:27:THR:O	1:AR:31:SER:N	2.15	0.78
1:r:27:THR:O	1:r:31:SER:N	2.15	0.78
1:AN:37:THR:O	1:AN:41:PHE:N	2.16	0.78
1:n:37:THR:O	1:n:41:PHE:N	2.16	0.78
1:D:37:THR:O	1:D:41:PHE:N	2.17	0.77
1:t:37:THR:O	1:t:41:PHE:N	2.17	0.77
1:L:139:CYS:CA	1:L:147:CYS:SG	2.73	0.77
1:P:139:CYS:CA	1:P:147:CYS:SG	2.73	0.77
1:X:139:CYS:CA	1:X:147:CYS:SG	2.73	0.77
1:b:139:CYS:CA	1:b:147:CYS:SG	2.73	0.77
1:z:139:CYS:CA	1:z:147:CYS:SG	2.73	0.77
1:4:139:CYS:CA	1:4:147:CYS:SG	2.73	0.77
1:H:139:CYS:CA	1:H:147:CYS:SG	2.73	0.77
1:Q:107:CYS:HB3	1:R:105:PRO:CB	2.15	0.77
1:V:139:CYS:CA	1:V:147:CYS:SG	2.73	0.77
1:Z:139:CYS:CA	1:Z:147:CYS:SG	2.73	0.77
1:5:107:CYS:HB3	1:6:105:PRO:CB	2.15	0.77
1:0:139:CYS:CA	1:0:147:CYS:SG	2.73	0.77
1:AB:139:CYS:CA	1:AB:147:CYS:SG	2.73	0.77
1:AD:139:CYS:CA	1:AD:147:CYS:SG	2.73	0.77
1:AM:107:CYS:HB3	1:AN:105:PRO:CB	2.15	0.77
1:P:27:THR:O	1:P:31:SER:N	2.17	0.77
1:m:107:CYS:HB3	1:n:105:PRO:CB	2.15	0.77
1:D:139:CYS:CA	1:D:147:CYS:SG	2.73	0.77
1:N:139:CYS:CA	1:N:147:CYS:SG	2.73	0.77
1:2:139:CYS:CA	1:2:147:CYS:SG	2.73	0.77
1:AB:37:THR:O	1:AB:41:PHE:N	2.17	0.77
1:A:121:CYS:SG	1:A:124:CYS:N	2.58	0.77
1:Z:37:THR:O	1:Z:41:PHE:N	2.17	0.77
1:n:139:CYS:CA	1:n:147:CYS:SG	2.73	0.77
1:t:139:CYS:CA	1:t:147:CYS:SG	2.73	0.77
1:4:27:THR:O	1:4:31:SER:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:139:CYS:CA	1:AN:147:CYS:SG	2.73	0.77
1:R:139:CYS:CA	1:R:147:CYS:SG	2.73	0.77
1:T:139:CYS:CA	1:T:147:CYS:SG	2.73	0.77
1:m:121:CYS:SG	1:m:124:CYS:N	2.58	0.77
1:8:139:CYS:CA	1:8:147:CYS:SG	2.73	0.77
1:AF:139:CYS:CA	1:AF:147:CYS:SG	2.73	0.77
1:AM:121:CYS:SG	1:AM:124:CYS:N	2.58	0.77
1:a:121:CYS:SG	1:a:124:CYS:N	2.58	0.77
1:h:139:CYS:CA	1:h:147:CYS:SG	2.73	0.77
1:6:139:CYS:CA	1:6:147:CYS:SG	2.73	0.77
1:V:27:THR:O	1:V:31:SER:N	2.15	0.76
1:p:139:CYS:CA	1:p:147:CYS:SG	2.73	0.76
1:3:27:THR:O	1:3:31:SER:N	2.17	0.76
1:AH:139:CYS:CA	1:AH:147:CYS:SG	2.73	0.76
1:AP:139:CYS:CA	1:AP:147:CYS:SG	2.73	0.76
1:f:139:CYS:CA	1:f:147:CYS:SG	2.73	0.76
1:AC:121:CYS:SG	1:AC:124:CYS:N	2.58	0.76
1:O:27:THR:O	1:O:31:SER:N	2.17	0.76
1:l:139:CYS:CA	1:l:147:CYS:SG	2.73	0.76
1:AL:139:CYS:CA	1:AL:147:CYS:SG	2.73	0.76
1:S:105:PRO:CB	1:S:152:ILE:CB	2.64	0.76
1:X:37:THR:O	1:X:41:PHE:N	2.18	0.76
1:7:105:PRO:CB	1:7:152:ILE:CB	2.64	0.76
1:0:27:THR:O	1:0:31:SER:N	2.15	0.76
1:B:27:THR:O	1:B:31:SER:N	2.18	0.76
1:B:37:THR:O	1:B:41:PHE:N	2.18	0.76
1:F:139:CYS:CA	1:F:147:CYS:SG	2.73	0.76
1:B:139:CYS:CA	1:B:147:CYS:SG	2.73	0.76
1:j:139:CYS:CA	1:j:147:CYS:SG	2.73	0.76
1:r:139:CYS:CA	1:r:147:CYS:SG	2.73	0.76
1:v:139:CYS:CA	1:v:147:CYS:SG	2.73	0.76
1:AJ:139:CYS:CA	1:AJ:147:CYS:SG	2.73	0.76
1:AR:139:CYS:CA	1:AR:147:CYS:SG	2.73	0.76
1:x:139:CYS:CA	1:x:147:CYS:SG	2.73	0.75
1:J:139:CYS:CA	1:J:147:CYS:SG	2.73	0.75
1:AK:27:THR:O	1:AK:31:SER:N	2.17	0.75
1:d:139:CYS:CA	1:d:147:CYS:SG	2.73	0.75
1:E:121:CYS:SG	1:E:124:CYS:N	2.58	0.75
1:k:27:THR:O	1:k:31:SER:N	2.17	0.75
1:u:121:CYS:SG	1:u:124:CYS:N	2.58	0.75
1:k:121:CYS:SG	1:k:124:CYS:N	2.58	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:121:CYS:SG	1:AK:124:CYS:N	2.58	0.75
1:C:121:CYS:SG	1:C:124:CYS:N	2.58	0.75
1:X:101:GLN:OE1	1:X:101:GLN:N	2.19	0.75
1:s:121:CYS:SG	1:s:124:CYS:N	2.58	0.75
1:w:121:CYS:SG	1:w:124:CYS:N	2.58	0.75
1:I:121:CYS:SG	1:I:124:CYS:N	2.58	0.75
1:o:105:PRO:CB	1:o:152:ILE:CB	2.64	0.75
1:q:121:CYS:SG	1:q:124:CYS:N	2.58	0.75
1:AO:105:PRO:CB	1:AO:152:ILE:CB	2.64	0.75
1:AQ:121:CYS:SG	1:AQ:124:CYS:N	2.58	0.75
1:K:156:TRP:CD1	1:K:156:TRP:O	2.40	0.75
1:M:121:CYS:SG	1:M:124:CYS:N	2.58	0.75
1:W:32:LEU:O	1:W:36:TRP:HD1	1.69	0.75
1:l:121:CYS:SG	1:l:124:CYS:N	2.58	0.75
1:AN:38:SER:O	1:AN:42:LEU:N	2.20	0.75
1:S:121:CYS:SG	1:S:124:CYS:N	2.58	0.75
1:n:38:SER:O	1:n:42:LEU:N	2.20	0.75
1:y:156:TRP:CD1	1:y:156:TRP:O	2.40	0.75
1:AL:27:THR:O	1:AL:31:SER:N	2.17	0.75
1:A:32:LEU:O	1:A:36:TRP:HD1	1.69	0.74
1:B:101:GLN:OE1	1:B:101:GLN:N	2.19	0.74
1:7:121:CYS:SG	1:7:124:CYS:N	2.58	0.74
1:l:27:THR:O	1:l:31:SER:N	2.17	0.74
1:o:121:CYS:SG	1:o:124:CYS:N	2.58	0.74
1:AO:121:CYS:SG	1:AO:124:CYS:N	2.58	0.74
1:R:38:SER:O	1:R:42:LEU:N	2.20	0.74
1:Y:106:VAL:CB	1:Y:158:PHE:O	2.36	0.74
1:6:38:SER:O	1:6:42:LEU:N	2.20	0.74
1:3:121:CYS:SG	1:3:124:CYS:N	2.58	0.74
1:AA:106:VAL:CB	1:AA:158:PHE:O	2.36	0.74
1:W:121:CYS:SG	1:W:124:CYS:N	2.58	0.74
1:g:156:TRP:O	1:g:156:TRP:CD1	2.40	0.74
1:x:98:LEU:O	1:x:101:GLN:HG2	1.88	0.74
1:AG:156:TRP:O	1:AG:156:TRP:CD1	2.40	0.74
1:J:98:LEU:O	1:J:101:GLN:HG2	1.88	0.74
1:b:27:THR:O	1:b:31:SER:N	2.19	0.74
1:f:98:LEU:O	1:f:101:GLN:HG2	1.88	0.74
1:O:121:CYS:SG	1:O:124:CYS:N	2.58	0.73
1:AD:27:THR:O	1:AD:31:SER:N	2.19	0.73
1:AF:98:LEU:O	1:AF:101:GLN:HG2	1.88	0.73
1:A:160:LYS:HA	1:A:163:TRP:NE1	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:121:CYS:SG	1:g:124:CYS:N	2.58	0.73
1:k:35:TRP:CH2	1:t:208:ILE:HA	2.24	0.73
1:AG:121:CYS:SG	1:AG:124:CYS:N	2.58	0.73
1:C:106:VAL:CB	1:C:158:PHE:O	2.36	0.73
1:D:208:ILE:HA	1:AK:35:TRP:CH2	2.24	0.73
1:Y:162:LEU:HA	1:Y:166:ALA:HB3	1.71	0.73
1:i:121:CYS:SG	1:i:124:CYS:N	2.58	0.73
1:s:106:VAL:CB	1:s:158:PHE:O	2.36	0.73
1:AA:162:LEU:HA	1:AA:166:ALA:HB3	1.71	0.73
1:AC:98:LEU:O	1:AC:101:GLN:HB2	1.88	0.73
1:AI:121:CYS:SG	1:AI:124:CYS:N	2.58	0.73
1:a:98:LEU:O	1:a:101:GLN:HB2	1.88	0.73
1:AO:27:THR:O	1:AO:31:SER:N	2.20	0.73
1:U:121:CYS:SG	1:U:124:CYS:N	2.58	0.73
1:c:121:CYS:SG	1:c:124:CYS:N	2.58	0.73
1:V:37:THR:O	1:V:41:PHE:N	2.22	0.73
1:o:27:THR:O	1:o:31:SER:N	2.20	0.73
1:9:121:CYS:SG	1:9:124:CYS:N	2.58	0.73
1:0:37:THR:O	1:0:41:PHE:N	2.22	0.73
1:AH:98:LEU:C	1:AH:101:GLN:HG2	2.11	0.73
1:E:27:THR:O	1:E:31:SER:N	2.16	0.73
1:h:98:LEU:C	1:h:101:GLN:HG2	2.11	0.73
1:L:98:LEU:C	1:L:101:GLN:HG2	2.11	0.72
1:E:98:LEU:O	1:E:101:GLN:HB2	1.88	0.72
1:G:121:CYS:SG	1:G:124:CYS:N	2.58	0.72
1:K:121:CYS:SG	1:K:124:CYS:N	2.58	0.72
1:O:35:TRP:CH2	1:AB:208:ILE:HA	2.24	0.72
1:y:121:CYS:SG	1:y:124:CYS:N	2.58	0.72
1:Z:208:ILE:HA	1:3:35:TRP:CH2	2.24	0.72
1:u:27:THR:O	1:u:31:SER:N	2.16	0.72
1:u:98:LEU:O	1:u:101:GLN:HB2	1.88	0.72
1:z:98:LEU:C	1:z:101:GLN:HG2	2.11	0.72
1:Y:121:CYS:SG	1:Y:124:CYS:N	2.58	0.72
1:e:121:CYS:SG	1:e:124:CYS:N	2.58	0.72
1:AE:121:CYS:SG	1:AE:124:CYS:N	2.58	0.72
1:Q:121:CYS:SG	1:Q:124:CYS:N	2.58	0.72
1:5:121:CYS:SG	1:5:124:CYS:N	2.58	0.72
1:AN:105:PRO:O	1:AN:107:CYS:N	2.23	0.72
1:W:160:LYS:HA	1:W:163:TRP:NE1	2.03	0.72
1:a:27:THR:O	1:a:31:SER:N	2.16	0.72
1:n:105:PRO:O	1:n:107:CYS:N	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:121:CYS:SG	1:AA:124:CYS:N	2.58	0.72
1:v:27:THR:O	1:v:31:SER:N	2.19	0.72
1:F:27:THR:O	1:F:31:SER:N	2.19	0.72
1:b:101:GLN:OE1	1:b:101:GLN:N	2.20	0.72
1:AD:101:GLN:OE1	1:AD:101:GLN:N	2.20	0.72
1:AR:37:THR:O	1:AR:41:PHE:N	2.22	0.72
1:r:37:THR:O	1:r:41:PHE:N	2.22	0.72
1:s:27:THR:O	1:s:31:SER:N	2.18	0.71
1:AC:27:THR:O	1:AC:31:SER:N	2.16	0.71
1:C:162:LEU:HA	1:C:166:ALA:HB3	1.71	0.71
1:X:27:THR:O	1:X:31:SER:N	2.18	0.71
1:C:27:THR:O	1:C:31:SER:N	2.18	0.71
1:N:56:PRO:C	1:N:58:SER:H	1.98	0.71
1:s:162:LEU:HA	1:s:166:ALA:HB3	1.71	0.71
1:2:56:PRO:C	1:2:58:SER:H	1.98	0.71
1:n:27:THR:O	1:n:31:SER:N	2.18	0.71
1:A:37:THR:O	1:A:41:PHE:N	2.23	0.71
1:r:32:LEU:HA	1:r:35:TRP:HD1	1.54	0.71
1:6:105:PRO:O	1:6:107:CYS:N	2.23	0.71
1:AN:27:THR:O	1:AN:31:SER:N	2.18	0.71
1:AJ:98:LEU:HA	1:AJ:101:GLN:CD	2.16	0.71
1:AR:32:LEU:HA	1:AR:35:TRP:HD1	1.54	0.71
1:R:105:PRO:O	1:R:107:CYS:N	2.23	0.71
1:j:98:LEU:HA	1:j:101:GLN:CD	2.16	0.71
1:AJ:56:PRO:C	1:AJ:58:SER:H	1.98	0.71
1:0:32:LEU:HA	1:0:35:TRP:HD1	1.54	0.71
1:W:37:THR:O	1:W:41:PHE:N	2.23	0.70
1:j:56:PRO:C	1:j:58:SER:H	1.98	0.70
1:AA:27:THR:O	1:AA:31:SER:N	2.18	0.70
1:H:16:GLN:O	1:H:19:PHE:HB3	1.91	0.70
1:V:32:LEU:HA	1:V:35:TRP:HD1	1.54	0.70
1:Y:27:THR:O	1:Y:31:SER:N	2.18	0.70
1:d:16:GLN:O	1:d:19:PHE:HB3	1.91	0.70
1:N:98:LEU:HA	1:N:101:GLN:CD	2.16	0.70
1:2:98:LEU:HA	1:2:101:GLN:CD	2.16	0.70
1:AQ:105:PRO:CB	1:AQ:152:ILE:CB	2.70	0.70
1:q:105:PRO:CB	1:q:152:ILE:CB	2.70	0.69
1:l:48:CYS:N	1:l:60:HIS:O	2.26	0.69
1:AL:48:CYS:N	1:AL:60:HIS:O	2.26	0.69
1:E:209:LEU:O	1:E:213:LEU:N	2.25	0.69
1:X:160:LYS:HA	1:X:163:TRP:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AC:209:LEU:O	1:AC:213:LEU:N	2.25	0.69
1:a:209:LEU:O	1:a:213:LEU:N	2.25	0.69
1:u:209:LEU:O	1:u:213:LEU:N	2.25	0.69
1:D:207:SER:C	1:AK:35:TRP:CH2	2.65	0.69
1:7:27:THR:O	1:7:31:SER:N	2.20	0.69
1:4:48:CYS:N	1:4:60:HIS:O	2.26	0.69
1:P:48:CYS:N	1:P:60:HIS:O	2.26	0.69
1:U:105:PRO:CB	1:U:152:ILE:CB	2.70	0.69
1:B:160:LYS:HA	1:B:163:TRP:HB3	1.73	0.69
1:S:27:THR:O	1:S:31:SER:N	2.20	0.69
1:9:105:PRO:CB	1:9:152:ILE:CB	2.70	0.69
1:F:156:TRP:O	1:F:158:PHE:N	2.26	0.69
1:R:106:VAL:CB	1:R:157:ALA:HB3	2.18	0.69
1:6:106:VAL:CB	1:6:157:ALA:HB3	2.18	0.69
1:b:156:TRP:O	1:b:158:PHE:N	2.26	0.68
1:v:156:TRP:O	1:v:158:PHE:N	2.26	0.68
1:k:35:TRP:CH2	1:t:207:SER:C	2.65	0.68
1:AD:156:TRP:O	1:AD:158:PHE:N	2.26	0.68
1:F:35:TRP:HH2	1:AM:208:ILE:HA	1.58	0.68
1:7:37:THR:O	1:7:41:PHE:N	2.23	0.68
1:Z:211:PRO:CB	1:3:35:TRP:CZ2	2.76	0.68
1:m:208:ILE:HA	1:v:35:TRP:HH2	1.58	0.68
1:O:35:TRP:CZ2	1:AB:211:PRO:CB	2.76	0.68
1:k:35:TRP:CZ2	1:t:211:PRO:CB	2.76	0.68
1:S:37:THR:O	1:S:41:PHE:N	2.23	0.68
1:D:211:PRO:CB	1:AK:35:TRP:CZ2	2.76	0.68
1:G:37:THR:O	1:G:41:PHE:N	2.24	0.68
1:X:101:GLN:HG2	1:X:103:MET:H	1.59	0.68
1:W:38:SER:O	1:W:42:LEU:N	2.20	0.67
1:k:35:TRP:NE1	1:t:211:PRO:CA	2.47	0.67
1:n:105:PRO:C	1:n:107:CYS:H	2.02	0.67
1:6:105:PRO:C	1:6:107:CYS:H	2.02	0.67
1:I:37:THR:O	1:I:41:PHE:N	2.27	0.67
1:R:105:PRO:C	1:R:107:CYS:H	2.02	0.67
1:w:37:THR:O	1:w:41:PHE:N	2.27	0.67
1:AN:105:PRO:C	1:AN:107:CYS:H	2.02	0.67
1:D:9:LEU:O	1:D:13:LEU:N	2.25	0.67
1:B:101:GLN:HG2	1:B:103:MET:H	1.59	0.67
1:m:27:THR:O	1:m:31:SER:N	2.26	0.67
1:t:9:LEU:O	1:t:13:LEU:N	2.25	0.67
1:F:101:GLN:OE1	1:F:101:GLN:N	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:35:TRP:NE1	1:AB:211:PRO:CA	2.47	0.67
1:Z:211:PRO:CA	1:3:35:TRP:NE1	2.47	0.67
1:b:35:TRP:HH2	1:5:208:ILE:HA	1.58	0.67
1:v:101:GLN:OE1	1:v:101:GLN:N	2.20	0.67
1:Q:208:ILE:HA	1:AD:35:TRP:HH2	1.58	0.67
1:AK:106:VAL:CB	1:AK:158:PHE:CB	2.73	0.67
1:k:106:VAL:CB	1:k:158:PHE:CB	2.73	0.66
1:AM:27:THR:O	1:AM:31:SER:N	2.26	0.66
1:C:37:THR:O	1:C:41:PHE:N	2.23	0.66
1:s:37:THR:O	1:s:41:PHE:N	2.23	0.66
1:D:32:LEU:HA	1:D:35:TRP:HD1	1.61	0.66
1:t:32:LEU:HA	1:t:35:TRP:HD1	1.61	0.66
1:AE:37:THR:O	1:AE:41:PHE:N	2.27	0.66
1:A:38:SER:O	1:A:42:LEU:N	2.20	0.66
1:D:27:THR:O	1:D:31:SER:N	2.16	0.66
1:t:27:THR:O	1:t:31:SER:N	2.16	0.66
1:Z:32:LEU:HA	1:Z:35:TRP:HD1	1.61	0.66
1:e:37:THR:O	1:e:41:PHE:N	2.27	0.66
1:AB:32:LEU:HA	1:AB:35:TRP:HD1	1.61	0.66
1:O:106:VAL:CB	1:O:158:PHE:CB	2.73	0.66
1:R:27:THR:O	1:R:31:SER:N	2.18	0.66
1:Z:9:LEU:O	1:Z:13:LEU:N	2.25	0.66
1:3:106:VAL:CB	1:3:158:PHE:CB	2.73	0.66
1:O:105:PRO:CB	1:O:152:ILE:CB	2.74	0.66
1:W:27:THR:O	1:W:31:SER:N	2.18	0.66
1:3:105:PRO:CB	1:3:152:ILE:CB	2.74	0.66
1:AA:37:THR:O	1:AA:41:PHE:N	2.23	0.66
1:J:98:LEU:O	1:J:101:GLN:CG	2.44	0.66
1:Y:37:THR:O	1:Y:41:PHE:N	2.23	0.66
1:x:98:LEU:O	1:x:101:GLN:CG	2.44	0.66
1:AO:37:THR:O	1:AO:41:PHE:N	2.23	0.66
1:V:38:SER:O	1:V:42:LEU:N	2.30	0.65
1:0:38:SER:O	1:0:42:LEU:N	2.30	0.65
1:AB:9:LEU:O	1:AB:13:LEU:N	2.25	0.65
1:AR:38:SER:O	1:AR:42:LEU:N	2.30	0.65
1:V:48:CYS:N	1:V:60:HIS:O	2.23	0.65
1:o:37:THR:O	1:o:41:PHE:N	2.23	0.65
1:r:38:SER:O	1:r:42:LEU:N	2.30	0.65
1:6:27:THR:O	1:6:31:SER:N	2.18	0.65
1:AF:98:LEU:O	1:AF:101:GLN:CG	2.44	0.65
1:f:98:LEU:O	1:f:101:GLN:CG	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:48:CYS:N	1:0:60:HIS:O	2.23	0.65
1:r:48:CYS:N	1:r:60:HIS:O	2.23	0.65
1:k:105:PRO:CB	1:k:152:ILE:CB	2.74	0.65
1:AK:105:PRO:CB	1:AK:152:ILE:CB	2.74	0.65
1:t:48:CYS:H	1:t:62:PRO:HA	1.61	0.65
1:AQ:209:LEU:O	1:AQ:213:LEU:N	2.29	0.64
1:AR:48:CYS:N	1:AR:60:HIS:O	2.23	0.64
1:D:48:CYS:H	1:D:62:PRO:HA	1.61	0.64
1:U:209:LEU:O	1:U:213:LEU:N	2.29	0.64
1:q:209:LEU:O	1:q:213:LEU:N	2.29	0.64
1:t:66:PRO:O	1:t:69:CYS:N	2.29	0.64
1:9:209:LEU:O	1:9:213:LEU:N	2.29	0.64
1:AB:48:CYS:H	1:AB:62:PRO:HA	1.61	0.64
1:D:66:PRO:O	1:D:69:CYS:N	2.29	0.64
1:c:179:PHE:HA	1:c:182:TRP:CD1	2.33	0.64
1:Z:48:CYS:H	1:Z:62:PRO:HA	1.61	0.64
1:Z:207:SER:C	1:3:35:TRP:CH2	2.65	0.64
1:j:37:THR:O	1:j:41:PHE:N	2.26	0.64
1:M:47:VAL:HA	1:M:61:SER:HA	1.80	0.64
1:c:185:GLY:O	1:c:186:LEU:C	2.40	0.64
1:j:48:CYS:HB3	1:j:60:HIS:HA	1.80	0.64
1:m:101:GLN:HG2	1:m:103:MET:H	1.63	0.64
1:AJ:48:CYS:HB3	1:AJ:60:HIS:HA	1.80	0.64
1:G:179:PHE:HA	1:G:182:TRP:CD1	2.33	0.64
1:Q:27:THR:O	1:Q:31:SER:N	2.26	0.64
1:Q:101:GLN:HG2	1:Q:103:MET:H	1.63	0.64
1:1:47:VAL:HA	1:1:61:SER:HA	1.80	0.64
1:AM:101:GLN:HG2	1:AM:103:MET:H	1.63	0.64
1:q:155:SER:C	1:q:157:ALA:H	2.06	0.64
1:5:27:THR:O	1:5:31:SER:N	2.26	0.64
1:5:101:GLN:HG2	1:5:103:MET:H	1.63	0.64
1:AQ:155:SER:C	1:AQ:157:ALA:H	2.06	0.64
1:T:48:CYS:N	1:T:60:HIS:O	2.30	0.64
1:AJ:37:THR:O	1:AJ:41:PHE:N	2.26	0.64
1:A:27:THR:O	1:A:31:SER:N	2.18	0.63
1:O:41:PHE:O	1:O:42:LEU:C	2.41	0.63
1:T:27:THR:O	1:T:31:SER:N	2.23	0.63
1:p:27:THR:O	1:p:31:SER:N	2.23	0.63
1:8:48:CYS:N	1:8:60:HIS:O	2.30	0.63
1:AE:209:LEU:O	1:AE:213:LEU:N	2.31	0.63
1:e:209:LEU:O	1:e:213:LEU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:41:PHE:O	1:3:42:LEU:C	2.41	0.63
1:AP:27:THR:O	1:AP:31:SER:N	2.23	0.63
1:N:48:CYS:HB3	1:N:60:HIS:HA	1.80	0.63
1:2:48:CYS:HB3	1:2:60:HIS:HA	1.80	0.63
1:AI:47:VAL:HA	1:AI:61:SER:HA	1.80	0.63
1:N:37:THR:O	1:N:41:PHE:N	2.26	0.63
1:O:35:TRP:CH2	1:AB:207:SER:C	2.65	0.63
1:c:37:THR:O	1:c:41:PHE:N	2.24	0.63
1:i:47:VAL:HA	1:i:61:SER:HA	1.80	0.63
1:n:106:VAL:CB	1:n:157:ALA:HB3	2.18	0.63
1:8:27:THR:O	1:8:31:SER:N	2.23	0.63
1:AN:106:VAL:CB	1:AN:157:ALA:HB3	2.18	0.63
1:2:37:THR:O	1:2:41:PHE:N	2.26	0.63
1:AP:48:CYS:N	1:AP:60:HIS:O	2.30	0.63
1:w:209:LEU:O	1:w:213:LEU:N	2.31	0.63
1:I:209:LEU:O	1:I:213:LEU:N	2.31	0.63
1:p:48:CYS:N	1:p:60:HIS:O	2.30	0.63
1:AK:41:PHE:O	1:AK:42:LEU:C	2.41	0.62
1:k:41:PHE:O	1:k:42:LEU:C	2.41	0.62
1:Z:27:THR:O	1:Z:31:SER:N	2.16	0.62
1:a:61:SER:O	1:a:65:CYS:N	2.32	0.62
1:AC:61:SER:O	1:AC:65:CYS:N	2.32	0.62
1:E:61:SER:O	1:E:65:CYS:N	2.32	0.62
1:G:185:GLY:O	1:G:186:LEU:C	2.40	0.62
1:g:105:PRO:CB	1:g:152:ILE:CB	2.78	0.62
1:u:61:SER:O	1:u:65:CYS:N	2.32	0.62
1:AG:105:PRO:CB	1:AG:152:ILE:CB	2.78	0.62
1:X:106:VAL:CB	1:X:158:PHE:HA	2.30	0.62
1:P:212:PHE:O	1:P:216:LEU:N	2.32	0.62
1:U:155:SER:C	1:U:157:ALA:H	2.06	0.62
1:4:212:PHE:O	1:4:216:LEU:N	2.32	0.62
1:AB:27:THR:O	1:AB:31:SER:N	2.16	0.62
1:AL:212:PHE:O	1:AL:216:LEU:N	2.32	0.62
1:l:212:PHE:O	1:l:216:LEU:N	2.32	0.62
1:P:99:ASP:O	1:P:104:LEU:CB	2.48	0.62
1:4:99:ASP:O	1:4:104:LEU:CB	2.48	0.62
1:9:155:SER:C	1:9:157:ALA:H	2.06	0.62
1:B:106:VAL:CB	1:B:158:PHE:HA	2.30	0.61
1:D:48:CYS:SG	1:D:65:CYS:N	2.73	0.61
1:b:179:PHE:HA	1:b:182:TRP:NE1	2.15	0.61
1:l:99:ASP:O	1:l:104:LEU:CB	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:48:CYS:SG	1:t:65:CYS:N	2.73	0.61
1:AB:66:PRO:O	1:AB:69:CYS:N	2.29	0.61
1:AD:179:PHE:HA	1:AD:182:TRP:NE1	2.15	0.61
1:U:55:SER:O	1:U:57:ILE:N	2.34	0.61
1:9:55:SER:O	1:9:57:ILE:N	2.34	0.61
1:Z:48:CYS:SG	1:Z:65:CYS:N	2.73	0.61
1:AL:99:ASP:O	1:AL:104:LEU:CB	2.48	0.61
1:K:105:PRO:CB	1:K:152:ILE:CB	2.78	0.61
1:Z:66:PRO:O	1:Z:69:CYS:N	2.29	0.61
1:y:105:PRO:CB	1:y:152:ILE:CB	2.78	0.61
1:AB:48:CYS:SG	1:AB:65:CYS:N	2.73	0.61
1:W:106:VAL:CB	1:W:158:PHE:CA	2.76	0.61
1:d:198:MET:O	1:d:202:GLY:N	2.33	0.60
1:AR:8:PHE:O	1:AR:12:LEU:N	2.33	0.60
1:A:106:VAL:CB	1:A:158:PHE:CA	2.76	0.60
1:F:179:PHE:HA	1:F:182:TRP:NE1	2.15	0.60
1:P:208:ILE:HA	1:e:35:TRP:HH2	1.66	0.60
1:r:8:PHE:O	1:r:12:LEU:N	2.33	0.60
1:v:179:PHE:HA	1:v:182:TRP:NE1	2.15	0.60
1:4:208:ILE:HA	1:AE:35:TRP:HH2	1.66	0.60
1:P:38:SER:O	1:P:42:LEU:N	2.35	0.60
1:4:38:SER:O	1:4:42:LEU:N	2.35	0.60
1:I:35:TRP:HH2	1:l:208:ILE:HA	1.66	0.60
1:w:35:TRP:HH2	1:AL:208:ILE:HA	1.66	0.60
1:H:198:MET:O	1:H:202:GLY:N	2.33	0.60
1:R:179:PHE:HA	1:R:182:TRP:CE2	2.37	0.60
1:6:179:PHE:HA	1:6:182:TRP:CE2	2.37	0.60
1:d:17:ALA:O	1:d:20:PHE:N	2.35	0.59
1:A:32:LEU:O	1:A:36:TRP:CD1	2.53	0.59
1:H:201:TRP:O	1:H:205:LEU:N	2.26	0.59
1:AQ:55:SER:O	1:AQ:57:ILE:N	2.34	0.59
1:H:17:ALA:O	1:H:20:PHE:N	2.35	0.59
1:i:209:LEU:O	1:i:213:LEU:N	2.35	0.59
1:AI:209:LEU:O	1:AI:213:LEU:N	2.35	0.59
1:q:55:SER:O	1:q:57:ILE:N	2.34	0.59
1:AJ:179:PHE:HA	1:AJ:182:TRP:CD1	2.37	0.59
1:B:35:TRP:HH2	1:J:208:ILE:HA	1.67	0.59
1:X:35:TRP:HH2	1:f:208:ILE:HA	1.67	0.59
1:j:179:PHE:HA	1:j:182:TRP:CD1	2.37	0.59
1:S:209:LEU:O	1:S:213:LEU:N	2.31	0.59
1:W:32:LEU:O	1:W:36:TRP:CD1	2.53	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:ARG:O	1:L:76:CYS:N	2.36	0.59
1:h:73:ARG:O	1:h:76:CYS:N	2.36	0.59
1:n:179:PHE:HA	1:n:182:TRP:CE2	2.37	0.59
1:AE:27:THR:O	1:AE:31:SER:N	2.23	0.59
1:AH:73:ARG:O	1:AH:76:CYS:N	2.36	0.59
1:AN:179:PHE:HA	1:AN:182:TRP:CE2	2.37	0.59
1:z:73:ARG:O	1:z:76:CYS:N	2.36	0.59
1:1:209:LEU:O	1:1:213:LEU:N	2.35	0.59
1:7:209:LEU:O	1:7:213:LEU:N	2.31	0.59
1:I:199:TRP:CG	1:I:200:TYR:H	2.21	0.59
1:J:201:TRP:O	1:J:205:LEU:N	2.25	0.59
1:M:209:LEU:O	1:M:213:LEU:N	2.35	0.59
1:w:199:TRP:CG	1:w:200:TYR:H	2.21	0.59
1:x:201:TRP:O	1:x:205:LEU:N	2.25	0.58
1:Q:208:ILE:HA	1:AD:35:TRP:CH2	2.37	0.58
1:e:27:THR:O	1:e:31:SER:N	2.23	0.58
1:W:101:GLN:HG2	1:W:103:MET:H	1.68	0.58
1:b:35:TRP:CH2	1:5:208:ILE:HA	2.37	0.58
1:l:38:SER:O	1:l:42:LEU:N	2.35	0.58
1:AL:38:SER:O	1:AL:42:LEU:N	2.35	0.58
1:N:179:PHE:HA	1:N:182:TRP:CD1	2.37	0.58
1:w:27:THR:O	1:w:31:SER:N	2.23	0.58
1:R:35:TRP:HH2	1:AA:208:ILE:HA	1.68	0.58
1:e:199:TRP:CG	1:e:200:TYR:H	2.21	0.58
1:m:208:ILE:HA	1:v:35:TRP:CH2	2.37	0.58
1:2:179:PHE:HA	1:2:182:TRP:CD1	2.37	0.58
1:AE:199:TRP:CG	1:AE:200:TYR:H	2.21	0.58
1:F:35:TRP:CH2	1:AM:208:ILE:HA	2.37	0.58
1:H:100:TYR:HD1	1:H:156:TRP:HB3	1.69	0.58
1:W:160:LYS:HA	1:W:163:TRP:CD1	2.38	0.58
1:Y:208:ILE:HA	1:6:35:TRP:HH2	1.68	0.58
1:M:100:TYR:CD2	1:M:100:TYR:O	2.56	0.58
1:d:100:TYR:HD1	1:d:156:TRP:HB3	1.69	0.58
1:1:100:TYR:O	1:1:100:TYR:CD2	2.56	0.58
1:AI:100:TYR:CD2	1:AI:100:TYR:O	2.56	0.58
1:I:27:THR:O	1:I:31:SER:N	2.23	0.58
1:i:100:TYR:O	1:i:100:TYR:CD2	2.56	0.58
1:A:101:GLN:HG2	1:A:103:MET:H	1.68	0.57
1:A:160:LYS:HA	1:A:163:TRP:CD1	2.38	0.57
1:C:208:ILE:HA	1:AN:35:TRP:HH2	1.68	0.57
1:n:35:TRP:HH2	1:s:208:ILE:HA	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:209:LEU:O	1:o:213:LEU:N	2.31	0.57
1:AN:8:PHE:O	1:AN:12:LEU:N	2.36	0.57
1:W:200:TYR:C	1:W:202:GLY:H	2.12	0.57
1:n:8:PHE:O	1:n:12:LEU:N	2.36	0.57
1:AF:38:SER:O	1:AF:42:LEU:HA	2.04	0.57
1:B:157:ALA:O	1:B:159:GLY:N	2.38	0.57
1:f:38:SER:O	1:f:42:LEU:HA	2.04	0.57
1:AO:209:LEU:O	1:AO:213:LEU:N	2.31	0.57
1:A:200:TYR:C	1:A:202:GLY:H	2.12	0.57
1:x:67:PRO:HA	1:x:72:TYR:HA	1.87	0.57
1:0:8:PHE:O	1:0:12:LEU:N	2.33	0.57
1:J:67:PRO:HA	1:J:72:TYR:HA	1.87	0.57
1:Q:72:TYR:O	1:Q:76:CYS:N	2.25	0.57
1:V:8:PHE:O	1:V:12:LEU:N	2.33	0.57
1:M:100:TYR:O	1:M:100:TYR:CG	2.59	0.56
1:Z:38:SER:O	1:Z:42:LEU:N	2.39	0.56
1:5:72:TYR:O	1:5:76:CYS:N	2.25	0.56
1:AB:38:SER:O	1:AB:42:LEU:N	2.39	0.56
1:1:100:TYR:O	1:1:100:TYR:CG	2.59	0.56
1:K:37:THR:O	1:K:41:PHE:N	2.39	0.56
1:x:38:SER:O	1:x:42:LEU:HA	2.04	0.56
1:y:37:THR:O	1:y:41:PHE:N	2.39	0.56
1:AK:179:PHE:HA	1:AK:182:TRP:CD1	2.40	0.56
1:D:38:SER:O	1:D:42:LEU:N	2.39	0.56
1:K:156:TRP:O	1:K:156:TRP:CG	2.58	0.56
1:O:179:PHE:HA	1:O:182:TRP:CD1	2.40	0.56
1:k:179:PHE:HA	1:k:182:TRP:CD1	2.40	0.56
1:J:38:SER:O	1:J:42:LEU:HA	2.04	0.56
1:g:37:THR:O	1:g:41:PHE:N	2.39	0.56
1:i:100:TYR:O	1:i:100:TYR:CG	2.59	0.56
1:t:38:SER:O	1:t:42:LEU:N	2.39	0.56
1:y:156:TRP:O	1:y:156:TRP:CG	2.58	0.56
1:AG:37:THR:O	1:AG:41:PHE:N	2.39	0.56
1:3:179:PHE:HA	1:3:182:TRP:CD1	2.40	0.56
1:AI:100:TYR:O	1:AI:100:TYR:CG	2.59	0.56
1:R:36:TRP:O	1:R:40:ASN:N	2.35	0.56
1:AJ:98:LEU:HA	1:AJ:101:GLN:HG2	1.88	0.56
1:X:157:ALA:O	1:X:159:GLY:N	2.38	0.56
1:j:98:LEU:HA	1:j:101:GLN:HG2	1.88	0.56
1:AF:67:PRO:HA	1:AF:72:TYR:HA	1.87	0.56
1:L:106:VAL:CB	1:L:157:ALA:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:106:VAL:CB	1:c:161:PHE:CA	2.81	0.55
1:f:67:PRO:HA	1:f:72:TYR:HA	1.87	0.55
1:z:106:VAL:CB	1:z:157:ALA:HA	2.36	0.55
1:6:36:TRP:O	1:6:40:ASN:N	2.35	0.55
1:AK:48:CYS:N	1:AK:60:HIS:O	2.32	0.55
1:g:156:TRP:O	1:g:156:TRP:CG	2.58	0.55
1:AG:156:TRP:O	1:AG:156:TRP:CG	2.58	0.55
1:Z:162:LEU:O	1:Z:166:ALA:N	2.34	0.55
1:f:179:PHE:HA	1:f:182:TRP:CD1	2.42	0.55
1:AF:179:PHE:HA	1:AF:182:TRP:CD1	2.42	0.55
1:E:196:TRP:HA	1:E:199:TRP:HB3	1.88	0.55
1:T:37:THR:O	1:T:41:PHE:N	2.29	0.55
1:Z:100:TYR:O	1:Z:102:GLY:N	2.38	0.55
1:8:37:THR:O	1:8:41:PHE:N	2.29	0.55
1:AI:157:ALA:O	1:AI:158:PHE:C	2.49	0.55
1:k:48:CYS:N	1:k:60:HIS:O	2.32	0.55
1:AB:100:TYR:O	1:AB:102:GLY:N	2.38	0.55
1:h:106:VAL:CB	1:h:157:ALA:HA	2.36	0.55
1:AB:162:LEU:O	1:AB:166:ALA:N	2.34	0.55
1:AH:106:VAL:CB	1:AH:157:ALA:HA	2.36	0.55
1:d:35:TRP:CH2	1:v:207:SER:C	2.64	0.55
1:H:35:TRP:CH2	1:AD:207:SER:C	2.64	0.55
1:G:106:VAL:CB	1:G:161:PHE:CA	2.81	0.54
1:2:56:PRO:C	1:2:58:SER:N	2.65	0.54
1:J:179:PHE:HA	1:J:182:TRP:CD1	2.42	0.54
1:N:56:PRO:C	1:N:58:SER:N	2.65	0.54
1:u:196:TRP:HA	1:u:199:TRP:HB3	1.89	0.54
1:S:160:LYS:HA	1:S:163:TRP:CD1	2.42	0.54
1:x:179:PHE:HA	1:x:182:TRP:CD1	2.42	0.54
1:N:98:LEU:HA	1:N:101:GLN:HG2	1.88	0.54
1:p:37:THR:O	1:p:41:PHE:N	2.29	0.54
1:2:98:LEU:HA	1:2:101:GLN:HG2	1.88	0.54
1:AC:157:ALA:O	1:AC:161:PHE:N	2.35	0.54
1:d:201:TRP:O	1:d:205:LEU:N	2.26	0.54
1:o:160:LYS:HA	1:o:163:TRP:CD1	2.42	0.54
1:7:160:LYS:HA	1:7:163:TRP:CD1	2.42	0.54
1:AO:160:LYS:HA	1:AO:163:TRP:CD1	2.42	0.54
1:a:157:ALA:O	1:a:161:PHE:N	2.35	0.54
1:d:100:TYR:CD1	1:d:156:TRP:HB3	2.42	0.54
1:n:32:LEU:HA	1:n:35:TRP:HB2	1.90	0.54
1:w:69:CYS:O	1:w:71:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:32:LEU:HA	1:AN:35:TRP:HB2	1.90	0.54
1:H:100:TYR:CD1	1:H:156:TRP:HB3	2.42	0.54
1:I:69:CYS:O	1:I:71:GLY:N	2.41	0.54
1:R:8:PHE:O	1:R:12:LEU:N	2.36	0.54
1:a:196:TRP:HA	1:a:199:TRP:HB3	1.89	0.54
1:6:8:PHE:O	1:6:12:LEU:N	2.36	0.54
1:D:100:TYR:O	1:D:102:GLY:N	2.38	0.54
1:D:179:PHE:HA	1:D:182:TRP:NE1	2.23	0.54
1:D:208:ILE:CA	1:AK:35:TRP:CH2	2.91	0.54
1:R:105:PRO:C	1:R:107:CYS:N	2.66	0.54
1:k:35:TRP:CH2	1:t:208:ILE:CA	2.91	0.54
1:t:162:LEU:O	1:t:166:ALA:N	2.34	0.54
1:t:179:PHE:HA	1:t:182:TRP:NE1	2.23	0.54
1:AP:37:THR:O	1:AP:41:PHE:N	2.29	0.54
1:6:105:PRO:C	1:6:107:CYS:N	2.66	0.54
1:D:162:LEU:O	1:D:166:ALA:N	2.34	0.53
1:D:211:PRO:CA	1:AK:35:TRP:NE1	2.47	0.53
1:t:100:TYR:O	1:t:102:GLY:N	2.38	0.53
1:AB:179:PHE:HA	1:AB:182:TRP:NE1	2.23	0.53
1:Y:57:ILE:O	1:Y:59:ASN:N	2.42	0.53
1:Z:179:PHE:HA	1:Z:182:TRP:NE1	2.23	0.53
1:e:199:TRP:CD1	1:e:200:TYR:H	2.26	0.53
1:k:35:TRP:CZ2	1:t:207:SER:O	2.61	0.53
1:AC:196:TRP:HA	1:AC:199:TRP:HB3	1.90	0.53
1:D:207:SER:O	1:AK:35:TRP:CZ2	2.61	0.53
1:AA:57:ILE:O	1:AA:59:ASN:N	2.42	0.53
1:AE:199:TRP:CD1	1:AE:200:TYR:H	2.26	0.53
1:s:57:ILE:O	1:s:59:ASN:N	2.42	0.53
1:AN:36:TRP:O	1:AN:40:ASN:N	2.35	0.53
1:C:57:ILE:O	1:C:59:ASN:N	2.42	0.53
1:n:36:TRP:O	1:n:40:ASN:N	2.35	0.53
1:l:179:PHE:HA	1:l:182:TRP:NE1	2.24	0.53
1:M:179:PHE:HA	1:M:182:TRP:NE1	2.24	0.53
1:Q:212:PHE:O	1:Q:216:LEU:N	2.36	0.53
1:AD:212:PHE:O	1:AD:216:LEU:N	2.41	0.53
1:D:179:PHE:HA	1:D:182:TRP:CD1	2.44	0.53
1:W:179:PHE:HA	1:W:182:TRP:CD1	2.44	0.53
1:b:212:PHE:O	1:b:216:LEU:N	2.41	0.53
1:E:157:ALA:O	1:E:161:PHE:N	2.35	0.53
1:r:32:LEU:HA	1:r:35:TRP:CD1	2.40	0.53
1:t:179:PHE:HA	1:t:182:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:212:PHE:O	1:5:216:LEU:N	2.36	0.53
1:AD:69:CYS:O	1:AD:71:GLY:N	2.42	0.53
1:AI:179:PHE:HA	1:AI:182:TRP:NE1	2.24	0.53
1:S:212:PHE:O	1:S:216:LEU:N	2.41	0.52
1:b:69:CYS:O	1:b:71:GLY:N	2.42	0.52
1:i:179:PHE:HA	1:i:182:TRP:NE1	2.24	0.52
1:7:212:PHE:O	1:7:216:LEU:N	2.41	0.52
1:l:139:CYS:HB3	1:l:147:CYS:SG	2.50	0.52
1:v:212:PHE:O	1:v:216:LEU:N	2.41	0.52
1:3:48:CYS:N	1:3:60:HIS:O	2.32	0.52
1:AR:32:LEU:HA	1:AR:35:TRP:CD1	2.40	0.52
1:F:69:CYS:O	1:F:71:GLY:N	2.42	0.52
1:F:212:PHE:O	1:F:216:LEU:N	2.41	0.52
1:R:32:LEU:HA	1:R:35:TRP:HB2	1.90	0.52
1:a:35:TRP:CH2	1:r:208:ILE:HA	2.45	0.52
1:e:69:CYS:O	1:e:71:GLY:N	2.41	0.52
1:AB:179:PHE:HA	1:AB:182:TRP:CD1	2.44	0.52
1:AC:35:TRP:CH2	1:AR:208:ILE:HA	2.45	0.52
1:F:199:TRP:O	1:F:201:TRP:N	2.43	0.52
1:Z:179:PHE:HA	1:Z:182:TRP:CD1	2.44	0.52
1:p:139:CYS:HB3	1:p:147:CYS:SG	2.49	0.52
1:v:69:CYS:O	1:v:71:GLY:N	2.42	0.52
1:v:199:TRP:O	1:v:201:TRP:N	2.43	0.52
1:2:98:LEU:HA	1:2:101:GLN:CG	2.40	0.52
1:6:32:LEU:HA	1:6:35:TRP:HB2	1.90	0.52
1:AE:69:CYS:O	1:AE:71:GLY:N	2.41	0.52
1:AP:139:CYS:HB3	1:AP:147:CYS:SG	2.49	0.52
1:N:98:LEU:HA	1:N:101:GLN:CG	2.40	0.52
1:Z:101:GLN:C	1:Z:103:MET:H	2.18	0.52
1:Z:208:ILE:CA	1:3:35:TRP:CH2	2.91	0.52
1:w:199:TRP:CD1	1:w:200:TYR:H	2.26	0.52
1:x:48:CYS:HA	1:x:62:PRO:HA	1.92	0.52
1:AB:101:GLN:C	1:AB:103:MET:H	2.18	0.52
1:A:98:LEU:O	1:A:101:GLN:HB2	2.09	0.52
1:I:199:TRP:CD1	1:I:200:TYR:H	2.26	0.52
1:J:48:CYS:HA	1:J:62:PRO:HA	1.92	0.52
1:O:35:TRP:CH2	1:AB:208:ILE:CA	2.91	0.52
1:O:48:CYS:N	1:O:60:HIS:O	2.32	0.52
1:W:98:LEU:O	1:W:101:GLN:HB2	2.09	0.52
1:W:200:TYR:O	1:W:202:GLY:N	2.43	0.52
1:D:31:SER:O	1:D:35:TRP:CD1	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:31:SER:O	1:V:35:TRP:CD1	2.63	0.52
1:t:31:SER:O	1:t:35:TRP:CD1	2.63	0.52
1:0:31:SER:O	1:0:35:TRP:CD1	2.63	0.52
1:1:9:LEU:O	1:1:13:LEU:N	2.36	0.52
1:AB:31:SER:O	1:AB:35:TRP:CD1	2.63	0.52
1:O:35:TRP:CZ2	1:AB:207:SER:O	2.61	0.52
1:Z:31:SER:O	1:Z:35:TRP:CD1	2.63	0.52
1:t:101:GLN:C	1:t:103:MET:H	2.18	0.52
1:u:35:TRP:CH2	1:0:208:ILE:HA	2.45	0.52
1:D:101:GLN:C	1:D:103:MET:H	2.18	0.51
1:E:35:TRP:CH2	1:V:208:ILE:HA	2.45	0.51
1:G:48:CYS:O	1:G:65:CYS:SG	2.69	0.51
1:M:9:LEU:O	1:M:13:LEU:N	2.36	0.51
1:V:32:LEU:HA	1:V:35:TRP:CD1	2.40	0.51
1:V:139:CYS:HB3	1:V:147:CYS:SG	2.50	0.51
1:r:139:CYS:HB3	1:r:147:CYS:SG	2.50	0.51
1:A:179:PHE:HA	1:A:182:TRP:CD1	2.44	0.51
1:Z:207:SER:O	1:3:35:TRP:CZ2	2.61	0.51
1:AO:212:PHE:O	1:AO:216:LEU:N	2.41	0.51
1:f:52:ASN:O	1:f:54:GLN:N	2.43	0.51
1:o:212:PHE:O	1:o:216:LEU:N	2.41	0.51
1:x:27:THR:O	1:x:31:SER:N	2.27	0.51
1:J:52:ASN:O	1:J:54:GLN:N	2.43	0.51
1:d:223:TRP:O	1:d:225:TYR:N	2.43	0.51
1:0:32:LEU:HA	1:0:35:TRP:CD1	2.40	0.51
1:0:139:CYS:HB3	1:0:147:CYS:SG	2.50	0.51
1:AR:139:CYS:HB3	1:AR:147:CYS:SG	2.50	0.51
1:P:208:ILE:HA	1:e:35:TRP:CH2	2.46	0.51
1:r:31:SER:O	1:r:35:TRP:CD1	2.63	0.51
1:t:100:TYR:C	1:t:102:GLY:H	2.19	0.51
1:x:52:ASN:O	1:x:54:GLN:N	2.43	0.51
1:4:208:ILE:HA	1:AE:35:TRP:CH2	2.46	0.51
1:AF:52:ASN:O	1:AF:54:GLN:N	2.43	0.51
1:AJ:98:LEU:HA	1:AJ:101:GLN:CG	2.40	0.51
1:AR:31:SER:O	1:AR:35:TRP:CD1	2.63	0.51
1:D:100:TYR:C	1:D:102:GLY:H	2.19	0.51
1:j:98:LEU:HA	1:j:101:GLN:CG	2.40	0.51
1:AF:48:CYS:HA	1:AF:62:PRO:HA	1.92	0.51
1:J:27:THR:O	1:J:31:SER:N	2.27	0.51
1:T:32:LEU:O	1:T:36:TRP:HD1	1.94	0.51
1:A:200:TYR:O	1:A:202:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:TRP:CH2	1:l:208:ILE:HA	2.46	0.51
1:b:139:CYS:HB3	1:b:147:CYS:SG	2.49	0.51
1:f:48:CYS:HA	1:f:62:PRO:HA	1.92	0.51
1:n:197:MET:O	1:n:201:TRP:HB2	2.11	0.51
1:w:35:TRP:CH2	1:AL:208:ILE:HA	2.46	0.51
1:8:32:LEU:O	1:8:36:TRP:HD1	1.94	0.51
1:AD:139:CYS:HB3	1:AD:147:CYS:SG	2.49	0.51
1:c:48:CYS:O	1:c:65:CYS:SG	2.69	0.51
1:m:212:PHE:O	1:m:216:LEU:N	2.36	0.51
1:AN:197:MET:O	1:AN:201:TRP:HB2	2.11	0.51
1:H:223:TRP:O	1:H:225:TYR:N	2.43	0.51
1:X:139:CYS:HB3	1:X:147:CYS:SG	2.50	0.51
1:Z:48:CYS:SG	1:Z:63:THR:N	2.84	0.51
1:p:32:LEU:O	1:p:36:TRP:HD1	1.94	0.50
1:AB:48:CYS:SG	1:AB:63:THR:N	2.84	0.50
1:AD:199:TRP:O	1:AD:201:TRP:N	2.43	0.50
1:AP:32:LEU:O	1:AP:36:TRP:HD1	1.94	0.50
1:k:179:PHE:HA	1:k:182:TRP:NE1	2.26	0.50
1:m:38:SER:O	1:m:42:LEU:N	2.45	0.50
1:0:9:LEU:O	1:0:13:LEU:N	2.38	0.50
1:AK:179:PHE:HA	1:AK:182:TRP:NE1	2.26	0.50
1:AM:38:SER:O	1:AM:42:LEU:N	2.45	0.50
1:AM:212:PHE:O	1:AM:216:LEU:N	2.36	0.50
1:H:139:CYS:HB3	1:H:147:CYS:SG	2.50	0.50
1:b:199:TRP:O	1:b:201:TRP:N	2.43	0.50
1:d:139:CYS:HB3	1:d:147:CYS:SG	2.50	0.50
1:AB:100:TYR:C	1:AB:102:GLY:H	2.19	0.50
1:AF:201:TRP:O	1:AF:205:LEU:N	2.25	0.50
1:D:48:CYS:SG	1:D:63:THR:N	2.84	0.50
1:Z:100:TYR:C	1:Z:102:GLY:H	2.19	0.50
1:f:201:TRP:O	1:f:205:LEU:N	2.25	0.50
1:t:48:CYS:SG	1:t:63:THR:N	2.84	0.50
1:AF:27:THR:O	1:AF:31:SER:N	2.27	0.50
1:U:155:SER:C	1:U:157:ALA:N	2.70	0.50
1:V:9:LEU:O	1:V:13:LEU:N	2.38	0.50
1:u:72:TYR:O	1:u:76:CYS:N	2.32	0.50
1:9:155:SER:C	1:9:157:ALA:N	2.70	0.50
1:N:139:CYS:HB3	1:N:147:CYS:SG	2.50	0.50
1:2:139:CYS:HB3	1:2:147:CYS:SG	2.50	0.50
1:R:197:MET:O	1:R:201:TRP:HB2	2.11	0.50
1:W:160:LYS:HA	1:W:163:TRP:HE1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:32:LEU:HA	1:Z:35:TRP:CD1	2.44	0.50
1:c:179:PHE:HA	1:c:182:TRP:NE1	2.26	0.50
1:z:98:LEU:O	1:z:101:GLN:CD	2.52	0.50
1:3:179:PHE:HA	1:3:182:TRP:NE1	2.26	0.50
1:6:197:MET:O	1:6:201:TRP:HB2	2.11	0.50
1:AN:106:VAL:CB	1:AN:157:ALA:O	2.60	0.50
1:E:72:TYR:O	1:E:76:CYS:N	2.32	0.50
1:O:179:PHE:HA	1:O:182:TRP:NE1	2.26	0.50
1:n:106:VAL:CB	1:n:157:ALA:O	2.60	0.50
1:AB:32:LEU:HA	1:AB:35:TRP:CD1	2.44	0.50
1:AL:9:LEU:O	1:AL:13:LEU:N	2.33	0.50
1:L:98:LEU:O	1:L:101:GLN:CD	2.52	0.50
1:AB:139:CYS:HB3	1:AB:147:CYS:SG	2.50	0.50
1:G:179:PHE:HA	1:G:182:TRP:NE1	2.26	0.49
1:Y:211:PRO:O	1:Y:215:LEU:N	2.40	0.49
1:f:27:THR:O	1:f:31:SER:N	2.27	0.49
1:8:139:CYS:HB3	1:8:147:CYS:SG	2.49	0.49
1:AC:35:TRP:CD1	1:AC:35:TRP:C	2.90	0.49
1:B:139:CYS:HB3	1:B:147:CYS:SG	2.50	0.49
1:a:35:TRP:CD1	1:a:35:TRP:C	2.90	0.49
1:l:9:LEU:O	1:l:13:LEU:N	2.33	0.49
1:u:157:ALA:O	1:u:161:PHE:N	2.35	0.49
1:AH:98:LEU:O	1:AH:101:GLN:CD	2.52	0.49
1:J:139:CYS:HB3	1:J:147:CYS:SG	2.50	0.49
1:P:9:LEU:O	1:P:13:LEU:N	2.33	0.49
1:T:139:CYS:HB3	1:T:147:CYS:SG	2.49	0.49
1:Y:48:CYS:HB3	1:Y:62:PRO:N	2.28	0.49
1:a:72:TYR:O	1:a:76:CYS:N	2.32	0.49
1:x:139:CYS:HB3	1:x:147:CYS:SG	2.50	0.49
1:AA:48:CYS:HB3	1:AA:62:PRO:N	2.28	0.49
1:AC:72:TYR:O	1:AC:76:CYS:N	2.32	0.49
1:d:3:ASN:HA	1:d:6:SER:CB	2.43	0.49
1:h:98:LEU:O	1:h:101:GLN:CD	2.52	0.49
1:m:72:TYR:O	1:m:76:CYS:N	2.25	0.49
1:4:9:LEU:O	1:4:13:LEU:N	2.33	0.49
1:O:61:SER:O	1:O:64:SER:N	2.45	0.49
1:R:139:CYS:HB3	1:R:147:CYS:SG	2.50	0.49
1:Z:139:CYS:HB3	1:Z:147:CYS:SG	2.50	0.49
1:5:38:SER:O	1:5:42:LEU:N	2.45	0.49
1:6:139:CYS:HB3	1:6:147:CYS:SG	2.50	0.49
1:AN:162:LEU:O	1:AN:166:ALA:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:38:SER:O	1:Q:42:LEU:N	2.45	0.49
1:c:32:LEU:HA	1:c:35:TRP:HE3	1.77	0.49
1:s:48:CYS:HB3	1:s:62:PRO:N	2.28	0.49
1:3:61:SER:O	1:3:64:SER:N	2.45	0.49
1:C:48:CYS:HB3	1:C:62:PRO:N	2.28	0.49
1:k:61:SER:O	1:k:64:SER:N	2.45	0.49
1:R:135:PRO:O	1:R:136:SER:C	2.56	0.49
1:n:162:LEU:O	1:n:166:ALA:N	2.39	0.49
1:6:135:PRO:O	1:6:136:SER:C	2.56	0.49
1:AI:9:LEU:O	1:AI:13:LEU:N	2.36	0.49
1:AK:61:SER:O	1:AK:64:SER:N	2.45	0.49
1:F:135:PRO:O	1:F:136:SER:C	2.56	0.49
1:T:106:VAL:CB	1:T:157:ALA:HB1	2.43	0.49
1:e:47:VAL:HA	1:e:61:SER:HA	1.95	0.49
1:v:135:PRO:O	1:v:136:SER:C	2.56	0.49
1:AE:47:VAL:HA	1:AE:61:SER:HA	1.95	0.49
1:AM:72:TYR:O	1:AM:76:CYS:N	2.25	0.49
1:D:212:PHE:O	1:D:216:LEU:N	2.46	0.48
1:i:9:LEU:O	1:i:13:LEU:N	2.36	0.48
1:i:179:PHE:HA	1:i:182:TRP:CD1	2.48	0.48
1:k:160:LYS:HA	1:k:163:TRP:CD1	2.48	0.48
1:l:135:PRO:O	1:l:136:SER:C	2.56	0.48
1:t:212:PHE:O	1:t:216:LEU:N	2.46	0.48
1:2:59:ASN:O	1:2:65:CYS:HB3	2.13	0.48
1:8:106:VAL:CB	1:8:157:ALA:HB1	2.43	0.48
1:AK:160:LYS:HA	1:AK:163:TRP:CD1	2.48	0.48
1:AL:135:PRO:O	1:AL:136:SER:C	2.56	0.48
1:E:35:TRP:CD1	1:E:35:TRP:C	2.90	0.48
1:N:56:PRO:O	1:N:58:SER:N	2.46	0.48
1:N:59:ASN:O	1:N:65:CYS:HB3	2.13	0.48
1:b:135:PRO:O	1:b:136:SER:C	2.56	0.48
1:j:135:PRO:O	1:j:136:SER:C	2.56	0.48
1:u:35:TRP:CD1	1:u:35:TRP:C	2.90	0.48
1:2:56:PRO:O	1:2:58:SER:N	2.46	0.48
1:AD:135:PRO:O	1:AD:136:SER:C	2.56	0.48
1:AI:179:PHE:HA	1:AI:182:TRP:CD1	2.48	0.48
1:AJ:135:PRO:O	1:AJ:136:SER:C	2.56	0.48
1:H:3:ASN:HA	1:H:6:SER:CB	2.43	0.48
1:H:135:PRO:O	1:H:136:SER:C	2.56	0.48
1:j:139:CYS:HB3	1:j:147:CYS:SG	2.50	0.48
1:AH:139:CYS:HB3	1:AH:147:CYS:SG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AJ:139:CYS:HB3	1:AJ:147:CYS:SG	2.50	0.48
1:D:199:TRP:O	1:D:201:TRP:N	2.46	0.48
1:G:32:LEU:HA	1:G:35:TRP:HE3	1.77	0.48
1:d:135:PRO:O	1:d:136:SER:C	2.56	0.48
1:e:139:CYS:N	1:e:147:CYS:SG	2.87	0.48
1:t:199:TRP:O	1:t:201:TRP:N	2.46	0.48
1:w:199:TRP:CG	1:w:200:TYR:N	2.82	0.48
1:AE:139:CYS:N	1:AE:147:CYS:SG	2.87	0.48
1:AH:135:PRO:O	1:AH:136:SER:C	2.56	0.48
1:I:199:TRP:CG	1:I:200:TYR:N	2.82	0.48
1:J:106:VAL:CB	1:J:157:ALA:C	2.87	0.48
1:h:135:PRO:O	1:h:136:SER:C	2.56	0.48
1:p:106:VAL:CB	1:p:157:ALA:HB1	2.43	0.48
1:s:211:PRO:O	1:s:215:LEU:N	2.40	0.48
1:x:106:VAL:CB	1:x:157:ALA:C	2.87	0.48
1:AP:106:VAL:CB	1:AP:157:ALA:HB1	2.43	0.48
1:J:135:PRO:O	1:J:136:SER:C	2.56	0.48
1:N:135:PRO:O	1:N:136:SER:C	2.56	0.48
1:O:160:LYS:HA	1:O:163:TRP:CD1	2.48	0.48
1:a:139:CYS:N	1:a:147:CYS:SG	2.87	0.48
1:r:35:TRP:CH2	1:3:208:ILE:HA	2.49	0.48
1:x:135:PRO:O	1:x:136:SER:C	2.56	0.48
1:2:135:PRO:O	1:2:136:SER:C	2.56	0.48
1:6:106:VAL:CB	1:6:157:ALA:O	2.60	0.48
1:AC:139:CYS:N	1:AC:147:CYS:SG	2.87	0.48
1:O:208:ILE:HA	1:AR:35:TRP:CH2	2.49	0.48
1:R:106:VAL:CB	1:R:157:ALA:O	2.60	0.48
1:Y:101:GLN:CG	1:Y:102:GLY:N	2.48	0.48
1:Z:212:PHE:O	1:Z:216:LEU:N	2.46	0.48
1:3:160:LYS:HA	1:3:163:TRP:CD1	2.48	0.48
1:AB:212:PHE:O	1:AB:216:LEU:N	2.46	0.48
1:C:211:PRO:O	1:C:215:LEU:N	2.40	0.48
1:K:43:GLY:O	1:L:50:GLY:N	2.40	0.48
1:M:179:PHE:HA	1:M:182:TRP:CD1	2.48	0.48
1:j:56:PRO:C	1:j:58:SER:N	2.65	0.48
1:3:139:CYS:N	1:3:147:CYS:SG	2.87	0.48
1:4:139:CYS:HB3	1:4:147:CYS:SG	2.50	0.48
1:AJ:56:PRO:C	1:AJ:58:SER:N	2.65	0.48
1:C:139:CYS:N	1:C:147:CYS:SG	2.87	0.48
1:G:139:CYS:N	1:G:147:CYS:SG	2.87	0.48
1:O:139:CYS:N	1:O:147:CYS:SG	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:98:LEU:C	1:f:101:GLN:HG2	2.39	0.48
1:f:106:VAL:CB	1:f:157:ALA:C	2.87	0.48
1:h:98:LEU:O	1:h:101:GLN:NE2	2.47	0.48
1:h:139:CYS:HB3	1:h:147:CYS:SG	2.49	0.48
1:k:208:ILE:HA	1:0:35:TRP:CH2	2.49	0.48
1:AH:98:LEU:O	1:AH:101:GLN:NE2	2.47	0.48
1:AR:135:PRO:O	1:AR:136:SER:C	2.56	0.48
1:I:165:TRP:O	1:I:169:ARG:N	2.47	0.48
1:S:139:CYS:N	1:S:147:CYS:SG	2.87	0.48
1:V:35:TRP:CH2	1:AK:208:ILE:HA	2.49	0.48
1:Z:135:PRO:O	1:Z:136:SER:C	2.56	0.48
1:j:56:PRO:O	1:j:58:SER:N	2.46	0.48
1:s:139:CYS:N	1:s:147:CYS:SG	2.87	0.48
1:t:48:CYS:H	1:t:62:PRO:CA	2.27	0.48
1:w:165:TRP:O	1:w:169:ARG:N	2.47	0.48
1:y:43:GLY:O	1:z:50:GLY:N	2.40	0.48
1:z:139:CYS:HB3	1:z:147:CYS:SG	2.49	0.48
1:1:179:PHE:HA	1:1:182:TRP:CD1	2.48	0.48
1:AF:98:LEU:C	1:AF:101:GLN:HG2	2.39	0.48
1:AF:106:VAL:CB	1:AF:157:ALA:C	2.87	0.48
1:A:139:CYS:N	1:A:147:CYS:SG	2.87	0.47
1:D:48:CYS:H	1:D:62:PRO:CA	2.27	0.47
1:E:35:TRP:HH2	1:V:208:ILE:HA	1.79	0.47
1:F:139:CYS:HB3	1:F:147:CYS:SG	2.49	0.47
1:e:199:TRP:CG	1:e:200:TYR:N	2.82	0.47
1:f:135:PRO:O	1:f:136:SER:C	2.56	0.47
1:j:59:ASN:O	1:j:65:CYS:HB3	2.13	0.47
1:r:135:PRO:O	1:r:136:SER:C	2.56	0.47
1:u:35:TRP:HH2	1:0:208:ILE:HA	1.79	0.47
1:v:139:CYS:HB3	1:v:147:CYS:SG	2.49	0.47
1:y:139:CYS:N	1:y:147:CYS:SG	2.87	0.47
1:z:98:LEU:O	1:z:101:GLN:NE2	2.47	0.47
1:7:139:CYS:N	1:7:147:CYS:SG	2.87	0.47
1:AJ:56:PRO:O	1:AJ:58:SER:N	2.46	0.47
1:D:66:PRO:O	1:D:68:THR:N	2.47	0.47
1:K:139:CYS:N	1:K:147:CYS:SG	2.87	0.47
1:L:98:LEU:O	1:L:101:GLN:NE2	2.47	0.47
1:W:139:CYS:N	1:W:147:CYS:SG	2.87	0.47
1:f:139:CYS:HB3	1:f:147:CYS:SG	2.50	0.47
1:i:139:CYS:N	1:i:147:CYS:SG	2.87	0.47
1:n:139:CYS:HB3	1:n:147:CYS:SG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:139:CYS:N	1:o:147:CYS:SG	2.87	0.47
1:AB:135:PRO:O	1:AB:136:SER:C	2.56	0.47
1:AF:135:PRO:O	1:AF:136:SER:C	2.56	0.47
1:AF:139:CYS:HB3	1:AF:147:CYS:SG	2.50	0.47
1:AK:139:CYS:N	1:AK:147:CYS:SG	2.87	0.47
1:AM:139:CYS:N	1:AM:147:CYS:SG	2.87	0.47
1:AN:139:CYS:HB3	1:AN:147:CYS:SG	2.50	0.47
1:AO:139:CYS:N	1:AO:147:CYS:SG	2.87	0.47
1:B:135:PRO:O	1:B:136:SER:C	2.56	0.47
1:J:98:LEU:C	1:J:101:GLN:HG2	2.39	0.47
1:k:139:CYS:N	1:k:147:CYS:SG	2.87	0.47
1:k:163:TRP:O	1:k:167:SER:N	2.42	0.47
1:m:139:CYS:N	1:m:147:CYS:SG	2.87	0.47
1:p:160:LYS:HA	1:p:163:TRP:CD1	2.50	0.47
1:t:66:PRO:O	1:t:68:THR:N	2.47	0.47
1:AA:101:GLN:CG	1:AA:102:GLY:N	2.48	0.47
1:AA:139:CYS:N	1:AA:147:CYS:SG	2.87	0.47
1:AI:139:CYS:N	1:AI:147:CYS:SG	2.87	0.47
1:AJ:59:ASN:O	1:AJ:65:CYS:HB3	2.13	0.47
1:AP:160:LYS:HA	1:AP:163:TRP:CD1	2.50	0.47
1:P:139:CYS:HB3	1:P:147:CYS:SG	2.50	0.47
1:t:139:CYS:HB3	1:t:147:CYS:SG	2.50	0.47
1:u:139:CYS:N	1:u:147:CYS:SG	2.87	0.47
1:x:98:LEU:C	1:x:101:GLN:HG2	2.39	0.47
1:6:162:LEU:O	1:6:166:ALA:N	2.39	0.47
1:AK:163:TRP:O	1:AK:167:SER:N	2.42	0.47
1:AQ:48:CYS:HA	1:AQ:62:PRO:HA	1.96	0.47
1:E:139:CYS:N	1:E:147:CYS:SG	2.87	0.47
1:U:48:CYS:HA	1:U:62:PRO:HA	1.96	0.47
1:X:98:LEU:O	1:X:101:GLN:NE2	2.30	0.47
1:d:216:LEU:C	1:d:218:ILE:H	2.23	0.47
1:q:48:CYS:HA	1:q:62:PRO:HA	1.96	0.47
1:w:47:VAL:HA	1:w:61:SER:HA	1.95	0.47
1:2:160:LYS:HA	1:2:163:TRP:CE2	2.50	0.47
1:9:48:CYS:HA	1:9:62:PRO:HA	1.96	0.47
1:AB:66:PRO:O	1:AB:68:THR:N	2.47	0.47
1:D:139:CYS:HB3	1:D:147:CYS:SG	2.50	0.47
1:I:47:VAL:HA	1:I:61:SER:HA	1.95	0.47
1:N:160:LYS:HA	1:N:163:TRP:CE2	2.50	0.47
1:Y:139:CYS:N	1:Y:147:CYS:SG	2.87	0.47
1:Z:66:PRO:O	1:Z:68:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:135:PRO:O	1:n:136:SER:C	2.56	0.47
1:H:216:LEU:C	1:H:218:ILE:H	2.23	0.47
1:L:139:CYS:HB3	1:L:147:CYS:SG	2.49	0.47
1:M:139:CYS:N	1:M:147:CYS:SG	2.87	0.47
1:T:160:LYS:HA	1:T:163:TRP:CD1	2.50	0.47
1:U:139:CYS:N	1:U:147:CYS:SG	2.87	0.47
1:j:162:LEU:HA	1:j:165:TRP:CZ2	2.50	0.47
1:q:139:CYS:N	1:q:147:CYS:SG	2.87	0.47
1:5:139:CYS:N	1:5:147:CYS:SG	2.87	0.47
1:8:160:LYS:HA	1:8:163:TRP:CD1	2.50	0.47
1:AJ:162:LEU:HA	1:AJ:165:TRP:CZ2	2.50	0.47
1:AN:135:PRO:O	1:AN:136:SER:C	2.56	0.47
1:AQ:139:CYS:N	1:AQ:147:CYS:SG	2.87	0.47
1:I:139:CYS:N	1:I:147:CYS:SG	2.87	0.47
1:P:28:ILE:O	1:P:32:LEU:CB	2.63	0.47
1:R:162:LEU:O	1:R:166:ALA:N	2.39	0.47
1:Y:22:LEU:O	1:Y:23:THR:C	2.58	0.47
1:j:27:THR:O	1:j:31:SER:N	2.26	0.47
1:q:156:TRP:C	1:q:158:PHE:H	2.23	0.47
1:1:139:CYS:N	1:1:147:CYS:SG	2.87	0.47
1:4:28:ILE:O	1:4:32:LEU:CB	2.63	0.47
1:7:163:TRP:O	1:7:167:SER:N	2.48	0.47
1:9:139:CYS:N	1:9:147:CYS:SG	2.87	0.47
1:AA:22:LEU:O	1:AA:23:THR:C	2.58	0.47
1:AJ:160:LYS:HA	1:AJ:163:TRP:CE2	2.50	0.47
1:AQ:8:PHE:O	1:AQ:12:LEU:N	2.41	0.47
1:L:135:PRO:O	1:L:136:SER:C	2.56	0.47
1:Q:139:CYS:N	1:Q:147:CYS:SG	2.87	0.47
1:S:163:TRP:O	1:S:167:SER:N	2.48	0.47
1:c:139:CYS:N	1:c:147:CYS:SG	2.87	0.47
1:h:106:VAL:CB	1:h:157:ALA:CA	2.93	0.47
1:j:160:LYS:HA	1:j:163:TRP:CE2	2.50	0.47
1:t:135:PRO:O	1:t:136:SER:C	2.56	0.47
1:AQ:156:TRP:C	1:AQ:158:PHE:H	2.23	0.47
1:D:135:PRO:O	1:D:136:SER:C	2.56	0.47
1:I:3:ASN:O	1:I:7:GLY:N	2.40	0.47
1:Z:48:CYS:H	1:Z:62:PRO:CA	2.27	0.47
1:p:124:CYS:HB3	1:p:125:THR:H	1.59	0.47
1:w:139:CYS:N	1:w:147:CYS:SG	2.87	0.47
1:z:135:PRO:O	1:z:136:SER:C	2.56	0.47
1:AH:106:VAL:CB	1:AH:157:ALA:CA	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:124:CYS:HB3	1:AP:125:THR:H	1.59	0.47
1:g:48:CYS:SG	1:g:62:PRO:HA	2.55	0.46
1:g:139:CYS:N	1:g:147:CYS:SG	2.87	0.46
1:q:8:PHE:O	1:q:12:LEU:N	2.41	0.46
1:r:28:ILE:O	1:r:32:LEU:CB	2.64	0.46
1:0:28:ILE:O	1:0:32:LEU:CB	2.64	0.46
1:AG:48:CYS:SG	1:AG:62:PRO:HA	2.55	0.46
1:AR:28:ILE:O	1:AR:32:LEU:CB	2.64	0.46
1:N:162:LEU:HA	1:N:165:TRP:CZ2	2.50	0.46
1:V:28:ILE:O	1:V:32:LEU:CB	2.64	0.46
1:V:197:MET:O	1:V:201:TRP:HB2	2.16	0.46
1:w:3:ASN:O	1:w:7:GLY:N	2.40	0.46
1:2:162:LEU:HA	1:2:165:TRP:CZ2	2.50	0.46
1:0:197:MET:O	1:0:201:TRP:HB2	2.16	0.46
1:AB:48:CYS:H	1:AB:62:PRO:CA	2.27	0.46
1:AD:124:CYS:HB3	1:AD:125:THR:H	1.59	0.46
1:AG:139:CYS:N	1:AG:147:CYS:SG	2.87	0.46
1:AJ:27:THR:O	1:AJ:31:SER:N	2.26	0.46
1:B:124:CYS:HB3	1:B:125:THR:H	1.59	0.46
1:L:106:VAL:CB	1:L:157:ALA:CA	2.93	0.46
1:U:156:TRP:C	1:U:158:PHE:H	2.23	0.46
1:l:28:ILE:O	1:l:32:LEU:CB	2.63	0.46
1:4:135:PRO:O	1:4:136:SER:C	2.56	0.46
1:P:135:PRO:O	1:P:136:SER:C	2.56	0.46
1:T:135:PRO:O	1:T:136:SER:C	2.56	0.46
1:U:8:PHE:O	1:U:12:LEU:N	2.41	0.46
1:j:153:PRO:CB	1:j:157:ALA:HB2	2.46	0.46
1:z:106:VAL:CB	1:z:157:ALA:CA	2.93	0.46
1:8:135:PRO:O	1:8:136:SER:C	2.56	0.46
1:9:8:PHE:O	1:9:12:LEU:N	2.41	0.46
1:AJ:153:PRO:CB	1:AJ:157:ALA:HB2	2.46	0.46
1:AL:28:ILE:O	1:AL:32:LEU:CB	2.63	0.46
1:A:160:LYS:HA	1:A:163:TRP:HE1	1.74	0.46
1:B:60:HIS:O	1:B:65:CYS:HA	2.16	0.46
1:B:98:LEU:O	1:B:101:GLN:NE2	2.30	0.46
1:c:188:PRO:O	1:c:192:LEU:N	2.49	0.46
1:p:135:PRO:O	1:p:136:SER:C	2.56	0.46
1:t:32:LEU:HA	1:t:35:TRP:CD1	2.44	0.46
1:AE:199:TRP:CG	1:AE:200:TYR:N	2.82	0.46
1:AP:135:PRO:O	1:AP:136:SER:C	2.56	0.46
1:X:135:PRO:O	1:X:136:SER:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:165:TRP:O	1:e:169:ARG:N	2.47	0.46
1:2:153:PRO:CB	1:2:157:ALA:HB2	2.46	0.46
1:9:156:TRP:C	1:9:158:PHE:H	2.23	0.46
1:AO:163:TRP:O	1:AO:167:SER:N	2.48	0.46
1:D:32:LEU:HA	1:D:35:TRP:CD1	2.44	0.46
1:K:48:CYS:SG	1:K:62:PRO:HA	2.55	0.46
1:L:67:PRO:O	1:L:71:GLY:HA3	2.16	0.46
1:N:153:PRO:CB	1:N:157:ALA:HB2	2.46	0.46
1:U:156:TRP:C	1:U:158:PHE:N	2.74	0.46
1:o:163:TRP:O	1:o:167:SER:N	2.48	0.46
1:y:48:CYS:SG	1:y:62:PRO:HA	2.55	0.46
1:z:67:PRO:O	1:z:71:GLY:HA3	2.16	0.46
1:9:156:TRP:C	1:9:158:PHE:N	2.74	0.46
1:b:124:CYS:HB3	1:b:125:THR:H	1.59	0.46
1:d:17:ALA:C	1:d:20:PHE:H	2.24	0.46
1:l:100:TYR:CE1	1:l:156:TRP:NE1	2.84	0.46
1:q:156:TRP:C	1:q:158:PHE:N	2.74	0.46
1:r:47:VAL:HA	1:r:61:SER:HA	1.98	0.46
1:AL:100:TYR:CE1	1:AL:156:TRP:NE1	2.84	0.46
1:AQ:156:TRP:C	1:AQ:158:PHE:N	2.74	0.46
1:AR:47:VAL:HA	1:AR:61:SER:HA	1.98	0.46
1:A:61:SER:HA	1:A:65:CYS:HA	1.98	0.46
1:N:27:THR:O	1:N:31:SER:N	2.26	0.46
1:V:47:VAL:HA	1:V:61:SER:HA	1.98	0.46
1:W:61:SER:HA	1:W:65:CYS:HA	1.98	0.46
1:AE:165:TRP:O	1:AE:169:ARG:N	2.47	0.46
1:O:47:VAL:HA	1:O:61:SER:HA	1.98	0.46
1:O:135:PRO:O	1:O:136:SER:C	2.56	0.46
1:M:157:ALA:O	1:M:158:PHE:C	2.59	0.45
1:5:48:CYS:HB3	1:5:60:HIS:O	2.16	0.45
1:P:162:LEU:O	1:P:166:ALA:N	2.37	0.45
1:Q:48:CYS:HB3	1:Q:60:HIS:O	2.16	0.45
1:V:135:PRO:O	1:V:136:SER:C	2.56	0.45
1:r:197:MET:O	1:r:201:TRP:HB2	2.16	0.45
1:AC:35:TRP:HH2	1:AR:208:ILE:HA	1.79	0.45
1:AG:43:GLY:O	1:AH:50:GLY:N	2.40	0.45
1:AL:139:CYS:HB3	1:AL:147:CYS:SG	2.50	0.45
1:C:21:LEU:O	1:C:22:LEU:C	2.60	0.45
1:C:22:LEU:O	1:C:23:THR:C	2.58	0.45
1:P:32:LEU:O	1:P:36:TRP:HD1	1.99	0.45
1:s:22:LEU:O	1:s:23:THR:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:27:THR:O	1:2:31:SER:N	2.26	0.45
1:4:32:LEU:O	1:4:36:TRP:HD1	1.99	0.45
1:AA:51:GLN:N	1:AA:65:CYS:SG	2.90	0.45
1:AM:48:CYS:HB3	1:AM:60:HIS:O	2.16	0.45
1:AR:197:MET:O	1:AR:201:TRP:HB2	2.16	0.45
1:W:200:TYR:C	1:W:202:GLY:N	2.75	0.45
1:Y:51:GLN:N	1:Y:65:CYS:SG	2.90	0.45
1:Y:161:PHE:O	1:Y:166:ALA:N	2.50	0.45
1:a:35:TRP:HH2	1:r:208:ILE:HA	1.79	0.45
1:m:48:CYS:HB3	1:m:60:HIS:O	2.16	0.45
1:s:21:LEU:O	1:s:22:LEU:C	2.60	0.45
1:AA:161:PHE:O	1:AA:166:ALA:N	2.50	0.45
1:AH:67:PRO:O	1:AH:71:GLY:HA3	2.16	0.45
1:X:60:HIS:O	1:X:65:CYS:HA	2.16	0.45
1:Z:199:TRP:O	1:Z:201:TRP:N	2.46	0.45
1:P:100:TYR:CE1	1:P:156:TRP:NE1	2.84	0.45
1:h:67:PRO:O	1:h:71:GLY:HA3	2.16	0.45
1:4:100:TYR:CE1	1:4:156:TRP:NE1	2.84	0.45
1:4:162:LEU:O	1:4:166:ALA:N	2.37	0.45
1:8:124:CYS:HB3	1:8:125:THR:H	1.59	0.45
1:W:155:SER:C	1:W:157:ALA:N	2.69	0.45
1:g:43:GLY:O	1:h:50:GLY:N	2.40	0.45
1:AB:199:TRP:O	1:AB:201:TRP:N	2.46	0.45
1:H:216:LEU:C	1:H:218:ILE:N	2.75	0.45
1:J:87:LEU:HA	1:J:90:CYS:SG	2.57	0.45
1:L:179:PHE:HA	1:L:182:TRP:CE3	2.52	0.45
1:T:124:CYS:HB3	1:T:125:THR:H	1.59	0.45
1:s:51:GLN:N	1:s:65:CYS:SG	2.90	0.45
1:C:51:GLN:N	1:C:65:CYS:SG	2.90	0.45
1:Y:21:LEU:O	1:Y:22:LEU:C	2.60	0.45
1:l:124:CYS:HB3	1:l:125:THR:H	1.59	0.45
1:z:179:PHE:HA	1:z:182:TRP:CE3	2.52	0.45
1:AL:124:CYS:HB3	1:AL:125:THR:H	1.59	0.45
1:d:216:LEU:C	1:d:218:ILE:N	2.75	0.45
1:q:155:SER:C	1:q:157:ALA:N	2.70	0.45
1:x:87:LEU:HA	1:x:90:CYS:SG	2.57	0.45
1:9:50:GLY:HA3	1:9:71:GLY:HA3	1.99	0.45
1:AA:21:LEU:O	1:AA:22:LEU:C	2.60	0.45
1:AQ:155:SER:C	1:AQ:157:ALA:N	2.70	0.45
1:D:208:ILE:CA	1:AK:35:TRP:HH2	2.30	0.44
1:U:50:GLY:HA3	1:U:71:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:87:LEU:HA	1:f:90:CYS:SG	2.57	0.44
1:h:179:PHE:HA	1:h:182:TRP:CE3	2.52	0.44
1:j:124:CYS:HB3	1:j:125:THR:H	1.59	0.44
1:k:35:TRP:HH2	1:t:208:ILE:CA	2.30	0.44
1:k:34:SER:HA	1:k:37:THR:CB	2.47	0.44
1:AF:87:LEU:HA	1:AF:90:CYS:SG	2.57	0.44
1:AH:179:PHE:HA	1:AH:182:TRP:CE3	2.52	0.44
1:H:17:ALA:C	1:H:20:PHE:H	2.24	0.44
1:AK:34:SER:HA	1:AK:37:THR:CB	2.47	0.44
1:G:188:PRO:O	1:G:192:LEU:N	2.49	0.44
1:r:9:LEU:O	1:r:13:LEU:N	2.38	0.44
1:O:34:SER:HA	1:O:37:THR:CB	2.47	0.44
1:l:32:LEU:O	1:l:36:TRP:HD1	1.99	0.44
1:AQ:50:GLY:HA3	1:AQ:71:GLY:HA3	1.99	0.44
1:D:63:THR:O	1:D:65:CYS:HB3	2.18	0.44
1:q:50:GLY:HA3	1:q:71:GLY:HA3	1.99	0.44
1:t:63:THR:O	1:t:65:CYS:HB3	2.18	0.44
1:4:163:TRP:O	1:4:167:SER:N	2.39	0.44
1:AL:32:LEU:O	1:AL:36:TRP:HD1	1.99	0.44
1:N:124:CYS:HB3	1:N:125:THR:H	1.59	0.44
1:3:34:SER:HA	1:3:37:THR:CB	2.47	0.44
1:AJ:124:CYS:HB3	1:AJ:125:THR:H	1.59	0.44
1:AK:160:LYS:HA	1:AK:163:TRP:NE1	2.33	0.44
1:j:104:LEU:O	1:j:105:PRO:C	2.61	0.44
1:k:160:LYS:HA	1:k:163:TRP:NE1	2.33	0.44
1:1:48:CYS:N	1:1:60:HIS:O	2.31	0.44
1:C:161:PHE:O	1:C:166:ALA:N	2.50	0.43
1:D:101:GLN:HG3	1:D:103:MET:H	1.83	0.43
1:H:100:TYR:CE1	1:H:156:TRP:HE3	2.36	0.43
1:O:35:TRP:HH2	1:AB:208:ILE:CA	2.30	0.43
1:O:163:TRP:O	1:O:167:SER:N	2.42	0.43
1:P:163:TRP:O	1:P:167:SER:N	2.39	0.43
1:Y:100:TYR:CE2	1:Y:156:TRP:CE2	3.06	0.43
1:Z:208:ILE:CA	1:3:35:TRP:HH2	2.30	0.43
1:t:101:GLN:HG3	1:t:103:MET:H	1.83	0.43
1:AA:100:TYR:CE2	1:AA:156:TRP:CE2	3.06	0.43
1:L:124:CYS:HB3	1:L:125:THR:H	1.59	0.43
1:T:156:TRP:O	1:T:157:ALA:C	2.61	0.43
1:d:100:TYR:CE1	1:d:156:TRP:HE3	2.36	0.43
1:s:161:PHE:O	1:s:166:ALA:N	2.50	0.43
1:H:100:TYR:HA	1:H:156:TRP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:101:GLN:HG3	1:Z:103:MET:H	1.83	0.43
1:z:124:CYS:HB3	1:z:125:THR:H	1.59	0.43
1:C:100:TYR:CE2	1:C:156:TRP:CE2	3.06	0.43
1:Y:4:ILE:O	1:Y:5:THR:C	2.61	0.43
1:Z:63:THR:O	1:Z:65:CYS:HB3	2.18	0.43
1:3:163:TRP:O	1:3:167:SER:N	2.42	0.43
1:AA:20:PHE:O	1:AA:21:LEU:C	2.62	0.43
1:AB:63:THR:O	1:AB:65:CYS:HB3	2.18	0.43
1:AB:101:GLN:HG3	1:AB:103:MET:H	1.83	0.43
1:M:65:CYS:HB3	1:M:69:CYS:O	2.19	0.43
1:Y:20:PHE:O	1:Y:21:LEU:C	2.62	0.43
1:b:156:TRP:C	1:b:158:PHE:N	2.77	0.43
1:d:100:TYR:HA	1:d:156:TRP:HA	2.00	0.43
1:k:61:SER:O	1:k:65:CYS:N	2.51	0.43
1:s:100:TYR:CE2	1:s:156:TRP:CE2	3.06	0.43
1:1:65:CYS:HB3	1:1:69:CYS:O	2.19	0.43
1:2:124:CYS:HB3	1:2:125:THR:H	1.59	0.43
1:2:179:PHE:HA	1:2:182:TRP:NE1	2.33	0.43
1:AA:4:ILE:O	1:AA:5:THR:C	2.61	0.43
1:AD:156:TRP:C	1:AD:158:PHE:N	2.77	0.43
1:M:48:CYS:N	1:M:60:HIS:O	2.31	0.43
1:N:179:PHE:HA	1:N:182:TRP:NE1	2.33	0.43
1:O:160:LYS:HA	1:O:163:TRP:NE1	2.33	0.43
1:f:48:CYS:CA	1:f:62:PRO:HA	2.48	0.43
1:AA:211:PRO:O	1:AA:215:LEU:N	2.40	0.43
1:AK:61:SER:O	1:AK:65:CYS:N	2.51	0.43
1:J:48:CYS:CA	1:J:62:PRO:HA	2.48	0.43
1:i:65:CYS:HB3	1:i:69:CYS:O	2.19	0.43
1:x:48:CYS:CA	1:x:62:PRO:HA	2.48	0.43
1:1:157:ALA:O	1:1:158:PHE:C	2.62	0.43
1:2:156:TRP:CD1	1:2:156:TRP:N	2.86	0.43
1:3:160:LYS:HA	1:3:163:TRP:NE1	2.33	0.43
1:AF:48:CYS:CA	1:AF:62:PRO:HA	2.48	0.43
1:AI:65:CYS:HB3	1:AI:69:CYS:O	2.19	0.43
1:N:156:TRP:CD1	1:N:156:TRP:N	2.86	0.43
1:AB:124:CYS:HB3	1:AB:125:THR:H	1.59	0.43
1:F:159:GLY:C	1:F:161:PHE:H	2.27	0.43
1:Z:124:CYS:HB3	1:Z:125:THR:H	1.59	0.43
1:c:53:SER:C	1:c:55:SER:H	2.27	0.43
1:n:105:PRO:C	1:n:107:CYS:N	2.66	0.43
1:s:20:PHE:O	1:s:21:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:159:GLY:C	1:v:161:PHE:H	2.27	0.43
1:AJ:179:PHE:HA	1:AJ:182:TRP:NE1	2.33	0.43
1:AL:163:TRP:O	1:AL:167:SER:N	2.39	0.43
1:AN:105:PRO:C	1:AN:107:CYS:N	2.66	0.43
1:C:20:PHE:O	1:C:21:LEU:C	2.62	0.42
1:O:61:SER:O	1:O:65:CYS:N	2.51	0.42
1:i:157:ALA:O	1:i:158:PHE:C	2.62	0.42
1:j:179:PHE:HA	1:j:182:TRP:NE1	2.33	0.42
1:3:61:SER:O	1:3:65:CYS:N	2.51	0.42
1:A:48:CYS:SG	1:A:63:THR:N	2.92	0.42
1:j:198:MET:O	1:j:202:GLY:N	2.52	0.42
1:n:46:THR:O	1:n:61:SER:HA	2.19	0.42
1:AN:46:THR:O	1:AN:61:SER:HA	2.19	0.42
1:AR:9:LEU:O	1:AR:13:LEU:N	2.38	0.42
1:F:156:TRP:C	1:F:158:PHE:N	2.77	0.42
1:R:179:PHE:HA	1:R:182:TRP:CZ2	2.55	0.42
1:l:162:LEU:O	1:l:166:ALA:N	2.37	0.42
1:v:156:TRP:C	1:v:158:PHE:N	2.77	0.42
1:l:157:ALA:C	1:l:159:GLY:N	2.77	0.42
1:6:179:PHE:HA	1:6:182:TRP:CZ2	2.55	0.42
1:AJ:198:MET:O	1:AJ:202:GLY:N	2.52	0.42
1:G:170:PHE:O	1:G:173:LEU:N	2.52	0.42
1:l:163:TRP:O	1:l:167:SER:N	2.39	0.42
1:AJ:156:TRP:CD1	1:AJ:156:TRP:N	2.86	0.42
1:l:212:PHE:O	1:l:216:LEU:N	2.53	0.42
1:6:124:CYS:HB3	1:6:125:THR:H	1.59	0.42
1:8:199:TRP:O	1:8:201:TRP:N	2.48	0.42
1:AL:156:TRP:CD1	1:AL:156:TRP:H	2.38	0.42
1:AP:199:TRP:O	1:AP:201:TRP:N	2.48	0.42
1:M:212:PHE:O	1:M:216:LEU:N	2.53	0.42
1:N:198:MET:O	1:N:202:GLY:N	2.52	0.42
1:T:199:TRP:O	1:T:201:TRP:N	2.48	0.42
1:j:156:TRP:N	1:j:156:TRP:CD1	2.86	0.42
1:l:156:TRP:CD1	1:l:156:TRP:H	2.38	0.42
1:z:137:CYS:SG	1:z:137:CYS:O	2.78	0.42
1:L:137:CYS:SG	1:L:137:CYS:O	2.78	0.42
1:P:165:TRP:O	1:P:169:ARG:HG2	2.20	0.42
1:p:199:TRP:O	1:p:201:TRP:N	2.48	0.42
1:4:165:TRP:O	1:4:169:ARG:HG2	2.20	0.42
1:B:137:CYS:SG	1:B:137:CYS:O	2.78	0.42
1:D:46:THR:O	1:D:63:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:46:THR:O	1:t:63:THR:HA	2.20	0.42
1:2:198:MET:O	1:2:202:GLY:N	2.52	0.42
1:AL:162:LEU:O	1:AL:166:ALA:N	2.37	0.42
1:N:137:CYS:SG	1:N:137:CYS:O	2.78	0.42
1:h:106:VAL:CB	1:h:157:ALA:C	2.93	0.42
1:AH:106:VAL:CB	1:AH:157:ALA:C	2.93	0.42
1:C:101:GLN:CG	1:C:102:GLY:N	2.48	0.41
1:J:137:CYS:O	1:J:137:CYS:SG	2.78	0.41
1:P:156:TRP:CD1	1:P:156:TRP:H	2.38	0.41
1:l:165:TRP:O	1:l:169:ARG:HG2	2.20	0.41
1:x:137:CYS:O	1:x:137:CYS:SG	2.78	0.41
1:2:137:CYS:O	1:2:137:CYS:SG	2.78	0.41
1:AL:165:TRP:O	1:AL:169:ARG:HG2	2.20	0.41
1:D:137:CYS:SG	1:D:137:CYS:O	2.78	0.41
1:H:137:CYS:O	1:H:137:CYS:SG	2.78	0.41
1:O:40:ASN:O	1:O:44:GLY:HA3	2.20	0.41
1:P:74:TRP:HA	1:P:74:TRP:CE3	2.56	0.41
1:b:159:GLY:C	1:b:161:PHE:H	2.27	0.41
1:f:137:CYS:SG	1:f:137:CYS:O	2.78	0.41
1:i:157:ALA:C	1:i:159:GLY:N	2.77	0.41
1:t:137:CYS:O	1:t:137:CYS:SG	2.78	0.41
1:3:40:ASN:O	1:3:44:GLY:HA3	2.20	0.41
1:4:74:TRP:HA	1:4:74:TRP:CE3	2.56	0.41
1:4:156:TRP:CD1	1:4:156:TRP:H	2.38	0.41
1:AD:159:GLY:C	1:AD:161:PHE:H	2.27	0.41
1:C:4:ILE:O	1:C:5:THR:C	2.61	0.41
1:R:124:CYS:HB3	1:R:125:THR:H	1.59	0.41
1:V:137:CYS:O	1:V:137:CYS:SG	2.78	0.41
1:X:137:CYS:O	1:X:137:CYS:SG	2.78	0.41
1:Z:137:CYS:SG	1:Z:137:CYS:O	2.78	0.41
1:b:61:SER:O	1:b:65:CYS:HB3	2.20	0.41
1:j:137:CYS:O	1:j:137:CYS:SG	2.78	0.41
1:p:137:CYS:O	1:p:137:CYS:SG	2.78	0.41
1:AB:137:CYS:SG	1:AB:137:CYS:O	2.78	0.41
1:AD:61:SER:O	1:AD:65:CYS:HB3	2.20	0.41
1:AF:137:CYS:SG	1:AF:137:CYS:O	2.78	0.41
1:G:53:SER:C	1:G:55:SER:H	2.27	0.41
1:K:31:SER:O	1:K:35:TRP:CE3	2.74	0.41
1:N:217:PRO:HA	1:N:220:PHE:CB	2.51	0.41
1:l:46:THR:O	1:l:61:SER:HA	2.20	0.41
1:y:31:SER:O	1:y:35:TRP:CE3	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:46:THR:O	1:6:61:SER:HA	2.19	0.41
1:AJ:137:CYS:SG	1:AJ:137:CYS:O	2.78	0.41
1:AK:40:ASN:O	1:AK:44:GLY:HA3	2.20	0.41
1:AL:137:CYS:O	1:AL:137:CYS:SG	2.78	0.41
1:AP:137:CYS:O	1:AP:137:CYS:SG	2.78	0.41
1:A:179:PHE:HA	1:A:182:TRP:NE1	2.36	0.41
1:H:212:PHE:HA	1:S:35:TRP:HZ2	1.85	0.41
1:K:198:MET:O	1:K:202:GLY:N	2.34	0.41
1:M:157:ALA:C	1:M:159:GLY:N	2.78	0.41
1:P:137:CYS:SG	1:P:137:CYS:O	2.78	0.41
1:R:137:CYS:O	1:R:137:CYS:SG	2.78	0.41
1:k:40:ASN:O	1:k:44:GLY:HA3	2.20	0.41
1:s:4:ILE:O	1:s:5:THR:C	2.61	0.41
1:2:217:PRO:HA	1:2:220:PHE:CB	2.51	0.41
1:4:137:CYS:O	1:4:137:CYS:SG	2.78	0.41
1:0:137:CYS:O	1:0:137:CYS:SG	2.78	0.41
1:AL:46:THR:O	1:AL:61:SER:HA	2.20	0.41
1:R:46:THR:O	1:R:61:SER:HA	2.19	0.41
1:d:137:CYS:SG	1:d:137:CYS:O	2.78	0.41
1:l:137:CYS:O	1:l:137:CYS:SG	2.78	0.41
1:y:198:MET:O	1:y:202:GLY:N	2.34	0.41
1:1:157:ALA:O	1:1:159:GLY:N	2.54	0.41
1:AL:74:TRP:HA	1:AL:74:TRP:CE3	2.56	0.41
1:X:124:CYS:HB3	1:X:125:THR:H	1.59	0.41
1:h:137:CYS:O	1:h:137:CYS:SG	2.78	0.41
1:i:157:ALA:O	1:i:159:GLY:N	2.54	0.41
1:l:74:TRP:HA	1:l:74:TRP:CE3	2.56	0.41
1:6:137:CYS:SG	1:6:137:CYS:O	2.78	0.41
1:AH:137:CYS:O	1:AH:137:CYS:SG	2.78	0.41
1:AJ:217:PRO:HA	1:AJ:220:PHE:CB	2.51	0.41
1:F:61:SER:O	1:F:65:CYS:HB3	2.20	0.41
1:j:217:PRO:HA	1:j:220:PHE:CB	2.51	0.41
1:n:179:PHE:HA	1:n:182:TRP:CZ2	2.55	0.41
1:r:137:CYS:O	1:r:137:CYS:SG	2.78	0.41
1:s:101:GLN:CG	1:s:102:GLY:N	2.48	0.41
1:v:61:SER:O	1:v:65:CYS:HB3	2.20	0.41
1:v:137:CYS:O	1:v:137:CYS:SG	2.78	0.41
1:AR:137:CYS:O	1:AR:137:CYS:SG	2.78	0.41
1:A:155:SER:C	1:A:157:ALA:N	2.69	0.41
1:A:225:TYR:OH	1:t:169:ARG:NE	2.54	0.41
1:F:137:CYS:O	1:F:137:CYS:SG	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:106:VAL:CB	1:L:157:ALA:C	2.93	0.41
1:S:48:CYS:HB2	1:S:62:PRO:HA	2.03	0.41
1:n:137:CYS:O	1:n:137:CYS:SG	2.78	0.41
1:z:106:VAL:CB	1:z:157:ALA:C	2.93	0.41
1:4:46:THR:O	1:4:61:SER:HA	2.20	0.41
1:7:48:CYS:HB2	1:7:62:PRO:HA	2.03	0.41
1:AN:137:CYS:O	1:AN:137:CYS:SG	2.78	0.41
1:AN:179:PHE:HA	1:AN:182:TRP:CZ2	2.55	0.41
1:P:46:THR:O	1:P:61:SER:HA	2.20	0.41
1:AD:137:CYS:O	1:AD:137:CYS:SG	2.78	0.41
1:AG:31:SER:O	1:AG:35:TRP:CE3	2.74	0.41
1:AI:212:PHE:O	1:AI:216:LEU:N	2.53	0.41
1:P:67:PRO:HA	1:P:72:TYR:CB	2.52	0.40
1:T:137:CYS:O	1:T:137:CYS:SG	2.78	0.40
1:b:137:CYS:O	1:b:137:CYS:SG	2.78	0.40
1:g:31:SER:O	1:g:35:TRP:CE3	2.74	0.40
1:i:212:PHE:O	1:i:216:LEU:N	2.53	0.40
1:4:67:PRO:HA	1:4:72:TYR:CB	2.52	0.40
1:H:212:PHE:CA	1:S:35:TRP:HZ2	2.34	0.40
1:d:212:PHE:CA	1:o:35:TRP:HZ2	2.34	0.40
1:v:163:TRP:O	1:v:167:SER:N	2.49	0.40
1:8:137:CYS:O	1:8:137:CYS:SG	2.78	0.40
1:AL:181:GLN:O	1:AL:185:GLY:N	2.49	0.40
1:W:179:PHE:HA	1:W:182:TRP:NE1	2.36	0.40
1:c:170:PHE:O	1:c:173:LEU:N	2.52	0.40
1:2:104:LEU:O	1:2:105:PRO:C	2.64	0.40
1:d:222:LEU:O	1:d:223:TRP:HB3	2.22	0.40
1:0:124:CYS:HB3	1:0:125:THR:H	1.59	0.40
1:E:8:PHE:O	1:E:12:LEU:N	2.46	0.40
1:F:163:TRP:O	1:F:167:SER:N	2.49	0.40
1:H:100:TYR:HE1	1:H:156:TRP:HE3	1.70	0.40
1:Z:46:THR:O	1:Z:63:THR:HA	2.20	0.40
1:u:8:PHE:O	1:u:12:LEU:N	2.46	0.40
1:v:124:CYS:HB3	1:v:125:THR:H	1.59	0.40
1:AN:124:CYS:HB3	1:AN:125:THR:H	1.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	224/226 (99%)	198 (88%)	25 (11%)	1 (0%)	30	67
1	1	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	2	224/226 (99%)	196 (88%)	25 (11%)	3 (1%)	9	42
1	3	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	4	224/226 (99%)	199 (89%)	22 (10%)	3 (1%)	9	42
1	5	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	67
1	6	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	67
1	7	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
1	8	224/226 (99%)	197 (88%)	25 (11%)	2 (1%)	14	51
1	9	224/226 (99%)	193 (86%)	29 (13%)	2 (1%)	14	51
1	A	224/226 (99%)	189 (84%)	26 (12%)	9 (4%)	2	18
1	AA	224/226 (99%)	189 (84%)	30 (13%)	5 (2%)	5	29
1	AB	224/226 (99%)	182 (81%)	38 (17%)	4 (2%)	6	34
1	AC	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	AD	224/226 (99%)	183 (82%)	33 (15%)	8 (4%)	2	20
1	AE	224/226 (99%)	185 (83%)	35 (16%)	4 (2%)	6	34
1	AF	224/226 (99%)	193 (86%)	28 (12%)	3 (1%)	9	42
1	AG	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	14	51
1	AH	224/226 (99%)	186 (83%)	35 (16%)	3 (1%)	9	42
1	AI	224/226 (99%)	194 (87%)	26 (12%)	4 (2%)	6	34
1	AJ	224/226 (99%)	196 (88%)	25 (11%)	3 (1%)	9	42
1	AK	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	AL	224/226 (99%)	199 (89%)	22 (10%)	3 (1%)	9	42
1	AM	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	67
1	AN	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AO	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
1	AP	224/226 (99%)	197 (88%)	25 (11%)	2 (1%)	14	51
1	AQ	224/226 (99%)	193 (86%)	29 (13%)	2 (1%)	14	51
1	AR	224/226 (99%)	198 (88%)	25 (11%)	1 (0%)	30	67
1	B	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	C	224/226 (99%)	190 (85%)	29 (13%)	5 (2%)	5	29
1	D	224/226 (99%)	182 (81%)	38 (17%)	4 (2%)	6	34
1	E	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	F	224/226 (99%)	183 (82%)	33 (15%)	8 (4%)	2	20
1	G	224/226 (99%)	186 (83%)	31 (14%)	7 (3%)	3	22
1	H	224/226 (99%)	183 (82%)	36 (16%)	5 (2%)	5	29
1	I	224/226 (99%)	185 (83%)	35 (16%)	4 (2%)	6	34
1	J	224/226 (99%)	193 (86%)	28 (12%)	3 (1%)	9	42
1	K	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	14	51
1	L	224/226 (99%)	186 (83%)	35 (16%)	3 (1%)	9	42
1	M	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	N	224/226 (99%)	196 (88%)	25 (11%)	3 (1%)	9	42
1	O	224/226 (99%)	193 (86%)	28 (12%)	3 (1%)	9	42
1	P	224/226 (99%)	199 (89%)	22 (10%)	3 (1%)	9	42
1	Q	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	67
1	R	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	67
1	S	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
1	T	224/226 (99%)	197 (88%)	26 (12%)	1 (0%)	30	67
1	U	224/226 (99%)	193 (86%)	29 (13%)	2 (1%)	14	51
1	V	224/226 (99%)	198 (88%)	25 (11%)	1 (0%)	30	67
1	W	224/226 (99%)	189 (84%)	26 (12%)	9 (4%)	2	18
1	X	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	Y	224/226 (99%)	189 (84%)	30 (13%)	5 (2%)	5	29
1	Z	224/226 (99%)	182 (81%)	38 (17%)	4 (2%)	6	34
1	a	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	b	224/226 (99%)	183 (82%)	33 (15%)	8 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	224/226 (99%)	186 (83%)	31 (14%)	7 (3%)	3	22
1	d	224/226 (99%)	183 (82%)	36 (16%)	5 (2%)	5	29
1	e	224/226 (99%)	186 (83%)	34 (15%)	4 (2%)	6	34
1	f	224/226 (99%)	193 (86%)	28 (12%)	3 (1%)	9	42
1	g	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	14	51
1	h	224/226 (99%)	186 (83%)	35 (16%)	3 (1%)	9	42
1	i	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	j	224/226 (99%)	196 (88%)	25 (11%)	3 (1%)	9	42
1	k	224/226 (99%)	194 (87%)	27 (12%)	3 (1%)	9	42
1	l	224/226 (99%)	199 (89%)	22 (10%)	3 (1%)	9	42
1	m	224/226 (99%)	195 (87%)	28 (12%)	1 (0%)	30	67
1	n	224/226 (99%)	196 (88%)	27 (12%)	1 (0%)	30	67
1	o	224/226 (99%)	204 (91%)	20 (9%)	0	100	100
1	p	224/226 (99%)	197 (88%)	25 (11%)	2 (1%)	14	51
1	q	224/226 (99%)	193 (86%)	29 (13%)	2 (1%)	14	51
1	r	224/226 (99%)	198 (88%)	25 (11%)	1 (0%)	30	67
1	s	224/226 (99%)	189 (84%)	30 (13%)	5 (2%)	5	29
1	t	224/226 (99%)	182 (81%)	38 (17%)	4 (2%)	6	34
1	u	224/226 (99%)	191 (85%)	29 (13%)	4 (2%)	6	34
1	v	224/226 (99%)	183 (82%)	33 (15%)	8 (4%)	2	20
1	w	224/226 (99%)	185 (83%)	35 (16%)	4 (2%)	6	34
1	x	224/226 (99%)	193 (86%)	28 (12%)	3 (1%)	9	42
1	y	224/226 (99%)	196 (88%)	26 (12%)	2 (1%)	14	51
1	z	224/226 (99%)	186 (83%)	35 (16%)	3 (1%)	9	42
All	All	17920/18080 (99%)	15383 (86%)	2279 (13%)	258 (1%)	11	40

All (258) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	62	PRO
1	A	66	PRO
1	A	67	PRO
1	A	70	PRO

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Mol	Chain	Res	Type
1	B	61	SER
1	B	62	PRO
1	B	70	PRO
1	C	58	SER
1	C	62	PRO
1	C	67	PRO
1	C	70	PRO
1	C	105	PRO
1	D	62	PRO
1	D	66	PRO
1	D	67	PRO
1	D	70	PRO
1	E	66	PRO
1	F	56	PRO
1	F	61	SER
1	F	62	PRO
1	F	66	PRO
1	F	67	PRO
1	F	70	PRO
1	F	157	ALA
1	G	66	PRO
1	G	67	PRO
1	G	156	TRP
1	H	62	PRO
1	H	67	PRO
1	H	70	PRO
1	I	62	PRO
1	I	70	PRO
1	J	56	PRO
1	J	156	TRP
1	K	66	PRO
1	K	68	THR
1	L	67	PRO
1	L	70	PRO
1	M	62	PRO
1	M	67	PRO
1	M	70	PRO
1	N	62	PRO
1	O	41	PHE
1	O	70	PRO
1	P	56	PRO
1	P	156	TRP

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Mol	Chain	Res	Type
1	R	106	VAL
1	T	56	PRO
1	U	56	PRO
1	V	56	PRO
1	W	61	SER
1	W	62	PRO
1	W	66	PRO
1	W	67	PRO
1	W	70	PRO
1	X	61	SER
1	X	62	PRO
1	X	70	PRO
1	Y	58	SER
1	Y	62	PRO
1	Y	67	PRO
1	Y	70	PRO
1	Z	62	PRO
1	Z	66	PRO
1	Z	67	PRO
1	Z	70	PRO
1	a	66	PRO
1	b	56	PRO
1	b	61	SER
1	b	62	PRO
1	b	66	PRO
1	b	67	PRO
1	b	70	PRO
1	b	157	ALA
1	c	66	PRO
1	c	67	PRO
1	c	156	TRP
1	d	62	PRO
1	d	67	PRO
1	d	70	PRO
1	e	62	PRO
1	e	70	PRO
1	f	56	PRO
1	f	156	TRP
1	g	66	PRO
1	g	68	THR
1	h	67	PRO
1	h	70	PRO

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Mol	Chain	Res	Type
1	i	62	PRO
1	i	67	PRO
1	i	70	PRO
1	j	62	PRO
1	k	41	PHE
1	k	70	PRO
1	l	56	PRO
1	l	156	TRP
1	n	106	VAL
1	p	56	PRO
1	p	156	TRP
1	q	56	PRO
1	r	56	PRO
1	s	58	SER
1	s	62	PRO
1	s	67	PRO
1	s	70	PRO
1	t	62	PRO
1	t	66	PRO
1	t	67	PRO
1	t	70	PRO
1	u	66	PRO
1	v	56	PRO
1	v	61	SER
1	v	62	PRO
1	v	66	PRO
1	v	67	PRO
1	v	70	PRO
1	v	157	ALA
1	w	62	PRO
1	w	70	PRO
1	x	56	PRO
1	x	156	TRP
1	y	66	PRO
1	y	68	THR
1	z	67	PRO
1	z	70	PRO
1	1	62	PRO
1	1	67	PRO
1	1	70	PRO
1	2	62	PRO
1	3	41	PHE

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Mol	Chain	Res	Type
1	3	70	PRO
1	4	56	PRO
1	4	156	TRP
1	6	106	VAL
1	8	56	PRO
1	8	156	TRP
1	9	56	PRO
1	0	56	PRO
1	AA	58	SER
1	AA	62	PRO
1	AA	67	PRO
1	AA	70	PRO
1	AB	62	PRO
1	AB	66	PRO
1	AB	67	PRO
1	AB	70	PRO
1	AC	66	PRO
1	AD	56	PRO
1	AD	61	SER
1	AD	62	PRO
1	AD	66	PRO
1	AD	67	PRO
1	AD	70	PRO
1	AD	157	ALA
1	AE	62	PRO
1	AE	70	PRO
1	AF	56	PRO
1	AF	156	TRP
1	AG	66	PRO
1	AG	68	THR
1	AH	67	PRO
1	AH	70	PRO
1	AI	62	PRO
1	AI	67	PRO
1	AI	70	PRO
1	AJ	62	PRO
1	AK	41	PHE
1	AK	70	PRO
1	AL	56	PRO
1	AL	156	TRP
1	AN	106	VAL
1	AP	56	PRO

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Mol	Chain	Res	Type
1	AP	156	TRP
1	AQ	56	PRO
1	AR	56	PRO
1	A	101	GLN
1	B	65	CYS
1	E	69	CYS
1	E	101	GLN
1	I	61	SER
1	J	105	PRO
1	N	57	ILE
1	P	106	VAL
1	W	101	GLN
1	X	65	CYS
1	Y	105	PRO
1	a	69	CYS
1	a	101	GLN
1	e	61	SER
1	j	57	ILE
1	l	106	VAL
1	u	69	CYS
1	u	101	GLN
1	w	61	SER
1	x	105	PRO
1	2	57	ILE
1	4	106	VAL
1	AA	105	PRO
1	AC	69	CYS
1	AC	101	GLN
1	AE	61	SER
1	AJ	57	ILE
1	AL	106	VAL
1	A	63	THR
1	F	187	SER
1	G	157	ALA
1	G	171	SER
1	O	156	TRP
1	W	63	THR
1	b	187	SER
1	c	157	ALA
1	c	171	SER
1	f	105	PRO
1	k	156	TRP

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Mol	Chain	Res	Type
1	s	105	PRO
1	v	187	SER
1	3	156	TRP
1	AD	187	SER
1	AF	105	PRO
1	AK	156	TRP
1	A	155	SER
1	E	195	ILE
1	G	47	VAL
1	I	101	GLN
1	Q	35	TRP
1	W	155	SER
1	a	195	ILE
1	c	47	VAL
1	e	101	GLN
1	m	35	TRP
1	u	195	ILE
1	w	101	GLN
1	5	35	TRP
1	AC	195	ILE
1	AE	101	GLN
1	AM	35	TRP
1	A	105	PRO
1	L	156	TRP
1	N	66	PRO
1	U	157	ALA
1	W	105	PRO
1	h	156	TRP
1	j	66	PRO
1	q	157	ALA
1	z	156	TRP
1	2	66	PRO
1	9	157	ALA
1	AH	156	TRP
1	AJ	66	PRO
1	AQ	157	ALA
1	G	188	PRO
1	c	188	PRO
1	H	102	GLY
1	H	224	VAL
1	d	102	GLY
1	d	224	VAL

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Mol	Chain	Res	Type
1	AI	159	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	24/206 (12%)	24 (100%)	0	100	100
1	1	21/206 (10%)	21 (100%)	0	100	100
1	2	20/206 (10%)	20 (100%)	0	100	100
1	3	24/206 (12%)	24 (100%)	0	100	100
1	4	24/206 (12%)	24 (100%)	0	100	100
1	5	22/206 (11%)	22 (100%)	0	100	100
1	6	26/206 (13%)	26 (100%)	0	100	100
1	7	24/206 (12%)	24 (100%)	0	100	100
1	8	23/206 (11%)	23 (100%)	0	100	100
1	9	23/206 (11%)	23 (100%)	0	100	100
1	A	23/206 (11%)	23 (100%)	0	100	100
1	AA	19/206 (9%)	19 (100%)	0	100	100
1	AB	23/206 (11%)	23 (100%)	0	100	100
1	AC	22/206 (11%)	22 (100%)	0	100	100
1	AD	23/206 (11%)	23 (100%)	0	100	100
1	AE	24/206 (12%)	24 (100%)	0	100	100
1	AF	21/206 (10%)	21 (100%)	0	100	100
1	AG	22/206 (11%)	22 (100%)	0	100	100
1	AH	17/206 (8%)	17 (100%)	0	100	100
1	AI	21/206 (10%)	21 (100%)	0	100	100
1	AJ	20/206 (10%)	20 (100%)	0	100	100
1	AK	24/206 (12%)	24 (100%)	0	100	100
1	AL	24/206 (12%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	22/206 (11%)	22 (100%)	0	100	100
1	AN	26/206 (13%)	26 (100%)	0	100	100
1	AO	24/206 (12%)	24 (100%)	0	100	100
1	AP	23/206 (11%)	23 (100%)	0	100	100
1	AQ	23/206 (11%)	23 (100%)	0	100	100
1	AR	24/206 (12%)	24 (100%)	0	100	100
1	B	23/206 (11%)	23 (100%)	0	100	100
1	C	19/206 (9%)	19 (100%)	0	100	100
1	D	23/206 (11%)	23 (100%)	0	100	100
1	E	22/206 (11%)	22 (100%)	0	100	100
1	F	23/206 (11%)	23 (100%)	0	100	100
1	G	23/206 (11%)	23 (100%)	0	100	100
1	H	22/206 (11%)	22 (100%)	0	100	100
1	I	24/206 (12%)	24 (100%)	0	100	100
1	J	21/206 (10%)	21 (100%)	0	100	100
1	K	22/206 (11%)	22 (100%)	0	100	100
1	L	17/206 (8%)	17 (100%)	0	100	100
1	M	21/206 (10%)	21 (100%)	0	100	100
1	N	20/206 (10%)	20 (100%)	0	100	100
1	O	24/206 (12%)	24 (100%)	0	100	100
1	P	24/206 (12%)	24 (100%)	0	100	100
1	Q	22/206 (11%)	22 (100%)	0	100	100
1	R	26/206 (13%)	26 (100%)	0	100	100
1	S	24/206 (12%)	24 (100%)	0	100	100
1	T	23/206 (11%)	23 (100%)	0	100	100
1	U	23/206 (11%)	23 (100%)	0	100	100
1	V	24/206 (12%)	24 (100%)	0	100	100
1	W	23/206 (11%)	23 (100%)	0	100	100
1	X	23/206 (11%)	23 (100%)	0	100	100
1	Y	19/206 (9%)	19 (100%)	0	100	100
1	Z	23/206 (11%)	23 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	22/206 (11%)	22 (100%)	0	100	100
1	b	23/206 (11%)	23 (100%)	0	100	100
1	c	23/206 (11%)	23 (100%)	0	100	100
1	d	22/206 (11%)	22 (100%)	0	100	100
1	e	24/206 (12%)	24 (100%)	0	100	100
1	f	21/206 (10%)	21 (100%)	0	100	100
1	g	22/206 (11%)	22 (100%)	0	100	100
1	h	17/206 (8%)	17 (100%)	0	100	100
1	i	21/206 (10%)	21 (100%)	0	100	100
1	j	20/206 (10%)	20 (100%)	0	100	100
1	k	24/206 (12%)	24 (100%)	0	100	100
1	l	24/206 (12%)	24 (100%)	0	100	100
1	m	22/206 (11%)	22 (100%)	0	100	100
1	n	26/206 (13%)	26 (100%)	0	100	100
1	o	24/206 (12%)	24 (100%)	0	100	100
1	p	23/206 (11%)	23 (100%)	0	100	100
1	q	23/206 (11%)	23 (100%)	0	100	100
1	r	24/206 (12%)	24 (100%)	0	100	100
1	s	19/206 (9%)	19 (100%)	0	100	100
1	t	23/206 (11%)	23 (100%)	0	100	100
1	u	22/206 (11%)	22 (100%)	0	100	100
1	v	23/206 (11%)	23 (100%)	0	100	100
1	w	24/206 (12%)	24 (100%)	0	100	100
1	x	21/206 (10%)	21 (100%)	0	100	100
1	y	22/206 (11%)	22 (100%)	0	100	100
1	z	17/206 (8%)	17 (100%)	0	100	100
All	All	1790/16480 (11%)	1790 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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](#)

There are no chain breaks in this entry.

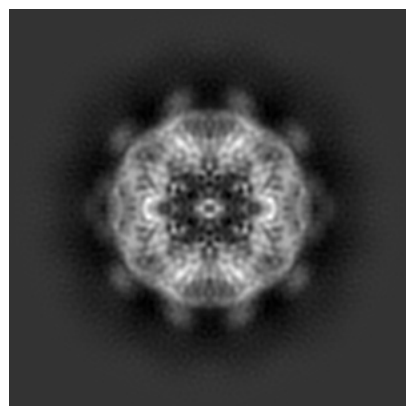
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39395. These allow visual inspection of the internal detail of the map and identification of artifacts.

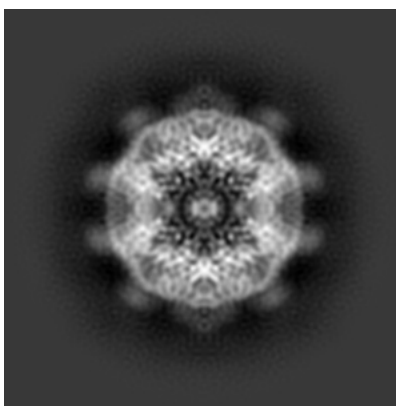
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

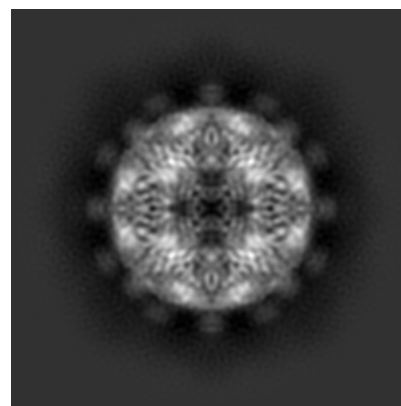
6.1.1 Primary map



X

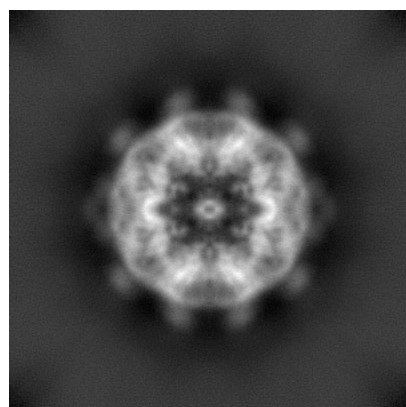


Y

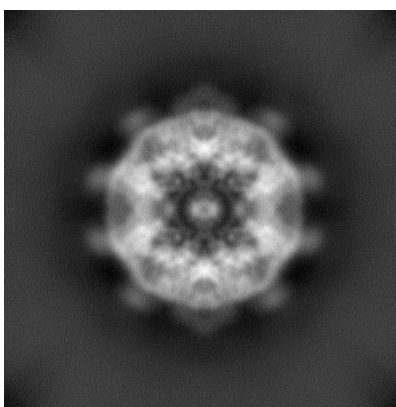


Z

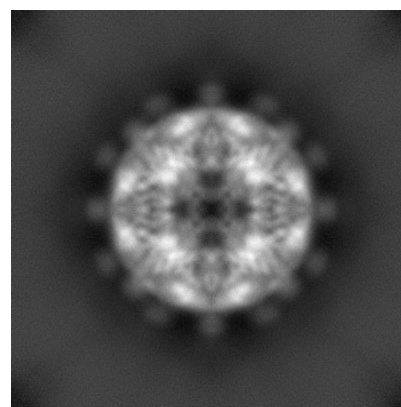
6.1.2 Raw map



X



Y

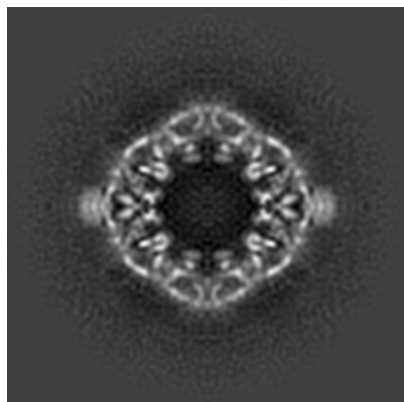


Z

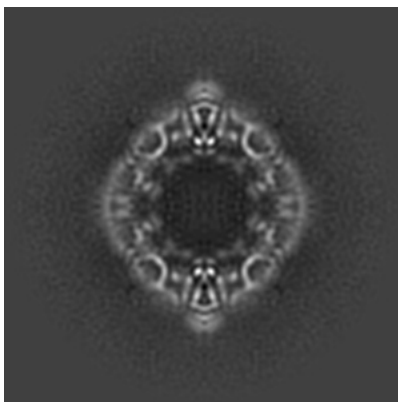
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

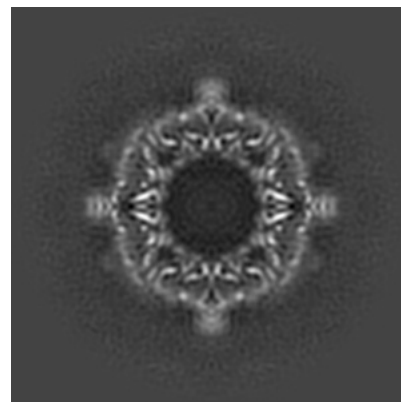
6.2.1 Primary map



X Index: 200

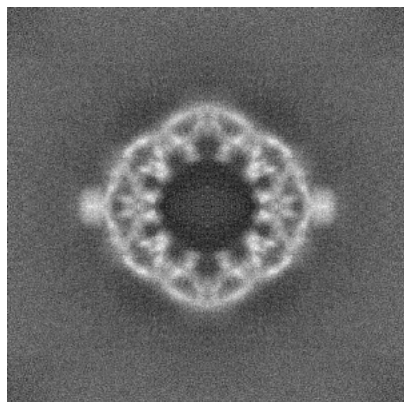


Y Index: 200

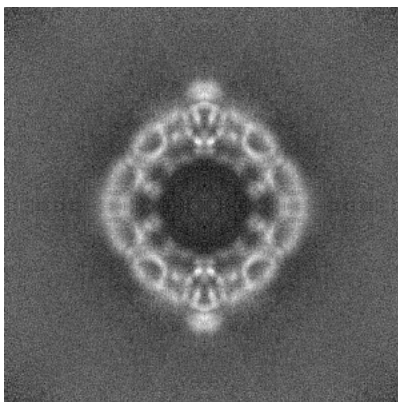


Z Index: 200

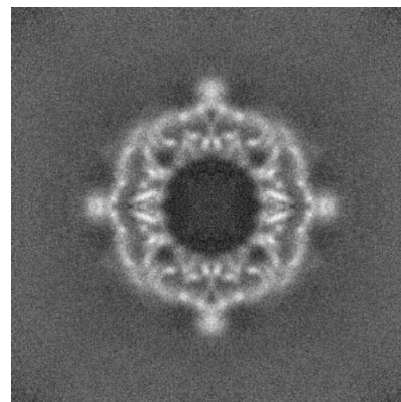
6.2.2 Raw map



X Index: 200



Y Index: 200

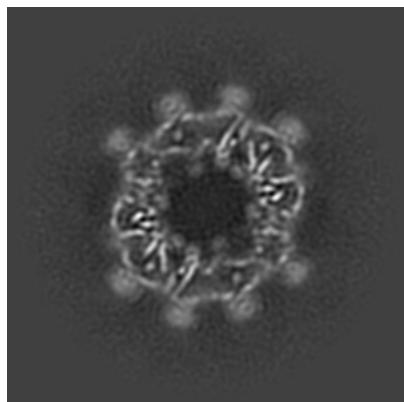


Z Index: 200

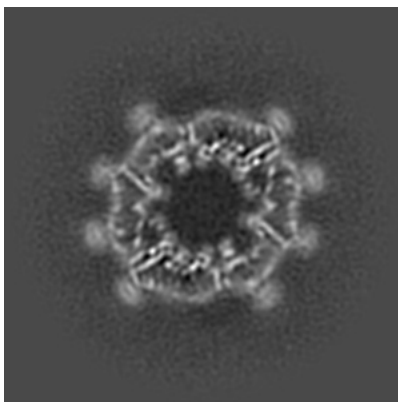
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

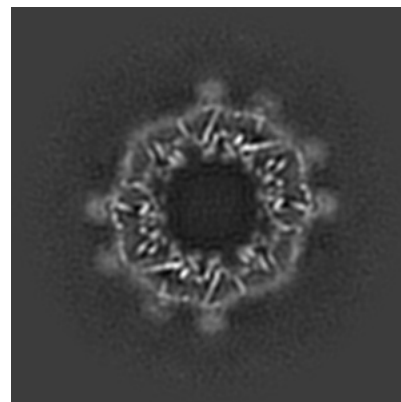
6.3.1 Primary map



X Index: 171

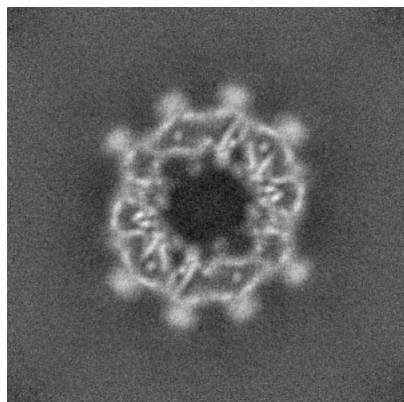


Y Index: 170

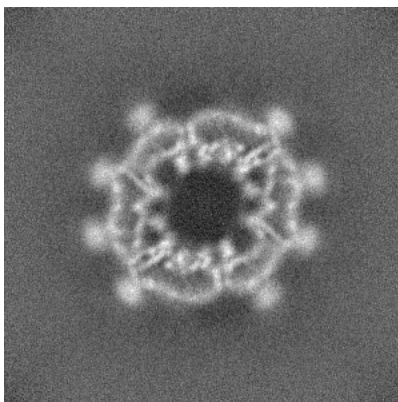


Z Index: 192

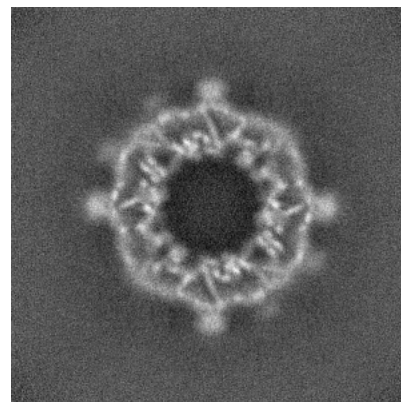
6.3.2 Raw map



X Index: 172



Y Index: 169

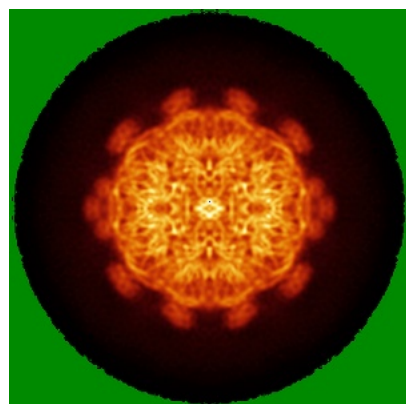


Z Index: 205

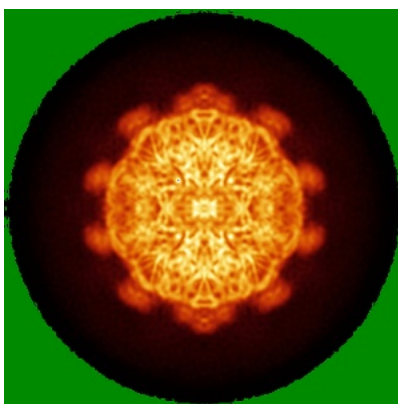
The images above show the largest variance slices of the map in three orthogonal directions.

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

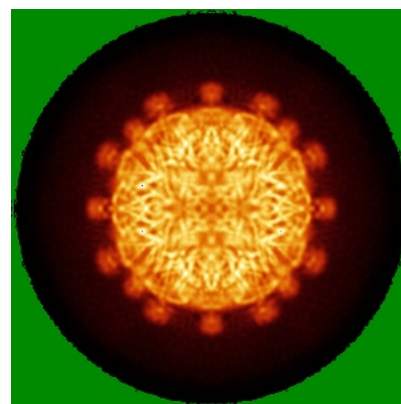
6.4.1 Primary map



X

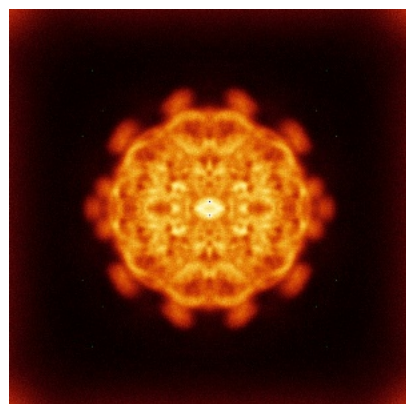


Y

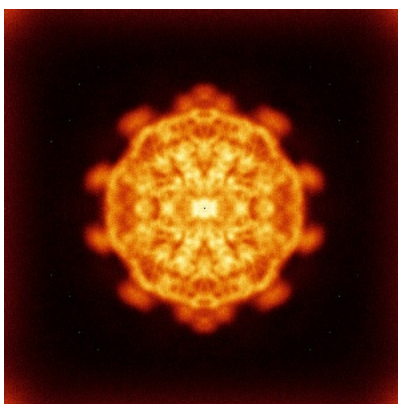


Z

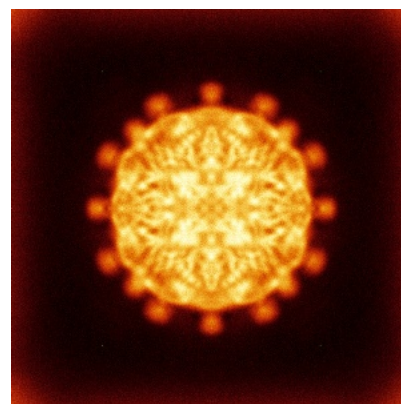
6.4.2 Raw map



X



Y

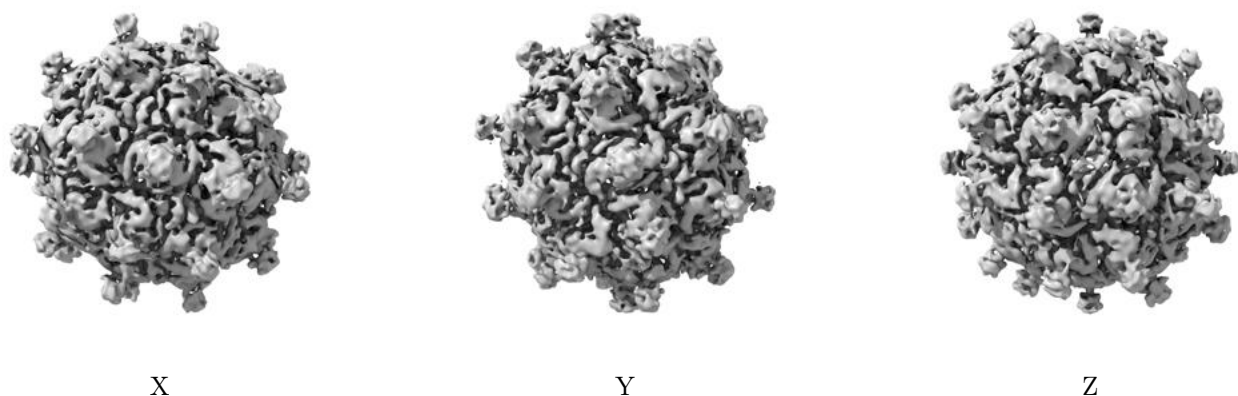


Z

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.

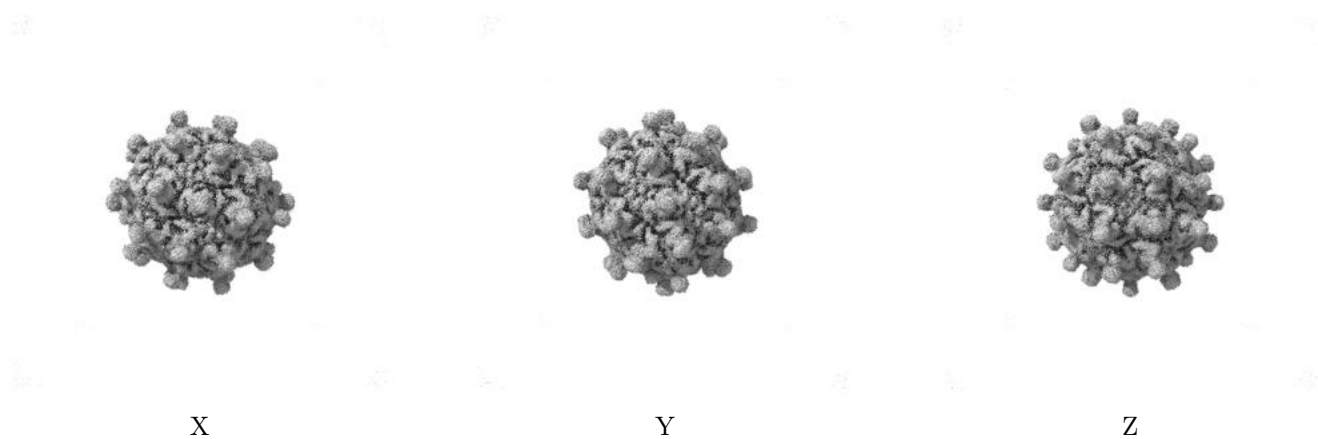
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

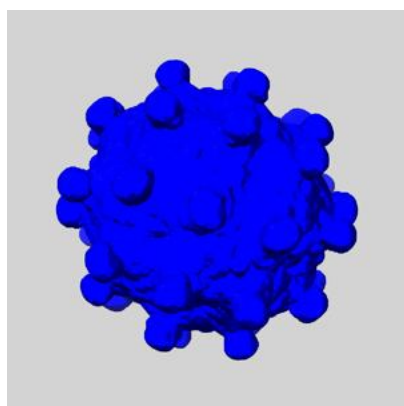
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

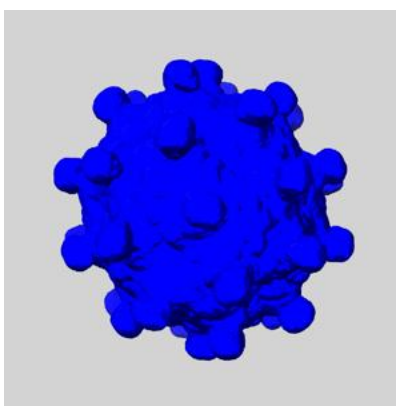
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

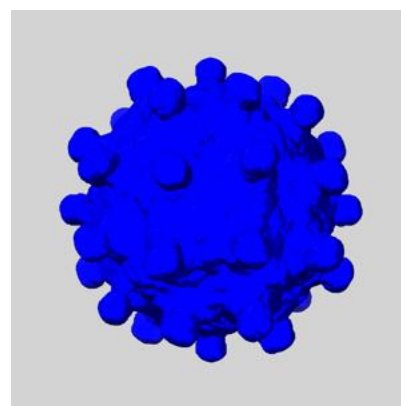
6.6.1 emd_39395_msk_1.map [i](#)



X



Y

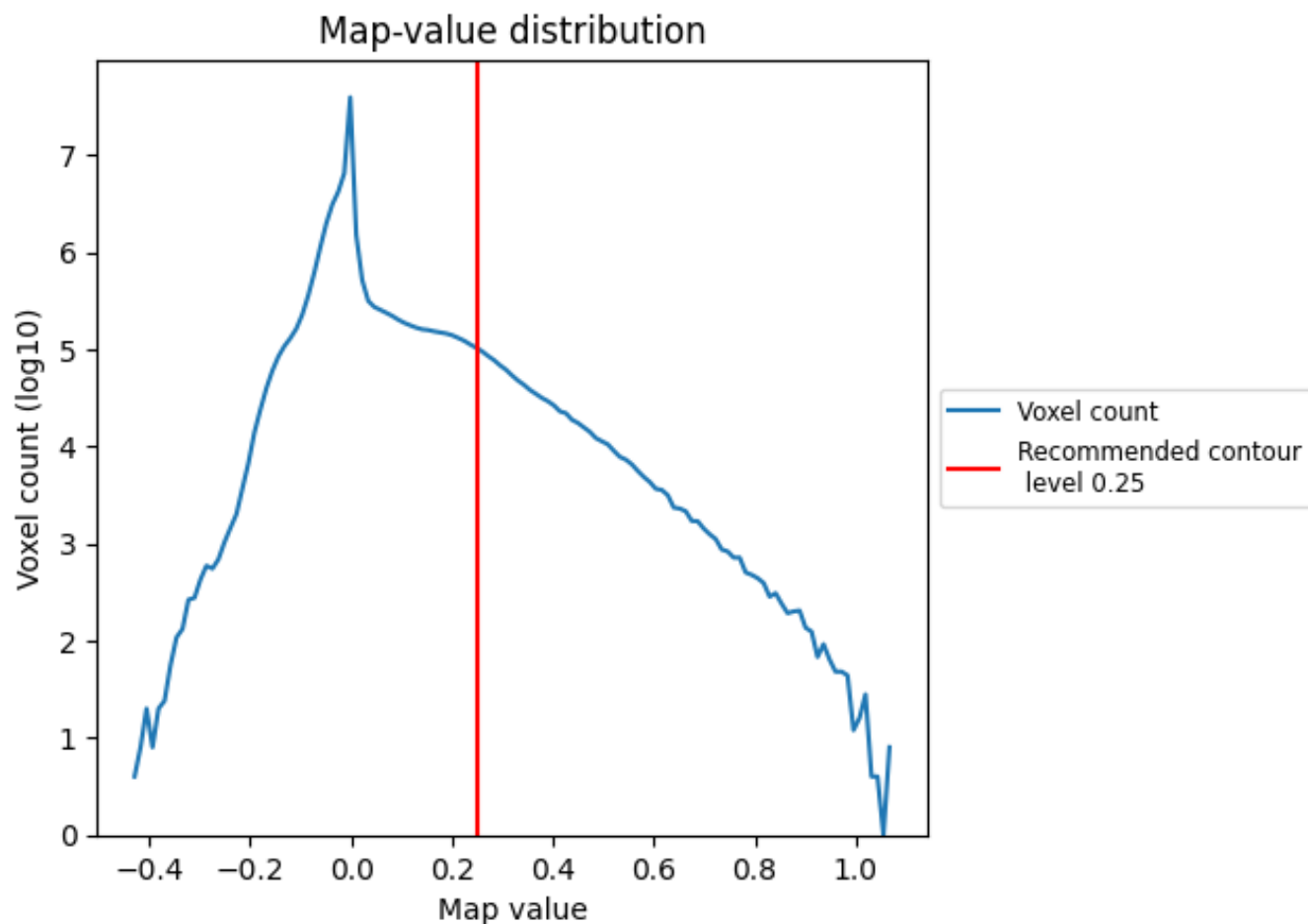


Z

7 Map analysis [i](#)

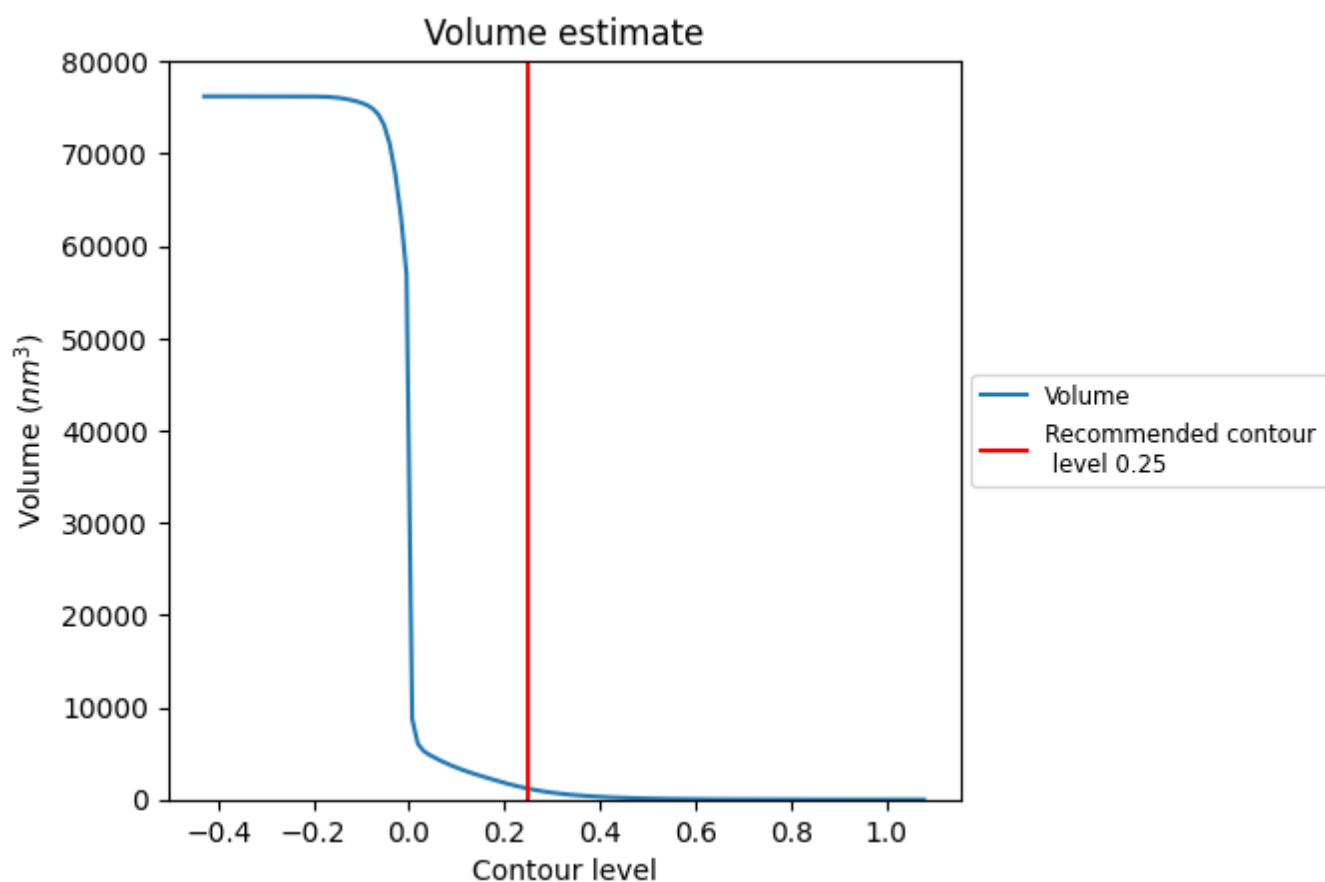
This section contains the results of statistical analysis of the map.

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.

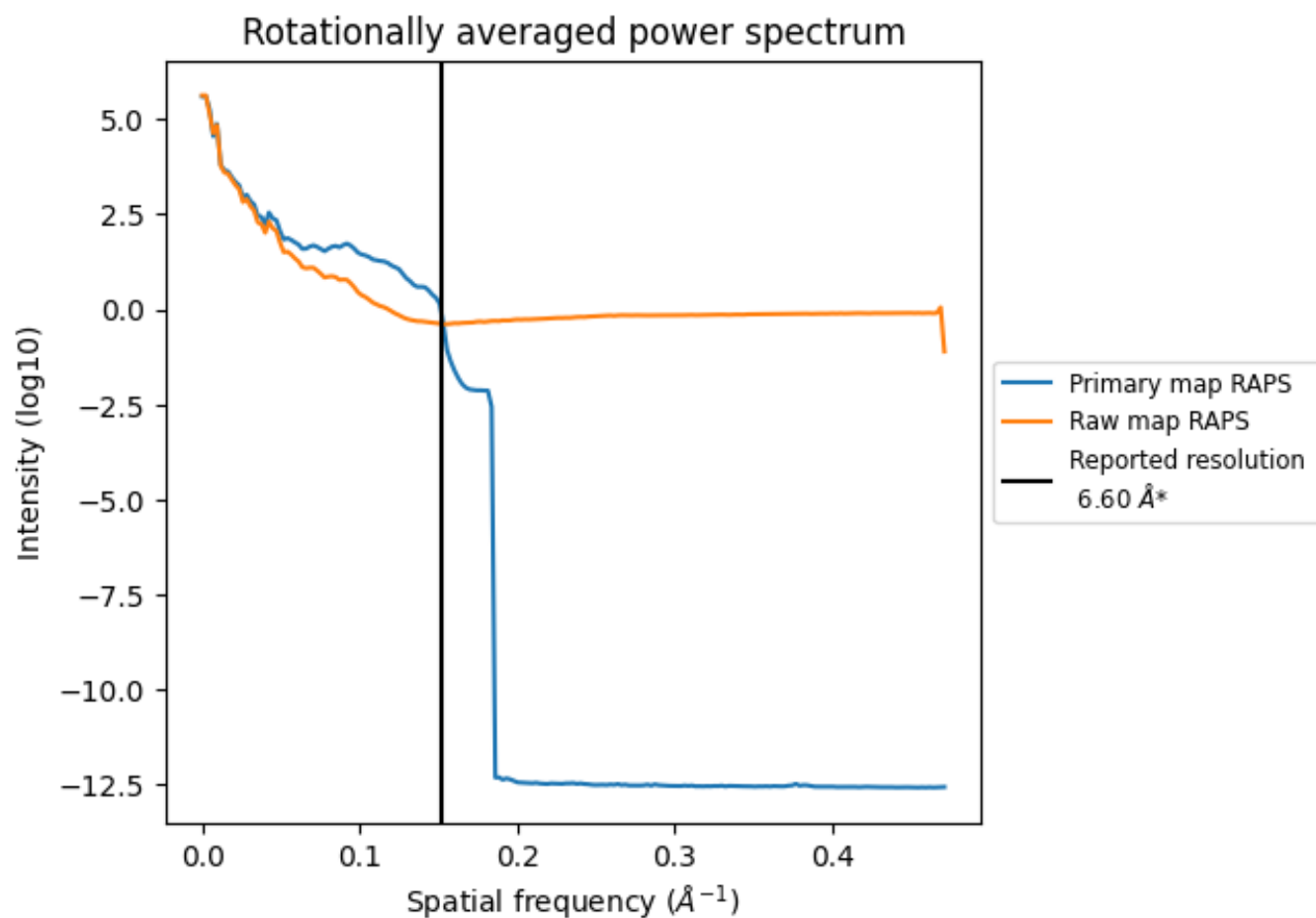
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1185 nm³; this corresponds to an approximate mass of 1070 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 ⓘ

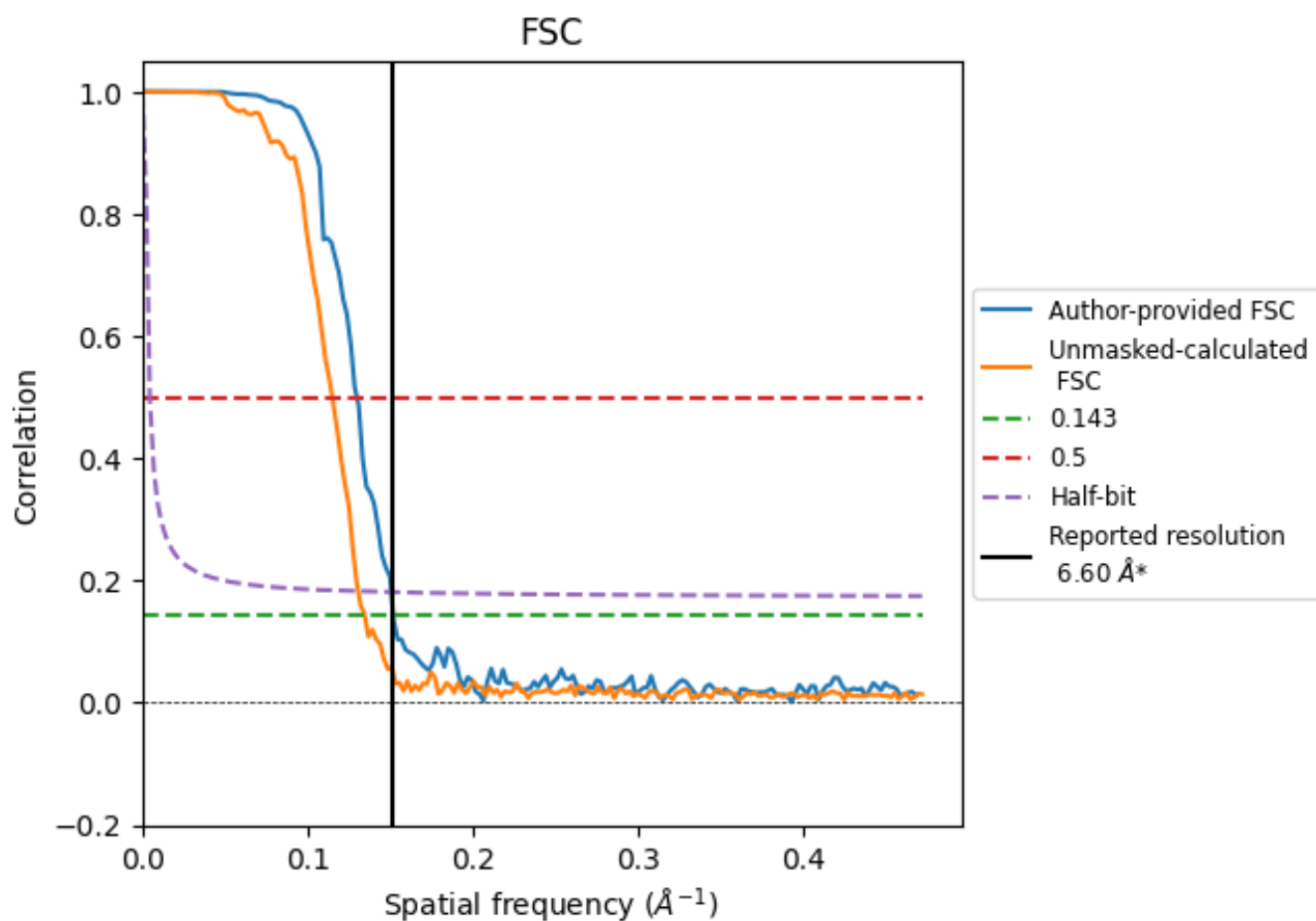


*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.152 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

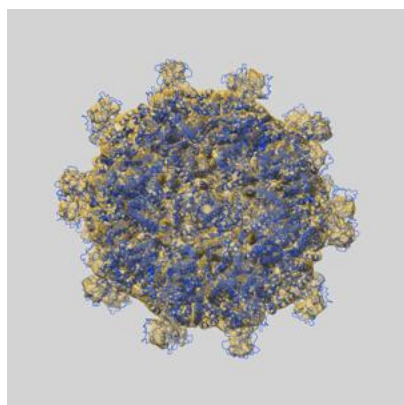
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.59	7.70	6.64
Unmasked-calculated*	7.43	8.70	7.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.43 differs from the reported value 6.6 by more than 10 %

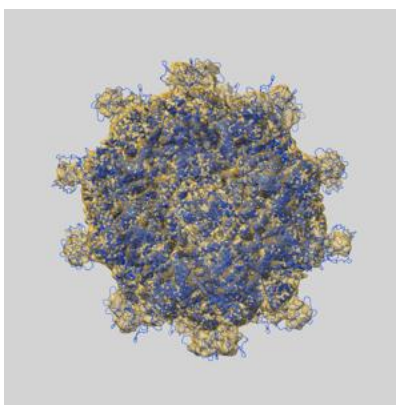
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39395 and PDB model 8YMJ. Per-residue inclusion information can be found in section 3 on page 11.

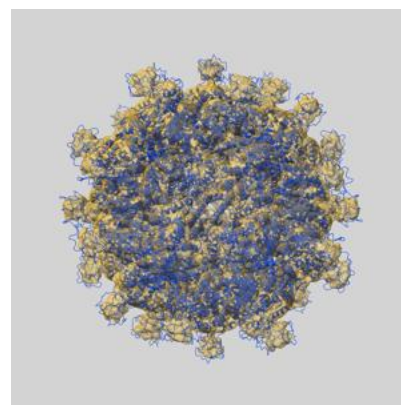
9.1 Map-model overlay [i](#)



X



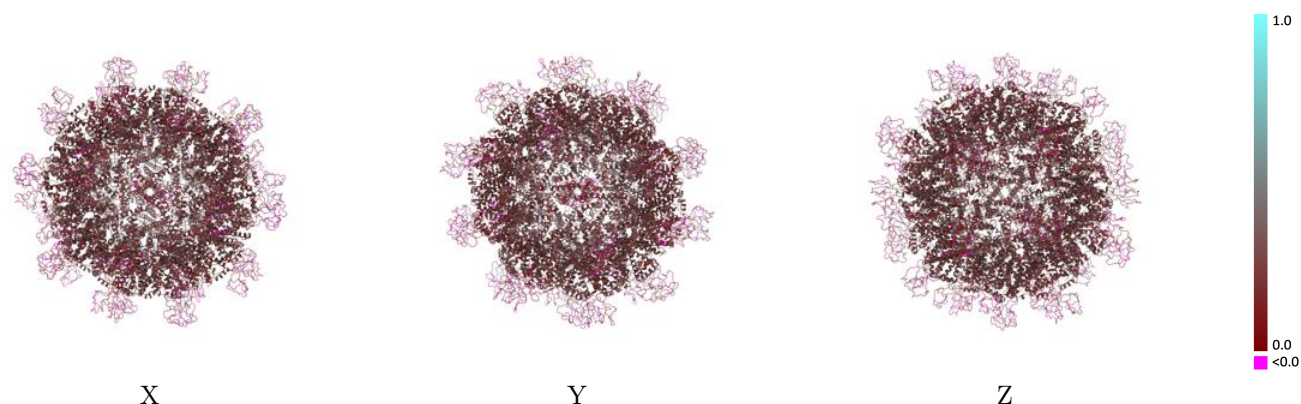
Y



Z

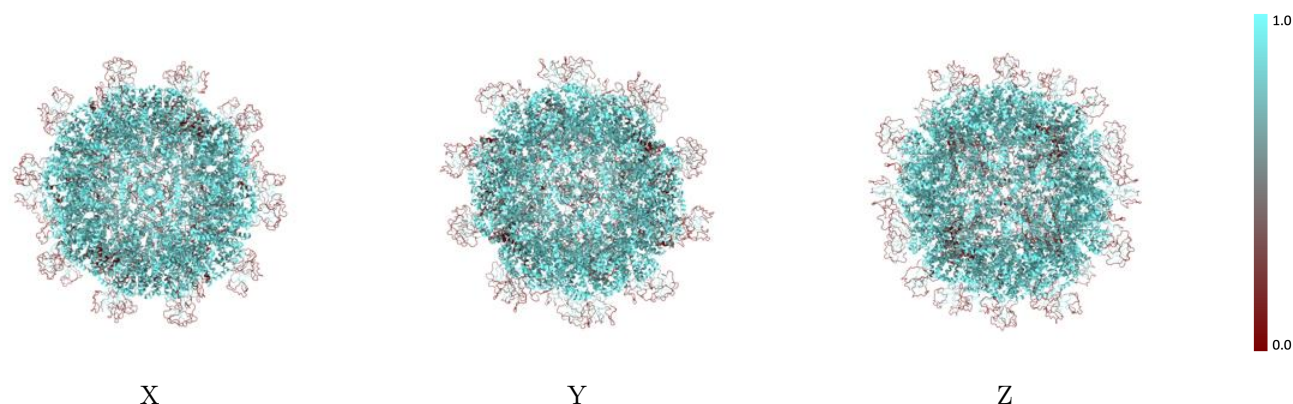
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



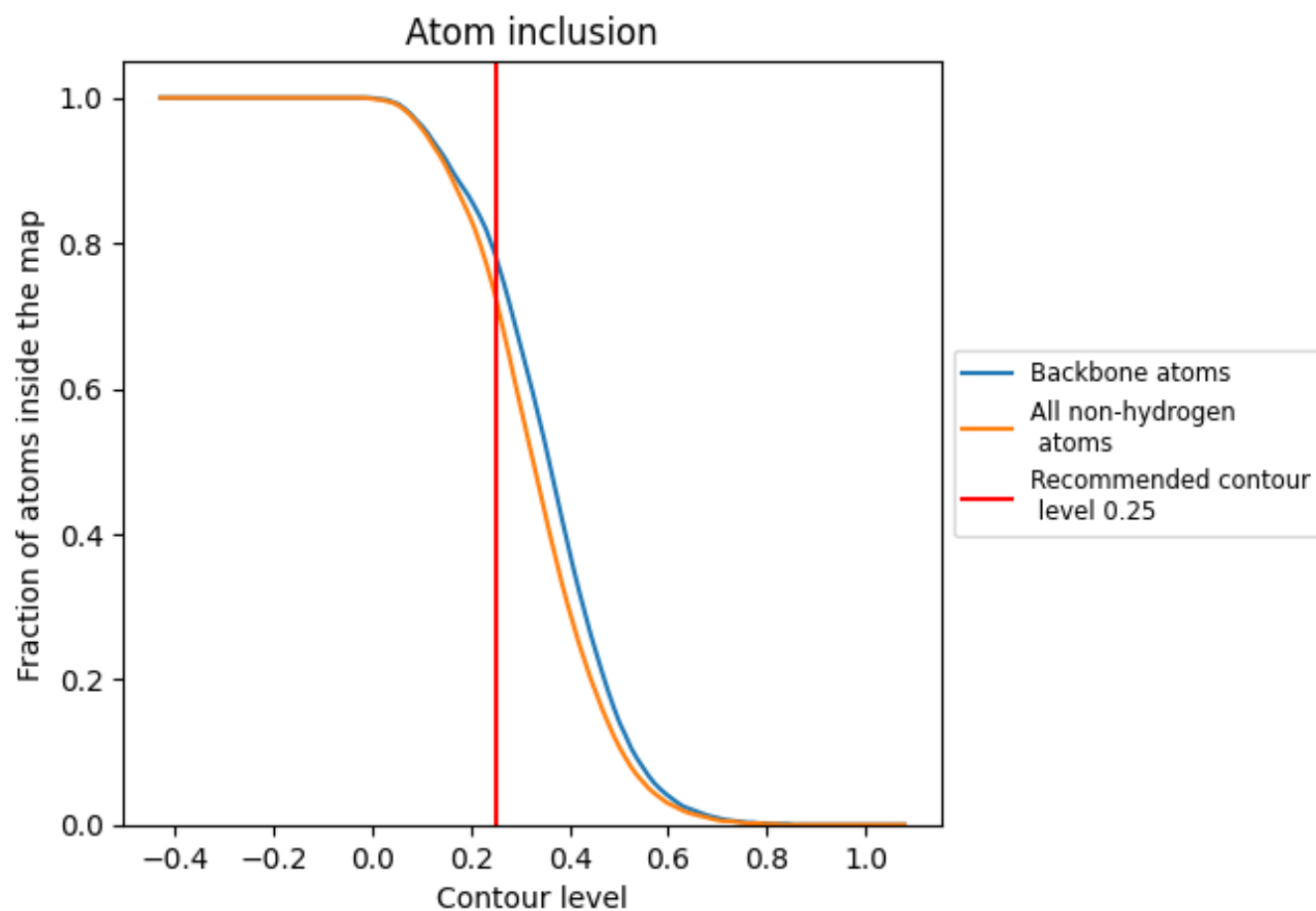
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.2330
0	 0.6980	 0.2280
1	 0.7030	 0.2270
2	 0.7150	 0.2220
3	 0.7630	 0.2420
4	 0.7440	 0.2380
5	 0.7190	 0.2280
6	 0.7350	 0.2340
7	 0.7450	 0.2370
8	 0.7260	 0.2350
9	 0.7470	 0.2340
A	 0.7830	 0.2480
AA	 0.7580	 0.2300
AB	 0.7360	 0.2390
AC	 0.7790	 0.2410
AD	 0.7710	 0.2370
AE	 0.6750	 0.2300
AF	 0.6540	 0.2260
AG	 0.6790	 0.2350
AH	 0.6690	 0.2250
AI	 0.7030	 0.2230
AJ	 0.7150	 0.2230
AK	 0.7630	 0.2420
AL	 0.7440	 0.2360
AM	 0.7190	 0.2300
AN	 0.7350	 0.2340
AO	 0.7450	 0.2370
AP	 0.7260	 0.2370
AQ	 0.7470	 0.2320
AR	 0.6980	 0.2260
B	 0.7880	 0.2460
C	 0.7580	 0.2330
D	 0.7360	 0.2360
E	 0.7790	 0.2380
F	 0.7710	 0.2390



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Chain	Atom inclusion	Q-score
G	 0.6990	 0.2280
H	 0.7390	 0.2300
I	 0.6750	 0.2310
J	 0.6540	 0.2230
K	 0.6790	 0.2340
L	 0.6690	 0.2230
M	 0.7030	 0.2260
N	 0.7150	 0.2240
O	 0.7630	 0.2410
P	 0.7440	 0.2380
Q	 0.7190	 0.2300
R	 0.7350	 0.2340
S	 0.7450	 0.2380
T	 0.7280	 0.2330
U	 0.7470	 0.2300
V	 0.6980	 0.2280
W	 0.7830	 0.2470
X	 0.7880	 0.2440
Y	 0.7580	 0.2320
Z	 0.7360	 0.2360
a	 0.7790	 0.2400
b	 0.7710	 0.2360
c	 0.6990	 0.2300
d	 0.7390	 0.2300
e	 0.6750	 0.2310
f	 0.6540	 0.2210
g	 0.6790	 0.2330
h	 0.6690	 0.2240
i	 0.7030	 0.2250
j	 0.7150	 0.2250
k	 0.7630	 0.2430
l	 0.7440	 0.2370
m	 0.7190	 0.2300
n	 0.7350	 0.2320
o	 0.7450	 0.2370
p	 0.7260	 0.2360
q	 0.7470	 0.2310
r	 0.6980	 0.2300
s	 0.7580	 0.2300
t	 0.7360	 0.2390
u	 0.7790	 0.2390
v	 0.7710	 0.2370

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Chain	Atom inclusion	Q-score
w	 0.6750	 0.2300
x	 0.6540	 0.2250
y	 0.6790	 0.2340
z	 0.6690	 0.2250