



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 6QZ9 / pdb_00006qz9
EMDB ID : EMD-4684
Title : The cryo-EM structure of the collar complex and tail axis in bacteriophage phi29
Authors : Xu, J.; Wang, D.; Gui, M.; Xiang, Y.
Deposited on : 2019-03-11
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

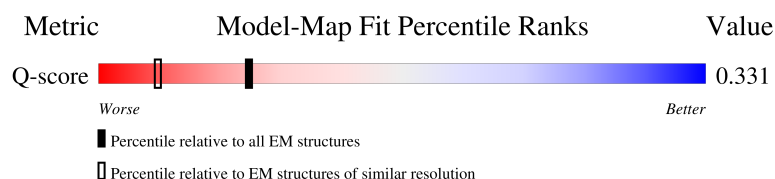
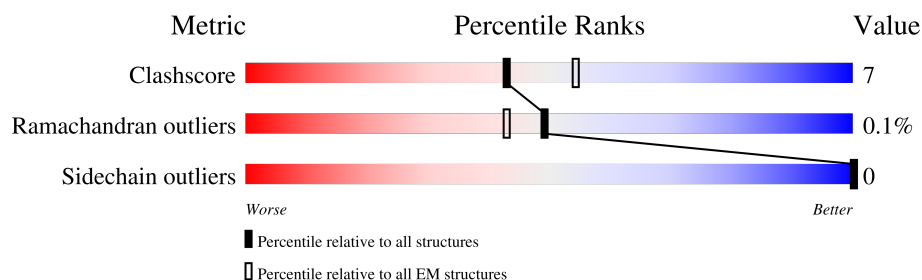
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	0a	309	50% 70% 15% 15%
1	0b	309	50% 70% 16% 15%
1	0c	309	50% 70% 16% 15%
1	0d	309	50% 69% 16% 15%

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Mol	Chain	Length	Quality of chain
1	0e	309	
1	0f	309	
1	0g	309	
1	0h	309	
1	0i	309	
1	0j	309	
1	0k	309	
1	0l	309	
2	0A	293	
2	0B	293	
2	0C	293	
2	0D	293	
2	0E	293	
2	0F	293	
2	0G	293	
2	0H	293	
2	0I	293	
2	0J	293	
2	0K	293	
2	0L	293	
3	A	854	
3	B	854	
3	C	854	
3	D	854	
3	E	854	

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Mol	Chain	Length	Quality of chain	
3	F	854		92%
3	G	854		94%
3	H	854		93%
3	I	854		92%
3	J	854		94%
3	K	854		93%
3	L	854		92%
3	M	854		94%
3	N	854		93%
3	O	854		92%
3	P	854		94%
3	Q	854		93%
3	R	854		92%
3	S	854		94%
3	T	854		93%
3	U	854		92%
3	V	854		94%
3	W	854		93%
3	X	854		92%
3	Y	854		94%
3	Z	854		93%
3	a	854		92%
3	b	854		94%
3	c	854		93%
3	d	854		92%

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Mol	Chain	Length	Quality of chain	
3	e	854		94%
3	f	854		93%
3	g	854		92%
3	h	854		94%
3	i	854		93%
3	j	854		92%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 71724 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	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0b	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0c	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0d	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0e	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0f	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0g	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0h	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0i	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0j	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0k	264	Total 2163	C 1384	N 360	O 412	S 7	0	0
1	0l	264	Total 2163	C 1384	N 360	O 412	S 7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0A	291	Total 2296	C 1414	N 396	O 478	S 8	0	0
2	0B	291	Total 2296	C 1414	N 396	O 478	S 8	0	0
2	0C	291	Total 2296	C 1414	N 396	O 478	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	0D	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0E	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0F	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0G	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0H	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0I	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0J	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0K	291	Total	C	N	O	S	0	0
			2296	1414	396	478	8		
2	0L	291	Total	C	N	O	S	0	0
			2296	1414	396	478	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	71	Total	C	N	O	S	0	0
			603	391	94	114	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	71	Total	C	N	O	S	0	0
			603	391	94	114	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	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	J	51	Total	C	N	O	S	0	0
			433	281	67	83	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	L	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	M	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	N	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	O	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	P	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	Q	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	R	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	S	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	T	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	U	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	V	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	W	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	X	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	Y	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	Z	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	a	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	b	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	c	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	d	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	e	51	Total	C	N	O	S	0	0
			433	281	67	83	2		

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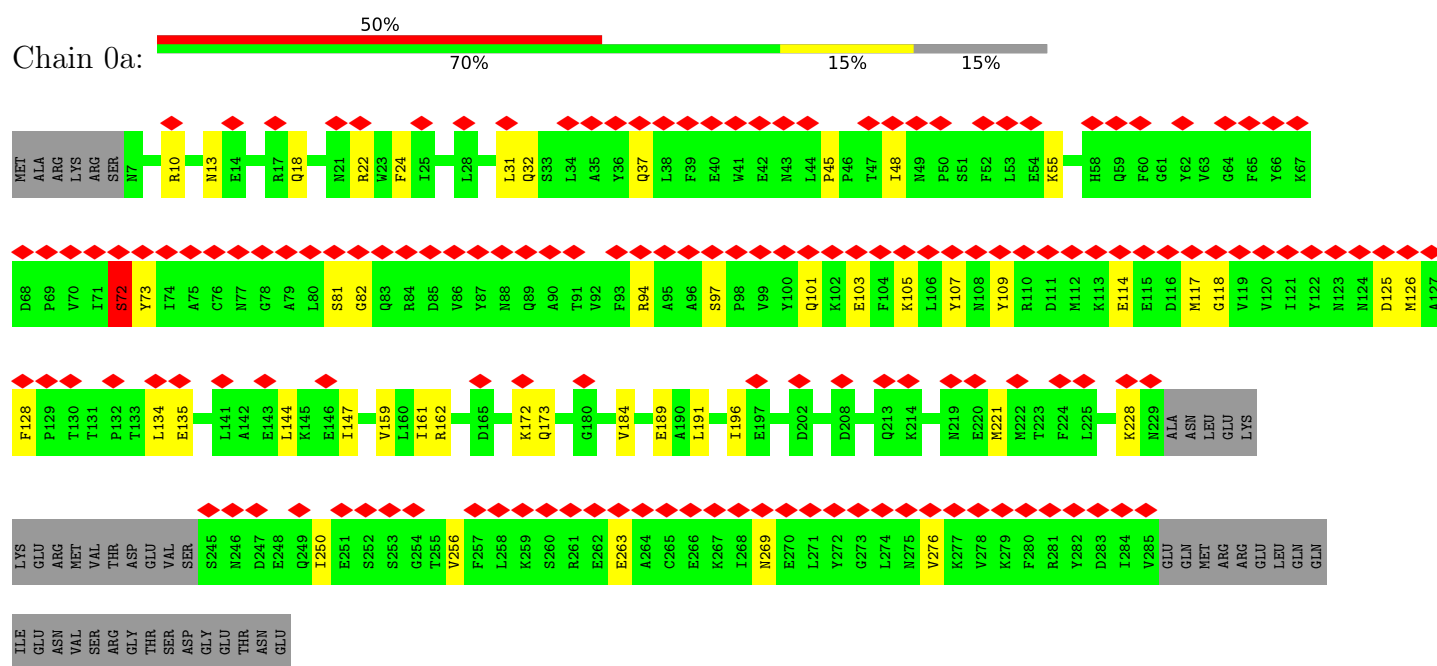
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	g	71	Total	C	N	O	S	0	0
			603	391	94	114	4		
3	h	51	Total	C	N	O	S	0	0
			433	281	67	83	2		
3	i	57	Total	C	N	O	S	0	0
			482	312	74	92	4		
3	j	71	Total	C	N	O	S	0	0
			603	391	94	114	4		

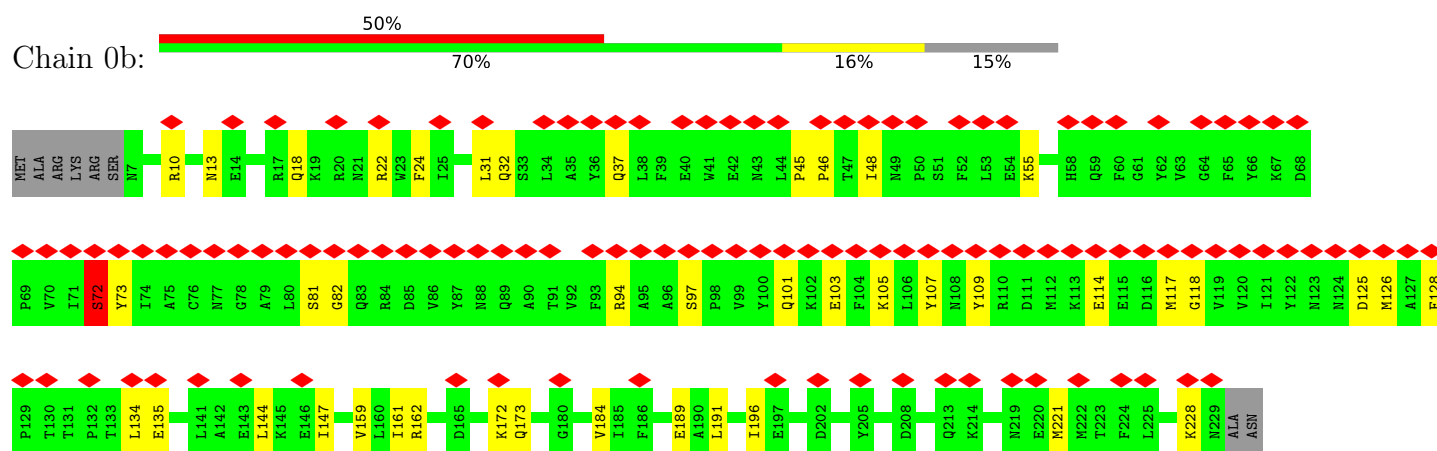
3 Residue-property plots [i](#)

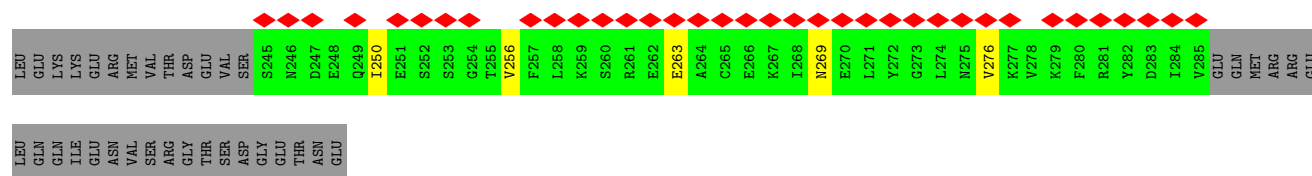
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

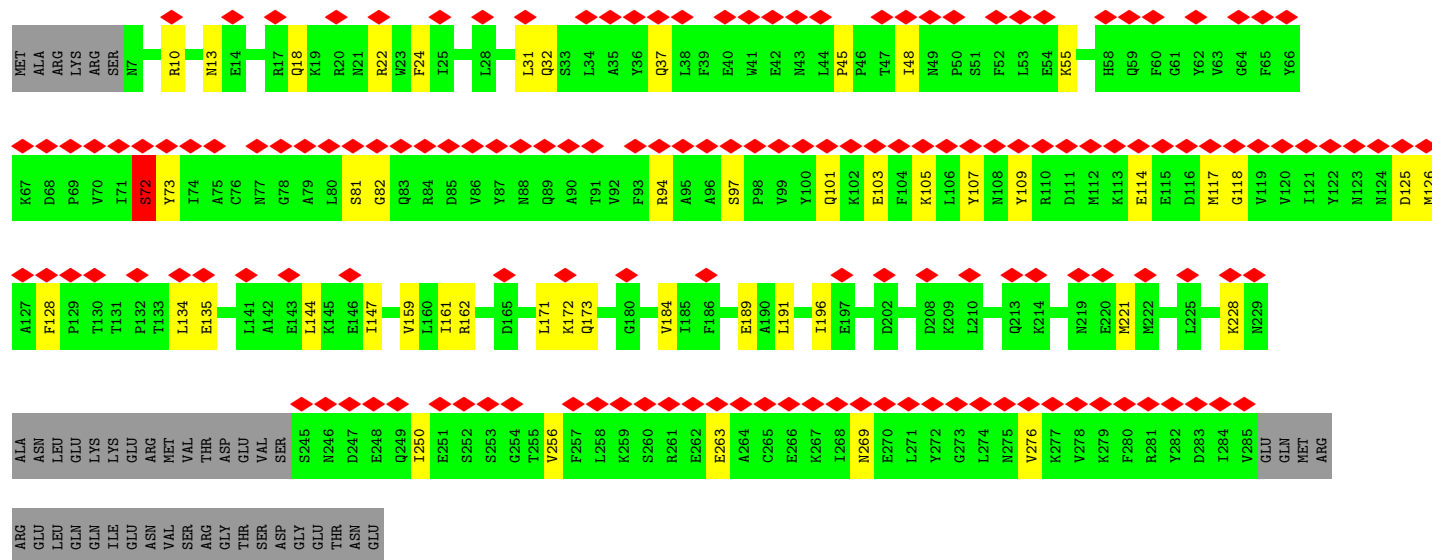


• Molecule 1: Portal protein

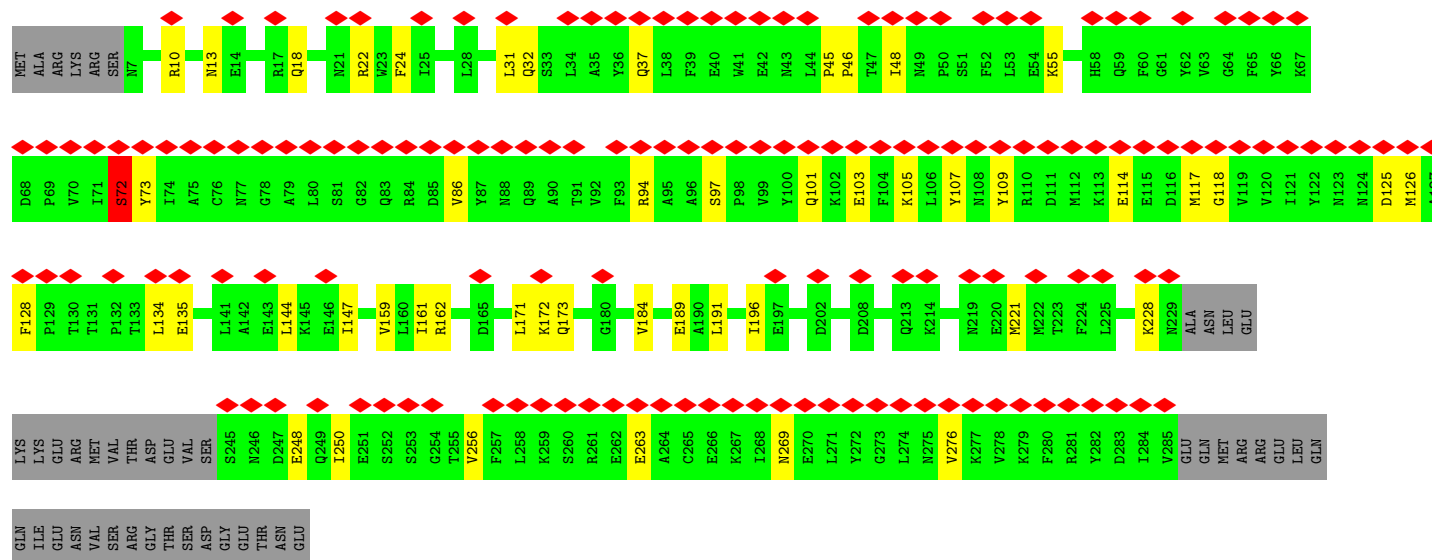




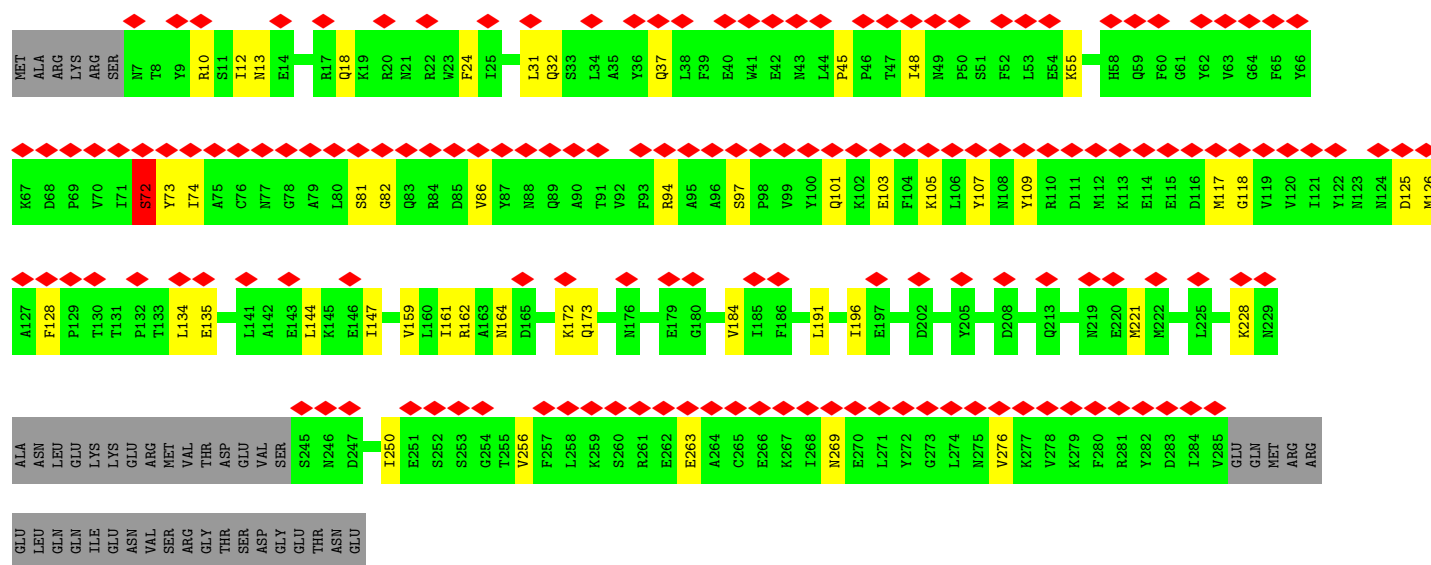
• Molecule 1: Portal protein



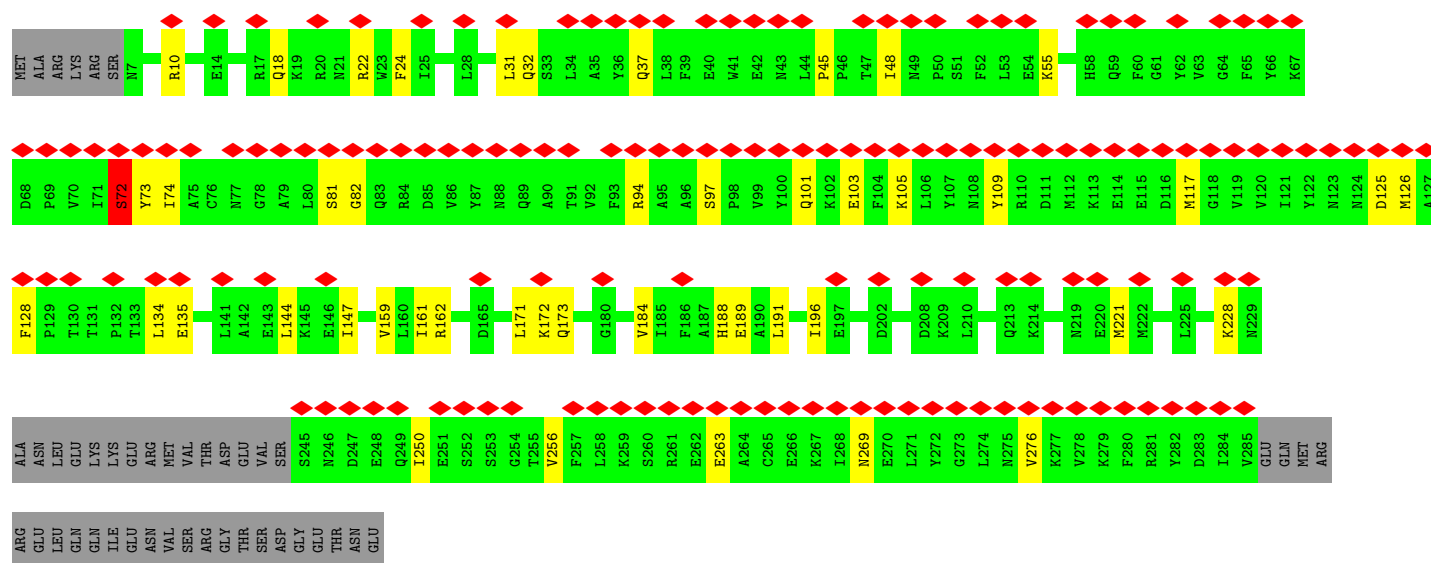
• Molecule 1: Portal protein



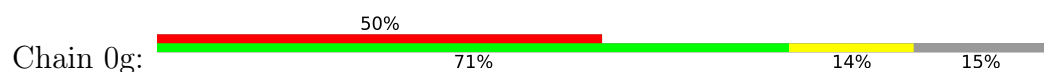
• Molecule 1: Portal protein

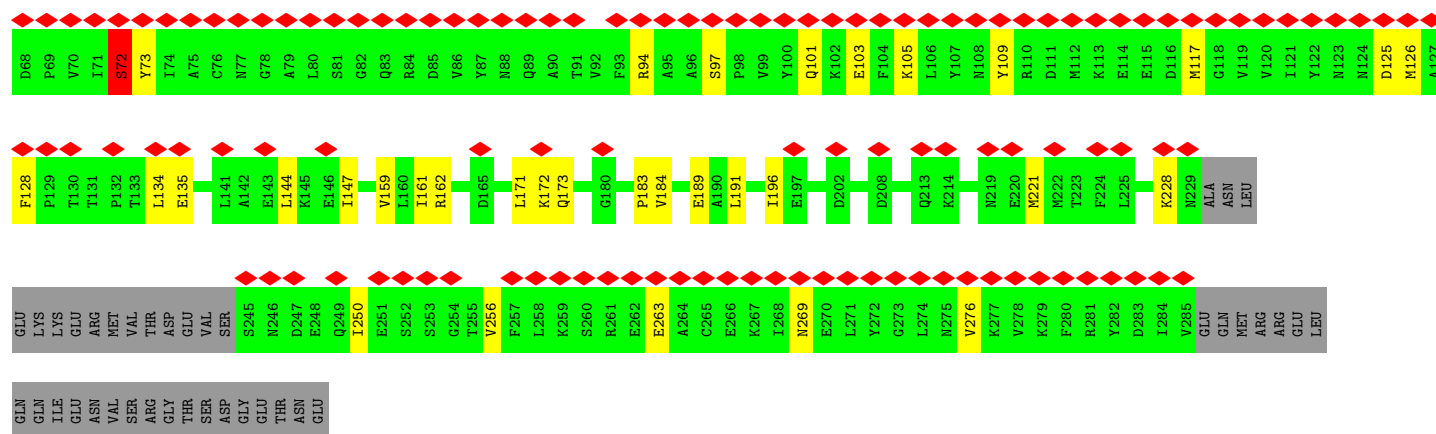


• Molecule 1: Portal protein

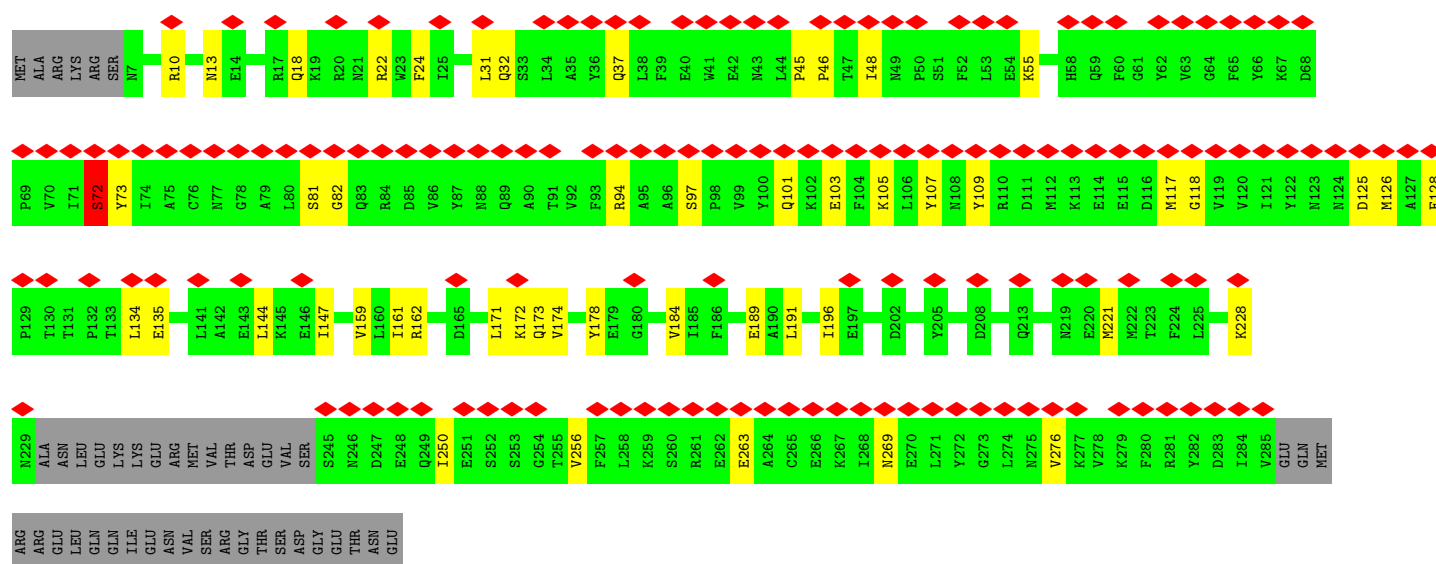


• Molecule 1: Portal protein

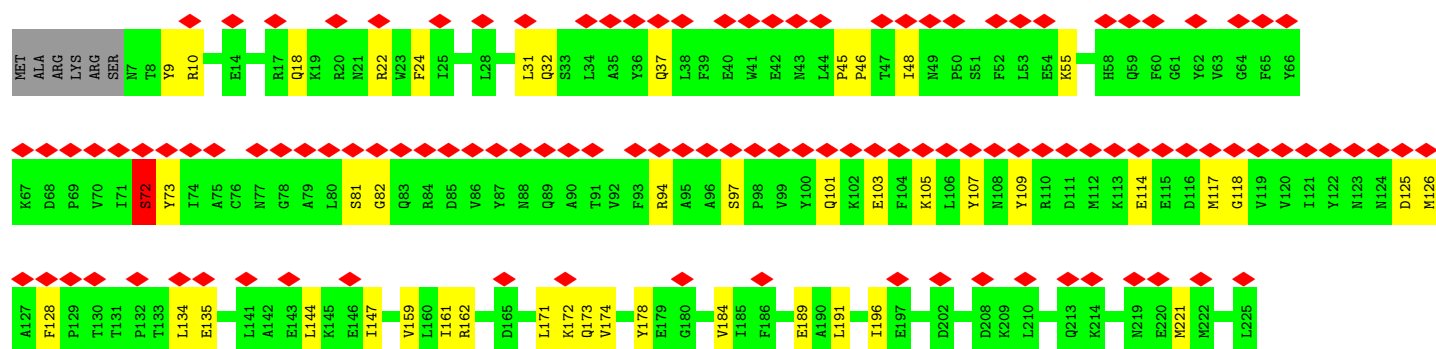


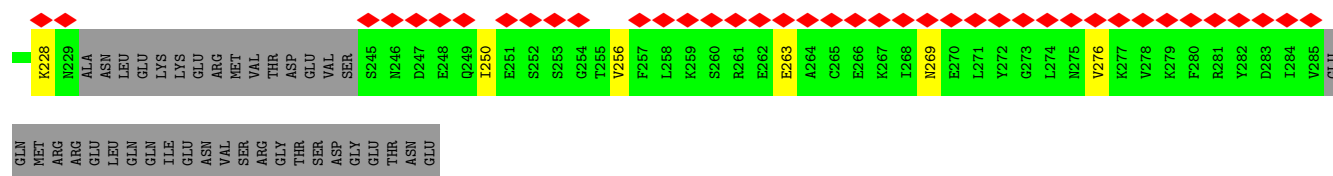


• Molecule 1: Portal protein

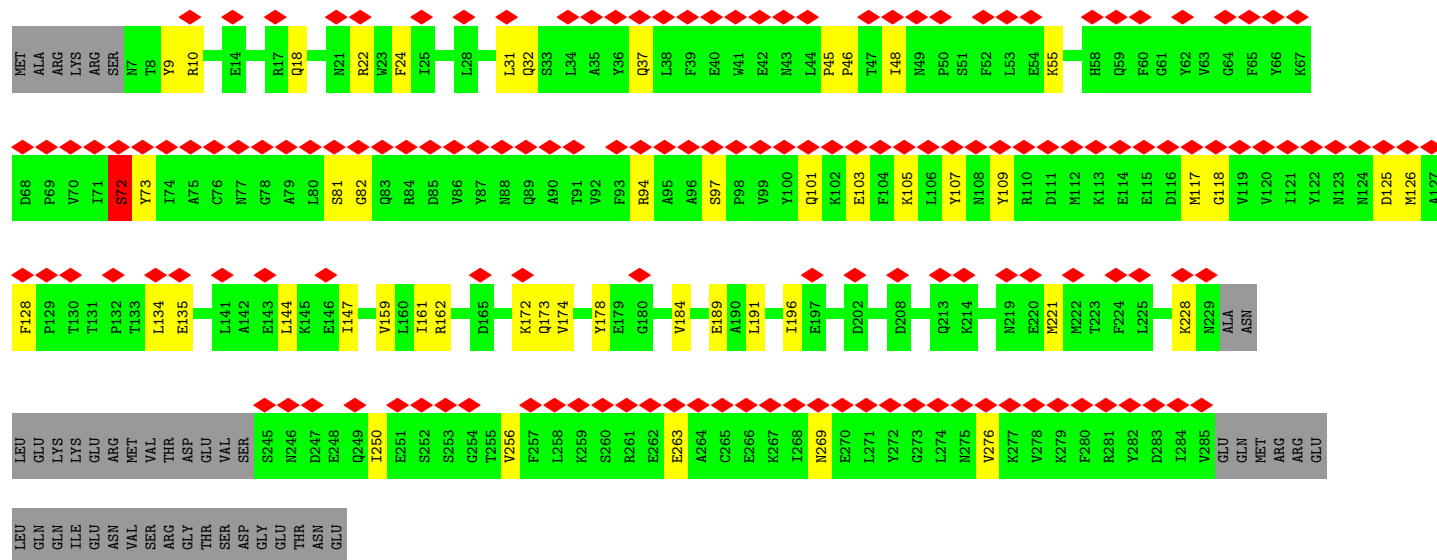


• Molecule 1: Portal protein

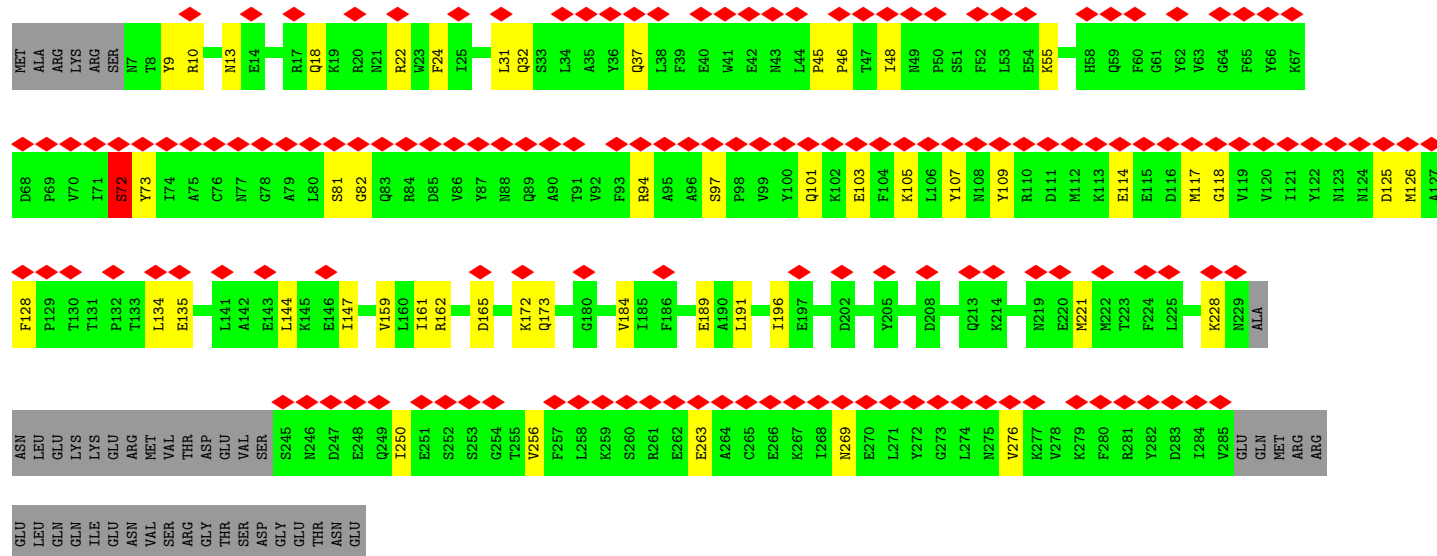




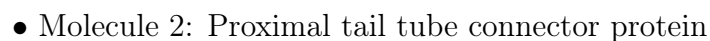
• Molecule 1: Portal protein

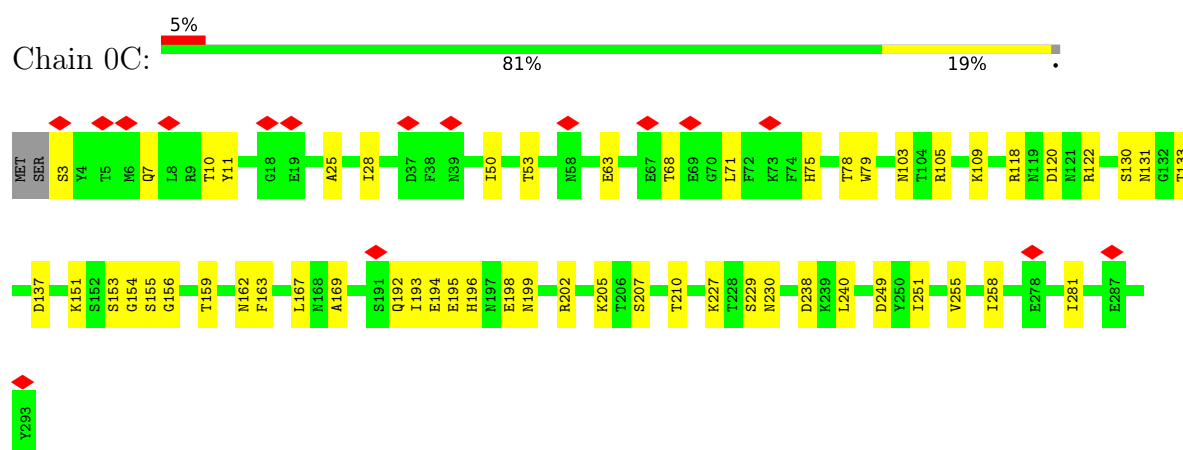


• Molecule 1: Portal protein

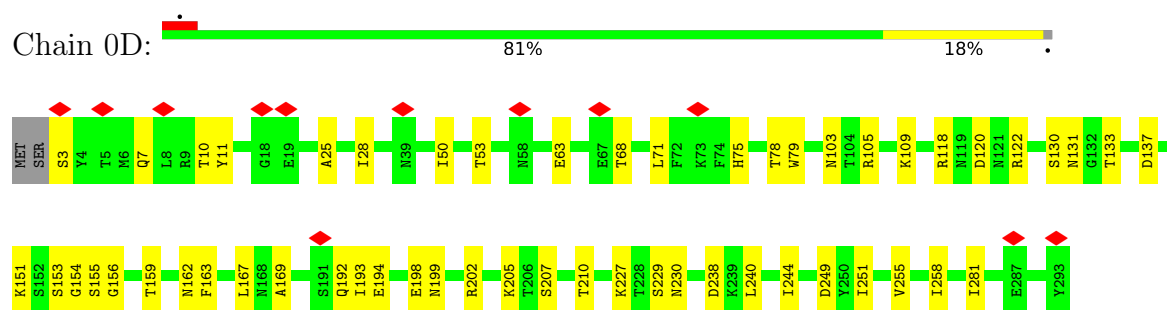


• Molecule 1: Portal protein

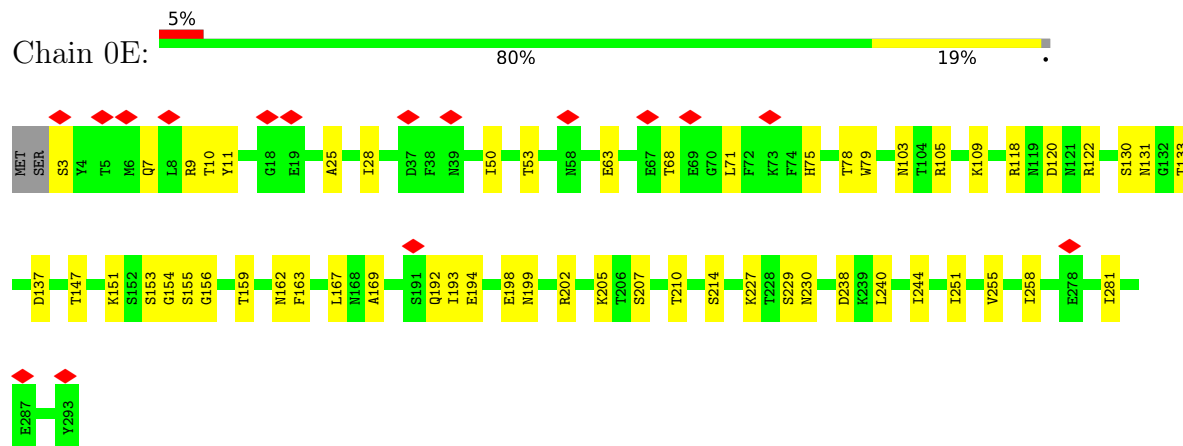




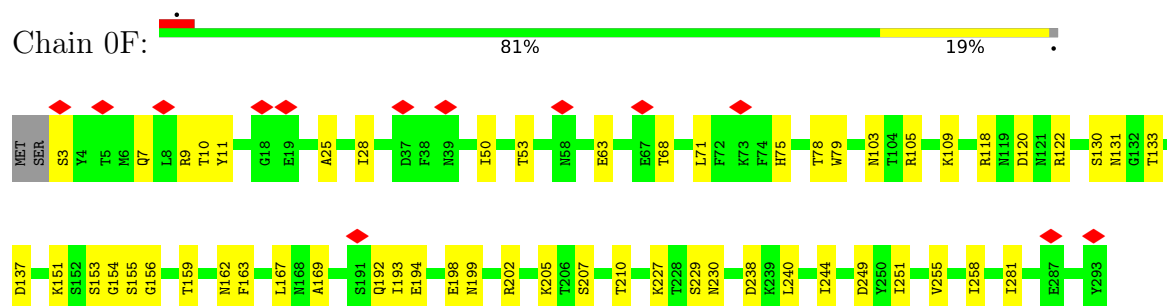
- Molecule 2: Proximal tail tube connector protein



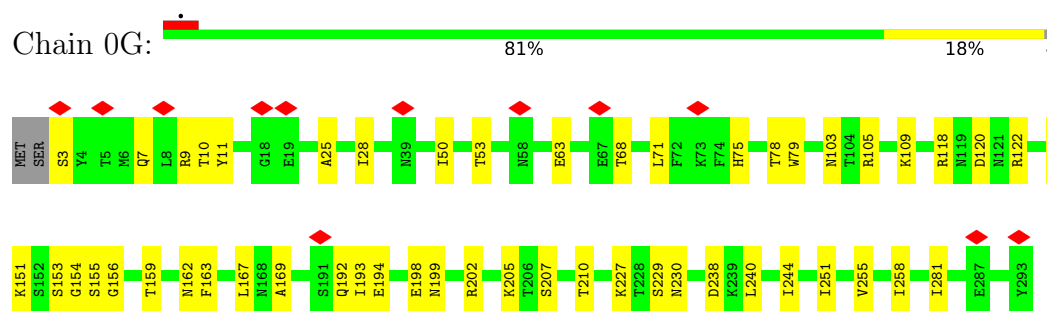
- Molecule 2: Proximal tail tube connector protein



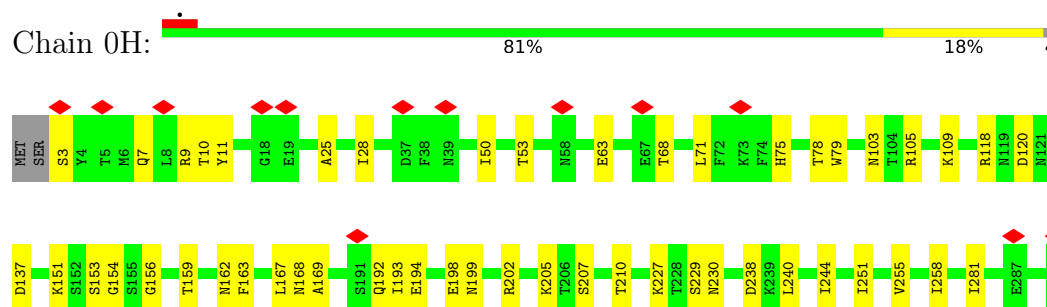
- Molecule 2: Proximal tail tube connector protein



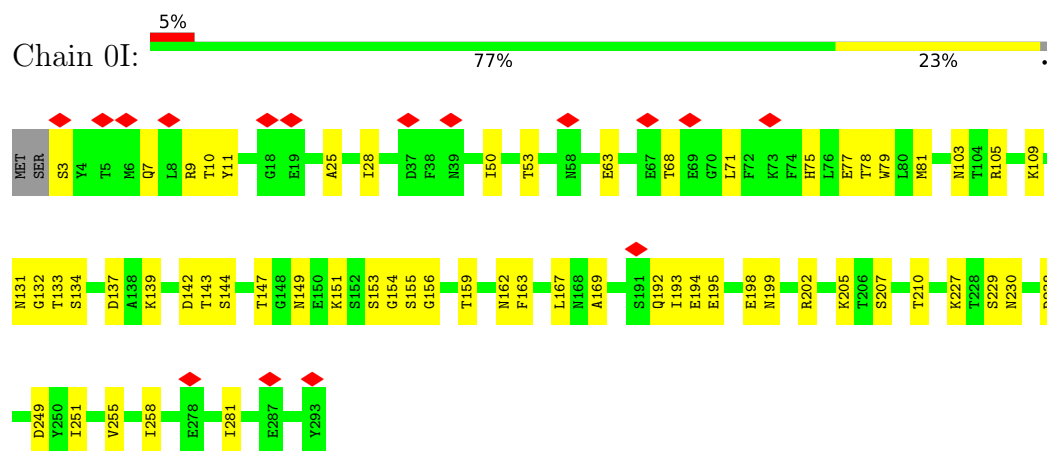
- Molecule 2: Proximal tail tube connector protein



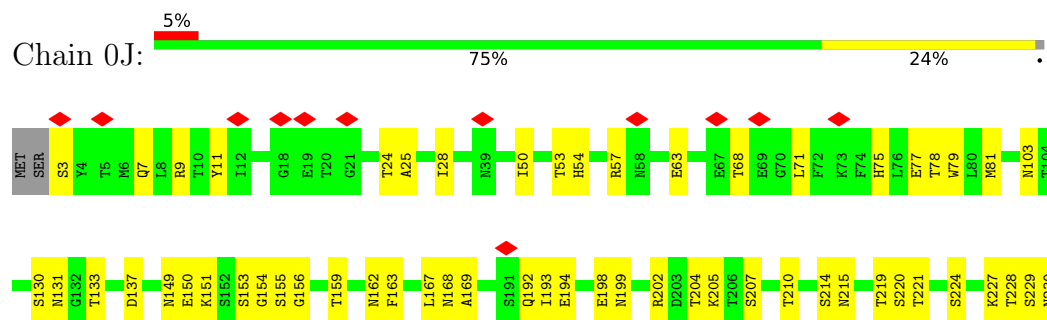
- Molecule 2: Proximal tail tube connector protein

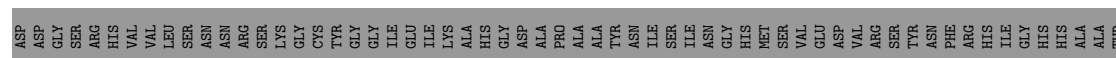


- Molecule 2: Proximal tail tube connector protein



- Molecule 2: Proximal tail tube connector protein









- Molecule 3: Pre-neck appendage protein

[illegible]

- Molecule 3: Pre-neck appendage protein

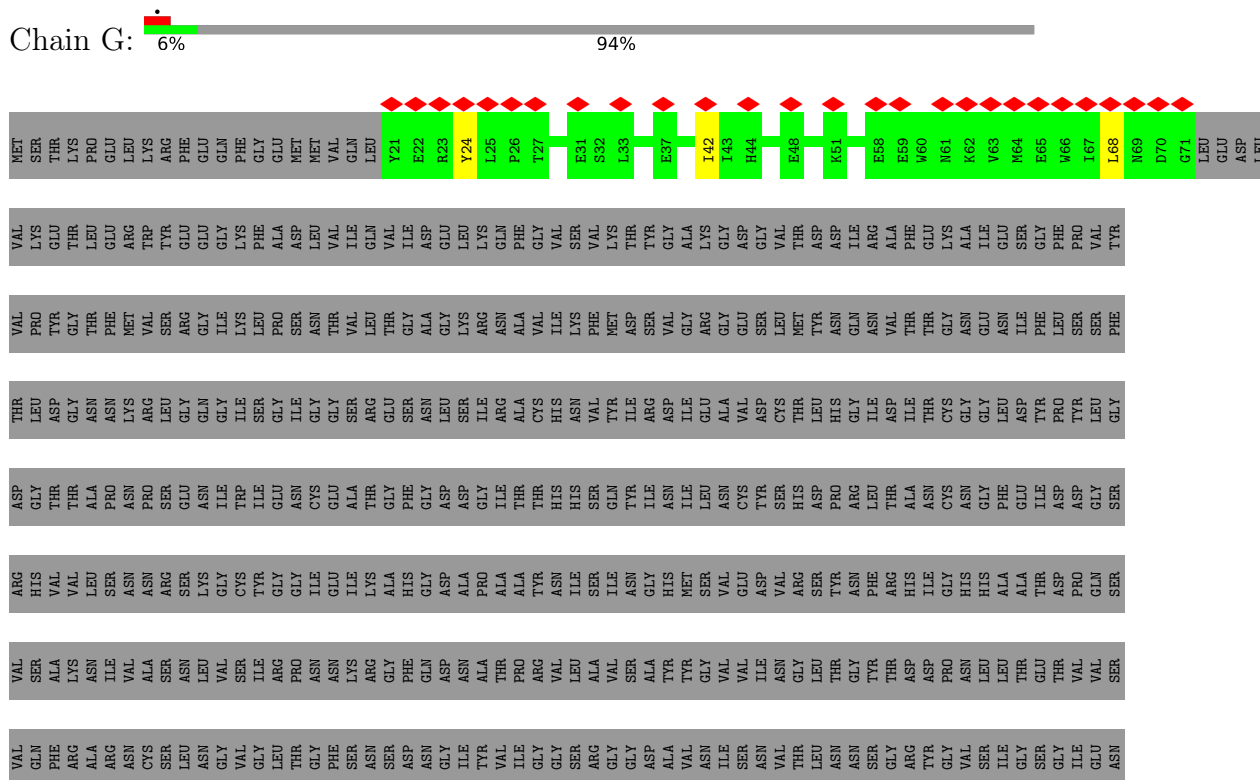




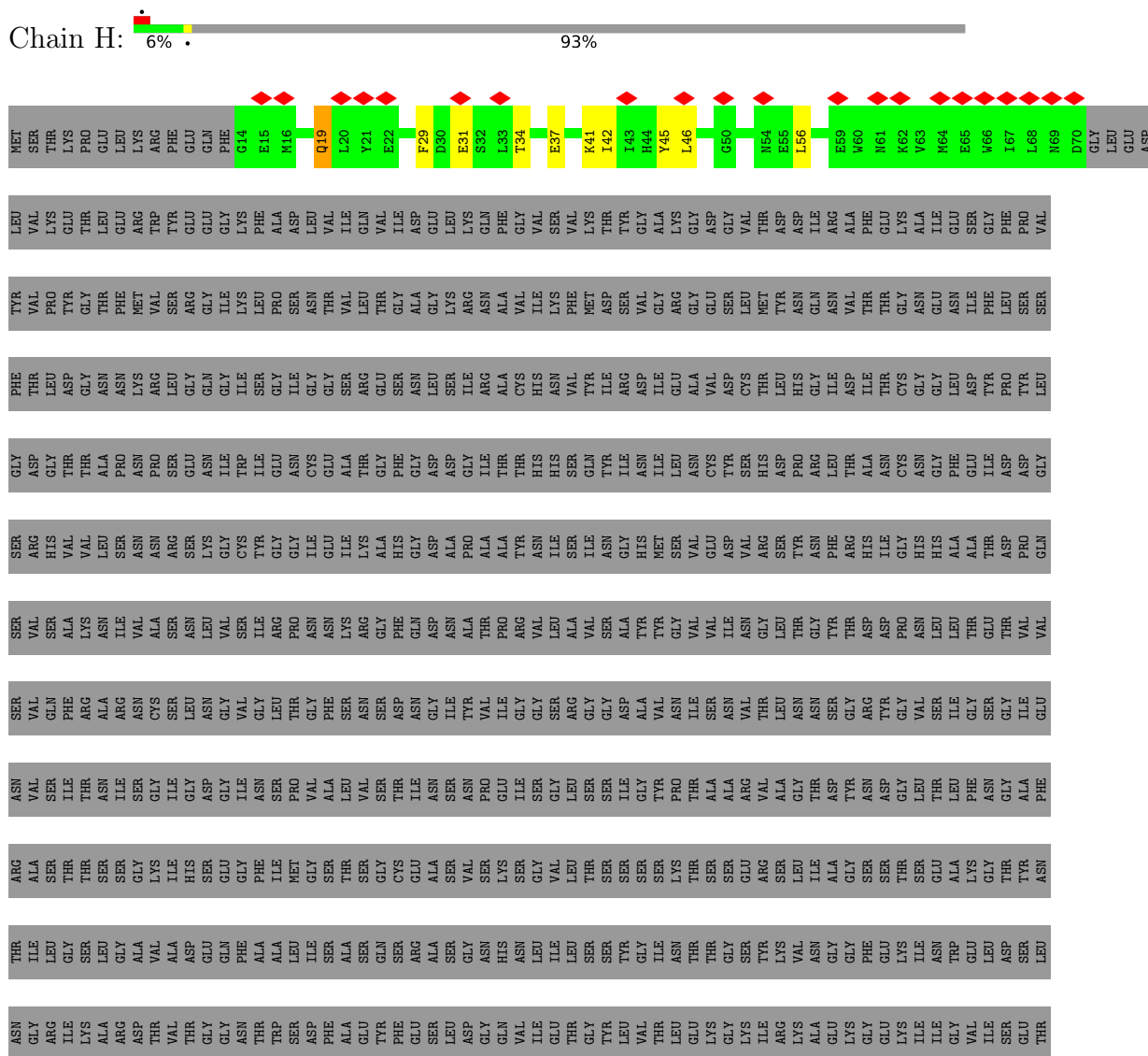
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THR										LEU										GLU										T3									
ASP										GLY										K4										T5									
ASN										PHE										THR										P5									
ASN										MET										GLU										E6									
ARG										VAL										TRP										L7									
LEU										SER										GLY										K8									
GLY										ARG										GLU										R9									
GLN										ILE										GLY										F10									
ILE										LYS										LYS										E11									
SER										LEU										PHE										Q12									
GLY										PRO										ALA										F13									
ILE										SER										ASP										G14									
GLY										ASN										LEU										E15									
GLY										THR										VAL										M16									
SER										VAL										ILE										M17									
ARG										LEU										GLN										L20									
GLU										THR										GLY										Y21									
SER										ASN										ALA										E22									
ASN										VAL										GLY										R23									
LEU										LYS										LEU										Y24									
SER										ILE										LYS										L25									
ILE										ARG										ASN										F29									
ARG										ALA										PHE										D30									
ALA										ILE										VAL										E31									
HIS										LYS										SER										S32									
ASN										PHE										VAL										L33									
VAL										MET										LYS										T34									
THR										ILE										THR										L35									
ARG										SER										ARG										L36									
ASP										VAL										GLY										L37									
ILE										GLY										ALA										L38									
GLU										ARG										LYS										L39									
ALA										GLY										GLY										L40									
VAL										GLU										ASP										L41									
ASP										SER										GLY										L42									
CYS										LEU										VAL										G50									
THR										MET										THR										K51									
LEU										TYR										ASP										V52									
HIS										ASN										ASP										T53									
GLY										GLN										ILE										M54									
ILE										ASN										ARG										E55									
ASP										VAL										ALA										L56									
THR										THR										PHE										I57									
THR										THR										GLU										L58									
CYS										GLY										LYS										E59									
GLY										ASN										ALA										W60									
GLY										GLU										GLU										M61									
THR										ASN										SER										L62									
ASP										PHE										GLY										M64									
PRO										LEU										PHE										E65									
TYR										SER										VAL										W66									
LEU										SER										VAL										I67									
THR										SER										VAL										L68									
SER										SER										VAL										W69									
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SER										SER										VAL										G71									
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SER										SER										VAL										A74									

[illegible]

- Molecule 3: Pre-neck appendage protein



- Molecule 3: Pre-neck appendage protein



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

- Molecule 3: Pre-neck appendage protein

[illegible]

- Molecule 3: Pre-neck appendage protein

Chain J:  6% 94%

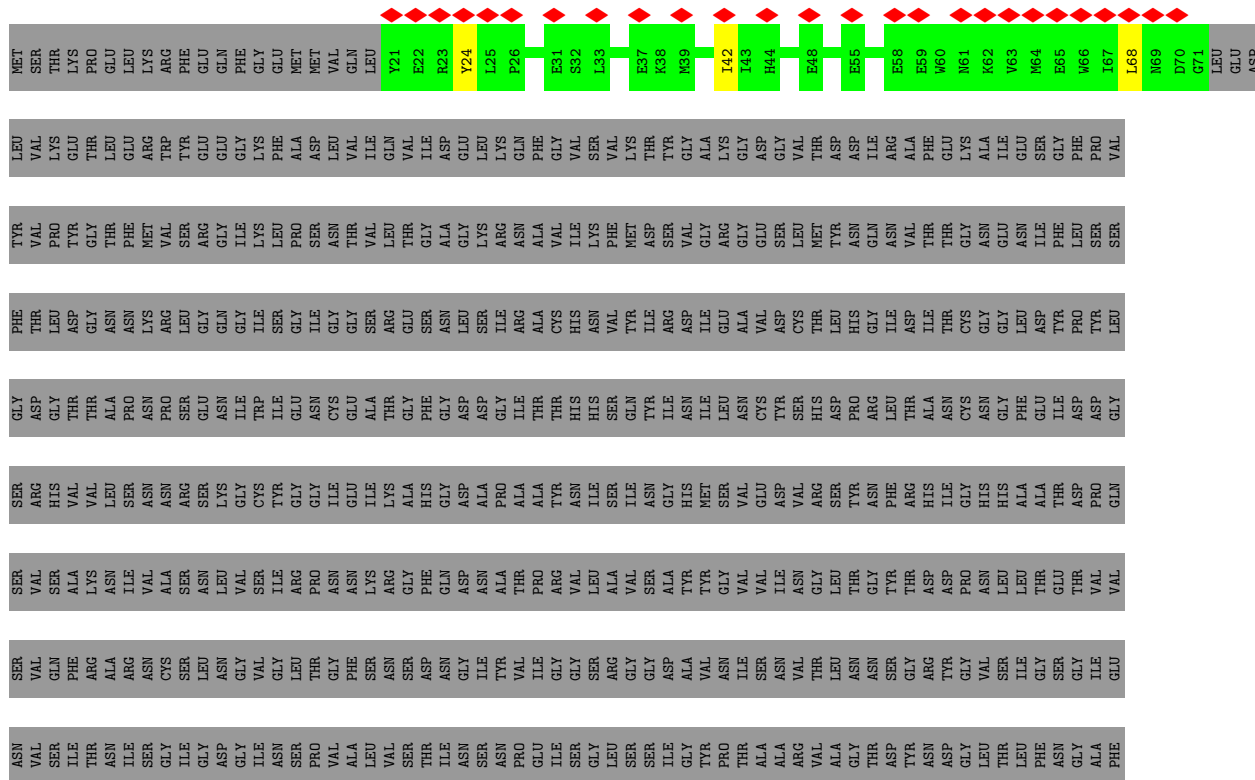
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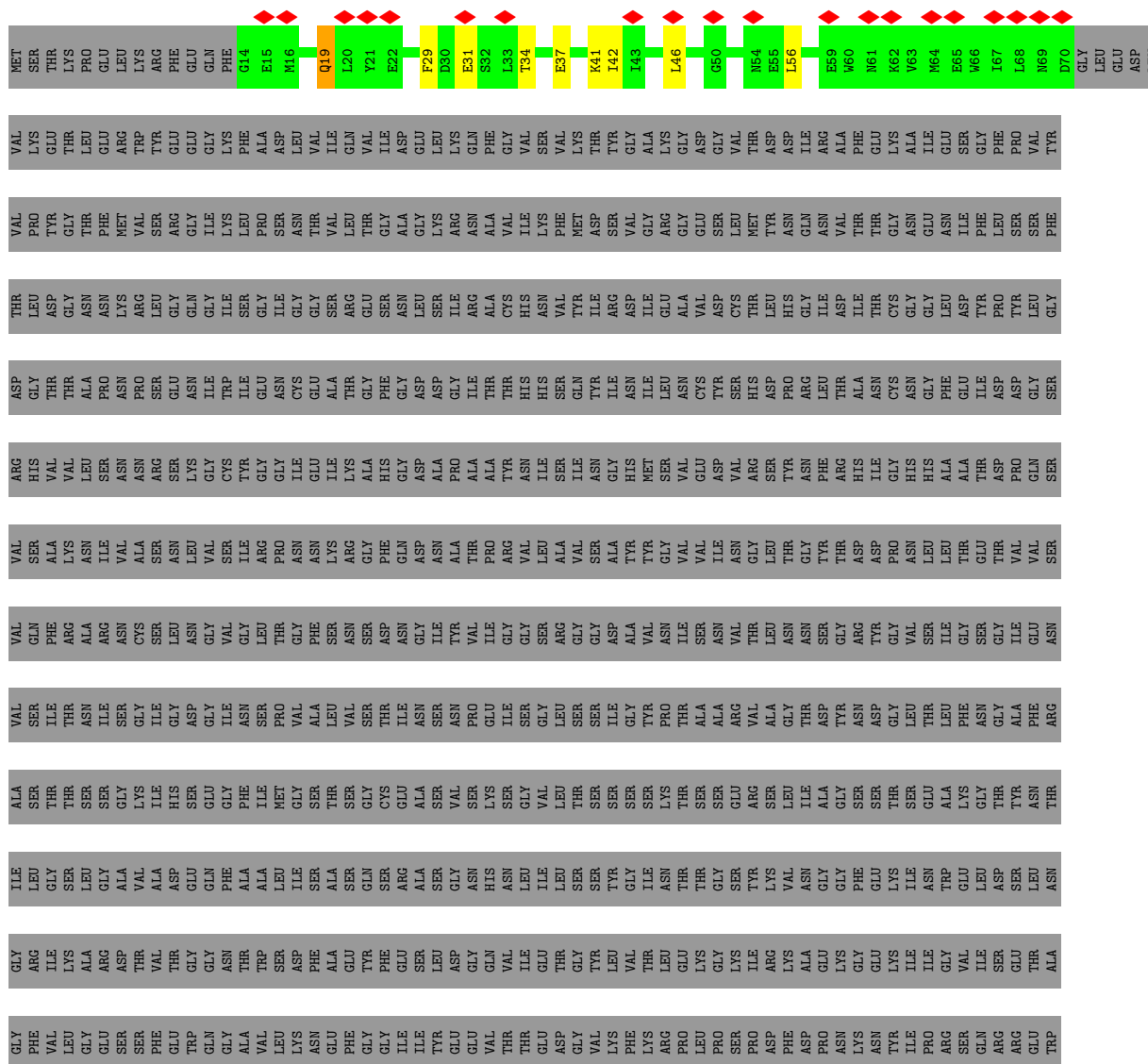
● Molecule 3: Pre-neck appendage protein

Chain K:  6% 93%

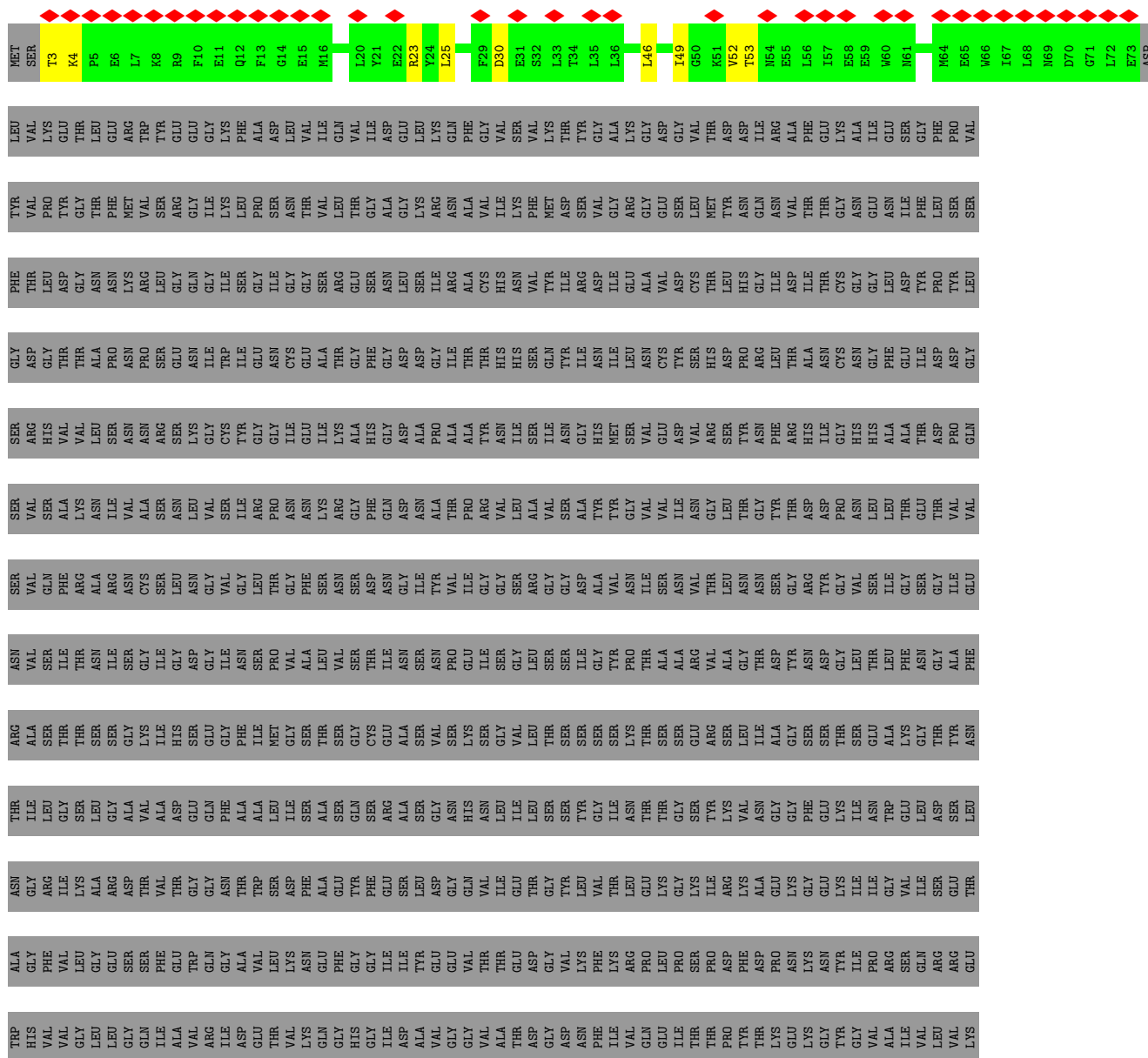
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VAL	LYS	GLU	THR	LEU	GLU	ARG	TRP	TYR	GLU	GLY	ILE	PHE	ALA	ASP	LEU	VAL	ILE	VAL	ILE	GLY	LEU	LYS	PHE	GLY	VAL	SER	VAL	LYS	THR	TYR	GLY	ALA	LYS	GLY	ASP	GLY	VAL	THR	ASP	ASP	ILE	ARG	ALA	PHE	GLU	LYS	ALA	ILE	GLU	SER	GLY	PHE	PRO	VAL	VAL	TYR



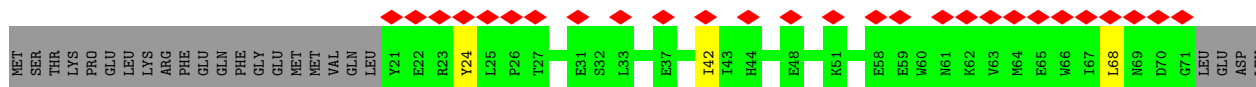




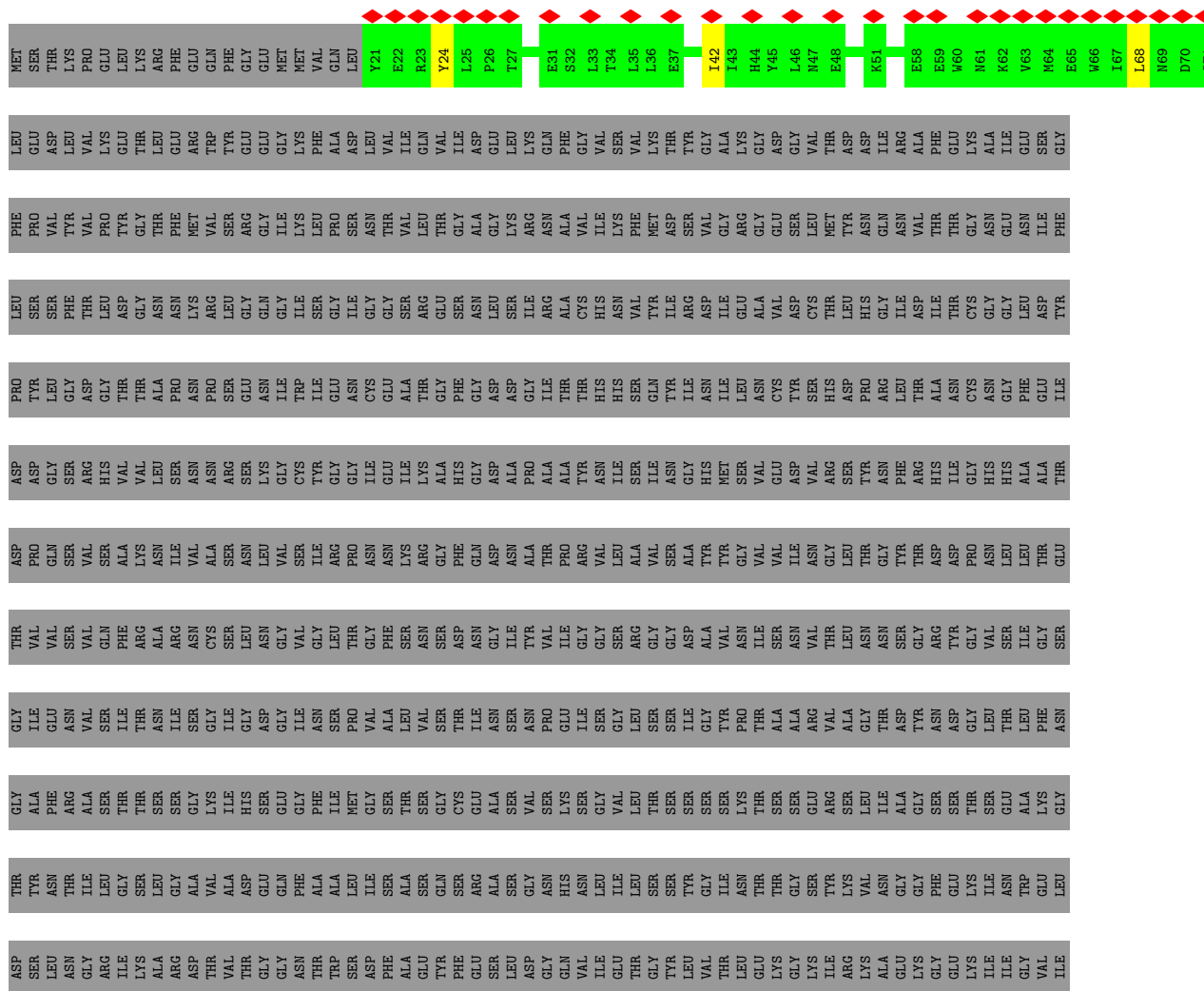
Chain 0: 7% 92%



Chain P: 6% 94%







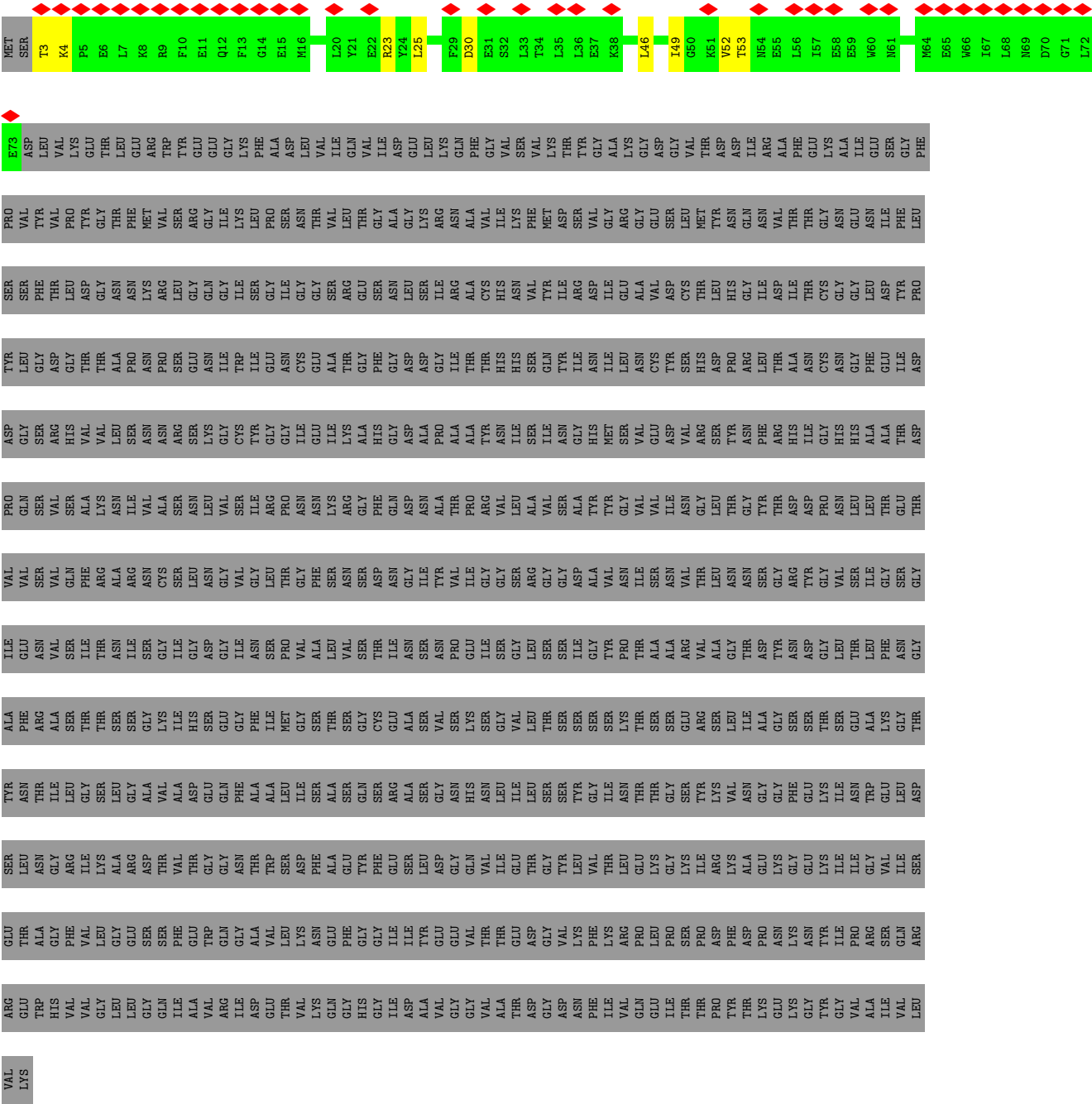
LEU
VAL
LYS

- Molecule 3: Pre-neck appendage protein

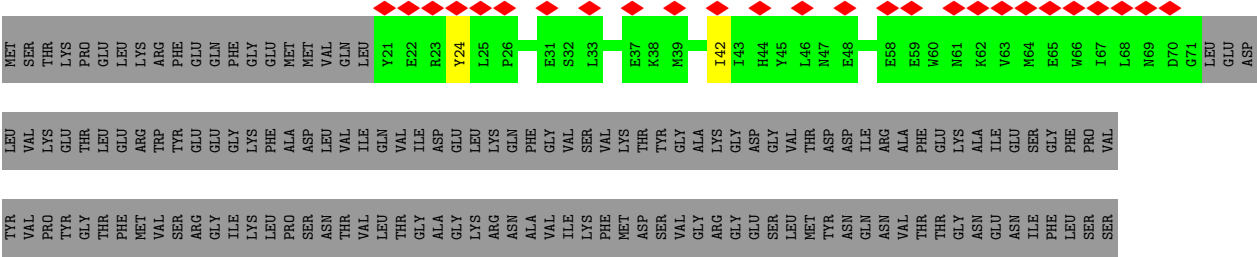
[illegible]

- Molecule 3: Pre-neck appendage protein



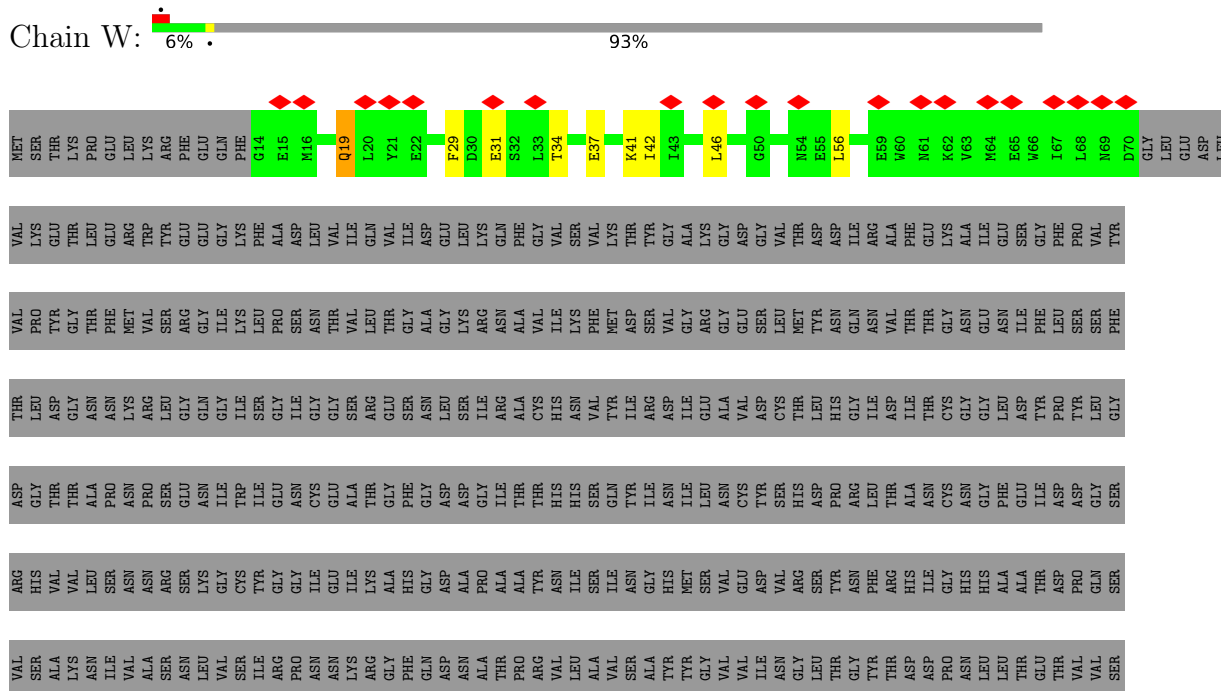


● Molecule 3: Pre-neck appendage protein



[illegible]

- Molecule 3: Pre-neck appendage protein





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

- Molecule 3: Pre-neck appendage protein

[illegible]

- Molecule 3: Pre-neck appendage protein



TRP	HIS	VAL	VAL	GLY	LEU	LEU	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</
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● Molecule 3: Pre-neck appendage protein

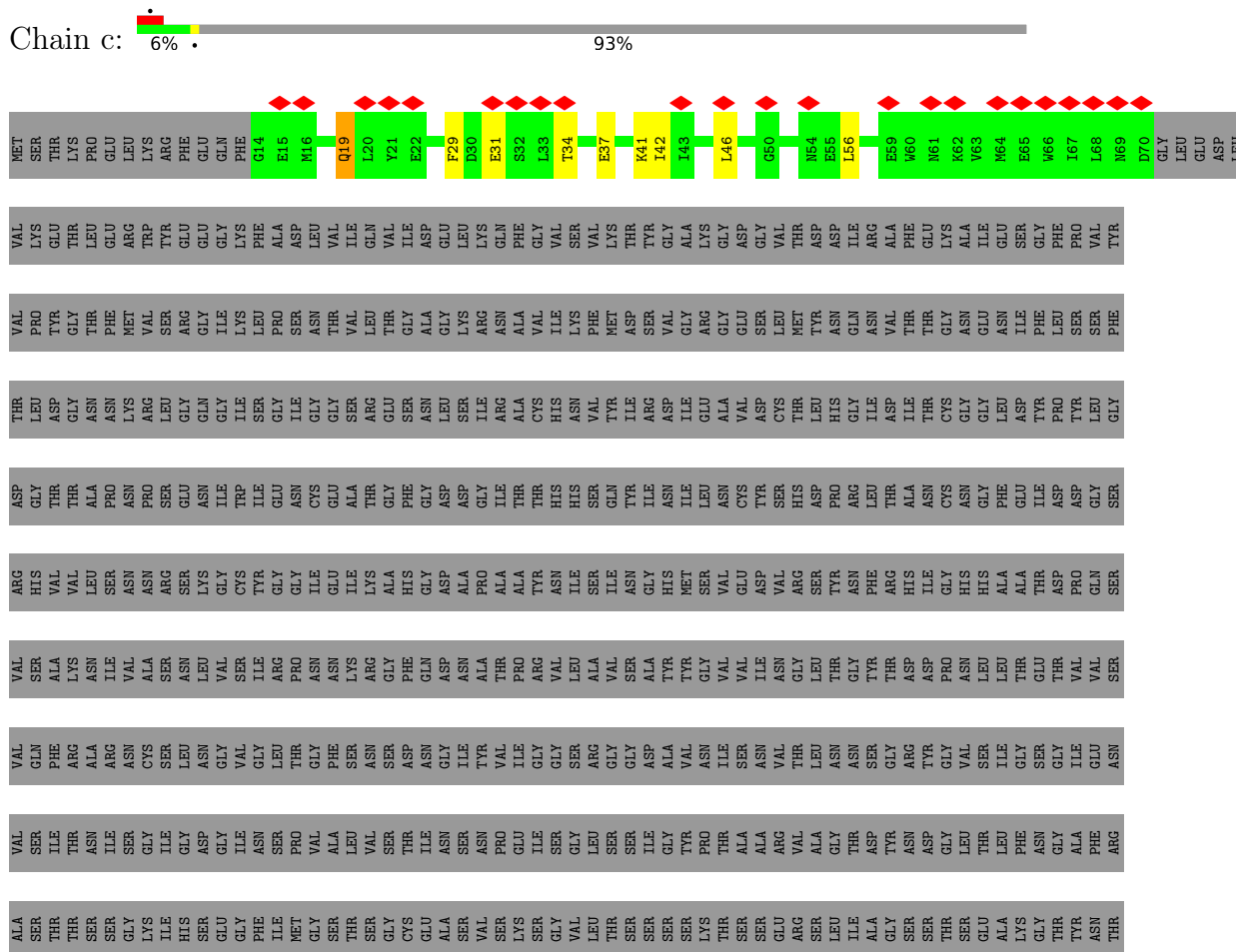
Chain a:  7% .  92%

MET	SER	T3	K4	P5	E6	L7	K8	R9	F10	E11	Q12	F13	G14	E15	M16	L20	Y21	E22	R23	Y24	L25	F29	D30	E31	S32	L33	T34	L35	L36	E37	K38	L46	I49	G50	N51	V52	T53	L56	I57	E58	E59	M60	N61	M64	E65	M66	I67	L68	N69	D70	G71	L72	E73
ASP	LEU	VAL	LYS	THR	LEU	GLU	ARG	TRP	TYR	GLU	GLY	LYS	PHE	ALA	ASP	LEU	VAL	ILE	GLN	VAL	GLY	LYS	GLN	PHE	GLY	VAL	THR	THR	TYR	GLY	ALA	LYS	GLY	ASP	GLY	VAL	THR	THR	PHE	GLU	GLY	LYS	ALA	ILE	GLU	ASN	GLU	ASN	GLY	PHE	LEU	PRO	
VAL	TYR	PRO	TYR	GLY	THR	THR	PHE	MET	VAL	SER	ARG	LYS	LEU	PRO	SER	THR	VAL	LEU	THR	GLY	ALA	ASN	ALA	VAL	VAL	LYS	THR	THR	THR	GLY	ARG	GLY	GLU	SER	GLY	LEU	THR	THR	THR	GLY	ASN	GLY	ASN	GLU	ASN	ILE	PHE	LEU	SER				
SER	PHE	THR	LEU	ASP	GLY	ASN	ASN	ARG	LEU	GLY	GLN	THR	GLY	ILE	THR	ARG	ASN	ALA	CYS	HIS	ASN	VAL	VAL	ILE	ARG	ASP	ASP	ILE	GLU	GLY	ALA	VAL	ASP	THR	CYS	THR	THR	ILE	THR	GLY	CYS	GLY	GLY	LEU	ASP	TYR	PRO	TYR					



[illegible]

- Molecule 3: Pre-neck appendage protein



[illegible]

LYS

● Molecule 3: Pre-neck appendage protein

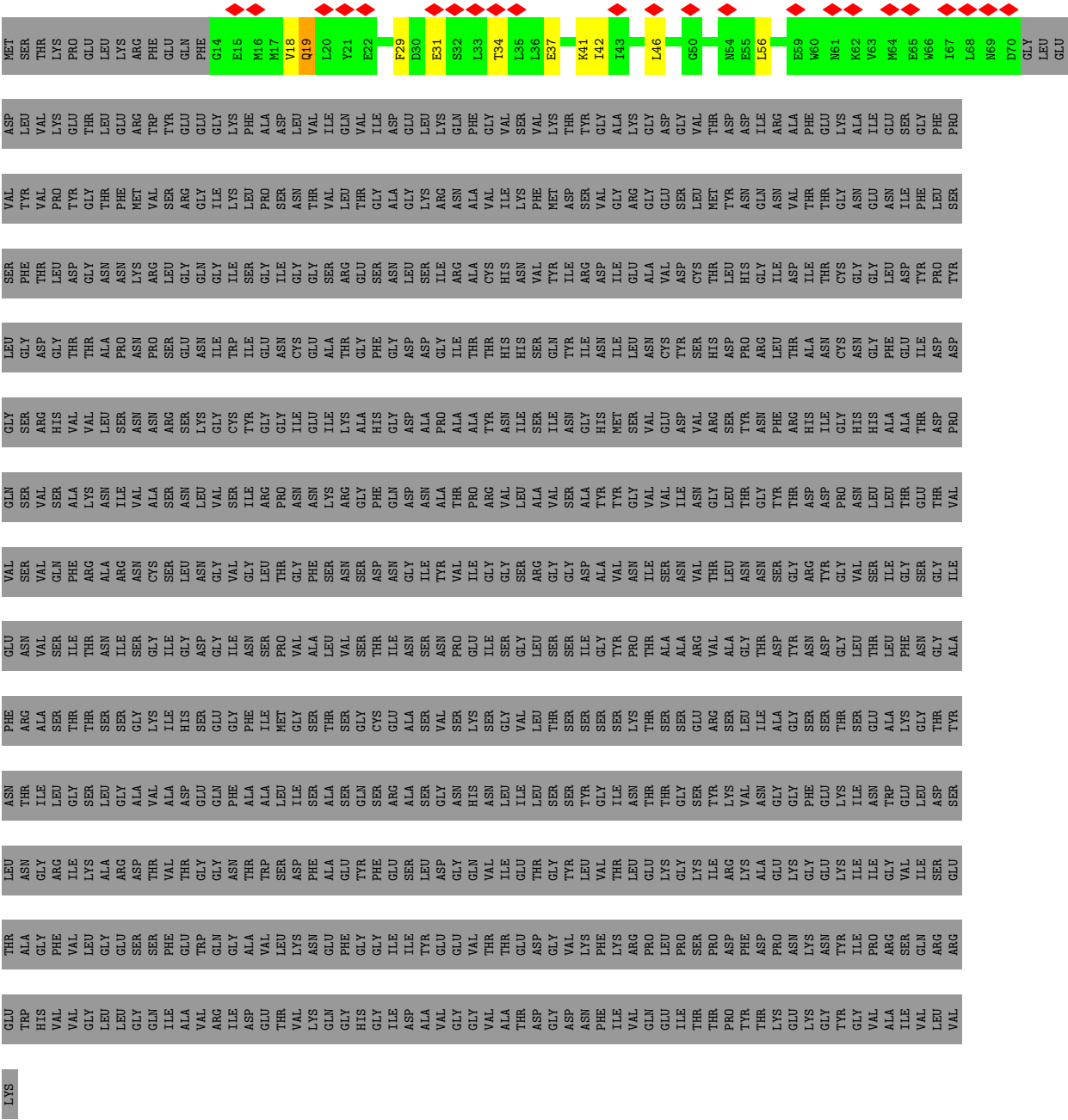


MET	THR	LYS	PRO	GLU	LEU	LYS	GLN	PHE	GLY	LEU	Y21	E22	R23	Y24	L25	P26	E31	S32	L33	E37	K38	M39	I42	I43	H44	Y45	L46	M47	E48	E55	E58	E59	W60	N61	K62	V63	M64	E65	W66	I67	L68	D70	G71	LEU			
GLU	ASP	LEU	VAL	THR	LYS	GLY	THR	GLY	LEU	THR	VAL	THR	GLN	ILE	ASP	GLY	LEU	GLN	PHE	GLY	VAL	THR	TYR	GLY	ALA	LYS	GLY	ASP	GLY	VAL	THR	ASP	ILE	ARG	ALA	PHE	THR	GLU	LYS	ALA	ILE	GLY	SER	GLY	PHE	LEU	
PRO	VAL	TYR	VAL	THR	LYS	GLY	THR	GLY	THR	THR	THR	THR	GLY	ILE	ALA	GLY	ASN	ALA	VAL	ILE	LYS	ASP	SER	VAL	GLY	ARG	GLY	GLY	SER	LEU	MET	TYR	ASN	GLN	ASN	VAL	THR	THR	GLY	LYS	ALA	ASN	GLY	ILE	ASN	PHE	LEU
SER	SER	PHE	THR	LEU	ASP	THR	ALA	ASN	ASN	GLY	GLY	ILE	ILE	SER	GLY	GLN	GLY	ILE	GLY	THR	VAL	THR	ILE	ARG	ASP	HIS	CYS	VAL	THR	MET	TYR	ASP	HIS	GLY	ILE	ASN	VAL	THR	THR	CYS	GLY	THR	ASP	ILE	TYR	PRO	
TYR	LEU	GLY	ASP	THR	THR	THR	ALA	ASN	PRO	PRO	GLY	TRP	ILE	SER	GLY	ASN	CYS	GLY	THR	THR	HIS	THR	ILE	ASP	ASN	ILE	LEU	ALA	ASN	VAL	THR	PRO	ARG	LEU	THR	THR	ARG	ILE	ASN	ALA	THR	GLY	ASP	ILE	ASP		
ASP	GLY	SER	ARG	HIS	VAL	VAL	LEU	ASN	ASN	ARG	SER	GLY	TYR	GLY	LYS	GLY	ILE	GLY	ASP	ALA	PRO	ILE	ALA	TYR	THR	ILE	LEU	VAL	VAL	GLY	ASP	VAL	ARG	THR	ASN	PHE	ARG	HIS	ILE	ASP	THR	ASP	GLY	THR	THR		
PRO	GLN	SER	VAL	ALA	VAL	GLN	ALA	ASN	VAL	ALA	ASN	VAL	ILE	GLY	LEU	ASN	PRO	ASN	GLY	ASP	ALA	THR	ALA	TYR	ARG	VAL	VAL	VAL	VAL	ILE	ASN	VAL	GLY	THR	TYR	THR	THR	ASP	ASP	THR	PRO	GLY	THR	LEU	THR		
VAL	VAL	SER	VAL	VAL	GLN	PHE	ARG	ALA	ASN	ASN	ASN	VAL	THR	THR	ASN	ASN	THR	ASN	GLY	ILE	THR	ILE	GLY	ASP	GLY	VAL	ILE	ILE	ASN	VAL	THR	ASN	GLY	THR	GLY	THR	THR	ARG	THR	THR	THR	THR	THR	GLY	THR		
ILE	GLU	VAL	ASN	ILE	THR	THR	ASN	ASN	GLY	ASP	GLY	ILE	ASN	ASN	ASP	ASP	PRO	VAL	PHE	ASN	ASN	ILE	THR	ILE	ASN	GLY	THR	VAL	THR	THR	ASN	THR	ASN	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY		
ALA	PHE	ARG	ALA	SER	THR	THR	SER	LYS	GLY	SER	GLY	PHE	ILE	GLY	GLY	GLY	ILE	GLY	GLY	THR	GLY	GLY	THR	ILE	ALA	VAL	THR	ASN	VAL	THR	ASN	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
TYR	ASN	ILE	THR	LEU	SER	GLY	THR	ALA	ASP	GLY	ILE	ALA	ALA	ALA	PHE	GLY	ASN	ASN	ASN	GLY	ASN	ASN	THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
SER	LEU	ASN	GLY	ILE	ARG	LYS	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
GLU	THR	ALA	GLY	PHE	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
ARG	GLU	TRP	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	

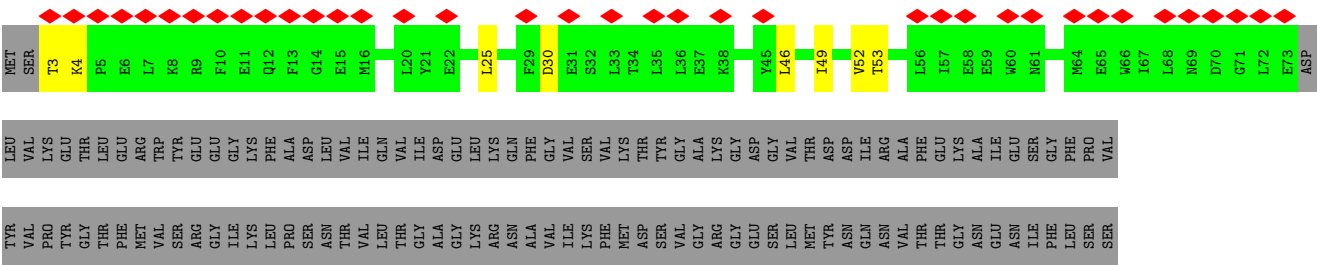
VAL
LYS

● Molecule 3: Pre-neck appendage protein





● Molecule 3: Pre-neck appendage protein





- 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	36370	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	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	120.855	Depositor
Minimum map value	-0.428	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.514	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	740.8544, 740.8544, 740.8544	wwPDB
Map dimensions	572, 572, 572	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2952, 1.2952, 1.2952	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	0.23	0/2211	0.57	1/2996 (0.0%)
1	0b	0.23	0/2211	0.57	1/2996 (0.0%)
1	0c	0.23	0/2211	0.57	1/2996 (0.0%)
1	0d	0.23	0/2211	0.57	1/2996 (0.0%)
1	0e	0.23	0/2211	0.57	1/2996 (0.0%)
1	0f	0.23	0/2211	0.57	1/2996 (0.0%)
1	0g	0.23	0/2211	0.57	1/2996 (0.0%)
1	0h	0.23	0/2211	0.57	1/2996 (0.0%)
1	0i	0.23	0/2211	0.57	1/2996 (0.0%)
1	0j	0.23	0/2211	0.57	1/2996 (0.0%)
1	0k	0.23	0/2211	0.57	1/2996 (0.0%)
1	0l	0.23	0/2211	0.57	1/2996 (0.0%)
2	0A	0.31	0/2331	0.60	0/3144
2	0B	0.32	0/2331	0.60	0/3144
2	0C	0.32	0/2331	0.60	0/3144
2	0D	0.31	0/2331	0.60	0/3144
2	0E	0.32	0/2331	0.60	0/3144
2	0F	0.32	0/2331	0.60	0/3144
2	0G	0.32	0/2331	0.60	0/3144
2	0H	0.32	0/2331	0.60	0/3144
2	0I	0.32	0/2331	0.60	0/3144
2	0J	0.32	0/2331	0.61	0/3144
2	0K	0.32	0/2331	0.60	0/3144
2	0L	0.32	0/2331	0.60	0/3144
3	A	0.29	0/442	0.69	0/598
3	B	0.33	0/491	0.69	2/663 (0.3%)
3	C	0.23	0/615	0.59	0/828
3	D	0.29	0/442	0.69	0/598
3	E	0.30	0/491	0.68	2/663 (0.3%)
3	F	0.23	0/615	0.59	0/828
3	G	0.29	0/442	0.69	0/598
3	H	0.32	0/491	0.68	2/663 (0.3%)
3	I	0.23	0/615	0.59	0/828
3	J	0.29	0/442	0.69	0/598

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	K	0.32	0/491	0.68	2/663 (0.3%)
3	L	0.23	0/615	0.59	0/828
3	M	0.30	0/442	0.69	0/598
3	N	0.32	0/491	0.68	2/663 (0.3%)
3	O	0.23	0/615	0.59	0/828
3	P	0.30	0/442	0.69	0/598
3	Q	0.32	0/491	0.68	2/663 (0.3%)
3	R	0.23	0/615	0.59	0/828
3	S	0.30	0/442	0.70	0/598
3	T	0.31	0/491	0.68	2/663 (0.3%)
3	U	0.23	0/615	0.59	0/828
3	V	0.29	0/442	0.70	0/598
3	W	0.31	0/491	0.68	2/663 (0.3%)
3	X	0.23	0/615	0.59	0/828
3	Y	0.30	0/442	0.69	0/598
3	Z	0.31	0/491	0.69	2/663 (0.3%)
3	a	0.23	0/615	0.59	0/828
3	b	0.29	0/442	0.69	0/598
3	c	0.32	0/491	0.69	2/663 (0.3%)
3	d	0.23	0/615	0.59	0/828
3	e	0.30	0/442	0.71	0/598
3	f	0.29	0/491	0.68	2/663 (0.3%)
3	g	0.23	0/615	0.59	0/828
3	h	0.29	0/442	0.70	0/598
3	i	0.30	0/491	0.68	2/663 (0.3%)
3	j	0.23	0/615	0.59	0/828
All	All	0.28	0/73080	0.60	36/98748 (0.0%)

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
1	0a	0	1
1	0b	0	1
1	0c	0	1
1	0d	0	1
1	0e	0	1
1	0f	0	1
1	0g	0	1
1	0h	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	0i	0	1
1	0j	0	1
1	0k	0	1
1	0l	0	1
3	B	0	1
3	f	0	1
All	All	0	14

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0e	72	SER	N-CA-C	5.89	118.61	109.60
1	0b	72	SER	N-CA-C	5.88	118.60	109.60
1	0k	72	SER	N-CA-C	5.88	118.60	109.60
1	0g	72	SER	N-CA-C	5.88	118.60	109.60
1	0d	72	SER	N-CA-C	5.88	118.59	109.60
1	0c	72	SER	N-CA-C	5.87	118.58	109.60
1	0f	72	SER	N-CA-C	5.87	118.58	109.60
1	0i	72	SER	N-CA-C	5.87	118.58	109.60
1	0j	72	SER	N-CA-C	5.87	118.57	109.60
1	0l	72	SER	N-CA-C	5.86	118.57	109.60
1	0a	72	SER	N-CA-C	5.86	118.56	109.60
1	0h	72	SER	N-CA-C	5.85	118.55	109.60
3	f	19	GLN	CA-C-N	5.47	131.98	121.54
3	f	19	GLN	C-N-CA	5.47	131.98	121.54
3	W	19	GLN	CA-C-N	5.46	131.97	121.54
3	W	19	GLN	C-N-CA	5.46	131.97	121.54
3	c	19	GLN	CA-C-N	5.46	131.96	121.54
3	c	19	GLN	C-N-CA	5.46	131.96	121.54
3	E	19	GLN	CA-C-N	5.44	131.94	121.54
3	E	19	GLN	C-N-CA	5.44	131.94	121.54
3	H	19	GLN	CA-C-N	5.44	131.94	121.54
3	H	19	GLN	C-N-CA	5.44	131.94	121.54
3	Q	19	GLN	CA-C-N	5.43	131.92	121.54
3	Q	19	GLN	C-N-CA	5.43	131.92	121.54
3	B	19	GLN	CA-C-N	5.43	131.91	121.54
3	B	19	GLN	C-N-CA	5.43	131.91	121.54
3	i	19	GLN	CA-C-N	5.43	131.91	121.54
3	i	19	GLN	C-N-CA	5.43	131.91	121.54
3	T	19	GLN	CA-C-N	5.43	131.91	121.54
3	T	19	GLN	C-N-CA	5.43	131.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	19	GLN	CA-C-N	5.43	131.91	121.54
3	K	19	GLN	C-N-CA	5.43	131.91	121.54
3	N	19	GLN	CA-C-N	5.42	131.90	121.54
3	N	19	GLN	C-N-CA	5.42	131.90	121.54
3	Z	19	GLN	CA-C-N	5.41	131.88	121.54
3	Z	19	GLN	C-N-CA	5.41	131.88	121.54

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0a	72	SER	Peptide
1	0b	72	SER	Peptide
1	0c	72	SER	Peptide
1	0d	72	SER	Peptide
1	0e	72	SER	Peptide
1	0f	72	SER	Peptide
1	0g	72	SER	Peptide
1	0h	72	SER	Peptide
1	0i	72	SER	Peptide
1	0j	72	SER	Peptide
1	0k	72	SER	Peptide
1	0l	72	SER	Peptide
3	B	18	VAL	Peptide
3	f	18	VAL	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	2163	0	2104	34	0
1	0b	2163	0	2104	36	0
1	0c	2163	0	2104	35	0
1	0d	2163	0	2104	35	0
1	0e	2163	0	2104	37	0
1	0f	2163	0	2104	35	0
1	0g	2163	0	2104	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0h	2163	0	2104	36	0
1	0i	2163	0	2104	37	0
1	0j	2163	0	2104	35	0
1	0k	2163	0	2104	37	0
1	0l	2163	0	2104	36	0
2	0A	2296	0	2143	56	0
2	0B	2296	0	2143	56	0
2	0C	2296	0	2143	38	0
2	0D	2296	0	2143	37	0
2	0E	2296	0	2143	38	0
2	0F	2296	0	2143	39	0
2	0G	2296	0	2143	37	0
2	0H	2296	0	2143	37	0
2	0I	2296	0	2143	51	0
2	0J	2296	0	2143	57	0
2	0K	2296	0	2143	47	0
2	0L	2296	0	2143	37	0
3	A	433	0	425	3	0
3	B	482	0	477	11	0
3	C	603	0	599	9	0
3	D	433	0	425	3	0
3	E	482	0	477	7	0
3	F	603	0	599	9	0
3	G	433	0	425	3	0
3	H	482	0	477	8	0
3	I	603	0	599	9	0
3	J	433	0	425	3	0
3	K	482	0	477	8	0
3	L	603	0	599	9	0
3	M	433	0	425	3	0
3	N	482	0	477	8	0
3	O	603	0	599	9	0
3	P	433	0	425	3	0
3	Q	482	0	477	8	0
3	R	603	0	599	9	0
3	S	433	0	425	3	0
3	T	482	0	477	9	0
3	U	603	0	599	9	0
3	V	433	0	425	2	0
3	W	482	0	477	8	0
3	X	603	0	599	9	0
3	Y	433	0	425	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	482	0	477	10	0
3	a	603	0	599	9	0
3	b	433	0	425	4	0
3	c	482	0	477	8	0
3	d	603	0	599	9	0
3	e	433	0	425	4	0
3	f	482	0	477	6	0
3	g	603	0	599	8	0
3	h	433	0	425	4	0
3	i	482	0	477	8	0
3	j	603	0	599	8	0
All	All	71724	0	68976	928	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 7.

All (928) 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)
2:0E:193:ILE:O	2:0E:194:GLU:HG3	1.88	0.74
2:0H:193:ILE:O	2:0H:194:GLU:HG3	1.88	0.74
2:0F:193:ILE:O	2:0F:194:GLU:HG3	1.88	0.74
2:0I:193:ILE:O	2:0I:194:GLU:HG3	1.88	0.74
2:0C:193:ILE:O	2:0C:194:GLU:HG3	1.88	0.73
2:0B:193:ILE:O	2:0B:194:GLU:HG3	1.88	0.73
2:0K:193:ILE:O	2:0K:194:GLU:HG3	1.88	0.73
2:0D:193:ILE:O	2:0D:194:GLU:HG3	1.88	0.73
2:0J:193:ILE:O	2:0J:194:GLU:HG3	1.88	0.73
2:0A:193:ILE:O	2:0A:194:GLU:HG3	1.88	0.73
2:0G:193:ILE:O	2:0G:194:GLU:HG3	1.88	0.73
2:0L:193:ILE:O	2:0L:194:GLU:HG3	1.88	0.73
1:0e:162:ARG:NH1	1:0f:191:LEU:O	2.26	0.68
1:0d:256:VAL:HA	1:0e:37:GLN:HG3	1.77	0.65
2:0K:159:THR:HB	2:0K:202:ARG:HB3	1.79	0.65
2:0J:159:THR:HB	2:0J:202:ARG:HB3	1.79	0.64
2:0A:159:THR:HB	2:0A:202:ARG:HB3	1.80	0.64
2:0B:163:PHE:HB2	2:0B:198:GLU:HB3	1.80	0.64
2:0G:163:PHE:HB2	2:0G:198:GLU:HB3	1.80	0.64
2:0B:159:THR:HB	2:0B:202:ARG:HB3	1.80	0.64
2:0E:163:PHE:HB2	2:0E:198:GLU:HB3	1.80	0.64
2:0G:159:THR:HB	2:0G:202:ARG:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0I:159:THR:HB	2:0I:202:ARG:HB3	1.80	0.64
1:0a:37:GLN:HG3	1:0l:256:VAL:HA	1.79	0.64
1:0a:256:VAL:HA	1:0b:37:GLN:HG3	1.79	0.64
1:0k:256:VAL:HA	1:0l:37:GLN:HG3	1.79	0.64
2:0E:159:THR:HB	2:0E:202:ARG:HB3	1.80	0.64
2:0L:159:THR:HB	2:0L:202:ARG:HB3	1.80	0.64
1:0j:256:VAL:HA	1:0k:37:GLN:HG3	1.79	0.64
2:0A:163:PHE:HB2	2:0A:198:GLU:HB3	1.80	0.64
2:0C:163:PHE:HB2	2:0C:198:GLU:HB3	1.80	0.64
2:0H:159:THR:HB	2:0H:202:ARG:HB3	1.80	0.64
2:0C:159:THR:HB	2:0C:202:ARG:HB3	1.80	0.64
2:0F:159:THR:HB	2:0F:202:ARG:HB3	1.80	0.64
2:0D:159:THR:HB	2:0D:202:ARG:HB3	1.80	0.64
2:0H:163:PHE:HB2	2:0H:198:GLU:HB3	1.80	0.64
1:0b:256:VAL:HA	1:0c:37:GLN:HG3	1.79	0.64
1:0i:256:VAL:HA	1:0j:37:GLN:HG3	1.79	0.63
1:0g:256:VAL:HA	1:0h:37:GLN:HG3	1.79	0.63
1:0f:256:VAL:HA	1:0g:37:GLN:HG3	1.79	0.63
2:0F:163:PHE:HB2	2:0F:198:GLU:HB3	1.80	0.63
1:0c:256:VAL:HA	1:0d:37:GLN:HG3	1.79	0.63
2:0L:163:PHE:HB2	2:0L:198:GLU:HB3	1.80	0.63
2:0B:168:ASN:ND2	2:0C:195:GLU:OE1	2.31	0.63
1:0h:256:VAL:HA	1:0i:37:GLN:HG3	1.79	0.63
2:0D:163:PHE:HB2	2:0D:198:GLU:HB3	1.80	0.63
2:0I:163:PHE:HB2	2:0I:198:GLU:HB3	1.80	0.63
2:0K:163:PHE:HB2	2:0K:198:GLU:HB3	1.80	0.62
2:0C:11:TYR:HA	3:H:29:PHE:HE2	1.64	0.62
2:0F:11:TYR:HA	3:N:29:PHE:HE2	1.64	0.62
3:b:68:LEU:O	3:g:4:LYS:NZ	2.33	0.62
2:0D:11:TYR:HA	3:K:29:PHE:HE2	1.64	0.62
2:0E:169:ALA:HB3	2:0E:192:GLN:CB	2.30	0.62
2:0J:163:PHE:HB2	2:0J:198:GLU:HB3	1.80	0.62
2:0L:169:ALA:HB3	2:0L:192:GLN:CB	2.30	0.62
1:0h:72:SER:OG	1:0h:73:TYR:N	2.33	0.62
2:0B:169:ALA:HB3	2:0B:192:GLN:CB	2.30	0.62
2:0C:169:ALA:HB3	2:0C:192:GLN:CB	2.30	0.62
2:0I:169:ALA:HB3	2:0I:192:GLN:CB	2.30	0.62
1:0g:72:SER:OG	1:0g:73:TYR:N	2.33	0.61
2:0H:169:ALA:HB3	2:0H:192:GLN:CB	2.30	0.61
2:0F:169:ALA:HB3	2:0F:192:GLN:CB	2.30	0.61
2:0E:11:TYR:HA	3:Q:29:PHE:HE2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:169:ALA:HB3	2:0K:192:GLN:CB	2.30	0.61
1:0i:72:SER:OG	1:0i:73:TYR:N	2.33	0.61
2:0A:139:LYS:HA	2:0B:224:SER:HA	1.83	0.61
1:0j:72:SER:OG	1:0j:73:TYR:N	2.33	0.61
2:0A:169:ALA:HB3	2:0A:192:GLN:CB	2.30	0.61
2:0G:169:ALA:HB3	2:0G:192:GLN:CB	2.30	0.61
2:0J:169:ALA:HB3	2:0J:192:GLN:CB	2.30	0.61
2:0A:11:TYR:HA	3:B:29:PHE:HE2	1.65	0.60
2:0D:169:ALA:HB3	2:0D:192:GLN:CB	2.30	0.60
1:0k:72:SER:OG	1:0k:73:TYR:N	2.33	0.60
2:0A:147:THR:OG1	2:0B:215:ASN:O	2.15	0.59
1:0j:162:ARG:NH1	1:0k:191:LEU:O	2.36	0.59
1:0l:72:SER:OG	1:0l:73:TYR:N	2.33	0.59
2:0J:151:LYS:HB3	2:0J:210:THR:HB	1.85	0.59
1:0i:162:ARG:NH1	1:0j:191:LEU:O	2.36	0.59
2:0I:151:LYS:HB3	2:0I:210:THR:HB	1.84	0.59
1:0c:162:ARG:NH1	1:0d:191:LEU:O	2.36	0.59
1:0g:162:ARG:NH1	1:0h:191:LEU:O	2.36	0.59
1:0k:162:ARG:NH1	1:0l:191:LEU:O	2.36	0.59
2:0K:151:LYS:HB3	2:0K:210:THR:HB	1.85	0.59
2:0L:151:LYS:HB3	2:0L:210:THR:HB	1.84	0.59
1:0a:72:SER:OG	1:0a:73:TYR:N	2.33	0.59
1:0b:72:SER:OG	1:0b:73:TYR:N	2.33	0.59
1:0b:162:ARG:NH1	1:0c:191:LEU:O	2.36	0.59
1:0f:162:ARG:NH1	1:0g:191:LEU:O	2.36	0.59
1:0a:191:LEU:O	1:0l:162:ARG:NH1	2.36	0.59
1:0h:162:ARG:NH1	1:0i:191:LEU:O	2.36	0.59
2:0H:11:TYR:HA	3:W:29:PHE:HE2	1.67	0.59
2:0K:162:ASN:ND2	2:0K:199:ASN:OD1	2.36	0.59
1:0a:162:ARG:NH1	1:0b:191:LEU:O	2.36	0.59
2:0J:162:ASN:ND2	2:0J:199:ASN:OD1	2.36	0.59
2:0L:11:TYR:HA	3:i:29:PHE:HE2	1.68	0.59
1:0d:172:LYS:HB3	3:L:25:LEU:HD23	1.85	0.59
1:0g:172:LYS:HB3	3:U:25:LEU:HD23	1.85	0.59
2:0L:162:ASN:ND2	2:0L:199:ASN:OD1	2.36	0.59
1:0c:172:LYS:HB3	3:I:25:LEU:HD23	1.85	0.59
1:0f:172:LYS:HB3	3:R:25:LEU:HD23	1.85	0.59
2:0A:151:LYS:HB3	2:0A:210:THR:HB	1.85	0.59
2:0D:151:LYS:HB3	2:0D:210:THR:HB	1.85	0.59
2:0F:151:LYS:HB3	2:0F:210:THR:HB	1.84	0.59
2:0G:11:TYR:HA	3:T:29:PHE:HE2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0b:172:LYS:HB3	3:F:25:LEU:HD23	1.85	0.58
2:0I:11:TYR:HA	3:Z:29:PHE:HE2	1.68	0.58
2:0F:162:ASN:ND2	2:0F:199:ASN:OD1	2.36	0.58
2:0H:151:LYS:HB3	2:0H:210:THR:HB	1.84	0.58
2:0H:162:ASN:ND2	2:0H:199:ASN:OD1	2.36	0.58
2:0I:162:ASN:ND2	2:0I:199:ASN:OD1	2.36	0.58
1:0j:172:LYS:HB3	3:d:25:LEU:HD23	1.85	0.58
2:0D:162:ASN:ND2	2:0D:199:ASN:OD1	2.36	0.58
1:0a:172:LYS:HB3	3:C:25:LEU:HD23	1.85	0.58
2:0A:134:SER:HA	2:0B:228:THR:HA	1.84	0.58
2:0A:162:ASN:ND2	2:0A:199:ASN:OD1	2.36	0.58
2:0C:151:LYS:HB3	2:0C:210:THR:HB	1.85	0.58
2:0E:162:ASN:ND2	2:0E:199:ASN:OD1	2.36	0.58
2:0E:151:LYS:HB3	2:0E:210:THR:HB	1.84	0.58
2:0G:162:ASN:ND2	2:0G:199:ASN:OD1	2.36	0.58
2:0C:162:ASN:ND2	2:0C:199:ASN:OD1	2.36	0.58
3:e:68:LEU:O	3:j:4:LYS:NZ	2.35	0.58
2:0B:151:LYS:HB3	2:0B:210:THR:HB	1.85	0.57
1:0e:256:VAL:HA	1:0f:37:GLN:HG3	1.85	0.57
1:0i:161:ILE:HG12	1:0i:196:ILE:HG12	1.87	0.57
3:C:4:LYS:NZ	3:h:68:LEU:O	2.37	0.57
2:0A:133:THR:N	2:0B:229:SER:O	2.33	0.57
2:0B:162:ASN:ND2	2:0B:199:ASN:OD1	2.36	0.57
2:0G:3:SER:N	3:U:30:ASP:OD2	2.36	0.57
1:0h:161:ILE:HG12	1:0h:196:ILE:HG12	1.87	0.57
1:0j:161:ILE:HG12	1:0j:196:ILE:HG12	1.87	0.57
1:0g:161:ILE:HG12	1:0g:196:ILE:HG12	1.87	0.57
3:A:68:LEU:O	3:F:4:LYS:NZ	2.37	0.57
3:E:42:ILE:HG23	3:F:46:LEU:HD11	1.87	0.57
2:0A:77:GLU:HB3	2:0B:57:ARG:HH22	1.69	0.57
2:0A:132:GLY:HA2	2:0B:230:ASN:HA	1.85	0.57
2:0G:151:LYS:HB3	2:0G:210:THR:HB	1.85	0.57
1:0k:161:ILE:HG12	1:0k:196:ILE:HG12	1.87	0.56
3:Y:68:LEU:O	3:d:4:LYS:NZ	2.37	0.56
3:i:42:ILE:HG23	3:j:46:LEU:HD11	1.87	0.56
3:G:68:LEU:O	3:L:4:LYS:NZ	2.37	0.56
3:J:68:LEU:O	3:O:4:LYS:NZ	2.37	0.56
1:0f:161:ILE:HG12	1:0f:196:ILE:HG12	1.87	0.56
2:0J:11:TYR:HA	3:c:29:PHE:HE2	1.69	0.56
3:H:42:ILE:HG23	3:I:46:LEU:HD11	1.87	0.56
3:e:42:ILE:HG12	3:f:46:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:42:ILE:HG23	3:C:46:LEU:HD11	1.88	0.56
3:D:68:LEU:O	3:I:4:LYS:NZ	2.38	0.56
2:0E:109:LYS:HG2	2:0E:251:ILE:HG12	1.88	0.56
2:0G:109:LYS:HG2	2:0G:251:ILE:HG12	1.87	0.56
2:0C:3:SER:N	3:I:30:ASP:OD2	2.39	0.56
2:0H:109:LYS:HG2	2:0H:251:ILE:HG12	1.88	0.56
2:0J:109:LYS:HG2	2:0J:251:ILE:HG12	1.88	0.56
1:0i:105:LYS:HB3	1:0i:117:MET:HE3	1.88	0.56
2:0D:3:SER:N	3:L:30:ASP:OD2	2.39	0.56
2:0D:109:LYS:HG2	2:0D:251:ILE:HG12	1.88	0.56
2:0F:109:LYS:HG2	2:0F:251:ILE:HG12	1.88	0.56
2:0I:109:LYS:HG2	2:0I:251:ILE:HG12	1.88	0.56
1:0l:105:LYS:HB3	1:0l:117:MET:HE3	1.88	0.56
3:Z:42:ILE:HG23	3:a:46:LEU:HD11	1.88	0.56
3:c:42:ILE:HG23	3:d:46:LEU:HD11	1.88	0.56
1:0c:161:ILE:HG12	1:0c:196:ILE:HG12	1.87	0.56
1:0e:228:LYS:HA	1:0e:250:ILE:HD13	1.88	0.56
1:0j:105:LYS:HB3	1:0j:117:MET:HE3	1.88	0.56
2:0A:3:SER:N	3:C:30:ASP:OD2	2.39	0.56
1:0a:105:LYS:HB3	1:0a:117:MET:HE3	1.88	0.56
1:0b:161:ILE:HG12	1:0b:196:ILE:HG12	1.87	0.56
1:0d:228:LYS:HA	1:0d:250:ILE:HD13	1.88	0.56
2:0A:143:THR:HA	2:0B:220:SER:HA	1.88	0.56
2:0K:109:LYS:HG2	2:0K:251:ILE:HG12	1.88	0.56
3:Q:42:ILE:HG23	3:R:46:LEU:HD11	1.87	0.56
3:f:42:ILE:HG23	3:g:46:LEU:HD11	1.88	0.56
1:0f:228:LYS:HA	1:0f:250:ILE:HD13	1.88	0.55
2:0C:103:ASN:ND2	2:0C:258:ILE:O	2.39	0.55
2:0J:103:ASN:ND2	2:0J:258:ILE:O	2.39	0.55
3:N:31:GLU:O	3:N:41:LYS:NZ	2.39	0.55
3:Q:31:GLU:O	3:Q:41:LYS:NZ	2.39	0.55
3:W:42:ILE:HG23	3:X:46:LEU:HD11	1.88	0.55
1:0d:161:ILE:HG12	1:0d:196:ILE:HG12	1.87	0.55
1:0l:161:ILE:HG12	1:0l:196:ILE:HG12	1.87	0.55
2:0C:109:LYS:HG2	2:0C:251:ILE:HG12	1.88	0.55
2:0F:133:THR:HA	2:0F:227:LYS:HA	1.89	0.55
3:B:31:GLU:O	3:B:41:LYS:NZ	2.39	0.55
3:K:42:ILE:HG23	3:L:46:LEU:HD11	1.88	0.55
1:0a:161:ILE:HG12	1:0a:196:ILE:HG12	1.87	0.55
2:0A:133:THR:HA	2:0A:227:LYS:HA	1.89	0.55
2:0C:105:ARG:HG3	2:0C:255:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0D:133:THR:HA	2:0D:227:LYS:HA	1.89	0.55
2:0L:133:THR:HA	2:0L:227:LYS:HA	1.89	0.55
1:0c:228:LYS:HA	1:0c:250:ILE:HD13	1.88	0.55
2:0E:133:THR:HA	2:0E:227:LYS:HA	1.89	0.55
2:0F:3:SER:N	3:O:30:ASP:OD2	2.39	0.55
2:0L:109:LYS:HG2	2:0L:251:ILE:HG12	1.88	0.55
1:0h:228:LYS:HA	1:0h:250:ILE:HD13	1.88	0.55
2:0B:131:ASN:HA	2:0B:229:SER:HA	1.89	0.55
2:0B:133:THR:HA	2:0B:227:LYS:HA	1.89	0.55
2:0E:131:ASN:HA	2:0E:229:SER:HA	1.89	0.55
2:0K:103:ASN:ND2	2:0K:258:ILE:O	2.39	0.55
3:N:42:ILE:HG23	3:O:46:LEU:HD11	1.87	0.55
2:0C:131:ASN:HA	2:0C:229:SER:HA	1.89	0.55
2:0G:131:ASN:HA	2:0G:229:SER:HA	1.89	0.55
2:0K:133:THR:HA	2:0K:227:LYS:HA	1.89	0.55
3:M:68:LEU:O	3:R:4:LYS:NZ	2.37	0.55
3:c:31:GLU:O	3:c:41:LYS:NZ	2.39	0.55
1:0g:228:LYS:HA	1:0g:250:ILE:HD13	1.88	0.55
2:0C:133:THR:HA	2:0C:227:LYS:HA	1.89	0.55
2:0F:131:ASN:HA	2:0F:229:SER:HA	1.89	0.55
2:0A:131:ASN:HA	2:0A:229:SER:HA	1.89	0.55
2:0B:109:LYS:HG2	2:0B:251:ILE:HG12	1.88	0.55
2:0C:122:ARG:HB2	2:0C:238:ASP:HB3	1.89	0.55
2:0D:131:ASN:HA	2:0D:229:SER:HA	1.89	0.55
2:0E:3:SER:N	3:R:30:ASP:OD2	2.39	0.55
2:0H:105:ARG:HG3	2:0H:255:VAL:HG12	1.88	0.55
2:0H:133:THR:HA	2:0H:227:LYS:HA	1.89	0.55
3:E:31:GLU:O	3:E:41:LYS:NZ	2.40	0.55
3:T:31:GLU:O	3:T:41:LYS:NZ	2.39	0.55
3:Z:31:GLU:O	3:Z:41:LYS:NZ	2.39	0.55
1:0k:105:LYS:HB3	1:0k:117:MET:HE3	1.88	0.55
2:0A:109:LYS:HG2	2:0A:251:ILE:HG12	1.88	0.55
2:0B:105:ARG:HG3	2:0B:255:VAL:HG12	1.88	0.55
2:0E:154:GLY:HA3	2:0E:207:SER:HA	1.89	0.55
2:0G:133:THR:HA	2:0G:227:LYS:HA	1.89	0.55
3:i:31:GLU:O	3:i:41:LYS:NZ	2.39	0.55
1:0h:105:LYS:HB3	1:0h:117:MET:HE3	1.88	0.55
1:0k:228:LYS:HA	1:0k:250:ILE:HD13	1.88	0.55
1:0l:228:LYS:HA	1:0l:250:ILE:HD13	1.88	0.55
2:0B:11:TYR:HA	3:E:29:PHE:HE2	1.72	0.55
2:0E:122:ARG:HB2	2:0E:238:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0F:154:GLY:HA3	2:0F:207:SER:HA	1.89	0.55
2:0H:131:ASN:HA	2:0H:229:SER:HA	1.89	0.55
2:0I:103:ASN:ND2	2:0I:258:ILE:O	2.39	0.55
2:0I:122:ARG:HB2	2:0I:238:ASP:HB3	1.89	0.55
2:0I:133:THR:HA	2:0I:227:LYS:HA	1.89	0.55
2:0J:133:THR:HA	2:0J:227:LYS:HA	1.89	0.55
3:T:42:ILE:HG23	3:U:46:LEU:HD11	1.89	0.55
3:h:42:ILE:HG12	3:i:46:LEU:HD11	1.88	0.55
1:0c:105:LYS:HB3	1:0c:117:MET:HE3	1.88	0.54
1:0e:161:ILE:HG12	1:0e:196:ILE:HG12	1.87	0.54
2:0I:105:ARG:HG3	2:0I:255:VAL:HG12	1.88	0.54
2:0K:3:SER:N	3:g:30:ASP:OD2	2.39	0.54
1:0f:105:LYS:HB3	1:0f:117:MET:HE3	1.88	0.54
1:0g:105:LYS:HB3	1:0g:117:MET:HE3	1.88	0.54
1:0i:228:LYS:HA	1:0i:250:ILE:HD13	1.88	0.54
2:0D:154:GLY:HA3	2:0D:207:SER:HA	1.89	0.54
2:0G:105:ARG:HG3	2:0G:255:VAL:HG12	1.88	0.54
2:0G:154:GLY:HA3	2:0G:207:SER:HA	1.89	0.54
2:0L:105:ARG:HG3	2:0L:255:VAL:HG12	1.88	0.54
2:0L:122:ARG:HB2	2:0L:238:ASP:HB3	1.89	0.54
2:0L:131:ASN:HA	2:0L:229:SER:HA	1.89	0.54
3:Y:42:ILE:HG12	3:Z:46:LEU:HD11	1.88	0.54
1:0j:228:LYS:HA	1:0j:250:ILE:HD13	1.88	0.54
2:0B:154:GLY:HA3	2:0B:207:SER:HA	1.89	0.54
2:0D:103:ASN:ND2	2:0D:258:ILE:O	2.39	0.54
2:0D:105:ARG:HG3	2:0D:255:VAL:HG12	1.88	0.54
2:0D:122:ARG:HB2	2:0D:238:ASP:HB3	1.89	0.54
2:0G:103:ASN:ND2	2:0G:258:ILE:O	2.39	0.54
2:0H:103:ASN:ND2	2:0H:258:ILE:O	2.39	0.54
3:f:56:LEU:HD22	3:g:53:THR:HG23	1.89	0.54
1:0b:125:ASP:HB3	1:0c:55:LYS:HD2	1.89	0.54
1:0b:228:LYS:HA	1:0b:250:ILE:HD13	1.88	0.54
1:0d:105:LYS:HB3	1:0d:117:MET:HE3	1.88	0.54
1:0f:97:SER:O	1:0f:101:GLN:NE2	2.41	0.54
1:0g:97:SER:O	1:0g:101:GLN:NE2	2.41	0.54
2:0A:122:ARG:HB2	2:0A:238:ASP:HB3	1.89	0.54
2:0E:103:ASN:ND2	2:0E:258:ILE:O	2.39	0.54
2:0H:154:GLY:HA3	2:0H:207:SER:HA	1.89	0.54
2:0I:131:ASN:HA	2:0I:229:SER:HA	1.89	0.54
2:0J:3:SER:N	3:d:30:ASP:OD2	2.41	0.54
2:0J:105:ARG:HG3	2:0J:255:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0e:97:SER:O	1:0e:101:GLN:NE2	2.41	0.54
1:0e:105:LYS:HB3	1:0e:117:MET:HE3	1.88	0.54
1:0h:97:SER:O	1:0h:101:GLN:NE2	2.41	0.54
1:0k:125:ASP:HB3	1:0l:55:LYS:HD2	1.89	0.54
2:0A:154:GLY:HA3	2:0A:207:SER:HA	1.89	0.54
2:0C:154:GLY:HA3	2:0C:207:SER:HA	1.89	0.54
2:0H:122:ARG:HB2	2:0H:238:ASP:HB3	1.89	0.54
2:0J:131:ASN:HA	2:0J:229:SER:HA	1.89	0.54
2:0K:131:ASN:HA	2:0K:229:SER:HA	1.89	0.54
3:K:31:GLU:O	3:K:41:LYS:NZ	2.40	0.54
1:0a:125:ASP:HB3	1:0b:55:LYS:HD2	1.89	0.54
1:0i:97:SER:O	1:0i:101:GLN:NE2	2.41	0.54
2:0A:103:ASN:ND2	2:0A:258:ILE:O	2.39	0.54
2:0G:122:ARG:HB2	2:0G:238:ASP:HB3	1.89	0.54
2:0K:105:ARG:HG3	2:0K:255:VAL:HG12	1.88	0.54
3:V:42:ILE:HG12	3:W:46:LEU:HD11	1.90	0.54
1:0a:55:LYS:HD2	1:0l:125:ASP:HB3	1.89	0.54
1:0a:97:SER:O	1:0a:101:GLN:NE2	2.41	0.54
1:0b:97:SER:O	1:0b:101:GLN:NE2	2.41	0.54
1:0b:105:LYS:HB3	1:0b:117:MET:HE3	1.88	0.54
2:0E:105:ARG:HG3	2:0E:255:VAL:HG12	1.88	0.54
1:0a:228:LYS:HA	1:0a:250:ILE:HD13	1.88	0.54
1:0c:125:ASP:HB3	1:0d:55:LYS:HD2	1.89	0.54
2:0J:122:ARG:HB2	2:0J:238:ASP:HB3	1.89	0.54
2:0L:103:ASN:ND2	2:0L:258:ILE:O	2.39	0.54
2:0L:154:GLY:HA3	2:0L:207:SER:HA	1.89	0.54
1:0c:97:SER:O	1:0c:101:GLN:NE2	2.41	0.54
1:0d:97:SER:O	1:0d:101:GLN:NE2	2.41	0.54
1:0j:97:SER:O	1:0j:101:GLN:NE2	2.41	0.54
2:0I:154:GLY:HA3	2:0I:207:SER:HA	1.89	0.54
3:f:31:GLU:O	3:f:41:LYS:NZ	2.41	0.54
1:0c:107:TYR:OH	1:0c:114:GLU:O	2.25	0.54
2:0A:105:ARG:HG3	2:0A:255:VAL:HG12	1.88	0.54
2:0B:103:ASN:ND2	2:0B:258:ILE:O	2.39	0.54
2:0F:105:ARG:HG3	2:0F:255:VAL:HG12	1.88	0.54
2:0F:122:ARG:HB2	2:0F:238:ASP:HB3	1.89	0.54
1:0f:125:ASP:HB3	1:0g:55:LYS:HD2	1.89	0.53
1:0j:125:ASP:HB3	1:0k:55:LYS:HD2	1.89	0.53
1:0k:97:SER:O	1:0k:101:GLN:NE2	2.41	0.53
1:0l:97:SER:O	1:0l:101:GLN:NE2	2.41	0.53
2:0L:3:SER:N	3:j:30:ASP:OD2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:31:GLU:O	3:W:41:LYS:NZ	2.39	0.53
2:0C:103:ASN:HB2	2:0C:258:ILE:H	1.74	0.53
2:0K:154:GLY:HA3	2:0K:207:SER:HA	1.89	0.53
1:0h:125:ASP:HB3	1:0i:55:LYS:HD2	1.89	0.53
1:0i:172:LYS:HB3	3:a:25:LEU:HD23	1.90	0.53
2:0D:103:ASN:HB2	2:0D:258:ILE:H	1.74	0.53
2:0I:130:SER:OG	2:0I:230:ASN:OD1	2.26	0.53
2:0G:103:ASN:HB2	2:0G:258:ILE:H	1.73	0.53
2:0H:130:SER:OG	2:0H:230:ASN:OD1	2.26	0.53
2:0J:154:GLY:HA3	2:0J:207:SER:HA	1.89	0.53
2:0L:103:ASN:HB2	2:0L:258:ILE:H	1.74	0.53
2:0A:273:ALA:O	2:0B:271:ARG:NH1	2.32	0.53
2:0B:122:ARG:HB2	2:0B:238:ASP:HB3	1.89	0.53
2:0E:103:ASN:HB2	2:0E:258:ILE:H	1.73	0.53
1:0f:72:SER:OG	1:0f:73:TYR:N	2.33	0.53
2:0C:130:SER:OG	2:0C:230:ASN:OD1	2.26	0.53
2:0D:130:SER:OG	2:0D:230:ASN:OD1	2.26	0.53
2:0K:122:ARG:HB2	2:0K:238:ASP:HB3	1.89	0.53
1:0e:72:SER:OG	1:0e:73:TYR:N	2.33	0.53
1:0i:125:ASP:HB3	1:0j:55:LYS:HD2	1.89	0.53
2:0H:103:ASN:HB2	2:0H:258:ILE:H	1.74	0.53
2:0L:137:ASP:OD1	2:0L:137:ASP:N	2.39	0.53
1:0b:107:TYR:OH	1:0b:114:GLU:O	2.25	0.53
1:0e:173:GLN:NE2	3:O:25:LEU:O	2.42	0.53
2:0A:103:ASN:HB2	2:0A:258:ILE:H	1.74	0.53
2:0F:130:SER:OG	2:0F:230:ASN:OD1	2.26	0.53
2:0A:142:ASP:N	2:0B:221:THR:O	2.42	0.53
2:0B:130:SER:OG	2:0B:230:ASN:OD1	2.26	0.53
2:0H:3:SER:N	3:X:30:ASP:OD2	2.42	0.53
2:0I:103:ASN:HB2	2:0I:258:ILE:H	1.74	0.53
2:0K:103:ASN:HB2	2:0K:258:ILE:H	1.74	0.53
1:0d:72:SER:OG	1:0d:73:TYR:N	2.33	0.52
3:Z:56:LEU:HD22	3:a:53:THR:HG23	1.91	0.52
2:0A:130:SER:OG	2:0A:230:ASN:OD1	2.26	0.52
2:0G:130:SER:OG	2:0G:230:ASN:OD1	2.26	0.52
2:0B:103:ASN:HB2	2:0B:258:ILE:H	1.74	0.52
2:0K:11:TYR:HA	3:f:29:PHE:HE2	1.75	0.52
3:T:56:LEU:HD22	3:U:53:THR:HG23	1.91	0.52
1:0g:125:ASP:HB3	1:0h:55:LYS:HD2	1.89	0.52
2:0F:103:ASN:ND2	2:0F:258:ILE:O	2.39	0.52
3:X:3:THR:HG22	3:X:4:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0L:130:SER:OG	2:0L:230:ASN:OD1	2.26	0.52
3:O:3:THR:HG22	3:O:4:LYS:HG2	1.92	0.52
3:U:3:THR:HG22	3:U:4:LYS:HG2	1.92	0.52
3:a:3:THR:HG22	3:a:4:LYS:HG2	1.92	0.52
2:0E:130:SER:OG	2:0E:230:ASN:OD1	2.26	0.52
2:0F:50:ILE:O	2:0F:53:THR:OG1	2.28	0.52
2:0J:103:ASN:HB2	2:0J:258:ILE:H	1.74	0.52
3:L:3:THR:HG22	3:L:4:LYS:HG2	1.92	0.52
3:R:3:THR:HG22	3:R:4:LYS:HG2	1.92	0.52
3:W:56:LEU:HD22	3:X:53:THR:HG23	1.92	0.52
1:0d:125:ASP:HB3	1:0e:55:LYS:HD2	1.91	0.52
1:0h:172:LYS:HB3	3:X:25:LEU:HD23	1.92	0.52
2:0B:3:SER:N	3:F:30:ASP:OD2	2.43	0.52
2:0I:132:GLY:HA2	2:0J:230:ASN:HA	1.92	0.52
3:I:3:THR:HG22	3:I:4:LYS:HG2	1.92	0.52
1:0d:162:ARG:NH1	1:0e:191:LEU:O	2.43	0.52
2:0A:144:SER:N	2:0B:219:THR:O	2.43	0.52
2:0B:167:LEU:HD22	2:0C:196:HIS:CD2	2.44	0.52
1:0l:172:LYS:HB3	3:j:25:LEU:HD23	1.91	0.51
2:0F:103:ASN:HB2	2:0F:258:ILE:H	1.74	0.51
3:P:42:ILE:HG12	3:Q:46:LEU:HD11	1.91	0.51
1:0e:135:GLU:OE1	1:0f:22:ARG:NH2	2.44	0.51
2:0B:50:ILE:O	2:0B:53:THR:OG1	2.28	0.51
3:d:3:THR:HG22	3:d:4:LYS:HG2	1.92	0.51
2:0I:134:SER:HA	2:0J:228:THR:HA	1.92	0.51
2:0K:130:SER:OG	2:0K:230:ASN:OD1	2.26	0.51
3:G:42:ILE:HG12	3:H:46:LEU:HD11	1.91	0.51
1:0a:107:TYR:OH	1:0a:114:GLU:O	2.25	0.51
1:0e:94:ARG:HA	1:0e:103:GLU:HA	1.93	0.51
2:0A:149:ASN:HA	2:0B:214:SER:HA	1.92	0.51
2:0K:137:ASP:OD1	2:0K:137:ASP:N	2.40	0.51
1:0i:10:ARG:NH1	1:0i:18:GLN:OE1	2.44	0.51
2:0D:50:ILE:O	2:0D:53:THR:OG1	2.28	0.51
2:0I:3:SER:N	3:a:30:ASP:OD2	2.43	0.51
3:F:3:THR:HG22	3:F:4:LYS:HG2	1.92	0.51
1:0b:10:ARG:NH1	1:0b:18:GLN:OE1	2.44	0.51
1:0d:94:ARG:HA	1:0d:103:GLU:HA	1.93	0.51
1:0e:162:ARG:HB3	1:0f:189:GLU:HA	1.93	0.51
2:0D:193:ILE:O	2:0D:194:GLU:CG	2.59	0.51
2:0E:193:ILE:C	2:0E:194:GLU:HG3	2.36	0.51
2:0K:24:THR:OG1	3:c:31:GLU:OE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:50:ILE:O	2:0K:53:THR:OG1	2.28	0.51
3:D:42:ILE:HG12	3:E:46:LEU:HD11	1.92	0.51
3:g:3:THR:HG22	3:g:4:LYS:HG2	1.92	0.51
1:0c:94:ARG:HA	1:0c:103:GLU:HA	1.93	0.51
1:0j:10:ARG:NH1	1:0j:18:GLN:OE1	2.44	0.51
2:0A:120:ASP:HB2	2:0A:240:LEU:HB3	1.93	0.51
2:0B:9:ARG:NH2	3:B:37:GLU:OE2	2.44	0.51
2:0D:193:ILE:C	2:0D:194:GLU:HG3	2.36	0.51
2:0G:193:ILE:O	2:0G:194:GLU:CG	2.59	0.51
2:0H:193:ILE:C	2:0H:194:GLU:HG3	2.36	0.51
3:C:3:THR:HG22	3:C:4:LYS:HG2	1.92	0.51
3:j:3:THR:HG22	3:j:4:LYS:HG2	1.92	0.51
1:0c:10:ARG:NH1	1:0c:18:GLN:OE1	2.44	0.51
2:0K:120:ASP:HB2	2:0K:240:LEU:HB3	1.93	0.51
2:0L:120:ASP:HB2	2:0L:240:LEU:HB3	1.93	0.51
3:b:42:ILE:HG12	3:c:46:LEU:HD11	1.92	0.51
3:i:56:LEU:HD22	3:j:53:THR:HG23	1.91	0.51
1:0f:94:ARG:HA	1:0f:103:GLU:HA	1.93	0.51
2:0B:120:ASP:HB2	2:0B:240:LEU:HB3	1.93	0.51
1:0a:10:ARG:NH1	1:0a:18:GLN:OE1	2.44	0.51
1:0b:94:ARG:HA	1:0b:103:GLU:HA	1.93	0.51
1:0d:10:ARG:NH1	1:0d:18:GLN:OE1	2.44	0.51
1:0e:172:LYS:HB3	3:O:25:LEU:HD23	1.93	0.51
1:0g:10:ARG:NH1	1:0g:18:GLN:OE1	2.44	0.51
2:0E:50:ILE:O	2:0E:53:THR:OG1	2.28	0.51
2:0J:120:ASP:HB2	2:0J:240:LEU:HB3	1.93	0.51
3:S:68:LEU:O	3:X:4:LYS:NZ	2.43	0.51
2:0A:193:ILE:C	2:0A:194:GLU:HG3	2.36	0.50
2:0C:193:ILE:C	2:0C:194:GLU:HG3	2.36	0.50
2:0I:120:ASP:HB2	2:0I:240:LEU:HB3	1.93	0.50
3:A:42:ILE:HG12	3:B:46:LEU:HD11	1.92	0.50
3:M:42:ILE:HG12	3:N:46:LEU:HD11	1.92	0.50
3:S:42:ILE:HG12	3:T:46:LEU:HD11	1.92	0.50
1:0e:10:ARG:NH1	1:0e:18:GLN:OE1	2.44	0.50
1:0f:10:ARG:NH1	1:0f:18:GLN:OE1	2.44	0.50
1:0h:10:ARG:NH1	1:0h:18:GLN:OE1	2.44	0.50
1:0l:10:ARG:NH1	1:0l:18:GLN:OE1	2.44	0.50
2:0K:193:ILE:C	2:0K:194:GLU:HG3	2.36	0.50
3:H:31:GLU:O	3:H:41:LYS:NZ	2.39	0.50
2:0A:193:ILE:O	2:0A:194:GLU:CG	2.59	0.50
2:0H:50:ILE:O	2:0H:53:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0H:120:ASP:HB2	2:0H:240:LEU:HB3	1.93	0.50
2:0I:193:ILE:C	2:0I:194:GLU:HG3	2.36	0.50
1:0g:94:ARG:HA	1:0g:103:GLU:HA	1.93	0.50
1:0k:10:ARG:NH1	1:0k:18:GLN:OE1	2.44	0.50
2:0J:130:SER:OG	2:0J:230:ASN:OD1	2.26	0.50
2:0L:193:ILE:O	2:0L:194:GLU:CG	2.59	0.50
2:0F:193:ILE:C	2:0F:194:GLU:HG3	2.36	0.50
2:0I:139:LYS:HA	2:0J:224:SER:HA	1.92	0.50
1:0a:94:ARG:HA	1:0a:103:GLU:HA	1.93	0.50
2:0A:81:MET:HB3	2:0B:54:HIS:NE2	2.26	0.50
2:0B:193:ILE:C	2:0B:194:GLU:HG3	2.36	0.50
2:0C:120:ASP:HB2	2:0C:240:LEU:HB3	1.93	0.50
2:0J:193:ILE:C	2:0J:194:GLU:HG3	2.36	0.50
2:0G:120:ASP:HB2	2:0G:240:LEU:HB3	1.93	0.50
1:0h:94:ARG:HA	1:0h:103:GLU:HA	1.93	0.50
2:0G:193:ILE:C	2:0G:194:GLU:HG3	2.36	0.50
3:Q:56:LEU:HD22	3:R:53:THR:HG23	1.94	0.50
1:0e:125:ASP:HB3	1:0f:55:LYS:HD2	1.93	0.50
1:0l:94:ARG:HA	1:0l:103:GLU:HA	1.93	0.50
2:0I:77:GLU:HB3	2:0J:57:ARG:HH22	1.77	0.50
2:0K:193:ILE:O	2:0K:194:GLU:CG	2.59	0.50
2:0C:137:ASP:OD1	2:0C:137:ASP:N	2.39	0.49
3:J:42:ILE:HG12	3:K:46:LEU:HD11	1.92	0.49
1:0g:173:GLN:NE2	3:U:25:LEU:O	2.45	0.49
2:0C:193:ILE:O	2:0C:194:GLU:CG	2.59	0.49
2:0L:50:ILE:O	2:0L:53:THR:OG1	2.28	0.49
1:0i:94:ARG:HA	1:0i:103:GLU:HA	1.93	0.49
2:0D:120:ASP:HB2	2:0D:240:LEU:HB3	1.93	0.49
1:0j:94:ARG:HA	1:0j:103:GLU:HA	1.93	0.49
1:0j:173:GLN:NE2	3:d:25:LEU:O	2.46	0.49
2:0A:50:ILE:O	2:0A:53:THR:OG1	2.28	0.49
2:0B:137:ASP:OD1	2:0B:137:ASP:N	2.39	0.49
2:0E:120:ASP:HB2	2:0E:240:LEU:HB3	1.93	0.49
1:0k:94:ARG:HA	1:0k:103:GLU:HA	1.93	0.49
2:0E:193:ILE:O	2:0E:194:GLU:CG	2.59	0.49
2:0F:120:ASP:HB2	2:0F:240:LEU:HB3	1.93	0.49
2:0J:149:ASN:HA	2:0K:214:SER:HA	1.94	0.49
1:0l:107:TYR:OH	1:0l:114:GLU:O	2.25	0.49
2:0J:50:ILE:O	2:0J:53:THR:OG1	2.28	0.49
2:0J:159:THR:HG23	2:0K:204:THR:HB	1.95	0.49
2:0J:193:ILE:O	2:0J:194:GLU:CG	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0L:193:ILE:C	2:0L:194:GLU:HG3	2.36	0.49
3:B:56:LEU:HD22	3:C:53:THR:HG23	1.94	0.49
3:N:56:LEU:HD22	3:O:53:THR:HG23	1.94	0.49
2:0D:193:ILE:HG12	2:0D:194:GLU:N	2.28	0.49
2:0J:24:THR:OG1	3:Z:31:GLU:OE2	2.28	0.49
1:0a:173:GLN:NE2	3:C:25:LEU:O	2.46	0.49
2:0A:135:SER:N	2:0B:227:LYS:O	2.45	0.49
2:0C:193:ILE:HG12	2:0C:194:GLU:N	2.28	0.49
2:0I:193:ILE:HG12	2:0I:194:GLU:N	2.28	0.49
3:W:34:THR:HG23	3:W:37:GLU:H	1.78	0.49
1:0i:173:GLN:NE2	3:a:25:LEU:O	2.46	0.49
2:0B:193:ILE:HG12	2:0B:194:GLU:N	2.28	0.49
3:H:56:LEU:HD22	3:I:53:THR:HG23	1.94	0.49
2:0E:193:ILE:HG12	2:0E:194:GLU:N	2.28	0.48
2:0K:193:ILE:HG12	2:0K:194:GLU:N	2.28	0.48
3:E:56:LEU:HD22	3:F:53:THR:HG23	1.94	0.48
3:K:56:LEU:HD22	3:L:53:THR:HG23	1.94	0.48
3:Z:34:THR:HG23	3:Z:37:GLU:H	1.78	0.48
1:0c:72:SER:OG	1:0c:73:TYR:N	2.33	0.48
1:0e:86:VAL:HG21	1:0f:74:ILE:HD11	1.95	0.48
2:0A:193:ILE:HG12	2:0A:194:GLU:N	2.28	0.48
3:T:34:THR:HG23	3:T:37:GLU:H	1.77	0.48
1:0d:13:ASN:HB3	3:R:23:ARG:HD3	1.95	0.48
1:0f:173:GLN:NE2	3:R:25:LEU:O	2.46	0.48
2:0D:167:LEU:O	2:0D:194:GLU:N	2.46	0.48
2:0F:193:ILE:HG12	2:0F:194:GLU:N	2.28	0.48
2:0G:193:ILE:HG12	2:0G:194:GLU:N	2.28	0.48
2:0L:193:ILE:HG12	2:0L:194:GLU:N	2.28	0.48
3:i:34:THR:HG23	3:i:37:GLU:H	1.77	0.48
1:0c:13:ASN:HB3	3:O:23:ARG:HD3	1.95	0.48
2:0H:193:ILE:HG12	2:0H:194:GLU:N	2.28	0.48
2:0J:9:ARG:NH2	3:Z:37:GLU:OE2	2.46	0.48
2:0J:137:ASP:OD1	2:0J:137:ASP:N	2.40	0.48
1:0b:173:GLN:NE2	3:F:25:LEU:O	2.46	0.48
1:0d:173:GLN:NE2	3:L:25:LEU:O	2.46	0.48
1:0g:159:VAL:HB	1:0h:184:VAL:HG22	1.96	0.48
1:0h:13:ASN:HB3	3:d:23:ARG:HD3	1.95	0.48
1:0h:159:VAL:HB	1:0i:184:VAL:HG22	1.96	0.48
2:0G:167:LEU:O	2:0G:194:GLU:N	2.46	0.48
3:K:34:THR:HG23	3:K:37:GLU:H	1.77	0.48
3:Q:34:THR:HG23	3:Q:37:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0k:172:LYS:HB3	3:g:25:LEU:HD23	1.95	0.48
2:0l:193:ILE:O	2:0l:194:GLU:CG	2.59	0.48
2:0J:167:LEU:O	2:0J:194:GLU:N	2.46	0.48
2:0C:167:LEU:O	2:0C:194:GLU:N	2.46	0.48
2:0l:167:LEU:O	2:0l:194:GLU:N	2.46	0.48
2:0J:77:GLU:HB3	2:0K:57:ARG:HH22	1.78	0.48
3:f:34:THR:HG23	3:f:37:GLU:H	1.79	0.48
1:0d:159:VAL:HB	1:0e:184:VAL:HG22	1.96	0.48
1:0f:159:VAL:HB	1:0g:184:VAL:HG22	1.96	0.48
1:0i:159:VAL:HB	1:0j:184:VAL:HG22	1.96	0.48
2:0A:167:LEU:O	2:0A:194:GLU:N	2.46	0.48
3:c:56:LEU:HD22	3:d:53:THR:HG23	1.94	0.48
1:0b:13:ASN:HB3	3:L:23:ARG:HD3	1.95	0.48
1:0c:159:VAL:HB	1:0d:184:VAL:HG22	1.96	0.48
2:0H:167:LEU:O	2:0H:194:GLU:N	2.47	0.48
1:0a:159:VAL:HB	1:0b:184:VAL:HG22	1.96	0.47
1:0a:184:VAL:HG22	1:0l:159:VAL:HB	1.96	0.47
1:0b:159:VAL:HB	1:0c:184:VAL:HG22	1.96	0.47
1:0l:13:ASN:HB3	3:F:23:ARG:HD3	1.95	0.47
1:0a:13:ASN:HB3	3:I:23:ARG:HD3	1.95	0.47
1:0c:173:GLN:NE2	3:I:25:LEU:O	2.46	0.47
1:0k:13:ASN:HB3	3:C:23:ARG:HD3	1.95	0.47
2:0A:133:THR:O	2:0B:228:THR:OG1	2.26	0.47
2:0J:193:ILE:HG12	2:0J:194:GLU:N	2.28	0.47
3:N:34:THR:HG23	3:N:37:GLU:H	1.77	0.47
1:0j:159:VAL:HB	1:0k:184:VAL:HG22	1.96	0.47
2:0F:167:LEU:O	2:0F:194:GLU:N	2.47	0.47
2:0l:50:ILE:O	2:0l:53:THR:OG1	2.28	0.47
2:0L:10:THR:HG22	3:i:29:PHE:HZ	1.79	0.47
1:0k:24:PHE:HZ	1:0k:135:GLU:HG2	1.80	0.47
1:0k:159:VAL:HB	1:0l:184:VAL:HG22	1.96	0.47
2:0G:137:ASP:N	2:0G:137:ASP:OD1	2.39	0.47
1:0c:24:PHE:HZ	1:0c:135:GLU:HG2	1.80	0.47
1:0l:173:GLN:NE2	3:j:25:LEU:O	2.48	0.47
2:0B:167:LEU:O	2:0B:194:GLU:N	2.47	0.47
2:0B:193:ILE:O	2:0B:194:GLU:CG	2.59	0.47
2:0K:168:ASN:ND2	2:0L:195:GLU:OE1	2.43	0.47
2:0L:167:LEU:O	2:0L:194:GLU:N	2.47	0.47
1:0b:24:PHE:HZ	1:0b:135:GLU:HG2	1.80	0.47
1:0b:72:SER:HG	1:0b:73:TYR:H	1.59	0.47
1:0d:24:PHE:HZ	1:0d:135:GLU:HG2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0l:24:PHE:HZ	1:0l:135:GLU:HG2	1.80	0.47
2:0B:24:THR:OG1	3:B:31:GLU:OE2	2.27	0.47
3:H:34:THR:HG23	3:H:37:GLU:H	1.77	0.47
1:0h:24:PHE:HZ	1:0h:135:GLU:HG2	1.80	0.47
2:0A:137:ASP:OD1	2:0A:137:ASP:N	2.39	0.47
1:0e:24:PHE:HZ	1:0e:135:GLU:HG2	1.80	0.47
1:0g:24:PHE:HZ	1:0g:135:GLU:HG2	1.80	0.47
1:0i:24:PHE:HZ	1:0i:135:GLU:HG2	1.80	0.47
1:0k:269:ASN:OD1	1:0k:276:VAL:N	2.48	0.47
2:0H:10:THR:HG22	3:W:29:PHE:HZ	1.80	0.47
2:0K:167:LEU:O	2:0K:194:GLU:N	2.47	0.47
1:0d:144:LEU:HD23	1:0d:147:ILE:HD12	1.97	0.47
1:0d:269:ASN:OD1	1:0d:276:VAL:N	2.48	0.47
1:0e:269:ASN:OD1	1:0e:276:VAL:N	2.48	0.47
1:0f:24:PHE:HZ	1:0f:135:GLU:HG2	1.80	0.47
2:0G:10:THR:HG22	3:T:29:PHE:HZ	1.80	0.47
3:B:34:THR:HG23	3:B:37:GLU:H	1.79	0.47
1:0c:144:LEU:HD23	1:0c:147:ILE:HD12	1.97	0.46
1:0e:144:LEU:HD23	1:0e:147:ILE:HD12	1.97	0.46
1:0j:269:ASN:OD1	1:0j:276:VAL:N	2.48	0.46
2:0A:10:THR:HG22	3:B:29:PHE:HZ	1.80	0.46
2:0F:193:ILE:O	2:0F:194:GLU:CG	2.59	0.46
2:0A:145:LYS:HA	2:0B:218:GLY:HA3	1.97	0.46
2:0E:167:LEU:O	2:0E:194:GLU:N	2.46	0.46
1:0d:248:GLU:OE2	1:0e:228:LYS:NZ	2.40	0.46
1:0l:269:ASN:OD1	1:0l:276:VAL:N	2.48	0.46
2:0I:10:THR:HG22	3:Z:29:PHE:HZ	1.79	0.46
2:0I:149:ASN:HA	2:0J:214:SER:HA	1.97	0.46
1:0b:144:LEU:HD23	1:0b:147:ILE:HD12	1.97	0.46
1:0f:144:LEU:HD23	1:0f:147:ILE:HD12	1.97	0.46
1:0h:109:TYR:OH	1:0h:263:GLU:OE2	2.34	0.46
1:0j:24:PHE:HZ	1:0j:135:GLU:HG2	1.80	0.46
1:0a:24:PHE:HZ	1:0a:135:GLU:HG2	1.80	0.46
1:0c:269:ASN:OD1	1:0c:276:VAL:N	2.48	0.46
1:0f:109:TYR:OH	1:0f:263:GLU:OE2	2.34	0.46
1:0i:109:TYR:OH	1:0i:263:GLU:OE2	2.34	0.46
1:0b:31:LEU:HD22	1:0b:221:MET:HE2	1.98	0.46
1:0e:109:TYR:OH	1:0e:263:GLU:OE2	2.34	0.46
1:0i:269:ASN:OD1	1:0i:276:VAL:N	2.48	0.46
1:0j:109:TYR:OH	1:0j:263:GLU:OE2	2.34	0.46
1:0k:31:LEU:HD22	1:0k:221:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0D:10:THR:HG22	3:K:29:PHE:HZ	1.81	0.46
2:0K:9:ARG:NH2	3:c:37:GLU:OE2	2.49	0.46
1:0g:109:TYR:OH	1:0g:263:GLU:OE2	2.34	0.46
2:0A:151:LYS:O	2:0A:210:THR:N	2.49	0.46
2:0D:153:SER:OG	2:0D:154:GLY:N	2.49	0.46
1:0a:31:LEU:HD22	1:0a:221:MET:HE2	1.98	0.46
1:0a:144:LEU:HD23	1:0a:147:ILE:HD12	1.97	0.46
1:0c:31:LEU:HD22	1:0c:221:MET:HE2	1.98	0.46
2:0D:151:LYS:O	2:0D:210:THR:N	2.49	0.46
2:0F:153:SER:OG	2:0F:154:GLY:N	2.49	0.46
2:0I:151:LYS:O	2:0I:210:THR:N	2.49	0.46
2:0J:151:LYS:O	2:0J:210:THR:N	2.49	0.46
1:0d:31:LEU:HD22	1:0d:221:MET:HE2	1.98	0.46
1:0k:135:GLU:OE1	1:0l:22:ARG:NH2	2.49	0.46
2:0E:137:ASP:OD1	2:0E:137:ASP:N	2.39	0.46
2:0H:193:ILE:O	2:0H:194:GLU:CG	2.59	0.46
1:0c:135:GLU:OE1	1:0d:22:ARG:NH2	2.49	0.46
1:0g:144:LEU:HD23	1:0g:147:ILE:HD12	1.98	0.46
1:0j:31:LEU:HD22	1:0j:221:MET:HE2	1.98	0.46
1:0l:31:LEU:HD22	1:0l:221:MET:HE2	1.98	0.46
2:0C:151:LYS:O	2:0C:210:THR:N	2.49	0.46
2:0C:153:SER:OG	2:0C:154:GLY:N	2.49	0.46
2:0H:151:LYS:O	2:0H:210:THR:N	2.49	0.46
1:0g:135:GLU:OE1	1:0h:22:ARG:NH2	2.49	0.45
1:0k:109:TYR:OH	1:0k:263:GLU:OE2	2.34	0.45
2:0C:10:THR:HG22	3:H:29:PHE:HZ	1.81	0.45
2:0F:10:THR:HG22	3:N:29:PHE:HZ	1.81	0.45
2:0F:151:LYS:O	2:0F:210:THR:N	2.49	0.45
1:0d:109:TYR:OH	1:0d:263:GLU:OE2	2.34	0.45
1:0i:31:LEU:HD22	1:0i:221:MET:HE2	1.98	0.45
1:0i:135:GLU:OE1	1:0j:22:ARG:NH2	2.49	0.45
2:0E:153:SER:OG	2:0E:154:GLY:N	2.49	0.45
3:c:34:THR:HG23	3:c:37:GLU:H	1.81	0.45
1:0a:22:ARG:NH2	1:0l:135:GLU:OE1	2.49	0.45
1:0a:135:GLU:OE1	1:0b:22:ARG:NH2	2.49	0.45
1:0d:107:TYR:OH	1:0d:114:GLU:O	2.25	0.45
1:0j:135:GLU:OE1	1:0k:22:ARG:NH2	2.49	0.45
2:0E:10:THR:HG22	3:Q:29:PHE:HZ	1.82	0.45
1:0h:144:LEU:HD23	1:0h:147:ILE:HD12	1.97	0.45
1:0l:144:LEU:HD23	1:0l:147:ILE:HD12	1.97	0.45
2:0A:118:ARG:HG3	2:0B:244:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:151:LYS:O	2:0K:210:THR:N	2.49	0.45
2:0L:151:LYS:O	2:0L:210:THR:N	2.49	0.45
1:0b:269:ASN:OD1	1:0b:276:VAL:N	2.48	0.45
2:0B:153:SER:OG	2:0B:154:GLY:N	2.49	0.45
2:0I:143:THR:HA	2:0J:220:SER:HA	1.98	0.45
1:0b:135:GLU:OE1	1:0c:22:ARG:NH2	2.49	0.45
1:0h:135:GLU:OE1	1:0i:22:ARG:NH2	2.49	0.45
1:0h:269:ASN:OD1	1:0h:276:VAL:N	2.48	0.45
1:0k:144:LEU:HD23	1:0k:147:ILE:HD12	1.97	0.45
2:0B:151:LYS:O	2:0B:210:THR:N	2.49	0.45
1:0c:109:TYR:OH	1:0c:263:GLU:OE2	2.34	0.45
1:0e:45:PRO:HD2	1:0e:48:ILE:HD12	1.99	0.45
1:0h:31:LEU:HD22	1:0h:221:MET:HE2	1.98	0.45
1:0i:144:LEU:HD23	1:0i:147:ILE:HD12	1.98	0.45
1:0l:109:TYR:OH	1:0l:263:GLU:OE2	2.34	0.45
2:0G:50:ILE:O	2:0G:53:THR:OG1	2.28	0.45
2:0I:118:ARG:HG3	2:0J:244:ILE:HG12	1.99	0.45
2:0J:168:ASN:ND2	2:0K:195:GLU:OE1	2.46	0.45
1:0d:45:PRO:HD2	1:0d:48:ILE:HD12	1.99	0.45
1:0e:31:LEU:HD22	1:0e:221:MET:HE2	1.98	0.45
1:0f:45:PRO:HD2	1:0f:48:ILE:HD12	1.99	0.45
1:0j:45:PRO:HD2	1:0j:48:ILE:HD12	1.99	0.45
1:0j:144:LEU:HD23	1:0j:147:ILE:HD12	1.97	0.45
2:0G:151:LYS:O	2:0G:210:THR:N	2.49	0.45
2:0G:153:SER:OG	2:0G:154:GLY:N	2.49	0.45
2:0L:153:SER:OG	2:0L:154:GLY:N	2.49	0.45
1:0a:109:TYR:OH	1:0a:263:GLU:OE2	2.34	0.45
1:0c:45:PRO:HD2	1:0c:48:ILE:HD12	1.99	0.45
1:0f:135:GLU:OE1	1:0g:22:ARG:NH2	2.49	0.45
2:0E:151:LYS:O	2:0E:210:THR:N	2.49	0.45
2:0I:133:THR:N	2:0J:229:SER:O	2.41	0.45
3:E:34:THR:HG23	3:E:37:GLU:H	1.80	0.45
1:0b:109:TYR:OH	1:0b:263:GLU:OE2	2.34	0.45
1:0f:31:LEU:HD22	1:0f:221:MET:HE2	1.98	0.45
1:0h:173:GLN:NE2	3:X:25:LEU:O	2.50	0.45
1:0i:45:PRO:HD2	1:0i:48:ILE:HD12	1.99	0.45
1:0k:45:PRO:HD2	1:0k:48:ILE:HD12	1.99	0.45
3:P:68:LEU:O	3:U:4:LYS:NZ	2.49	0.45
1:0b:45:PRO:HD2	1:0b:48:ILE:HD12	1.99	0.44
1:0f:269:ASN:OD1	1:0f:276:VAL:N	2.48	0.44
1:0g:31:LEU:HD22	1:0g:221:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:153:SER:OG	2:0K:154:GLY:N	2.49	0.44
1:0c:126:MET:HG3	1:0c:128:PHE:HB2	2.00	0.44
1:0j:45:PRO:HA	1:0j:46:PRO:HD3	1.88	0.44
2:0I:153:SER:OG	2:0I:154:GLY:N	2.49	0.44
1:0f:126:MET:HG3	1:0f:128:PHE:HB2	2.00	0.44
1:0g:126:MET:HG3	1:0g:128:PHE:HB2	2.00	0.44
2:0A:153:SER:OG	2:0A:154:GLY:N	2.49	0.44
2:0H:153:SER:OG	2:0H:154:GLY:N	2.49	0.44
1:0a:45:PRO:HD2	1:0a:48:ILE:HD12	1.99	0.44
1:0b:126:MET:HG3	1:0b:128:PHE:HB2	2.00	0.44
1:0h:126:MET:HG3	1:0h:128:PHE:HB2	2.00	0.44
2:0J:153:SER:OG	2:0J:154:GLY:N	2.49	0.44
1:0d:126:MET:HG3	1:0d:128:PHE:HB2	2.00	0.44
1:0g:45:PRO:HD2	1:0g:48:ILE:HD12	1.99	0.44
2:0I:137:ASP:OD1	2:0I:137:ASP:N	2.39	0.44
3:R:49:ILE:HA	3:R:52:VAL:HG12	2.00	0.44
1:0a:126:MET:HG3	1:0a:128:PHE:HB2	2.00	0.44
1:0a:269:ASN:OD1	1:0a:276:VAL:N	2.48	0.44
1:0g:269:ASN:OD1	1:0g:276:VAL:N	2.48	0.44
1:0j:126:MET:HG3	1:0j:128:PHE:HB2	2.00	0.44
2:0I:147:THR:OG1	2:0J:215:ASN:O	2.28	0.44
2:0J:150:GLU:N	2:0K:213:THR:O	2.42	0.44
3:I:49:ILE:HA	3:I:52:VAL:HG12	2.00	0.44
3:U:49:ILE:HA	3:U:52:VAL:HG12	2.00	0.44
1:0e:126:MET:HG3	1:0e:128:PHE:HB2	2.00	0.44
1:0i:45:PRO:HA	1:0i:46:PRO:HD3	1.88	0.44
1:0i:126:MET:HG3	1:0i:128:PHE:HB2	2.00	0.44
1:0l:126:MET:HG3	1:0l:128:PHE:HB2	2.00	0.44
2:0C:7:GLN:HA	2:0C:63:GLU:HA	2.00	0.44
2:0F:7:GLN:HA	2:0F:63:GLU:HA	2.00	0.44
2:0I:81:MET:HB3	2:0J:54:HIS:NE2	2.33	0.44
1:0h:45:PRO:HD2	1:0h:48:ILE:HD12	1.99	0.44
1:0k:126:MET:HG3	1:0k:128:PHE:HB2	2.00	0.44
2:0D:7:GLN:HA	2:0D:63:GLU:HA	2.00	0.44
3:L:49:ILE:HA	3:L:52:VAL:HG12	2.00	0.44
3:O:49:ILE:HA	3:O:52:VAL:HG12	2.00	0.44
3:X:49:ILE:HA	3:X:52:VAL:HG12	2.00	0.44
1:0k:107:TYR:OH	1:0k:114:GLU:O	2.25	0.44
1:0l:45:PRO:HD2	1:0l:48:ILE:HD12	1.99	0.44
2:0E:7:GLN:HA	2:0E:63:GLU:HA	2.00	0.44
1:0a:189:GLU:HA	1:0l:162:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0k:45:PRO:HA	1:0k:46:PRO:HD3	1.88	0.43
2:0B:7:GLN:HA	2:0B:63:GLU:HA	2.00	0.43
2:0G:7:GLN:HA	2:0G:63:GLU:HA	2.00	0.43
2:0H:7:GLN:HA	2:0H:63:GLU:HA	2.00	0.43
2:0I:7:GLN:HA	2:0I:63:GLU:HA	2.00	0.43
1:0b:45:PRO:HA	1:0b:46:PRO:HD3	1.88	0.43
2:0J:7:GLN:HA	2:0J:63:GLU:HA	2.00	0.43
3:F:49:ILE:HA	3:F:52:VAL:HG12	2.00	0.43
2:0A:7:GLN:HA	2:0A:63:GLU:HA	2.00	0.43
2:0A:151:LYS:HA	2:0B:212:THR:HA	2.00	0.43
2:0A:159:THR:HG23	2:0B:204:THR:HB	1.99	0.43
2:0L:7:GLN:HA	2:0L:63:GLU:HA	2.00	0.43
1:0g:13:ASN:HB3	3:a:23:ARG:HD3	2.00	0.43
1:0i:107:TYR:OH	1:0i:114:GLU:O	2.25	0.43
2:0K:7:GLN:HA	2:0K:63:GLU:HA	2.00	0.43
1:0k:162:ARG:HB3	1:0l:189:GLU:HA	2.01	0.43
2:0E:68:THR:HG23	2:0E:71:LEU:H	1.84	0.43
2:0F:137:ASP:OD1	2:0F:137:ASP:N	2.39	0.43
2:0H:68:THR:HG23	2:0H:71:LEU:H	1.84	0.43
2:0J:68:THR:HG23	2:0J:71:LEU:H	1.84	0.43
3:a:49:ILE:HA	3:a:52:VAL:HG12	2.00	0.43
1:0a:162:ARG:HB3	1:0b:189:GLU:HA	2.01	0.43
1:0e:159:VAL:HB	1:0f:184:VAL:HG22	2.01	0.43
1:0f:162:ARG:HB3	1:0g:189:GLU:HA	2.01	0.43
2:0A:68:THR:HG23	2:0A:71:LEU:H	1.84	0.43
2:0D:25:ALA:HA	2:0D:28:ILE:HD12	2.00	0.43
2:0D:68:THR:HG23	2:0D:71:LEU:H	1.84	0.43
2:0G:79:TRP:HH2	2:0G:281:ILE:HG23	1.84	0.43
2:0J:25:ALA:HA	2:0J:28:ILE:HD12	2.00	0.43
3:X:59:GLU:HG3	3:a:9:ARG:HG2	2.01	0.43
1:0l:45:PRO:HA	1:0l:46:PRO:HD3	1.88	0.43
2:0F:25:ALA:HA	2:0F:28:ILE:HD12	2.00	0.43
2:0J:81:MET:HB3	2:0K:54:HIS:NE2	2.34	0.43
3:C:49:ILE:HA	3:C:52:VAL:HG12	2.00	0.43
2:0C:75:HIS:HA	2:0C:78:THR:HB	2.01	0.43
2:0D:75:HIS:HA	2:0D:78:THR:HB	2.01	0.43
2:0E:25:ALA:HA	2:0E:28:ILE:HD12	2.00	0.43
2:0G:25:ALA:HA	2:0G:28:ILE:HD12	2.00	0.43
2:0G:75:HIS:HA	2:0G:78:THR:HB	2.01	0.43
1:0b:162:ARG:HB3	1:0c:189:GLU:HA	2.01	0.43
2:0A:25:ALA:HA	2:0A:28:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0B:68:THR:HG23	2:0B:71:LEU:H	1.84	0.43
2:0B:75:HIS:HA	2:0B:78:THR:HB	2.01	0.43
2:0C:68:THR:HG23	2:0C:71:LEU:H	1.84	0.43
2:0H:75:HIS:HA	2:0H:78:THR:HB	2.01	0.43
2:0L:68:THR:HG23	2:0L:71:LEU:H	1.84	0.43
1:0g:162:ARG:HB3	1:0h:189:GLU:HA	2.01	0.42
3:d:49:ILE:HA	3:d:52:VAL:HG12	2.00	0.42
1:0e:12:ILE:HD11	1:0g:183:PRO:HD2	2.01	0.42
1:0j:162:ARG:HB3	1:0k:189:GLU:HA	2.01	0.42
2:0C:25:ALA:HA	2:0C:28:ILE:HD12	2.00	0.42
2:0E:75:HIS:HA	2:0E:78:THR:HB	2.01	0.42
2:0E:156:GLY:HA2	2:0E:205:LYS:HA	2.01	0.42
2:0I:75:HIS:HA	2:0I:78:THR:HB	2.01	0.42
2:0J:79:TRP:HH2	2:0J:281:ILE:HG23	1.84	0.42
2:0K:25:ALA:HA	2:0K:28:ILE:HD12	2.00	0.42
1:0h:45:PRO:HA	1:0h:46:PRO:HD3	1.88	0.42
2:0A:75:HIS:HA	2:0A:78:THR:HB	2.01	0.42
2:0F:75:HIS:HA	2:0F:78:THR:HB	2.01	0.42
2:0F:156:GLY:HA2	2:0F:205:LYS:HA	2.01	0.42
2:0H:25:ALA:HA	2:0H:28:ILE:HD12	2.00	0.42
2:0H:79:TRP:HH2	2:0H:281:ILE:HG23	1.84	0.42
2:0J:75:HIS:HA	2:0J:78:THR:HB	2.01	0.42
2:0K:75:HIS:HA	2:0K:78:THR:HB	2.01	0.42
3:j:49:ILE:HA	3:j:52:VAL:HG12	2.00	0.42
1:0b:107:TYR:N	1:0b:118:GLY:O	2.52	0.42
2:0A:244:ILE:HG12	2:0L:118:ARG:HG3	2.02	0.42
2:0G:156:GLY:HA2	2:0G:205:LYS:HA	2.01	0.42
2:0K:68:THR:HG23	2:0K:71:LEU:H	1.84	0.42
1:0c:171:LEU:HD23	1:0c:171:LEU:HA	1.90	0.42
2:0D:156:GLY:HA2	2:0D:205:LYS:HA	2.01	0.42
2:0F:79:TRP:HH2	2:0F:281:ILE:HG23	1.84	0.42
2:0H:137:ASP:N	2:0H:137:ASP:OD1	2.39	0.42
2:0L:75:HIS:HA	2:0L:78:THR:HB	2.01	0.42
3:g:49:ILE:HA	3:g:52:VAL:HG12	2.00	0.42
1:0c:162:ARG:HB3	1:0d:189:GLU:HA	2.01	0.42
1:0d:45:PRO:HA	1:0d:46:PRO:HD3	1.88	0.42
1:0h:162:ARG:HB3	1:0i:189:GLU:HA	2.01	0.42
2:0E:79:TRP:HH2	2:0E:281:ILE:HG23	1.84	0.42
2:0H:156:GLY:HA2	2:0H:205:LYS:HA	2.01	0.42
2:0I:25:ALA:HA	2:0I:28:ILE:HD12	2.00	0.42
2:0I:79:TRP:HH2	2:0I:281:ILE:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0J:151:LYS:HA	2:0K:212:THR:HA	2.01	0.42
2:0L:25:ALA:HA	2:0L:28:ILE:HD12	2.00	0.42
1:0a:107:TYR:N	1:0a:118:GLY:O	2.52	0.42
1:0c:107:TYR:N	1:0c:118:GLY:O	2.53	0.42
1:0j:81:SER:OG	1:0j:82:GLY:N	2.53	0.42
2:0A:158:ILE:HD11	2:0B:205:LYS:HE2	2.02	0.42
2:0K:147:THR:O	2:0K:214:SER:N	2.44	0.42
1:0i:24:PHE:HB2	3:b:24:TYR:CE1	2.55	0.42
1:0i:81:SER:OG	1:0i:82:GLY:N	2.53	0.42
1:0j:107:TYR:N	1:0j:118:GLY:O	2.52	0.42
2:0C:156:GLY:HA2	2:0C:205:LYS:HA	2.01	0.42
2:0G:155:SER:OG	2:0G:156:GLY:N	2.53	0.42
2:0I:68:THR:HG23	2:0I:71:LEU:H	1.84	0.42
1:0b:24:PHE:HB2	3:G:24:TYR:CE1	2.55	0.42
1:0k:24:PHE:HB2	3:h:24:TYR:CE1	2.55	0.42
1:0k:107:TYR:N	1:0k:118:GLY:O	2.52	0.42
1:0l:24:PHE:HB2	3:A:24:TYR:CE1	2.55	0.42
2:0B:25:ALA:HA	2:0B:28:ILE:HD12	2.00	0.42
2:0D:79:TRP:HH2	2:0D:281:ILE:HG23	1.84	0.42
2:0F:68:THR:HG23	2:0F:71:LEU:H	1.84	0.42
2:0G:68:THR:HG23	2:0G:71:LEU:H	1.84	0.42
1:0a:24:PHE:HB2	3:D:24:TYR:CE1	2.55	0.42
1:0b:81:SER:OG	1:0b:82:GLY:N	2.53	0.42
1:0e:13:ASN:HB3	3:U:23:ARG:HD3	2.02	0.42
1:0e:164:ASN:HA	1:0f:188:HIS:NE2	2.35	0.42
2:0A:79:TRP:HH2	2:0A:281:ILE:HG23	1.84	0.42
2:0A:195:GLU:OE1	2:0L:168:ASN:ND2	2.48	0.42
2:0F:155:SER:OG	2:0F:156:GLY:N	2.53	0.42
2:0I:144:SER:N	2:0J:219:THR:O	2.52	0.42
2:0L:79:TRP:HH2	2:0L:281:ILE:HG23	1.84	0.42
1:0e:24:PHE:HB2	3:P:24:TYR:CE1	2.55	0.41
1:0j:32:GLN:HA	1:0j:134:LEU:HD13	2.02	0.41
1:0k:81:SER:OG	1:0k:82:GLY:N	2.53	0.41
2:0I:156:GLY:HA2	2:0I:205:LYS:HA	2.01	0.41
1:0d:107:TYR:N	1:0d:118:GLY:O	2.52	0.41
1:0h:107:TYR:N	1:0h:118:GLY:O	2.52	0.41
2:0I:142:ASP:N	2:0J:221:THR:O	2.52	0.41
2:0I:155:SER:OG	2:0I:156:GLY:N	2.53	0.41
2:0I:159:THR:HG23	2:0J:204:THR:HB	2.01	0.41
1:0a:32:GLN:HA	1:0a:134:LEU:HD13	2.03	0.41
1:0c:24:PHE:HB2	3:J:24:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0c:81:SER:OG	1:0c:82:GLY:N	2.53	0.41
1:0i:32:GLN:HA	1:0i:134:LEU:HD13	2.03	0.41
1:0i:107:TYR:N	1:0i:118:GLY:O	2.52	0.41
1:0l:32:GLN:HA	1:0l:134:LEU:HD13	2.03	0.41
2:0B:79:TRP:HH2	2:0B:281:ILE:HG23	1.84	0.41
2:0B:156:GLY:HA2	2:0B:205:LYS:HA	2.01	0.41
2:0C:50:ILE:O	2:0C:53:THR:OG1	2.28	0.41
2:0C:118:ARG:HG3	2:0D:244:ILE:HG12	2.02	0.41
2:0D:137:ASP:OD1	2:0D:137:ASP:N	2.39	0.41
2:0K:79:TRP:HH2	2:0K:281:ILE:HG23	1.84	0.41
1:0h:171:LEU:HD23	1:0h:171:LEU:HA	1.90	0.41
1:0k:32:GLN:HA	1:0k:134:LEU:HD13	2.02	0.41
2:0A:24:THR:OG1	3:i:31:GLU:OE2	2.38	0.41
2:0B:9:ARG:HH12	3:B:33:LEU:HB2	1.86	0.41
2:0J:156:GLY:HA2	2:0J:205:LYS:HA	2.01	0.41
1:0a:81:SER:OG	1:0a:82:GLY:N	2.53	0.41
1:0b:32:GLN:HA	1:0b:134:LEU:HD13	2.03	0.41
2:0A:156:GLY:HA2	2:0A:205:LYS:HA	2.01	0.41
2:0H:168:ASN:ND2	2:0I:195:GLU:OE1	2.50	0.41
2:0K:249:ASP:OD1	2:0K:249:ASP:N	2.54	0.41
3:E:42:ILE:HA	3:E:45:TYR:HD2	1.85	0.41
1:0f:81:SER:OG	1:0f:82:GLY:N	2.53	0.41
1:0g:24:PHE:HB2	3:V:24:TYR:CE1	2.55	0.41
1:0h:32:GLN:HA	1:0h:134:LEU:HD13	2.03	0.41
1:0h:81:SER:OG	1:0h:82:GLY:N	2.53	0.41
1:0l:81:SER:OG	1:0l:82:GLY:N	2.53	0.41
1:0l:107:TYR:N	1:0l:118:GLY:O	2.53	0.41
2:0D:155:SER:OG	2:0D:156:GLY:N	2.53	0.41
2:0J:155:SER:OG	2:0J:156:GLY:N	2.53	0.41
2:0J:249:ASP:OD1	2:0J:249:ASP:N	2.54	0.41
1:0j:24:PHE:HB2	3:e:24:TYR:CE1	2.55	0.41
2:0D:118:ARG:HG3	2:0F:244:ILE:HG12	2.02	0.41
2:0E:155:SER:OG	2:0E:156:GLY:N	2.53	0.41
3:Z:42:ILE:HA	3:Z:45:TYR:HD2	1.86	0.41
1:0c:32:GLN:HA	1:0c:134:LEU:HD13	2.03	0.41
1:0d:171:LEU:HD23	1:0d:171:LEU:HA	1.90	0.41
1:0g:32:GLN:HA	1:0g:134:LEU:HD13	2.03	0.41
1:0h:24:PHE:HB2	3:Y:24:TYR:CE1	2.55	0.41
1:0k:165:ASP:OD2	2:0K:62:ARG:HD2	2.20	0.41
2:0C:155:SER:OG	2:0C:156:GLY:N	2.53	0.41
2:0E:9:ARG:NH2	3:N:37:GLU:OE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0K:156:GLY:HA2	2:0K:205:LYS:HA	2.01	0.41
2:0L:156:GLY:HA2	2:0L:205:LYS:HA	2.01	0.41
1:0d:24:PHE:HB2	3:M:24:TYR:CE1	2.55	0.41
1:0d:32:GLN:HA	1:0d:134:LEU:HD13	2.03	0.41
1:0e:32:GLN:HA	1:0e:134:LEU:HD13	2.03	0.41
1:0f:32:GLN:HA	1:0f:134:LEU:HD13	2.03	0.41
1:0g:171:LEU:HD23	1:0g:171:LEU:HA	1.90	0.41
1:0i:9:TYR:HD1	3:Y:31:GLU:HB2	1.86	0.41
1:0i:162:ARG:HB3	1:0j:189:GLU:HA	2.01	0.41
1:0i:171:LEU:HD23	1:0i:171:LEU:HA	1.90	0.41
2:0C:79:TRP:HH2	2:0C:281:ILE:HG23	1.84	0.41
2:0E:147:THR:O	2:0E:214:SER:N	2.44	0.41
2:0E:244:ILE:HG12	2:0F:118:ARG:HG3	2.02	0.41
2:0L:249:ASP:OD1	2:0L:249:ASP:N	2.54	0.41
1:0e:81:SER:OG	1:0e:82:GLY:N	2.53	0.41
1:0l:9:TYR:HD1	3:h:31:GLU:HB2	1.86	0.41
2:0K:155:SER:OG	2:0K:156:GLY:N	2.53	0.41
3:T:50:GLY:O	3:T:54:ASN:ND2	2.54	0.41
2:0E:118:ARG:HG3	2:0G:244:ILE:HG12	2.02	0.40
2:0F:169:ALA:CB	2:0F:192:GLN:CB	2.99	0.40
2:0H:9:ARG:NH2	3:T:37:GLU:OE2	2.55	0.40
2:0H:118:ARG:HG3	2:0I:244:ILE:HG12	2.02	0.40
1:0f:171:LEU:HD23	1:0f:171:LEU:HA	1.90	0.40
1:0j:9:TYR:HD1	3:b:31:GLU:HB2	1.87	0.40
2:0A:155:SER:OG	2:0A:156:GLY:N	2.53	0.40
2:0F:9:ARG:NH2	3:K:37:GLU:OE2	2.54	0.40
1:0e:107:TYR:N	1:0e:118:GLY:O	2.53	0.40
2:0G:118:ARG:HG3	2:0H:244:ILE:HG12	2.02	0.40
2:0I:249:ASP:OD1	2:0I:249:ASP:N	2.54	0.40
1:0e:125:ASP:OD2	1:0f:37:GLN:NE2	2.43	0.40
1:0i:174:VAL:O	1:0i:178:TYR:N	2.51	0.40
1:0k:9:TYR:HD1	3:e:31:GLU:HB2	1.87	0.40
1:0k:173:GLN:NE2	3:g:25:LEU:O	2.55	0.40
2:0D:249:ASP:N	2:0D:249:ASP:OD1	2.54	0.40
2:0F:249:ASP:N	2:0F:249:ASP:OD1	2.54	0.40
2:0G:9:ARG:NH2	3:Q:37:GLU:OE2	2.54	0.40
2:0I:9:ARG:NH2	3:W:37:GLU:OE2	2.54	0.40
3:B:50:GLY:O	3:B:54:ASN:ND2	2.55	0.40
3:H:42:ILE:HA	3:H:45:TYR:HD2	1.86	0.40
1:0d:86:VAL:HG21	1:0e:74:ILE:HD11	2.04	0.40
1:0f:24:PHE:HB2	3:S:24:TYR:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0h:174:VAL:O	1:0h:178:TYR:N	2.51	0.40
1:0j:174:VAL:O	1:0j:178:TYR:N	2.51	0.40
2:0C:249:ASP:N	2:0C:249:ASP:OD1	2.54	0.40
2:0J:273:ALA:O	2:0K:271:ARG:NH1	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0a	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0b	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0c	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0d	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0e	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0f	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0g	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0h	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0i	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0j	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0k	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
1	0l	260/309 (84%)	243 (94%)	17 (6%)	0	100	100
2	0A	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0B	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0C	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0D	289/293 (99%)	272 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0E	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0F	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0G	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0H	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0I	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0J	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0K	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
2	0L	289/293 (99%)	272 (94%)	17 (6%)	0	100	100
3	A	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	B	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	C	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	D	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	E	55/854 (6%)	51 (93%)	3 (6%)	1 (2%)	6	29
3	F	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	G	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	H	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	I	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	J	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	K	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	L	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	M	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	N	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	O	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	P	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	Q	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	R	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	S	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	T	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	U	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	V	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	W	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	X	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	Y	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	Z	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	a	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	b	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	c	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	d	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	e	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	f	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	g	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
3	h	49/854 (6%)	42 (86%)	7 (14%)	0	100	100
3	i	55/854 (6%)	52 (94%)	2 (4%)	1 (2%)	6	29
3	j	69/854 (8%)	63 (91%)	6 (9%)	0	100	100
All	All	8664/37968 (23%)	8063 (93%)	589 (7%)	12 (0%)	49	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	19	GLN
3	E	19	GLN
3	H	19	GLN
3	K	19	GLN
3	N	19	GLN
3	Q	19	GLN
3	T	19	GLN
3	W	19	GLN
3	Z	19	GLN
3	c	19	GLN
3	f	19	GLN
3	i	19	GLN

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	236/277 (85%)	236 (100%)	0	100	100
1	0b	236/277 (85%)	236 (100%)	0	100	100
1	0c	236/277 (85%)	236 (100%)	0	100	100
1	0d	236/277 (85%)	236 (100%)	0	100	100
1	0e	236/277 (85%)	236 (100%)	0	100	100
1	0f	236/277 (85%)	236 (100%)	0	100	100
1	0g	236/277 (85%)	236 (100%)	0	100	100
1	0h	236/277 (85%)	236 (100%)	0	100	100
1	0i	236/277 (85%)	236 (100%)	0	100	100
1	0j	236/277 (85%)	236 (100%)	0	100	100
1	0k	236/277 (85%)	236 (100%)	0	100	100
1	0l	236/277 (85%)	236 (100%)	0	100	100
2	0A	249/270 (92%)	249 (100%)	0	100	100
2	0B	249/270 (92%)	249 (100%)	0	100	100
2	0C	249/270 (92%)	249 (100%)	0	100	100
2	0D	249/270 (92%)	249 (100%)	0	100	100
2	0E	249/270 (92%)	249 (100%)	0	100	100
2	0F	249/270 (92%)	249 (100%)	0	100	100
2	0G	249/270 (92%)	249 (100%)	0	100	100
2	0H	249/270 (92%)	249 (100%)	0	100	100
2	0I	249/270 (92%)	249 (100%)	0	100	100
2	0J	249/270 (92%)	249 (100%)	0	100	100
2	0K	249/270 (92%)	249 (100%)	0	100	100
2	0L	249/270 (92%)	249 (100%)	0	100	100
3	A	48/706 (7%)	48 (100%)	0	100	100
3	B	54/706 (8%)	54 (100%)	0	100	100
3	C	67/706 (10%)	67 (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	67/706 (10%)	67 (100%)	0	100	100
3	G	48/706 (7%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	54/706 (8%)	54 (100%)	0	100	100
3	I	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (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	67/706 (10%)	67 (100%)	0	100	100
3	h	48/706 (7%)	48 (100%)	0	100	100
3	i	54/706 (8%)	54 (100%)	0	100	100
3	j	67/706 (10%)	67 (100%)	0	100	100
All	All	7848/31980 (24%)	7848 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	0a	16	GLN
1	0a	173	GLN
1	0b	16	GLN
1	0b	173	GLN
1	0c	16	GLN
1	0d	16	GLN
1	0d	168	GLN
1	0d	173	GLN
1	0e	16	GLN
1	0e	168	GLN
1	0f	16	GLN
1	0g	16	GLN
1	0g	168	GLN
1	0h	16	GLN
1	0h	21	ASN
1	0h	168	GLN
1	0i	16	GLN
1	0i	168	GLN
1	0j	16	GLN
1	0j	173	GLN
1	0k	16	GLN
1	0k	168	GLN
1	0l	16	GLN
1	0l	168	GLN
2	0A	7	GLN
2	0A	126	GLN
2	0A	162	ASN
2	0A	196	HIS
2	0A	279	GLN
2	0B	7	GLN
2	0B	126	GLN
2	0B	162	ASN
2	0B	196	HIS
2	0C	7	GLN
2	0C	126	GLN
2	0C	141	ASN
2	0C	162	ASN
2	0C	196	HIS
2	0C	199	ASN
2	0C	279	GLN
2	0D	7	GLN

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Mol	Chain	Res	Type
2	0D	126	GLN
2	0D	141	ASN
2	0D	162	ASN
2	0D	196	HIS
2	0D	279	GLN
2	0E	7	GLN
2	0E	126	GLN
2	0E	162	ASN
2	0E	196	HIS
2	0E	279	GLN
2	0F	7	GLN
2	0F	126	GLN
2	0F	162	ASN
2	0F	196	HIS
2	0F	199	ASN
2	0F	279	GLN
2	0G	7	GLN
2	0G	126	GLN
2	0G	162	ASN
2	0G	196	HIS
2	0G	279	GLN
2	0H	7	GLN
2	0H	126	GLN
2	0H	141	ASN
2	0H	162	ASN
2	0H	196	HIS
2	0H	199	ASN
2	0H	279	GLN
2	0I	7	GLN
2	0I	162	ASN
2	0I	196	HIS
2	0I	199	ASN
2	0I	279	GLN
2	0J	7	GLN
2	0J	126	GLN
2	0J	141	ASN
2	0J	162	ASN
2	0J	196	HIS
2	0K	7	GLN
2	0K	103	ASN
2	0K	126	GLN
2	0K	162	ASN

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Mol	Chain	Res	Type
2	0K	196	HIS
2	0K	199	ASN
2	0L	7	GLN
2	0L	126	GLN
2	0L	141	ASN
2	0L	162	ASN
2	0L	196	HIS
2	0L	279	GLN
3	A	61	ASN
3	B	54	ASN
3	B	61	ASN
3	D	61	ASN
3	E	54	ASN
3	E	61	ASN
3	H	54	ASN
3	H	61	ASN
3	J	61	ASN
3	K	54	ASN
3	K	61	ASN
3	M	61	ASN
3	N	54	ASN
3	N	61	ASN
3	P	61	ASN
3	Q	54	ASN
3	Q	61	ASN
3	S	61	ASN
3	T	54	ASN
3	T	61	ASN
3	V	61	ASN
3	W	54	ASN
3	W	61	ASN
3	Y	61	ASN
3	Z	54	ASN
3	Z	61	ASN
3	a	19	GLN
3	b	61	ASN
3	c	54	ASN
3	c	61	ASN
3	e	61	ASN
3	f	54	ASN
3	f	61	ASN
3	h	61	ASN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

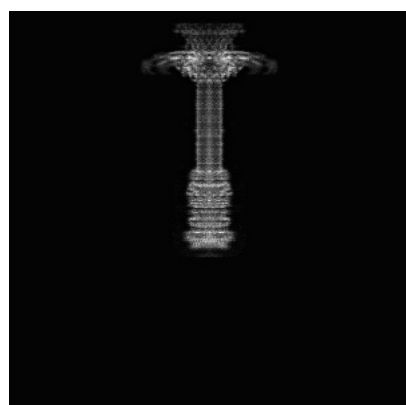
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4684. These allow visual inspection of the internal detail of the map and identification of artifacts.

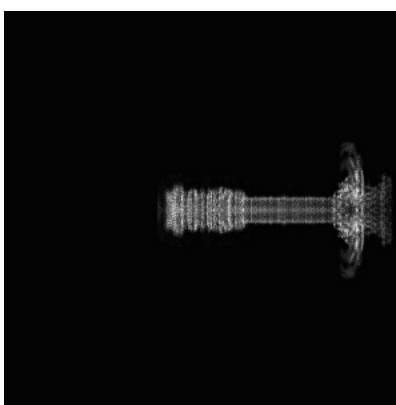
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

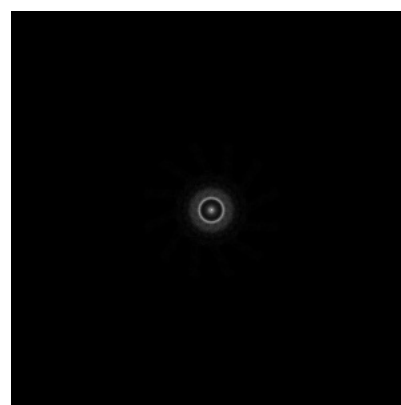
6.1.1 Primary map



X



Y

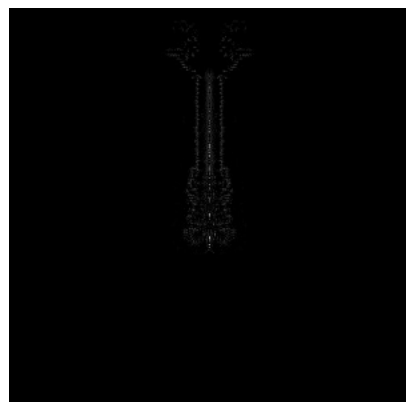


Z

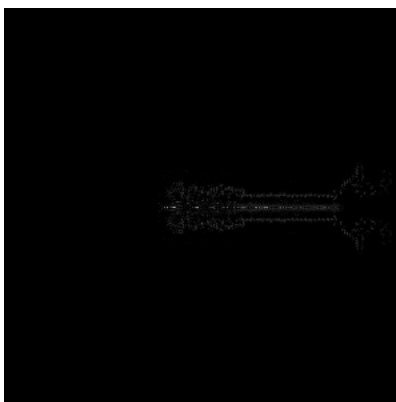
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

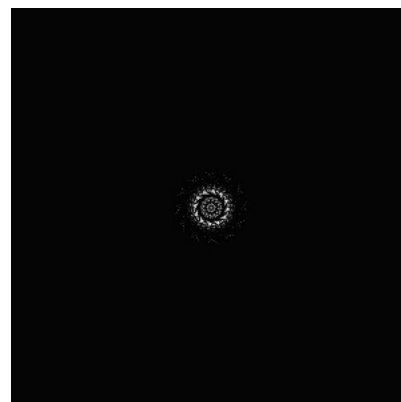
6.2.1 Primary map



X Index: 286



Y Index: 286

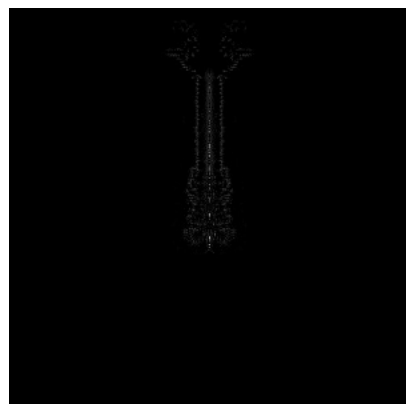


Z Index: 286

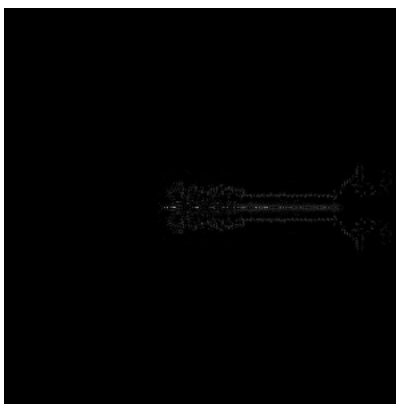
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

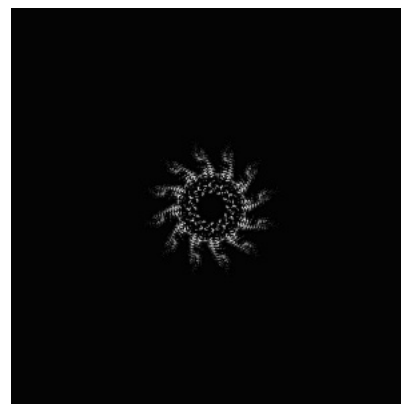
6.3.1 Primary map



X Index: 286



Y Index: 286

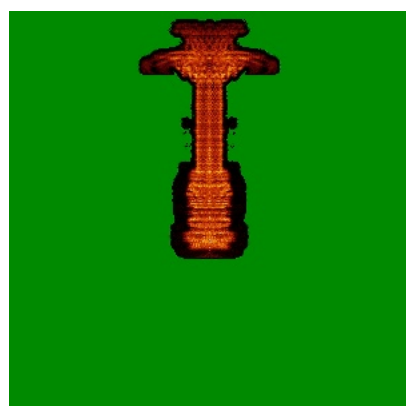


Z Index: 504

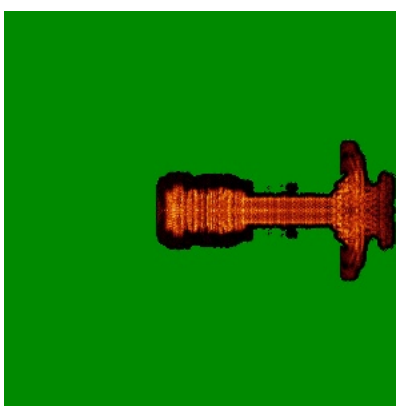
The images above show the largest variance slices of the map in three orthogonal directions.

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

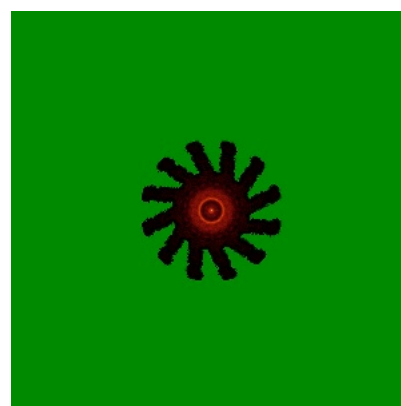
6.4.1 Primary map



X



Y

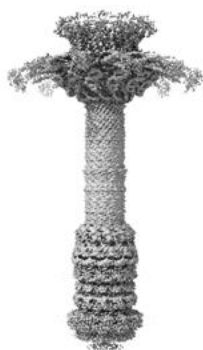


Z

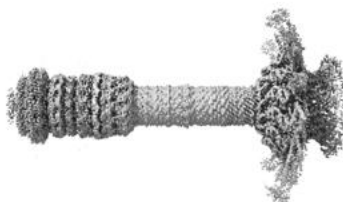
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

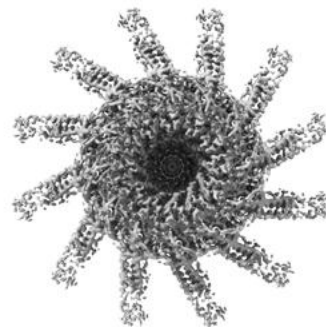
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

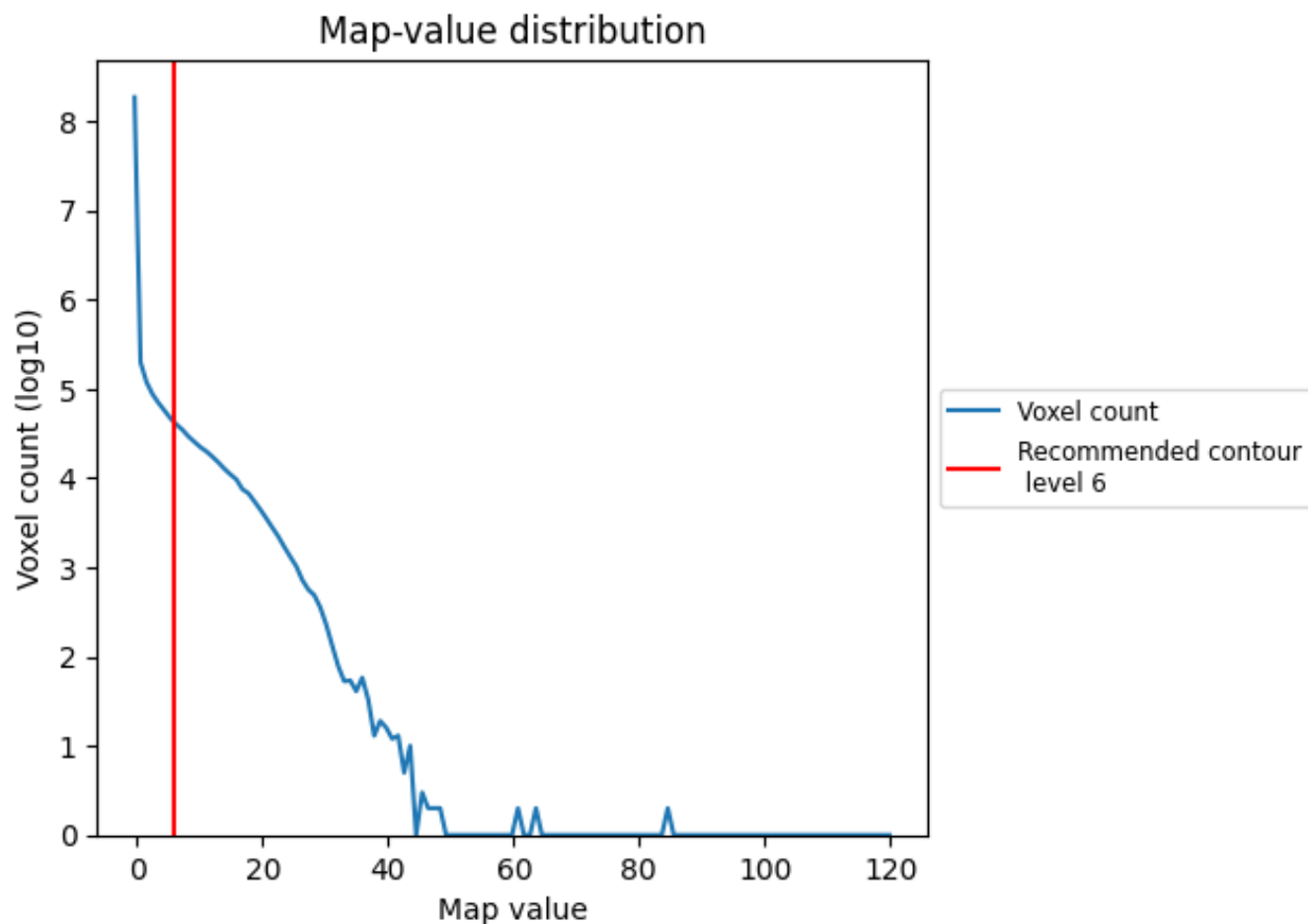
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

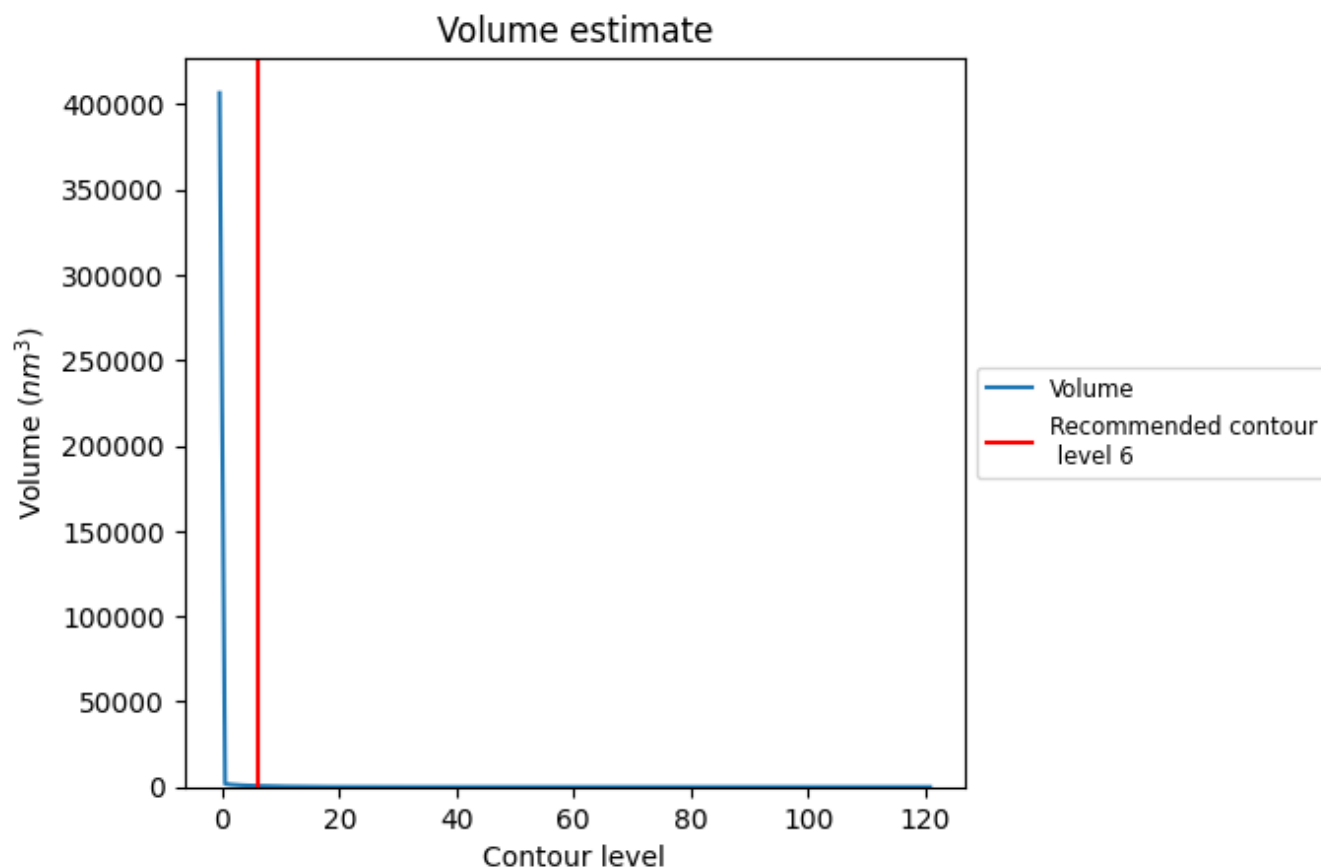
This section contains the results of statistical analysis of the map.

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.

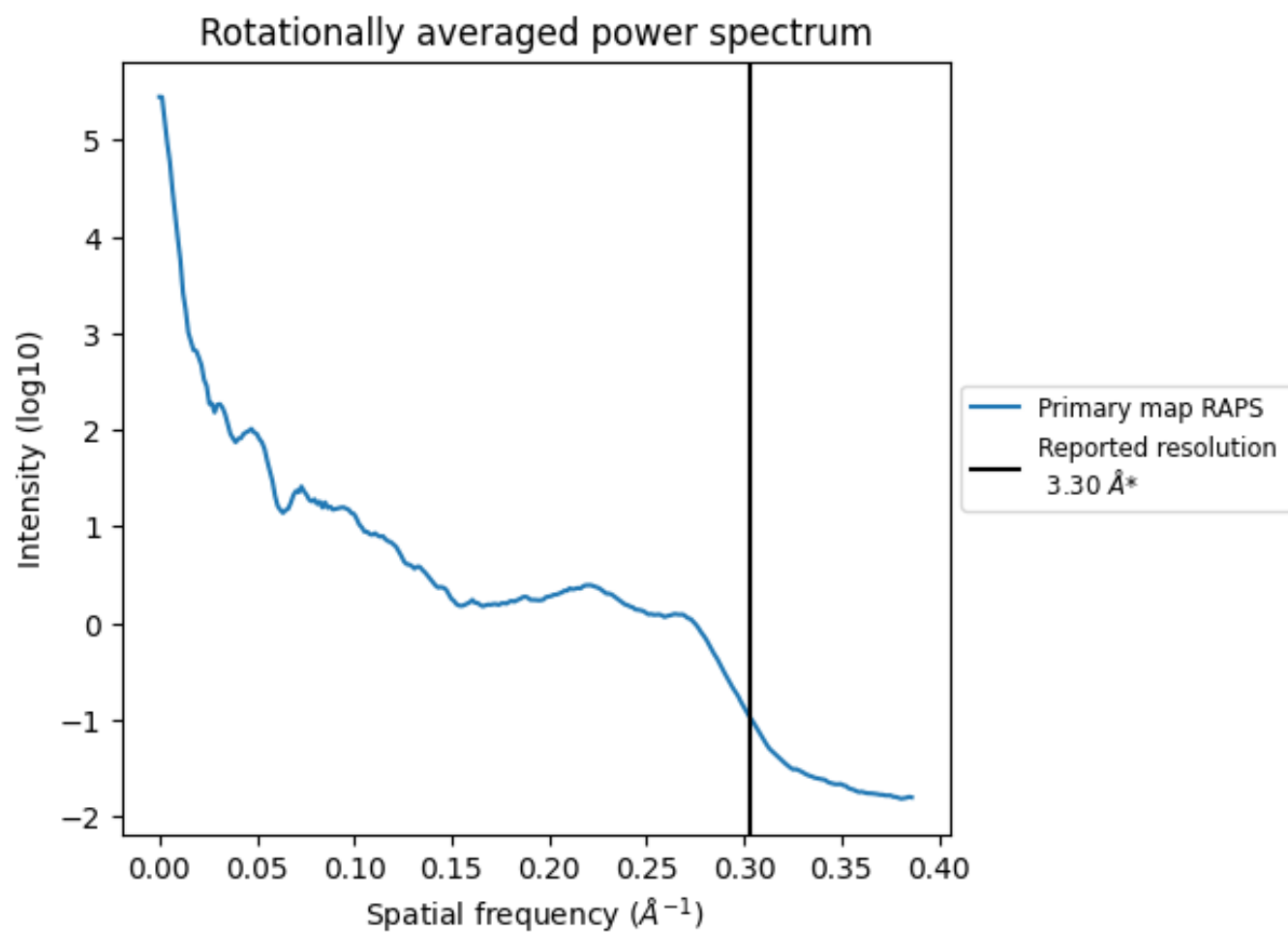
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 630 nm^3 ; this corresponds to an approximate mass of 569 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 0.303 Å⁻¹

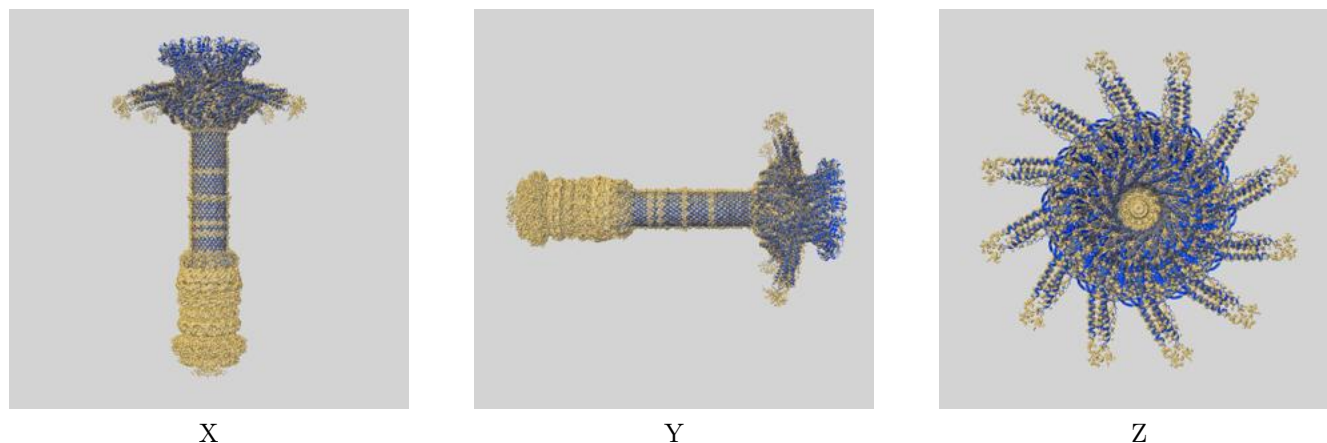
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

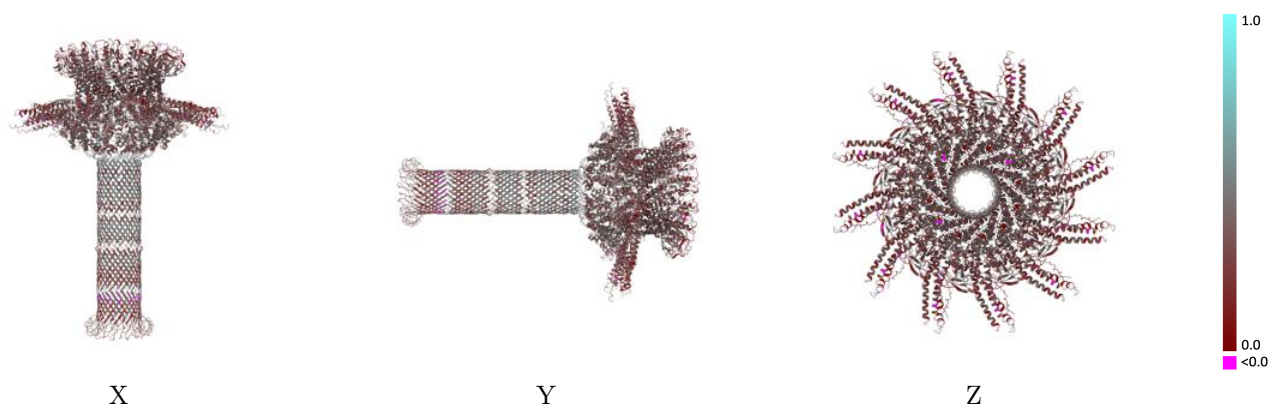
This section contains information regarding the fit between EMDB map EMD-4684 and PDB model 6QZ9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 6.0 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](#)

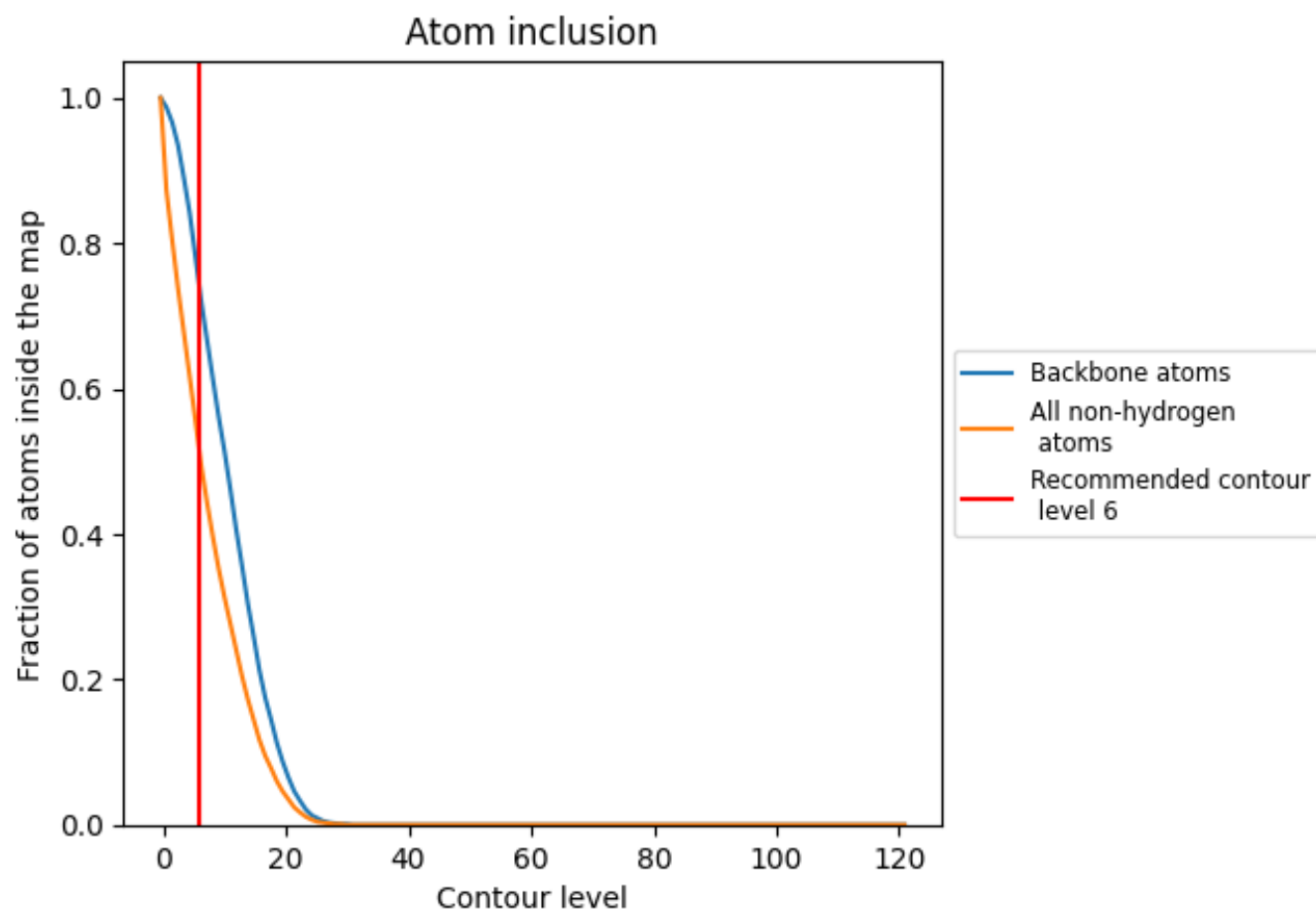


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 51% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5070	0.3310
0A	0.7320	0.3750
0B	0.7270	0.3720
0C	0.7330	0.3750
0D	0.7320	0.3750
0E	0.7330	0.3750
0F	0.7340	0.3740
0G	0.7320	0.3730
0H	0.7330	0.3730
0I	0.7320	0.3730
0J	0.7300	0.3730
0K	0.7250	0.3710
0L	0.7330	0.3740
0a	0.3370	0.3190
0b	0.3360	0.3170
0c	0.3380	0.3160
0d	0.3370	0.3180
0e	0.3370	0.3170
0f	0.3380	0.3160
0g	0.3370	0.3180
0h	0.3360	0.3180
0i	0.3370	0.3170
0j	0.3370	0.3190
0k	0.3360	0.3180
0l	0.3370	0.3180
A	0.4250	0.2620
B	0.4590	0.2920
C	0.3620	0.3070
D	0.4200	0.2620
E	0.4590	0.2880
F	0.3650	0.3080
G	0.4270	0.2610
H	0.4550	0.2910
I	0.3590	0.3070
J	0.4250	0.2650



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Chain	Atom inclusion	Q-score
K	 0.4610	 0.2900
L	 0.3620	 0.3050
M	 0.4220	 0.2610
N	 0.4610	 0.2880
O	 0.3650	 0.3060
P	 0.4300	 0.2600
Q	 0.4530	 0.2880
R	 0.3590	 0.3040
S	 0.4250	 0.2640
T	 0.4610	 0.2910
U	 0.3640	 0.3030
V	 0.4200	 0.2600
W	 0.4610	 0.2870
X	 0.3670	 0.3060
Y	 0.4270	 0.2600
Z	 0.4480	 0.2880
a	 0.3640	 0.3020
b	 0.4200	 0.2580
c	 0.4610	 0.2880
d	 0.3620	 0.3060
e	 0.4150	 0.2610
f	 0.4550	 0.2880
g	 0.3720	 0.3020
h	 0.4270	 0.2570
i	 0.4530	 0.2910
j	 0.3620	 0.3050