



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:27 PM UTC

PDB ID : 6QZF / pdb_00006qzf
EMDB ID : EMD-4685
Title : The cryo-EM structure of the collar complex and tail axis in genome emptied bacteriophage phi29
Authors : Xu, J.; Wang, D.; Gui, M.; Xiang, Y.
Deposited on : 2019-03-11
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

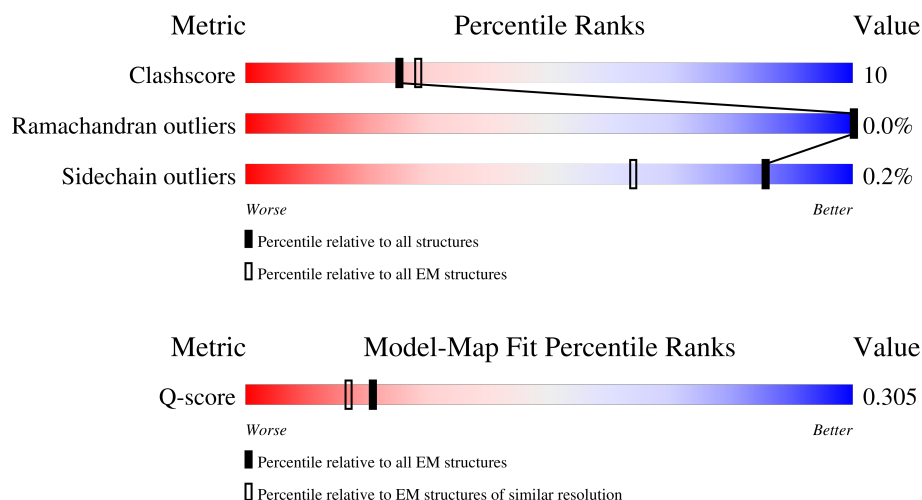
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	0a	309	74% 69% 22% 9%
1	0b	309	75% 68% 23% 9%
1	0c	309	75% 70% 21% 9%
1	0d	309	74% 69% 22% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	0e	309	74% 69% 22% 9%
1	0f	309	75% 67% 24% 9%
1	0g	309	74% 67% 23% 9%
1	0h	309	75% 69% 22% 9%
1	0i	309	75% 69% 22% 9%
1	0j	309	75% 69% 22% 9%
1	0k	309	74% 68% 23% 9%
1	0l	309	75% 69% 22% 9%
2	0A	293	9% 70% 29% ..
2	0B	293	9% 67% 32% .
2	0C	293	9% 62% 37% ..
2	0D	293	9% 65% 34% ..
2	0E	293	9% 68% 31% ..
2	0F	293	9% 65% 34% ..
2	0G	293	10% 66% 33% ..
2	0H	293	10% 69% 30% ..
2	0I	293	9% 68% 31% ..
2	0J	293	9% 69% 30% ..
2	0K	293	9% 68% 30% ..
2	0L	293	9% 67% 32% ..
3	A	854	5% 5% . 94%
3	B	854	5% 5% . 93%
3	C	854	6% 6% . 93%
3	D	854	5% 5% . 94%
3	E	854	5% 5% . 93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
3	F	854		93%
3	G	854		94%
3	H	854		93%
3	I	854		93%
3	J	854		94%
3	K	854		93%
3	L	854		93%
3	M	854		94%
3	N	854		93%
3	O	854		93%
3	P	854		94%
3	Q	854		93%
3	R	854		93%
3	S	854		94%
3	T	854		93%
3	U	854		93%
3	V	854		94%
3	W	854		93%
3	X	854		93%
3	Y	854		94%
3	Z	854		93%
3	a	854		93%
3	b	854		94%
3	c	854		93%
3	d	854		93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
3	e	854	5% 5%	94%
3	f	854	5% 5%	93%
3	g	854	6% 6%	93%
3	h	854	5% 5%	94%
3	i	854	5% 5%	93%
3	j	854	6% 6%	93%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 71628 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0a	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0b	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0c	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0d	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0e	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0f	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0g	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0h	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0i	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0j	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0k	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		
1	0l	280	Total	C	N	O	S	0	0
			2240	1429	376	428	7		

- Molecule 2 is a protein called Proximal tail tube connector protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0A	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0B	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0C	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0D	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0E	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0F	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0G	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0H	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0I	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0J	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0K	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		
2	0L	291	Total	C	N	O	S	0	0
			2300	1416	397	479	8		

- Molecule 3 is a protein called Pre-neck appendage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	B	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	C	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	D	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	E	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	F	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	G	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	H	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	I	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	J	51	Total	C	N	O	S	0	0
			433	281	67	83	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	L	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	M	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	N	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	O	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	P	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	Q	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	R	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	S	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	T	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	U	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	V	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	W	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	X	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	Y	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	Z	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	a	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	b	51	Total 433	C 281	N 67	O 83	S 2	0	0
3	c	57	Total 482	C 312	N 74	O 92	S 4	0	0
3	d	61	Total 514	C 334	N 78	O 98	S 4	0	0
3	e	51	Total 433	C 281	N 67	O 83	S 2	0	0

Continued on next page...

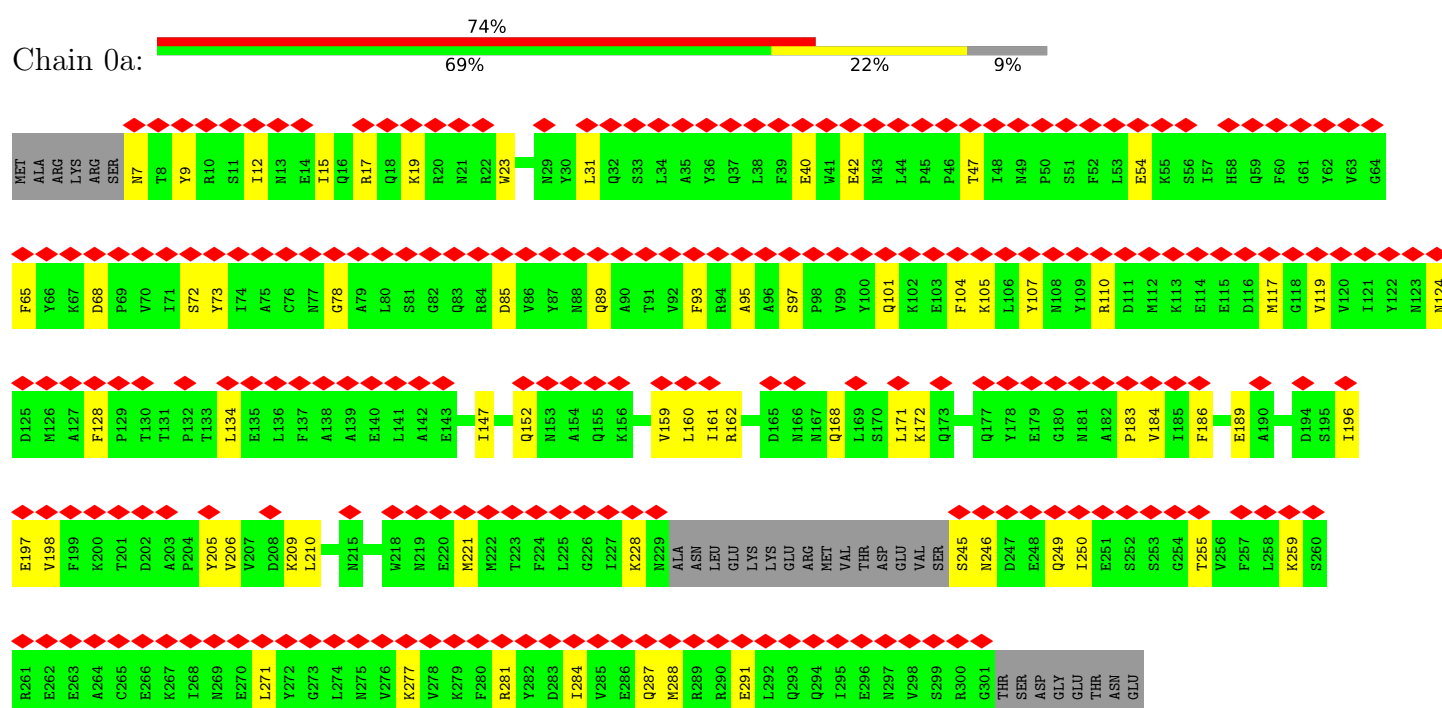
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	g	61	Total	C	N	O	S	0	0
			514	334	78	98	4		
3	h	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	i	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	j	61	Total	C	N	O	S	0	0
			514	334	78	98	4		

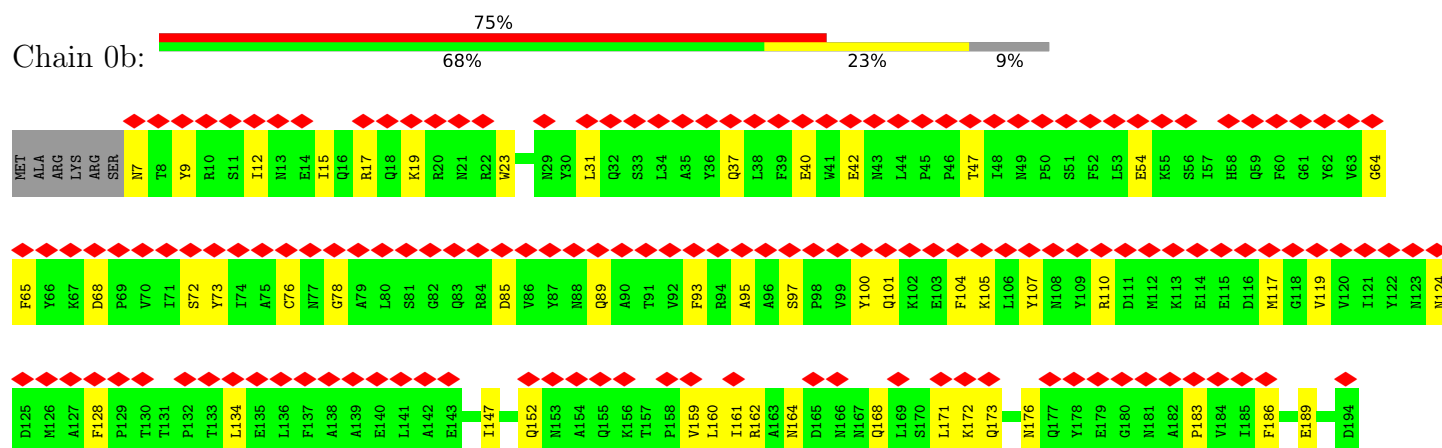
3 Residue-property plots

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: Portal protein

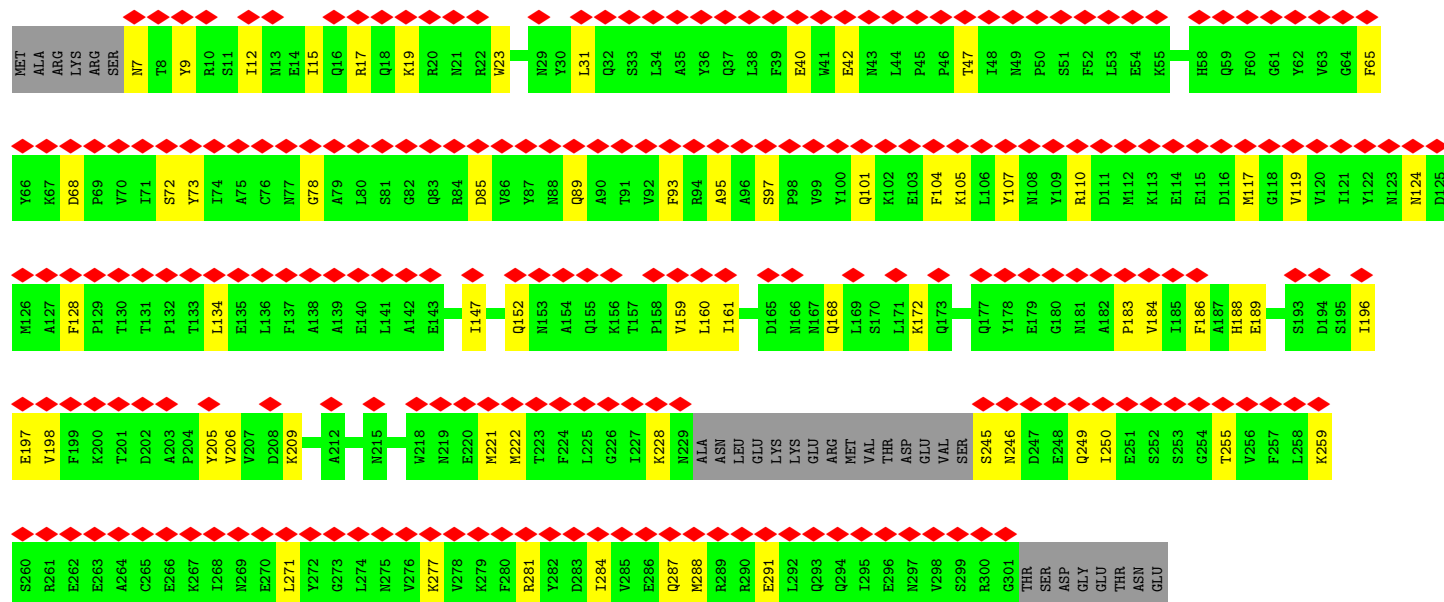
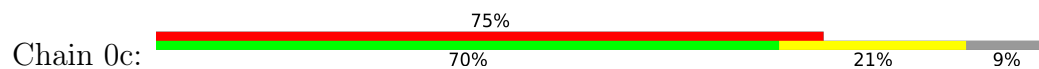


• Molecule 1: Portal protein

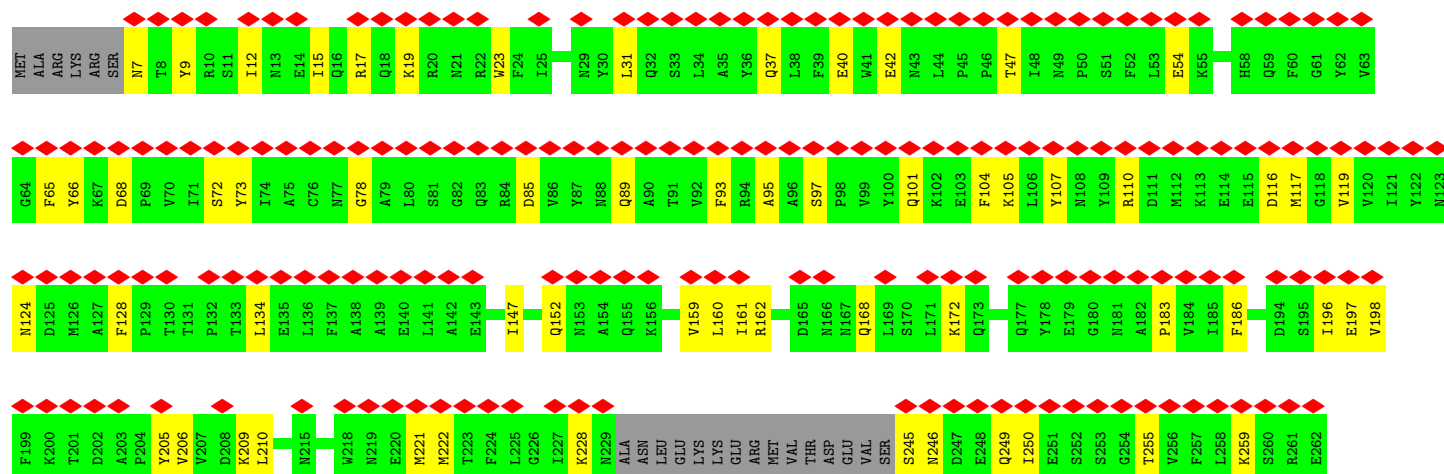
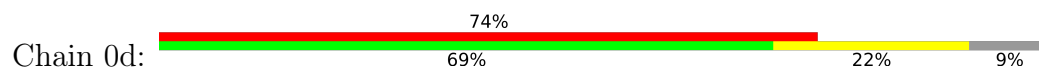




• Molecule 1: Portal protein

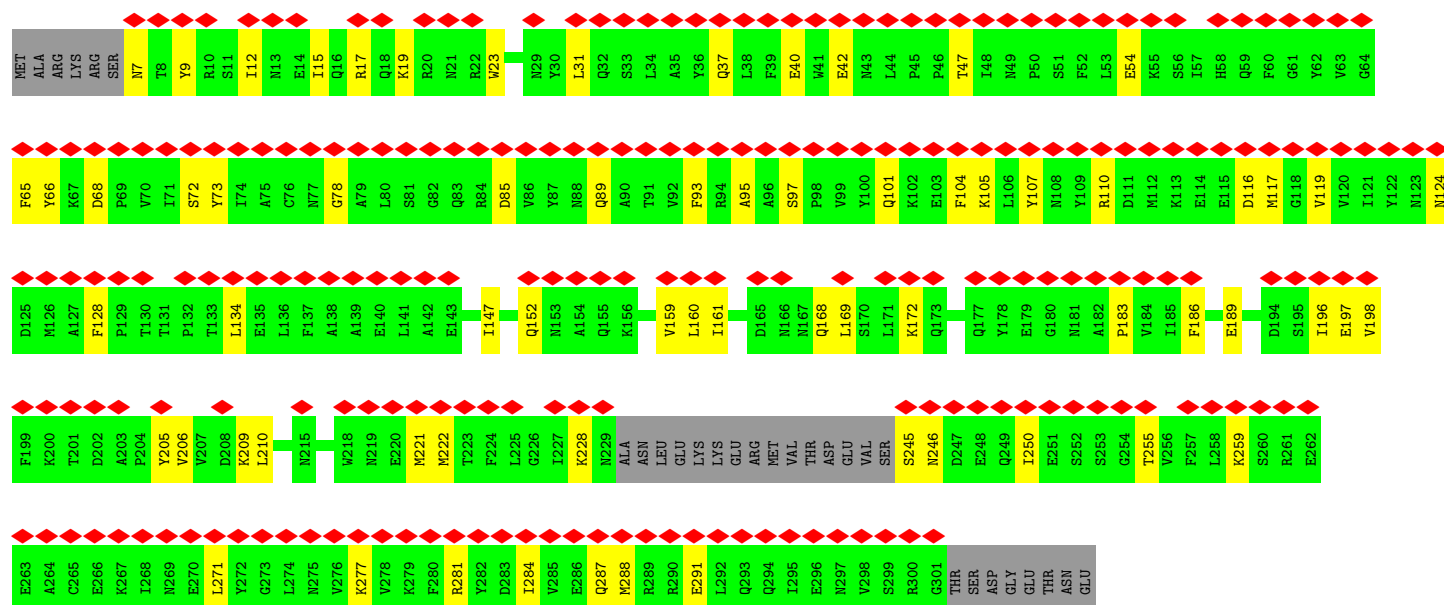
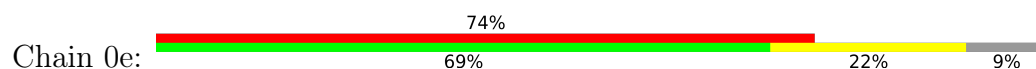


• Molecule 1: Portal protein

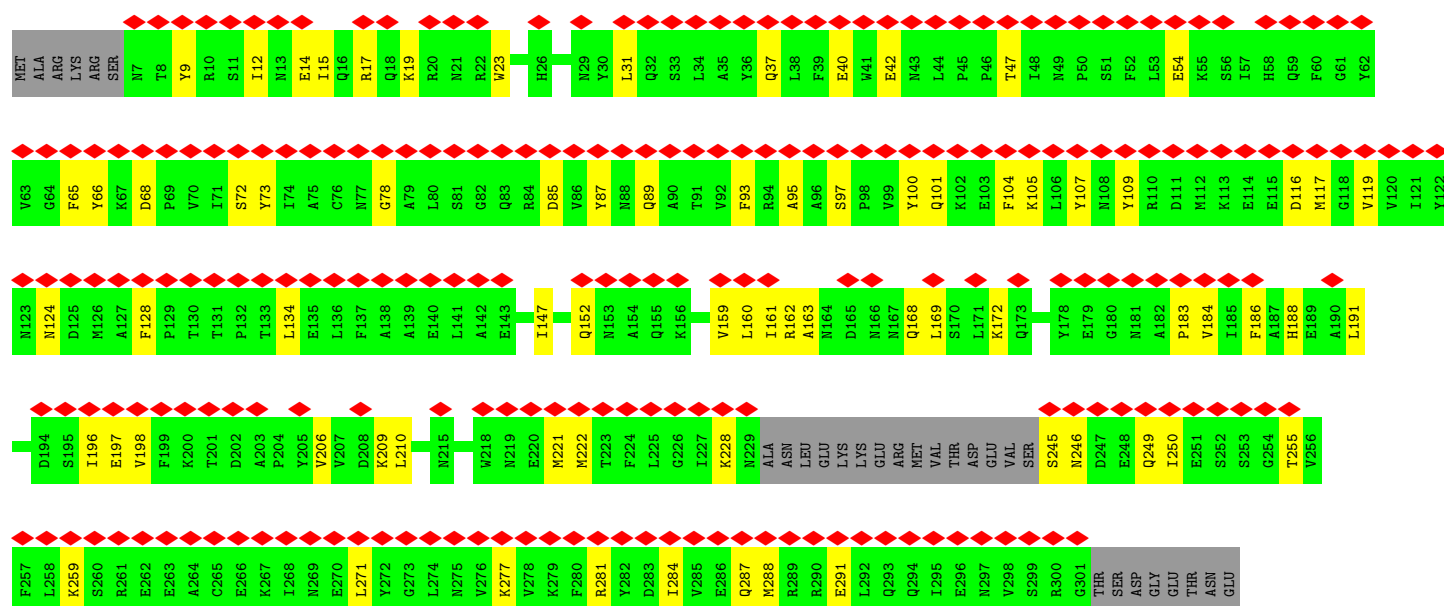
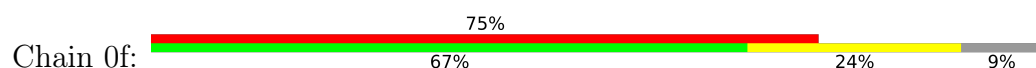




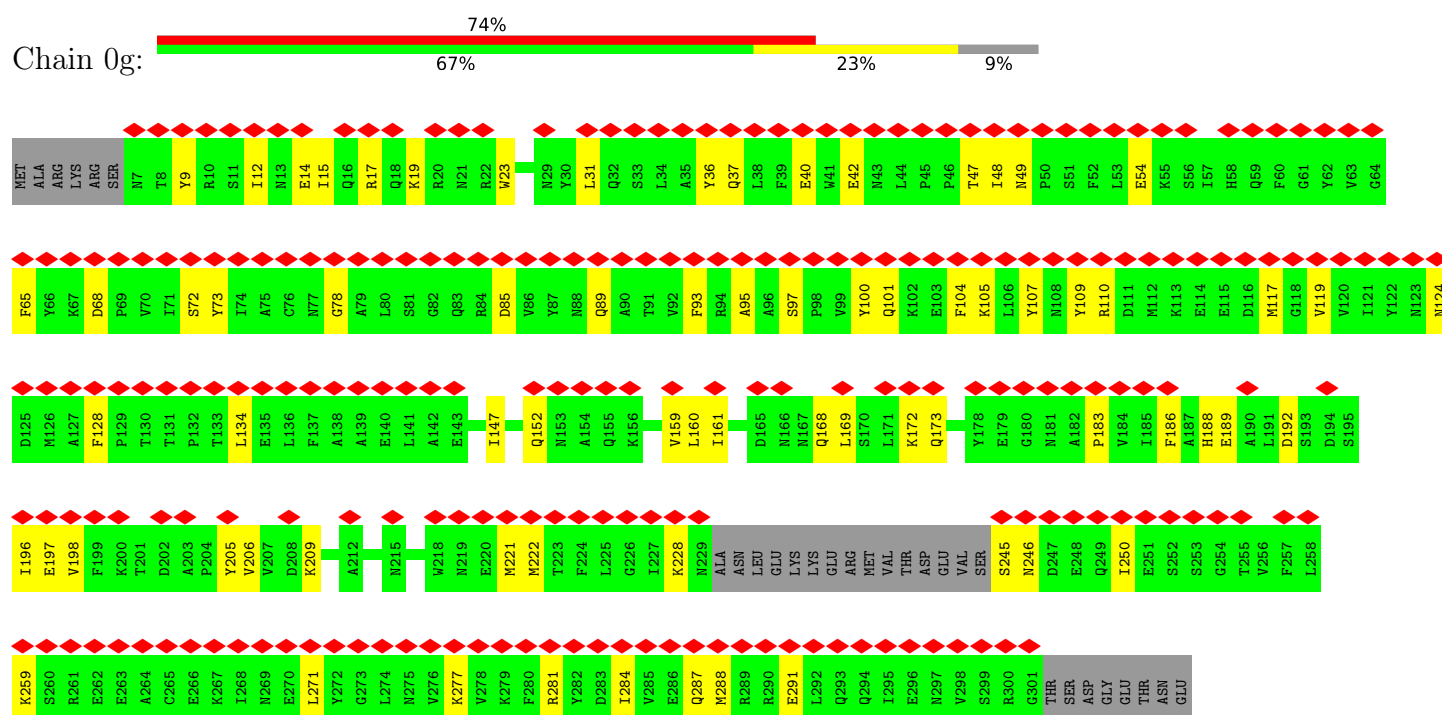
• Molecule 1: Portal protein



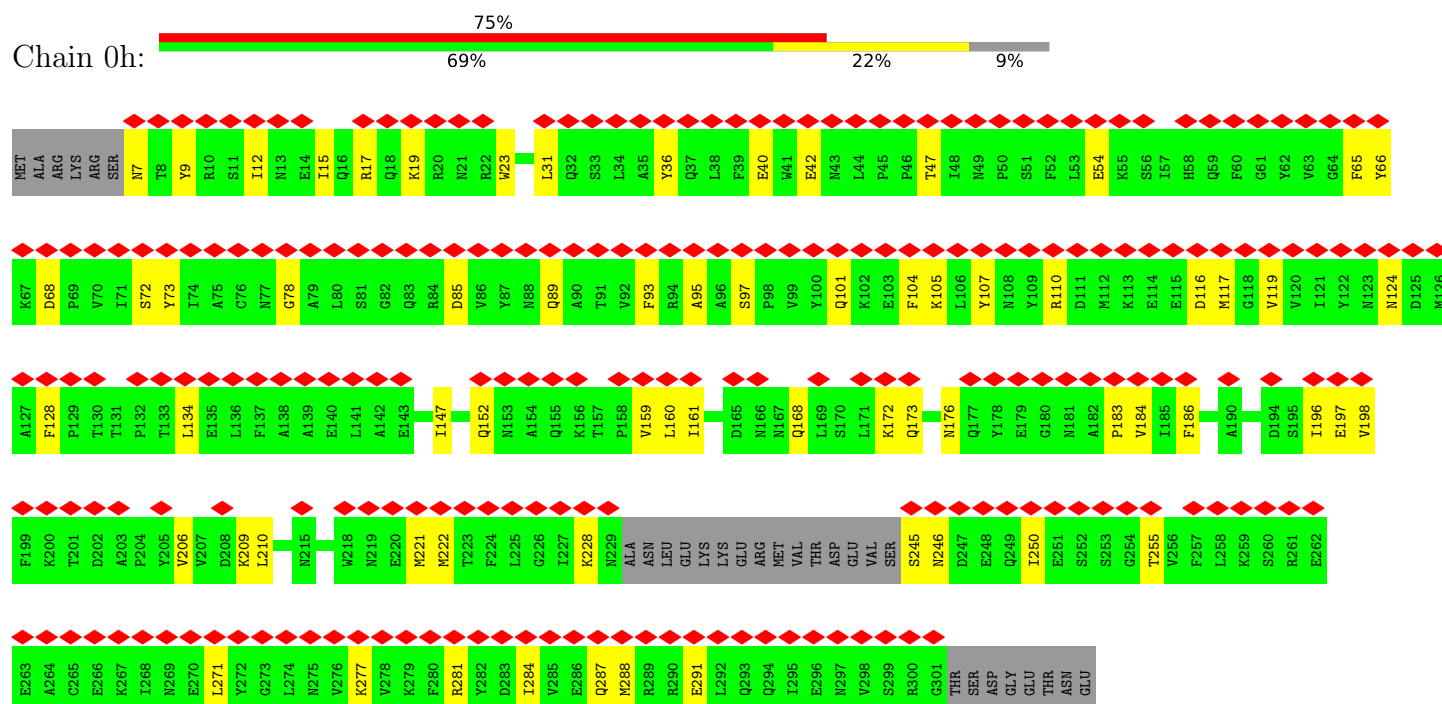
• Molecule 1: Portal protein



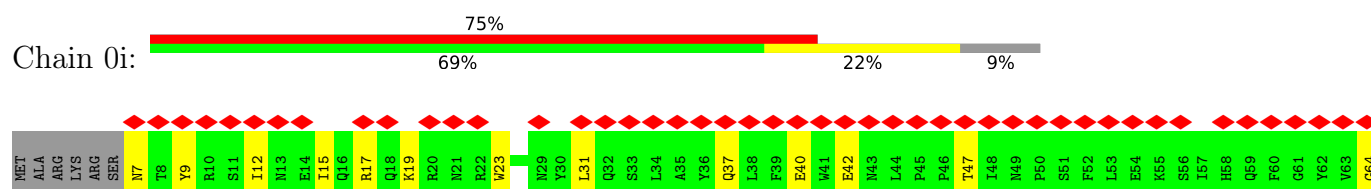
• Molecule 1: Portal protein

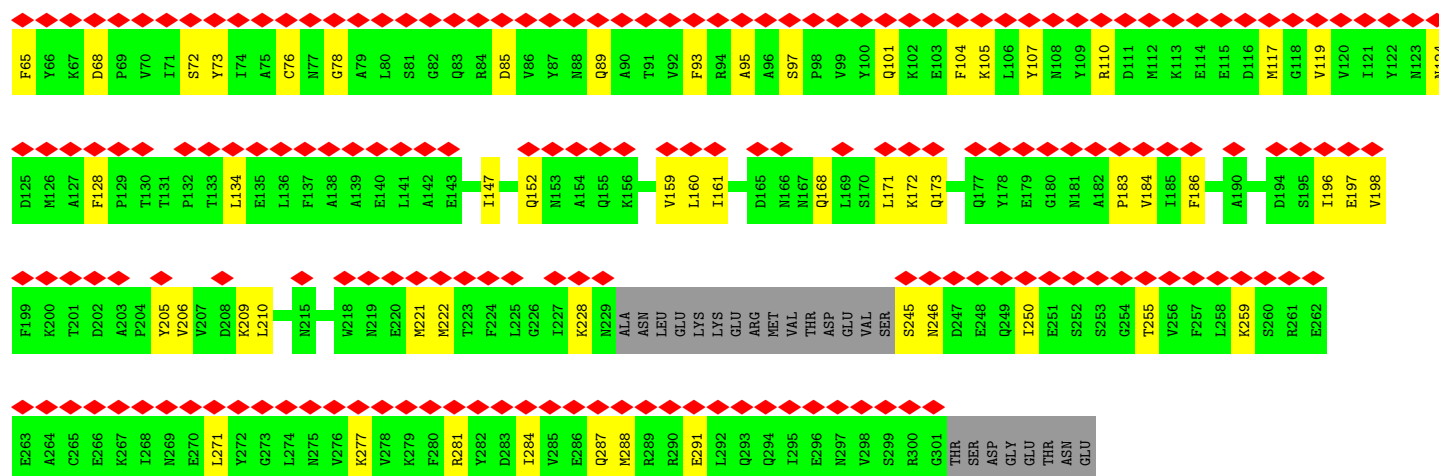


• Molecule 1: Portal protein

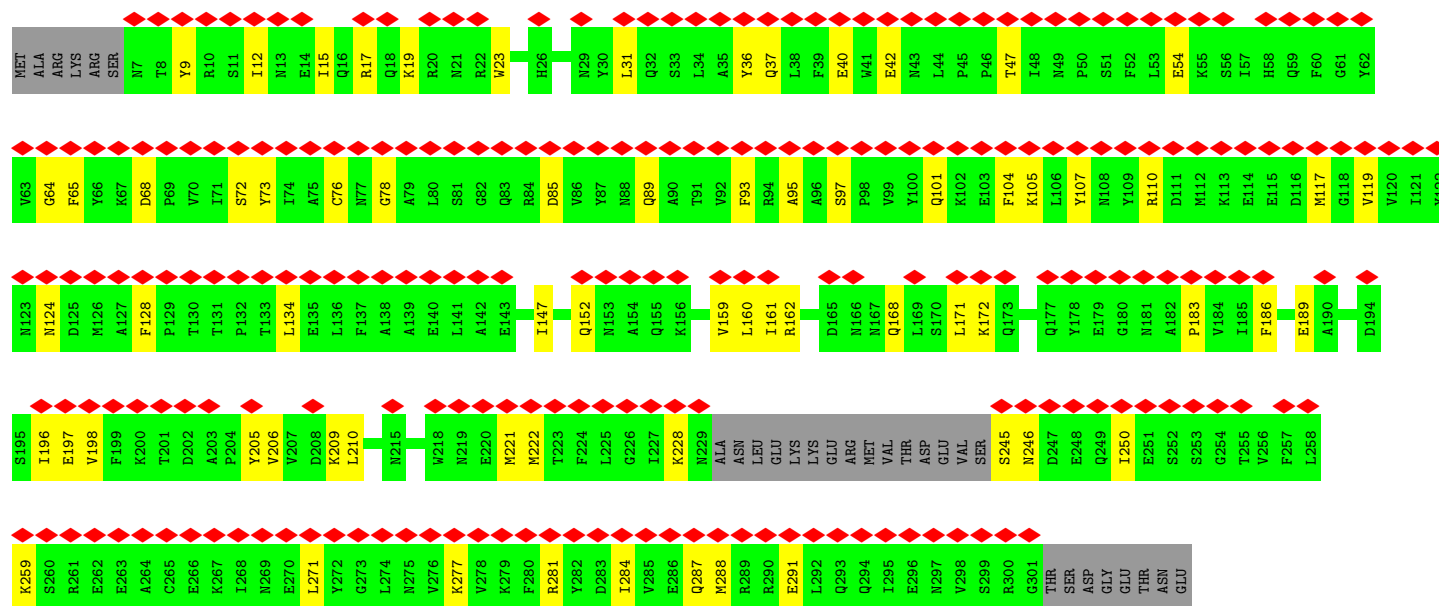
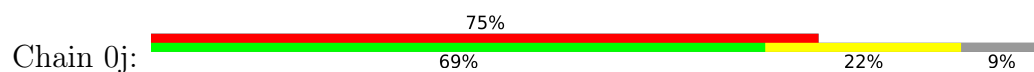


• Molecule 1: Portal protein

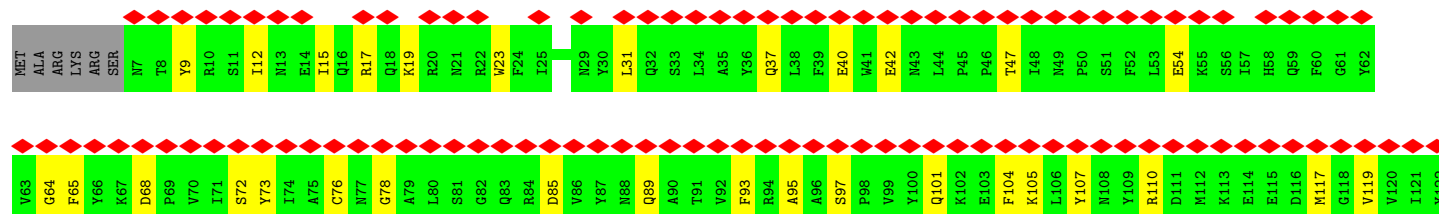
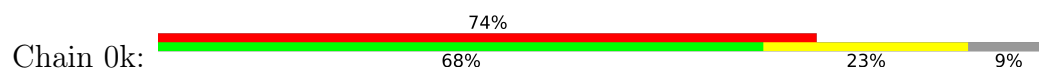


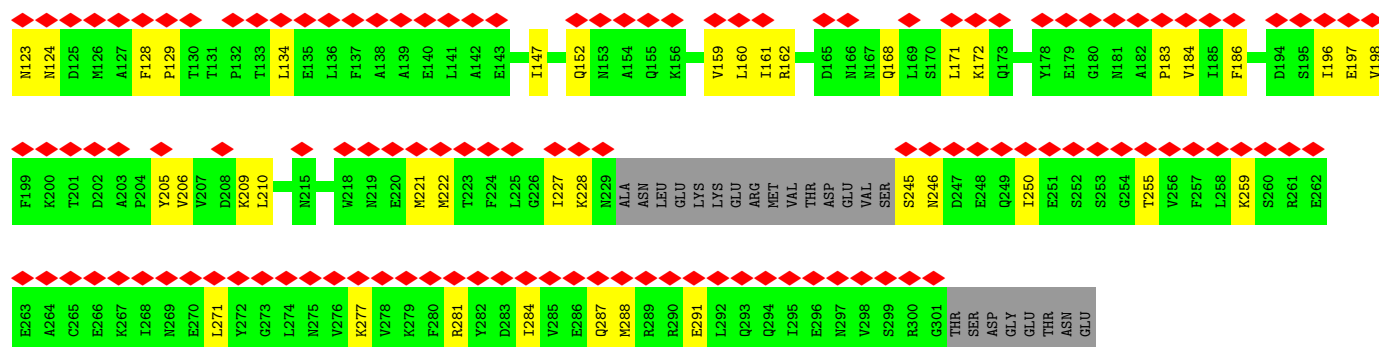


• Molecule 1: Portal protein

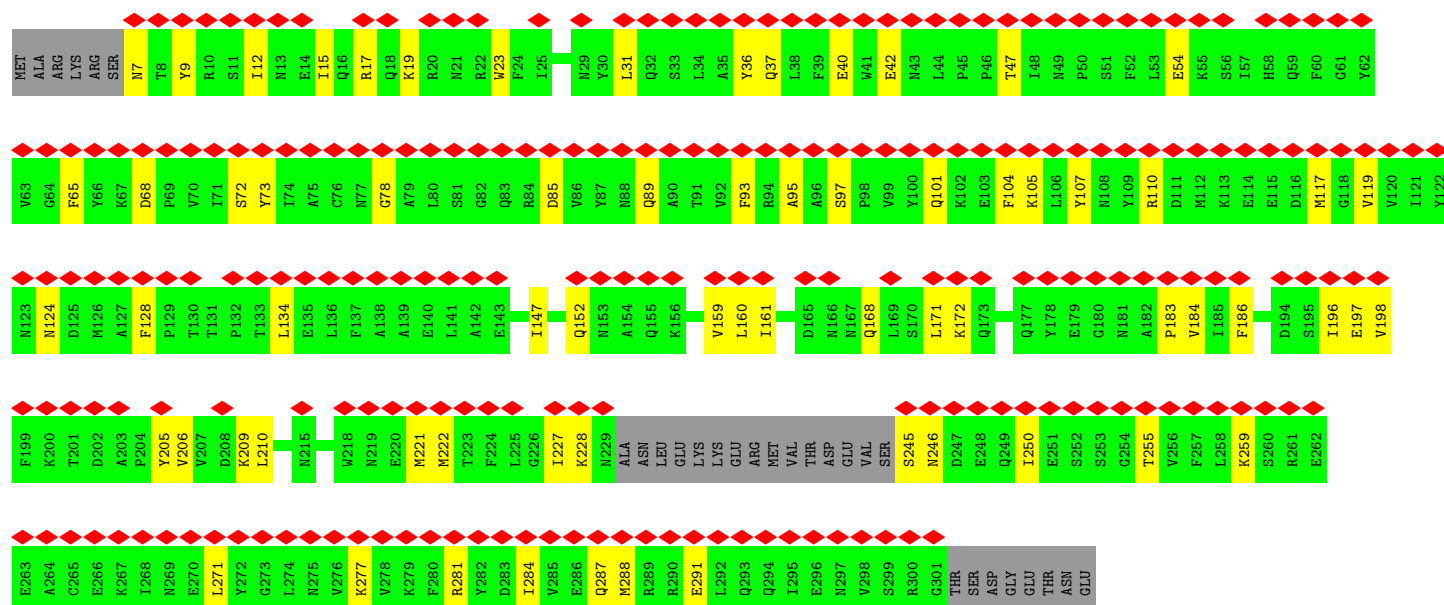
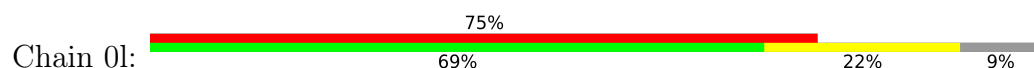


• Molecule 1: Portal protein

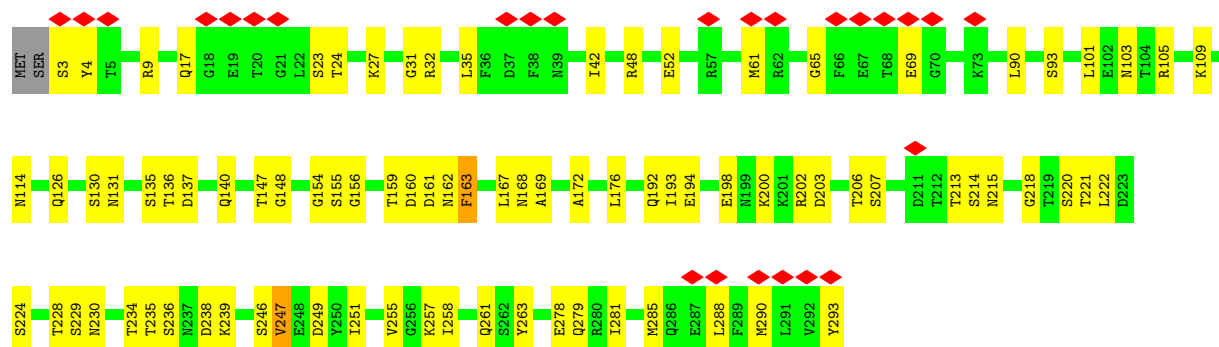




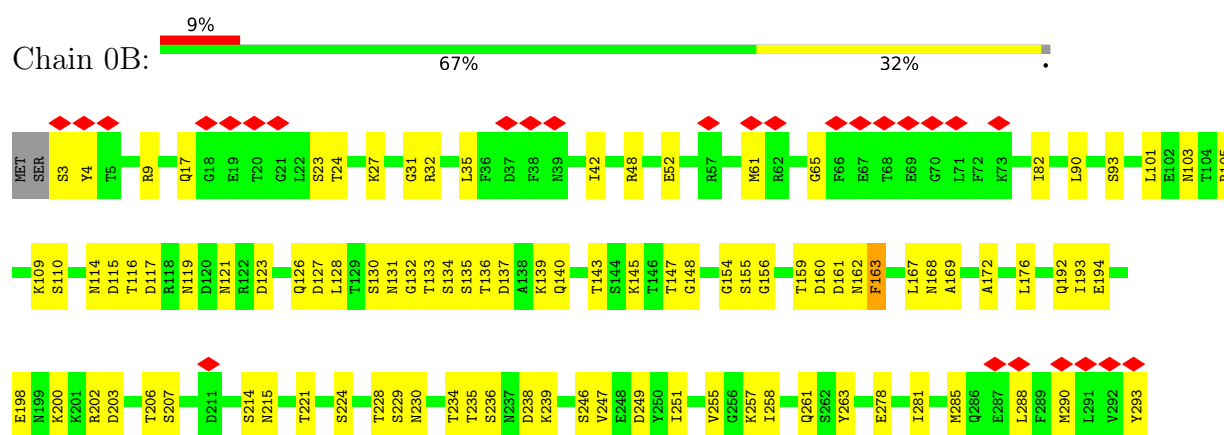
• Molecule 1: Portal protein



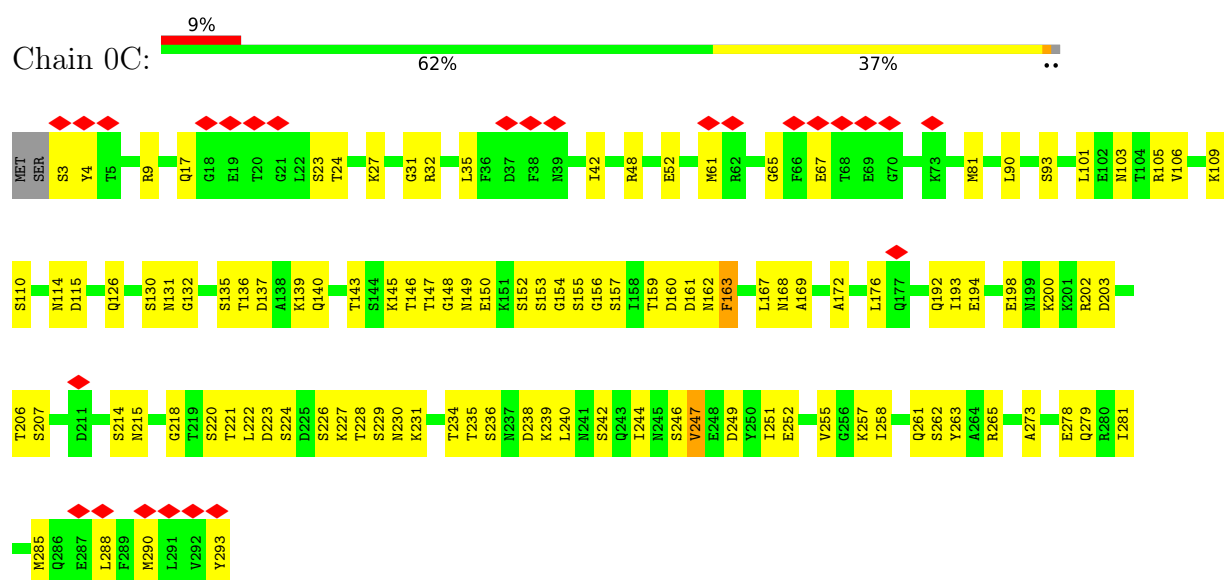
• Molecule 2: Proximal tail tube connector protein



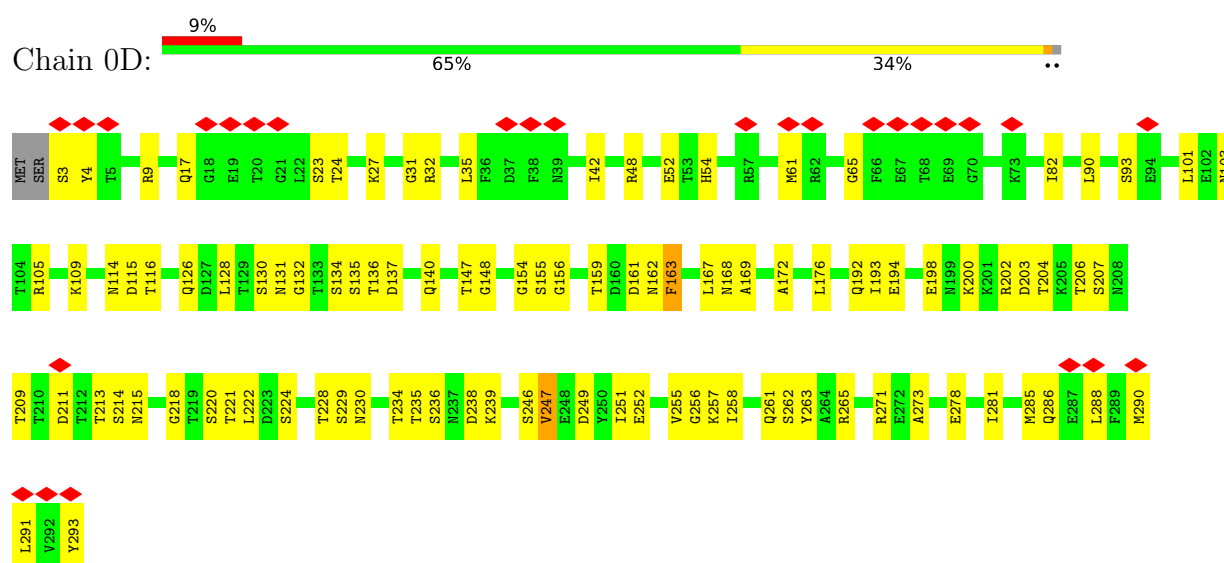
• Molecule 2: Proximal tail tube connector protein



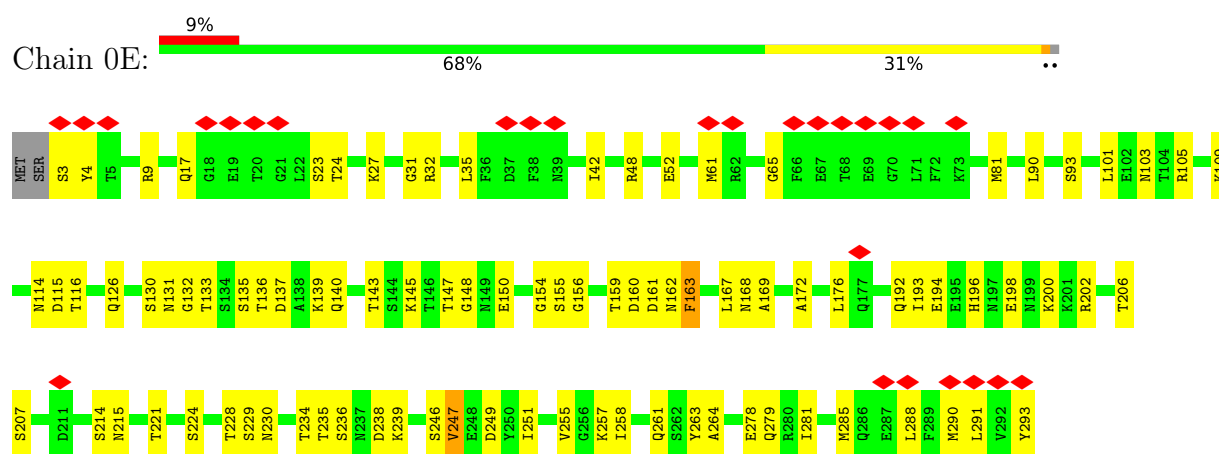
• Molecule 2: Proximal tail tube connector protein



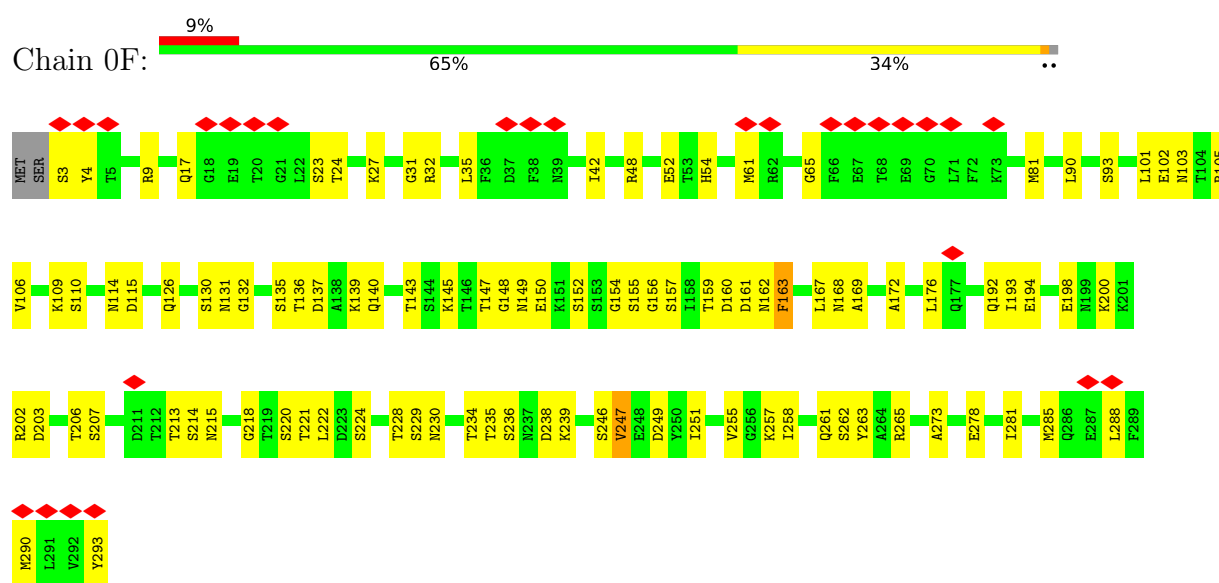
• Molecule 2: Proximal tail tube connector protein



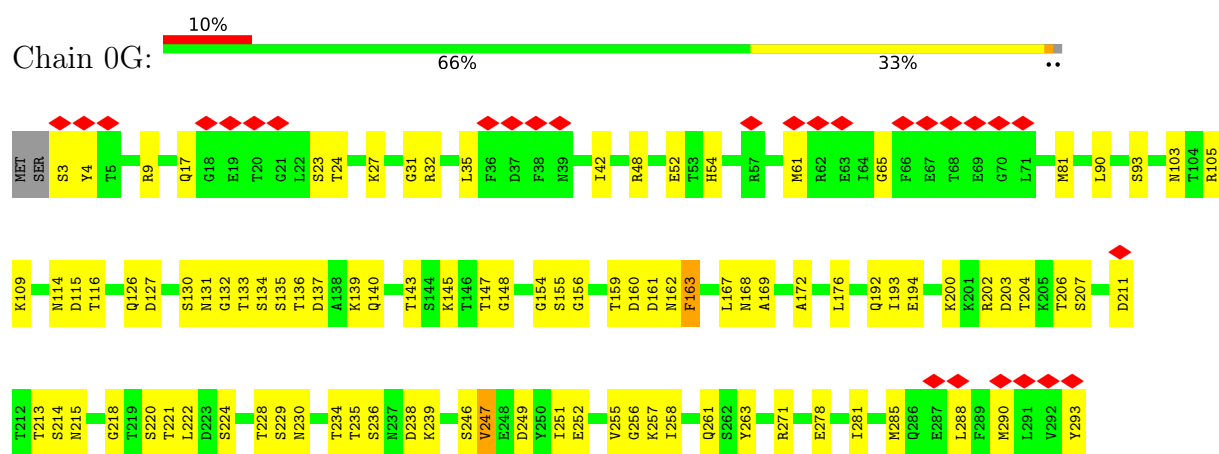
• Molecule 2: Proximal tail tube connector protein



• Molecule 2: Proximal tail tube connector protein

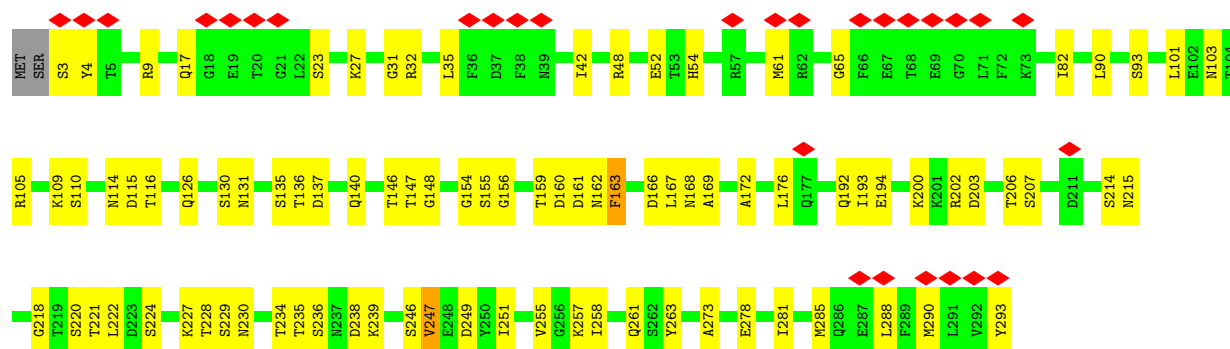


• Molecule 2: Proximal tail tube connector protein

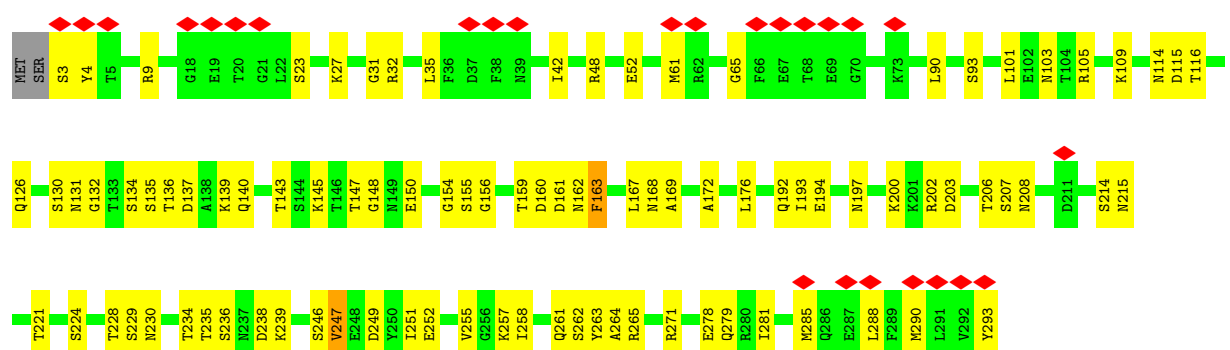


• Molecule 2: Proximal tail tube connector protein

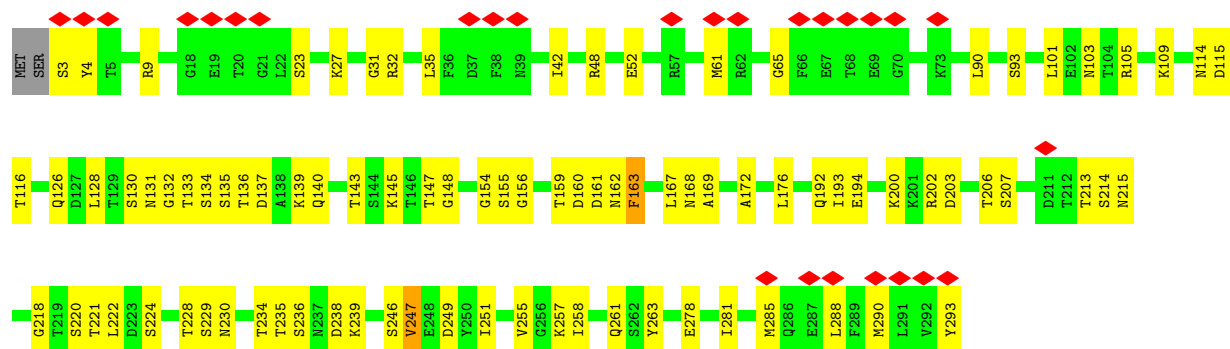




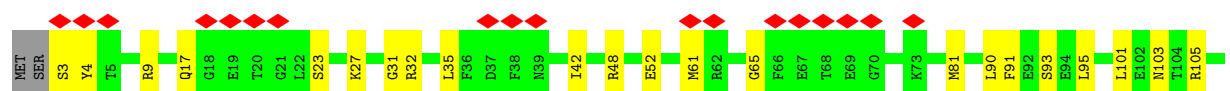
• Molecule 2: Proximal tail tube connector protein

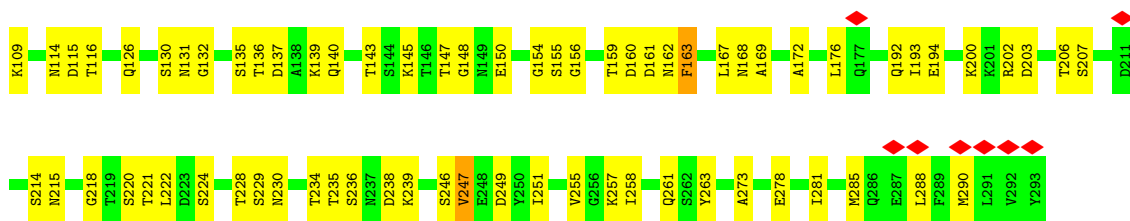


• Molecule 2: Proximal tail tube connector protein

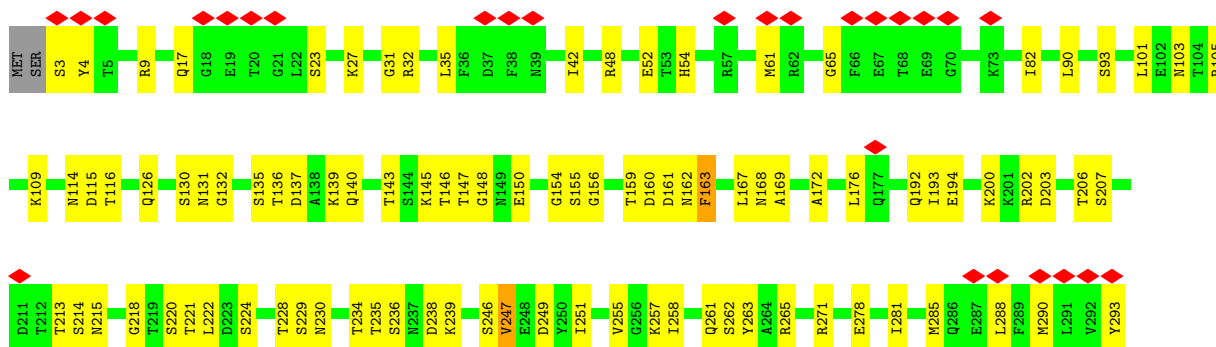


• Molecule 2: Proximal tail tube connector protein

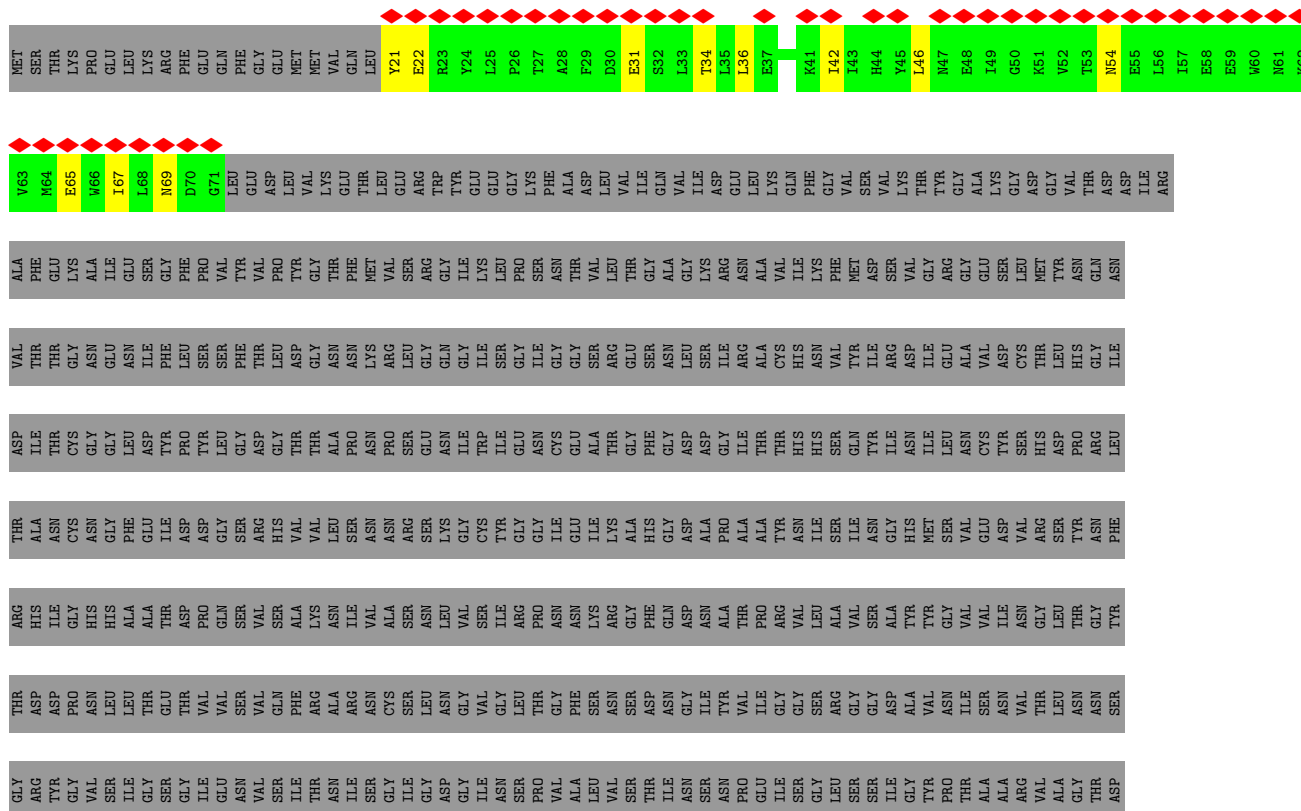




• Molecule 2: Proximal tail tube connector protein

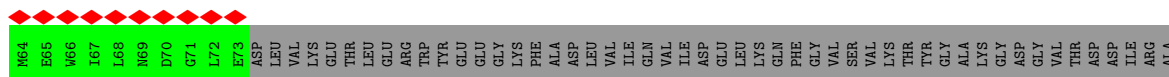


• Molecule 3: Pre-neck appendage protein



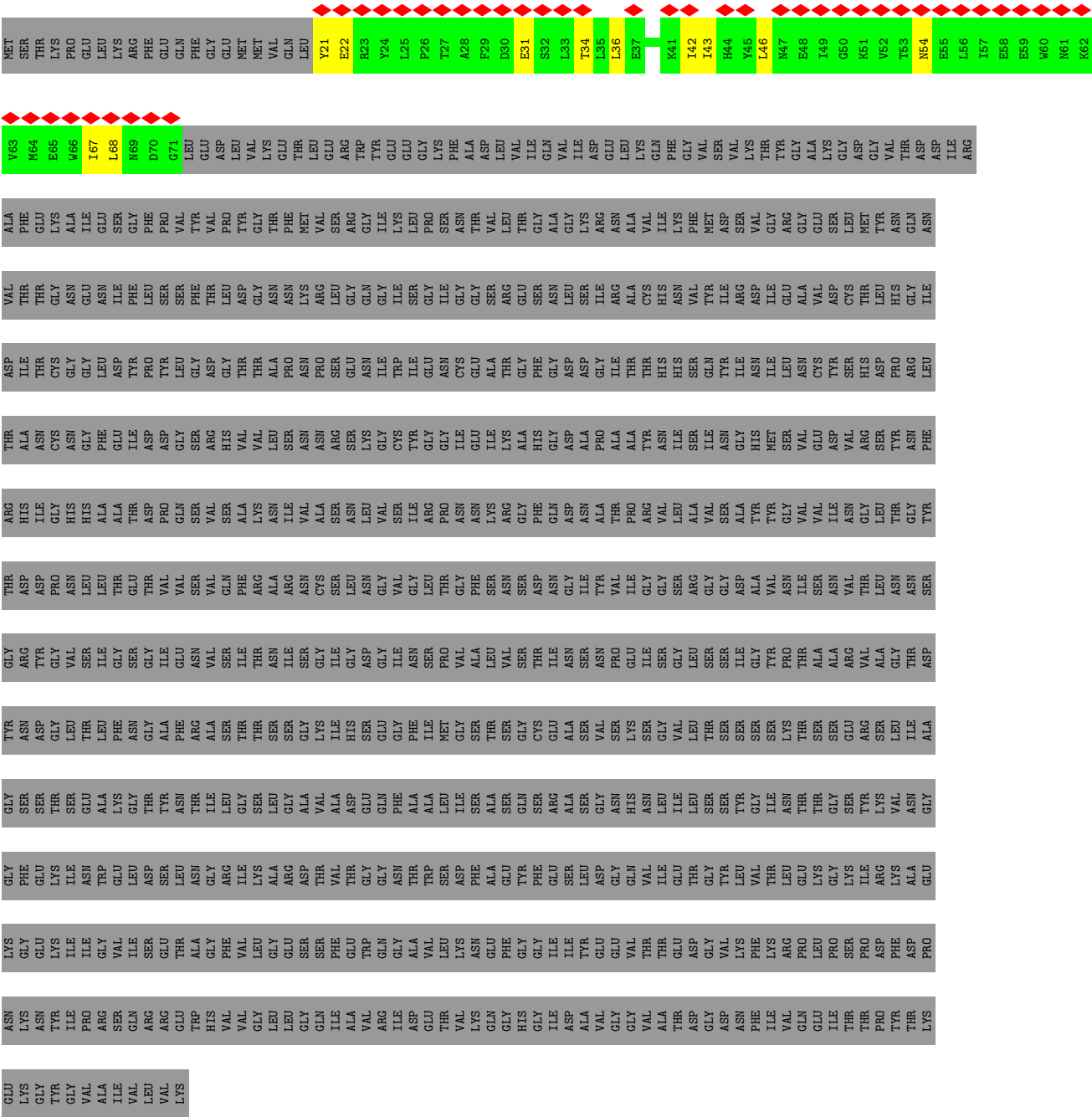
GLY
VAL
ALA
ILE
VAL
LEU
VAL
LYS

Chain C: 6% 6% 93%

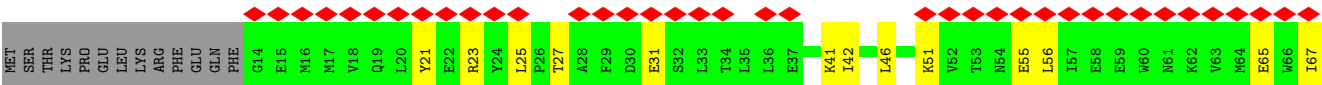


LYS
GLY
TYR
GLY
VAL
ALA
ILE
VAL
LEU
VAL
LYS

● Molecule 3: Pre-neck appendage protein



● Molecule 3: Pre-neck appendage protein







- Molecule 3: Pre-neck appendage protein

[illegible]

ASN	TYR	SER	ILE	GLY	PRO	ARG	SER	GLN	ARG	GLU	TRP	HIS	VAL	VAL	GLY	LEU	GLY	GLN	ILE	ALA	VAL	ARG	ILE	ASP	GLU	THR	VAL	LYS	GLN	GLY	HIS	GLY	ILE	ASP	ALA	VAL	GLY	VAL	VAL	GLY	VAL	VAL	LYS	
GLY	TYR	GLY	VAL	ALA	ALA	ILE	ILE	VAL	VAL	VAL	LYS																																	

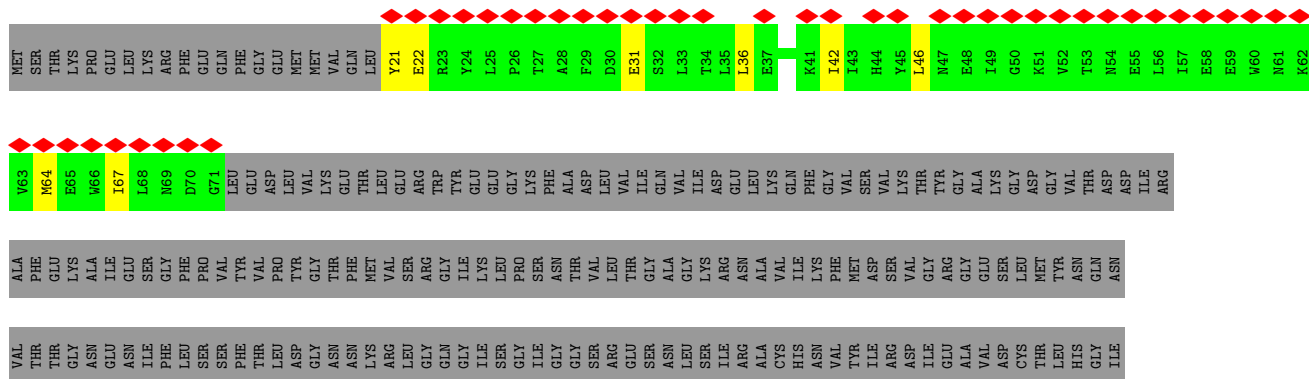
● Molecule 3: Pre-neck appendage protein



GLU	ASN	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

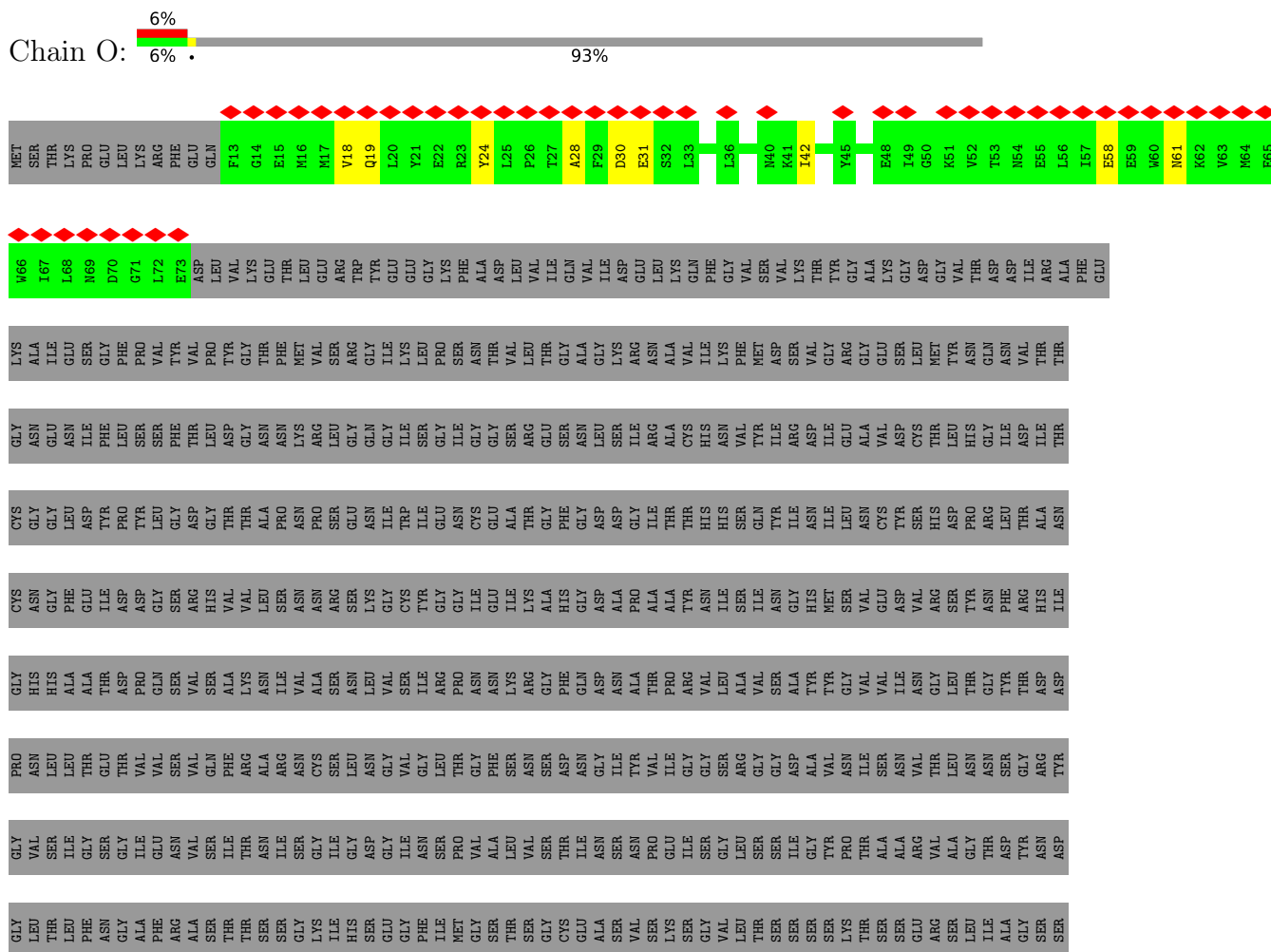
● Molecule 3: Pre-neck appendage protein

- Molecule 3: Pre-neck appendage protein



[illegible]

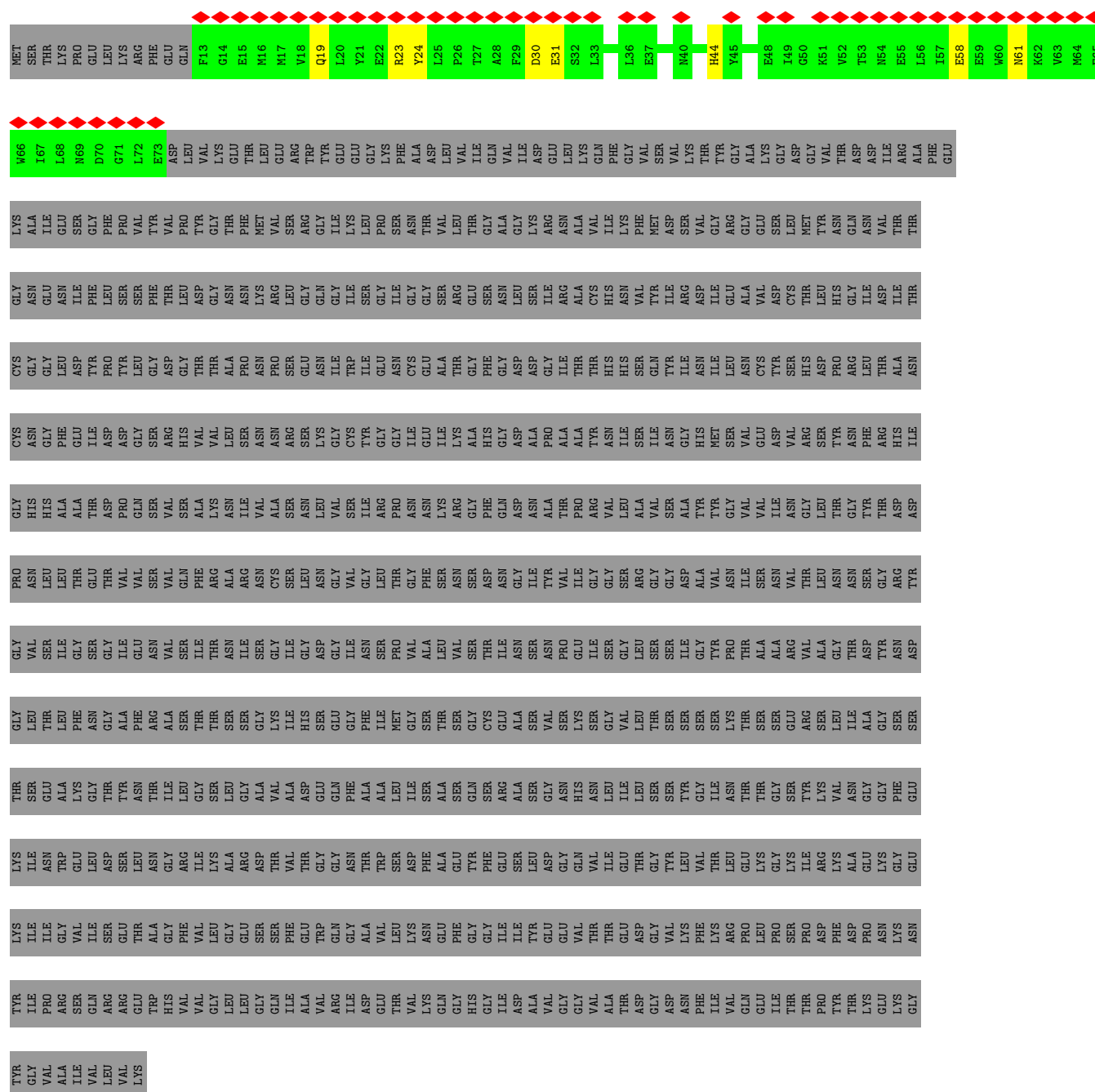
- Molecule 3: Pre-neck appendage protein



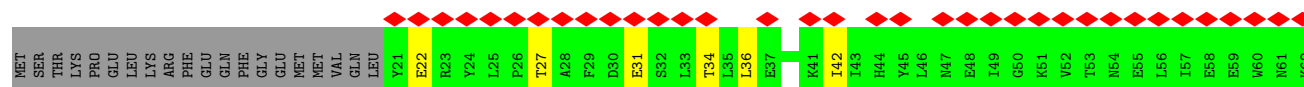
- Molecule 3: Pre-neck appendage protein

[illegible]

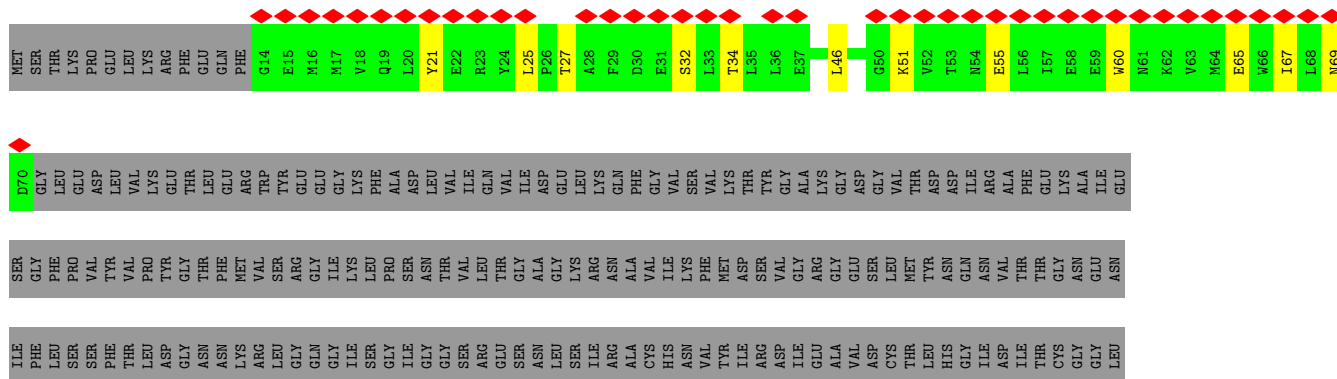
- Molecule 3: Pre-neck appendage protein



Chain S:



- Molecule 3: Pre-neck appendage protein





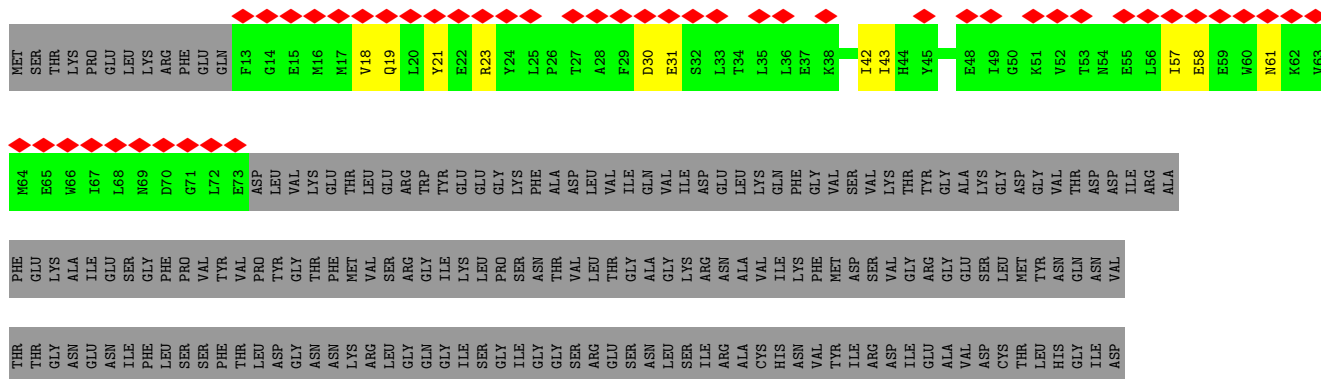
PRO	ARG	SER	GLN	ARG	ARG	GLU	TRP	HIS	VAL	VAL	GLY	LEU	LEU	GLY	GLN	ILE	ALA	VAL	ARG	ILE	ASP	GLU	THR	VAL	LYS	GLN	GLY	HIS	GLY	ILE	ASP	ALA	VAL	GLY	VAL	VAL	ALA	THR	ASP	GLY	ASN	ASN	PHE	ILE	VAL	GLN	GLU	ILE	THR	THR	PRO	THR	LYS	LYS	GLY	TYR	GLY
VAL	ALA	ILE	VAL	LEU	VAL	LYS																																																			

● Molecule 3: Pre-neck appendage protein



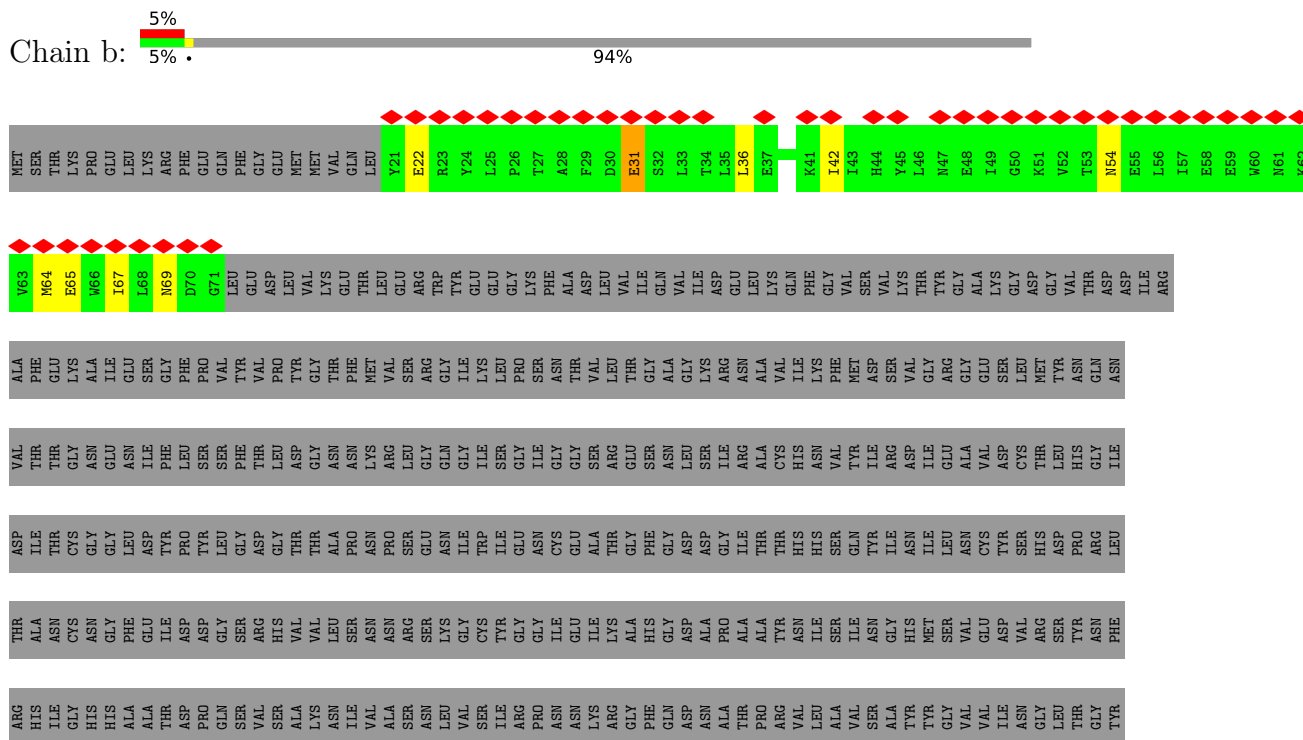
GLY	TYR	ASN	GLU	LYS	GLU	SER	ASP	GLY	TYR	ASP	ILE	GLY	CYS	ASN	THR	THR	THR	GLY	GLY	ASP	E65
ILE	ILE	ILE	ILE	ILE	ILE	SER	LEU	VAL	ASN	ASN	HIS	ASN	GLY	ASN	GLY	ASN	W66	ILE	ALA	ALA	W66
ARG	ARG	ARG	GLY	GLY	TRP	ALA	LEU	THR	GLU	LEU	ALA	PHE	LEU	GLY	ASN	ASN	I67	ILE	GLU	GLU	I67
SER	GLN	SER	VAL	VAL	GLU	GLY	ASN	GLY	LYS	THR	ALA	GLU	ASP	THR	ILE	ASN	L68	SER	GLY	SER	L68
ARG	ARG	ARG	GLU	GLU	ASP	THR	GLY	GLY	ASP	THR	THR	THR	PRO	PRO	PHE	LEU	M69	PHE	GLY	PHE	M69
GLY	GLY	GLY	THR	THR	LEU	ASN	PHE	GLY	VAL	VAL	GLN	GLY	ASN	SER	SER	VAL	G71	SER	PRO	PRO	G71
TRP	HIS	TRP	ALA	ALA	ASN	THR	ARG	GLY	ASN	SER	THR	SER	ASN	ASN	PHE	THR	L72	SER	VAL	VAL	L72
ASN	GLN	GLY	GLY	SER	ASP	ALA	ALA	SER	ASN	ASN	VAL	SER	ASN	ASN	THR	TYR	E73	THR	VAL	VAL	E73
VAL	VAL	VAL	PHE	PHE	ARG	GLY	SER	THR	ILE	GLN	SER	HIS	ASN	THR	GLY	PRO	ASP	LEU	PRO	VAL	ASP
VAL	VAL	VAL	VAL	VAL	VAL	GLY	THR	THR	ILE	THR	ALA	VAL	GLY	THR	ASP	TYR	LEU	THR	TYR	VAL	LEU
GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	ASN	VAL	GLY	THR	GLY	GLY	LYS	GLY	GLY	GLY	F13
LEU	LEU	LEU	LEU	LEU	LEU	SER	THR	THR	THR	THR	ASN	ASN	ASN	ASN	THR	ASN	LYS	LYS	THR	THR	G14
LEU	LEU	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E15
LEU	LEU	LEU	LEU	LEU	LEU	GLY	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M16
LEU	LEU	LEU	LEU	LEU	LEU	GLY	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M17
LEU	LEU	LEU	LEU	LEU	LEU	GLY	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	V18
LYS	LYS	LYS	LYS	LYS	LYS	GLY	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	Q19
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	L20
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	Y21
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E22
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	R23
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	Y24
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	L25
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	P26
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	A28
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	F29
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	D30
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E31
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	S32
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	I33
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	T34
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	L35
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	L36
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M39
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M39
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	I42
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	I43
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	H44
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	Y45
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	I49
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	G50
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	K51
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	V52
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	T53
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	N54
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E55
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	L56
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	I57
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E58
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	E59
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	W60
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M61
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	K62
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	V63
GLY	GLY	GLY	GLY	GLY	GLY	ASN	THR	THR	THR	THR	THR	ASN	ASN	ASN	THR	THR	THR	THR	THR	THR	M64

● Molecule 3: Pre-neck appendage protein



[illegible]

- Molecule 3: Pre-neck appendage protein



- Molecule 3: Pre-neck appendage protein

[illegible]

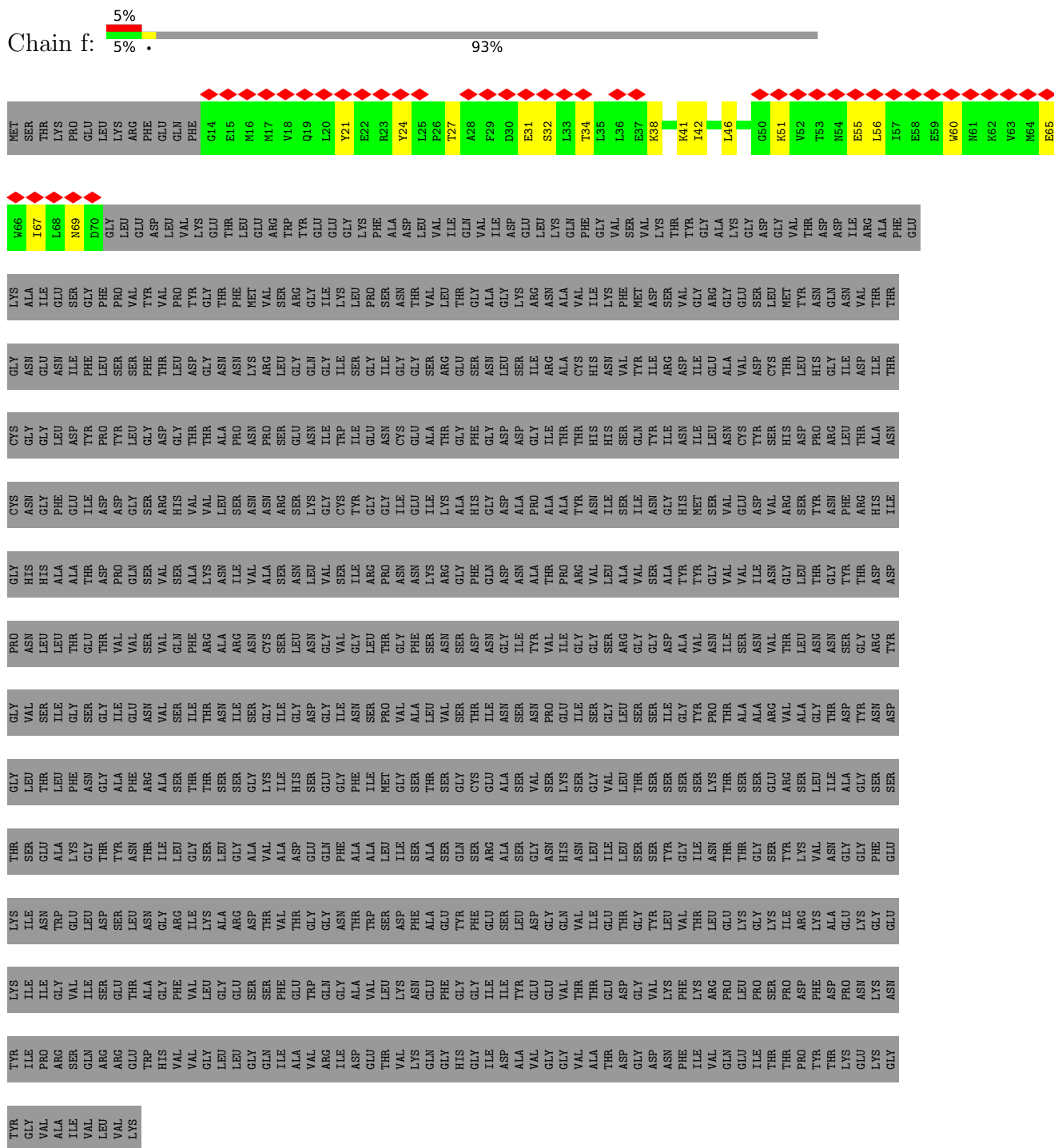
ASN	TYR	ILE	PRO	ARG	SER	GLN	ARG	GLU	TRP	HIS	VAL	VAL	GLY	GLY	LYS	LEU	ARG	VAL	LYS
GLY	TYR	GLY	VAL	ALA	ILE	VAL	VAL	VAL	LYS										

● Molecule 3: Pre-neck appendage protein

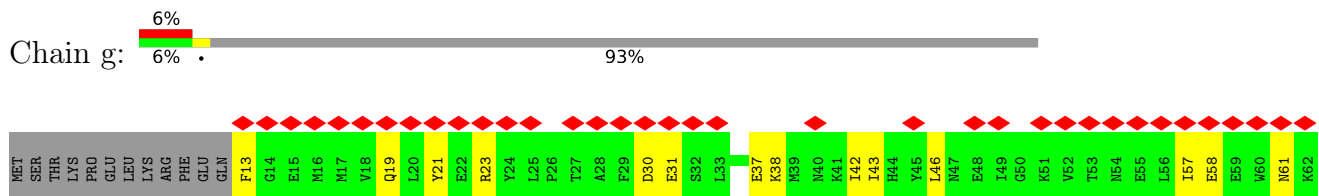


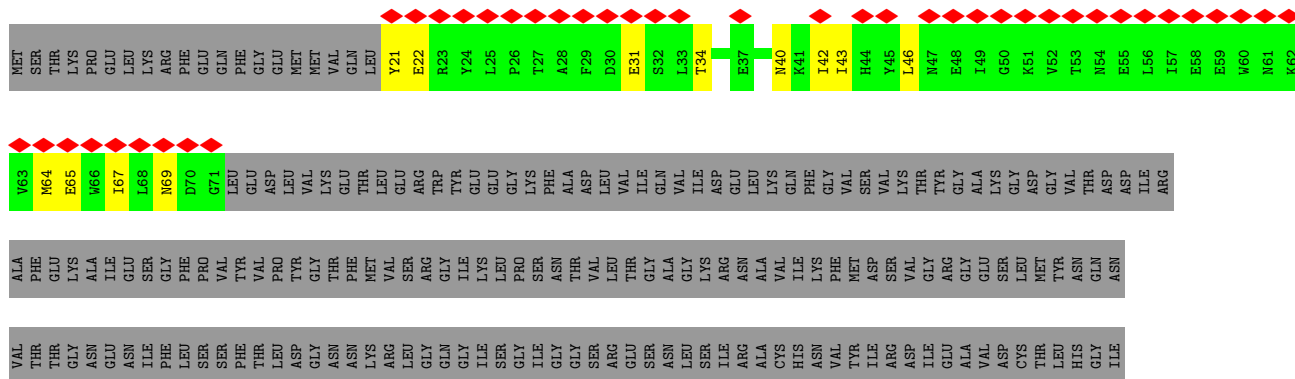
MET	SER	THR	LYS	PRO	GLU	LEU	LYS	ARG	GLU	TRP	HIS	VAL	VAL	GLY	GLY	LYS	LEU	ARG	VAL
M64	E65	M66	I67	L68	M69	D70	G71	LEU	GLU	ASP	ASP	PRO	THR	VAL	GLY	LYS	LEU	ARG	VAL
PHE	GLU	LYS	ALA	ILE	GLU	SER	GLY	LEU	ASP	PRO	THR	VAL	VAL	GLY	GLY	LYS	LEU	ARG	VAL
THR	THR	GLY	ASN	GLU	GLY	ILE	ASP	PHE	LEU	SER	THR	VAL	VAL	GLY	GLY	LYS	LEU	ARG	VAL
ILE	THR	CYS	GLY	GLY	LEU	ASP	TYR	PHE	LEU	ASP	PRO	THR	VAL	VAL	GLY	GLY	LYS	LEU	ARG
ALA	ASN	CYS	GLY	PHE	GLU	ILE	ASP	GLY	LEU	ASP	PRO	THR	VAL	VAL	GLY	GLY	LYS	LEU	ARG
HIS	ILE	GLY	HIS	ALA	THR	THR	THR	GLN	SER	VAL	VAL	SER	VAL	SER	VAL	VAL	VAL	VAL	THR
ASP	ASP	PRO	ASN	LEU	THR	GLU	THR	VAL	GLN	VAL	VAL	GLN	VAL	GLY	VAL	VAL	VAL	VAL	THR
ARG	TYR	GLY	VAL	SER	ILE	GLY	GLY	VAL	ASP	GLY	VAL	SER	SER	GLY	GLY	GLY	GLY	GLY	TYR
ASN	ASP	GLY	THR	LEU	PHE	ASN	ASN	ARG	ASN	GLY	VAL	SER	SER	GLY	VAL	VAL	VAL	VAL	GLY
SER	SER	THR	GLU	ALA	LYS	THR	THR	VAL	GLN	VAL	VAL	GLY	GLY	ILE	THR	THR	THR	THR	GLY
PHE	GLU	LYS	ILE	ASN	GLU	ASP	THR	ARG	GLY	THR	THR	VAL	VAL	GLY	GLY	GLY	GLY	GLY	LYS
GLY	GLU	LYS	ILE	THR	VAL	SER	THR	VAL	GLY	THR	THR	VAL	VAL	GLY	GLY	GLY	GLY	GLY	LYS
LYS	ASN	TYR	ILE	PRO	ARG	SER	GLN	THR	TRP	HIS	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLU
LYS	GLY	TYR	GLY	VAL	ALA	ILE	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL

● Molecule 3: Pre-neck appendage protein



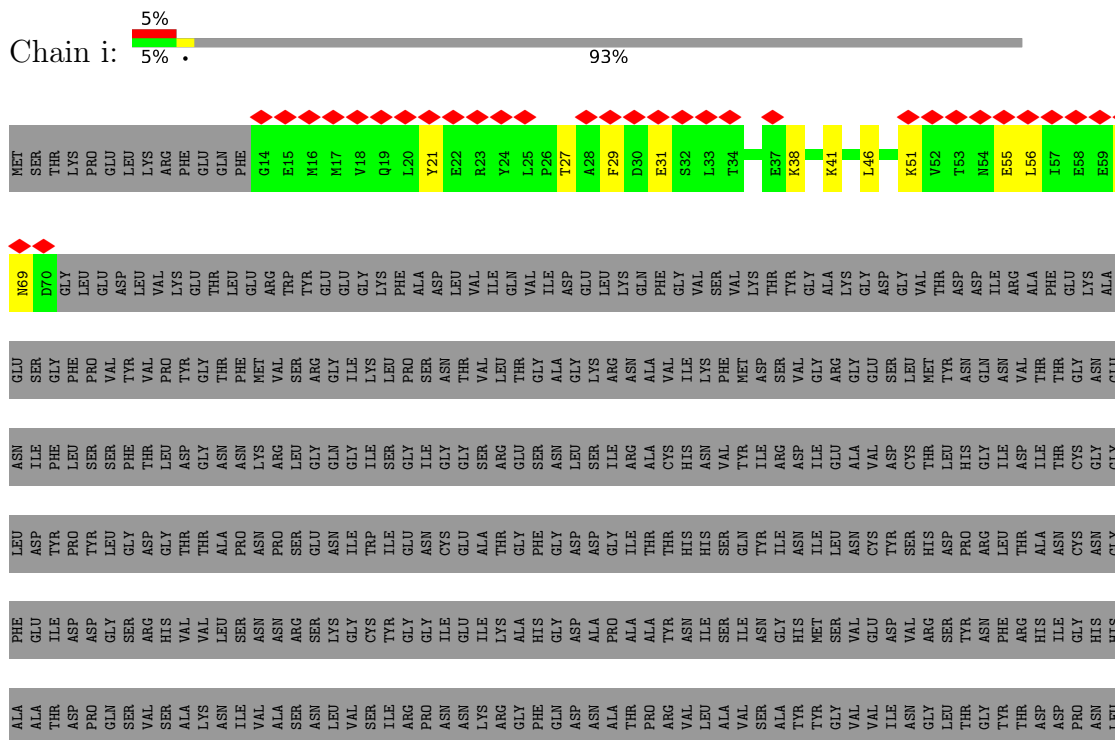
- Molecule 3: Pre-neck appendage protein





[illegible]

- Molecule 3: Pre-neck appendage protein



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	22.011	Depositor
Minimum map value	-4.860	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.233	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	734.4, 734.4, 734.4	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0a	0.36	0/2288	0.52	0/3103
1	0b	0.36	0/2288	0.52	0/3103
1	0c	0.36	0/2288	0.52	0/3103
1	0d	0.36	0/2288	0.53	0/3103
1	0e	0.36	0/2288	0.53	0/3103
1	0f	0.36	0/2288	0.53	0/3103
1	0g	0.36	0/2288	0.53	0/3103
1	0h	0.36	0/2288	0.53	0/3103
1	0i	0.36	0/2288	0.52	0/3103
1	0j	0.36	0/2288	0.53	0/3103
1	0k	0.36	0/2288	0.52	0/3103
1	0l	0.36	0/2288	0.52	0/3103
2	0A	0.62	0/2335	0.75	0/3149
2	0B	0.62	0/2335	0.75	0/3149
2	0C	0.62	0/2335	0.75	0/3149
2	0D	0.62	0/2335	0.75	0/3149
2	0E	0.62	0/2335	0.75	0/3149
2	0F	0.62	0/2335	0.75	0/3149
2	0G	0.62	0/2335	0.75	0/3149
2	0H	0.62	0/2335	0.75	0/3149
2	0I	0.62	0/2335	0.75	0/3149
2	0J	0.62	0/2335	0.75	0/3149
2	0K	0.62	0/2335	0.75	0/3149
2	0L	0.62	0/2335	0.75	0/3149
3	A	0.34	0/442	0.66	0/598
3	B	0.41	0/491	0.59	0/663
3	C	0.36	0/524	0.64	0/707
3	D	0.34	0/442	0.65	0/598
3	E	0.39	0/491	0.60	0/663
3	F	0.36	0/524	0.64	0/707
3	G	0.34	0/442	0.65	0/598
3	H	0.40	0/491	0.60	0/663
3	I	0.36	0/524	0.64	0/707
3	J	0.33	0/442	0.66	0/598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	K	0.40	0/491	0.60	0/663
3	L	0.36	0/524	0.64	0/707
3	M	0.32	0/442	0.65	0/598
3	N	0.38	0/491	0.57	0/663
3	O	0.36	0/524	0.64	0/707
3	P	0.31	0/442	0.66	0/598
3	Q	0.37	0/491	0.58	0/663
3	R	0.36	0/524	0.64	0/707
3	S	0.32	0/442	0.66	0/598
3	T	0.37	0/491	0.57	0/663
3	U	0.36	0/524	0.64	0/707
3	V	0.32	0/442	0.65	0/598
3	W	0.39	0/491	0.57	0/663
3	X	0.36	0/524	0.64	0/707
3	Y	0.33	0/442	0.65	0/598
3	Z	0.38	0/491	0.56	0/663
3	a	0.36	0/524	0.64	0/707
3	b	0.32	0/442	0.65	0/598
3	c	0.38	0/491	0.57	0/663
3	d	0.36	0/524	0.64	0/707
3	e	0.34	0/442	0.67	0/598
3	f	0.38	0/491	0.59	0/663
3	g	0.36	0/524	0.64	0/707
3	h	0.38	0/442	0.66	0/598
3	i	0.41	0/491	0.59	0/663
3	j	0.36	0/524	0.64	0/707
All	All	0.48	0/72960	0.64	0/98640

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	0A	0	3
2	0B	0	3
2	0C	0	3
2	0D	0	3
2	0E	0	3
2	0F	0	3
2	0G	0	3
2	0H	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	0I	0	3
2	0J	0	3
2	0K	0	3
2	0L	0	3
All	All	0	36

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0A	163	PHE	Peptide
2	0A	172	ALA	Peptide
2	0A	176	LEU	Peptide
2	0B	163	PHE	Peptide
2	0B	172	ALA	Peptide
2	0B	176	LEU	Peptide
2	0C	163	PHE	Peptide
2	0C	172	ALA	Peptide
2	0C	176	LEU	Peptide
2	0D	163	PHE	Peptide
2	0D	172	ALA	Peptide
2	0D	176	LEU	Peptide
2	0E	163	PHE	Peptide
2	0E	172	ALA	Peptide
2	0E	176	LEU	Peptide
2	0F	163	PHE	Peptide
2	0F	172	ALA	Peptide
2	0F	176	LEU	Peptide
2	0G	163	PHE	Peptide
2	0G	172	ALA	Peptide
2	0G	176	LEU	Peptide
2	0H	163	PHE	Peptide
2	0H	172	ALA	Peptide
2	0H	176	LEU	Peptide
2	0I	163	PHE	Peptide
2	0I	172	ALA	Peptide
2	0I	176	LEU	Peptide
2	0J	163	PHE	Peptide
2	0J	172	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	0J	176	LEU	Peptide
2	0K	163	PHE	Peptide
2	0K	172	ALA	Peptide
2	0K	176	LEU	Peptide
2	0L	163	PHE	Peptide
2	0L	172	ALA	Peptide
2	0L	176	LEU	Peptide

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	0a	2240	0	2130	55	0
1	0b	2240	0	2130	61	0
1	0c	2240	0	2130	51	0
1	0d	2240	0	2130	53	0
1	0e	2240	0	2130	52	0
1	0f	2240	0	2130	65	0
1	0g	2240	0	2130	67	0
1	0h	2240	0	2130	55	0
1	0i	2240	0	2130	55	0
1	0j	2240	0	2130	51	0
1	0k	2240	0	2130	59	0
1	0l	2240	0	2130	52	0
2	0A	2300	0	2149	63	0
2	0B	2300	0	2149	76	0
2	0C	2300	0	2149	95	0
2	0D	2300	0	2149	83	0
2	0E	2300	0	2149	70	0
2	0F	2300	0	2149	83	0
2	0G	2300	0	2149	80	0
2	0H	2300	0	2149	73	0
2	0I	2300	0	2149	66	0
2	0J	2300	0	2149	66	0
2	0K	2300	0	2149	68	0
2	0L	2300	0	2149	69	0
3	A	433	0	425	11	0
3	B	482	0	477	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	514	0	506	11	0
3	D	433	0	425	11	0
3	E	482	0	477	13	0
3	F	514	0	506	12	0
3	G	433	0	425	11	0
3	H	482	0	477	13	0
3	I	514	0	506	13	0
3	J	433	0	425	10	0
3	K	482	0	477	13	0
3	L	514	0	506	13	0
3	M	433	0	425	9	0
3	N	482	0	477	12	0
3	O	514	0	506	8	0
3	P	433	0	425	10	0
3	Q	482	0	477	11	0
3	R	514	0	506	8	0
3	S	433	0	425	10	0
3	T	482	0	477	11	0
3	U	514	0	506	11	0
3	V	433	0	425	10	0
3	W	482	0	477	10	0
3	X	514	0	506	10	0
3	Y	433	0	425	9	0
3	Z	482	0	477	11	0
3	a	514	0	506	11	0
3	b	433	0	425	9	0
3	c	482	0	477	11	0
3	d	514	0	506	6	0
3	e	433	0	425	10	0
3	f	482	0	477	15	0
3	g	514	0	506	17	0
3	h	433	0	425	11	0
3	i	482	0	477	14	0
3	j	514	0	506	13	0
All	All	71628	0	68244	1455	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 10.

All (1455) 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)
1:0h:17:ARG:HE	3:X:23:ARG:HB2	1.46	0.80
2:0H:160:ASP:HB2	2:0I:203:ASP:HB3	1.67	0.76
1:0k:17:ARG:HE	3:g:23:ARG:HB2	1.52	0.75
2:0B:132:GLY:HA3	2:0C:230:ASN:HA	1.68	0.74
1:0g:17:ARG:HH12	3:P:22:GLU:HB2	1.55	0.72
2:0C:160:ASP:HB2	2:0D:203:ASP:HB3	1.72	0.72
2:0H:167:LEU:HB2	2:0H:194:GLU:HB2	1.72	0.72
2:0I:167:LEU:HB2	2:0I:194:GLU:HB2	1.72	0.72
2:0G:167:LEU:HB2	2:0G:194:GLU:HB2	1.72	0.71
2:0J:167:LEU:HB2	2:0J:194:GLU:HB2	1.72	0.71
2:0F:167:LEU:HB2	2:0F:194:GLU:HB2	1.72	0.71
2:0E:167:LEU:HB2	2:0E:194:GLU:HB2	1.72	0.71
2:0K:167:LEU:HB2	2:0K:194:GLU:HB2	1.72	0.71
2:0D:167:LEU:HB2	2:0D:194:GLU:HB2	1.72	0.70
2:0L:167:LEU:HB2	2:0L:194:GLU:HB2	1.72	0.70
2:0A:167:LEU:HB2	2:0A:194:GLU:HB2	1.72	0.70
2:0B:167:LEU:HB2	2:0B:194:GLU:HB2	1.72	0.70
2:0C:167:LEU:HB2	2:0C:194:GLU:HB2	1.72	0.70
1:0k:17:ARG:HH21	3:g:23:ARG:HG3	1.57	0.69
2:0A:160:ASP:HB2	2:0B:203:ASP:HB3	1.75	0.68
2:0F:160:ASP:HB2	2:0G:203:ASP:HB3	1.75	0.68
1:0c:17:ARG:HH12	3:D:22:GLU:HB2	1.58	0.68
1:0j:17:ARG:HH12	3:e:22:GLU:HB2	1.60	0.67
1:0e:168:GLN:NE2	2:0D:293:TYR:O	2.28	0.67
2:0D:126:GLN:NE2	2:0E:235:THR:O	2.28	0.66
1:0b:17:ARG:HH12	3:A:22:GLU:HB2	1.60	0.66
1:0b:124:ASN:HD21	1:0b:128:PHE:HB3	1.61	0.66
1:0c:124:ASN:HD21	1:0c:128:PHE:HB3	1.61	0.66
1:0g:124:ASN:HD21	1:0g:128:PHE:HB3	1.61	0.66
1:0i:124:ASN:HD21	1:0i:128:PHE:HB3	1.61	0.66
1:0e:124:ASN:HD21	1:0e:128:PHE:HB3	1.61	0.65
1:0k:124:ASN:HD21	1:0k:128:PHE:HB3	1.61	0.65
3:D:54:ASN:HD21	3:I:13:PHE:HB2	1.61	0.65
2:0C:114:ASN:HB3	2:0C:246:SER:HB3	1.79	0.65
1:0a:124:ASN:HD21	1:0a:128:PHE:HB3	1.61	0.65
2:0F:114:ASN:HB3	2:0F:246:SER:HB3	1.79	0.65
1:0l:124:ASN:HD21	1:0l:128:PHE:HB3	1.61	0.65
2:0D:114:ASN:HB3	2:0D:246:SER:HB3	1.79	0.65
2:0G:114:ASN:HB3	2:0G:246:SER:HB3	1.79	0.65
1:0d:124:ASN:HD21	1:0d:128:PHE:HB3	1.61	0.65
1:0i:17:ARG:HH12	3:V:22:GLU:HB2	1.62	0.65
2:0E:114:ASN:HB3	2:0E:246:SER:HB3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0k:17:ARG:HH12	3:b:22:GLU:HB2	1.62	0.64
1:0f:124:ASN:HD21	1:0f:128:PHE:HB3	1.61	0.64
1:0h:124:ASN:HD21	1:0h:128:PHE:HB3	1.61	0.64
1:0j:124:ASN:HD21	1:0j:128:PHE:HB3	1.61	0.64
2:0B:114:ASN:HB3	2:0B:246:SER:HB3	1.79	0.64
2:0E:139:LYS:HE3	2:0F:222:LEU:HD11	1.80	0.64
3:K:21:TYR:OH	3:L:31:GLU:O	2.14	0.64
2:0H:114:ASN:HB3	2:0H:246:SER:HB3	1.79	0.64
1:0h:17:ARG:HH21	3:X:23:ARG:HG3	1.63	0.64
2:0A:114:ASN:HB3	2:0A:246:SER:HB3	1.79	0.64
2:0I:114:ASN:HB3	2:0I:246:SER:HB3	1.79	0.64
1:0e:17:ARG:HH12	3:J:22:GLU:HB2	1.62	0.64
1:0l:17:ARG:HH12	3:Y:22:GLU:HB2	1.62	0.64
1:0f:17:ARG:HH12	3:M:22:GLU:HB2	1.61	0.64
2:0G:139:LYS:HE3	2:0H:222:LEU:HD11	1.80	0.64
2:0J:114:ASN:HB3	2:0J:246:SER:HB3	1.79	0.64
2:0K:114:ASN:HB3	2:0K:246:SER:HB3	1.79	0.64
2:0L:114:ASN:HB3	2:0L:246:SER:HB3	1.79	0.64
1:0b:210:LEU:HD22	1:0c:152:GLN:HE22	1.62	0.64
2:0B:116:THR:HA	2:0C:246:SER:HA	1.80	0.64
2:0E:160:ASP:HB2	2:0F:203:ASP:HB3	1.79	0.63
1:0h:17:ARG:HH12	3:S:22:GLU:HB2	1.63	0.63
2:0A:103:ASN:ND2	2:0A:258:ILE:O	2.32	0.63
2:0E:147:THR:OG1	2:0F:215:ASN:O	2.16	0.63
2:0L:103:ASN:ND2	2:0L:258:ILE:O	2.32	0.63
3:f:21:TYR:OH	3:g:31:GLU:O	2.15	0.63
2:0B:103:ASN:ND2	2:0B:258:ILE:O	2.32	0.63
2:0H:103:ASN:ND2	2:0H:258:ILE:O	2.32	0.63
2:0F:103:ASN:ND2	2:0F:258:ILE:O	2.32	0.62
2:0C:103:ASN:ND2	2:0C:258:ILE:O	2.32	0.62
2:0E:103:ASN:ND2	2:0E:258:ILE:O	2.32	0.62
2:0K:103:ASN:ND2	2:0K:258:ILE:O	2.32	0.62
2:0I:103:ASN:ND2	2:0I:258:ILE:O	2.32	0.62
2:0J:132:GLY:HA3	2:0K:230:ASN:HA	1.80	0.62
2:0G:103:ASN:ND2	2:0G:258:ILE:O	2.32	0.62
1:0d:17:ARG:HH12	3:G:22:GLU:HB2	1.64	0.62
2:0B:134:SER:HA	2:0C:228:THR:HA	1.80	0.62
2:0D:103:ASN:ND2	2:0D:258:ILE:O	2.32	0.62
3:i:38:LYS:HZ1	3:j:43:ILE:HD12	1.65	0.62
1:0d:12:ILE:HD11	1:0f:183:PRO:HD2	1.82	0.61
2:0J:103:ASN:ND2	2:0J:258:ILE:O	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:54:ASN:HD21	3:L:13:PHE:HB2	1.64	0.61
1:0a:17:ARG:HH12	3:h:22:GLU:HB2	1.64	0.61
2:0H:135:SER:HB3	2:0H:137:ASP:HB2	1.82	0.61
3:C:18:VAL:HA	3:h:43:ILE:HD13	1.82	0.61
3:S:36:LEU:HD22	3:X:19:GLN:HG2	1.83	0.61
2:0G:135:SER:HB3	2:0G:137:ASP:HB2	1.82	0.61
2:0K:160:ASP:HB2	2:0L:203:ASP:HB3	1.83	0.61
2:0I:135:SER:HB3	2:0I:137:ASP:HB2	1.82	0.61
2:0H:140:GLN:HA	2:0H:221:THR:HA	1.83	0.60
2:0E:140:GLN:HA	2:0E:221:THR:HA	1.83	0.60
3:Z:21:TYR:OH	3:a:31:GLU:O	2.19	0.60
2:0A:203:ASP:HB3	2:0L:160:ASP:HB2	1.82	0.60
2:0G:140:GLN:HA	2:0G:221:THR:HA	1.83	0.60
2:0I:140:GLN:HA	2:0I:221:THR:HA	1.83	0.60
2:0F:140:GLN:HA	2:0F:221:THR:HA	1.84	0.60
2:0B:135:SER:HB3	2:0B:137:ASP:HB2	1.82	0.60
2:0K:135:SER:HB3	2:0K:137:ASP:HB2	1.82	0.60
2:0C:135:SER:HB3	2:0C:137:ASP:HB2	1.82	0.60
2:0A:135:SER:HB3	2:0A:137:ASP:HB2	1.82	0.60
2:0D:140:GLN:HA	2:0D:221:THR:HA	1.84	0.60
3:E:21:TYR:OH	3:F:31:GLU:O	2.19	0.60
2:0L:135:SER:HB3	2:0L:137:ASP:HB2	1.82	0.60
2:0J:140:GLN:HA	2:0J:221:THR:HA	1.84	0.60
2:0F:135:SER:HB3	2:0F:137:ASP:HB2	1.82	0.59
3:B:21:TYR:OH	3:C:31:GLU:O	2.18	0.59
1:0d:206:VAL:HA	1:0d:209:LYS:HD3	1.85	0.59
1:0g:9:TYR:HB3	3:M:31:GLU:HB2	1.83	0.59
2:0C:140:GLN:HA	2:0C:221:THR:HA	1.83	0.59
1:0a:17:ARG:NH1	3:h:21:TYR:O	2.35	0.59
1:0d:42:GLU:HB2	1:0d:277:LYS:HB2	1.84	0.59
2:0D:135:SER:HB3	2:0D:137:ASP:HB2	1.82	0.59
2:0J:135:SER:HB3	2:0J:137:ASP:HB2	1.82	0.59
3:A:54:ASN:HD21	3:F:13:PHE:HB2	1.67	0.59
3:S:42:ILE:HG12	3:T:46:LEU:HD11	1.85	0.59
1:0e:42:GLU:HB2	1:0e:277:LYS:HB2	1.85	0.59
1:0c:206:VAL:HA	1:0c:209:LYS:HD3	1.85	0.59
1:0e:206:VAL:HA	1:0e:209:LYS:HD3	1.85	0.59
1:0f:42:GLU:HB2	1:0f:277:LYS:HB2	1.84	0.59
1:0j:206:VAL:HA	1:0j:209:LYS:HD3	1.84	0.59
2:0E:135:SER:HB3	2:0E:137:ASP:HB2	1.82	0.59
2:0K:140:GLN:HA	2:0K:221:THR:HA	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:54:ASN:HD21	3:g:13:PHE:HB2	1.67	0.59
1:0c:42:GLU:HB2	1:0c:277:LYS:HB2	1.84	0.59
1:0k:159:VAL:HG22	1:0k:198:VAL:HG22	1.85	0.59
1:0g:159:VAL:HG22	1:0g:198:VAL:HG22	1.85	0.59
1:0j:159:VAL:HG22	1:0j:198:VAL:HG22	1.85	0.59
3:H:21:TYR:OH	3:I:31:GLU:O	2.17	0.59
1:0h:42:GLU:HB2	1:0h:277:LYS:HB2	1.84	0.59
3:P:42:ILE:HG12	3:Q:46:LEU:HD11	1.85	0.59
3:Y:42:ILE:HG12	3:Z:46:LEU:HD11	1.85	0.59
1:0a:159:VAL:HG22	1:0a:198:VAL:HG22	1.85	0.59
1:0a:206:VAL:HA	1:0a:209:LYS:HD3	1.85	0.59
1:0f:169:LEU:HD13	3:L:28:ALA:HB2	1.85	0.59
1:0h:159:VAL:HG22	1:0h:198:VAL:HG22	1.85	0.59
2:0B:140:GLN:HA	2:0B:221:THR:HA	1.84	0.59
2:0L:140:GLN:HA	2:0L:221:THR:HA	1.83	0.59
1:0f:209:LYS:HB3	1:0g:205:TYR:CZ	2.38	0.59
1:0g:42:GLU:HB2	1:0g:277:LYS:HB2	1.84	0.59
1:0i:159:VAL:HG22	1:0i:198:VAL:HG22	1.85	0.59
1:0l:159:VAL:HG22	1:0l:198:VAL:HG22	1.85	0.59
1:0k:206:VAL:HA	1:0k:209:LYS:HD3	1.85	0.58
2:0A:140:GLN:HA	2:0A:221:THR:HA	1.83	0.58
3:b:42:ILE:HG12	3:c:46:LEU:HD11	1.85	0.58
3:e:42:ILE:HG12	3:f:46:LEU:HD11	1.85	0.58
3:A:42:ILE:HG12	3:B:46:LEU:HD11	1.85	0.58
1:0f:159:VAL:HG22	1:0f:198:VAL:HG22	1.85	0.58
1:0i:42:GLU:HB2	1:0i:277:LYS:HB2	1.84	0.58
2:0G:132:GLY:HA3	2:0H:230:ASN:HA	1.85	0.58
1:0b:42:GLU:HB2	1:0b:277:LYS:HB2	1.84	0.58
1:0b:159:VAL:HG22	1:0b:198:VAL:HG22	1.85	0.58
1:0f:206:VAL:HA	1:0f:209:LYS:HD3	1.85	0.58
1:0l:206:VAL:HA	1:0l:209:LYS:HD3	1.85	0.58
2:0C:17:GLN:HE22	3:E:27:THR:H	1.50	0.58
1:0i:206:VAL:HA	1:0i:209:LYS:HD3	1.85	0.58
3:M:42:ILE:HG12	3:N:46:LEU:HD11	1.86	0.58
1:0e:159:VAL:HG22	1:0e:198:VAL:HG22	1.85	0.58
2:0A:222:LEU:HD11	2:0L:139:LYS:HE3	1.85	0.58
2:0F:145:LYS:HA	2:0G:218:GLY:HA3	1.85	0.58
3:G:42:ILE:HG12	3:H:46:LEU:HD11	1.85	0.58
1:0h:206:VAL:HA	1:0h:209:LYS:HD3	1.85	0.58
1:0l:42:GLU:HB2	1:0l:277:LYS:HB2	1.84	0.58
1:0b:206:VAL:HA	1:0b:209:LYS:HD3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0k:42:GLU:HB2	1:0k:277:LYS:HB2	1.84	0.58
2:0F:143:THR:HA	2:0G:220:SER:HA	1.85	0.58
2:0L:249:ASP:N	2:0L:249:ASP:OD1	2.37	0.58
3:h:42:ILE:HG12	3:i:46:LEU:HD11	1.86	0.58
1:0c:159:VAL:HG22	1:0c:198:VAL:HG22	1.85	0.58
2:0H:249:ASP:N	2:0H:249:ASP:OD1	2.37	0.58
1:0a:42:GLU:HB2	1:0a:277:LYS:HB2	1.84	0.57
1:0d:159:VAL:HG22	1:0d:198:VAL:HG22	1.85	0.57
2:0K:168:ASN:OD1	2:0K:168:ASN:N	2.37	0.57
3:J:42:ILE:HG12	3:K:46:LEU:HD11	1.86	0.57
3:N:21:TYR:OH	3:O:31:GLU:O	2.20	0.57
2:0K:249:ASP:OD1	2:0K:249:ASP:N	2.37	0.57
1:0d:209:LYS:HB3	1:0e:205:TYR:CZ	2.39	0.57
2:0B:135:SER:O	2:0C:227:LYS:N	2.34	0.57
3:H:65:GLU:OE2	3:H:69:ASN:ND2	2.37	0.57
2:0C:139:LYS:HE3	2:0D:222:LEU:HD11	1.86	0.57
1:0g:206:VAL:HA	1:0g:209:LYS:HD3	1.85	0.57
1:0j:42:GLU:HB2	1:0j:277:LYS:HB2	1.84	0.57
2:0H:168:ASN:N	2:0H:168:ASN:OD1	2.37	0.57
2:0I:160:ASP:HB2	2:0J:203:ASP:HB3	1.86	0.57
2:0I:168:ASN:OD1	2:0I:168:ASN:N	2.37	0.57
2:0I:249:ASP:N	2:0I:249:ASP:OD1	2.37	0.57
2:0L:168:ASN:N	2:0L:168:ASN:OD1	2.37	0.57
3:i:65:GLU:OE2	3:i:69:ASN:ND2	2.37	0.57
2:0J:168:ASN:OD1	2:0J:168:ASN:N	2.37	0.57
1:0b:72:SER:OG	1:0b:73:TYR:N	2.38	0.57
1:0c:147:ILE:HG21	1:0d:152:GLN:HE21	1.70	0.57
2:0E:143:THR:HA	2:0F:220:SER:HA	1.87	0.57
1:0k:72:SER:OG	1:0k:73:TYR:N	2.38	0.57
3:B:65:GLU:OE2	3:B:69:ASN:ND2	2.37	0.56
1:0c:72:SER:OG	1:0c:73:TYR:N	2.38	0.56
1:0f:109:TYR:HB2	1:0g:47:THR:HA	1.87	0.56
1:0g:72:SER:OG	1:0g:73:TYR:N	2.38	0.56
3:c:65:GLU:OE2	3:c:69:ASN:ND2	2.38	0.56
1:0d:17:ARG:NH1	3:G:21:TYR:O	2.36	0.56
2:0B:139:LYS:HE3	2:0C:222:LEU:HD11	1.85	0.56
2:0B:147:THR:OG1	2:0C:215:ASN:O	2.22	0.56
2:0J:249:ASP:OD1	2:0J:249:ASP:N	2.37	0.56
3:E:65:GLU:OE2	3:E:69:ASN:ND2	2.38	0.56
3:Q:21:TYR:OH	3:R:31:GLU:O	2.23	0.56
3:V:42:ILE:HG12	3:W:46:LEU:HD11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:21:TYR:OH	3:d:31:GLU:O	2.24	0.56
2:0G:168:ASN:OD1	2:0G:168:ASN:N	2.36	0.56
2:0I:139:LYS:HE3	2:0J:222:LEU:HD11	1.87	0.56
3:Z:65:GLU:OE2	3:Z:69:ASN:ND2	2.39	0.56
1:0a:72:SER:OG	1:0a:73:TYR:N	2.38	0.56
1:0f:72:SER:OG	1:0f:73:TYR:N	2.38	0.56
1:0g:147:ILE:HG21	1:0h:152:GLN:HE21	1.71	0.56
3:Q:65:GLU:OE2	3:Q:69:ASN:ND2	2.38	0.56
3:h:46:LEU:HD11	3:j:42:ILE:HG23	1.86	0.56
1:0b:17:ARG:HE	3:F:23:ARG:HB2	1.70	0.56
1:0c:110:ARG:HB3	1:0d:47:THR:HG22	1.87	0.56
2:0D:17:GLN:NE2	3:H:25:LEU:O	2.38	0.56
3:K:65:GLU:OE2	3:K:69:ASN:ND2	2.37	0.56
3:b:36:LEU:HD22	3:g:19:GLN:HG2	1.88	0.56
3:c:38:LYS:HZ1	3:d:43:ILE:HD12	1.70	0.56
1:0h:72:SER:OG	1:0h:73:TYR:N	2.38	0.56
1:0j:72:SER:OG	1:0j:73:TYR:N	2.38	0.56
2:0A:285:MET:HE1	2:0A:288:LEU:HD12	1.88	0.56
2:0B:17:GLN:HE22	3:B:27:THR:H	1.53	0.56
2:0B:126:GLN:NE2	2:0C:235:THR:O	2.38	0.56
3:D:42:ILE:HG12	3:E:46:LEU:HD11	1.88	0.56
3:G:36:LEU:HD22	3:L:19:GLN:HG2	1.88	0.56
3:T:65:GLU:OE2	3:T:69:ASN:ND2	2.38	0.56
3:f:65:GLU:OE2	3:f:69:ASN:ND2	2.39	0.56
1:0j:9:TYR:HB3	3:b:31:GLU:HB2	1.88	0.56
2:0B:285:MET:HE1	2:0B:288:LEU:HD12	1.88	0.56
2:0C:143:THR:HA	2:0D:220:SER:HA	1.86	0.56
2:0F:249:ASP:OD1	2:0F:249:ASP:N	2.37	0.56
2:0L:285:MET:HE1	2:0L:288:LEU:HD12	1.88	0.56
1:0g:259:LYS:NZ	1:0h:36:TYR:O	2.36	0.56
1:0k:9:TYR:HB3	3:Y:31:GLU:HB2	1.87	0.56
1:0a:152:GLN:HE22	1:0j:210:LEU:HD22	1.70	0.55
1:0c:12:ILE:HD11	1:0e:183:PRO:HD2	1.86	0.55
1:0l:72:SER:OG	1:0l:73:TYR:N	2.38	0.55
2:0G:147:THR:OG1	2:0H:215:ASN:O	2.21	0.55
3:e:43:ILE:HD13	3:j:18:VAL:HA	1.87	0.55
1:0f:209:LYS:O	1:0g:205:TYR:OH	2.23	0.55
1:0i:72:SER:OG	1:0i:73:TYR:N	2.38	0.55
2:0A:168:ASN:OD1	2:0A:168:ASN:N	2.37	0.55
2:0E:132:GLY:HA3	2:0F:230:ASN:HA	1.87	0.55
3:W:65:GLU:OE2	3:W:69:ASN:ND2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:i:21:TYR:OH	3:j:31:GLU:O	2.23	0.55
1:0d:72:SER:OG	1:0d:73:TYR:N	2.38	0.55
1:0f:188:HIS:CE1	2:0D:286:GLN:HG2	2.41	0.55
2:0C:285:MET:HE1	2:0C:288:LEU:HD12	1.88	0.55
2:0K:285:MET:HE1	2:0K:288:LEU:HD12	1.88	0.55
1:0i:9:TYR:HB3	3:S:31:GLU:HB2	1.88	0.55
2:0B:168:ASN:OD1	2:0B:168:ASN:N	2.37	0.55
3:N:65:GLU:OE2	3:N:69:ASN:ND2	2.39	0.55
2:0D:132:GLY:HA3	2:0E:230:ASN:HA	1.89	0.55
1:0b:17:ARG:NH1	3:A:21:TYR:O	2.40	0.55
1:0i:110:ARG:HB3	1:0l:47:THR:HG22	1.89	0.55
1:0l:9:TYR:HB3	3:V:31:GLU:HB2	1.88	0.55
1:0d:210:LEU:HD22	1:0e:152:GLN:HE22	1.71	0.55
2:0C:168:ASN:N	2:0C:168:ASN:OD1	2.37	0.55
2:0F:17:GLN:HE22	3:N:27:THR:H	1.55	0.55
2:0D:17:GLN:HE22	3:H:27:THR:H	1.52	0.55
2:0G:249:ASP:OD1	2:0G:249:ASP:N	2.37	0.55
2:0D:168:ASN:N	2:0D:168:ASN:OD1	2.37	0.54
1:0h:168:GLN:NE2	2:0G:293:TYR:O	2.39	0.54
2:0C:155:SER:OG	2:0D:207:SER:OG	2.15	0.54
2:0F:168:ASN:OD1	2:0F:168:ASN:N	2.37	0.54
1:0i:97:SER:O	1:0i:101:GLN:NE2	2.41	0.54
2:0B:82:ILE:HG21	2:0C:279:GLN:HE21	1.72	0.54
2:0B:127:ASP:O	2:0C:234:THR:OG1	2.14	0.54
2:0C:147:THR:OG1	2:0D:215:ASN:O	2.16	0.54
2:0E:168:ASN:OD1	2:0E:168:ASN:N	2.37	0.54
2:0J:285:MET:HE1	2:0J:288:LEU:HD12	1.88	0.54
1:0b:284:ILE:O	1:0b:288:MET:N	2.41	0.54
1:0h:97:SER:O	1:0h:101:GLN:NE2	2.41	0.54
1:0h:110:ARG:HB3	1:0i:47:THR:HG22	1.89	0.54
2:0A:3:SER:N	3:j:30:ASP:OD1	2.41	0.54
2:0C:249:ASP:OD1	2:0C:249:ASP:N	2.37	0.54
2:0D:285:MET:HE1	2:0D:288:LEU:HD12	1.88	0.54
2:0G:285:MET:HE1	2:0G:288:LEU:HD12	1.88	0.54
3:A:36:LEU:HD22	3:F:19:GLN:HG2	1.90	0.54
1:0a:210:LEU:HD22	1:0b:152:GLN:HE22	1.70	0.54
1:0e:97:SER:O	1:0e:101:GLN:NE2	2.41	0.54
2:0C:145:LYS:HA	2:0D:218:GLY:HA3	1.88	0.54
2:0H:82:ILE:HG21	2:0I:279:GLN:HE21	1.73	0.54
1:0e:12:ILE:HD11	1:0g:183:PRO:HD2	1.89	0.54
1:0k:17:ARG:HB2	3:g:23:ARG:HD2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0k:168:GLN:NE2	2:0J:293:TYR:O	2.40	0.54
1:0l:284:ILE:O	1:0l:288:MET:N	2.40	0.54
2:0H:285:MET:HE1	2:0H:288:LEU:HD12	1.88	0.54
2:0J:126:GLN:NE2	2:0K:235:THR:O	2.41	0.54
1:0e:72:SER:OG	1:0e:73:TYR:N	2.38	0.54
1:0l:97:SER:O	1:0l:101:GLN:NE2	2.41	0.54
2:0F:285:MET:HE1	2:0F:288:LEU:HD12	1.88	0.54
1:0g:169:LEU:HD13	3:O:28:ALA:HB2	1.88	0.54
2:0D:249:ASP:N	2:0D:249:ASP:OD1	2.37	0.54
2:0E:145:LYS:HA	2:0F:218:GLY:HA3	1.90	0.54
1:0a:209:LYS:HB3	1:0b:205:TYR:CZ	2.43	0.54
1:0f:9:TYR:HB3	3:J:31:GLU:HB2	1.90	0.54
1:0j:152:GLN:HE22	1:0k:210:LEU:HD22	1.72	0.54
2:0F:81:MET:HB3	2:0G:54:HIS:NE2	2.23	0.54
1:0d:17:ARG:HH21	3:L:23:ARG:HG3	1.73	0.54
1:0d:97:SER:O	1:0d:101:GLN:NE2	2.41	0.54
1:0f:97:SER:O	1:0f:101:GLN:NE2	2.41	0.54
1:0j:97:SER:O	1:0j:101:GLN:NE2	2.41	0.54
1:0a:97:SER:O	1:0a:101:GLN:NE2	2.41	0.53
1:0f:255:THR:OG1	1:0g:37:GLN:NE2	2.41	0.53
2:0I:132:GLY:HA3	2:0J:230:ASN:HA	1.89	0.53
3:W:21:TYR:OH	3:X:31:GLU:O	2.25	0.53
3:Y:43:ILE:HD13	3:d:18:VAL:HA	1.90	0.53
1:0d:284:ILE:O	1:0d:288:MET:N	2.40	0.53
1:0e:147:ILE:HG21	1:0f:152:GLN:HE21	1.72	0.53
2:0B:249:ASP:OD1	2:0B:249:ASP:N	2.37	0.53
3:f:38:LYS:HZ1	3:g:43:ILE:HD12	1.72	0.53
1:0b:110:ARG:HB3	1:0c:47:THR:HG22	1.90	0.53
1:0g:14:GLU:OE2	3:U:23:ARG:N	2.37	0.53
1:0g:110:ARG:HB3	1:0h:47:THR:HG22	1.90	0.53
1:0k:47:THR:HG22	1:0l:110:ARG:HB3	1.91	0.53
1:0k:284:ILE:O	1:0k:288:MET:N	2.40	0.53
2:0A:249:ASP:N	2:0A:249:ASP:OD1	2.37	0.53
2:0I:285:MET:HE1	2:0I:288:LEU:HD12	1.88	0.53
1:0c:97:SER:O	1:0c:101:GLN:NE2	2.41	0.53
1:0j:47:THR:HG22	1:0k:110:ARG:HB3	1.90	0.53
1:0k:97:SER:O	1:0k:101:GLN:NE2	2.41	0.53
2:0E:285:MET:HE1	2:0E:288:LEU:HD12	1.88	0.53
2:0H:126:GLN:NE2	2:0I:235:THR:O	2.41	0.53
1:0f:147:ILE:HG21	1:0g:152:GLN:HE21	1.73	0.53
1:0g:259:LYS:NZ	1:0h:54:GLU:OE1	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0B:160:ASP:HB2	2:0C:203:ASP:HB3	1.89	0.53
1:0b:12:ILE:HD11	1:0d:183:PRO:HD2	1.91	0.53
1:0g:97:SER:O	1:0g:101:GLN:NE2	2.41	0.53
2:0A:215:ASN:O	2:0L:147:THR:OG1	2.19	0.53
2:0F:273:ALA:O	2:0G:271:ARG:NH1	2.36	0.53
1:0b:97:SER:O	1:0b:101:GLN:NE2	2.41	0.53
1:0h:284:ILE:O	1:0h:288:MET:N	2.41	0.53
2:0B:128:LEU:HG	2:0C:234:THR:HB	1.91	0.53
2:0F:147:THR:OG1	2:0G:215:ASN:O	2.18	0.53
2:0H:17:GLN:HE22	3:T:27:THR:H	1.57	0.53
3:A:46:LEU:HD11	3:C:42:ILE:HG23	1.89	0.53
1:0a:168:GLN:HE21	1:0a:172:LYS:HE2	1.74	0.53
1:0h:9:TYR:HB3	3:P:31:GLU:HB2	1.90	0.53
2:0A:23:SER:O	2:0A:27:LYS:N	2.40	0.53
2:0J:139:LYS:HE3	2:0K:222:LEU:HD11	1.91	0.53
1:0b:168:GLN:HE21	1:0b:172:LYS:HE2	1.74	0.53
1:0f:284:ILE:O	1:0f:288:MET:N	2.41	0.53
1:0g:168:GLN:HE21	1:0g:172:LYS:HE2	1.74	0.53
1:0h:168:GLN:HE21	1:0h:172:LYS:HE2	1.74	0.53
2:0A:17:GLN:HE22	3:i:27:THR:H	1.56	0.53
2:0B:143:THR:HA	2:0C:220:SER:HA	1.91	0.53
1:0i:168:GLN:HE21	1:0i:172:LYS:HE2	1.74	0.53
2:0E:249:ASP:N	2:0E:249:ASP:OD1	2.37	0.53
2:0F:139:LYS:HE3	2:0G:222:LEU:HD11	1.91	0.53
1:0c:168:GLN:HE21	1:0c:172:LYS:HE2	1.74	0.52
1:0d:168:GLN:HE21	1:0d:172:LYS:HE2	1.74	0.52
1:0e:168:GLN:HE21	1:0e:172:LYS:HE2	1.74	0.52
1:0h:210:LEU:HD22	1:0i:152:GLN:HE22	1.74	0.52
2:0B:121:ASN:O	2:0C:240:LEU:HA	2.09	0.52
2:0I:31:GLY:O	2:0I:35:LEU:N	2.38	0.52
2:0L:169:ALA:H	2:0L:192:GLN:HE21	1.58	0.52
3:Z:38:LYS:HZ1	3:a:43:ILE:HD12	1.74	0.52
1:0a:284:ILE:O	1:0a:288:MET:N	2.40	0.52
1:0i:284:ILE:O	1:0i:288:MET:N	2.40	0.52
2:0C:31:GLY:O	2:0C:35:LEU:N	2.38	0.52
2:0E:17:GLN:HE22	3:K:27:THR:H	1.55	0.52
2:0G:169:ALA:H	2:0G:192:GLN:HE21	1.58	0.52
2:0I:169:ALA:H	2:0I:192:GLN:HE21	1.58	0.52
2:0J:169:ALA:H	2:0J:192:GLN:HE21	1.58	0.52
1:0j:168:GLN:HE21	1:0j:172:LYS:HE2	1.74	0.52
2:0B:31:GLY:O	2:0B:35:LEU:N	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0B:145:LYS:HA	2:0C:218:GLY:HA3	1.90	0.52
2:0I:147:THR:OG1	2:0J:215:ASN:O	2.20	0.52
2:0K:126:GLN:NE2	2:0L:235:THR:O	2.42	0.52
2:0K:169:ALA:H	2:0K:192:GLN:HE21	1.58	0.52
1:0i:210:LEU:HD22	1:0l:152:GLN:HE22	1.75	0.52
1:0k:168:GLN:HE21	1:0k:172:LYS:HE2	1.74	0.52
1:0l:168:GLN:HE21	1:0l:172:LYS:HE2	1.74	0.52
1:0e:9:TYR:HB3	3:G:31:GLU:HB2	1.92	0.52
1:0f:168:GLN:HE21	1:0f:172:LYS:HE2	1.74	0.52
1:0i:17:ARG:HE	3:a:23:ARG:HB2	1.74	0.52
2:0A:169:ALA:H	2:0A:192:GLN:HE21	1.58	0.52
2:0D:31:GLY:O	2:0D:35:LEU:N	2.38	0.52
1:0f:259:LYS:NZ	1:0g:36:TYR:O	2.38	0.52
2:0B:169:ALA:H	2:0B:192:GLN:HE21	1.58	0.52
2:0E:23:SER:O	2:0E:27:LYS:N	2.40	0.52
2:0F:206:THR:OG1	2:0F:207:SER:N	2.43	0.52
2:0H:169:ALA:H	2:0H:192:GLN:HE21	1.58	0.52
2:0I:206:THR:OG1	2:0I:207:SER:N	2.43	0.52
2:0K:42:ILE:HG21	2:0K:48:ARG:HB2	1.92	0.52
2:0D:116:THR:HA	2:0E:246:SER:HA	1.92	0.52
2:0H:206:THR:OG1	2:0H:207:SER:N	2.43	0.52
1:0d:172:LYS:HG2	1:0e:186:PHE:HE2	1.75	0.52
2:0A:31:GLY:O	2:0A:35:LEU:N	2.38	0.52
2:0I:23:SER:O	2:0I:27:LYS:N	2.40	0.52
2:0K:206:THR:OG1	2:0K:207:SER:N	2.43	0.52
3:D:46:LEU:HD11	3:F:42:ILE:HG23	1.92	0.52
1:0c:172:LYS:HG2	1:0d:186:PHE:HE2	1.75	0.52
2:0A:167:LEU:O	2:0A:194:GLU:N	2.42	0.52
2:0C:159:THR:HA	2:0D:204:THR:HA	1.92	0.52
2:0E:169:ALA:H	2:0E:192:GLN:HE21	1.58	0.52
2:0F:169:ALA:H	2:0F:192:GLN:HE21	1.57	0.52
2:0H:42:ILE:HG21	2:0H:48:ARG:HB2	1.92	0.52
2:0K:147:THR:OG1	2:0L:215:ASN:O	2.27	0.51
1:0g:284:ILE:O	1:0g:288:MET:N	2.40	0.51
2:0B:42:ILE:HG21	2:0B:48:ARG:HB2	1.92	0.51
2:0B:115:ASP:HB2	2:0C:247:VAL:HG13	1.91	0.51
2:0C:169:ALA:H	2:0C:192:GLN:HE21	1.58	0.51
2:0D:167:LEU:O	2:0D:194:GLU:N	2.42	0.51
2:0D:169:ALA:H	2:0D:192:GLN:HE21	1.58	0.51
2:0E:31:GLY:O	2:0E:35:LEU:N	2.38	0.51
1:0g:159:VAL:HB	1:0h:184:VAL:HG22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0J:42:ILE:HG21	2:0J:48:ARG:HB2	1.92	0.51
3:T:21:TYR:OH	3:U:31:GLU:O	2.26	0.51
1:0b:17:ARG:HH21	3:F:23:ARG:HG3	1.75	0.51
1:0b:168:GLN:NE2	2:0A:293:TYR:O	2.43	0.51
2:0G:126:GLN:NE2	2:0H:235:THR:O	2.43	0.51
2:0L:42:ILE:HG21	2:0L:48:ARG:HB2	1.92	0.51
1:0a:172:LYS:HG2	1:0b:186:PHE:HE2	1.75	0.51
2:0C:167:LEU:O	2:0C:194:GLU:N	2.42	0.51
2:0D:206:THR:OG1	2:0D:207:SER:N	2.43	0.51
2:0E:206:THR:OG1	2:0E:207:SER:N	2.43	0.51
2:0F:31:GLY:O	2:0F:35:LEU:N	2.38	0.51
1:0c:17:ARG:NH1	3:D:21:TYR:O	2.44	0.51
1:0d:17:ARG:HE	3:L:23:ARG:HB2	1.74	0.51
1:0e:110:ARG:HB3	1:0f:47:THR:HG22	1.91	0.51
3:K:38:LYS:HZ1	3:L:43:ILE:HD12	1.75	0.51
2:0B:133:THR:O	2:0C:228:THR:OG1	2.22	0.51
2:0G:42:ILE:HG21	2:0G:48:ARG:HB2	1.92	0.51
2:0J:134:SER:HA	2:0K:228:THR:HA	1.93	0.51
1:0c:284:ILE:O	1:0c:288:MET:N	2.40	0.51
2:0A:206:THR:OG1	2:0A:207:SER:N	2.43	0.51
2:0C:206:THR:OG1	2:0C:207:SER:N	2.43	0.51
2:0I:42:ILE:HG21	2:0I:48:ARG:HB2	1.92	0.51
1:0g:14:GLU:CD	3:U:23:ARG:H	2.19	0.51
2:0A:42:ILE:HG21	2:0A:48:ARG:HB2	1.92	0.51
2:0F:106:VAL:HA	2:0G:256:GLY:HA3	1.92	0.51
1:0f:259:LYS:NZ	1:0g:54:GLU:OE1	2.38	0.51
2:0A:32:ARG:NH1	2:0A:52:GLU:OE1	2.44	0.51
2:0C:153:SER:OG	2:0D:209:THR:O	2.20	0.51
2:0D:23:SER:O	2:0D:27:LYS:N	2.40	0.51
2:0H:155:SER:OG	2:0I:207:SER:OG	2.23	0.51
2:0I:143:THR:HA	2:0J:220:SER:HA	1.92	0.51
2:0I:145:LYS:HA	2:0J:218:GLY:HA3	1.93	0.51
2:0K:32:ARG:NH1	2:0K:52:GLU:OE1	2.44	0.51
2:0L:32:ARG:NH1	2:0L:52:GLU:OE1	2.44	0.51
3:J:46:LEU:HD11	3:L:42:ILE:HG23	1.93	0.51
1:0d:255:THR:OG1	1:0e:37:GLN:NE2	2.43	0.50
1:0k:152:GLN:HE22	1:0l:210:LEU:HD22	1.75	0.50
2:0E:42:ILE:HG21	2:0E:48:ARG:HB2	1.92	0.50
1:0a:9:TYR:HB3	3:e:31:GLU:HB2	1.92	0.50
1:0a:47:THR:HG22	1:0j:110:ARG:HB3	1.93	0.50
2:0B:32:ARG:NH1	2:0B:52:GLU:OE1	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0C:42:ILE:HG21	2:0C:48:ARG:HB2	1.92	0.50
2:0E:133:THR:O	2:0F:228:THR:OG1	2.26	0.50
2:0H:31:GLY:O	2:0H:35:LEU:N	2.38	0.50
2:0H:167:LEU:O	2:0H:194:GLU:N	2.42	0.50
2:0L:23:SER:O	2:0L:27:LYS:N	2.40	0.50
1:0d:105:LYS:HB2	1:0d:117:MET:HG2	1.94	0.50
1:0e:17:ARG:NH1	3:J:21:TYR:O	2.44	0.50
1:0e:105:LYS:HB2	1:0e:117:MET:HG2	1.94	0.50
1:0f:172:LYS:HG2	1:0g:186:PHE:HE2	1.76	0.50
2:0B:17:GLN:NE2	3:B:25:LEU:O	2.44	0.50
2:0L:31:GLY:O	2:0L:35:LEU:N	2.38	0.50
2:0L:206:THR:OG1	2:0L:207:SER:N	2.43	0.50
3:W:38:LYS:HZ1	3:X:43:ILE:HD12	1.77	0.50
2:0B:206:THR:OG1	2:0B:207:SER:N	2.43	0.50
2:0J:32:ARG:NH1	2:0J:52:GLU:OE1	2.44	0.50
3:Y:46:LEU:HD11	3:a:42:ILE:HG23	1.92	0.50
1:0c:105:LYS:HB2	1:0c:117:MET:HG2	1.94	0.50
1:0e:284:ILE:O	1:0e:288:MET:N	2.40	0.50
2:0K:167:LEU:O	2:0K:194:GLU:N	2.42	0.50
3:B:38:LYS:HZ1	3:C:43:ILE:HD12	1.76	0.50
1:0g:12:ILE:HD11	1:0i:183:PRO:HD2	1.93	0.50
1:0i:12:ILE:HD11	1:0k:183:PRO:HD2	1.94	0.50
2:0I:32:ARG:NH1	2:0I:52:GLU:OE1	2.44	0.50
1:0f:105:LYS:HB2	1:0f:117:MET:HG2	1.94	0.50
2:0D:42:ILE:HG21	2:0D:48:ARG:HB2	1.92	0.50
2:0F:32:ARG:NH1	2:0F:52:GLU:OE1	2.44	0.50
2:0F:132:GLY:HA3	2:0G:230:ASN:HA	1.94	0.50
2:0G:32:ARG:NH1	2:0G:52:GLU:OE1	2.44	0.50
3:i:31:GLU:O	3:i:41:LYS:NZ	2.37	0.50
2:0D:105:ARG:HG3	2:0D:255:VAL:HG12	1.94	0.50
2:0E:32:ARG:NH1	2:0E:52:GLU:OE1	2.44	0.50
2:0F:42:ILE:HG21	2:0F:48:ARG:HB2	1.92	0.50
2:0G:81:MET:HB3	2:0H:54:HIS:CE1	2.47	0.50
2:0J:90:LEU:O	2:0J:93:SER:OG	2.27	0.50
2:0J:228:THR:OG1	2:0J:229:SER:N	2.45	0.50
2:0K:139:LYS:HE3	2:0L:222:LEU:HD11	1.94	0.50
2:0L:105:ARG:HG3	2:0L:255:VAL:HG12	1.94	0.50
1:0c:7:ASN:HA	3:A:34:THR:HG21	1.94	0.50
2:0A:105:ARG:HG3	2:0A:255:VAL:HG12	1.94	0.50
2:0A:228:THR:OG1	2:0A:229:SER:N	2.45	0.50
2:0C:228:THR:OG1	2:0C:229:SER:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:105:ARG:HG3	2:0K:255:VAL:HG12	1.94	0.50
1:0b:105:LYS:HB2	1:0b:117:MET:HG2	1.94	0.49
1:0h:12:ILE:HD11	1:0l:183:PRO:HD2	1.94	0.49
2:0A:126:GLN:NE2	2:0B:235:THR:O	2.45	0.49
2:0A:220:SER:HA	2:0L:143:THR:HA	1.93	0.49
2:0B:105:ARG:HG3	2:0B:255:VAL:HG12	1.94	0.49
2:0C:105:ARG:HG3	2:0C:255:VAL:HG12	1.94	0.49
2:0E:278:GLU:HA	2:0E:281:ILE:HD12	1.94	0.49
2:0G:228:THR:OG1	2:0G:229:SER:N	2.45	0.49
2:0L:228:THR:OG1	2:0L:229:SER:N	2.45	0.49
1:0h:17:ARG:NH2	3:X:23:ARG:HG3	2.27	0.49
2:0B:168:ASN:HB3	2:0B:193:ILE:HG13	1.94	0.49
2:0G:160:ASP:HB2	2:0H:203:ASP:HB3	1.93	0.49
2:0H:23:SER:O	2:0H:27:LYS:N	2.40	0.49
2:0J:278:GLU:HA	2:0J:281:ILE:HD12	1.94	0.49
2:0L:167:LEU:O	2:0L:194:GLU:N	2.42	0.49
3:G:46:LEU:HD11	3:I:42:ILE:HG23	1.94	0.49
3:W:32:SER:OG	3:W:34:THR:O	2.30	0.49
1:0a:110:ARG:HB3	1:0b:47:THR:HG22	1.94	0.49
1:0l:15:ILE:O	1:0l:19:LYS:N	2.34	0.49
2:0A:168:ASN:HB3	2:0A:193:ILE:HG13	1.94	0.49
2:0B:228:THR:OG1	2:0B:229:SER:N	2.45	0.49
2:0B:278:GLU:HA	2:0B:281:ILE:HD12	1.94	0.49
2:0C:32:ARG:NH1	2:0C:52:GLU:OE1	2.45	0.49
2:0F:167:LEU:O	2:0F:194:GLU:N	2.42	0.49
2:0G:161:ASP:OD1	2:0G:162:ASN:N	2.45	0.49
2:0H:32:ARG:NH1	2:0H:52:GLU:OE1	2.44	0.49
2:0J:105:ARG:HG3	2:0J:255:VAL:HG12	1.94	0.49
1:0g:105:LYS:HB2	1:0g:117:MET:HG2	1.94	0.49
2:0C:262:SER:HG	2:0C:265:ARG:H	1.59	0.49
2:0D:32:ARG:NH1	2:0D:52:GLU:OE1	2.44	0.49
2:0E:105:ARG:HG3	2:0E:255:VAL:HG12	1.94	0.49
2:0G:168:ASN:HB3	2:0G:193:ILE:HG13	1.94	0.49
2:0H:161:ASP:OD1	2:0H:162:ASN:N	2.45	0.49
2:0I:228:THR:OG1	2:0I:229:SER:N	2.45	0.49
2:0K:278:GLU:HA	2:0K:281:ILE:HD12	1.95	0.49
1:0a:105:LYS:HB2	1:0a:117:MET:HG2	1.94	0.49
2:0A:161:ASP:OD1	2:0A:162:ASN:N	2.45	0.49
2:0A:278:GLU:HA	2:0A:281:ILE:HD12	1.94	0.49
2:0B:90:LEU:O	2:0B:93:SER:OG	2.27	0.49
2:0H:168:ASN:HB3	2:0H:193:ILE:HG13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0H:228:THR:OG1	2:0H:229:SER:N	2.45	0.49
1:0a:134:LEU:HD22	1:0a:221:MET:HE1	1.95	0.49
1:0h:105:LYS:HB2	1:0h:117:MET:HG2	1.94	0.49
1:0j:284:ILE:O	1:0j:288:MET:N	2.40	0.49
1:0k:15:ILE:O	1:0k:19:LYS:N	2.34	0.49
2:0B:161:ASP:OD1	2:0B:162:ASN:N	2.45	0.49
2:0D:278:GLU:HA	2:0D:281:ILE:HD12	1.95	0.49
2:0E:228:THR:OG1	2:0E:229:SER:N	2.45	0.49
2:0F:105:ARG:HG3	2:0F:255:VAL:HG12	1.94	0.49
2:0H:278:GLU:HA	2:0H:281:ILE:HD12	1.94	0.49
2:0I:105:ARG:HG3	2:0I:255:VAL:HG12	1.94	0.49
2:0L:161:ASP:OD1	2:0L:162:ASN:N	2.45	0.49
1:0j:134:LEU:HD22	1:0j:221:MET:HE1	1.95	0.49
2:0C:168:ASN:HB3	2:0C:193:ILE:HG13	1.94	0.49
2:0G:278:GLU:HA	2:0G:281:ILE:HD12	1.94	0.49
2:0L:130:SER:OG	2:0L:230:ASN:OD1	2.31	0.49
2:0L:262:SER:HG	2:0L:265:ARG:H	1.61	0.49
3:D:36:LEU:HD22	3:I:19:GLN:HG2	1.94	0.49
1:0b:134:LEU:HD22	1:0b:221:MET:HE1	1.95	0.49
1:0d:134:LEU:HD22	1:0d:221:MET:HE1	1.95	0.49
1:0k:105:LYS:HB2	1:0k:117:MET:HG2	1.94	0.49
1:0l:105:LYS:HB2	1:0l:117:MET:HG2	1.94	0.49
2:0A:130:SER:OG	2:0A:230:ASN:OD1	2.31	0.49
2:0E:130:SER:OG	2:0E:230:ASN:OD1	2.31	0.49
2:0F:130:SER:OG	2:0F:230:ASN:OD1	2.31	0.49
2:0F:161:ASP:OD1	2:0F:162:ASN:N	2.45	0.49
2:0G:105:ARG:HG3	2:0G:255:VAL:HG12	1.94	0.49
2:0G:130:SER:OG	2:0G:230:ASN:OD1	2.31	0.49
2:0H:105:ARG:HG3	2:0H:255:VAL:HG12	1.94	0.49
2:0I:130:SER:OG	2:0I:230:ASN:OD1	2.31	0.49
2:0L:168:ASN:HB3	2:0L:193:ILE:HG13	1.94	0.49
1:0b:7:ASN:HA	3:h:34:THR:HG21	1.93	0.49
1:0c:134:LEU:HD22	1:0c:221:MET:HE1	1.95	0.49
1:0f:14:GLU:OE2	3:R:23:ARG:N	2.38	0.49
1:0g:110:ARG:H	1:0h:47:THR:HA	1.77	0.49
1:0j:65:PHE:HB3	1:0j:119:VAL:HB	1.95	0.49
1:0k:160:LEU:N	1:0k:197:GLU:O	2.46	0.49
2:0D:130:SER:OG	2:0D:230:ASN:OD1	2.31	0.49
2:0F:23:SER:O	2:0F:27:LYS:N	2.40	0.49
2:0H:130:SER:OG	2:0H:230:ASN:OD1	2.31	0.49
2:0K:130:SER:OG	2:0K:230:ASN:OD1	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:161:ASP:OD1	2:0K:162:ASN:N	2.45	0.49
1:0c:65:PHE:HB3	1:0c:119:VAL:HB	1.95	0.49
1:0i:105:LYS:HB2	1:0i:117:MET:HG2	1.94	0.49
1:0j:37:GLN:NE2	1:0k:255:THR:OG1	2.46	0.49
1:0j:105:LYS:HB2	1:0j:117:MET:HG2	1.94	0.49
2:0B:130:SER:OG	2:0B:230:ASN:OD1	2.31	0.49
2:0B:167:LEU:O	2:0B:194:GLU:N	2.42	0.49
2:0I:161:ASP:OD1	2:0I:162:ASN:N	2.45	0.49
2:0J:130:SER:OG	2:0J:230:ASN:OD1	2.31	0.49
2:0J:168:ASN:HB3	2:0J:193:ILE:HG13	1.94	0.49
1:0a:147:ILE:HG21	1:0b:152:GLN:HE21	1.78	0.48
1:0f:87:TYR:OH	1:0g:47:THR:O	2.20	0.48
1:0l:160:LEU:N	1:0l:197:GLU:O	2.46	0.48
2:0C:130:SER:OG	2:0C:230:ASN:OD1	2.31	0.48
2:0C:161:ASP:OD1	2:0C:162:ASN:N	2.45	0.48
2:0D:161:ASP:OD1	2:0D:162:ASN:N	2.45	0.48
2:0E:168:ASN:HB3	2:0E:193:ILE:HG13	1.94	0.48
2:0F:155:SER:OG	2:0F:156:GLY:N	2.46	0.48
3:B:31:GLU:O	3:B:41:LYS:NZ	2.41	0.48
1:0c:255:THR:OG1	1:0d:37:GLN:NE2	2.46	0.48
1:0c:259:LYS:NZ	1:0d:54:GLU:OE1	2.41	0.48
1:0i:15:ILE:O	1:0i:19:LYS:N	2.34	0.48
1:0i:65:PHE:HB3	1:0i:119:VAL:HB	1.95	0.48
1:0l:65:PHE:HB3	1:0l:119:VAL:HB	1.95	0.48
2:0D:128:LEU:HG	2:0E:234:THR:HB	1.95	0.48
2:0E:167:LEU:O	2:0E:194:GLU:N	2.42	0.48
2:0H:155:SER:OG	2:0H:156:GLY:N	2.46	0.48
2:0J:161:ASP:OD1	2:0J:162:ASN:N	2.45	0.48
3:E:31:GLU:O	3:E:41:LYS:NZ	2.40	0.48
3:e:46:LEU:HD11	3:g:42:ILE:HG23	1.94	0.48
1:0a:65:PHE:HB3	1:0a:119:VAL:HB	1.95	0.48
1:0b:173:GLN:HE22	3:j:24:TYR:HA	1.77	0.48
1:0e:134:LEU:HD22	1:0e:221:MET:HE1	1.95	0.48
1:0k:134:LEU:HD22	1:0k:221:MET:HE1	1.95	0.48
2:0C:278:GLU:HA	2:0C:281:ILE:HD12	1.94	0.48
2:0D:168:ASN:HB3	2:0D:193:ILE:HG13	1.94	0.48
2:0K:115:ASP:HB2	2:0L:247:VAL:HG13	1.96	0.48
1:0j:205:TYR:CZ	1:0k:209:LYS:HB3	2.47	0.48
2:0C:23:SER:O	2:0C:27:LYS:N	2.40	0.48
2:0D:228:THR:OG1	2:0D:229:SER:N	2.45	0.48
2:0F:228:THR:OG1	2:0F:229:SER:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0G:90:LEU:O	2:0G:93:SER:OG	2.27	0.48
2:0G:167:LEU:O	2:0G:194:GLU:N	2.41	0.48
2:0I:9:ARG:NE	2:0I:61:MET:SD	2.83	0.48
2:0J:167:LEU:O	2:0J:194:GLU:N	2.42	0.48
2:0K:168:ASN:HB3	2:0K:193:ILE:HG13	1.94	0.48
3:T:32:SER:OG	3:T:34:THR:O	2.32	0.48
1:0f:134:LEU:HD22	1:0f:221:MET:HE1	1.95	0.48
1:0j:183:PRO:HD2	1:0l:12:ILE:HD11	1.95	0.48
2:0E:161:ASP:OD1	2:0E:162:ASN:N	2.45	0.48
2:0F:24:THR:OG1	3:K:31:GLU:OE2	2.28	0.48
2:0I:126:GLN:NE2	2:0J:235:THR:O	2.46	0.48
2:0K:31:GLY:O	2:0K:35:LEU:N	2.38	0.48
2:0K:228:THR:OG1	2:0K:229:SER:N	2.45	0.48
1:0b:65:PHE:HB3	1:0b:119:VAL:HB	1.95	0.48
1:0f:209:LYS:HB3	1:0g:205:TYR:CE2	2.48	0.48
1:0j:15:ILE:O	1:0j:19:LYS:N	2.34	0.48
2:0A:218:GLY:HA3	2:0L:145:LYS:HA	1.94	0.48
2:0D:155:SER:OG	2:0D:156:GLY:N	2.46	0.48
2:0G:31:GLY:O	2:0G:35:LEU:N	2.38	0.48
2:0B:133:THR:HG22	2:0C:229:SER:HB3	1.94	0.48
2:0C:17:GLN:NE2	3:E:27:THR:H	2.11	0.48
2:0H:110:SER:HA	2:0I:252:GLU:HA	1.96	0.48
2:0I:167:LEU:O	2:0I:194:GLU:N	2.42	0.48
2:0I:168:ASN:HB3	2:0I:193:ILE:HG13	1.94	0.48
2:0I:278:GLU:HA	2:0I:281:ILE:HD12	1.95	0.48
2:0L:9:ARG:NE	2:0L:61:MET:SD	2.83	0.48
3:Z:32:SER:OG	3:Z:34:THR:O	2.31	0.48
1:0g:134:LEU:HD22	1:0g:221:MET:HE1	1.95	0.48
2:0D:115:ASP:HB2	2:0E:247:VAL:HG13	1.95	0.48
1:0b:161:ILE:HD12	1:0c:186:PHE:HE1	1.79	0.48
1:0b:209:LYS:HB3	1:0c:205:TYR:CZ	2.49	0.48
1:0f:65:PHE:HB3	1:0f:119:VAL:HB	1.95	0.48
1:0i:160:LEU:N	1:0i:197:GLU:O	2.46	0.48
1:0k:65:PHE:HB3	1:0k:119:VAL:HB	1.95	0.48
2:0F:278:GLU:HA	2:0F:281:ILE:HD12	1.95	0.48
2:0L:278:GLU:HA	2:0L:281:ILE:HD12	1.94	0.48
1:0c:160:LEU:N	1:0c:197:GLU:O	2.46	0.48
1:0d:65:PHE:HB3	1:0d:119:VAL:HB	1.95	0.48
1:0h:134:LEU:HD22	1:0h:221:MET:HE1	1.95	0.48
1:0l:134:LEU:HD22	1:0l:221:MET:HE1	1.95	0.48
2:0A:24:THR:OG1	3:f:31:GLU:OE2	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:51:LYS:NZ	3:T:55:GLU:OE2	2.46	0.48
1:0d:9:TYR:HB3	3:D:31:GLU:HB2	1.95	0.47
1:0e:160:LEU:N	1:0e:197:GLU:O	2.46	0.47
2:0B:238:ASP:OD1	2:0B:239:LYS:N	2.48	0.47
2:0J:160:ASP:HB2	2:0K:203:ASP:HB3	1.96	0.47
1:0d:147:ILE:HG21	1:0e:152:GLN:HE21	1.79	0.47
1:0e:255:THR:OG1	1:0f:37:GLN:NE2	2.47	0.47
1:0k:17:ARG:NH2	3:g:23:ARG:HG3	2.27	0.47
2:0F:150:GLU:O	2:0G:213:THR:OG1	2.28	0.47
2:0F:159:THR:HA	2:0G:204:THR:HA	1.96	0.47
2:0G:143:THR:HA	2:0H:220:SER:HA	1.96	0.47
2:0I:155:SER:OG	2:0I:156:GLY:N	2.47	0.47
3:H:31:GLU:O	3:H:41:LYS:NZ	2.43	0.47
3:Q:32:SER:OG	3:Q:34:THR:O	2.33	0.47
3:b:65:GLU:OE2	3:b:69:ASN:ND2	2.45	0.47
1:0d:110:ARG:HB3	1:0e:47:THR:HG22	1.96	0.47
2:0A:238:ASP:OD1	2:0A:239:LYS:N	2.48	0.47
2:0C:238:ASP:OD1	2:0C:239:LYS:N	2.48	0.47
2:0E:150:GLU:O	2:0F:213:THR:OG1	2.32	0.47
2:0F:168:ASN:HB3	2:0F:193:ILE:HG13	1.94	0.47
2:0H:115:ASP:HB2	2:0I:247:VAL:HG13	1.95	0.47
2:0J:206:THR:OG1	2:0J:207:SER:N	2.43	0.47
1:0d:168:GLN:NE2	2:0C:293:TYR:O	2.48	0.47
1:0e:172:LYS:HG2	1:0f:186:PHE:HE2	1.80	0.47
1:0g:65:PHE:HB3	1:0g:119:VAL:HB	1.95	0.47
1:0i:134:LEU:HD22	1:0i:221:MET:HE1	1.95	0.47
1:0k:54:GLU:OE1	1:0l:259:LYS:NZ	2.44	0.47
2:0G:155:SER:OG	2:0G:156:GLY:N	2.46	0.47
2:0J:238:ASP:OD1	2:0J:239:LYS:N	2.48	0.47
2:0K:23:SER:O	2:0K:27:LYS:N	2.40	0.47
2:0K:238:ASP:OD1	2:0K:239:LYS:N	2.48	0.47
3:V:36:LEU:HD22	3:a:19:GLN:HG2	1.95	0.47
1:0c:9:TYR:HB3	3:A:31:GLU:HB2	1.96	0.47
1:0d:7:ASN:HA	3:D:34:THR:HG21	1.97	0.47
1:0g:173:GLN:HE22	3:O:24:TYR:HA	1.79	0.47
2:0J:3:SER:OG	2:0J:4:TYR:N	2.48	0.47
2:0L:238:ASP:OD1	2:0L:239:LYS:N	2.48	0.47
3:V:43:ILE:HD13	3:a:18:VAL:HA	1.97	0.47
3:e:67:ILE:HG12	3:f:67:ILE:HB	1.96	0.47
2:0D:238:ASP:OD1	2:0D:239:LYS:N	2.48	0.47
1:0c:68:ASP:N	1:0c:72:SER:O	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0e:65:PHE:HB3	1:0e:119:VAL:HB	1.95	0.47
1:0e:159:VAL:HB	1:0f:184:VAL:HG22	1.97	0.47
1:0e:259:LYS:NZ	1:0f:54:GLU:OE1	2.40	0.47
1:0h:65:PHE:HB3	1:0h:119:VAL:HB	1.95	0.47
2:0A:230:ASN:HA	2:0L:132:GLY:HA3	1.96	0.47
2:0E:17:GLN:NE2	3:K:27:THR:H	2.13	0.47
2:0K:90:LEU:O	2:0K:93:SER:OG	2.27	0.47
3:K:31:GLU:O	3:K:41:LYS:NZ	2.42	0.47
3:P:65:GLU:OE2	3:P:69:ASN:ND2	2.45	0.47
1:0f:12:ILE:HD11	1:0h:183:PRO:HD2	1.97	0.47
1:0g:17:ARG:HE	3:U:23:ARG:HB2	1.79	0.47
1:0g:168:GLN:NE2	2:0F:293:TYR:O	2.48	0.47
1:0h:15:ILE:O	1:0h:19:LYS:N	2.34	0.47
2:0B:9:ARG:NE	2:0B:61:MET:SD	2.83	0.47
2:0C:90:LEU:O	2:0C:93:SER:OG	2.27	0.47
2:0F:81:MET:HB3	2:0G:54:HIS:CE1	2.49	0.47
2:0J:23:SER:O	2:0J:27:LYS:N	2.40	0.47
3:V:65:GLU:OE2	3:V:69:ASN:ND2	2.45	0.47
1:0b:68:ASP:N	1:0b:72:SER:O	2.48	0.47
1:0b:160:LEU:N	1:0b:197:GLU:O	2.46	0.47
1:0d:160:LEU:N	1:0d:197:GLU:O	2.46	0.47
1:0h:160:LEU:N	1:0h:197:GLU:O	2.46	0.47
2:0C:131:ASN:HA	2:0C:229:SER:HA	1.97	0.47
2:0C:150:GLU:O	2:0D:213:THR:OG1	2.30	0.47
2:0G:17:GLN:HE22	3:Q:27:THR:H	1.63	0.47
2:0I:238:ASP:OD1	2:0I:239:LYS:N	2.48	0.47
2:0K:3:SER:OG	2:0K:4:TYR:N	2.48	0.47
1:0d:85:ASP:OD1	1:0d:89:GLN:N	2.48	0.47
1:0l:68:ASP:N	1:0l:72:SER:O	2.48	0.47
2:0A:90:LEU:O	2:0A:93:SER:OG	2.27	0.47
2:0C:132:GLY:HA3	2:0D:230:ASN:HA	1.96	0.47
2:0C:157:SER:HA	2:0D:206:THR:HA	1.96	0.47
3:h:40:ASN:HA	3:h:43:ILE:HD12	1.96	0.47
1:0d:209:LYS:O	1:0e:205:TYR:OH	2.29	0.46
1:0g:161:ILE:HD12	1:0h:186:PHE:HE1	1.80	0.46
1:0i:68:ASP:N	1:0i:72:SER:O	2.48	0.46
2:0E:238:ASP:OD1	2:0E:239:LYS:N	2.48	0.46
2:0F:126:GLN:NE2	2:0G:235:THR:O	2.48	0.46
2:0G:145:LYS:HA	2:0H:218:GLY:HA3	1.97	0.46
1:0a:68:ASP:N	1:0a:72:SER:O	2.48	0.46
1:0d:68:ASP:N	1:0d:72:SER:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0f:19:LYS:HE2	1:0f:23:TRP:HE1	1.80	0.46
2:0G:23:SER:O	2:0G:27:LYS:N	2.40	0.46
3:H:51:LYS:NZ	3:H:55:GLU:OE2	2.47	0.46
3:J:36:LEU:HD22	3:O:19:GLN:HG2	1.96	0.46
1:0a:189:GLU:HA	1:0j:162:ARG:HB3	1.97	0.46
1:0e:85:ASP:OD1	1:0e:89:GLN:N	2.49	0.46
2:0B:131:ASN:HA	2:0B:229:SER:HA	1.97	0.46
2:0F:9:ARG:NE	2:0F:61:MET:SD	2.83	0.46
2:0F:131:ASN:HA	2:0F:229:SER:HA	1.97	0.46
2:0G:136:THR:O	2:0G:224:SER:OG	2.34	0.46
2:0H:136:THR:O	2:0H:224:SER:OG	2.34	0.46
2:0I:136:THR:O	2:0I:224:SER:OG	2.34	0.46
3:Y:67:ILE:HG12	3:Z:67:ILE:HB	1.97	0.46
1:0c:17:ARG:HH21	3:I:23:ARG:HG3	1.80	0.46
1:0h:68:ASP:N	1:0h:72:SER:O	2.48	0.46
1:0i:19:LYS:HE2	1:0i:23:TRP:HE1	1.80	0.46
1:0j:85:ASP:OD1	1:0j:89:GLN:N	2.49	0.46
1:0k:152:GLN:HE21	1:0l:147:ILE:HG21	1.80	0.46
1:0k:186:PHE:HE2	1:0l:172:LYS:HG2	1.80	0.46
2:0B:17:GLN:NE2	3:B:27:THR:H	2.13	0.46
2:0B:147:THR:OG1	2:0B:148:GLY:N	2.49	0.46
2:0D:131:ASN:HA	2:0D:229:SER:HA	1.97	0.46
2:0E:147:THR:OG1	2:0E:148:GLY:N	2.49	0.46
2:0J:143:THR:HA	2:0K:220:SER:HA	1.97	0.46
2:0J:214:SER:OG	2:0J:215:ASN:N	2.49	0.46
2:0K:214:SER:OG	2:0K:215:ASN:N	2.49	0.46
2:0L:131:ASN:HA	2:0L:229:SER:HA	1.97	0.46
3:K:51:LYS:NZ	3:K:55:GLU:OE2	2.47	0.46
1:0a:15:ILE:O	1:0a:19:LYS:N	2.34	0.46
1:0b:162:ARG:HB3	1:0c:189:GLU:HA	1.96	0.46
1:0c:19:LYS:HE2	1:0c:23:TRP:HE1	1.80	0.46
1:0f:85:ASP:OD1	1:0f:89:GLN:N	2.48	0.46
1:0f:287:GLN:O	1:0f:291:GLU:N	2.49	0.46
1:0g:85:ASP:OD1	1:0g:89:GLN:N	2.48	0.46
1:0h:287:GLN:O	1:0h:291:GLU:N	2.49	0.46
1:0i:17:ARG:NH2	3:a:21:TYR:OH	2.48	0.46
1:0i:147:ILE:HG21	1:0l:152:GLN:HE21	1.80	0.46
2:0E:155:SER:OG	2:0E:156:GLY:N	2.46	0.46
2:0G:206:THR:OG1	2:0G:207:SER:N	2.43	0.46
2:0I:214:SER:OG	2:0I:215:ASN:N	2.49	0.46
2:0J:136:THR:O	2:0J:224:SER:OG	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0L:3:SER:OG	2:0L:4:TYR:N	2.48	0.46
3:H:56:LEU:HD13	3:I:57:ILE:HD11	1.97	0.46
1:0d:19:LYS:HE2	1:0d:23:TRP:HE1	1.80	0.46
2:0F:136:THR:O	2:0F:224:SER:OG	2.34	0.46
2:0F:238:ASP:OD1	2:0F:239:LYS:N	2.48	0.46
2:0H:238:ASP:OD1	2:0H:239:LYS:N	2.48	0.46
2:0L:214:SER:OG	2:0L:215:ASN:N	2.49	0.46
3:P:67:ILE:HG12	3:Q:67:ILE:HB	1.97	0.46
1:0b:19:LYS:HE2	1:0b:23:TRP:HE1	1.81	0.46
1:0c:168:GLN:NE2	2:0B:293:TYR:O	2.49	0.46
1:0d:287:GLN:O	1:0d:291:GLU:N	2.49	0.46
1:0i:173:GLN:HE22	3:U:24:TYR:HA	1.80	0.46
1:0k:287:GLN:O	1:0k:291:GLU:N	2.49	0.46
1:0l:245:SER:OG	1:0l:246:ASN:N	2.49	0.46
2:0A:147:THR:OG1	2:0A:148:GLY:N	2.49	0.46
2:0F:17:GLN:NE2	3:N:27:THR:H	2.14	0.46
2:0H:214:SER:OG	2:0H:215:ASN:N	2.49	0.46
2:0L:147:THR:OG1	2:0L:148:GLY:N	2.49	0.46
3:G:67:ILE:HG12	3:H:67:ILE:HB	1.97	0.46
3:M:46:LEU:HD11	3:O:42:ILE:HG23	1.98	0.46
3:Z:51:LYS:NZ	3:Z:55:GLU:OE2	2.49	0.46
1:0b:85:ASP:OD1	1:0b:89:GLN:N	2.49	0.46
1:0f:66:TYR:OH	1:0f:116:ASP:OD1	2.22	0.46
1:0i:245:SER:OG	1:0i:246:ASN:N	2.49	0.46
1:0j:186:PHE:HE2	1:0k:172:LYS:HG2	1.80	0.46
1:0k:205:TYR:CZ	1:0l:209:LYS:HB3	2.51	0.46
2:0B:23:SER:O	2:0B:27:LYS:N	2.40	0.46
2:0B:24:THR:OG1	3:i:31:GLU:OE2	2.29	0.46
2:0G:214:SER:OG	2:0G:215:ASN:N	2.49	0.46
2:0J:145:LYS:HA	2:0K:218:GLY:HA3	1.96	0.46
1:0a:19:LYS:HE2	1:0a:23:TRP:HE1	1.80	0.46
1:0h:85:ASP:OD1	1:0h:89:GLN:N	2.48	0.46
1:0i:172:LYS:HG2	1:0l:186:PHE:HE2	1.80	0.46
1:0i:287:GLN:O	1:0i:291:GLU:N	2.49	0.46
1:0j:68:ASP:N	1:0j:72:SER:O	2.48	0.46
2:0D:65:GLY:HA2	2:0D:290:MET:HG2	1.98	0.46
2:0E:65:GLY:HA2	2:0E:290:MET:HG2	1.98	0.46
2:0E:131:ASN:HA	2:0E:229:SER:HA	1.97	0.46
2:0E:136:THR:O	2:0E:224:SER:OG	2.34	0.46
2:0K:9:ARG:NE	2:0K:61:MET:SD	2.83	0.46
3:D:67:ILE:HG12	3:E:67:ILE:HB	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0b:228:LYS:HD3	1:0b:250:ILE:HG21	1.98	0.46
1:0e:66:TYR:OH	1:0e:116:ASP:OD1	2.22	0.46
1:0e:68:ASP:N	1:0e:72:SER:O	2.48	0.46
1:0f:168:GLN:NE2	2:0E:293:TYR:O	2.49	0.46
1:0g:19:LYS:HE2	1:0g:23:TRP:HE1	1.80	0.46
1:0h:19:LYS:HE2	1:0h:23:TRP:HE1	1.80	0.46
1:0k:245:SER:OG	1:0k:246:ASN:N	2.49	0.46
2:0A:214:SER:OG	2:0A:215:ASN:N	2.49	0.46
2:0C:65:GLY:HA2	2:0C:290:MET:HG2	1.98	0.46
2:0D:9:ARG:NE	2:0D:61:MET:SD	2.83	0.46
2:0D:147:THR:OG1	2:0D:148:GLY:N	2.49	0.46
2:0G:238:ASP:OD1	2:0G:239:LYS:N	2.48	0.46
2:0K:136:THR:O	2:0K:224:SER:OG	2.33	0.46
3:Q:51:LYS:NZ	3:Q:55:GLU:OE2	2.47	0.46
3:c:51:LYS:NZ	3:c:55:GLU:OE2	2.49	0.46
1:0a:7:ASN:HA	3:e:34:THR:HG21	1.98	0.45
1:0a:228:LYS:HD3	1:0a:250:ILE:HG21	1.98	0.45
1:0c:287:GLN:O	1:0c:291:GLU:N	2.49	0.45
1:0f:160:LEU:N	1:0f:197:GLU:O	2.46	0.45
1:0g:15:ILE:O	1:0g:19:LYS:N	2.34	0.45
1:0g:287:GLN:O	1:0g:291:GLU:N	2.49	0.45
1:0h:245:SER:OG	1:0h:246:ASN:N	2.49	0.45
1:0l:85:ASP:OD1	1:0l:89:GLN:N	2.48	0.45
2:0A:131:ASN:HA	2:0A:229:SER:HA	1.97	0.45
2:0A:155:SER:OG	2:0B:207:SER:OG	2.23	0.45
2:0A:235:THR:O	2:0L:126:GLN:NE2	2.49	0.45
2:0C:81:MET:HB3	2:0D:54:HIS:CE1	2.51	0.45
2:0G:115:ASP:HB2	2:0H:247:VAL:HG13	1.98	0.45
2:0G:131:ASN:HA	2:0G:229:SER:HA	1.97	0.45
2:0G:147:THR:OG1	2:0G:148:GLY:N	2.49	0.45
2:0K:131:ASN:HA	2:0K:229:SER:HA	1.97	0.45
2:0K:147:THR:OG1	2:0K:148:GLY:N	2.49	0.45
3:N:31:GLU:O	3:N:41:LYS:NZ	2.44	0.45
1:0e:19:LYS:HE2	1:0e:23:TRP:HE1	1.80	0.45
1:0e:287:GLN:O	1:0e:291:GLU:N	2.49	0.45
1:0f:162:ARG:NH2	1:0g:192:ASP:OD1	2.49	0.45
1:0g:68:ASP:N	1:0g:72:SER:O	2.48	0.45
1:0h:228:LYS:HD3	1:0h:250:ILE:HG21	1.98	0.45
1:0i:228:LYS:HD3	1:0i:250:ILE:HG21	1.98	0.45
1:0j:36:TYR:O	1:0k:259:LYS:NZ	2.45	0.45
1:0l:287:GLN:O	1:0l:291:GLU:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0A:136:THR:O	2:0A:224:SER:OG	2.34	0.45
2:0F:214:SER:OG	2:0F:215:ASN:N	2.49	0.45
2:0I:65:GLY:HA2	2:0I:290:MET:HG2	1.98	0.45
2:0I:131:ASN:HA	2:0I:229:SER:HA	1.97	0.45
2:0I:147:THR:OG1	2:0I:148:GLY:N	2.49	0.45
2:0J:31:GLY:O	2:0J:35:LEU:N	2.38	0.45
2:0J:65:GLY:HA2	2:0J:290:MET:HG2	1.98	0.45
2:0J:147:THR:OG1	2:0J:148:GLY:N	2.49	0.45
3:N:51:LYS:NZ	3:N:55:GLU:OE2	2.48	0.45
2:0F:65:GLY:HA2	2:0F:290:MET:HG2	1.98	0.45
2:0H:65:GLY:HA2	2:0H:290:MET:HG2	1.98	0.45
1:0a:160:LEU:N	1:0a:197:GLU:O	2.46	0.45
1:0c:228:LYS:HD3	1:0c:250:ILE:HG21	1.98	0.45
1:0f:172:LYS:HG2	1:0g:186:PHE:CE2	2.51	0.45
1:0h:209:LYS:HB3	1:0i:205:TYR:CZ	2.52	0.45
1:0i:255:THR:OG1	1:0l:37:GLN:NE2	2.48	0.45
1:0j:19:LYS:HE2	1:0j:23:TRP:HE1	1.80	0.45
1:0j:228:LYS:HD3	1:0j:250:ILE:HG21	1.98	0.45
1:0j:245:SER:OG	1:0j:246:ASN:N	2.49	0.45
1:0k:85:ASP:OD1	1:0k:89:GLN:N	2.49	0.45
2:0A:3:SER:OG	2:0A:4:TYR:N	2.48	0.45
2:0G:134:SER:HA	2:0H:228:THR:HA	1.98	0.45
1:0a:65:PHE:N	1:0a:119:VAL:O	2.37	0.45
1:0a:85:ASP:OD1	1:0a:89:GLN:N	2.49	0.45
1:0c:245:SER:OG	1:0c:246:ASN:N	2.49	0.45
1:0f:68:ASP:N	1:0f:72:SER:O	2.48	0.45
1:0f:87:TYR:CD2	1:0g:49:ASN:HB2	2.52	0.45
1:0h:147:ILE:HG21	1:0i:152:GLN:HE21	1.81	0.45
1:0j:152:GLN:HE21	1:0k:147:ILE:HG21	1.82	0.45
2:0C:214:SER:OG	2:0C:215:ASN:N	2.49	0.45
2:0L:136:THR:O	2:0L:224:SER:OG	2.34	0.45
3:i:51:LYS:NZ	3:i:55:GLU:OE2	2.50	0.45
1:0b:287:GLN:O	1:0b:291:GLU:N	2.49	0.45
1:0g:160:LEU:N	1:0g:197:GLU:O	2.46	0.45
1:0h:172:LYS:HG2	1:0i:186:PHE:HE2	1.81	0.45
1:0i:17:ARG:HH21	3:a:23:ARG:HG3	1.82	0.45
2:0B:136:THR:O	2:0B:224:SER:OG	2.34	0.45
2:0C:17:GLN:NE2	3:E:25:LEU:O	2.50	0.45
2:0C:155:SER:OG	2:0C:156:GLY:N	2.46	0.45
2:0D:42:ILE:HG12	2:0D:48:ARG:HA	1.98	0.45
2:0D:214:SER:OG	2:0D:215:ASN:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0E:42:ILE:HG12	2:0E:48:ARG:HA	1.98	0.45
2:0H:9:ARG:NE	2:0H:61:MET:SD	2.83	0.45
2:0H:90:LEU:O	2:0H:93:SER:OG	2.27	0.45
3:N:32:SER:OG	3:N:34:THR:O	2.35	0.45
1:0a:259:LYS:NZ	1:0b:54:GLU:OE1	2.46	0.45
1:0b:245:SER:OG	1:0b:246:ASN:N	2.49	0.45
1:0d:78:GLY:HA3	1:0d:95:ALA:HA	1.99	0.45
1:0d:228:LYS:HD3	1:0d:250:ILE:HG21	1.98	0.45
1:0d:245:SER:OG	1:0d:246:ASN:N	2.49	0.45
1:0f:87:TYR:OH	1:0g:48:ILE:HA	2.17	0.45
1:0g:245:SER:OG	1:0g:246:ASN:N	2.49	0.45
1:0i:209:LYS:HB3	1:0l:205:TYR:CZ	2.51	0.45
1:0l:19:LYS:HE2	1:0l:23:TRP:HE1	1.80	0.45
1:0l:228:LYS:HD3	1:0l:250:ILE:HG21	1.98	0.45
2:0B:119:ASN:O	2:0C:242:SER:HA	2.15	0.45
2:0C:81:MET:HB3	2:0D:54:HIS:NE2	2.32	0.45
2:0D:136:THR:O	2:0D:224:SER:OG	2.34	0.45
2:0E:214:SER:OG	2:0E:215:ASN:N	2.49	0.45
2:0H:147:THR:OG1	2:0H:148:GLY:N	2.49	0.45
2:0J:42:ILE:HG12	2:0J:48:ARG:HA	1.98	0.45
3:V:67:ILE:HG12	3:W:67:ILE:HB	1.98	0.45
3:b:67:ILE:HG12	3:c:67:ILE:HB	1.99	0.45
1:0a:287:GLN:O	1:0a:291:GLU:N	2.49	0.45
1:0c:85:ASP:OD1	1:0c:89:GLN:N	2.48	0.45
1:0f:245:SER:OG	1:0f:246:ASN:N	2.49	0.45
1:0k:68:ASP:N	1:0k:72:SER:O	2.48	0.45
2:0B:214:SER:OG	2:0B:215:ASN:N	2.49	0.45
2:0C:147:THR:OG1	2:0C:148:GLY:N	2.49	0.45
2:0K:65:GLY:HA2	2:0K:290:MET:HG2	1.98	0.45
3:W:51:LYS:NZ	3:W:55:GLU:OE2	2.49	0.45
1:0c:78:GLY:HA3	1:0c:95:ALA:HA	1.99	0.45
1:0e:7:ASN:HA	3:G:34:THR:HG21	1.99	0.45
1:0e:93:PHE:HB3	1:0e:104:PHE:HB2	1.99	0.45
1:0f:162:ARG:HB3	1:0g:189:GLU:HA	1.97	0.45
1:0g:109:TYR:HB2	1:0h:47:THR:HA	1.99	0.45
1:0i:85:ASP:OD1	1:0i:89:GLN:N	2.49	0.45
1:0k:19:LYS:HE2	1:0k:23:TRP:HE1	1.80	0.45
1:0k:228:LYS:HD3	1:0k:250:ILE:HG21	1.98	0.45
2:0B:155:SER:OG	2:0B:156:GLY:N	2.46	0.45
2:0C:42:ILE:HG12	2:0C:48:ARG:HA	1.99	0.45
2:0D:24:THR:OG1	3:E:31:GLU:OE2	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0D:134:SER:HA	2:0E:228:THR:HA	1.97	0.45
2:0F:115:ASP:HB2	2:0G:247:VAL:HG13	1.97	0.45
2:0G:65:GLY:HA2	2:0G:290:MET:HG2	1.98	0.45
1:0a:245:SER:OG	1:0a:246:ASN:N	2.49	0.45
1:0e:245:SER:OG	1:0e:246:ASN:N	2.49	0.45
1:0g:93:PHE:HB3	1:0g:104:PHE:HB2	1.99	0.45
1:0h:7:ASN:HA	3:P:34:THR:HG21	1.99	0.45
1:0h:78:GLY:HA3	1:0h:95:ALA:HA	1.99	0.45
1:0j:287:GLN:O	1:0j:291:GLU:N	2.49	0.45
2:0C:3:SER:OG	2:0C:4:TYR:N	2.48	0.45
2:0C:115:ASP:HB2	2:0D:247:VAL:HG13	1.98	0.45
2:0H:131:ASN:HA	2:0H:229:SER:HA	1.97	0.45
2:0H:162:ASN:HD22	2:0H:163:PHE:N	2.15	0.45
2:0I:42:ILE:HG12	2:0I:48:ARG:HA	1.99	0.45
2:0J:131:ASN:HA	2:0J:229:SER:HA	1.97	0.45
3:S:67:ILE:HG12	3:T:67:ILE:HB	1.99	0.45
1:0b:78:GLY:HA3	1:0b:95:ALA:HA	1.99	0.44
1:0d:162:ARG:HB3	1:0e:189:GLU:HA	1.99	0.44
1:0f:93:PHE:HB3	1:0f:104:PHE:HB2	2.00	0.44
1:0h:93:PHE:HB3	1:0h:104:PHE:HB2	1.99	0.44
1:0h:173:GLN:HE22	3:R:24:TYR:HA	1.81	0.44
1:0i:78:GLY:HA3	1:0i:95:ALA:HA	1.99	0.44
1:0i:93:PHE:HB3	1:0i:104:PHE:HB2	1.99	0.44
1:0k:37:GLN:NE2	1:0l:255:THR:OG1	2.49	0.44
2:0B:65:GLY:HA2	2:0B:290:MET:HG2	1.98	0.44
2:0C:136:THR:O	2:0C:224:SER:OG	2.34	0.44
2:0D:90:LEU:O	2:0D:93:SER:OG	2.27	0.44
2:0F:42:ILE:HG12	2:0F:48:ARG:HA	1.98	0.44
2:0G:24:THR:OG1	3:N:31:GLU:OE2	2.32	0.44
3:A:65:GLU:OE2	3:A:69:ASN:ND2	2.47	0.44
3:H:32:SER:OG	3:H:34:THR:O	2.34	0.44
3:S:64:MET:HB2	3:T:60:TRP:HH2	1.81	0.44
1:0d:93:PHE:HB3	1:0d:104:PHE:HB2	1.99	0.44
1:0e:78:GLY:HA3	1:0e:95:ALA:HA	1.99	0.44
1:0f:17:ARG:NH1	3:M:21:TYR:O	2.50	0.44
1:0g:188:HIS:N	2:0E:291:LEU:O	2.50	0.44
1:0g:228:LYS:HD3	1:0g:250:ILE:HG21	1.98	0.44
2:0G:162:ASN:HD22	2:0G:163:PHE:N	2.15	0.44
2:0I:162:ASN:HD22	2:0I:163:PHE:N	2.15	0.44
2:0K:81:MET:HB3	2:0L:54:HIS:CE1	2.52	0.44
2:0K:132:GLY:HA3	2:0L:230:ASN:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:58:GLU:HA	3:I:61:ASN:HB2	2.00	0.44
3:J:64:MET:HB2	3:K:60:TRP:HH2	1.82	0.44
3:J:67:ILE:HG12	3:K:67:ILE:HB	1.99	0.44
3:Y:64:MET:HB2	3:Z:60:TRP:HH2	1.81	0.44
3:f:31:GLU:O	3:f:41:LYS:NZ	2.44	0.44
3:j:58:GLU:HA	3:j:61:ASN:HB2	2.00	0.44
1:0i:171:LEU:HD23	1:0i:171:LEU:HA	1.83	0.44
1:0k:93:PHE:HB3	1:0k:104:PHE:HB2	1.99	0.44
1:0l:93:PHE:HB3	1:0l:104:PHE:HB2	1.99	0.44
2:0A:42:ILE:HG12	2:0A:48:ARG:HA	1.98	0.44
2:0A:65:GLY:HA2	2:0A:290:MET:HG2	1.98	0.44
2:0F:162:ASN:HD22	2:0F:163:PHE:N	2.15	0.44
2:0I:116:THR:HA	2:0J:246:SER:HA	2.00	0.44
2:0J:133:THR:O	2:0K:228:THR:OG1	2.31	0.44
2:0L:42:ILE:HG12	2:0L:48:ARG:HA	1.98	0.44
3:M:67:ILE:HG12	3:N:67:ILE:HB	1.98	0.44
3:f:42:ILE:HG23	3:g:46:LEU:HD11	1.99	0.44
3:h:67:ILE:HG12	3:i:67:ILE:HB	1.99	0.44
1:0b:15:ILE:O	1:0b:19:LYS:N	2.34	0.44
1:0c:93:PHE:HB3	1:0c:104:PHE:HB2	1.99	0.44
1:0c:209:LYS:HB3	1:0d:205:TYR:CZ	2.52	0.44
1:0e:15:ILE:O	1:0e:19:LYS:N	2.34	0.44
1:0j:93:PHE:HB3	1:0j:104:PHE:HB2	1.99	0.44
1:0k:78:GLY:HA3	1:0k:95:ALA:HA	1.99	0.44
2:0C:110:SER:HA	2:0D:252:GLU:HA	2.00	0.44
2:0C:152:SER:O	2:0D:211:ASP:N	2.50	0.44
2:0L:65:GLY:HA2	2:0L:290:MET:HG2	1.98	0.44
3:D:43:ILE:HD13	3:I:18:VAL:HA	1.99	0.44
3:L:30:ASP:N	3:L:30:ASP:OD1	2.51	0.44
3:g:58:GLU:HA	3:g:61:ASN:HB2	2.00	0.44
1:0a:93:PHE:HB3	1:0a:104:PHE:HB2	1.99	0.44
1:0a:205:TYR:CZ	1:0j:209:LYS:HB3	2.53	0.44
1:0b:9:TYR:HB3	3:h:31:GLU:HB2	1.99	0.44
1:0b:93:PHE:HB3	1:0b:104:PHE:HB2	1.99	0.44
1:0f:163:ALA:O	1:0g:189:GLU:N	2.40	0.44
1:0j:78:GLY:HA3	1:0j:95:ALA:HA	1.99	0.44
1:0j:160:LEU:N	1:0j:197:GLU:O	2.46	0.44
1:0l:168:GLN:NE2	2:0I:293:TYR:O	2.49	0.44
2:0A:213:THR:OG1	2:0L:150:GLU:O	2.32	0.44
2:0I:115:ASP:HB2	2:0J:247:VAL:HG13	1.99	0.44
2:0J:162:ASN:HD22	2:0J:163:PHE:N	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:38:LYS:NZ	3:j:17:MET:O	2.36	0.44
1:0e:161:ILE:HG12	1:0e:196:ILE:HG23	2.00	0.44
1:0e:228:LYS:HD3	1:0e:250:ILE:HG21	1.98	0.44
1:0f:78:GLY:HA3	1:0f:95:ALA:HA	1.99	0.44
1:0g:78:GLY:HA3	1:0g:95:ALA:HA	1.99	0.44
1:0i:7:ASN:HA	3:S:34:THR:HG21	2.00	0.44
2:0B:42:ILE:HG12	2:0B:48:ARG:HA	1.98	0.44
2:0B:109:LYS:HG2	2:0B:251:ILE:HG23	2.00	0.44
2:0C:24:THR:OG1	3:B:31:GLU:OE2	2.28	0.44
2:0E:162:ASN:HD22	2:0E:163:PHE:N	2.15	0.44
2:0G:3:SER:OG	2:0G:4:TYR:N	2.48	0.44
2:0G:42:ILE:HG12	2:0G:48:ARG:HA	1.98	0.44
2:0G:116:THR:HA	2:0H:246:SER:HA	1.99	0.44
2:0J:115:ASP:HB2	2:0K:247:VAL:HG13	2.00	0.44
2:0K:109:LYS:HG2	2:0K:251:ILE:HG23	2.00	0.44
3:F:58:GLU:HA	3:F:61:ASN:HB2	2.00	0.44
3:M:64:MET:HB2	3:N:60:TRP:HH2	1.83	0.44
3:R:58:GLU:HA	3:R:61:ASN:HB2	2.00	0.44
1:0a:78:GLY:HA3	1:0a:95:ALA:HA	1.99	0.44
1:0i:259:LYS:NZ	1:0l:54:GLU:OE1	2.44	0.44
2:0A:109:LYS:HG2	2:0A:251:ILE:HG23	2.00	0.44
2:0C:109:LYS:HG2	2:0C:251:ILE:HG23	2.00	0.44
2:0D:167:LEU:HD22	2:0E:196:HIS:CD2	2.52	0.44
2:0J:109:LYS:HG2	2:0J:251:ILE:HG23	2.00	0.44
2:0L:109:LYS:HG2	2:0L:251:ILE:HG23	2.00	0.44
3:I:30:ASP:OD1	3:I:30:ASP:N	2.51	0.44
3:U:30:ASP:OD1	3:U:30:ASP:N	2.51	0.44
3:a:58:GLU:HA	3:a:61:ASN:HB2	2.00	0.44
1:0b:161:ILE:HG12	1:0b:196:ILE:HG23	2.00	0.44
1:0d:66:TYR:OH	1:0d:116:ASP:OD1	2.23	0.44
1:0d:161:ILE:HG12	1:0d:196:ILE:HG23	2.00	0.44
1:0i:168:GLN:NE2	2:0H:293:TYR:O	2.51	0.44
2:0F:3:SER:OG	2:0F:4:TYR:N	2.48	0.44
2:0I:109:LYS:HG2	2:0I:251:ILE:HG23	2.00	0.44
2:0K:42:ILE:HG12	2:0K:48:ARG:HA	1.98	0.44
2:0K:235:THR:OG1	2:0K:236:SER:N	2.51	0.44
2:0L:257:LYS:HZ1	2:0L:261:GLN:HB2	1.83	0.44
3:B:51:LYS:NZ	3:B:55:GLU:OE2	2.50	0.44
3:S:27:THR:OG1	3:X:23:ARG:NH1	2.49	0.44
1:0a:161:ILE:HG12	1:0a:196:ILE:HG23	2.00	0.44
1:0f:228:LYS:HD3	1:0f:250:ILE:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0A:155:SER:OG	2:0A:156:GLY:N	2.46	0.44
2:0G:109:LYS:HG2	2:0G:251:ILE:HG23	2.00	0.44
2:0H:109:LYS:HG2	2:0H:251:ILE:HG23	2.00	0.44
2:0K:143:THR:HA	2:0L:220:SER:HA	1.99	0.44
3:H:42:ILE:HG23	3:I:46:LEU:HD11	1.99	0.44
3:M:36:LEU:HD22	3:R:19:GLN:HG2	1.99	0.44
3:c:42:ILE:HG23	3:d:46:LEU:HD11	1.99	0.44
3:e:65:GLU:OE2	3:e:69:ASN:ND2	2.46	0.44
1:0i:259:LYS:NZ	1:0l:36:TYR:O	2.46	0.43
2:0C:161:ASP:HB3	2:0C:200:LYS:HB2	2.01	0.43
2:0J:235:THR:OG1	2:0J:236:SER:N	2.51	0.43
2:0K:162:ASN:HD22	2:0K:163:PHE:N	2.15	0.43
2:0L:90:LEU:O	2:0L:93:SER:OG	2.27	0.43
3:E:56:LEU:HD13	3:F:57:ILE:HD11	1.99	0.43
3:L:58:GLU:HA	3:L:61:ASN:HB2	2.00	0.43
1:0a:54:GLU:OE1	1:0j:259:LYS:NZ	2.46	0.43
1:0f:191:LEU:HB2	2:0D:291:LEU:HD13	1.99	0.43
1:0h:255:THR:OG1	1:0i:37:GLN:NE2	2.50	0.43
2:0D:109:LYS:HG2	2:0D:251:ILE:HG23	2.00	0.43
2:0D:235:THR:OG1	2:0D:236:SER:N	2.51	0.43
2:0E:109:LYS:HG2	2:0E:251:ILE:HG23	2.00	0.43
2:0H:3:SER:OG	2:0H:4:TYR:N	2.48	0.43
2:0H:42:ILE:HG12	2:0H:48:ARG:HA	1.98	0.43
2:0J:116:THR:HA	2:0K:246:SER:HA	2.00	0.43
2:0L:235:THR:OG1	2:0L:236:SER:N	2.51	0.43
3:O:58:GLU:HA	3:O:61:ASN:HB2	2.00	0.43
3:P:36:LEU:HD22	3:U:19:GLN:HG2	1.98	0.43
1:0a:31:LEU:HB3	1:0a:221:MET:HE2	2.01	0.43
1:0a:209:LYS:O	1:0b:205:TYR:OH	2.35	0.43
1:0b:171:LEU:HD23	1:0b:171:LEU:HA	1.83	0.43
1:0j:54:GLU:OE1	1:0k:259:LYS:NZ	2.42	0.43
1:0l:78:GLY:HA3	1:0l:95:ALA:HA	1.99	0.43
2:0B:235:THR:OG1	2:0B:236:SER:N	2.51	0.43
2:0C:235:THR:OG1	2:0C:236:SER:N	2.51	0.43
2:0D:162:ASN:HD22	2:0D:163:PHE:N	2.15	0.43
2:0F:157:SER:HA	2:0G:206:THR:HA	2.00	0.43
2:0H:17:GLN:NE2	3:T:27:THR:H	2.16	0.43
2:0J:155:SER:OG	2:0J:156:GLY:N	2.47	0.43
2:0K:145:LYS:HA	2:0L:218:GLY:HA3	1.99	0.43
2:0L:17:GLN:HE22	3:f:27:THR:H	1.66	0.43
3:f:51:LYS:NZ	3:f:55:GLU:OE2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0f:31:LEU:HB3	1:0f:221:MET:HE2	2.01	0.43
1:0h:161:ILE:HG12	1:0h:196:ILE:HG23	2.00	0.43
2:0B:3:SER:OG	2:0B:4:TYR:N	2.48	0.43
2:0F:109:LYS:HG2	2:0F:251:ILE:HG23	2.00	0.43
2:0F:161:ASP:HB3	2:0F:200:LYS:HB2	2.01	0.43
2:0H:116:THR:HA	2:0I:246:SER:HA	1.99	0.43
2:0K:17:GLN:HE22	3:c:27:THR:H	1.64	0.43
1:0b:31:LEU:HB3	1:0b:221:MET:HE2	2.01	0.43
1:0f:15:ILE:O	1:0f:19:LYS:N	2.34	0.43
1:0g:31:LEU:HB3	1:0g:221:MET:HE2	2.01	0.43
1:0g:161:ILE:HG12	1:0g:196:ILE:HG23	2.00	0.43
2:0A:247:VAL:HG13	2:0L:115:ASP:HB2	2.01	0.43
2:0B:257:LYS:HZ1	2:0B:261:GLN:HB2	1.84	0.43
2:0E:126:GLN:NE2	2:0F:235:THR:O	2.51	0.43
2:0E:235:THR:OG1	2:0E:236:SER:N	2.51	0.43
2:0F:152:SER:O	2:0G:211:ASP:N	2.51	0.43
2:0G:127:ASP:O	2:0H:234:THR:OG1	2.25	0.43
2:0G:133:THR:O	2:0H:228:THR:OG1	2.29	0.43
2:0I:235:THR:OG1	2:0I:236:SER:N	2.51	0.43
2:0J:128:LEU:HG	2:0K:234:THR:HB	2.01	0.43
1:0h:65:PHE:N	1:0h:119:VAL:O	2.37	0.43
1:0j:31:LEU:HB3	1:0j:221:MET:HE2	2.01	0.43
1:0k:17:ARG:HE	3:g:23:ARG:CB	2.27	0.43
2:0B:162:ASN:HD22	2:0B:163:PHE:N	2.15	0.43
2:0C:67:GLU:OE1	3:I:28:ALA:N	2.52	0.43
2:0C:273:ALA:O	2:0D:271:ARG:NH1	2.37	0.43
2:0J:147:THR:OG1	2:0K:215:ASN:O	2.29	0.43
2:0L:162:ASN:HD22	2:0L:163:PHE:N	2.15	0.43
3:A:67:ILE:HG12	3:B:67:ILE:HB	2.00	0.43
3:B:56:LEU:HD13	3:C:57:ILE:HD11	2.01	0.43
3:S:42:ILE:HG23	3:T:46:LEU:HD21	2.00	0.43
1:0a:186:PHE:HE2	1:0j:172:LYS:HG2	1.84	0.43
1:0b:172:LYS:HG2	1:0c:186:PHE:HE2	1.83	0.43
1:0f:161:ILE:HG12	1:0f:196:ILE:HG23	2.00	0.43
1:0h:31:LEU:HB3	1:0h:221:MET:HE2	2.01	0.43
1:0l:171:LEU:HA	1:0l:171:LEU:HD23	1.83	0.43
2:0A:162:ASN:HD22	2:0A:163:PHE:N	2.15	0.43
2:0B:117:ASP:O	2:0C:244:ILE:HA	2.19	0.43
2:0E:3:SER:OG	2:0E:4:TYR:N	2.48	0.43
2:0E:161:ASP:HB3	2:0E:200:LYS:HB2	2.01	0.43
2:0J:257:LYS:HZ1	2:0J:261:GLN:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:HA	3:C:61:ASN:HB2	2.00	0.43
3:F:30:ASP:OD1	3:F:30:ASP:N	2.51	0.43
3:J:43:ILE:HD13	3:O:18:VAL:HA	1.99	0.43
3:R:30:ASP:OD1	3:R:30:ASP:N	2.51	0.43
1:0a:12:ILE:HD11	1:0c:183:PRO:HD2	2.01	0.43
1:0c:31:LEU:HB3	1:0c:221:MET:HE2	2.01	0.43
1:0i:31:LEU:HB3	1:0i:221:MET:HE2	2.01	0.43
1:0k:161:ILE:HG12	1:0k:196:ILE:HG23	2.00	0.43
2:0A:9:ARG:NE	2:0A:61:MET:SD	2.83	0.43
2:0A:235:THR:OG1	2:0A:236:SER:N	2.51	0.43
2:0B:136:THR:HA	2:0C:226:SER:HA	2.01	0.43
2:0C:106:VAL:HA	2:0D:256:GLY:HA3	2.01	0.43
2:0C:126:GLN:NE2	2:0D:235:THR:O	2.51	0.43
2:0F:147:THR:OG1	2:0F:148:GLY:N	2.49	0.43
2:0H:161:ASP:HB3	2:0H:200:LYS:HB2	2.01	0.43
2:0I:161:ASP:HB3	2:0I:200:LYS:HB2	2.01	0.43
2:0L:161:ASP:HB3	2:0L:200:LYS:HB2	2.01	0.43
3:U:58:GLU:HA	3:U:61:ASN:HB2	2.00	0.43
3:V:64:MET:HB2	3:W:60:TRP:HH2	1.83	0.43
3:X:58:GLU:HA	3:X:61:ASN:HB2	2.00	0.43
1:0a:255:THR:OG1	1:0b:37:GLN:NE2	2.50	0.43
1:0d:40:GLU:OE1	1:0d:281:ARG:NH1	2.52	0.43
1:0e:31:LEU:HB3	1:0e:221:MET:HE2	2.01	0.43
1:0k:31:LEU:HB3	1:0k:221:MET:HE2	2.01	0.43
1:0k:40:GLU:OE1	1:0k:281:ARG:NH1	2.52	0.43
2:0C:162:ASN:HD22	2:0C:163:PHE:N	2.15	0.43
2:0F:235:THR:OG1	2:0F:236:SER:N	2.51	0.43
3:E:51:LYS:NZ	3:E:55:GLU:OE2	2.51	0.43
1:0b:183:PRO:HD2	1:0j:12:ILE:HD11	2.00	0.43
1:0d:31:LEU:HB3	1:0d:221:MET:HE2	2.01	0.43
1:0g:97:SER:OG	1:0g:100:TYR:O	2.32	0.43
1:0i:40:GLU:OE1	1:0i:281:ARG:NH1	2.52	0.43
2:0B:161:ASP:HB3	2:0B:200:LYS:HB2	2.01	0.43
2:0D:82:ILE:HG21	2:0E:279:GLN:HE21	1.83	0.43
2:0D:161:ASP:HB3	2:0D:200:LYS:HB2	2.01	0.43
3:J:68:LEU:HD13	3:L:63:VAL:HG21	2.01	0.43
3:j:30:ASP:OD1	3:j:30:ASP:N	2.51	0.43
1:0b:164:ASN:HA	1:0c:188:HIS:CD2	2.54	0.42
1:0c:15:ILE:O	1:0c:19:LYS:N	2.34	0.42
1:0c:161:ILE:HG12	1:0c:196:ILE:HG23	2.00	0.42
1:0e:40:GLU:OE1	1:0e:281:ARG:NH1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0f:65:PHE:N	1:0f:119:VAL:O	2.37	0.42
1:0l:31:LEU:HB3	1:0l:221:MET:HE2	2.01	0.42
2:0F:110:SER:HA	2:0G:252:GLU:HA	2.01	0.42
2:0G:17:GLN:NE2	3:Q:25:LEU:O	2.52	0.42
2:0G:235:THR:OG1	2:0G:236:SER:N	2.51	0.42
3:W:31:GLU:O	3:W:41:LYS:NZ	2.46	0.42
3:d:30:ASP:N	3:d:30:ASP:OD1	2.51	0.42
3:g:30:ASP:N	3:g:30:ASP:OD1	2.51	0.42
1:0b:159:VAL:HB	1:0c:184:VAL:HG22	2.01	0.42
1:0c:40:GLU:OE1	1:0c:281:ARG:NH1	2.52	0.42
1:0f:210:LEU:HD22	1:0g:152:GLN:HE22	1.83	0.42
1:0h:66:TYR:OH	1:0h:116:ASP:OD1	2.23	0.42
1:0l:161:ILE:HG12	1:0l:196:ILE:HG23	2.00	0.42
2:0D:257:LYS:HZ1	2:0D:261:GLN:HB2	1.84	0.42
2:0H:17:GLN:NE2	3:T:25:LEU:O	2.52	0.42
3:Y:65:GLU:OE2	3:Y:69:ASN:ND2	2.45	0.42
1:0a:40:GLU:OE1	1:0a:281:ARG:NH1	2.52	0.42
1:0g:17:ARG:NH2	3:U:21:TYR:OH	2.52	0.42
1:0j:40:GLU:OE1	1:0j:281:ARG:NH1	2.52	0.42
2:0A:161:ASP:HB3	2:0A:200:LYS:HB2	2.01	0.42
2:0G:9:ARG:NE	2:0G:61:MET:SD	2.83	0.42
2:0H:235:THR:OG1	2:0H:236:SER:N	2.51	0.42
3:D:68:LEU:HD13	3:F:63:VAL:HG21	2.01	0.42
3:c:32:SER:OG	3:c:34:THR:O	2.37	0.42
3:d:58:GLU:HA	3:d:61:ASN:HB2	2.00	0.42
1:0a:152:GLN:HE21	1:0j:147:ILE:HG21	1.84	0.42
1:0b:40:GLU:OE1	1:0b:281:ARG:NH1	2.52	0.42
2:0A:69:GLU:HG3	3:i:29:PHE:HB3	2.00	0.42
2:0B:123:ASP:O	2:0C:238:ASP:HA	2.18	0.42
2:0D:262:SER:HG	2:0D:265:ARG:H	1.66	0.42
2:0F:90:LEU:O	2:0F:93:SER:OG	2.27	0.42
2:0F:106:VAL:HG12	2:0G:257:LYS:H	1.84	0.42
2:0G:161:ASP:HB3	2:0G:200:LYS:HB2	2.01	0.42
2:0I:3:SER:OG	2:0I:4:TYR:N	2.48	0.42
1:0a:17:ARG:HH21	3:C:23:ARG:HG3	1.84	0.42
1:0b:65:PHE:N	1:0b:119:VAL:O	2.37	0.42
1:0f:188:HIS:HB3	2:0D:291:LEU:HD22	2.02	0.42
1:0g:17:ARG:HH21	3:U:23:ARG:HG3	1.84	0.42
1:0g:40:GLU:OE1	1:0g:281:ARG:NH1	2.52	0.42
1:0k:171:LEU:HD23	1:0k:171:LEU:HA	1.83	0.42
2:0I:154:GLY:HA3	2:0I:207:SER:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0J:154:GLY:HA3	2:0J:207:SER:HA	2.02	0.42
2:0K:154:GLY:HA3	2:0K:207:SER:HA	2.02	0.42
3:A:42:ILE:HG23	3:B:46:LEU:HD21	2.02	0.42
3:C:30:ASP:OD1	3:C:30:ASP:N	2.51	0.42
3:P:64:MET:HB2	3:Q:60:TRP:HH2	1.84	0.42
3:a:30:ASP:OD1	3:a:30:ASP:N	2.51	0.42
1:0d:249:GLN:NE2	1:0e:222:MET:SD	2.92	0.42
1:0e:169:LEU:HD13	3:I:28:ALA:HB2	2.02	0.42
1:0f:188:HIS:N	2:0D:291:LEU:O	2.53	0.42
2:0A:17:GLN:NE2	3:i:27:THR:H	2.16	0.42
2:0A:246:SER:HA	2:0L:116:THR:HA	2.02	0.42
2:0F:159:THR:HB	2:0F:202:ARG:HB3	2.02	0.42
2:0H:154:GLY:HA3	2:0H:207:SER:HA	2.02	0.42
2:0K:161:ASP:HB3	2:0K:200:LYS:HB2	2.01	0.42
2:0L:154:GLY:HA3	2:0L:207:SER:HA	2.02	0.42
2:0L:155:SER:OG	2:0L:156:GLY:N	2.46	0.42
1:0a:186:PHE:HE1	1:0j:161:ILE:HD12	1.85	0.42
1:0f:40:GLU:OE1	1:0f:281:ARG:NH1	2.52	0.42
1:0h:159:VAL:HB	1:0i:184:VAL:HG22	2.00	0.42
1:0i:159:VAL:HB	1:0l:184:VAL:HG22	2.02	0.42
2:0A:154:GLY:HA3	2:0A:207:SER:HA	2.02	0.42
2:0B:154:GLY:HA3	2:0B:207:SER:HA	2.02	0.42
2:0F:154:GLY:HA3	2:0F:207:SER:HA	2.02	0.42
2:0H:146:THR:OG1	2:0H:215:ASN:OD1	2.36	0.42
2:0L:159:THR:HB	2:0L:202:ARG:HB3	2.02	0.42
3:B:46:LEU:HD23	3:C:46:LEU:HD21	2.02	0.42
1:0a:168:GLN:NE2	2:0L:293:TYR:O	2.52	0.42
1:0h:40:GLU:OE1	1:0h:281:ARG:NH1	2.52	0.42
1:0i:161:ILE:HG12	1:0i:196:ILE:HG23	2.00	0.42
2:0A:159:THR:HB	2:0A:202:ARG:HB3	2.02	0.42
2:0B:101:LEU:HD22	2:0B:263:TYR:HD1	1.85	0.42
2:0B:159:THR:HB	2:0B:202:ARG:HB3	2.02	0.42
2:0C:154:GLY:HA3	2:0C:207:SER:HA	2.02	0.42
2:0D:154:GLY:HA3	2:0D:207:SER:HA	2.02	0.42
2:0E:90:LEU:O	2:0E:93:SER:OG	2.27	0.42
2:0G:159:THR:HB	2:0G:202:ARG:HB3	2.02	0.42
3:C:24:TYR:OH	3:j:35:LEU:N	2.51	0.42
3:e:42:ILE:HG23	3:f:46:LEU:HD21	2.02	0.42
3:i:56:LEU:HD13	3:j:57:ILE:HD11	2.01	0.42
1:0j:161:ILE:HG12	1:0j:196:ILE:HG23	2.00	0.42
2:0C:101:LEU:HD22	2:0C:263:TYR:HD1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0D:159:THR:HB	2:0D:202:ARG:HB3	2.02	0.42
2:0E:154:GLY:HA3	2:0E:207:SER:HA	2.02	0.42
2:0H:3:SER:N	3:U:30:ASP:OD1	2.52	0.42
2:0I:150:GLU:O	2:0J:213:THR:OG1	2.32	0.42
2:0K:159:THR:HB	2:0K:202:ARG:HB3	2.02	0.42
3:F:52:VAL:HG11	3:I:13:PHE:HZ	1.85	0.42
3:S:65:GLU:OE2	3:S:69:ASN:ND2	2.45	0.42
3:b:64:MET:HB2	3:c:60:TRP:HH2	1.83	0.42
2:0A:234:THR:OG1	2:0A:235:THR:N	2.53	0.42
2:0E:159:THR:HB	2:0E:202:ARG:HB3	2.02	0.42
2:0G:154:GLY:HA3	2:0G:207:SER:HA	2.02	0.42
2:0J:234:THR:OG1	2:0J:235:THR:N	2.53	0.42
2:0A:101:LEU:HD22	2:0A:263:TYR:HD1	1.85	0.41
2:0C:159:THR:HB	2:0C:202:ARG:HB3	2.02	0.41
2:0D:101:LEU:HD22	2:0D:263:TYR:HD1	1.85	0.41
2:0F:114:ASN:N	2:0F:246:SER:O	2.53	0.41
2:0H:273:ALA:HB2	2:0I:264:ALA:HB1	2.02	0.41
2:0K:116:THR:HA	2:0L:246:SER:HA	2.02	0.41
1:0d:15:ILE:O	1:0d:19:LYS:N	2.34	0.41
1:0j:171:LEU:HD23	1:0j:171:LEU:HA	1.83	0.41
1:0k:184:VAL:HG22	1:0l:159:VAL:HB	2.02	0.41
2:0A:114:ASN:N	2:0A:246:SER:O	2.54	0.41
2:0B:110:SER:HA	2:0C:252:GLU:HA	2.03	0.41
2:0D:114:ASN:N	2:0D:246:SER:O	2.54	0.41
2:0H:159:THR:HB	2:0H:202:ARG:HB3	2.02	0.41
2:0J:114:ASN:N	2:0J:246:SER:O	2.54	0.41
2:0J:161:ASP:HB3	2:0J:200:LYS:HB2	2.01	0.41
3:M:42:ILE:HG23	3:N:46:LEU:HD21	2.02	0.41
3:h:65:GLU:OE2	3:h:69:ASN:ND2	2.47	0.41
1:0a:171:LEU:HD23	1:0a:171:LEU:HA	1.83	0.41
1:0d:107:TYR:CZ	1:0d:271:LEU:HD13	2.55	0.41
1:0d:259:LYS:NZ	1:0e:54:GLU:OE1	2.41	0.41
1:0f:221:MET:HG3	1:0f:222:MET:HE2	2.03	0.41
1:0i:64:GLY:N	1:0i:76:CYS:O	2.53	0.41
1:0j:64:GLY:N	1:0j:76:CYS:O	2.54	0.41
1:0j:65:PHE:N	1:0j:119:VAL:O	2.37	0.41
1:0l:40:GLU:OE1	1:0l:281:ARG:NH1	2.52	0.41
2:0B:114:ASN:N	2:0B:246:SER:O	2.54	0.41
2:0D:3:SER:OG	2:0D:4:TYR:N	2.48	0.41
2:0D:90:LEU:HD23	2:0D:90:LEU:HA	1.94	0.41
2:0E:116:THR:HA	2:0F:246:SER:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0I:262:SER:HG	2:0I:265:ARG:H	1.65	0.41
2:0K:257:LYS:HZ1	2:0K:261:GLN:HB2	1.85	0.41
1:0f:107:TYR:CZ	1:0f:271:LEU:HD13	2.56	0.41
1:0h:221:MET:HG3	1:0h:222:MET:HE2	2.03	0.41
2:0G:234:THR:OG1	2:0G:235:THR:N	2.53	0.41
2:0G:257:LYS:HZ1	2:0G:261:GLN:HB2	1.86	0.41
2:0H:114:ASN:N	2:0H:246:SER:O	2.54	0.41
2:0I:90:LEU:O	2:0I:93:SER:OG	2.27	0.41
2:0I:114:ASN:N	2:0I:246:SER:O	2.54	0.41
2:0I:159:THR:HB	2:0I:202:ARG:HB3	2.02	0.41
2:0J:9:ARG:NE	2:0J:61:MET:SD	2.83	0.41
2:0L:101:LEU:HD22	2:0L:263:TYR:HD1	1.85	0.41
3:G:42:ILE:HG23	3:H:46:LEU:HD21	2.03	0.41
1:0e:221:MET:HG3	1:0e:222:MET:HE2	2.03	0.41
1:0g:107:TYR:CZ	1:0g:271:LEU:HD13	2.55	0.41
1:0i:221:MET:HG3	1:0i:222:MET:HE2	2.03	0.41
1:0l:221:MET:HG3	1:0l:222:MET:HE2	2.03	0.41
2:0A:257:LYS:HZ1	2:0A:261:GLN:HB2	1.85	0.41
2:0C:257:LYS:HZ1	2:0C:261:GLN:HB2	1.84	0.41
2:0E:234:THR:OG1	2:0E:235:THR:N	2.53	0.41
3:B:42:ILE:HG23	3:C:46:LEU:HD11	2.02	0.41
3:E:42:ILE:HG23	3:F:46:LEU:HD11	2.02	0.41
3:G:65:GLU:OE2	3:G:69:ASN:ND2	2.49	0.41
1:0f:97:SER:OG	1:0f:100:TYR:O	2.32	0.41
1:0k:17:ARG:NH2	3:g:21:TYR:OH	2.53	0.41
2:0C:163:PHE:HB2	2:0C:198:GLU:HB3	2.03	0.41
2:0E:81:MET:HB3	2:0F:54:HIS:CE1	2.56	0.41
2:0F:234:THR:OG1	2:0F:235:THR:N	2.53	0.41
2:0F:273:ALA:C	2:0G:271:ARG:HH12	2.27	0.41
2:0H:155:SER:HB3	2:0I:208:ASN:HA	2.01	0.41
2:0L:114:ASN:N	2:0L:246:SER:O	2.54	0.41
2:0L:146:THR:OG1	2:0L:215:ASN:OD1	2.36	0.41
3:K:56:LEU:HD13	3:L:57:ILE:HD11	2.02	0.41
3:b:42:ILE:HG23	3:c:46:LEU:HD21	2.02	0.41
1:0e:107:TYR:CZ	1:0e:271:LEU:HD13	2.56	0.41
1:0l:228:LYS:HA	1:0l:250:ILE:HD13	2.03	0.41
2:0F:262:SER:HG	2:0F:265:ARG:H	1.67	0.41
2:0I:234:THR:OG1	2:0I:235:THR:N	2.53	0.41
2:0J:159:THR:HB	2:0J:202:ARG:HB3	2.02	0.41
2:0L:234:THR:OG1	2:0L:235:THR:N	2.53	0.41
3:V:46:LEU:HD11	3:X:42:ILE:HG23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0b:161:ILE:HB	1:0c:186:PHE:CD1	2.56	0.41
1:0c:249:GLN:NE2	1:0d:222:MET:SD	2.94	0.41
1:0g:221:MET:HG3	1:0g:222:MET:HE2	2.03	0.41
2:0E:101:LEU:HD22	2:0E:263:TYR:HD1	1.85	0.41
2:0H:234:THR:OG1	2:0H:235:THR:N	2.53	0.41
3:K:24:TYR:HB3	3:L:37:GLU:OE2	2.20	0.41
1:0a:184:VAL:HG22	1:0j:159:VAL:HB	2.02	0.41
1:0b:147:ILE:HG21	1:0c:152:GLN:HE21	1.86	0.41
1:0b:176:ASN:HD21	3:j:23:ARG:HG2	1.86	0.41
1:0b:228:LYS:HA	1:0b:250:ILE:HD13	2.03	0.41
1:0d:221:MET:HG3	1:0d:222:MET:HE2	2.03	0.41
1:0g:228:LYS:HA	1:0g:250:ILE:HD13	2.03	0.41
1:0h:107:TYR:CZ	1:0h:271:LEU:HD13	2.56	0.41
1:0h:176:ASN:HD21	3:R:23:ARG:HG2	1.86	0.41
1:0j:107:TYR:CZ	1:0j:271:LEU:HD13	2.55	0.41
1:0j:189:GLU:HA	1:0k:162:ARG:HB3	2.02	0.41
1:0k:107:TYR:CZ	1:0k:271:LEU:HD13	2.56	0.41
1:0k:227:ILE:HD12	1:0k:227:ILE:HA	1.99	0.41
1:0k:228:LYS:HA	1:0k:250:ILE:HD13	2.03	0.41
2:0C:9:ARG:NE	2:0C:61:MET:SD	2.83	0.41
2:0C:90:LEU:HD23	2:0C:90:LEU:HA	1.94	0.41
2:0D:234:THR:OG1	2:0D:235:THR:N	2.53	0.41
2:0D:273:ALA:HB2	2:0E:264:ALA:HB1	2.03	0.41
2:0I:101:LEU:HD22	2:0I:263:TYR:HD1	1.85	0.41
2:0K:114:ASN:N	2:0K:246:SER:O	2.54	0.41
2:0K:234:THR:OG1	2:0K:235:THR:N	2.53	0.41
3:P:42:ILE:HG23	3:Q:46:LEU:HD21	2.02	0.41
3:Q:26:PRO:HB2	3:R:44:HIS:CD2	2.56	0.41
3:Z:56:LEU:HD13	3:a:57:ILE:HD11	2.03	0.41
3:e:64:MET:HB2	3:f:60:TRP:HH2	1.85	0.41
3:f:56:LEU:HD13	3:g:57:ILE:HD11	2.02	0.41
1:0f:249:GLN:NE2	1:0g:222:MET:SD	2.94	0.41
1:0i:65:PHE:N	1:0i:119:VAL:O	2.37	0.41
1:0k:221:MET:HG3	1:0k:222:MET:HE2	2.03	0.41
1:0l:7:ASN:HA	3:V:34:THR:HG21	2.03	0.41
2:0B:131:ASN:OD1	2:0C:231:LYS:HB3	2.20	0.41
2:0E:9:ARG:NE	2:0E:61:MET:SD	2.83	0.41
2:0E:115:ASP:HB2	2:0F:247:VAL:HG13	2.02	0.41
2:0E:155:SER:OG	2:0F:207:SER:OG	2.22	0.41
2:0F:102:GLU:HB3	2:0G:263:TYR:HE2	1.85	0.41
2:0F:239:LYS:HE3	2:0F:239:LYS:HB2	1.91	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0G:114:ASN:N	2:0G:246:SER:O	2.54	0.41
3:f:32:SER:OG	3:f:34:THR:O	2.38	0.41
1:0a:228:LYS:HA	1:0a:250:ILE:HD13	2.03	0.40
1:0b:64:GLY:N	1:0b:76:CYS:O	2.54	0.40
1:0l:227:ILE:HD12	1:0l:227:ILE:HA	1.99	0.40
2:0B:234:THR:OG1	2:0B:235:THR:N	2.53	0.40
2:0E:24:THR:OG1	3:H:31:GLU:OE2	2.30	0.40
2:0F:257:LYS:HZ1	2:0F:261:GLN:HB2	1.85	0.40
2:0I:134:SER:HA	2:0J:228:THR:HA	2.03	0.40
2:0J:101:LEU:HD22	2:0J:263:TYR:HD1	1.85	0.40
2:0K:101:LEU:HD22	2:0K:263:TYR:HD1	1.85	0.40
3:Y:42:ILE:HG23	3:Z:46:LEU:HD21	2.03	0.40
1:0a:107:TYR:CZ	1:0a:271:LEU:HD13	2.55	0.40
1:0b:97:SER:OG	1:0b:100:TYR:O	2.32	0.40
1:0h:228:LYS:HA	1:0h:250:ILE:HD13	2.03	0.40
1:0k:64:GLY:N	1:0k:76:CYS:O	2.54	0.40
2:0A:279:GLN:HE21	2:0L:82:ILE:HG21	1.86	0.40
2:0D:163:PHE:HB2	2:0D:198:GLU:HB3	2.03	0.40
2:0E:114:ASN:N	2:0E:246:SER:O	2.53	0.40
2:0F:101:LEU:HD22	2:0F:263:TYR:HD1	1.85	0.40
2:0F:163:PHE:HB2	2:0F:198:GLU:HB3	2.03	0.40
2:0H:101:LEU:HD22	2:0H:263:TYR:HD1	1.85	0.40
2:0H:257:LYS:HZ1	2:0H:261:GLN:HB2	1.86	0.40
2:0I:257:LYS:HZ1	2:0I:261:GLN:HB2	1.86	0.40
2:0K:273:ALA:O	2:0L:271:ARG:NH1	2.40	0.40
3:W:50:GLY:HA3	3:Z:16:MET:HG3	2.03	0.40
1:0c:107:TYR:CZ	1:0c:271:LEU:HD13	2.56	0.40
1:0c:221:MET:HG3	1:0c:222:MET:HE2	2.03	0.40
1:0e:210:LEU:HD23	1:0e:210:LEU:HA	1.92	0.40
1:0i:107:TYR:CZ	1:0i:271:LEU:HD13	2.56	0.40
1:0l:107:TYR:CZ	1:0l:271:LEU:HD13	2.55	0.40
2:0B:90:LEU:HD23	2:0B:90:LEU:HA	1.94	0.40
2:0B:139:LYS:HG2	2:0C:223:ASP:O	2.22	0.40
2:0C:9:ARG:HH22	3:E:23:ARG:HH22	1.68	0.40
2:0C:146:THR:OG1	2:0C:215:ASN:OD1	2.36	0.40
2:0D:239:LYS:HE3	2:0D:239:LYS:HB2	1.90	0.40
2:0E:163:PHE:HB2	2:0E:198:GLU:HB3	2.03	0.40
2:0E:257:LYS:HZ1	2:0E:261:GLN:HB2	1.87	0.40
2:0F:149:ASN:HA	2:0G:214:SER:HA	2.02	0.40
2:0H:93:SER:CB	2:0I:271:ARG:HE	2.35	0.40
2:0H:166:ASP:O	2:0I:197:ASN:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:30:ASP:N	3:O:30:ASP:OD1	2.51	0.40
3:i:46:LEU:HD23	3:j:46:LEU:HD21	2.04	0.40
1:0a:162:ARG:HB3	1:0b:189:GLU:HA	2.03	0.40
1:0a:183:PRO:HD2	1:0k:12:ILE:HD11	2.03	0.40
1:0b:107:TYR:CZ	1:0b:271:LEU:HD13	2.56	0.40
1:0k:123:ASN:HD22	1:0k:129:PRO:HA	1.87	0.40
2:0C:149:ASN:HA	2:0D:214:SER:HA	2.03	0.40
2:0G:135:SER:O	2:0H:227:LYS:N	2.47	0.40
2:0K:91:PHE:O	2:0K:95:LEU:N	2.55	0.40
2:0K:150:GLU:O	2:0L:213:THR:OG1	2.37	0.40
3:h:64:MET:HB2	3:i:60:TRP:HH2	1.86	0.40
1:0a:249:GLN:NE2	1:0b:222:MET:SD	2.95	0.40
1:0j:221:MET:HG3	1:0j:222:MET:HE2	2.03	0.40
2:0A:163:PHE:HB2	2:0A:198:GLU:HB3	2.03	0.40
2:0B:163:PHE:HB2	2:0B:198:GLU:HB3	2.03	0.40
2:0K:155:SER:OG	2:0K:156:GLY:N	2.46	0.40
3:P:51:LYS:NZ	3:P:55:GLU:OE2	2.45	0.40
3:X:30:ASP:OD1	3:X:30:ASP:N	2.51	0.40
3:f:24:TYR:HB3	3:g:37:GLU:OE2	2.22	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	0a	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0b	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0c	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0d	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0e	276/309 (89%)	258 (94%)	18 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0f	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0g	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0h	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0i	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0j	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0k	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
1	0l	276/309 (89%)	258 (94%)	18 (6%)	0	100	100
2	0A	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0B	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0C	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0D	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0E	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0F	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0G	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0H	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0I	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0J	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
2	0K	289/293 (99%)	248 (86%)	41 (14%)	0	100	100
2	0L	289/293 (99%)	249 (86%)	40 (14%)	0	100	100
3	A	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	B	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	C	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	D	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	E	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	F	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	G	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	H	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	I	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	J	49/854 (6%)	43 (88%)	5 (10%)	1 (2%)	6	32
3	K	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	L	59/854 (7%)	54 (92%)	5 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	N	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	O	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	P	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	Q	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	R	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	S	49/854 (6%)	43 (88%)	6 (12%)	0	100	100
3	T	55/854 (6%)	53 (96%)	2 (4%)	0	100	100
3	U	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	V	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	W	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	X	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	Y	49/854 (6%)	43 (88%)	5 (10%)	1 (2%)	6	32
3	Z	55/854 (6%)	51 (93%)	4 (7%)	0	100	100
3	a	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	b	49/854 (6%)	44 (90%)	4 (8%)	1 (2%)	6	32
3	c	55/854 (6%)	53 (96%)	2 (4%)	0	100	100
3	d	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	e	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	f	55/854 (6%)	51 (93%)	4 (7%)	0	100	100
3	g	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
3	h	49/854 (6%)	44 (90%)	5 (10%)	0	100	100
3	i	55/854 (6%)	52 (94%)	3 (6%)	0	100	100
3	j	59/854 (7%)	54 (92%)	5 (8%)	0	100	100
All	All	8736/37968 (23%)	7874 (90%)	859 (10%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	31	GLU
3	Y	31	GLU
3	b	31	GLU

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	0a	235/277 (85%)	235 (100%)	0	100	100
1	0b	235/277 (85%)	235 (100%)	0	100	100
1	0c	235/277 (85%)	235 (100%)	0	100	100
1	0d	235/277 (85%)	235 (100%)	0	100	100
1	0e	235/277 (85%)	235 (100%)	0	100	100
1	0f	235/277 (85%)	235 (100%)	0	100	100
1	0g	235/277 (85%)	235 (100%)	0	100	100
1	0h	235/277 (85%)	235 (100%)	0	100	100
1	0i	235/277 (85%)	235 (100%)	0	100	100
1	0j	235/277 (85%)	235 (100%)	0	100	100
1	0k	235/277 (85%)	235 (100%)	0	100	100
1	0l	235/277 (85%)	235 (100%)	0	100	100
2	0A	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0B	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0C	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0D	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0E	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0F	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0G	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0H	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0I	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0J	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0K	250/270 (93%)	249 (100%)	1 (0%)	84	83
2	0L	250/270 (93%)	249 (100%)	1 (0%)	84	83
3	A	48/706 (7%)	48 (100%)	0	100	100
3	B	54/706 (8%)	54 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	57/706 (8%)	57 (100%)	0	100	100
3	D	48/706 (7%)	48 (100%)	0	100	100
3	E	54/706 (8%)	54 (100%)	0	100	100
3	F	57/706 (8%)	57 (100%)	0	100	100
3	G	48/706 (7%)	48 (100%)	0	100	100
3	H	54/706 (8%)	54 (100%)	0	100	100
3	I	57/706 (8%)	57 (100%)	0	100	100
3	J	48/706 (7%)	48 (100%)	0	100	100
3	K	54/706 (8%)	54 (100%)	0	100	100
3	L	57/706 (8%)	57 (100%)	0	100	100
3	M	48/706 (7%)	48 (100%)	0	100	100
3	N	54/706 (8%)	54 (100%)	0	100	100
3	O	57/706 (8%)	57 (100%)	0	100	100
3	P	48/706 (7%)	48 (100%)	0	100	100
3	Q	54/706 (8%)	54 (100%)	0	100	100
3	R	57/706 (8%)	57 (100%)	0	100	100
3	S	48/706 (7%)	48 (100%)	0	100	100
3	T	54/706 (8%)	54 (100%)	0	100	100
3	U	57/706 (8%)	57 (100%)	0	100	100
3	V	48/706 (7%)	48 (100%)	0	100	100
3	W	54/706 (8%)	54 (100%)	0	100	100
3	X	57/706 (8%)	57 (100%)	0	100	100
3	Y	48/706 (7%)	48 (100%)	0	100	100
3	Z	54/706 (8%)	54 (100%)	0	100	100
3	a	57/706 (8%)	57 (100%)	0	100	100
3	b	48/706 (7%)	48 (100%)	0	100	100
3	c	54/706 (8%)	54 (100%)	0	100	100
3	d	57/706 (8%)	57 (100%)	0	100	100
3	e	48/706 (7%)	48 (100%)	0	100	100
3	f	54/706 (8%)	54 (100%)	0	100	100
3	g	57/706 (8%)	57 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	h	48/706 (7%)	48 (100%)	0	100	100
3	i	54/706 (8%)	54 (100%)	0	100	100
3	j	57/706 (8%)	57 (100%)	0	100	100
All	All	7728/31980 (24%)	7716 (100%)	12 (0%)	85	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	0A	247	VAL
2	0B	247	VAL
2	0C	247	VAL
2	0D	247	VAL
2	0E	247	VAL
2	0F	247	VAL
2	0G	247	VAL
2	0H	247	VAL
2	0I	247	VAL
2	0J	247	VAL
2	0K	247	VAL
2	0L	247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	0a	123	ASN
1	0a	152	GLN
1	0a	168	GLN
1	0a	269	ASN
1	0b	59	GLN
1	0b	123	ASN
1	0b	152	GLN
1	0b	168	GLN
1	0b	269	ASN
1	0c	59	GLN
1	0c	123	ASN
1	0c	152	GLN
1	0c	168	GLN
1	0c	269	ASN
1	0d	59	GLN
1	0d	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0d	152	GLN
1	0d	168	GLN
1	0d	269	ASN
1	0e	59	GLN
1	0e	123	ASN
1	0e	152	GLN
1	0e	168	GLN
1	0e	269	ASN
1	0f	59	GLN
1	0f	123	ASN
1	0f	152	GLN
1	0f	168	GLN
1	0f	269	ASN
1	0g	26	HIS
1	0g	59	GLN
1	0g	123	ASN
1	0g	152	GLN
1	0g	168	GLN
1	0g	269	ASN
1	0h	26	HIS
1	0h	59	GLN
1	0h	123	ASN
1	0h	152	GLN
1	0h	168	GLN
1	0h	269	ASN
1	0i	59	GLN
1	0i	123	ASN
1	0i	152	GLN
1	0i	168	GLN
1	0i	269	ASN
1	0j	59	GLN
1	0j	123	ASN
1	0j	152	GLN
1	0j	168	GLN
1	0j	269	ASN
1	0k	59	GLN
1	0k	123	ASN
1	0k	152	GLN
1	0k	168	GLN
1	0k	269	ASN
1	0l	123	ASN
1	0l	152	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0I	168	GLN
1	0I	269	ASN
2	0A	17	GLN
2	0A	103	ASN
2	0A	126	GLN
2	0A	162	ASN
2	0A	192	GLN
2	0A	261	GLN
2	0A	279	GLN
2	0B	17	GLN
2	0B	103	ASN
2	0B	162	ASN
2	0B	192	GLN
2	0B	196	HIS
2	0C	17	GLN
2	0C	83	ASN
2	0C	103	ASN
2	0C	126	GLN
2	0C	162	ASN
2	0C	192	GLN
2	0C	196	HIS
2	0C	279	GLN
2	0D	17	GLN
2	0D	103	ASN
2	0D	162	ASN
2	0D	192	GLN
2	0E	17	GLN
2	0E	103	ASN
2	0E	126	GLN
2	0E	162	ASN
2	0E	192	GLN
2	0E	196	HIS
2	0E	279	GLN
2	0F	17	GLN
2	0F	103	ASN
2	0F	126	GLN
2	0F	162	ASN
2	0F	192	GLN
2	0G	17	GLN
2	0G	103	ASN
2	0G	126	GLN
2	0G	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	0G	192	GLN
2	0G	261	GLN
2	0H	17	GLN
2	0H	103	ASN
2	0H	126	GLN
2	0H	162	ASN
2	0H	192	GLN
2	0H	196	HIS
2	0I	17	GLN
2	0I	103	ASN
2	0I	126	GLN
2	0I	162	ASN
2	0I	192	GLN
2	0I	196	HIS
2	0I	279	GLN
2	0J	17	GLN
2	0J	103	ASN
2	0J	126	GLN
2	0J	162	ASN
2	0J	192	GLN
2	0J	279	GLN
2	0K	17	GLN
2	0K	103	ASN
2	0K	126	GLN
2	0K	162	ASN
2	0K	192	GLN
2	0K	196	HIS
2	0K	261	GLN
2	0L	17	GLN
2	0L	103	ASN
2	0L	126	GLN
2	0L	162	ASN
2	0L	192	GLN
2	0L	261	GLN
3	A	54	ASN
3	B	54	ASN
3	B	61	ASN
3	C	61	ASN
3	D	54	ASN
3	E	61	ASN
3	F	61	ASN
3	G	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	61	ASN
3	I	61	ASN
3	J	54	ASN
3	K	54	ASN
3	K	61	ASN
3	L	19	GLN
3	L	61	ASN
3	N	40	ASN
3	N	54	ASN
3	N	61	ASN
3	O	19	GLN
3	O	61	ASN
3	Q	61	ASN
3	R	19	GLN
3	R	44	HIS
3	R	61	ASN
3	S	54	ASN
3	T	40	ASN
3	T	54	ASN
3	T	61	ASN
3	U	19	GLN
3	U	61	ASN
3	W	40	ASN
3	W	54	ASN
3	W	61	ASN
3	X	61	ASN
3	Y	54	ASN
3	Z	40	ASN
3	Z	54	ASN
3	Z	61	ASN
3	a	61	ASN
3	b	54	ASN
3	c	40	ASN
3	c	54	ASN
3	c	61	ASN
3	d	19	GLN
3	d	61	ASN
3	f	61	ASN
3	g	19	GLN
3	g	61	ASN
3	h	47	ASN
3	h	54	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	i	54	ASN
3	i	61	ASN
3	j	19	GLN
3	j	61	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

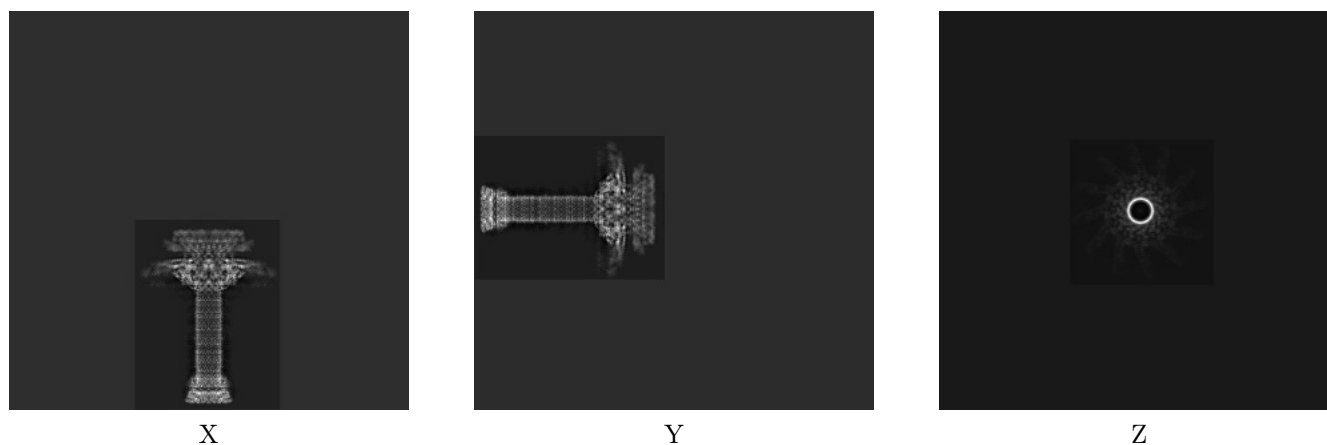
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4685. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

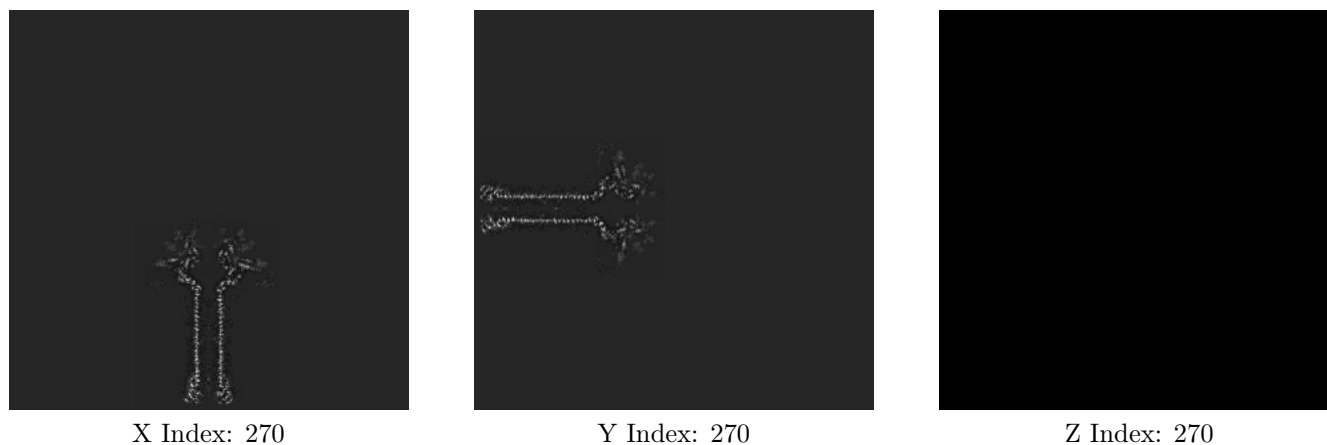
6.1.1 Primary map



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

6.2 Central slices [i](#)

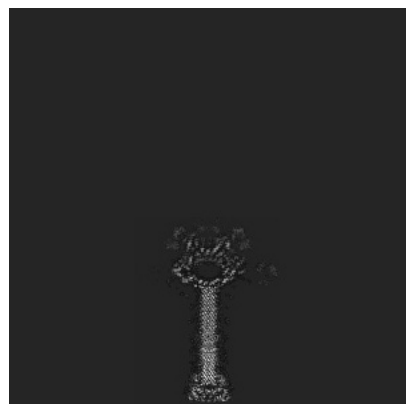
6.2.1 Primary map



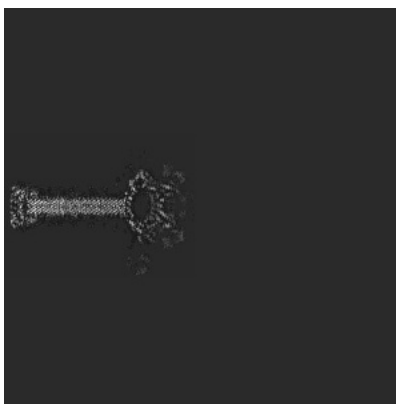
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

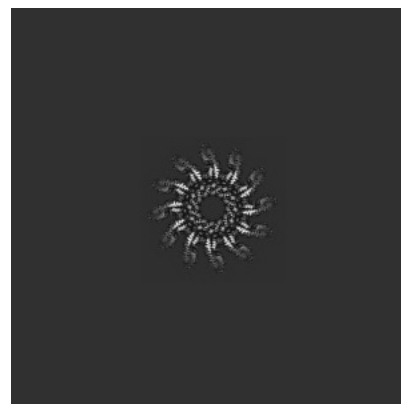
6.3.1 Primary map



X Index: 256



Y Index: 254

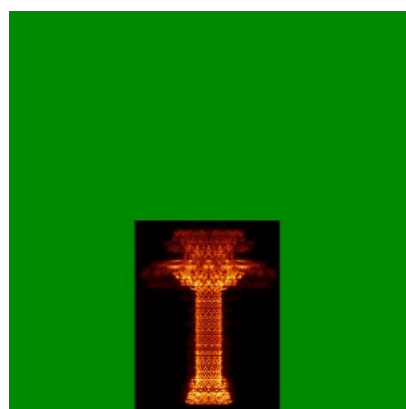


Z Index: 194

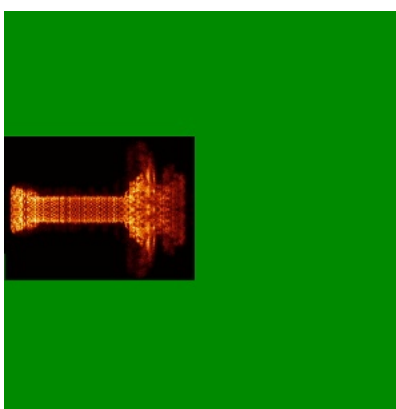
The images above show the largest variance slices of the map in three orthogonal directions.

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

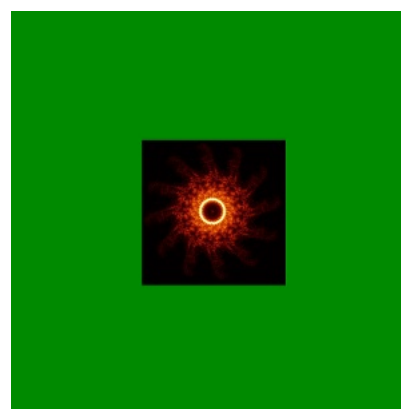
6.4.1 Primary map



X



Y

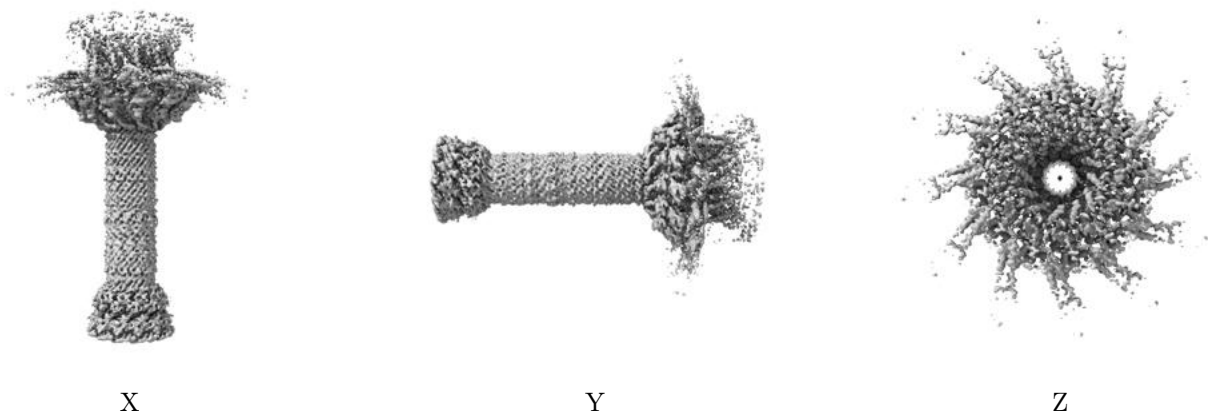


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

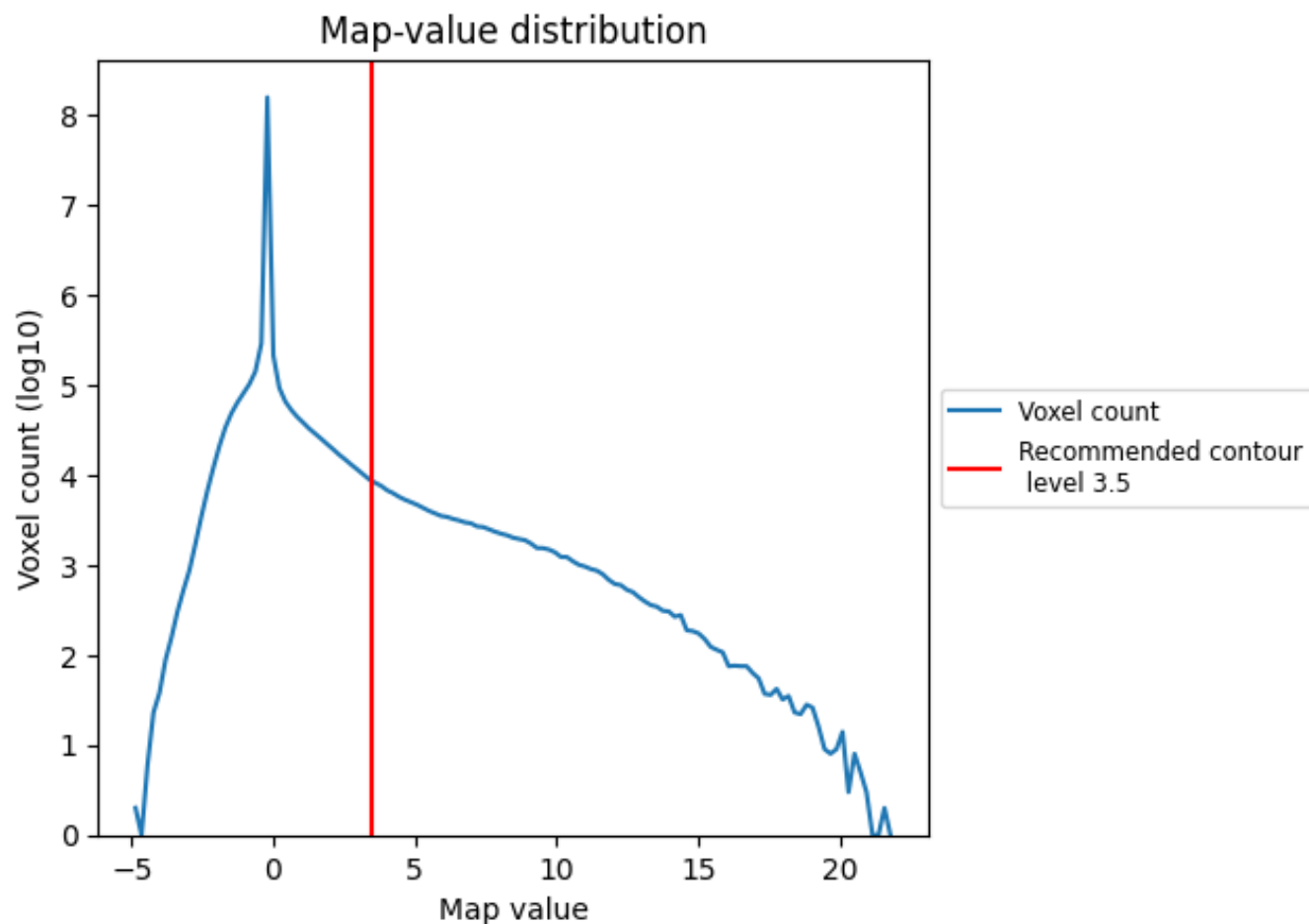
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

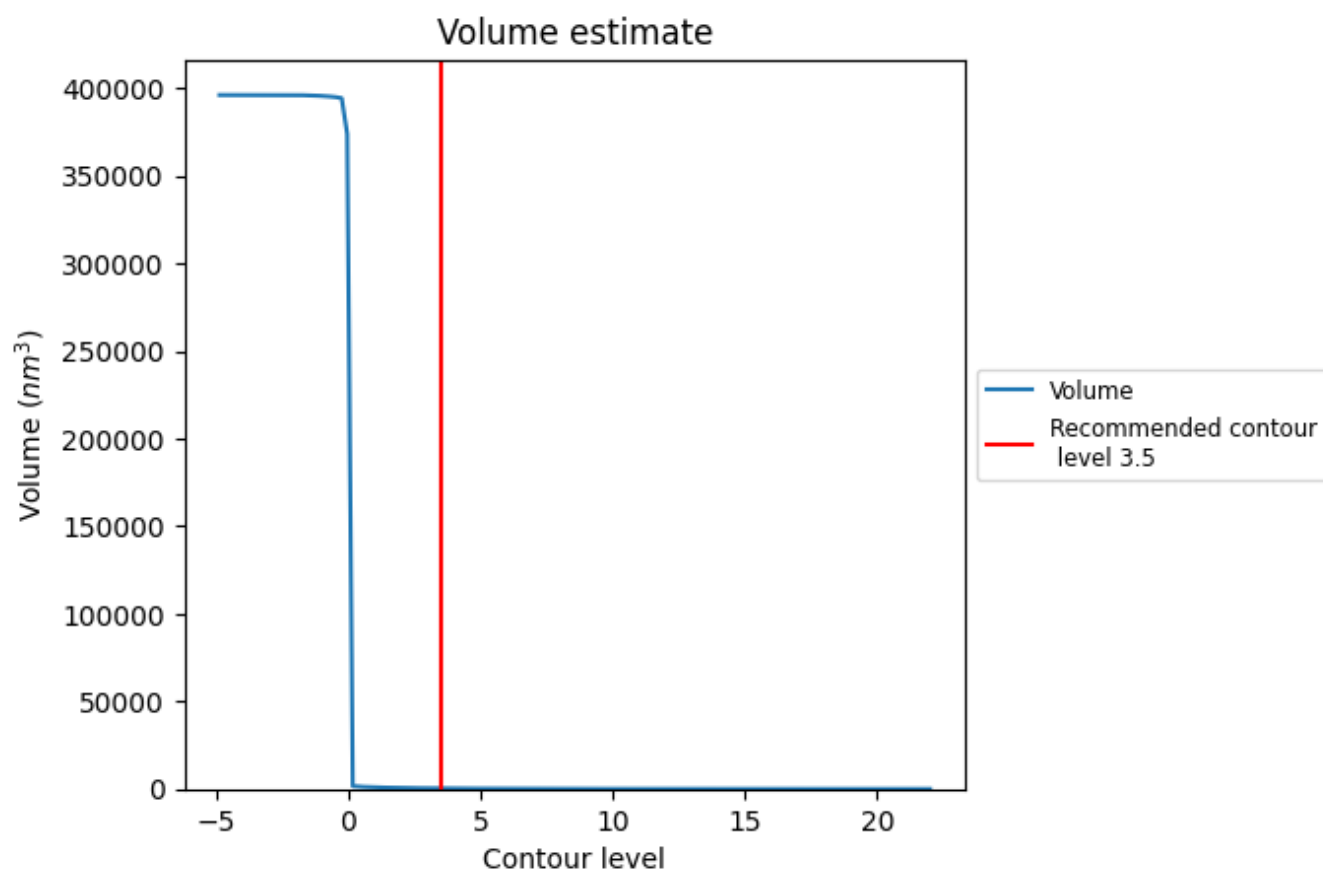
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

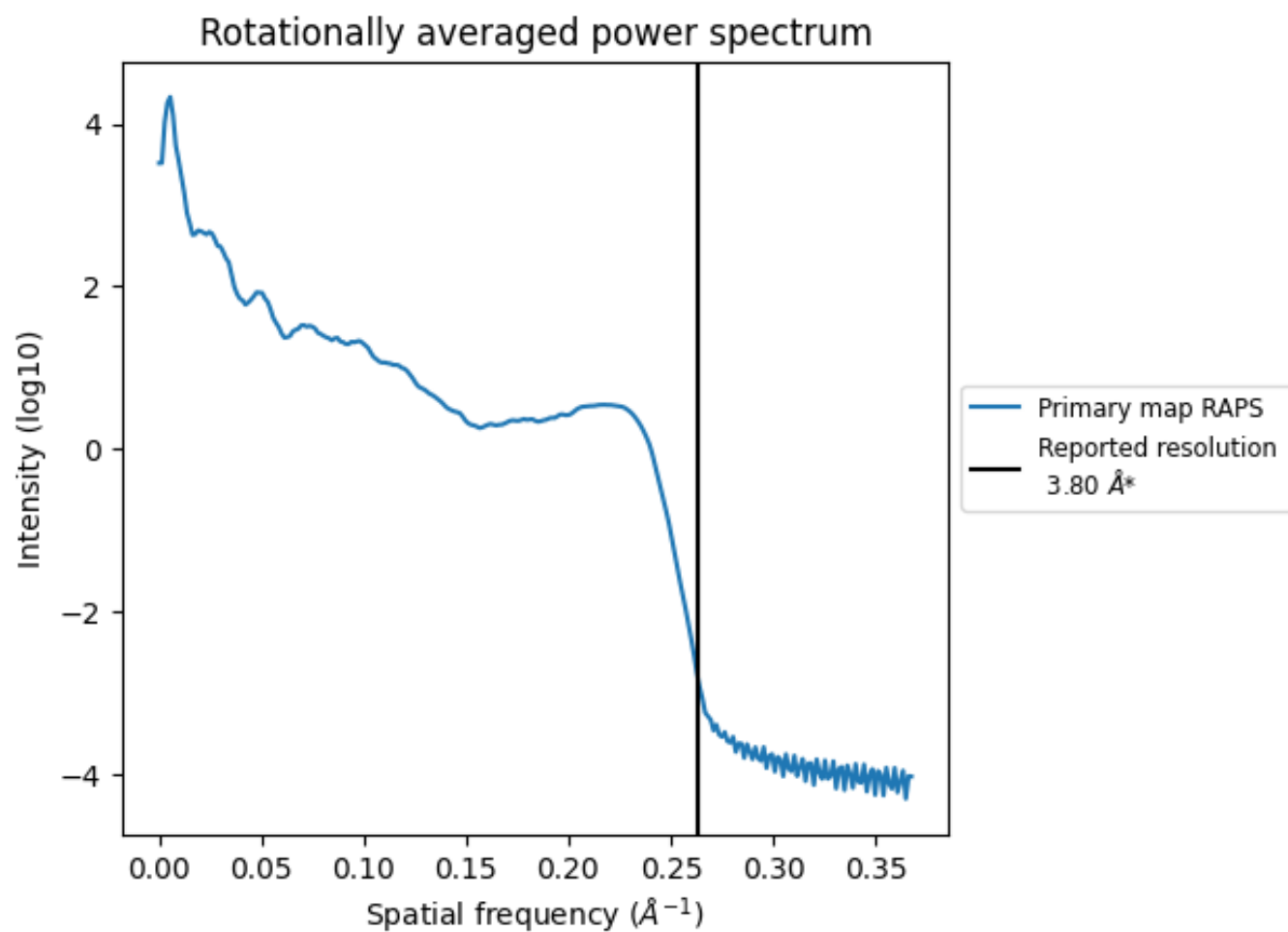
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 323 nm^3 ; this corresponds to an approximate mass of 291 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 0.263 Å⁻¹

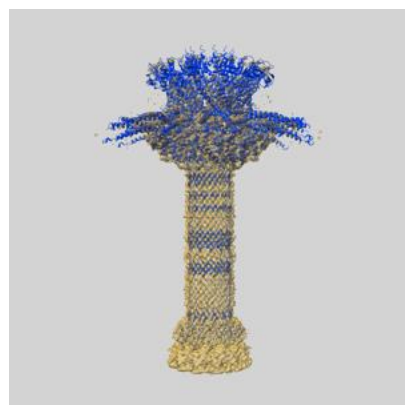
8 Fourier-Shell correlation

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

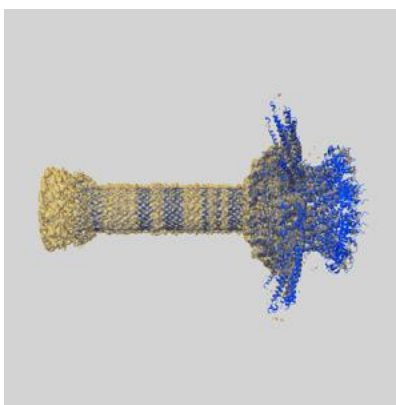
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4685 and PDB model 6QZF. Per-residue inclusion information can be found in section 3 on page 10.

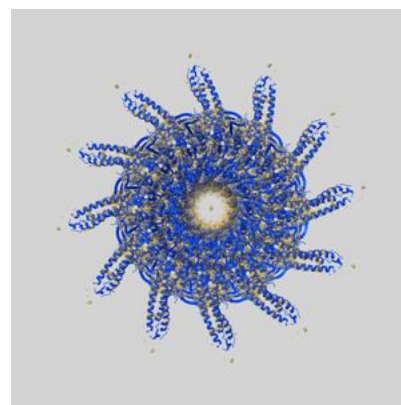
9.1 Map-model overlay [i](#)



X



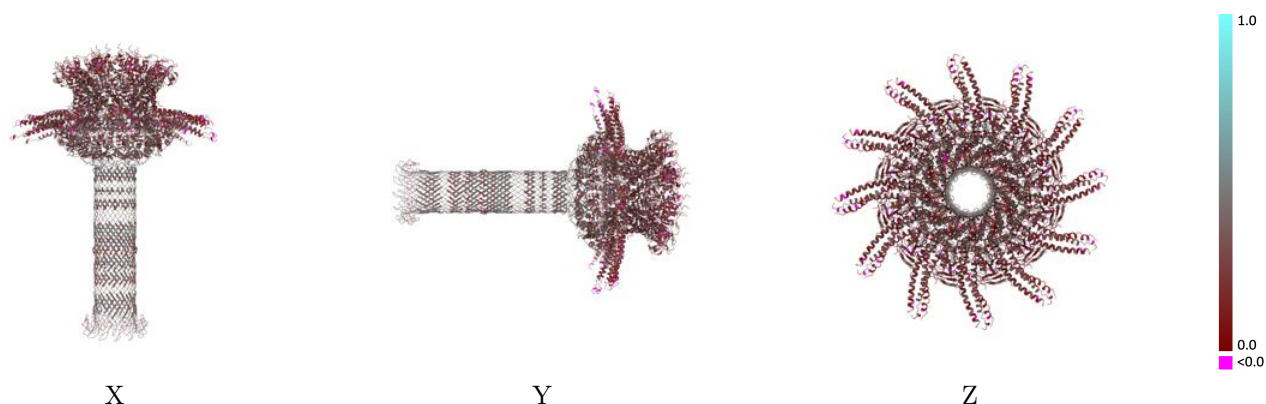
Y



Z

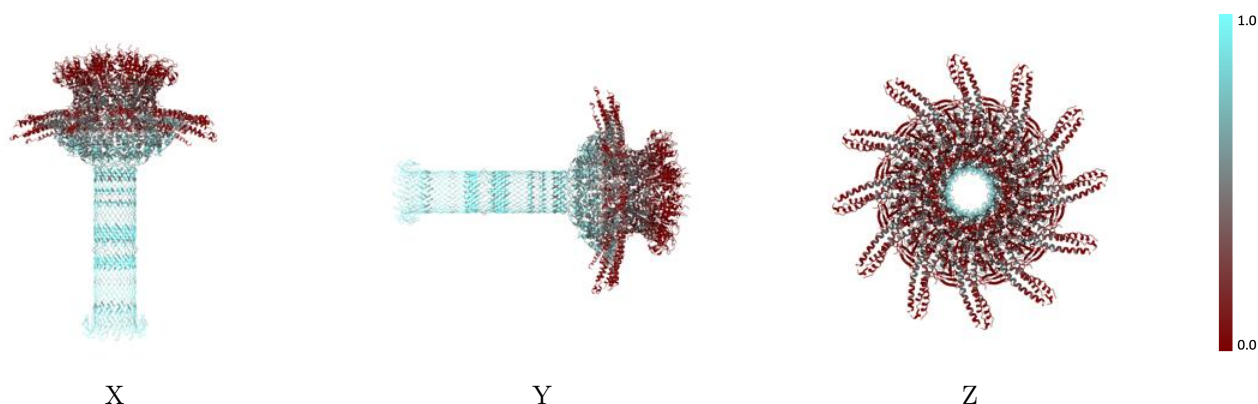
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



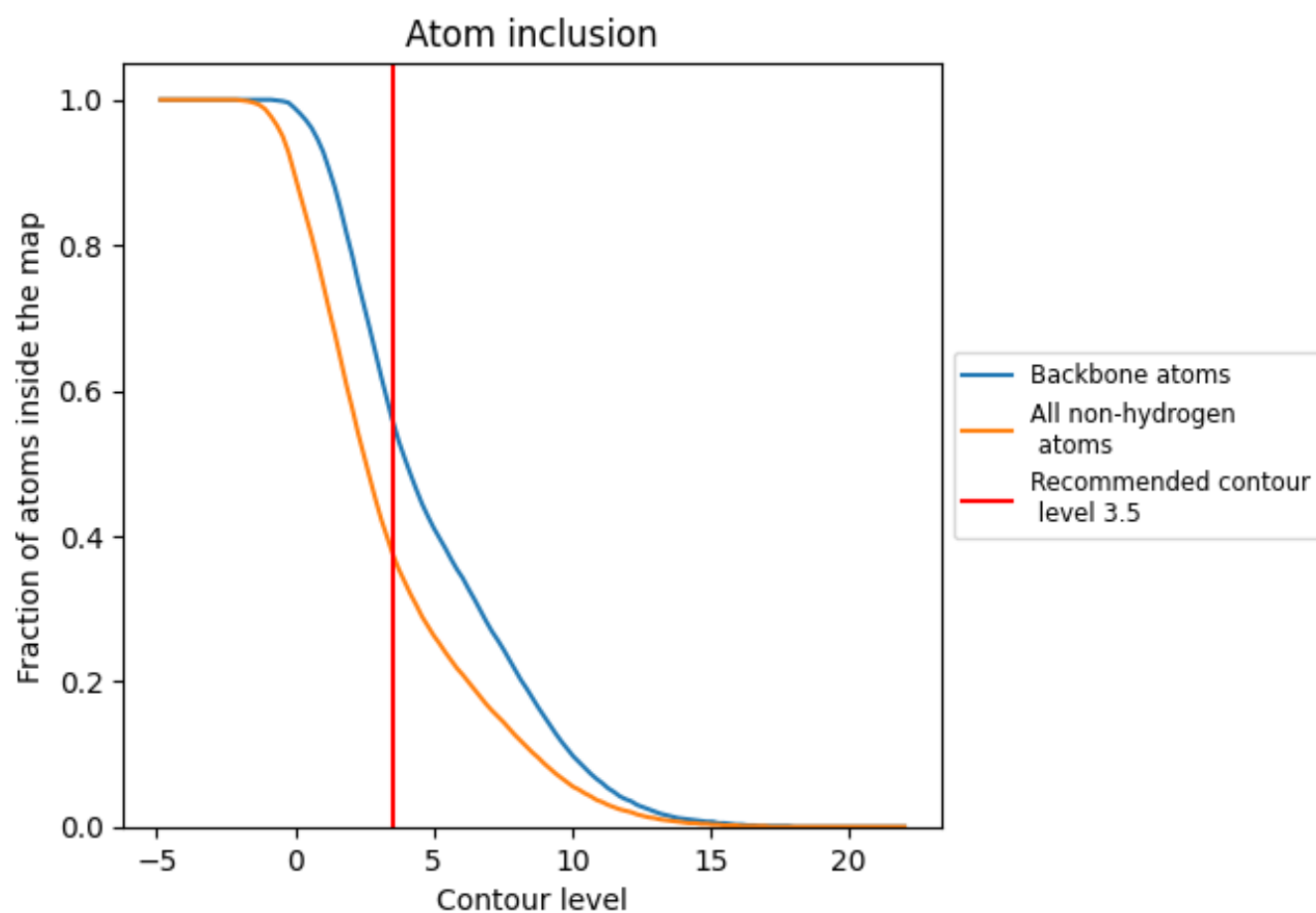
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 38% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3780	 0.3050
0A	 0.6740	 0.3690
0B	 0.6740	 0.3690
0C	 0.6760	 0.3730
0D	 0.6760	 0.3720
0E	 0.6780	 0.3720
0F	 0.6770	 0.3740
0G	 0.6740	 0.3720
0H	 0.6780	 0.3730
0I	 0.6750	 0.3730
0J	 0.6760	 0.3720
0K	 0.6770	 0.3700
0L	 0.6720	 0.3710
0a	 0.1890	 0.2840
0b	 0.1910	 0.2840
0c	 0.1910	 0.2840
0d	 0.1920	 0.2820
0e	 0.1930	 0.2860
0f	 0.1870	 0.2830
0g	 0.1880	 0.2820
0h	 0.1910	 0.2850
0i	 0.1900	 0.2850
0j	 0.1880	 0.2830
0k	 0.1870	 0.2830
0l	 0.1880	 0.2850
A	 0.1740	 0.2080
B	 0.2270	 0.2470
C	 0.1870	 0.2480
D	 0.1670	 0.2090
E	 0.2320	 0.2420
F	 0.1930	 0.2530
G	 0.1620	 0.2100
H	 0.2300	 0.2390
I	 0.1870	 0.2500
J	 0.1670	 0.2020



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
K	 0.2230	 0.2330
L	 0.1910	 0.2470
M	 0.1690	 0.2010
N	 0.2190	 0.2330
O	 0.1930	 0.2490
P	 0.1690	 0.2010
Q	 0.2190	 0.2310
R	 0.1910	 0.2420
S	 0.1710	 0.2040
T	 0.2210	 0.2340
U	 0.1870	 0.2500
V	 0.1740	 0.2080
W	 0.2190	 0.2260
X	 0.1810	 0.2400
Y	 0.1690	 0.2010
Z	 0.2210	 0.2290
a	 0.1810	 0.2430
b	 0.1670	 0.2000
c	 0.2170	 0.2290
d	 0.1930	 0.2480
e	 0.1690	 0.1960
f	 0.2210	 0.2390
g	 0.1770	 0.2390
h	 0.1710	 0.1950
i	 0.2230	 0.2390
j	 0.1890	 0.2500