



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:47 PM UTC

PDB ID : 9FN9 / pdb_00009fn9
EMDB ID : EMD-50585
Title : Icosahedral Encapsulin with a closed pore state
Authors : Capper, M.J.; Kohhnke, J.
Deposited on : 2024-06-09
Resolution : 2.81 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:

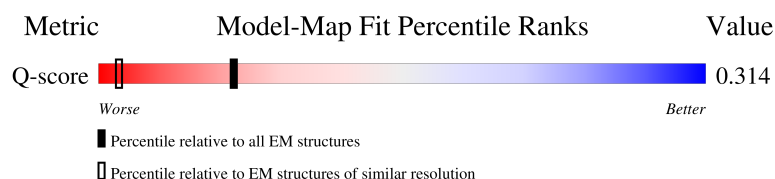
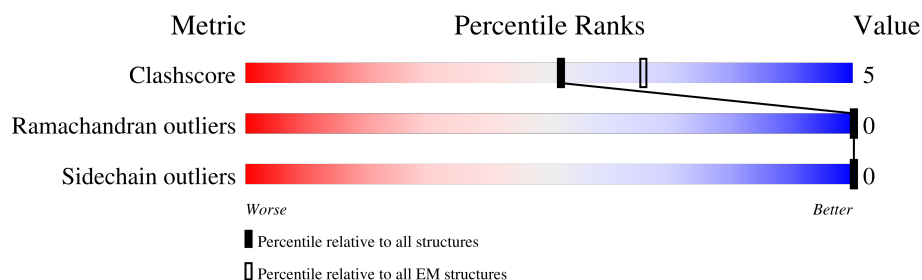
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.81 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	11740 (2.31 - 3.31)

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

Mol	Chain	Length	Quality of chain
1	A	275	
1	AA	275	
1	AB	275	
1	B	275	

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Mol	Chain	Length	Quality of chain
1	BA	275	72% 87% 9%
1	BB	275	96% 87% 9%
1	C	275	96% 87% 9%
1	CA	275	86% 10%
1	CB	275	96% 87% 9%
1	D	275	96% 87% 9%
1	DA	275	93% 86% 10%
1	DB	275	96% 87% 9%
1	E	275	70% 86% 10%
1	EA	275	96% 87% 9%
1	EB	275	96% 86% 10%
1	F	275	96% 86% 10%
1	FA	275	96% 87% 9%
1	FB	275	96% 86% 10%
1	G	275	96% 86% 10%
1	GA	275	94% 86% 10%
1	GB	275	96% 87% 9%
1	H	275	95% 87% 9%
1	HA	275	96% 86% 10%
1	HB	275	96% 87% 9%
1	I	275	96% 86% 10%
1	IA	275	96% 86% 10%
1	IB	275	96% 86% 10%
1	J	275	96% 86% 10%
1	JA	275	96% 86% 10%

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Mol	Chain	Length	Quality of chain
1	K	275	68% 86%10%.
1	KA	275	96% 87%9%.
1	L	275	. 86%10%.
1	LA	275	96% 86%10%.
1	M	275	91% 87%9%.
1	MA	275	96% 86%10%.
1	N	275	96% 86%10%.
1	NA	275	96% 86%10%.
1	O	275	96% 86%10%.
1	OA	275	95% 86%10%.
1	P	275	96% 87%9%.
1	PA	275	41% 86%10%.
1	Q	275	96% 87%9%.
1	QA	275	41% 87%9%.
1	R	275	96% 87%9%.
1	RA	275	41% 87%9%.
1	S	275	95% 87%9%.
1	SA	275	43% 87%9%.
1	T	275	96% 86%10%.
1	TA	275	39% 87%9%.
1	UA	275	96% 86%10%.
1	V	275	92% 87%9%.
1	VA	275	96% 86%10%.
1	W	275	96% 87%9%.
1	WA	275	70% 87%9%.

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Mol	Chain	Length	Quality of chain
1	X	275	96% 86% 10%
1	XA	275	86% 10%
1	Y	275	71% 86% 10%
1	YA	275	92% 86% 10%
1	Z	275	87% 9%
1	ZA	275	95% 86% 10%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 121020 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 29 kDa antigen Cfp29.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	AA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	AB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	B	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	BA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	BB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	C	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	CA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	CB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	D	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	DA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	DB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	E	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	EA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	EB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	F	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	FA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	G	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	GA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	GB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	H	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	HA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	HB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	I	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	IA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	IB	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	J	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	JA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	K	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	KA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	L	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	LA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	M	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	MA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	N	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	NA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	O	264	Total 2017	C 1266	N 349	O 399	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	OA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	P	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	PA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	Q	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	QA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	R	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	RA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	S	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	SA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	T	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	TA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	UA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	V	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	VA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	W	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	WA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	X	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	XA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	Y	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	YA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0
1	Z	264	Total 2017	C 1266	N 349	O 399	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ZA	264	Total 2017	C 1266	N 349	O 399	S 3	0	0

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	GLU	-	expression tag	UNP A0R4H0
A	267	LEU	-	expression tag	UNP A0R4H0
A	268	TRP	-	expression tag	UNP A0R4H0
A	269	SER	-	expression tag	UNP A0R4H0
A	270	HIS	-	expression tag	UNP A0R4H0
A	271	PRO	-	expression tag	UNP A0R4H0
A	272	GLN	-	expression tag	UNP A0R4H0
A	273	PHE	-	expression tag	UNP A0R4H0
A	274	GLU	-	expression tag	UNP A0R4H0
A	275	LYS	-	expression tag	UNP A0R4H0
AA	266	GLU	-	expression tag	UNP A0R4H0
AA	267	LEU	-	expression tag	UNP A0R4H0
AA	268	TRP	-	expression tag	UNP A0R4H0
AA	269	SER	-	expression tag	UNP A0R4H0
AA	270	HIS	-	expression tag	UNP A0R4H0
AA	271	PRO	-	expression tag	UNP A0R4H0
AA	272	GLN	-	expression tag	UNP A0R4H0
AA	273	PHE	-	expression tag	UNP A0R4H0
AA	274	GLU	-	expression tag	UNP A0R4H0
AA	275	LYS	-	expression tag	UNP A0R4H0
AB	266	GLU	-	expression tag	UNP A0R4H0
AB	267	LEU	-	expression tag	UNP A0R4H0
AB	268	TRP	-	expression tag	UNP A0R4H0
AB	269	SER	-	expression tag	UNP A0R4H0
AB	270	HIS	-	expression tag	UNP A0R4H0
AB	271	PRO	-	expression tag	UNP A0R4H0
AB	272	GLN	-	expression tag	UNP A0R4H0
AB	273	PHE	-	expression tag	UNP A0R4H0
AB	274	GLU	-	expression tag	UNP A0R4H0
AB	275	LYS	-	expression tag	UNP A0R4H0
B	266	GLU	-	expression tag	UNP A0R4H0
B	267	LEU	-	expression tag	UNP A0R4H0
B	268	TRP	-	expression tag	UNP A0R4H0
B	269	SER	-	expression tag	UNP A0R4H0
B	270	HIS	-	expression tag	UNP A0R4H0
B	271	PRO	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	272	GLN	-	expression tag	UNP A0R4H0
B	273	PHE	-	expression tag	UNP A0R4H0
B	274	GLU	-	expression tag	UNP A0R4H0
B	275	LYS	-	expression tag	UNP A0R4H0
BA	266	GLU	-	expression tag	UNP A0R4H0
BA	267	LEU	-	expression tag	UNP A0R4H0
BA	268	TRP	-	expression tag	UNP A0R4H0
BA	269	SER	-	expression tag	UNP A0R4H0
BA	270	HIS	-	expression tag	UNP A0R4H0
BA	271	PRO	-	expression tag	UNP A0R4H0
BA	272	GLN	-	expression tag	UNP A0R4H0
BA	273	PHE	-	expression tag	UNP A0R4H0
BA	274	GLU	-	expression tag	UNP A0R4H0
BA	275	LYS	-	expression tag	UNP A0R4H0
BB	266	GLU	-	expression tag	UNP A0R4H0
BB	267	LEU	-	expression tag	UNP A0R4H0
BB	268	TRP	-	expression tag	UNP A0R4H0
BB	269	SER	-	expression tag	UNP A0R4H0
BB	270	HIS	-	expression tag	UNP A0R4H0
BB	271	PRO	-	expression tag	UNP A0R4H0
BB	272	GLN	-	expression tag	UNP A0R4H0
BB	273	PHE	-	expression tag	UNP A0R4H0
BB	274	GLU	-	expression tag	UNP A0R4H0
BB	275	LYS	-	expression tag	UNP A0R4H0
C	266	GLU	-	expression tag	UNP A0R4H0
C	267	LEU	-	expression tag	UNP A0R4H0
C	268	TRP	-	expression tag	UNP A0R4H0
C	269	SER	-	expression tag	UNP A0R4H0
C	270	HIS	-	expression tag	UNP A0R4H0
C	271	PRO	-	expression tag	UNP A0R4H0
C	272	GLN	-	expression tag	UNP A0R4H0
C	273	PHE	-	expression tag	UNP A0R4H0
C	274	GLU	-	expression tag	UNP A0R4H0
C	275	LYS	-	expression tag	UNP A0R4H0
CA	266	GLU	-	expression tag	UNP A0R4H0
CA	267	LEU	-	expression tag	UNP A0R4H0
CA	268	TRP	-	expression tag	UNP A0R4H0
CA	269	SER	-	expression tag	UNP A0R4H0
CA	270	HIS	-	expression tag	UNP A0R4H0
CA	271	PRO	-	expression tag	UNP A0R4H0
CA	272	GLN	-	expression tag	UNP A0R4H0
CA	273	PHE	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	274	GLU	-	expression tag	UNP A0R4H0
CA	275	LYS	-	expression tag	UNP A0R4H0
CB	266	GLU	-	expression tag	UNP A0R4H0
CB	267	LEU	-	expression tag	UNP A0R4H0
CB	268	TRP	-	expression tag	UNP A0R4H0
CB	269	SER	-	expression tag	UNP A0R4H0
CB	270	HIS	-	expression tag	UNP A0R4H0
CB	271	PRO	-	expression tag	UNP A0R4H0
CB	272	GLN	-	expression tag	UNP A0R4H0
CB	273	PHE	-	expression tag	UNP A0R4H0
CB	274	GLU	-	expression tag	UNP A0R4H0
CB	275	LYS	-	expression tag	UNP A0R4H0
D	266	GLU	-	expression tag	UNP A0R4H0
D	267	LEU	-	expression tag	UNP A0R4H0
D	268	TRP	-	expression tag	UNP A0R4H0
D	269	SER	-	expression tag	UNP A0R4H0
D	270	HIS	-	expression tag	UNP A0R4H0
D	271	PRO	-	expression tag	UNP A0R4H0
D	272	GLN	-	expression tag	UNP A0R4H0
D	273	PHE	-	expression tag	UNP A0R4H0
D	274	GLU	-	expression tag	UNP A0R4H0
D	275	LYS	-	expression tag	UNP A0R4H0
DA	266	GLU	-	expression tag	UNP A0R4H0
DA	267	LEU	-	expression tag	UNP A0R4H0
DA	268	TRP	-	expression tag	UNP A0R4H0
DA	269	SER	-	expression tag	UNP A0R4H0
DA	270	HIS	-	expression tag	UNP A0R4H0
DA	271	PRO	-	expression tag	UNP A0R4H0
DA	272	GLN	-	expression tag	UNP A0R4H0
DA	273	PHE	-	expression tag	UNP A0R4H0
DA	274	GLU	-	expression tag	UNP A0R4H0
DA	275	LYS	-	expression tag	UNP A0R4H0
DB	266	GLU	-	expression tag	UNP A0R4H0
DB	267	LEU	-	expression tag	UNP A0R4H0
DB	268	TRP	-	expression tag	UNP A0R4H0
DB	269	SER	-	expression tag	UNP A0R4H0
DB	270	HIS	-	expression tag	UNP A0R4H0
DB	271	PRO	-	expression tag	UNP A0R4H0
DB	272	GLN	-	expression tag	UNP A0R4H0
DB	273	PHE	-	expression tag	UNP A0R4H0
DB	274	GLU	-	expression tag	UNP A0R4H0
DB	275	LYS	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	266	GLU	-	expression tag	UNP A0R4H0
E	267	LEU	-	expression tag	UNP A0R4H0
E	268	TRP	-	expression tag	UNP A0R4H0
E	269	SER	-	expression tag	UNP A0R4H0
E	270	HIS	-	expression tag	UNP A0R4H0
E	271	PRO	-	expression tag	UNP A0R4H0
E	272	GLN	-	expression tag	UNP A0R4H0
E	273	PHE	-	expression tag	UNP A0R4H0
E	274	GLU	-	expression tag	UNP A0R4H0
E	275	LYS	-	expression tag	UNP A0R4H0
EA	266	GLU	-	expression tag	UNP A0R4H0
EA	267	LEU	-	expression tag	UNP A0R4H0
EA	268	TRP	-	expression tag	UNP A0R4H0
EA	269	SER	-	expression tag	UNP A0R4H0
EA	270	HIS	-	expression tag	UNP A0R4H0
EA	271	PRO	-	expression tag	UNP A0R4H0
EA	272	GLN	-	expression tag	UNP A0R4H0
EA	273	PHE	-	expression tag	UNP A0R4H0
EA	274	GLU	-	expression tag	UNP A0R4H0
EA	275	LYS	-	expression tag	UNP A0R4H0
EB	266	GLU	-	expression tag	UNP A0R4H0
EB	267	LEU	-	expression tag	UNP A0R4H0
EB	268	TRP	-	expression tag	UNP A0R4H0
EB	269	SER	-	expression tag	UNP A0R4H0
EB	270	HIS	-	expression tag	UNP A0R4H0
EB	271	PRO	-	expression tag	UNP A0R4H0
EB	272	GLN	-	expression tag	UNP A0R4H0
EB	273	PHE	-	expression tag	UNP A0R4H0
EB	274	GLU	-	expression tag	UNP A0R4H0
EB	275	LYS	-	expression tag	UNP A0R4H0
F	266	GLU	-	expression tag	UNP A0R4H0
F	267	LEU	-	expression tag	UNP A0R4H0
F	268	TRP	-	expression tag	UNP A0R4H0
F	269	SER	-	expression tag	UNP A0R4H0
F	270	HIS	-	expression tag	UNP A0R4H0
F	271	PRO	-	expression tag	UNP A0R4H0
F	272	GLN	-	expression tag	UNP A0R4H0
F	273	PHE	-	expression tag	UNP A0R4H0
F	274	GLU	-	expression tag	UNP A0R4H0
F	275	LYS	-	expression tag	UNP A0R4H0
FA	266	GLU	-	expression tag	UNP A0R4H0
FA	267	LEU	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	268	TRP	-	expression tag	UNP A0R4H0
FA	269	SER	-	expression tag	UNP A0R4H0
FA	270	HIS	-	expression tag	UNP A0R4H0
FA	271	PRO	-	expression tag	UNP A0R4H0
FA	272	GLN	-	expression tag	UNP A0R4H0
FA	273	PHE	-	expression tag	UNP A0R4H0
FA	274	GLU	-	expression tag	UNP A0R4H0
FA	275	LYS	-	expression tag	UNP A0R4H0
FB	266	GLU	-	expression tag	UNP A0R4H0
FB	267	LEU	-	expression tag	UNP A0R4H0
FB	268	TRP	-	expression tag	UNP A0R4H0
FB	269	SER	-	expression tag	UNP A0R4H0
FB	270	HIS	-	expression tag	UNP A0R4H0
FB	271	PRO	-	expression tag	UNP A0R4H0
FB	272	GLN	-	expression tag	UNP A0R4H0
FB	273	PHE	-	expression tag	UNP A0R4H0
FB	274	GLU	-	expression tag	UNP A0R4H0
FB	275	LYS	-	expression tag	UNP A0R4H0
G	266	GLU	-	expression tag	UNP A0R4H0
G	267	LEU	-	expression tag	UNP A0R4H0
G	268	TRP	-	expression tag	UNP A0R4H0
G	269	SER	-	expression tag	UNP A0R4H0
G	270	HIS	-	expression tag	UNP A0R4H0
G	271	PRO	-	expression tag	UNP A0R4H0
G	272	GLN	-	expression tag	UNP A0R4H0
G	273	PHE	-	expression tag	UNP A0R4H0
G	274	GLU	-	expression tag	UNP A0R4H0
G	275	LYS	-	expression tag	UNP A0R4H0
GA	266	GLU	-	expression tag	UNP A0R4H0
GA	267	LEU	-	expression tag	UNP A0R4H0
GA	268	TRP	-	expression tag	UNP A0R4H0
GA	269	SER	-	expression tag	UNP A0R4H0
GA	270	HIS	-	expression tag	UNP A0R4H0
GA	271	PRO	-	expression tag	UNP A0R4H0
GA	272	GLN	-	expression tag	UNP A0R4H0
GA	273	PHE	-	expression tag	UNP A0R4H0
GA	274	GLU	-	expression tag	UNP A0R4H0
GA	275	LYS	-	expression tag	UNP A0R4H0
GB	266	GLU	-	expression tag	UNP A0R4H0
GB	267	LEU	-	expression tag	UNP A0R4H0
GB	268	TRP	-	expression tag	UNP A0R4H0
GB	269	SER	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
GB	270	HIS	-	expression tag	UNP A0R4H0
GB	271	PRO	-	expression tag	UNP A0R4H0
GB	272	GLN	-	expression tag	UNP A0R4H0
GB	273	PHE	-	expression tag	UNP A0R4H0
GB	274	GLU	-	expression tag	UNP A0R4H0
GB	275	LYS	-	expression tag	UNP A0R4H0
H	266	GLU	-	expression tag	UNP A0R4H0
H	267	LEU	-	expression tag	UNP A0R4H0
H	268	TRP	-	expression tag	UNP A0R4H0
H	269	SER	-	expression tag	UNP A0R4H0
H	270	HIS	-	expression tag	UNP A0R4H0
H	271	PRO	-	expression tag	UNP A0R4H0
H	272	GLN	-	expression tag	UNP A0R4H0
H	273	PHE	-	expression tag	UNP A0R4H0
H	274	GLU	-	expression tag	UNP A0R4H0
H	275	LYS	-	expression tag	UNP A0R4H0
HA	266	GLU	-	expression tag	UNP A0R4H0
HA	267	LEU	-	expression tag	UNP A0R4H0
HA	268	TRP	-	expression tag	UNP A0R4H0
HA	269	SER	-	expression tag	UNP A0R4H0
HA	270	HIS	-	expression tag	UNP A0R4H0
HA	271	PRO	-	expression tag	UNP A0R4H0
HA	272	GLN	-	expression tag	UNP A0R4H0
HA	273	PHE	-	expression tag	UNP A0R4H0
HA	274	GLU	-	expression tag	UNP A0R4H0
HA	275	LYS	-	expression tag	UNP A0R4H0
HB	266	GLU	-	expression tag	UNP A0R4H0
HB	267	LEU	-	expression tag	UNP A0R4H0
HB	268	TRP	-	expression tag	UNP A0R4H0
HB	269	SER	-	expression tag	UNP A0R4H0
HB	270	HIS	-	expression tag	UNP A0R4H0
HB	271	PRO	-	expression tag	UNP A0R4H0
HB	272	GLN	-	expression tag	UNP A0R4H0
HB	273	PHE	-	expression tag	UNP A0R4H0
HB	274	GLU	-	expression tag	UNP A0R4H0
HB	275	LYS	-	expression tag	UNP A0R4H0
I	266	GLU	-	expression tag	UNP A0R4H0
I	267	LEU	-	expression tag	UNP A0R4H0
I	268	TRP	-	expression tag	UNP A0R4H0
I	269	SER	-	expression tag	UNP A0R4H0
I	270	HIS	-	expression tag	UNP A0R4H0
I	271	PRO	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	272	GLN	-	expression tag	UNP A0R4H0
I	273	PHE	-	expression tag	UNP A0R4H0
I	274	GLU	-	expression tag	UNP A0R4H0
I	275	LYS	-	expression tag	UNP A0R4H0
IA	266	GLU	-	expression tag	UNP A0R4H0
IA	267	LEU	-	expression tag	UNP A0R4H0
IA	268	TRP	-	expression tag	UNP A0R4H0
IA	269	SER	-	expression tag	UNP A0R4H0
IA	270	HIS	-	expression tag	UNP A0R4H0
IA	271	PRO	-	expression tag	UNP A0R4H0
IA	272	GLN	-	expression tag	UNP A0R4H0
IA	273	PHE	-	expression tag	UNP A0R4H0
IA	274	GLU	-	expression tag	UNP A0R4H0
IA	275	LYS	-	expression tag	UNP A0R4H0
IB	266	GLU	-	expression tag	UNP A0R4H0
IB	267	LEU	-	expression tag	UNP A0R4H0
IB	268	TRP	-	expression tag	UNP A0R4H0
IB	269	SER	-	expression tag	UNP A0R4H0
IB	270	HIS	-	expression tag	UNP A0R4H0
IB	271	PRO	-	expression tag	UNP A0R4H0
IB	272	GLN	-	expression tag	UNP A0R4H0
IB	273	PHE	-	expression tag	UNP A0R4H0
IB	274	GLU	-	expression tag	UNP A0R4H0
IB	275	LYS	-	expression tag	UNP A0R4H0
J	266	GLU	-	expression tag	UNP A0R4H0
J	267	LEU	-	expression tag	UNP A0R4H0
J	268	TRP	-	expression tag	UNP A0R4H0
J	269	SER	-	expression tag	UNP A0R4H0
J	270	HIS	-	expression tag	UNP A0R4H0
J	271	PRO	-	expression tag	UNP A0R4H0
J	272	GLN	-	expression tag	UNP A0R4H0
J	273	PHE	-	expression tag	UNP A0R4H0
J	274	GLU	-	expression tag	UNP A0R4H0
J	275	LYS	-	expression tag	UNP A0R4H0
JA	266	GLU	-	expression tag	UNP A0R4H0
JA	267	LEU	-	expression tag	UNP A0R4H0
JA	268	TRP	-	expression tag	UNP A0R4H0
JA	269	SER	-	expression tag	UNP A0R4H0
JA	270	HIS	-	expression tag	UNP A0R4H0
JA	271	PRO	-	expression tag	UNP A0R4H0
JA	272	GLN	-	expression tag	UNP A0R4H0
JA	273	PHE	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	274	GLU	-	expression tag	UNP A0R4H0
JA	275	LYS	-	expression tag	UNP A0R4H0
K	266	GLU	-	expression tag	UNP A0R4H0
K	267	LEU	-	expression tag	UNP A0R4H0
K	268	TRP	-	expression tag	UNP A0R4H0
K	269	SER	-	expression tag	UNP A0R4H0
K	270	HIS	-	expression tag	UNP A0R4H0
K	271	PRO	-	expression tag	UNP A0R4H0
K	272	GLN	-	expression tag	UNP A0R4H0
K	273	PHE	-	expression tag	UNP A0R4H0
K	274	GLU	-	expression tag	UNP A0R4H0
K	275	LYS	-	expression tag	UNP A0R4H0
KA	266	GLU	-	expression tag	UNP A0R4H0
KA	267	LEU	-	expression tag	UNP A0R4H0
KA	268	TRP	-	expression tag	UNP A0R4H0
KA	269	SER	-	expression tag	UNP A0R4H0
KA	270	HIS	-	expression tag	UNP A0R4H0
KA	271	PRO	-	expression tag	UNP A0R4H0
KA	272	GLN	-	expression tag	UNP A0R4H0
KA	273	PHE	-	expression tag	UNP A0R4H0
KA	274	GLU	-	expression tag	UNP A0R4H0
KA	275	LYS	-	expression tag	UNP A0R4H0
L	266	GLU	-	expression tag	UNP A0R4H0
L	267	LEU	-	expression tag	UNP A0R4H0
L	268	TRP	-	expression tag	UNP A0R4H0
L	269	SER	-	expression tag	UNP A0R4H0
L	270	HIS	-	expression tag	UNP A0R4H0
L	271	PRO	-	expression tag	UNP A0R4H0
L	272	GLN	-	expression tag	UNP A0R4H0
L	273	PHE	-	expression tag	UNP A0R4H0
L	274	GLU	-	expression tag	UNP A0R4H0
L	275	LYS	-	expression tag	UNP A0R4H0
LA	266	GLU	-	expression tag	UNP A0R4H0
LA	267	LEU	-	expression tag	UNP A0R4H0
LA	268	TRP	-	expression tag	UNP A0R4H0
LA	269	SER	-	expression tag	UNP A0R4H0
LA	270	HIS	-	expression tag	UNP A0R4H0
LA	271	PRO	-	expression tag	UNP A0R4H0
LA	272	GLN	-	expression tag	UNP A0R4H0
LA	273	PHE	-	expression tag	UNP A0R4H0
LA	274	GLU	-	expression tag	UNP A0R4H0
LA	275	LYS	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	266	GLU	-	expression tag	UNP A0R4H0
M	267	LEU	-	expression tag	UNP A0R4H0
M	268	TRP	-	expression tag	UNP A0R4H0
M	269	SER	-	expression tag	UNP A0R4H0
M	270	HIS	-	expression tag	UNP A0R4H0
M	271	PRO	-	expression tag	UNP A0R4H0
M	272	GLN	-	expression tag	UNP A0R4H0
M	273	PHE	-	expression tag	UNP A0R4H0
M	274	GLU	-	expression tag	UNP A0R4H0
M	275	LYS	-	expression tag	UNP A0R4H0
MA	266	GLU	-	expression tag	UNP A0R4H0
MA	267	LEU	-	expression tag	UNP A0R4H0
MA	268	TRP	-	expression tag	UNP A0R4H0
MA	269	SER	-	expression tag	UNP A0R4H0
MA	270	HIS	-	expression tag	UNP A0R4H0
MA	271	PRO	-	expression tag	UNP A0R4H0
MA	272	GLN	-	expression tag	UNP A0R4H0
MA	273	PHE	-	expression tag	UNP A0R4H0
MA	274	GLU	-	expression tag	UNP A0R4H0
MA	275	LYS	-	expression tag	UNP A0R4H0
N	266	GLU	-	expression tag	UNP A0R4H0
N	267	LEU	-	expression tag	UNP A0R4H0
N	268	TRP	-	expression tag	UNP A0R4H0
N	269	SER	-	expression tag	UNP A0R4H0
N	270	HIS	-	expression tag	UNP A0R4H0
N	271	PRO	-	expression tag	UNP A0R4H0
N	272	GLN	-	expression tag	UNP A0R4H0
N	273	PHE	-	expression tag	UNP A0R4H0
N	274	GLU	-	expression tag	UNP A0R4H0
N	275	LYS	-	expression tag	UNP A0R4H0
NA	266	GLU	-	expression tag	UNP A0R4H0
NA	267	LEU	-	expression tag	UNP A0R4H0
NA	268	TRP	-	expression tag	UNP A0R4H0
NA	269	SER	-	expression tag	UNP A0R4H0
NA	270	HIS	-	expression tag	UNP A0R4H0
NA	271	PRO	-	expression tag	UNP A0R4H0
NA	272	GLN	-	expression tag	UNP A0R4H0
NA	273	PHE	-	expression tag	UNP A0R4H0
NA	274	GLU	-	expression tag	UNP A0R4H0
NA	275	LYS	-	expression tag	UNP A0R4H0
O	266	GLU	-	expression tag	UNP A0R4H0
O	267	LEU	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
O	268	TRP	-	expression tag	UNP A0R4H0
O	269	SER	-	expression tag	UNP A0R4H0
O	270	HIS	-	expression tag	UNP A0R4H0
O	271	PRO	-	expression tag	UNP A0R4H0
O	272	GLN	-	expression tag	UNP A0R4H0
O	273	PHE	-	expression tag	UNP A0R4H0
O	274	GLU	-	expression tag	UNP A0R4H0
O	275	LYS	-	expression tag	UNP A0R4H0
OA	266	GLU	-	expression tag	UNP A0R4H0
OA	267	LEU	-	expression tag	UNP A0R4H0
OA	268	TRP	-	expression tag	UNP A0R4H0
OA	269	SER	-	expression tag	UNP A0R4H0
OA	270	HIS	-	expression tag	UNP A0R4H0
OA	271	PRO	-	expression tag	UNP A0R4H0
OA	272	GLN	-	expression tag	UNP A0R4H0
OA	273	PHE	-	expression tag	UNP A0R4H0
OA	274	GLU	-	expression tag	UNP A0R4H0
OA	275	LYS	-	expression tag	UNP A0R4H0
P	266	GLU	-	expression tag	UNP A0R4H0
P	267	LEU	-	expression tag	UNP A0R4H0
P	268	TRP	-	expression tag	UNP A0R4H0
P	269	SER	-	expression tag	UNP A0R4H0
P	270	HIS	-	expression tag	UNP A0R4H0
P	271	PRO	-	expression tag	UNP A0R4H0
P	272	GLN	-	expression tag	UNP A0R4H0
P	273	PHE	-	expression tag	UNP A0R4H0
P	274	GLU	-	expression tag	UNP A0R4H0
P	275	LYS	-	expression tag	UNP A0R4H0
PA	266	GLU	-	expression tag	UNP A0R4H0
PA	267	LEU	-	expression tag	UNP A0R4H0
PA	268	TRP	-	expression tag	UNP A0R4H0
PA	269	SER	-	expression tag	UNP A0R4H0
PA	270	HIS	-	expression tag	UNP A0R4H0
PA	271	PRO	-	expression tag	UNP A0R4H0
PA	272	GLN	-	expression tag	UNP A0R4H0
PA	273	PHE	-	expression tag	UNP A0R4H0
PA	274	GLU	-	expression tag	UNP A0R4H0
PA	275	LYS	-	expression tag	UNP A0R4H0
Q	266	GLU	-	expression tag	UNP A0R4H0
Q	267	LEU	-	expression tag	UNP A0R4H0
Q	268	TRP	-	expression tag	UNP A0R4H0
Q	269	SER	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	270	HIS	-	expression tag	UNP A0R4H0
Q	271	PRO	-	expression tag	UNP A0R4H0
Q	272	GLN	-	expression tag	UNP A0R4H0
Q	273	PHE	-	expression tag	UNP A0R4H0
Q	274	GLU	-	expression tag	UNP A0R4H0
Q	275	LYS	-	expression tag	UNP A0R4H0
QA	266	GLU	-	expression tag	UNP A0R4H0
QA	267	LEU	-	expression tag	UNP A0R4H0
QA	268	TRP	-	expression tag	UNP A0R4H0
QA	269	SER	-	expression tag	UNP A0R4H0
QA	270	HIS	-	expression tag	UNP A0R4H0
QA	271	PRO	-	expression tag	UNP A0R4H0
QA	272	GLN	-	expression tag	UNP A0R4H0
QA	273	PHE	-	expression tag	UNP A0R4H0
QA	274	GLU	-	expression tag	UNP A0R4H0
QA	275	LYS	-	expression tag	UNP A0R4H0
R	266	GLU	-	expression tag	UNP A0R4H0
R	267	LEU	-	expression tag	UNP A0R4H0
R	268	TRP	-	expression tag	UNP A0R4H0
R	269	SER	-	expression tag	UNP A0R4H0
R	270	HIS	-	expression tag	UNP A0R4H0
R	271	PRO	-	expression tag	UNP A0R4H0
R	272	GLN	-	expression tag	UNP A0R4H0
R	273	PHE	-	expression tag	UNP A0R4H0
R	274	GLU	-	expression tag	UNP A0R4H0
R	275	LYS	-	expression tag	UNP A0R4H0
RA	266	GLU	-	expression tag	UNP A0R4H0
RA	267	LEU	-	expression tag	UNP A0R4H0
RA	268	TRP	-	expression tag	UNP A0R4H0
RA	269	SER	-	expression tag	UNP A0R4H0
RA	270	HIS	-	expression tag	UNP A0R4H0
RA	271	PRO	-	expression tag	UNP A0R4H0
RA	272	GLN	-	expression tag	UNP A0R4H0
RA	273	PHE	-	expression tag	UNP A0R4H0
RA	274	GLU	-	expression tag	UNP A0R4H0
RA	275	LYS	-	expression tag	UNP A0R4H0
S	266	GLU	-	expression tag	UNP A0R4H0
S	267	LEU	-	expression tag	UNP A0R4H0
S	268	TRP	-	expression tag	UNP A0R4H0
S	269	SER	-	expression tag	UNP A0R4H0
S	270	HIS	-	expression tag	UNP A0R4H0
S	271	PRO	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
S	272	GLN	-	expression tag	UNP A0R4H0
S	273	PHE	-	expression tag	UNP A0R4H0
S	274	GLU	-	expression tag	UNP A0R4H0
S	275	LYS	-	expression tag	UNP A0R4H0
SA	266	GLU	-	expression tag	UNP A0R4H0
SA	267	LEU	-	expression tag	UNP A0R4H0
SA	268	TRP	-	expression tag	UNP A0R4H0
SA	269	SER	-	expression tag	UNP A0R4H0
SA	270	HIS	-	expression tag	UNP A0R4H0
SA	271	PRO	-	expression tag	UNP A0R4H0
SA	272	GLN	-	expression tag	UNP A0R4H0
SA	273	PHE	-	expression tag	UNP A0R4H0
SA	274	GLU	-	expression tag	UNP A0R4H0
SA	275	LYS	-	expression tag	UNP A0R4H0
T	266	GLU	-	expression tag	UNP A0R4H0
T	267	LEU	-	expression tag	UNP A0R4H0
T	268	TRP	-	expression tag	UNP A0R4H0
T	269	SER	-	expression tag	UNP A0R4H0
T	270	HIS	-	expression tag	UNP A0R4H0
T	271	PRO	-	expression tag	UNP A0R4H0
T	272	GLN	-	expression tag	UNP A0R4H0
T	273	PHE	-	expression tag	UNP A0R4H0
T	274	GLU	-	expression tag	UNP A0R4H0
T	275	LYS	-	expression tag	UNP A0R4H0
TA	266	GLU	-	expression tag	UNP A0R4H0
TA	267	LEU	-	expression tag	UNP A0R4H0
TA	268	TRP	-	expression tag	UNP A0R4H0
TA	269	SER	-	expression tag	UNP A0R4H0
TA	270	HIS	-	expression tag	UNP A0R4H0
TA	271	PRO	-	expression tag	UNP A0R4H0
TA	272	GLN	-	expression tag	UNP A0R4H0
TA	273	PHE	-	expression tag	UNP A0R4H0
TA	274	GLU	-	expression tag	UNP A0R4H0
TA	275	LYS	-	expression tag	UNP A0R4H0
UA	266	GLU	-	expression tag	UNP A0R4H0
UA	267	LEU	-	expression tag	UNP A0R4H0
UA	268	TRP	-	expression tag	UNP A0R4H0
UA	269	SER	-	expression tag	UNP A0R4H0
UA	270	HIS	-	expression tag	UNP A0R4H0
UA	271	PRO	-	expression tag	UNP A0R4H0
UA	272	GLN	-	expression tag	UNP A0R4H0
UA	273	PHE	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
UA	274	GLU	-	expression tag	UNP A0R4H0
UA	275	LYS	-	expression tag	UNP A0R4H0
V	266	GLU	-	expression tag	UNP A0R4H0
V	267	LEU	-	expression tag	UNP A0R4H0
V	268	TRP	-	expression tag	UNP A0R4H0
V	269	SER	-	expression tag	UNP A0R4H0
V	270	HIS	-	expression tag	UNP A0R4H0
V	271	PRO	-	expression tag	UNP A0R4H0
V	272	GLN	-	expression tag	UNP A0R4H0
V	273	PHE	-	expression tag	UNP A0R4H0
V	274	GLU	-	expression tag	UNP A0R4H0
V	275	LYS	-	expression tag	UNP A0R4H0
VA	266	GLU	-	expression tag	UNP A0R4H0
VA	267	LEU	-	expression tag	UNP A0R4H0
VA	268	TRP	-	expression tag	UNP A0R4H0
VA	269	SER	-	expression tag	UNP A0R4H0
VA	270	HIS	-	expression tag	UNP A0R4H0
VA	271	PRO	-	expression tag	UNP A0R4H0
VA	272	GLN	-	expression tag	UNP A0R4H0
VA	273	PHE	-	expression tag	UNP A0R4H0
VA	274	GLU	-	expression tag	UNP A0R4H0
VA	275	LYS	-	expression tag	UNP A0R4H0
W	266	GLU	-	expression tag	UNP A0R4H0
W	267	LEU	-	expression tag	UNP A0R4H0
W	268	TRP	-	expression tag	UNP A0R4H0
W	269	SER	-	expression tag	UNP A0R4H0
W	270	HIS	-	expression tag	UNP A0R4H0
W	271	PRO	-	expression tag	UNP A0R4H0
W	272	GLN	-	expression tag	UNP A0R4H0
W	273	PHE	-	expression tag	UNP A0R4H0
W	274	GLU	-	expression tag	UNP A0R4H0
W	275	LYS	-	expression tag	UNP A0R4H0
WA	266	GLU	-	expression tag	UNP A0R4H0
WA	267	LEU	-	expression tag	UNP A0R4H0
WA	268	TRP	-	expression tag	UNP A0R4H0
WA	269	SER	-	expression tag	UNP A0R4H0
WA	270	HIS	-	expression tag	UNP A0R4H0
WA	271	PRO	-	expression tag	UNP A0R4H0
WA	272	GLN	-	expression tag	UNP A0R4H0
WA	273	PHE	-	expression tag	UNP A0R4H0
WA	274	GLU	-	expression tag	UNP A0R4H0
WA	275	LYS	-	expression tag	UNP A0R4H0

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Chain	Residue	Modelled	Actual	Comment	Reference
X	266	GLU	-	expression tag	UNP A0R4H0
X	267	LEU	-	expression tag	UNP A0R4H0
X	268	TRP	-	expression tag	UNP A0R4H0
X	269	SER	-	expression tag	UNP A0R4H0
X	270	HIS	-	expression tag	UNP A0R4H0
X	271	PRO	-	expression tag	UNP A0R4H0
X	272	GLN	-	expression tag	UNP A0R4H0
X	273	PHE	-	expression tag	UNP A0R4H0
X	274	GLU	-	expression tag	UNP A0R4H0
X	275	LYS	-	expression tag	UNP A0R4H0
XA	266	GLU	-	expression tag	UNP A0R4H0
XA	267	LEU	-	expression tag	UNP A0R4H0
XA	268	TRP	-	expression tag	UNP A0R4H0
XA	269	SER	-	expression tag	UNP A0R4H0
XA	270	HIS	-	expression tag	UNP A0R4H0
XA	271	PRO	-	expression tag	UNP A0R4H0
XA	272	GLN	-	expression tag	UNP A0R4H0
XA	273	PHE	-	expression tag	UNP A0R4H0
XA	274	GLU	-	expression tag	UNP A0R4H0
XA	275	LYS	-	expression tag	UNP A0R4H0
Y	266	GLU	-	expression tag	UNP A0R4H0
Y	267	LEU	-	expression tag	UNP A0R4H0
Y	268	TRP	-	expression tag	UNP A0R4H0
Y	269	SER	-	expression tag	UNP A0R4H0
Y	270	HIS	-	expression tag	UNP A0R4H0
Y	271	PRO	-	expression tag	UNP A0R4H0
Y	272	GLN	-	expression tag	UNP A0R4H0
Y	273	PHE	-	expression tag	UNP A0R4H0
Y	274	GLU	-	expression tag	UNP A0R4H0
Y	275	LYS	-	expression tag	UNP A0R4H0
YA	266	GLU	-	expression tag	UNP A0R4H0
YA	267	LEU	-	expression tag	UNP A0R4H0
YA	268	TRP	-	expression tag	UNP A0R4H0
YA	269	SER	-	expression tag	UNP A0R4H0
YA	270	HIS	-	expression tag	UNP A0R4H0
YA	271	PRO	-	expression tag	UNP A0R4H0
YA	272	GLN	-	expression tag	UNP A0R4H0
YA	273	PHE	-	expression tag	UNP A0R4H0
YA	274	GLU	-	expression tag	UNP A0R4H0
YA	275	LYS	-	expression tag	UNP A0R4H0
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Z	267	LEU	-	expression tag	UNP A0R4H0

Continued on next page...

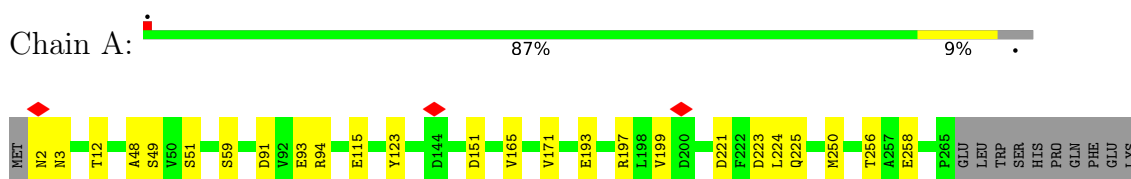
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Chain	Residue	Modelled	Actual	Comment	Reference
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Z	270	HIS	-	expression tag	UNP A0R4H0
Z	271	PRO	-	expression tag	UNP A0R4H0
Z	272	GLN	-	expression tag	UNP A0R4H0
Z	273	PHE	-	expression tag	UNP A0R4H0
Z	274	GLU	-	expression tag	UNP A0R4H0
Z	275	LYS	-	expression tag	UNP A0R4H0
ZA	266	GLU	-	expression tag	UNP A0R4H0
ZA	267	LEU	-	expression tag	UNP A0R4H0
ZA	268	TRP	-	expression tag	UNP A0R4H0
ZA	269	SER	-	expression tag	UNP A0R4H0
ZA	270	HIS	-	expression tag	UNP A0R4H0
ZA	271	PRO	-	expression tag	UNP A0R4H0
ZA	272	GLN	-	expression tag	UNP A0R4H0
ZA	273	PHE	-	expression tag	UNP A0R4H0
ZA	274	GLU	-	expression tag	UNP A0R4H0
ZA	275	LYS	-	expression tag	UNP A0R4H0

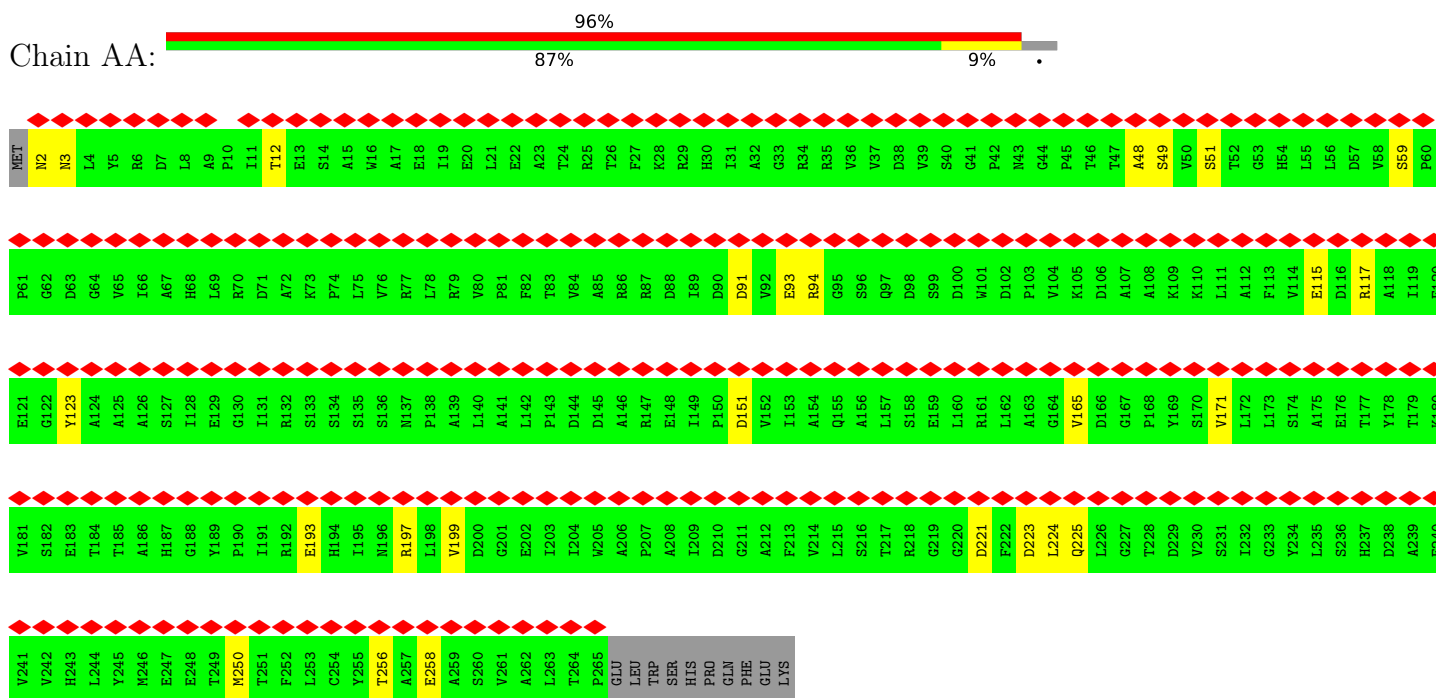
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

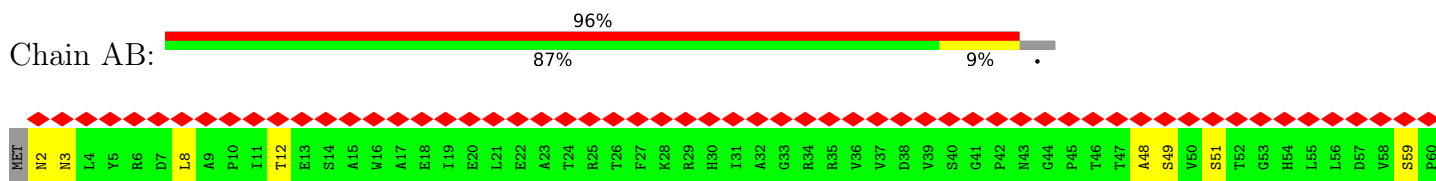
• Molecule 1: 29 kDa antigen Cfp29

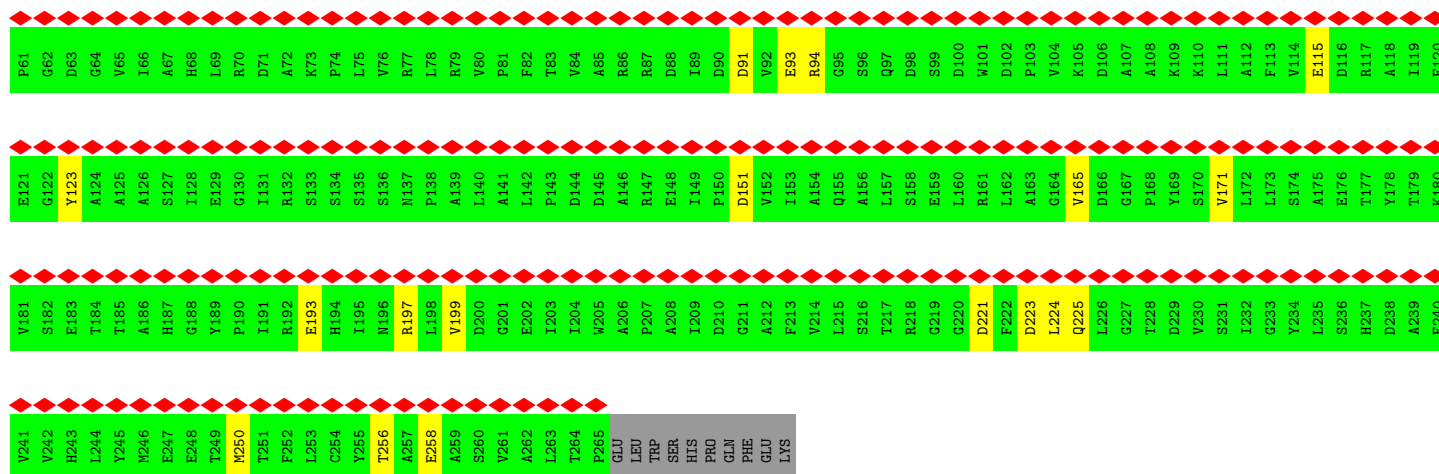


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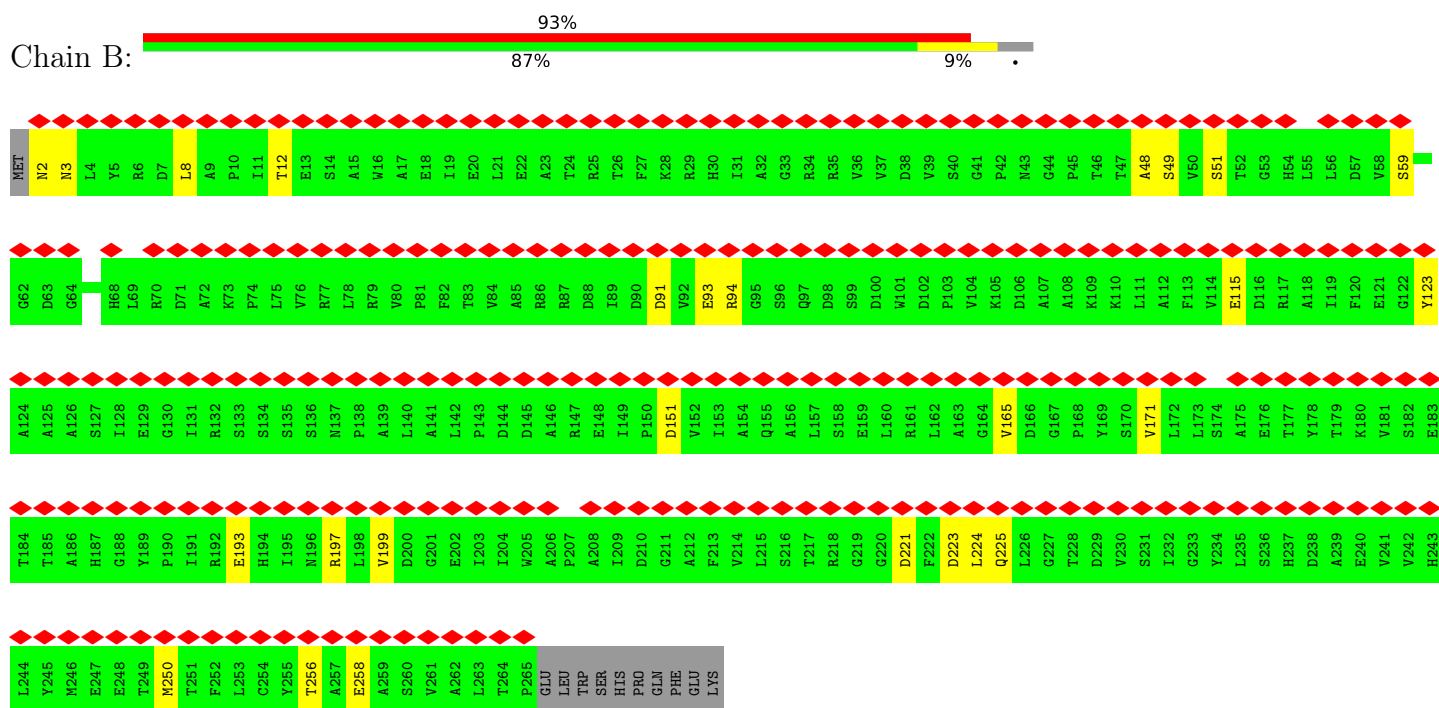


• Molecule 1: 29 kDa antigen Cfp29

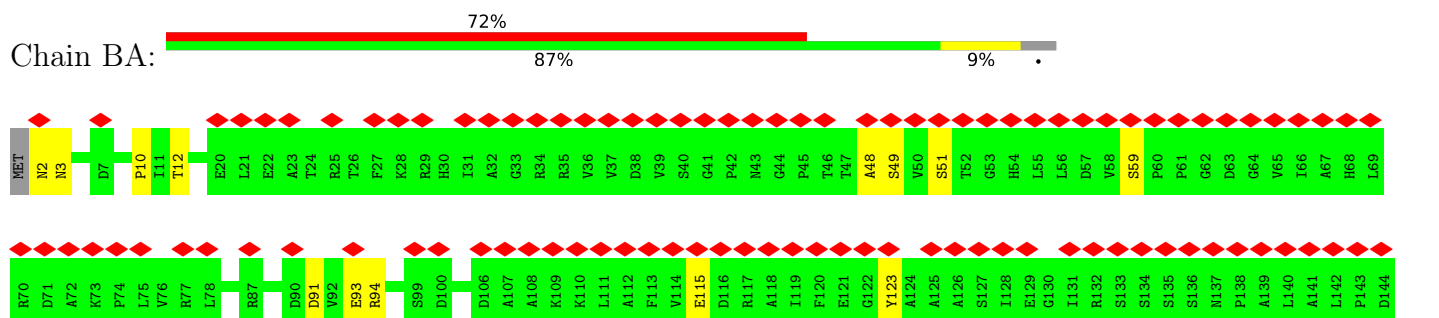


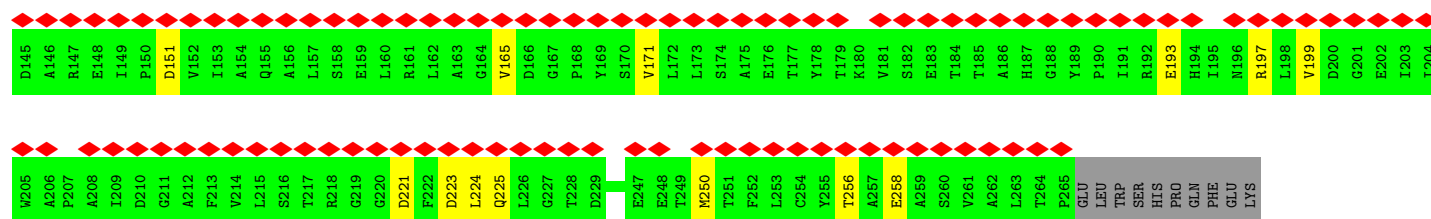


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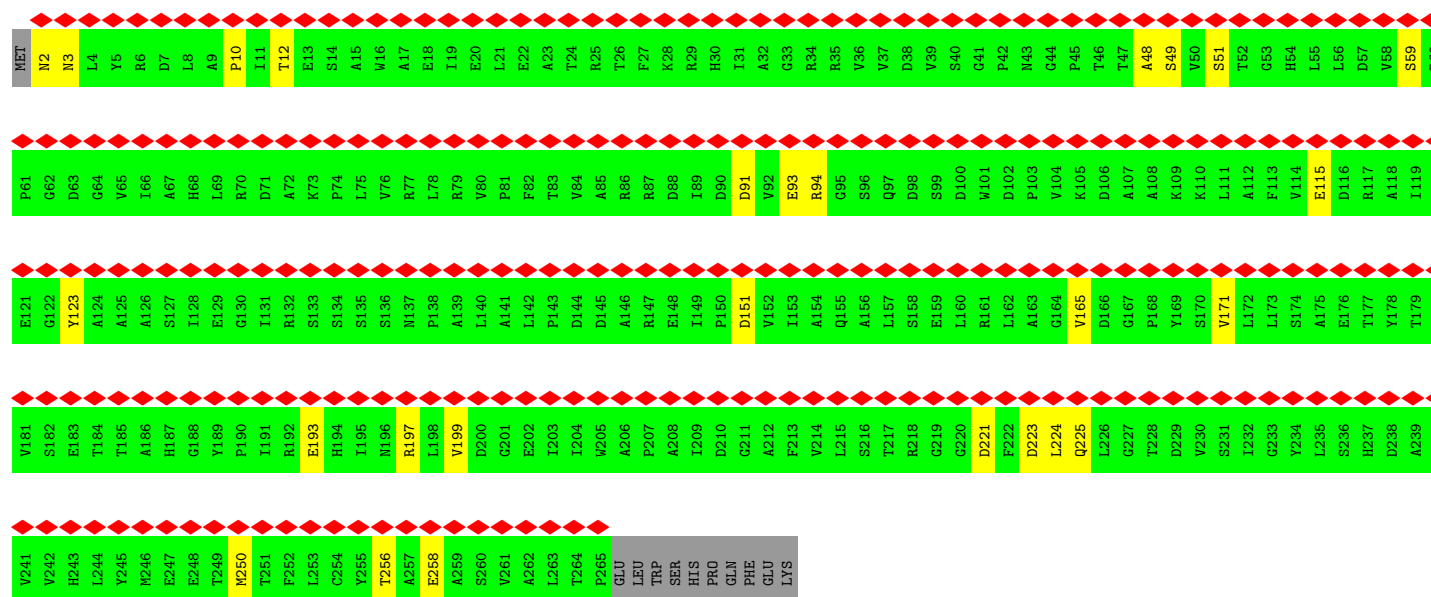


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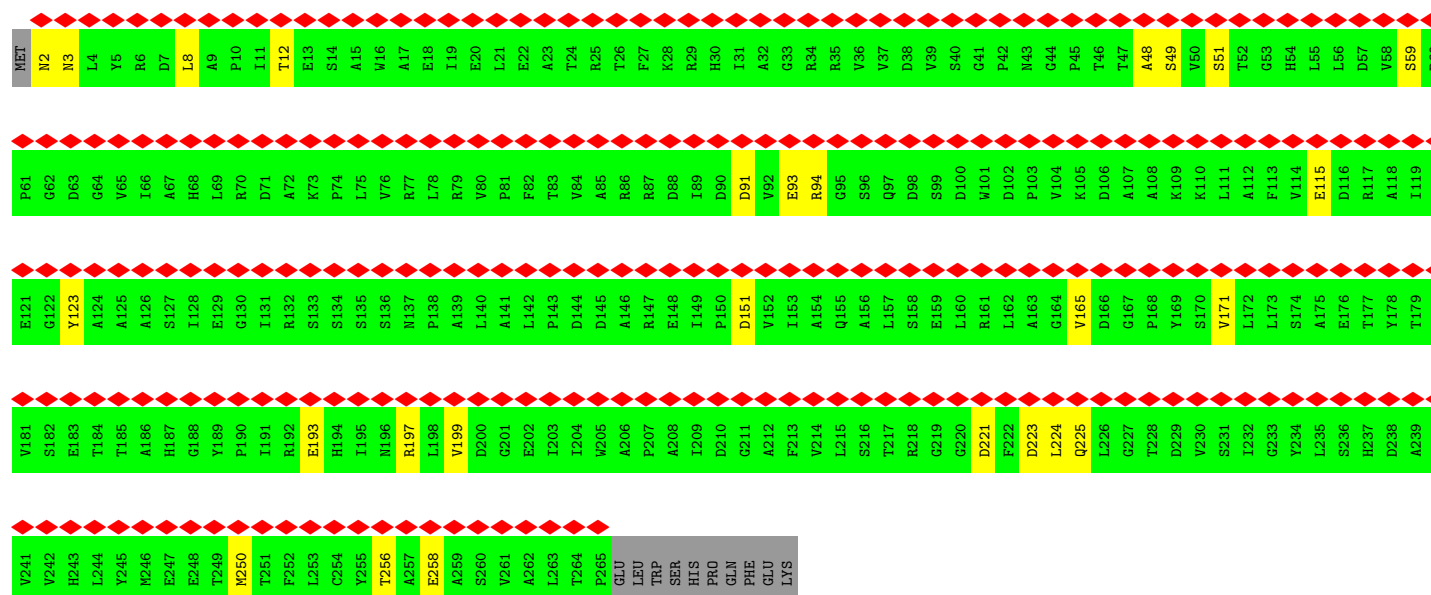
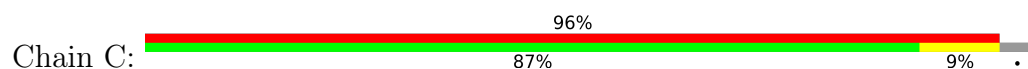




• Molecule 1: 29 kDa antigen Cfp29



• Molecule 1: 29 kDa antigen Cfp29



Chain CA:

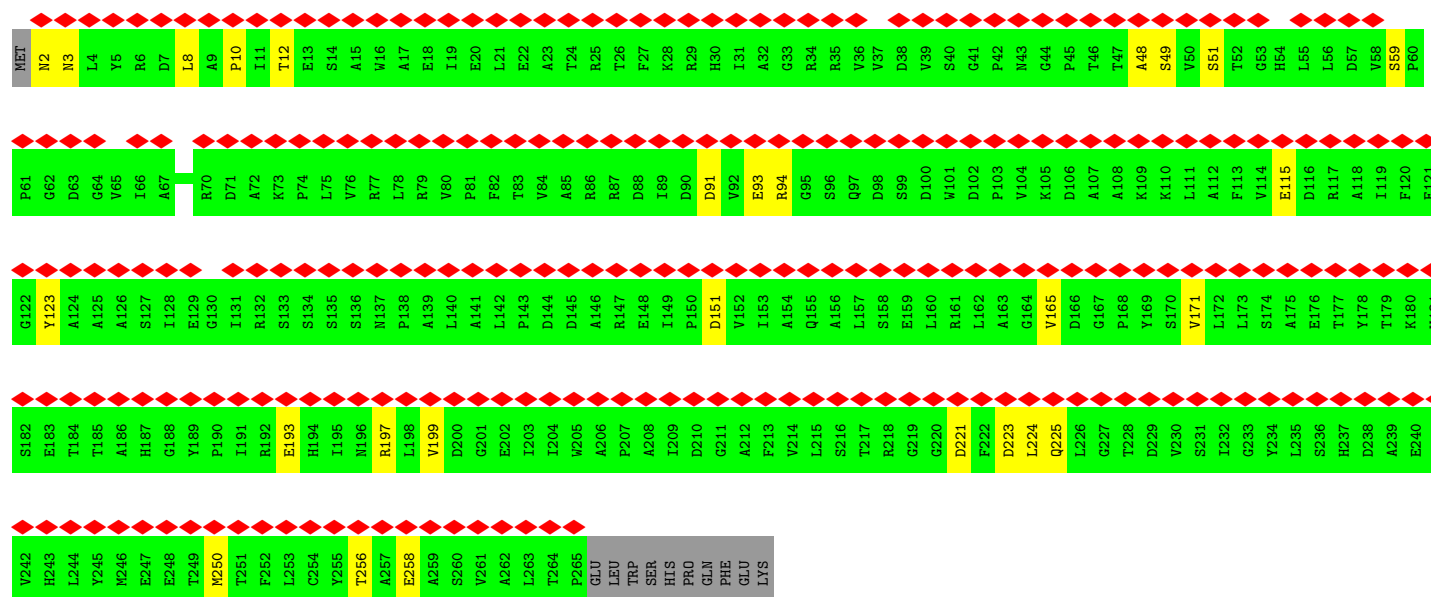
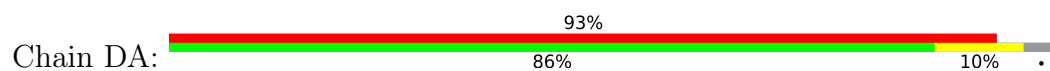
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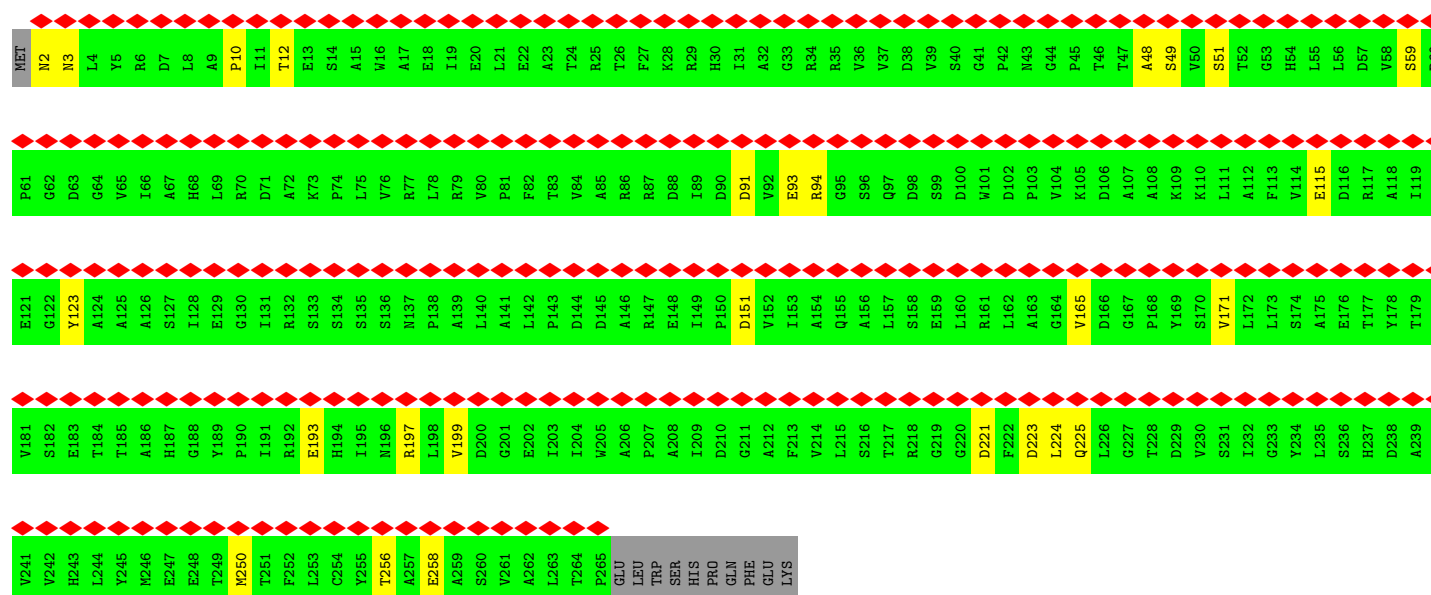
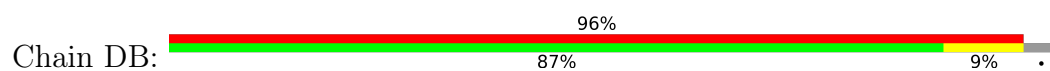
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E183	E183	D63	N3
T184	T184	G64	N4
T185	T185	V65	Y5
A186	A186	T66	R6
H187	H187	A67	D7
G188	G188	H68	L8
Y189	Y189	L69	A9
P190	P190	R70	P10
I191	I191	D71	I11
R192	R192	A72	T12
E193	E193	K73	E13
H194	H194	P74	S14
I195	I195	L75	A15
N196	N196	V76	W16
R197	R197	R77	A17
L198	L198	L78	E18
V199	V199	R79	I19
D200	D200	W80	E20
G201	G201	P81	L21
E202	E202	F82	E22
I203	I203	T83	A23
I204	I204	W84	T24
W205	W205	A85	R25
A206	A206	R86	T26
P207	P207	R87	F27
A208	A208	D88	K28
I209	I209	I89	R29
D210	D210	D90	H30
G211	G211	D91	T31
A212	A212	V92	A32
F213	F213	E93	G33
V214	V214	R94	R34
L215	L215	G95	R35
S216	S216	S96	V36
T217	T217	Q97	V37
R218	R218	D98	D38
G219	G219	S99	V39
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F222	F222	L102	P42
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			G44



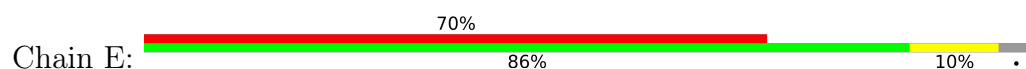
- Molecule 1: 29 kDa antigen Cfp29

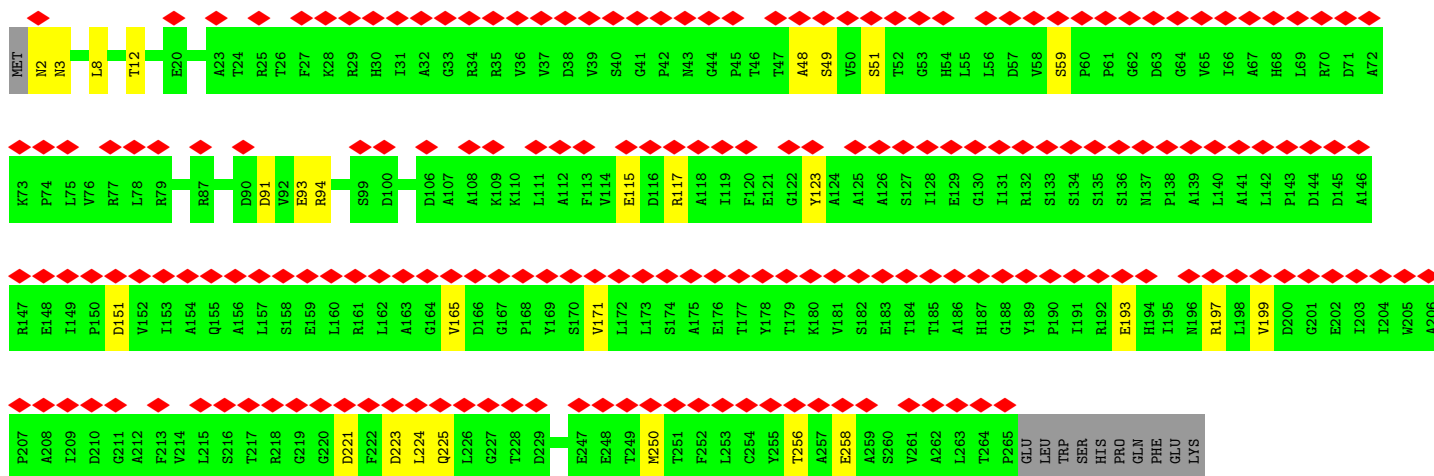


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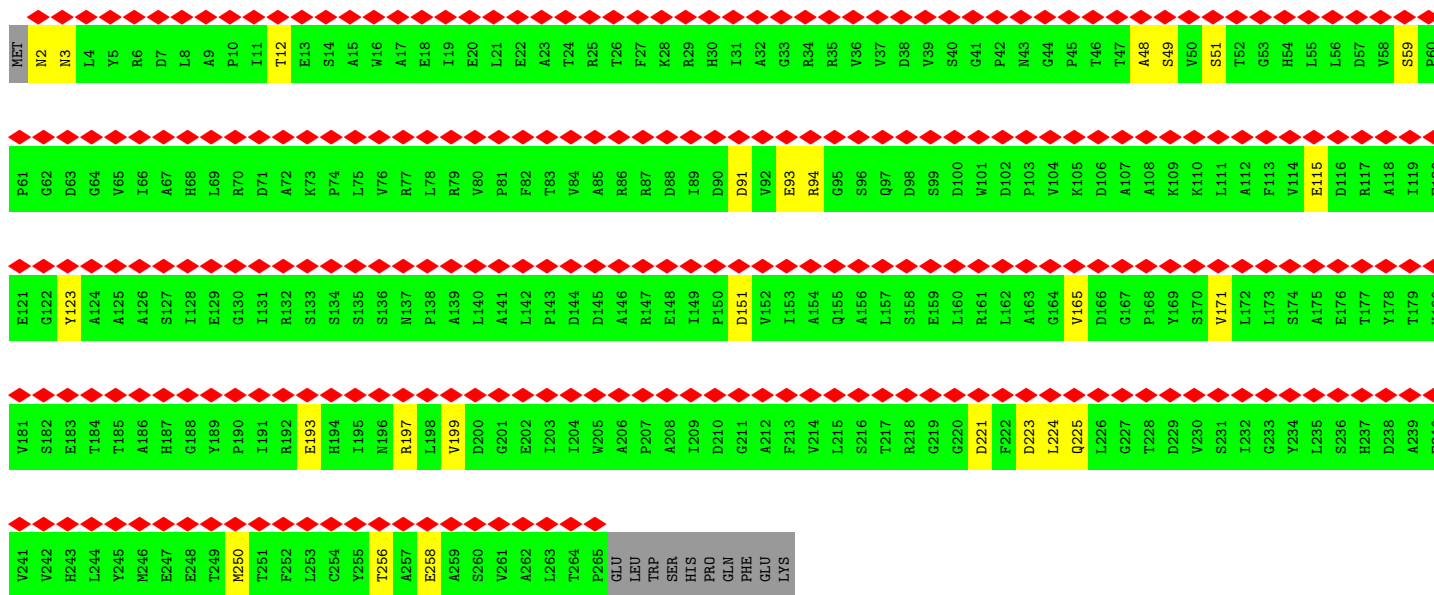
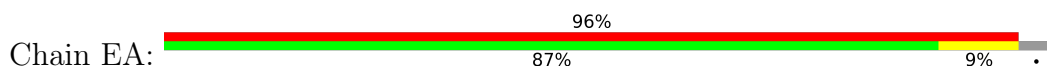


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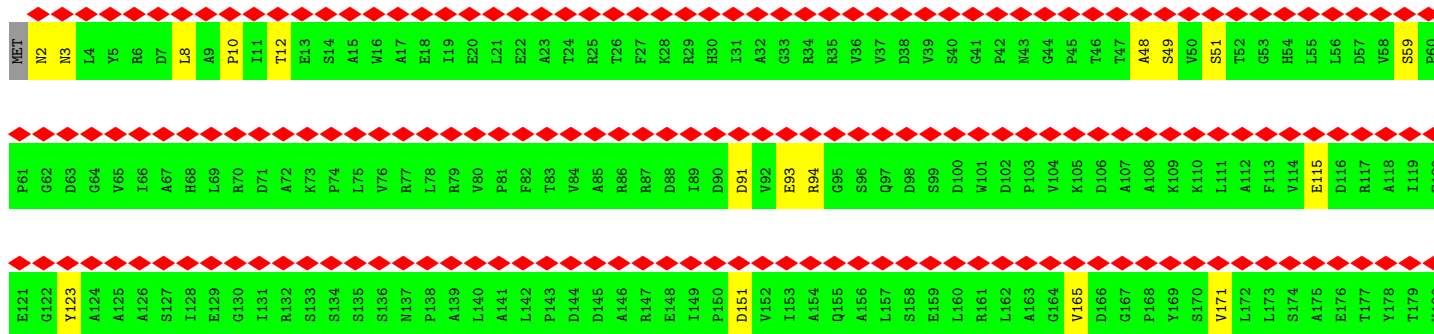
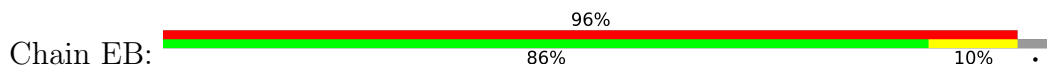


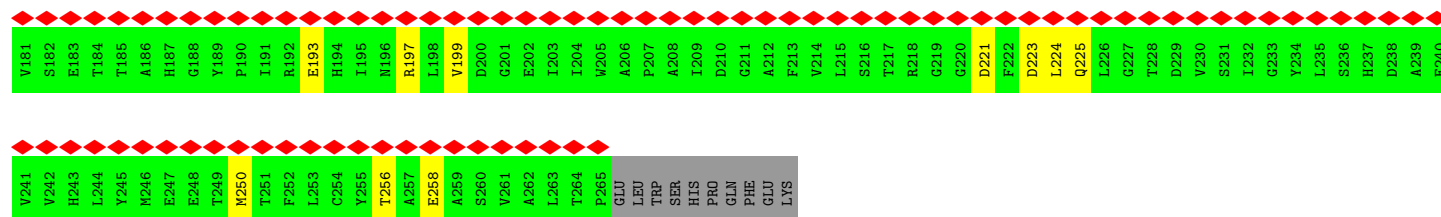


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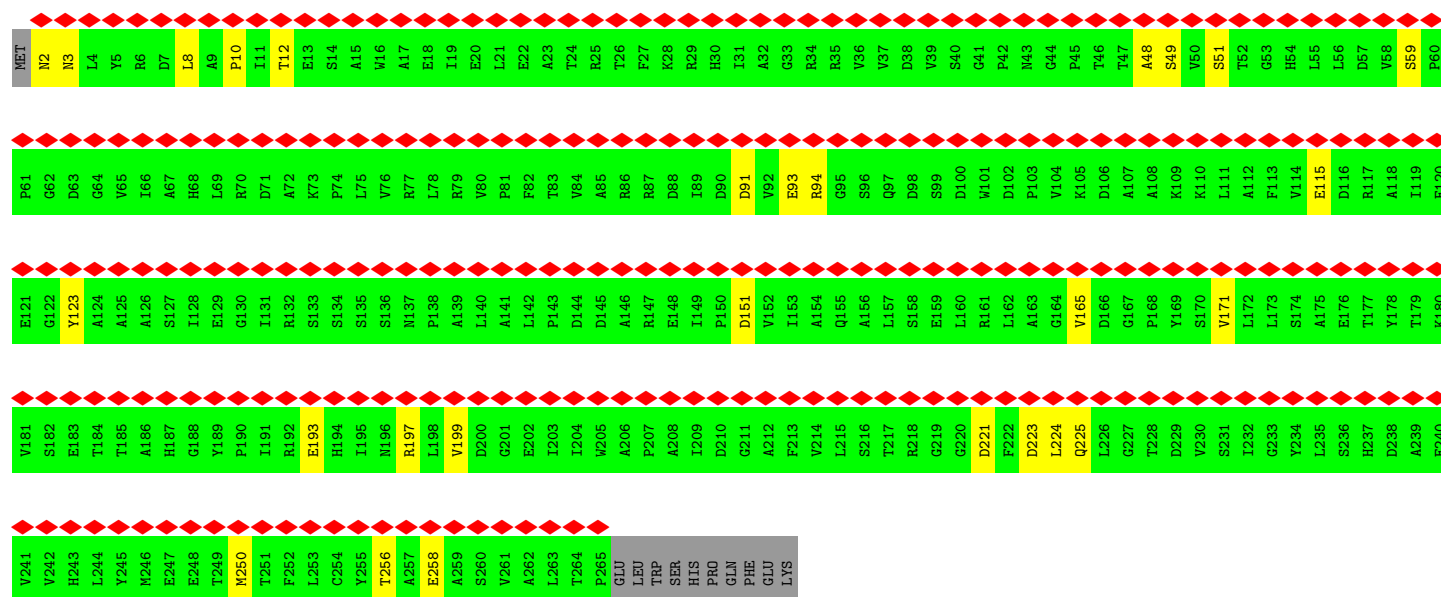
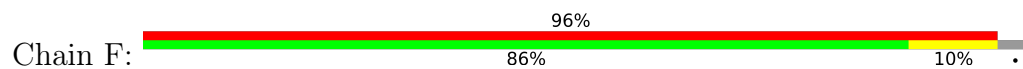


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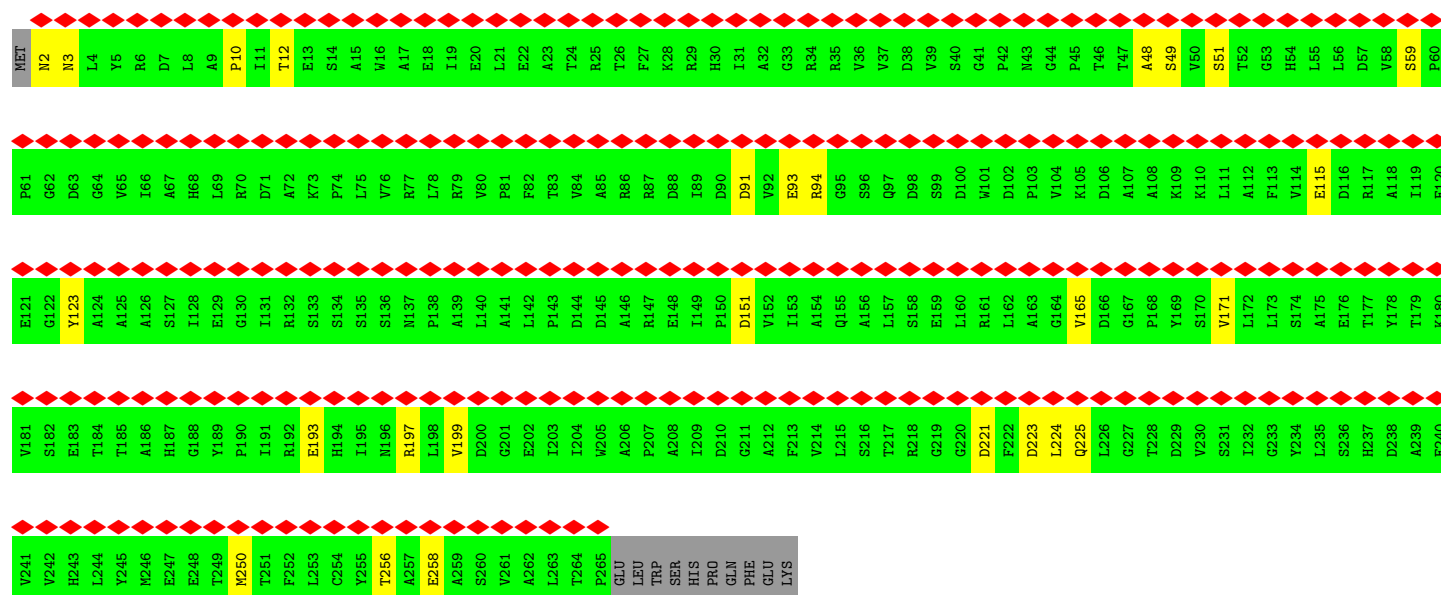


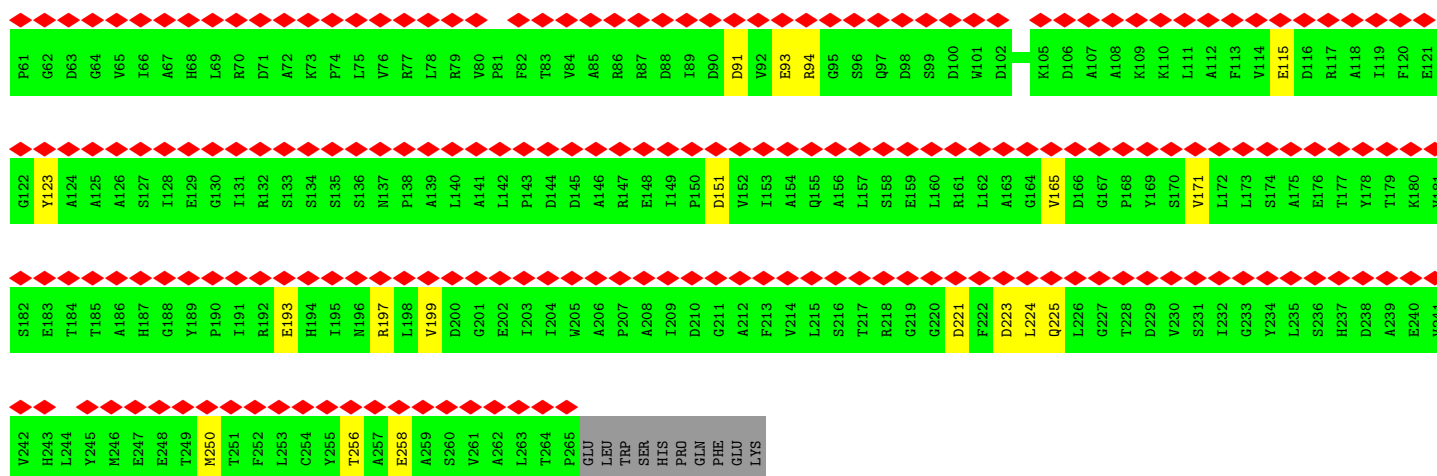


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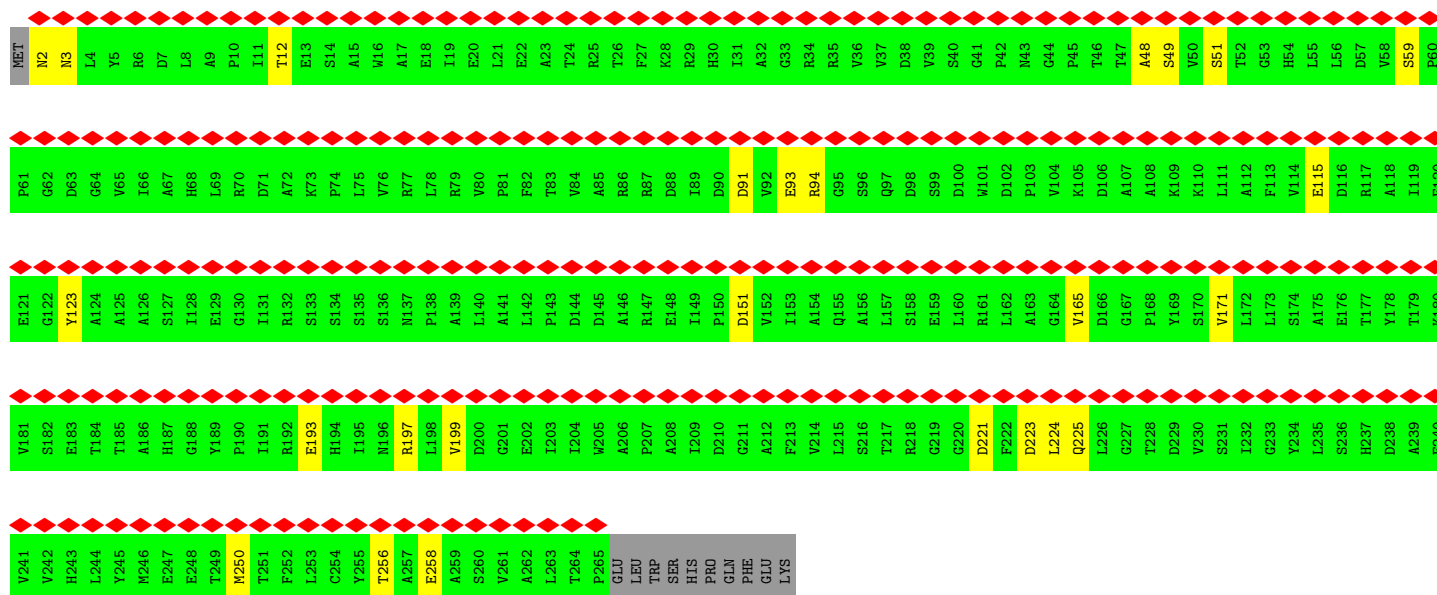
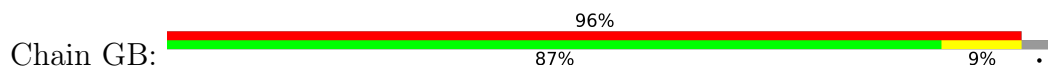


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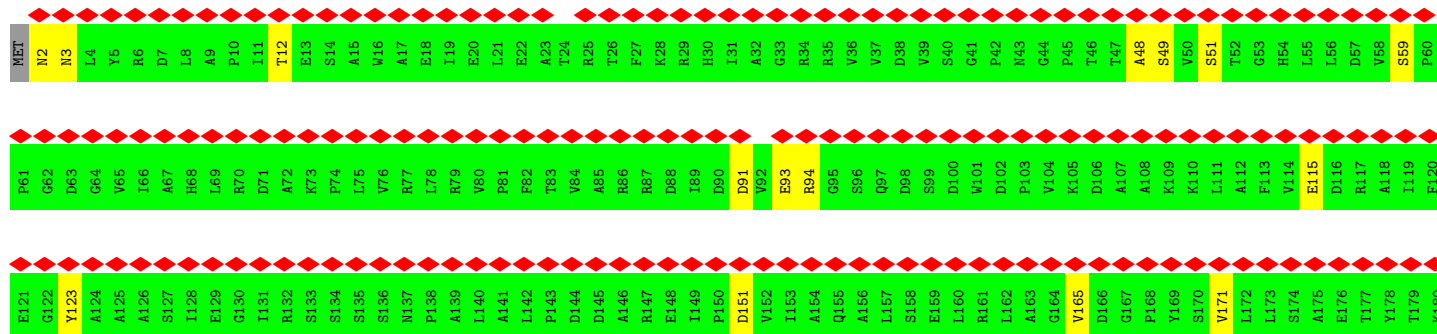
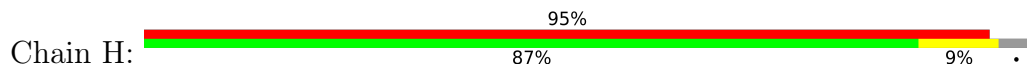


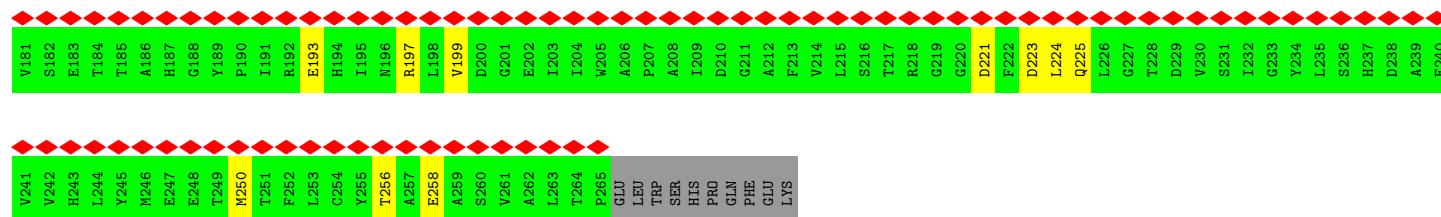


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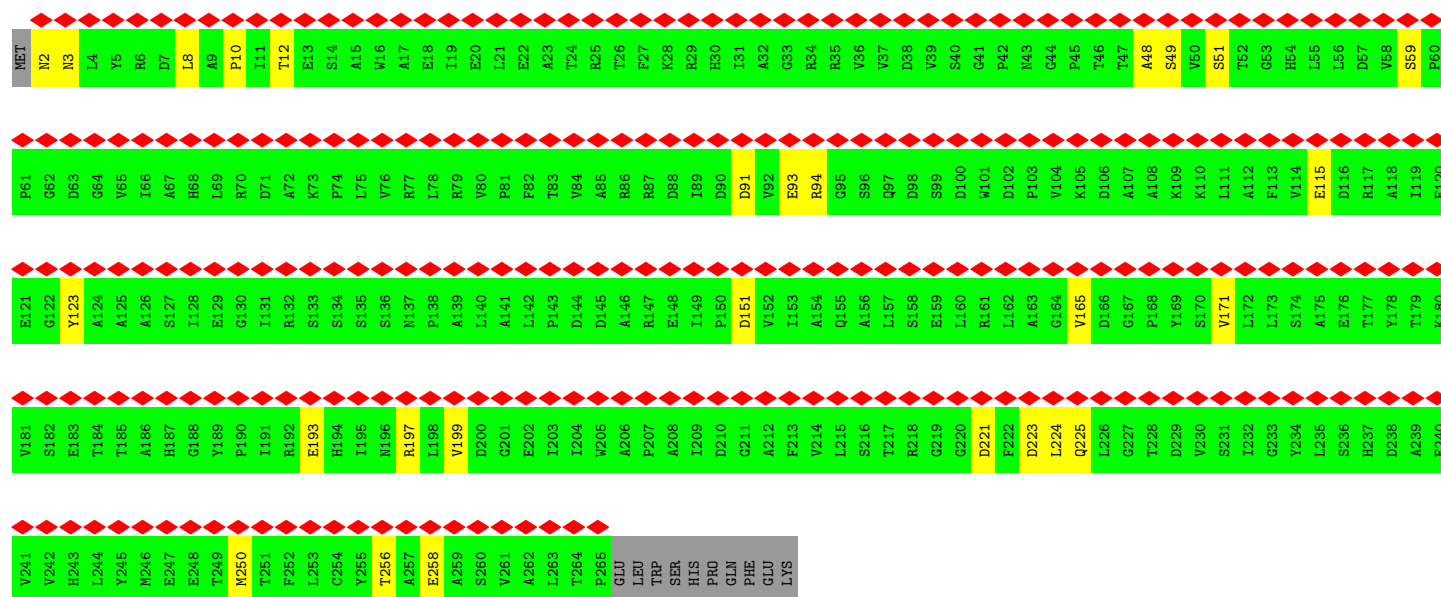
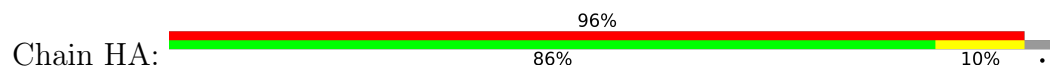


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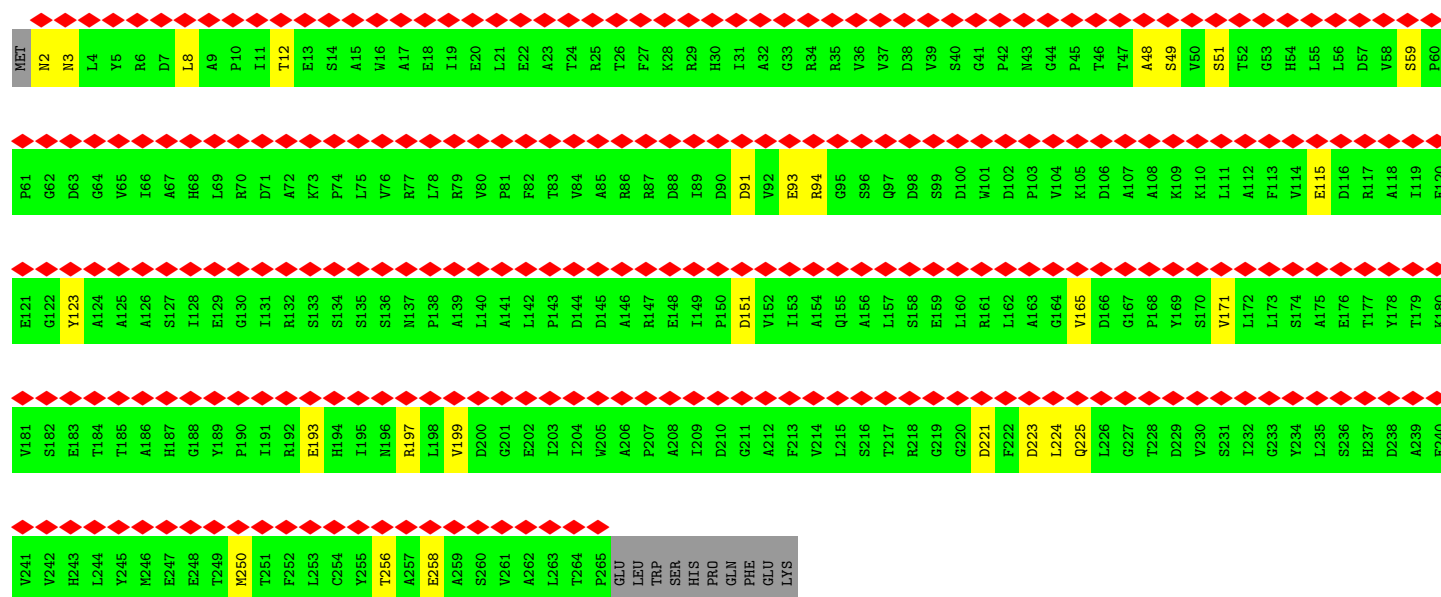
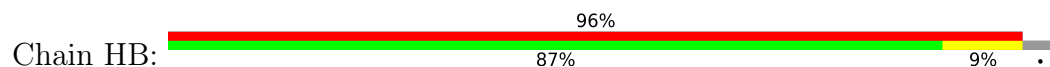


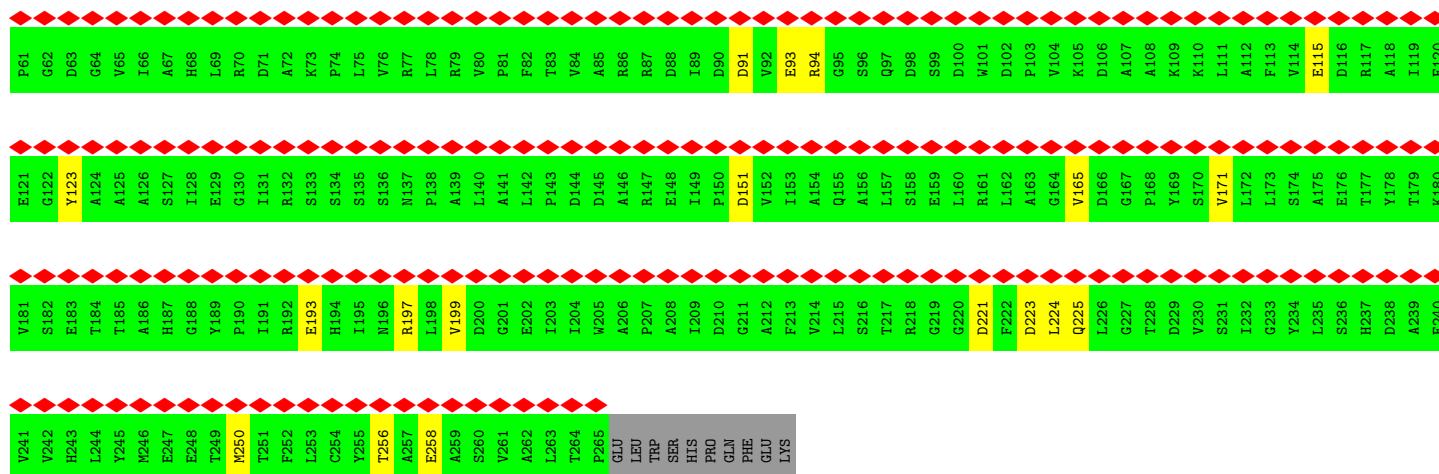


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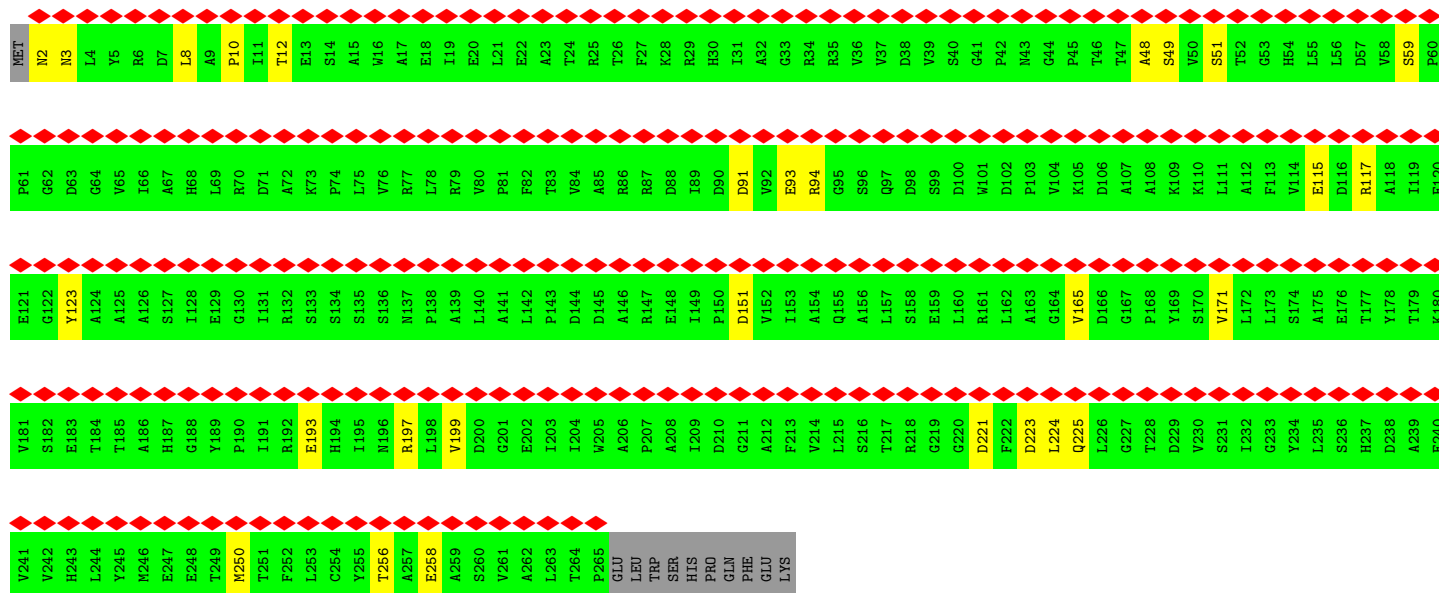
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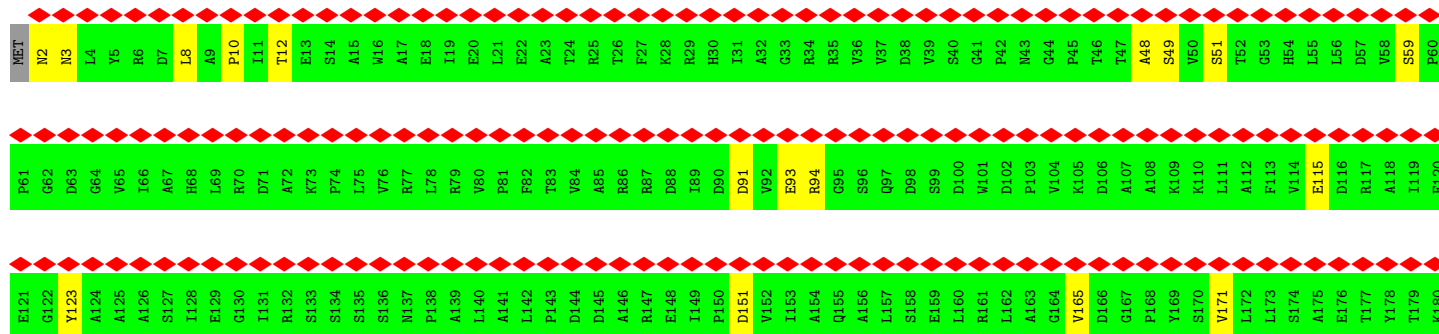
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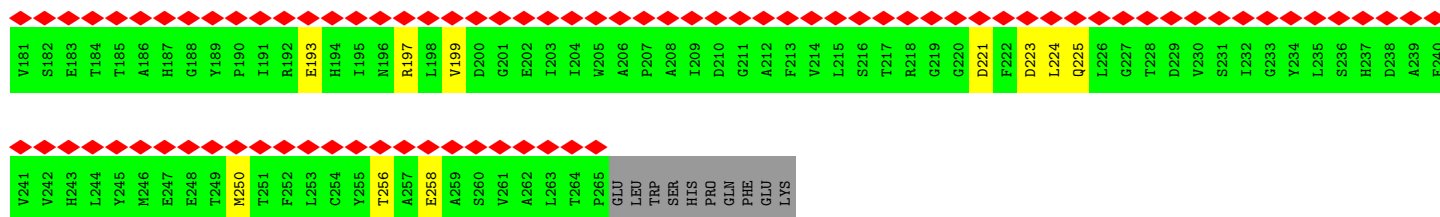
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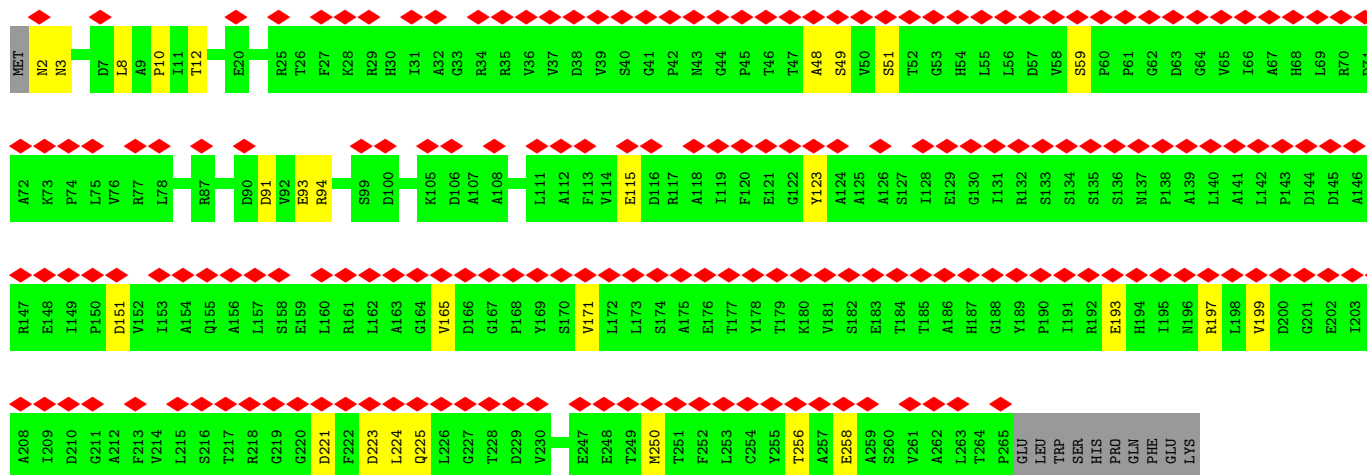
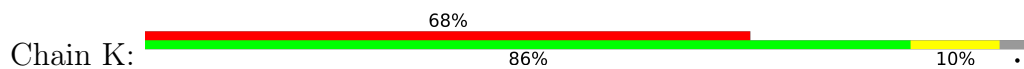
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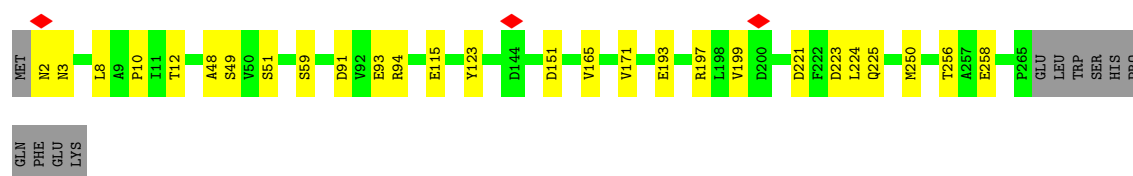




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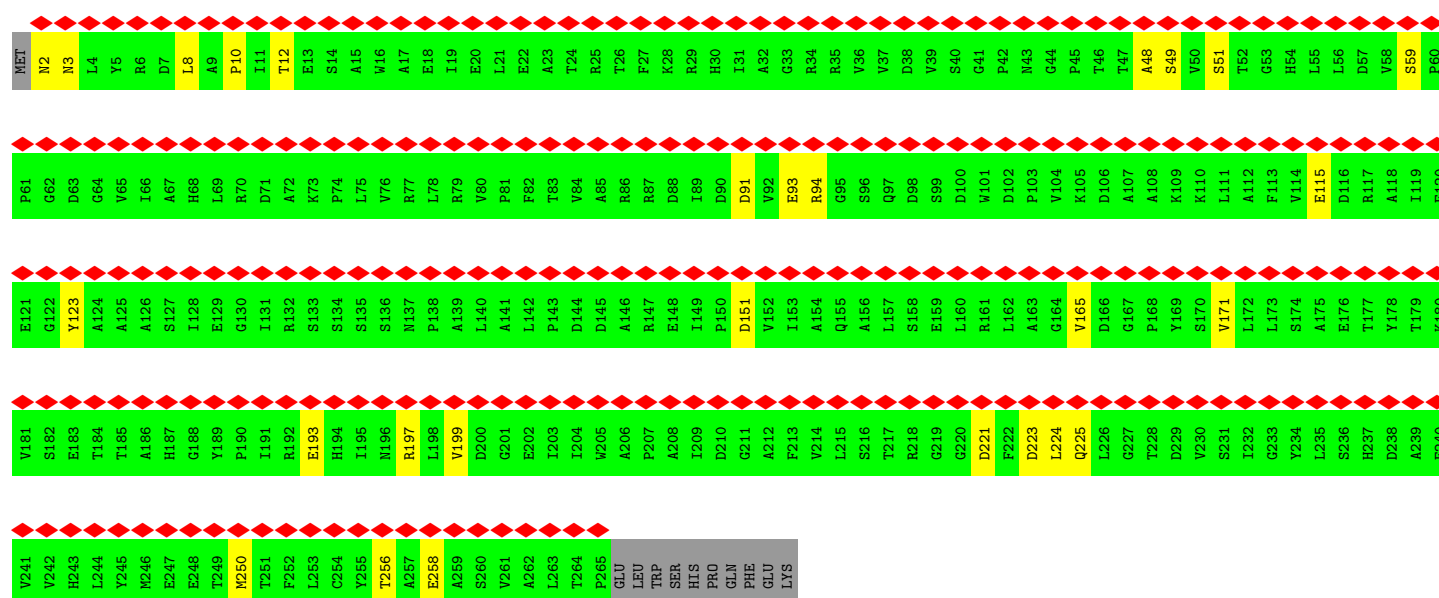


Chain L: 

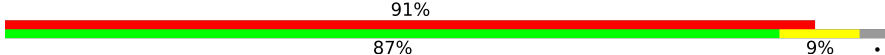


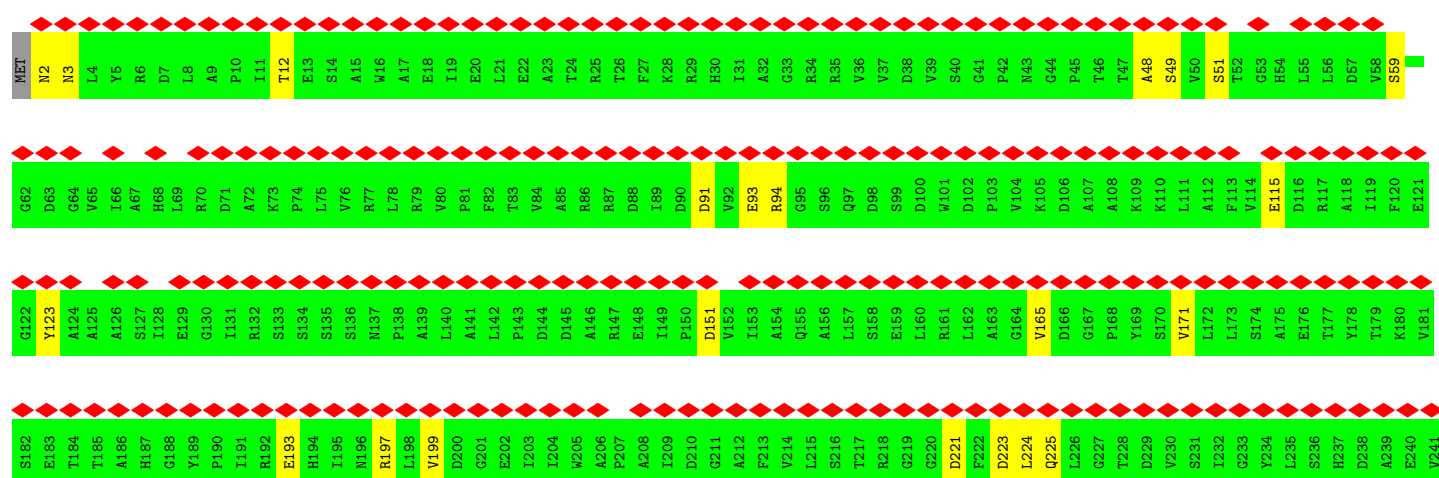
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Chain LA: 



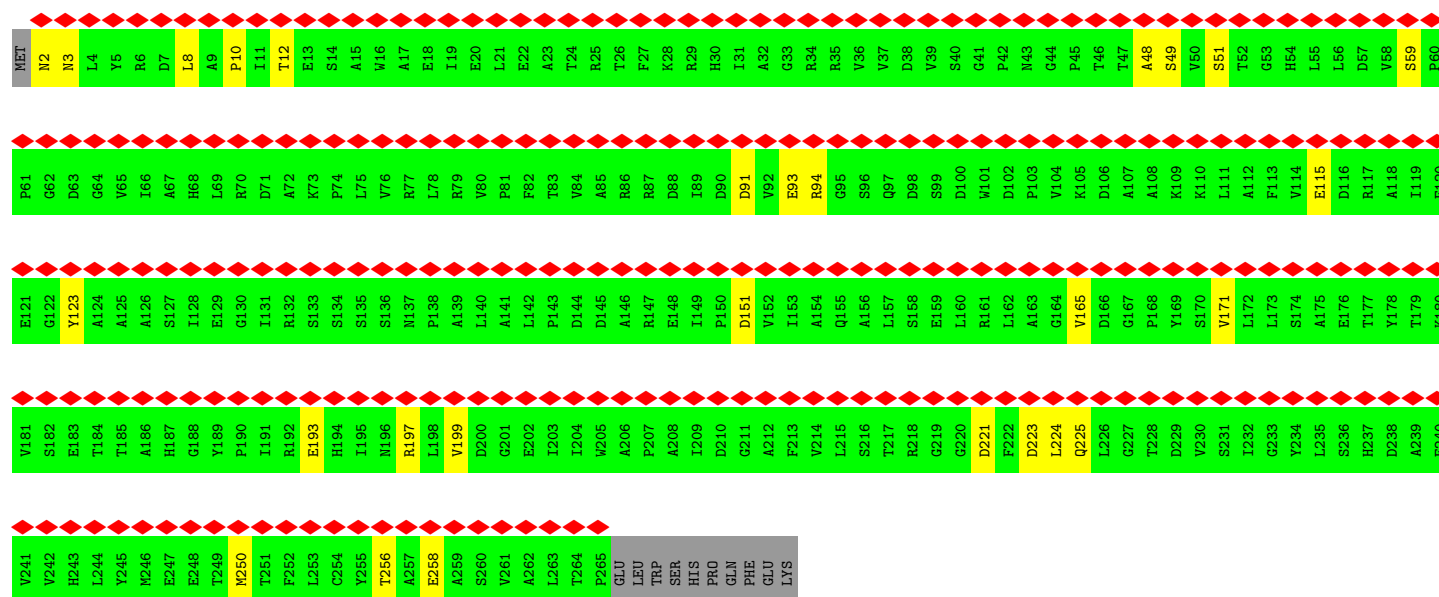
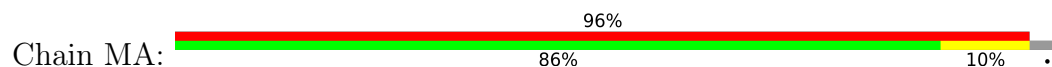
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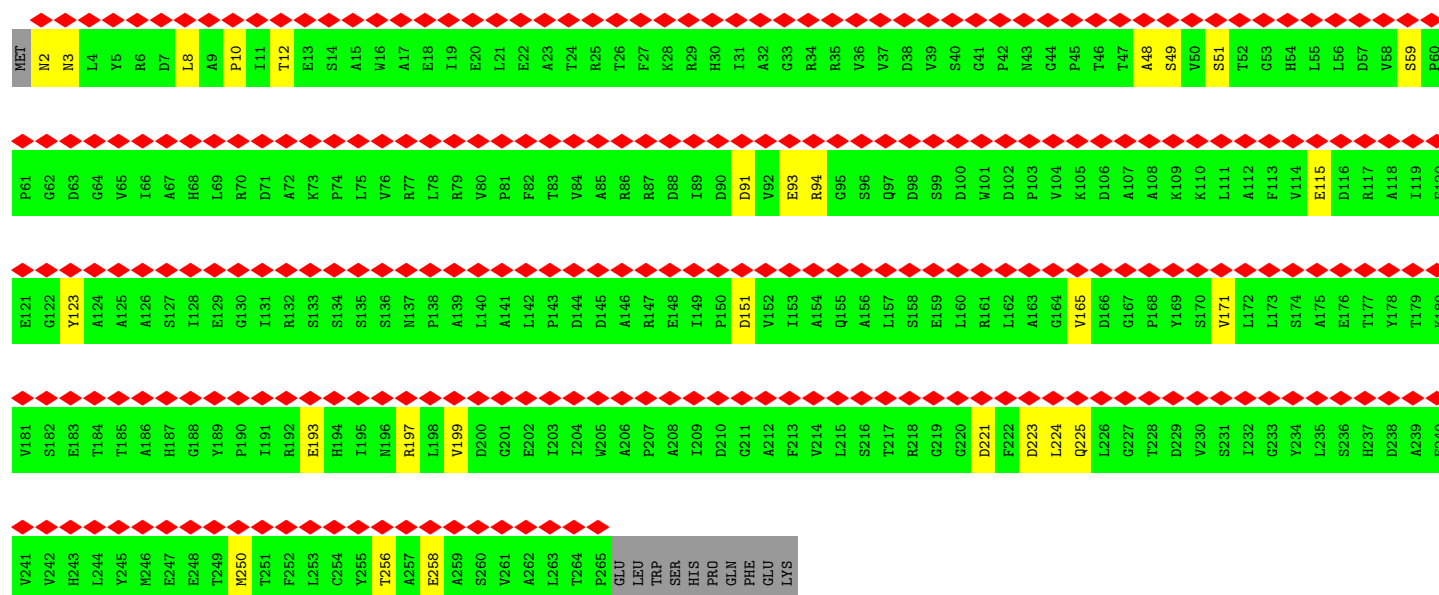
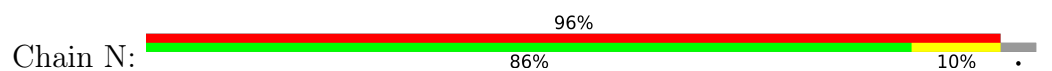




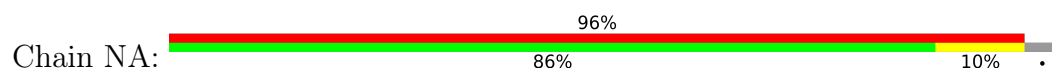
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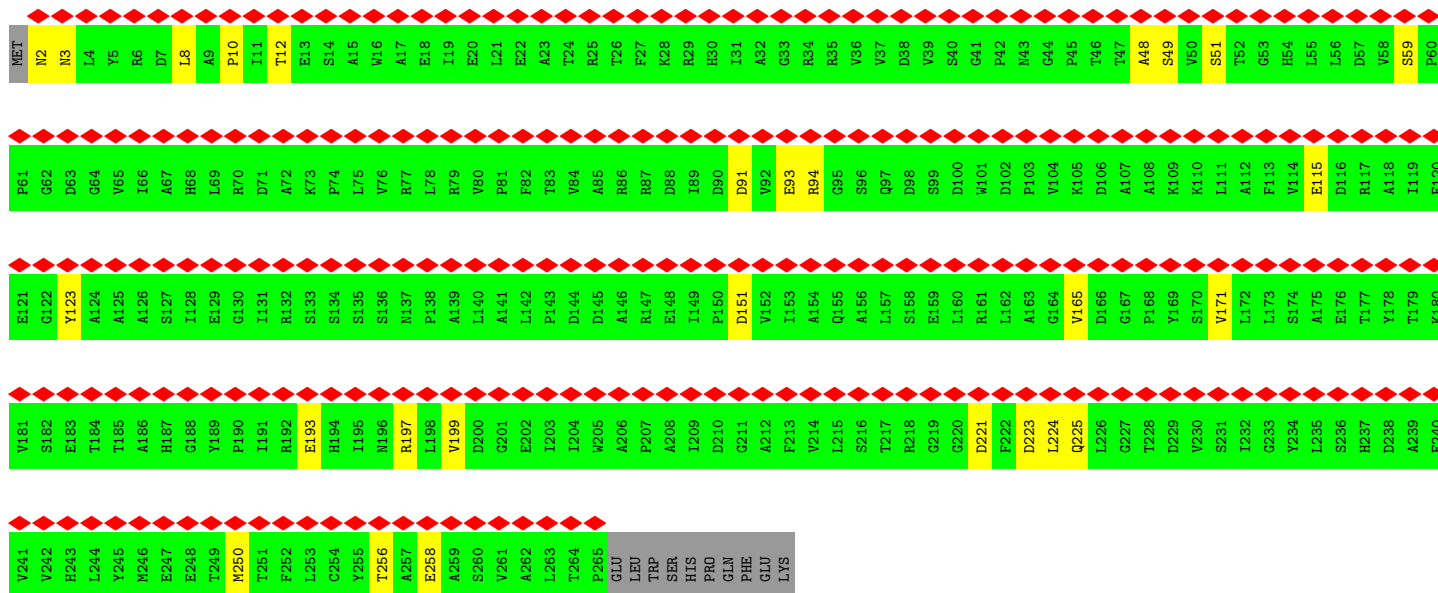


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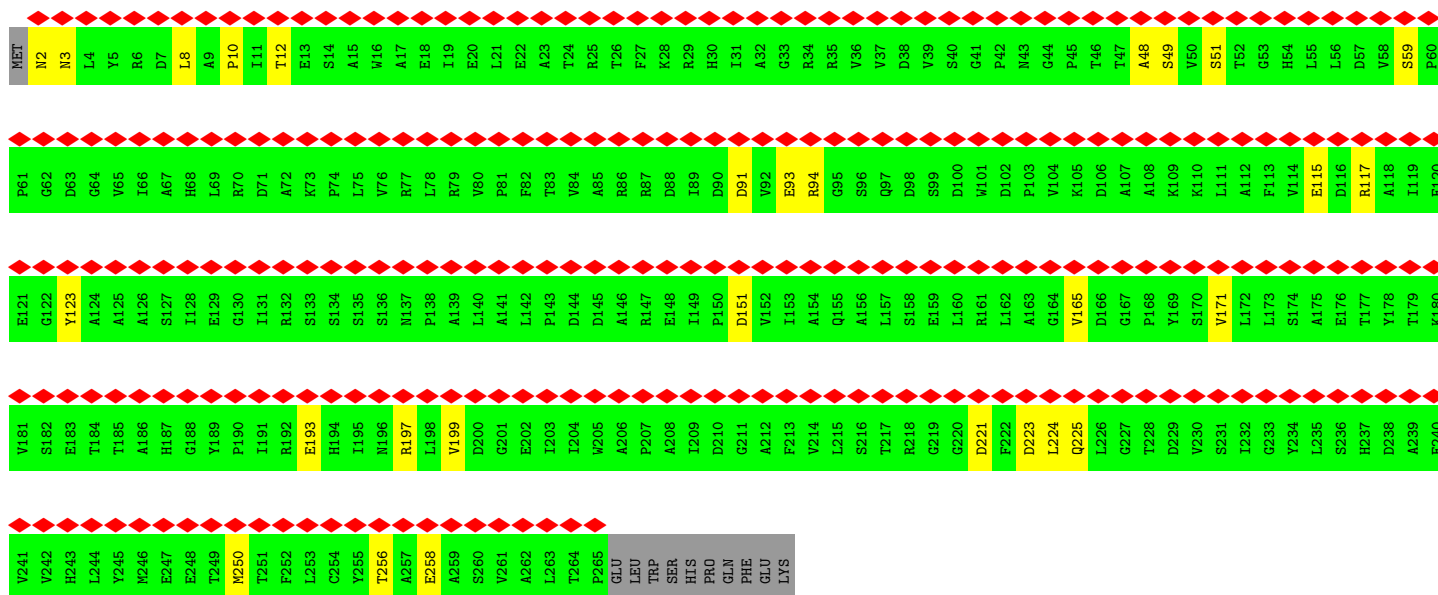
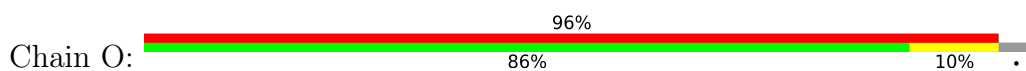


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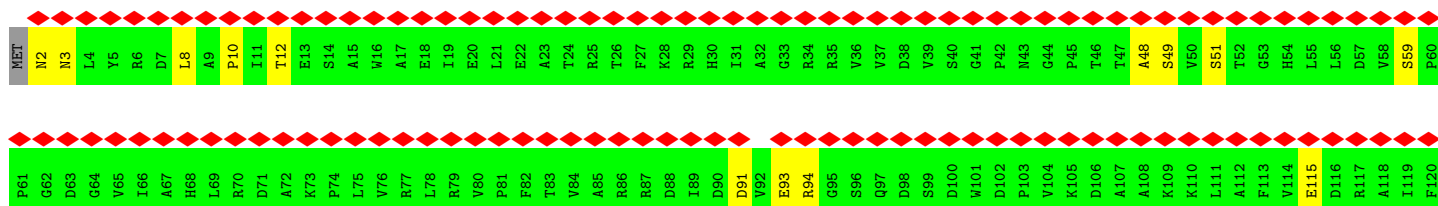
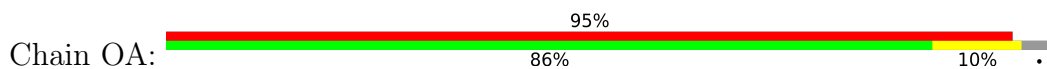


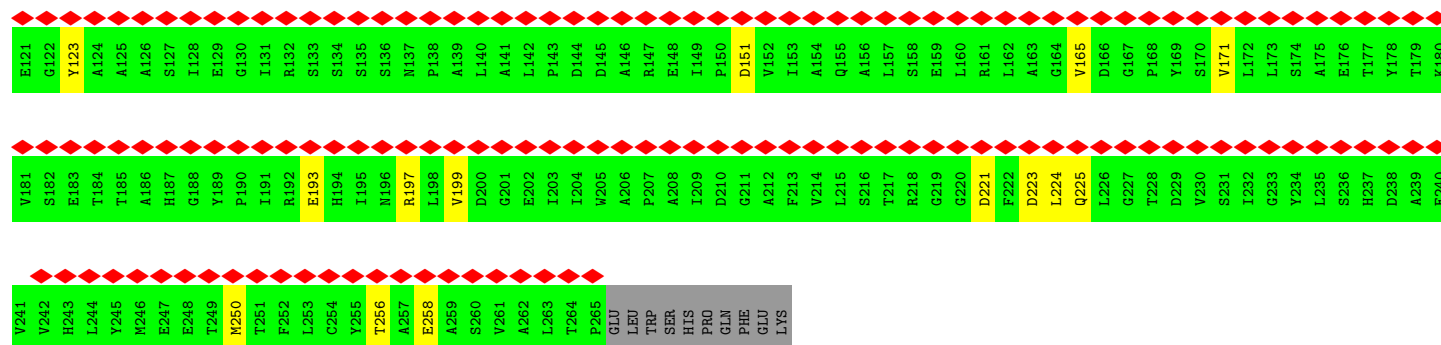


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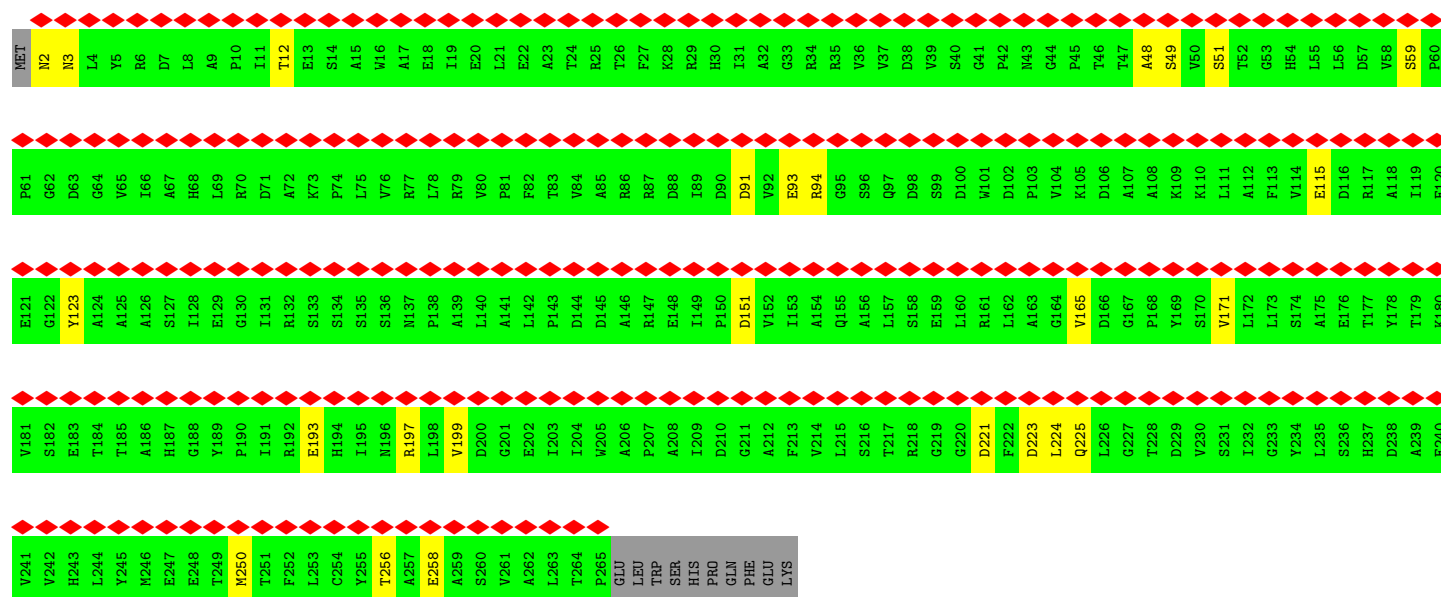


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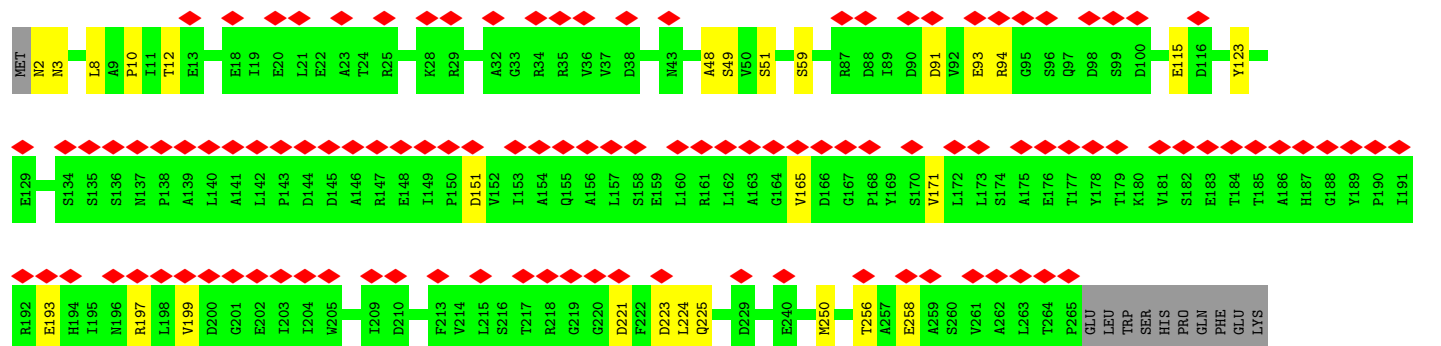




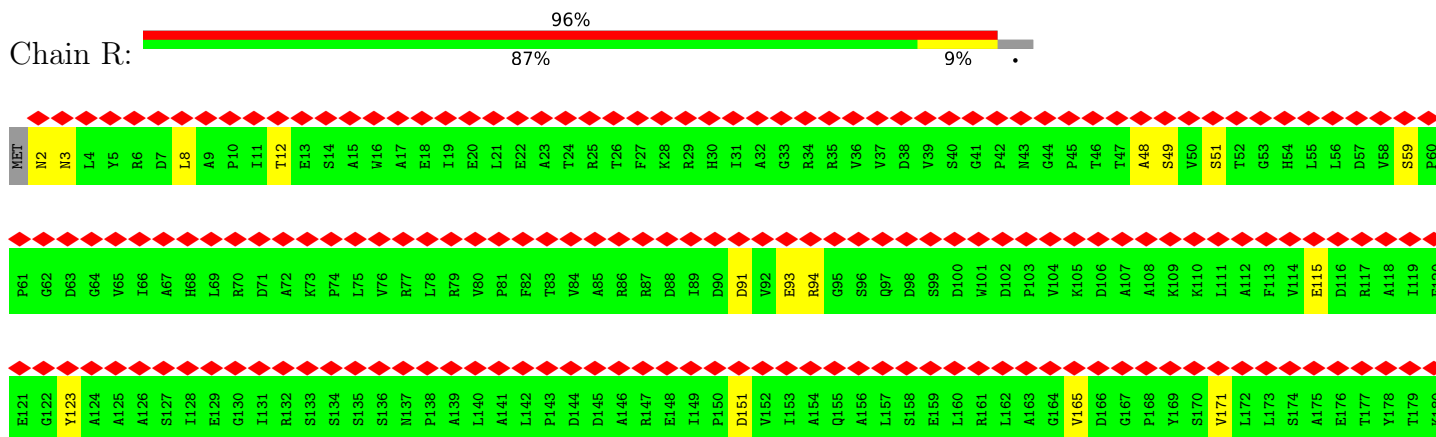
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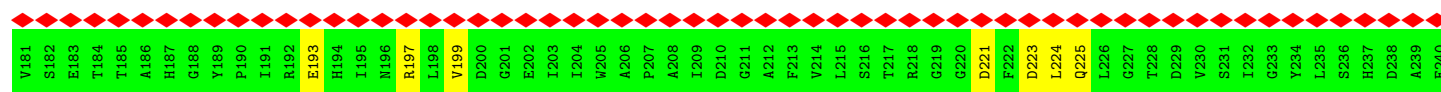


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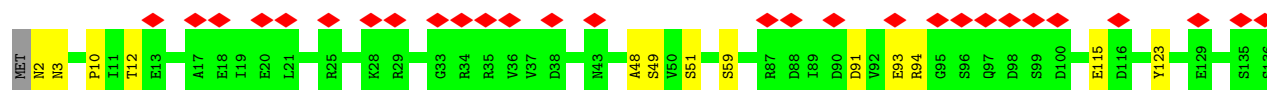
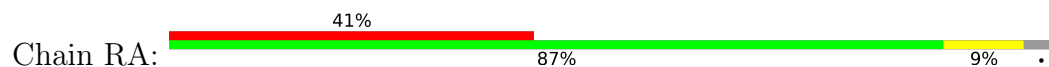


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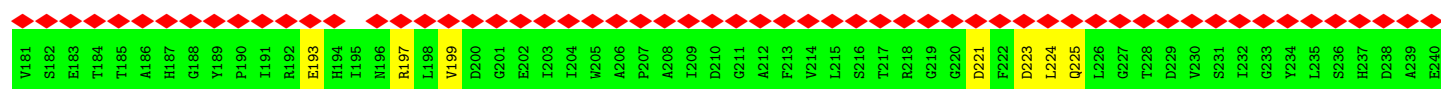
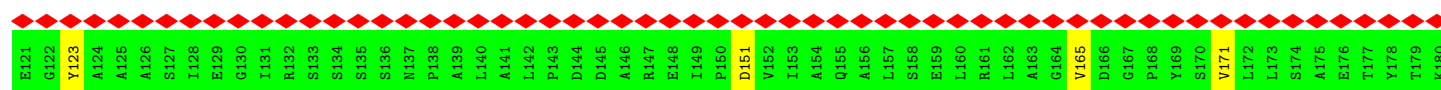
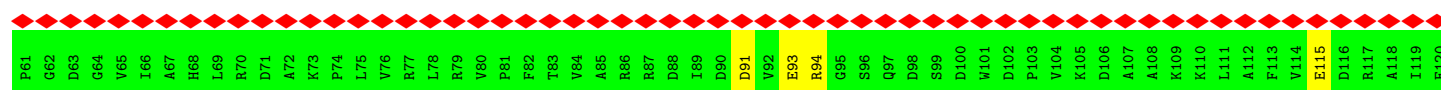
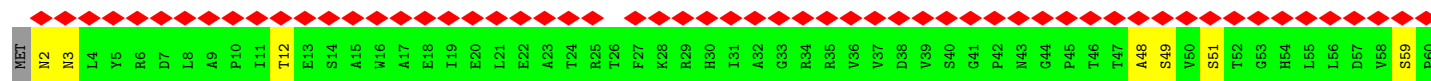
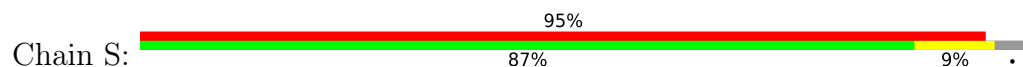




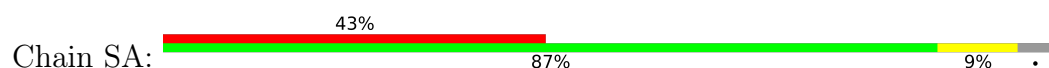
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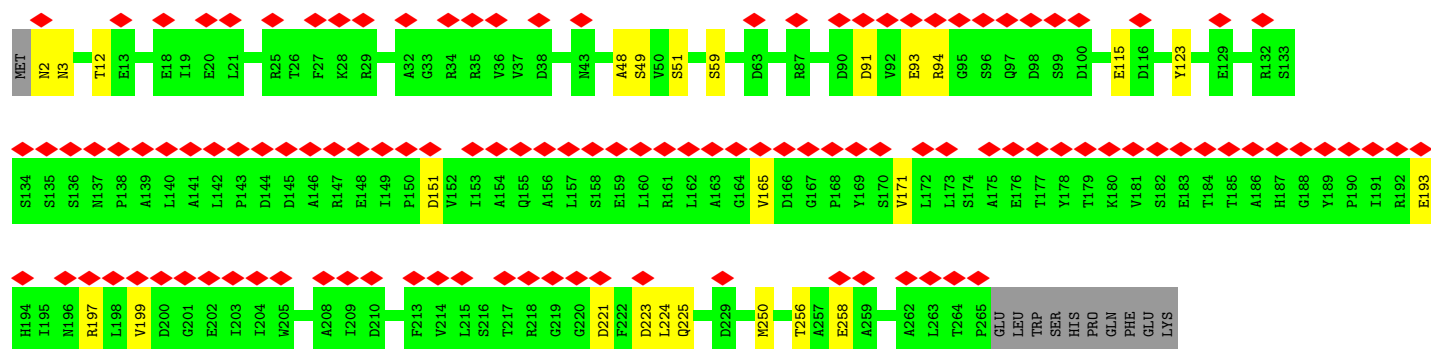


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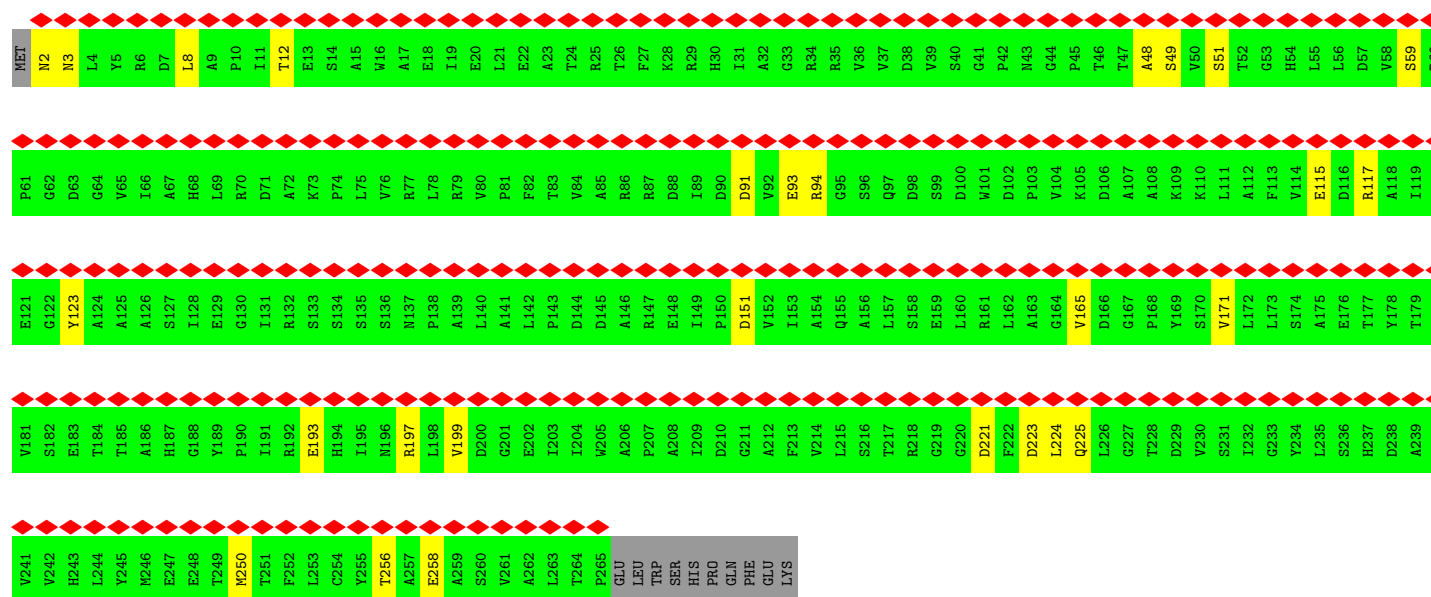


• Molecule 1: 29 kDa antigen Cfp29

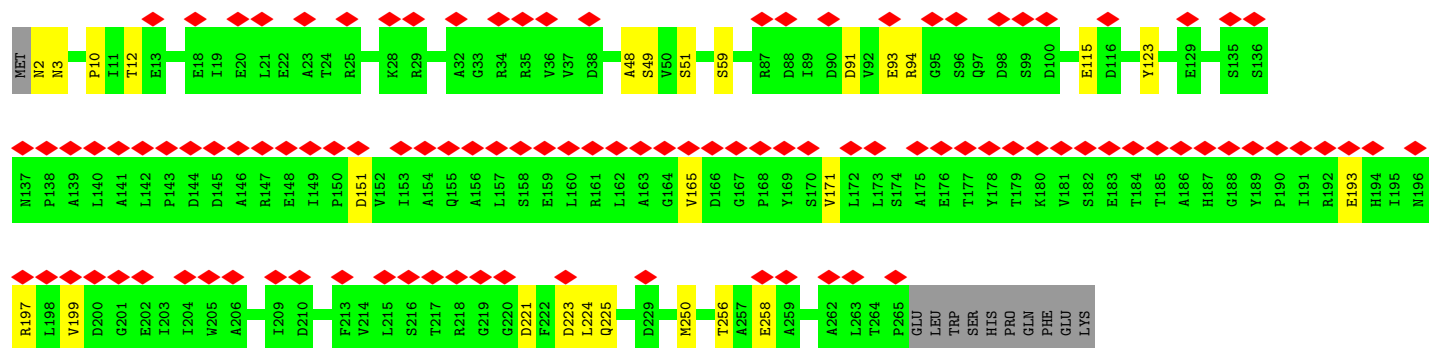
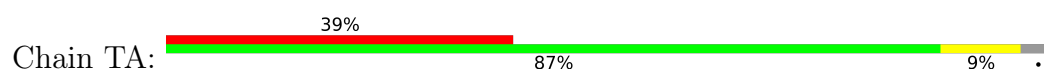




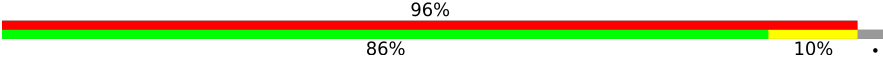
- Molecule 1: 29 kDa antigen Cfp29

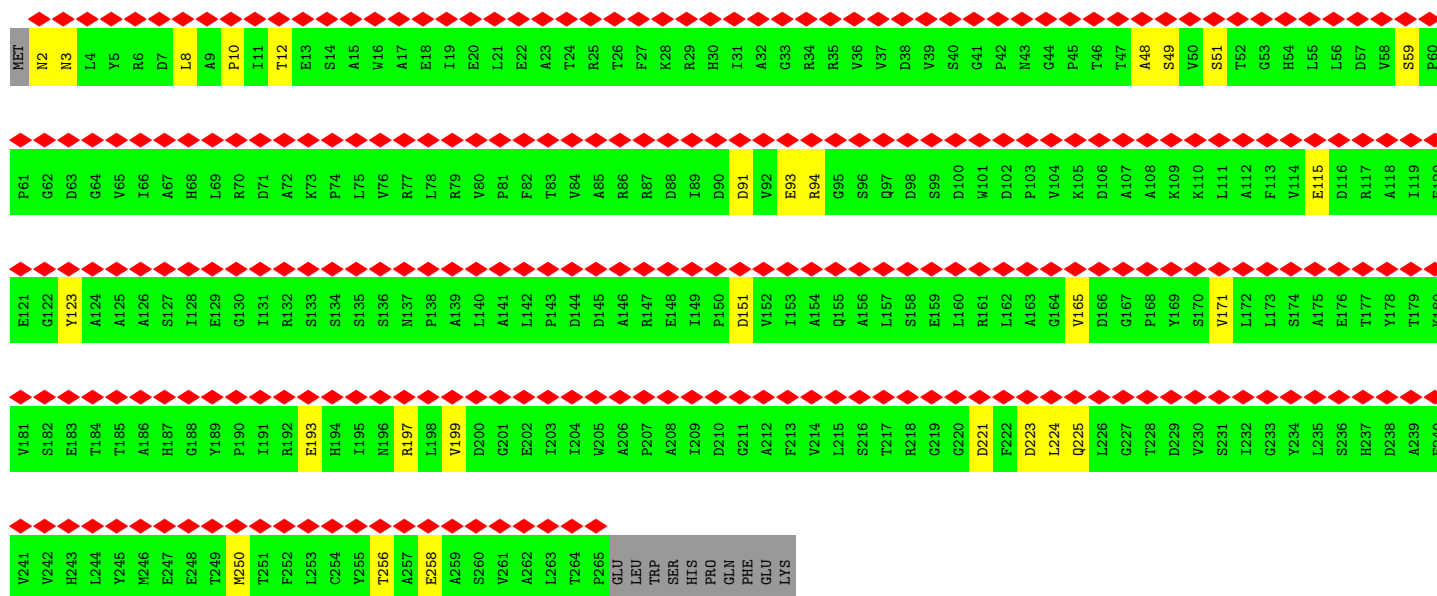


- Molecule 1: 29 kDa antigen Cfp29

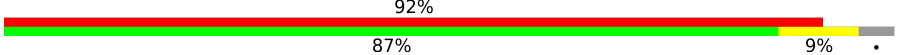


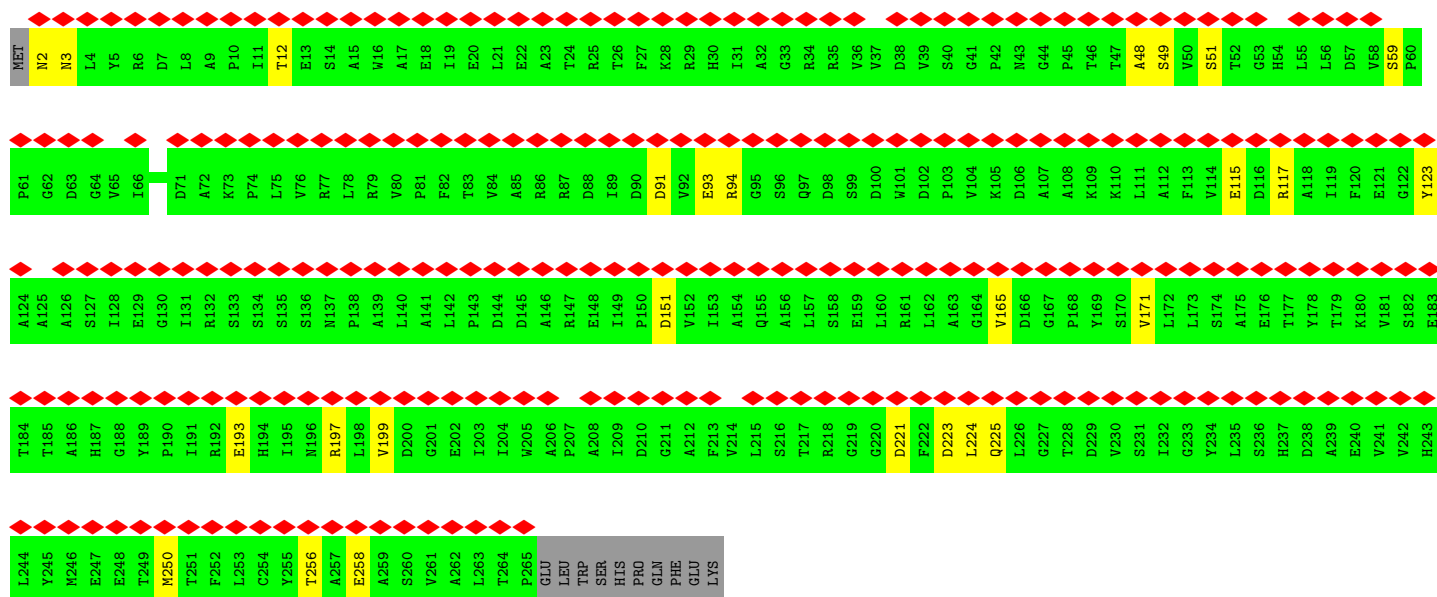
- Molecule 1: 29 kDa antigen Cfp29

Chain UA: 



• Molecule 1: 29 kDa antigen Cfp29

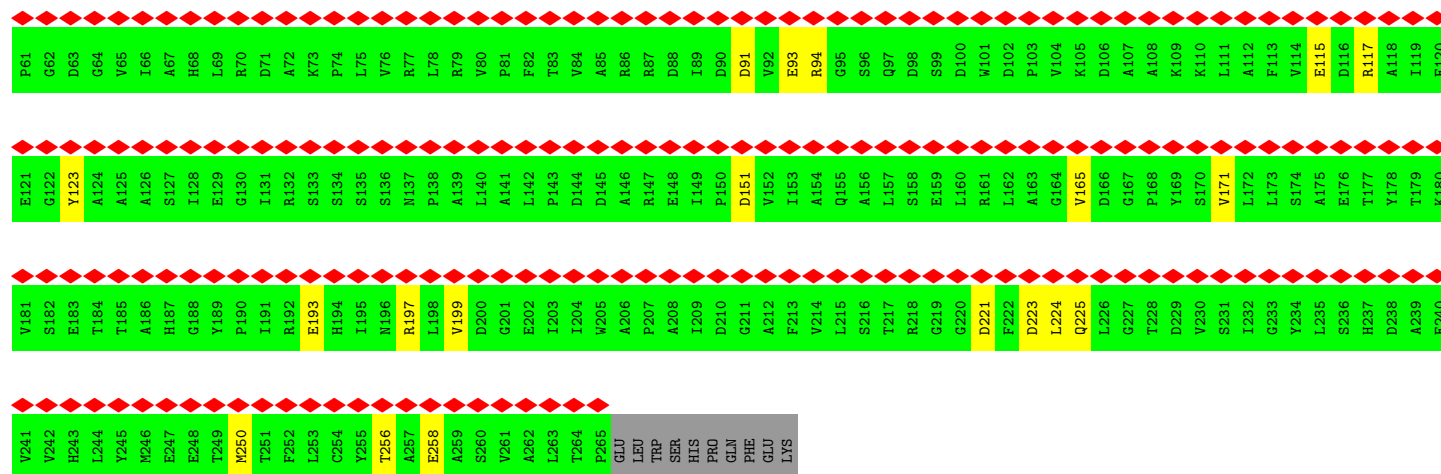
Chain V: 



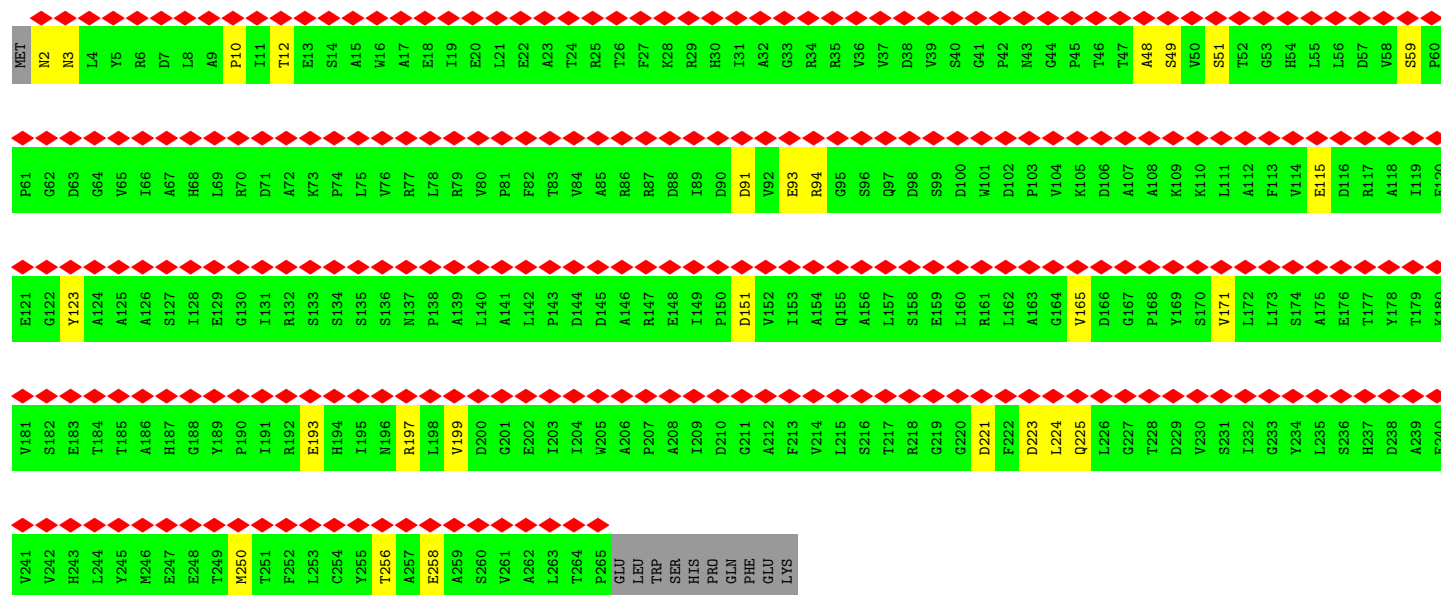
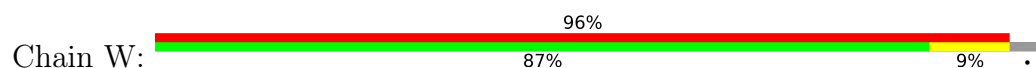
• Molecule 1: 29 kDa antigen Cfp29

Chain VA: 

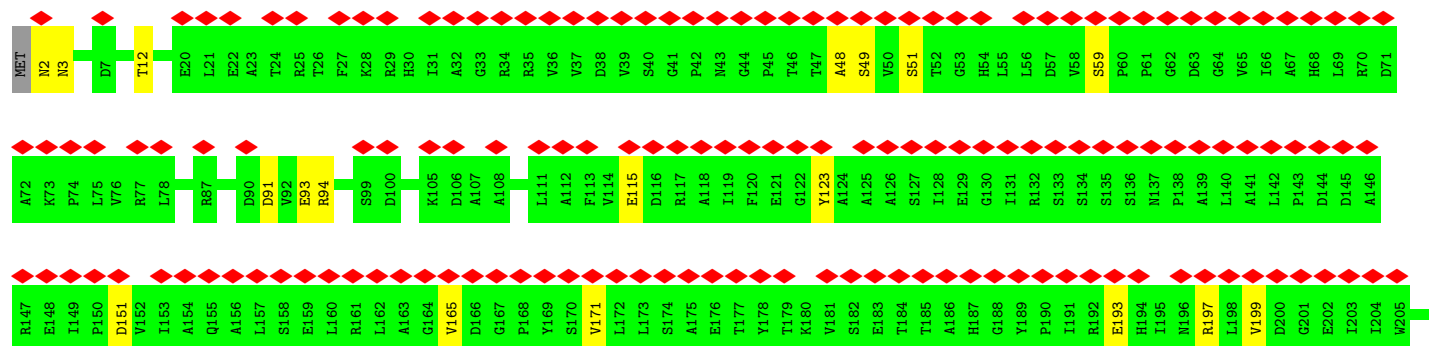
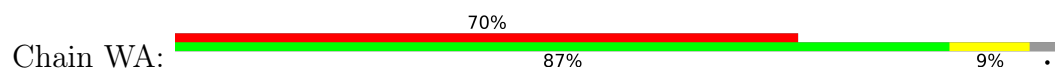


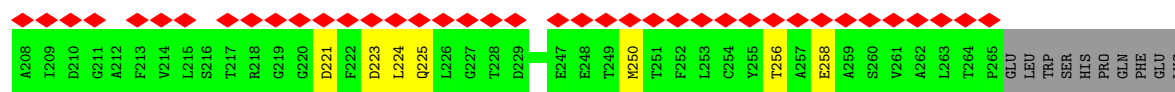


• Molecule 1: 29 kDa antigen Cfp29

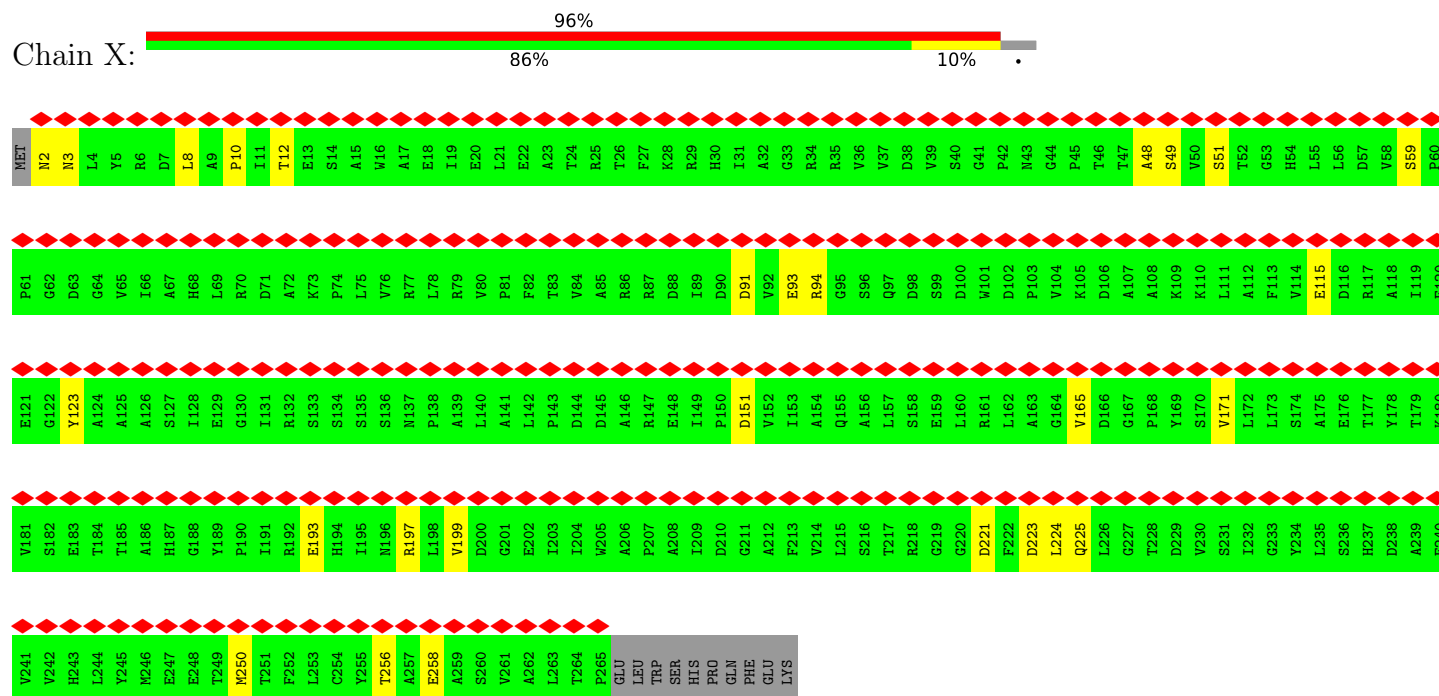


• Molecule 1: 29 kDa antigen Cfp29

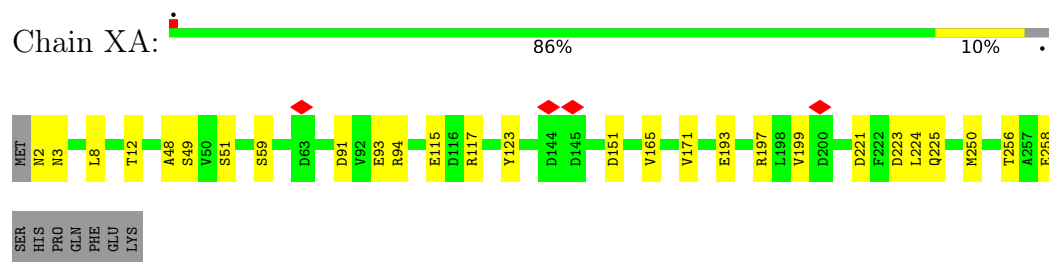




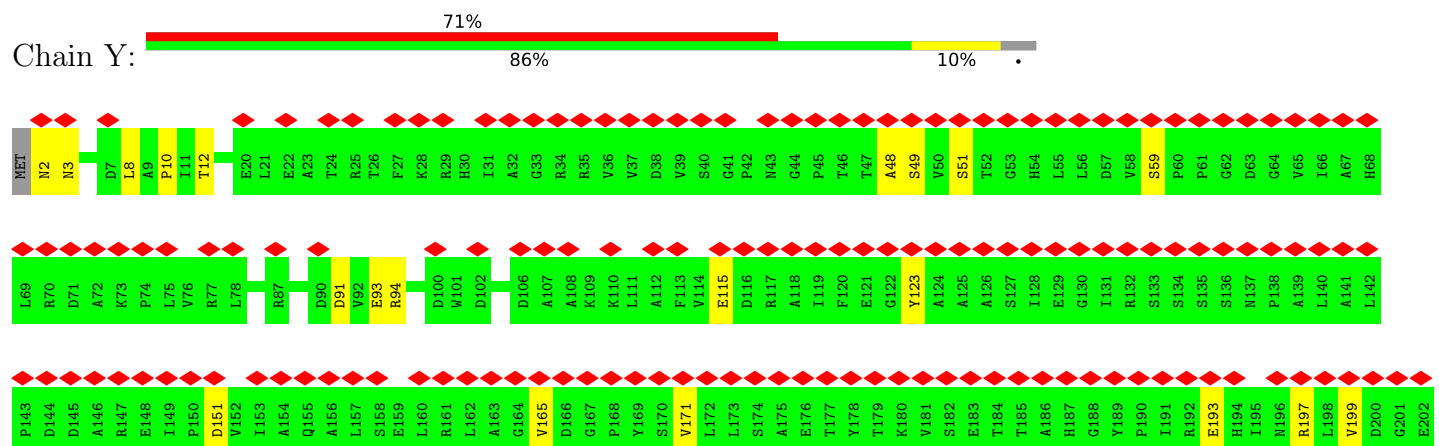
- Molecule 1: 29 kDa antigen Cfp29

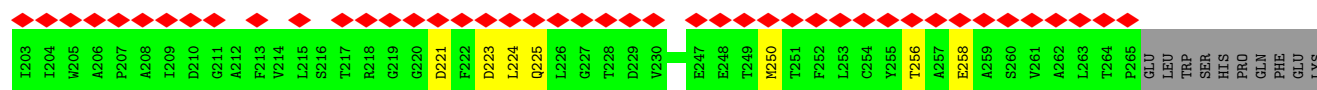


- Molecule 1: 29 kDa antigen Cfp29

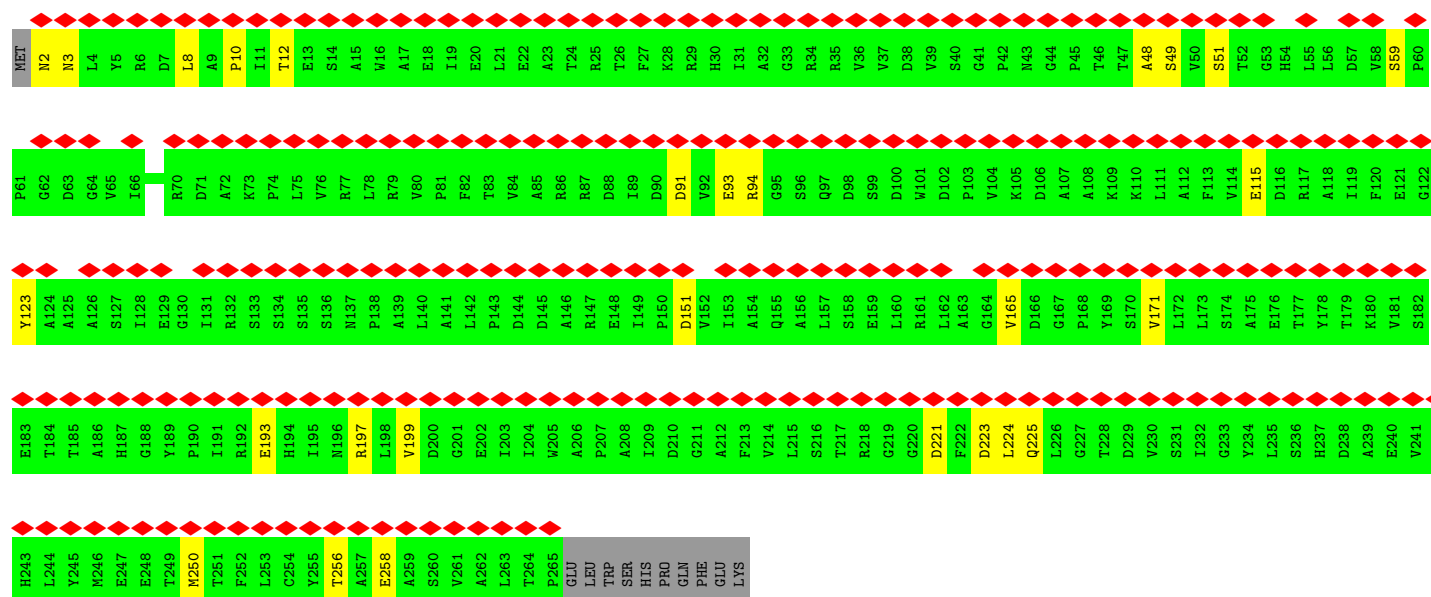
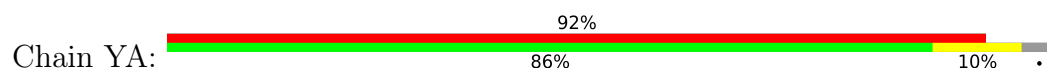


- Molecule 1: 29 kDa antigen Cfp29

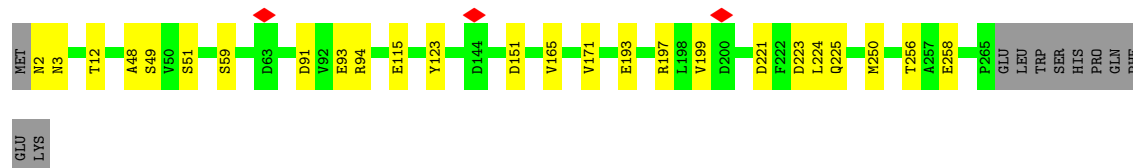
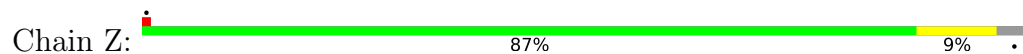




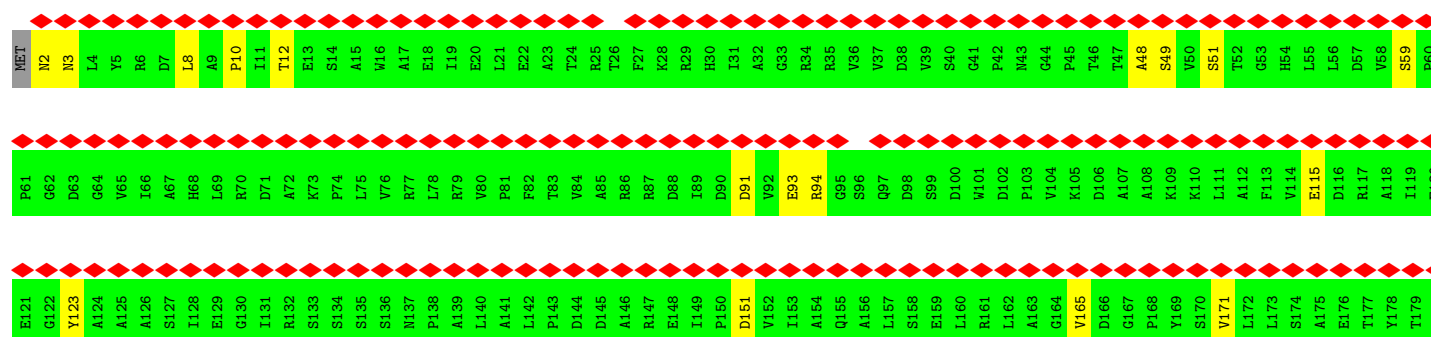
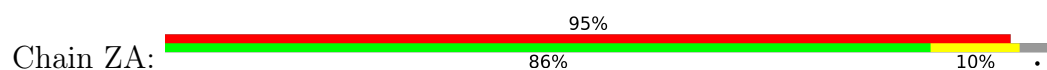
• Molecule 1: 29 kDa antigen Cfp29



• Molecule 1: 29 kDa antigen Cfp29



• Molecule 1: 29 kDa antigen Cfp29





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	308711	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	80000	Depositor
Image detector	DIRECT ELECTRON APOLLO (4k x 4k)	Depositor
Maximum map value	0.402	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	400.9984, 400.9984, 400.9984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7832, 0.7832, 0.7832	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/2059	0.27	0/2810
1	AA	0.11	0/2059	0.27	0/2810
1	AB	0.12	0/2059	0.27	0/2810
1	B	0.12	0/2059	0.27	0/2810
1	BA	0.12	0/2059	0.27	0/2810
1	BB	0.12	0/2059	0.27	0/2810
1	C	0.12	0/2059	0.27	0/2810
1	CA	0.12	0/2059	0.27	0/2810
1	CB	0.12	0/2059	0.27	0/2810
1	D	0.12	0/2059	0.27	0/2810
1	DA	0.12	0/2059	0.27	0/2810
1	DB	0.12	0/2059	0.27	0/2810
1	E	0.12	0/2059	0.27	0/2810
1	EA	0.12	0/2059	0.27	0/2810
1	EB	0.11	0/2059	0.27	0/2810
1	F	0.11	0/2059	0.27	0/2810
1	FA	0.11	0/2059	0.27	0/2810
1	FB	0.12	0/2059	0.27	0/2810
1	G	0.12	0/2059	0.27	0/2810
1	GA	0.12	0/2059	0.27	0/2810
1	GB	0.12	0/2059	0.27	0/2810
1	H	0.12	0/2059	0.27	0/2810
1	HA	0.12	0/2059	0.27	0/2810
1	HB	0.12	0/2059	0.27	0/2810
1	I	0.12	0/2059	0.27	0/2810
1	IA	0.12	0/2059	0.27	0/2810
1	IB	0.12	0/2059	0.27	0/2810
1	J	0.12	0/2059	0.27	0/2810
1	JA	0.12	0/2059	0.27	0/2810
1	K	0.11	0/2059	0.27	0/2810
1	KA	0.11	0/2059	0.27	0/2810
1	L	0.12	0/2059	0.27	0/2810
1	LA	0.12	0/2059	0.27	0/2810
1	M	0.12	0/2059	0.27	0/2810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	MA	0.12	0/2059	0.27	0/2810
1	N	0.12	0/2059	0.27	0/2810
1	NA	0.12	0/2059	0.27	0/2810
1	O	0.12	0/2059	0.27	0/2810
1	OA	0.12	0/2059	0.27	0/2810
1	P	0.11	0/2059	0.27	0/2810
1	PA	0.11	0/2059	0.27	0/2810
1	Q	0.12	0/2059	0.27	0/2810
1	QA	0.12	0/2059	0.27	0/2810
1	R	0.12	0/2059	0.27	0/2810
1	RA	0.12	0/2059	0.27	0/2810
1	S	0.12	0/2059	0.27	0/2810
1	SA	0.12	0/2059	0.27	0/2810
1	T	0.12	0/2059	0.27	0/2810
1	TA	0.12	0/2059	0.27	0/2810
1	UA	0.11	0/2059	0.27	0/2810
1	V	0.11	0/2059	0.27	0/2810
1	VA	0.12	0/2059	0.27	0/2810
1	W	0.12	0/2059	0.27	0/2810
1	WA	0.12	0/2059	0.27	0/2810
1	X	0.12	0/2059	0.27	0/2810
1	XA	0.12	0/2059	0.27	0/2810
1	Y	0.12	0/2059	0.27	0/2810
1	YA	0.12	0/2059	0.27	0/2810
1	Z	0.12	0/2059	0.27	0/2810
1	ZA	0.11	0/2059	0.27	0/2810
All	All	0.12	0/123540	0.27	0/168600

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2017	0	1972	32	0
1	AA	2017	0	1972	33	0
1	AB	2017	0	1972	33	0
1	B	2017	0	1972	33	0
1	BA	2017	0	1972	33	0
1	BB	2017	0	1972	33	0
1	C	2017	0	1972	33	0
1	CA	2017	0	1972	34	0
1	CB	2017	0	1972	32	0
1	D	2017	0	1972	33	0
1	DA	2017	0	1972	35	0
1	DB	2017	0	1972	33	0
1	E	2017	0	1972	34	0
1	EA	2017	0	1972	32	0
1	EB	2017	0	1972	34	0
1	F	2017	0	1972	34	0
1	FA	2017	0	1972	34	0
1	FB	2017	0	1972	34	0
1	G	2017	0	1972	34	0
1	GA	2017	0	1972	34	0
1	GB	2017	0	1972	32	0
1	H	2017	0	1972	33	0
1	HA	2017	0	1972	35	0
1	HB	2017	0	1972	33	0
1	I	2017	0	1972	35	0
1	IA	2017	0	1972	34	0
1	IB	2017	0	1972	34	0
1	J	2017	0	1972	36	0
1	JA	2017	0	1972	34	0
1	K	2017	0	1972	34	0
1	KA	2017	0	1972	33	0
1	L	2017	0	1972	34	0
1	LA	2017	0	1972	34	0
1	M	2017	0	1972	32	0
1	MA	2017	0	1972	34	0
1	N	2017	0	1972	34	0
1	NA	2017	0	1972	34	0
1	O	2017	0	1972	35	0
1	OA	2017	0	1972	34	0
1	P	2017	0	1972	32	0
1	PA	2017	0	1972	34	0
1	Q	2017	0	1972	33	0
1	QA	2017	0	1972	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2017	0	1972	33	0
1	RA	2017	0	1972	33	0
1	S	2017	0	1972	32	0
1	SA	2017	0	1972	32	0
1	T	2017	0	1972	34	0
1	TA	2017	0	1972	33	0
1	UA	2017	0	1972	34	0
1	V	2017	0	1972	33	0
1	VA	2017	0	1972	35	0
1	W	2017	0	1972	34	0
1	WA	2017	0	1972	32	0
1	X	2017	0	1972	34	0
1	XA	2017	0	1972	34	0
1	Y	2017	0	1972	35	0
1	YA	2017	0	1972	34	0
1	Z	2017	0	1972	32	0
1	ZA	2017	0	1972	34	0
All	All	121020	0	118320	1280	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 5.

All (1280) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:197:ARG:NH1	1:PA:193:GLU:OE2	1.98	0.97
1:EA:197:ARG:NH1	1:X:193:GLU:OE2	1.98	0.97
1:LA:197:ARG:NH1	1:N:193:GLU:OE2	1.98	0.97
1:Y:197:ARG:NH1	1:ZA:193:GLU:OE2	1.98	0.97
1:CA:193:GLU:OE2	1:Z:197:ARG:NH1	1.98	0.96
1:CB:197:ARG:NH1	1:F:193:GLU:OE2	1.98	0.96
1:GA:197:ARG:NH1	1:I:193:GLU:OE2	1.98	0.96
1:K:193:GLU:OE2	1:SA:197:ARG:NH1	1.98	0.96
1:CA:197:ARG:NH1	1:L:193:GLU:OE2	1.98	0.96
1:DB:197:ARG:NH1	1:GB:193:GLU:OE2	1.98	0.96
1:G:193:GLU:OE2	1:X:197:ARG:NH1	1.98	0.96
1:TA:197:ARG:NH1	1:WA:193:GLU:OE2	1.98	0.96
1:M:193:GLU:OE2	1:T:197:ARG:NH1	1.98	0.96
1:E:193:GLU:OE2	1:PA:197:ARG:NH1	1.99	0.96
1:E:197:ARG:NH1	1:H:193:GLU:OE2	1.98	0.96
1:IA:197:ARG:NH1	1:UA:193:GLU:OE2	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:ARG:NH1	1:JA:193:GLU:OE2	1.99	0.96
1:K:197:ARG:NH1	1:OA:193:GLU:OE2	1.99	0.96
1:T:193:GLU:OE2	1:ZA:197:ARG:NH1	1.99	0.96
1:CB:193:GLU:OE2	1:Q:197:ARG:NH1	1.98	0.96
1:A:193:GLU:OE2	1:XA:197:ARG:NH1	1.98	0.96
1:B:197:ARG:NH1	1:SA:193:GLU:OE2	1.98	0.96
1:BB:193:GLU:OE2	1:IB:197:ARG:NH1	1.98	0.96
1:EB:193:GLU:OE2	1:NA:197:ARG:NH1	1.98	0.96
1:EB:197:ARG:NH1	1:J:193:GLU:OE2	1.99	0.96
1:HB:197:ARG:NH1	1:P:193:GLU:OE2	1.98	0.96
1:O:193:GLU:OE2	1:UA:197:ARG:NH1	1.99	0.96
1:RA:193:GLU:OE2	1:YA:197:ARG:NH1	1.98	0.96
1:AB:193:GLU:OE2	1:H:197:ARG:NH1	1.98	0.96
1:M:197:ARG:NH1	1:QA:193:GLU:OE2	1.98	0.96
1:C:193:GLU:OE2	1:J:197:ARG:NH1	1.98	0.96
1:O:197:ARG:NH1	1:R:193:GLU:OE2	1.98	0.95
1:D:197:ARG:NH1	1:FA:193:GLU:OE2	1.98	0.95
1:KA:193:GLU:OE2	1:S:197:ARG:NH1	1.98	0.95
1:KA:197:ARG:NH1	1:YA:193:GLU:OE2	1.99	0.95
1:AA:197:ARG:NH1	1:DB:193:GLU:OE2	1.99	0.95
1:FA:197:ARG:NH1	1:IB:193:GLU:OE2	1.99	0.95
1:GB:197:ARG:NH1	1:LA:193:GLU:OE2	1.98	0.95
1:TA:193:GLU:OE2	1:V:197:ARG:NH1	1.99	0.95
1:B:193:GLU:OE2	1:HA:197:ARG:NH1	1.98	0.95
1:D:193:GLU:OE2	1:W:197:ARG:NH1	1.98	0.95
1:GA:193:GLU:OE2	1:WA:197:ARG:NH1	1.98	0.95
1:MA:197:ARG:NH1	1:Q:193:GLU:OE2	1.98	0.95
1:FB:197:ARG:NH1	1:IA:193:GLU:OE2	1.98	0.95
1:HA:193:GLU:OE2	1:OA:197:ARG:NH1	1.98	0.95
1:L:197:ARG:NH1	1:XA:193:GLU:OE2	1.98	0.95
1:NA:193:GLU:OE2	1:VA:197:ARG:NH1	1.98	0.95
1:BA:197:ARG:NH1	1:S:193:GLU:OE2	1.98	0.95
1:FB:193:GLU:OE2	1:R:197:ARG:NH1	1.98	0.95
1:JA:197:ARG:NH1	1:MA:193:GLU:OE2	1.98	0.95
1:AA:193:GLU:OE2	1:N:197:ARG:NH1	1.98	0.95
1:BB:197:ARG:NH1	1:W:193:GLU:OE2	1.98	0.95
1:C:197:ARG:NH1	1:VA:193:GLU:OE2	1.98	0.95
1:G:197:ARG:NH1	1:HB:193:GLU:OE2	1.98	0.95
1:I:197:ARG:NH1	1:V:193:GLU:OE2	1.98	0.95
1:BA:193:GLU:OE2	1:RA:197:ARG:NH1	1.98	0.95
1:AB:197:ARG:NH1	1:DA:193:GLU:OE2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:193:GLU:OE2	1:P:197:ARG:NH1	1.99	0.94
1:QA:197:ARG:NH1	1:Y:193:GLU:OE2	1.98	0.94
1:A:197:ARG:NH1	1:Z:193:GLU:OE2	1.99	0.94
1:BB:193:GLU:CD	1:IB:197:ARG:NH1	2.28	0.84
1:F:197:ARG:NH1	1:JA:193:GLU:CD	2.28	0.84
1:K:197:ARG:NH1	1:OA:193:GLU:CD	2.28	0.84
1:RA:193:GLU:CD	1:YA:197:ARG:NH1	2.28	0.84
1:GB:49:SER:OG	1:Q:49:SER:OG	1.96	0.83
1:K:49:SER:OG	1:YA:49:SER:OG	1.96	0.83
1:F:49:SER:OG	1:IB:49:SER:OG	1.96	0.83
1:B:197:ARG:NH1	1:SA:193:GLU:CD	2.28	0.83
1:BA:49:SER:OG	1:M:49:SER:OG	1.96	0.83
1:H:49:SER:OG	1:W:49:SER:OG	1.96	0.83
1:BB:49:SER:OG	1:G:49:SER:OG	1.96	0.83
1:HA:49:SER:OG	1:VA:49:SER:OG	1.96	0.83
1:FB:49:SER:OG	1:MA:49:SER:OG	1.96	0.83
1:L:49:SER:OG	1:RA:49:SER:OG	1.96	0.83
1:T:193:GLU:CD	1:ZA:197:ARG:NH1	2.28	0.83
1:CB:193:GLU:CD	1:Q:197:ARG:NH1	2.28	0.83
1:DB:49:SER:OG	1:P:49:SER:OG	1.96	0.83
1:FA:49:SER:OG	1:J:49:SER:OG	1.96	0.83
1:KA:49:SER:OG	1:O:49:SER:OG	1.96	0.83
1:N:49:SER:OG	1:S:49:SER:OG	1.96	0.83
1:D:49:SER:OG	1:I:49:SER:OG	1.96	0.83
1:E:193:GLU:CD	1:PA:197:ARG:NH1	2.28	0.83
1:A:49:SER:OG	1:TA:49:SER:OG	1.96	0.82
1:EA:49:SER:OG	1:ZA:49:SER:OG	1.96	0.82
1:FA:197:ARG:NH1	1:IB:193:GLU:CD	2.28	0.82
1:IA:49:SER:OG	1:NA:49:SER:OG	1.96	0.82
1:PA:49:SER:OG	1:Z:49:SER:OG	1.96	0.82
1:LA:49:SER:OG	1:R:49:SER:OG	1.96	0.82
1:CA:49:SER:OG	1:QA:49:SER:OG	1.96	0.82
1:CB:49:SER:OG	1:HB:49:SER:OG	1.96	0.82
1:O:193:GLU:CD	1:UA:197:ARG:NH1	2.28	0.82
1:C:49:SER:OG	1:GA:49:SER:OG	1.96	0.82
1:SA:49:SER:OG	1:XA:49:SER:OG	1.96	0.82
1:AB:49:SER:OG	1:X:49:SER:OG	1.96	0.82
1:KA:197:ARG:NH1	1:YA:193:GLU:CD	2.28	0.82
1:MA:197:ARG:NH1	1:Q:193:GLU:CD	2.28	0.82
1:O:197:ARG:NH1	1:R:193:GLU:CD	2.28	0.82
1:C:193:GLU:CD	1:J:197:ARG:NH1	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:SER:OG	1:WA:49:SER:OG	1.96	0.82
1:E:49:SER:OG	1:V:49:SER:OG	1.96	0.82
1:EB:197:ARG:NH1	1:J:193:GLU:CD	2.28	0.82
1:B:193:GLU:CD	1:HA:197:ARG:NH1	2.28	0.82
1:AA:49:SER:OG	1:T:49:SER:OG	1.96	0.81
1:TA:197:ARG:NH1	1:WA:193:GLU:CD	2.28	0.81
1:DB:197:ARG:NH1	1:GB:193:GLU:CD	2.28	0.81
1:DA:49:SER:OG	1:Y:49:SER:OG	1.96	0.81
1:CA:197:ARG:NH1	1:L:193:GLU:CD	2.28	0.81
1:OA:49:SER:OG	1:UA:49:SER:OG	1.96	0.81
1:EB:49:SER:OG	1:JA:49:SER:OG	1.96	0.81
1:G:193:GLU:CD	1:X:197:ARG:NH1	2.28	0.81
1:G:197:ARG:NH1	1:HB:193:GLU:CD	2.28	0.81
1:A:197:ARG:NH1	1:Z:193:GLU:CD	2.28	0.80
1:EA:193:GLU:CD	1:P:197:ARG:NH1	2.28	0.80
1:EB:193:GLU:CD	1:NA:197:ARG:NH1	2.28	0.80
1:IA:197:ARG:NH1	1:UA:193:GLU:CD	2.28	0.80
1:L:197:ARG:NH1	1:XA:193:GLU:CD	2.28	0.80
1:C:197:ARG:NH1	1:VA:193:GLU:CD	2.28	0.80
1:FB:193:GLU:CD	1:R:197:ARG:NH1	2.28	0.80
1:M:193:GLU:CD	1:T:197:ARG:NH1	2.28	0.80
1:AB:193:GLU:CD	1:H:197:ARG:NH1	2.28	0.80
1:D:193:GLU:CD	1:W:197:ARG:NH1	2.28	0.80
1:E:197:ARG:NH1	1:H:193:GLU:CD	2.28	0.80
1:D:197:ARG:NH1	1:FA:193:GLU:CD	2.28	0.79
1:M:197:ARG:NH1	1:QA:193:GLU:CD	2.28	0.79
1:KA:193:GLU:CD	1:S:197:ARG:NH1	2.28	0.79
1:NA:193:GLU:CD	1:VA:197:ARG:NH1	2.28	0.79
1:FB:197:ARG:NH1	1:IA:193:GLU:CD	2.28	0.78
1:HB:197:ARG:NH1	1:P:193:GLU:CD	2.28	0.78
1:I:197:ARG:NH1	1:V:193:GLU:CD	2.28	0.78
1:A:193:GLU:CD	1:XA:197:ARG:NH1	2.28	0.78
1:AA:193:GLU:CD	1:N:197:ARG:NH1	2.28	0.78
1:K:193:GLU:CD	1:SA:197:ARG:NH1	2.28	0.78
1:Y:197:ARG:NH1	1:ZA:193:GLU:CD	2.28	0.78
1:BA:193:GLU:CD	1:RA:197:ARG:NH1	2.28	0.77
1:DA:197:ARG:NH1	1:PA:193:GLU:CD	2.28	0.77
1:AB:197:ARG:NH1	1:DA:193:GLU:CD	2.28	0.77
1:JA:197:ARG:NH1	1:MA:193:GLU:CD	2.28	0.77
1:LA:197:ARG:NH1	1:N:193:GLU:CD	2.28	0.77
1:CB:197:ARG:NH1	1:F:193:GLU:CD	2.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GA:197:ARG:NH1	1:I:193:GLU:CD	2.28	0.77
1:QA:197:ARG:NH1	1:Y:193:GLU:CD	2.28	0.77
1:BB:197:ARG:NH1	1:W:193:GLU:CD	2.28	0.77
1:HA:193:GLU:CD	1:OA:197:ARG:NH1	2.28	0.77
1:TA:193:GLU:CD	1:V:197:ARG:NH1	2.28	0.76
1:D:91:ASP:OD1	1:D:94:ARG:NH2	2.19	0.76
1:J:91:ASP:OD1	1:J:94:ARG:NH2	2.20	0.76
1:O:91:ASP:OD1	1:O:94:ARG:NH2	2.20	0.76
1:Q:91:ASP:OD1	1:Q:94:ARG:NH2	2.19	0.76
1:S:91:ASP:OD1	1:S:94:ARG:NH2	2.19	0.76
1:B:91:ASP:OD1	1:B:94:ARG:NH2	2.20	0.75
1:BA:91:ASP:OD1	1:BA:94:ARG:NH2	2.19	0.75
1:G:91:ASP:OD1	1:G:94:ARG:NH2	2.19	0.75
1:GA:91:ASP:OD1	1:GA:94:ARG:NH2	2.19	0.75
1:JA:91:ASP:OD1	1:JA:94:ARG:NH2	2.20	0.75
1:L:91:ASP:OD1	1:L:94:ARG:NH2	2.19	0.75
1:LA:91:ASP:OD1	1:LA:94:ARG:NH2	2.19	0.75
1:AA:197:ARG:NH1	1:DB:193:GLU:CD	2.28	0.75
1:BB:91:ASP:OD1	1:BB:94:ARG:NH2	2.20	0.75
1:F:91:ASP:OD1	1:F:94:ARG:NH2	2.19	0.75
1:IA:91:ASP:OD1	1:IA:94:ARG:NH2	2.19	0.75
1:MA:91:ASP:OD1	1:MA:94:ARG:NH2	2.19	0.75
1:OA:91:ASP:OD1	1:OA:94:ARG:NH2	2.20	0.75
1:RA:91:ASP:OD1	1:RA:94:ARG:NH2	2.20	0.75
1:V:91:ASP:OD1	1:V:94:ARG:NH2	2.19	0.75
1:W:91:ASP:OD1	1:W:94:ARG:NH2	2.19	0.75
1:A:91:ASP:OD1	1:A:94:ARG:NH2	2.19	0.75
1:AA:91:ASP:OD1	1:AA:94:ARG:NH2	2.19	0.75
1:CB:91:ASP:OD1	1:CB:94:ARG:NH2	2.19	0.75
1:HA:91:ASP:OD1	1:HA:94:ARG:NH2	2.20	0.75
1:K:91:ASP:OD1	1:K:94:ARG:NH2	2.19	0.75
1:NA:91:ASP:OD1	1:NA:94:ARG:NH2	2.20	0.75
1:T:91:ASP:OD1	1:T:94:ARG:NH2	2.19	0.75
1:WA:91:ASP:OD1	1:WA:94:ARG:NH2	2.19	0.75
1:E:91:ASP:OD1	1:E:94:ARG:NH2	2.20	0.75
1:FB:91:ASP:OD1	1:FB:94:ARG:NH2	2.20	0.75
1:GB:91:ASP:OD1	1:GB:94:ARG:NH2	2.19	0.75
1:P:91:ASP:OD1	1:P:94:ARG:NH2	2.19	0.75
1:SA:91:ASP:OD1	1:SA:94:ARG:NH2	2.19	0.75
1:VA:91:ASP:OD1	1:VA:94:ARG:NH2	2.19	0.75
1:CA:193:GLU:CD	1:Z:197:ARG:NH1	2.28	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:91:ASP:OD1	1:DA:94:ARG:NH2	2.19	0.75
1:Y:91:ASP:OD1	1:Y:94:ARG:NH2	2.19	0.75
1:ZA:91:ASP:OD1	1:ZA:94:ARG:NH2	2.19	0.75
1:C:91:ASP:OD1	1:C:94:ARG:NH2	2.19	0.75
1:HB:91:ASP:OD1	1:HB:94:ARG:NH2	2.20	0.75
1:PA:91:ASP:OD1	1:PA:94:ARG:NH2	2.19	0.75
1:R:91:ASP:OD1	1:R:94:ARG:NH2	2.19	0.75
1:XA:91:ASP:OD1	1:XA:94:ARG:NH2	2.20	0.75
1:TA:91:ASP:OD1	1:TA:94:ARG:NH2	2.20	0.75
1:DB:91:ASP:OD1	1:DB:94:ARG:NH2	2.20	0.74
1:EA:197:ARG:NH1	1:X:193:GLU:CD	2.28	0.74
1:H:91:ASP:OD1	1:H:94:ARG:NH2	2.19	0.74
1:I:91:ASP:OD1	1:I:94:ARG:NH2	2.19	0.74
1:M:91:ASP:OD1	1:M:94:ARG:NH2	2.20	0.74
1:N:91:ASP:OD1	1:N:94:ARG:NH2	2.20	0.74
1:BA:197:ARG:NH1	1:S:193:GLU:CD	2.28	0.74
1:AB:91:ASP:OD1	1:AB:94:ARG:NH2	2.19	0.74
1:EB:91:ASP:OD1	1:EB:94:ARG:NH2	2.19	0.74
1:QA:91:ASP:OD1	1:QA:94:ARG:NH2	2.20	0.74
1:UA:91:ASP:OD1	1:UA:94:ARG:NH2	2.19	0.74
1:FA:91:ASP:OD1	1:FA:94:ARG:NH2	2.19	0.74
1:KA:91:ASP:OD1	1:KA:94:ARG:NH2	2.19	0.74
1:CA:91:ASP:OD1	1:CA:94:ARG:NH2	2.19	0.74
1:IB:91:ASP:OD1	1:IB:94:ARG:NH2	2.20	0.74
1:X:91:ASP:OD1	1:X:94:ARG:NH2	2.19	0.74
1:Z:91:ASP:OD1	1:Z:94:ARG:NH2	2.20	0.74
1:EA:91:ASP:OD1	1:EA:94:ARG:NH2	2.19	0.74
1:YA:91:ASP:OD1	1:YA:94:ARG:NH2	2.20	0.74
1:A:12:THR:HG22	1:SA:2:ASN:HB3	1.70	0.73
1:B:12:THR:HG22	1:VA:2:ASN:HB3	1.70	0.73
1:GB:197:ARG:NH1	1:LA:193:GLU:CD	2.28	0.73
1:FB:2:ASN:HB3	1:Q:12:THR:HG22	1.70	0.73
1:CB:12:THR:HG22	1:GB:2:ASN:HB3	1.70	0.73
1:GA:193:GLU:CD	1:WA:197:ARG:NH1	2.28	0.73
1:K:2:ASN:HB3	1:RA:12:THR:HG22	1.70	0.73
1:NA:2:ASN:HB3	1:UA:12:THR:HG22	1.70	0.73
1:CB:2:ASN:HB3	1:P:12:THR:HG22	1.71	0.73
1:DB:2:ASN:HB3	1:EA:12:THR:HG22	1.70	0.73
1:EB:12:THR:HG22	1:IA:2:ASN:HB3	1.70	0.73
1:TA:2:ASN:HB3	1:Z:12:THR:HG22	1.70	0.73
1:BA:12:THR:HG22	1:L:2:ASN:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:12:THR:HG22	1:F:2:ASN:HB3	1.71	0.73
1:DB:12:THR:HG22	1:T:2:ASN:HB3	1.70	0.73
1:E:2:ASN:HB3	1:TA:12:THR:HG22	1.70	0.73
1:G:2:ASN:HB3	1:W:12:THR:HG22	1.70	0.73
1:SA:12:THR:HG22	1:WA:2:ASN:HB3	1.71	0.73
1:B:2:ASN:HB3	1:GA:12:THR:HG22	1.70	0.73
1:CA:2:ASN:HB3	1:Y:12:THR:HG22	1.71	0.73
1:DA:12:THR:HG22	1:X:2:ASN:HB3	1.70	0.73
1:LA:12:THR:HG22	1:Q:2:ASN:HB3	1.70	0.73
1:EB:2:ASN:HB3	1:MA:12:THR:HG22	1.70	0.72
1:FA:12:THR:HG22	1:I:2:ASN:HB3	1.70	0.72
1:HA:2:ASN:HB3	1:NA:12:THR:HG22	1.70	0.72
1:E:12:THR:HG22	1:Z:2:ASN:HB3	1.70	0.72
1:HA:12:THR:HG22	1:UA:2:ASN:HB3	1.70	0.72
1:IA:12:THR:HG22	1:MA:2:ASN:HB3	1.71	0.72
1:EA:2:ASN:HB3	1:T:12:THR:HG22	1.70	0.72
1:KA:12:THR:HG22	1:N:2:ASN:HB3	1.70	0.72
1:AB:12:THR:HG22	1:W:2:ASN:HB3	1.71	0.72
1:GB:12:THR:HG22	1:P:2:ASN:HB3	1.71	0.72
1:IB:12:THR:HG22	1:J:2:ASN:HB3	1.70	0.72
1:PA:12:THR:HG22	1:Y:2:ASN:HB3	1.70	0.72
1:A:2:ASN:HB3	1:WA:12:THR:HG22	1.71	0.72
1:BA:2:ASN:HB3	1:QA:12:THR:HG22	1.70	0.72
1:DA:2:ASN:HB3	1:ZA:12:THR:HG22	1.71	0.72
1:F:12:THR:HG22	1:HB:2:ASN:HB3	1.70	0.72
1:O:2:ASN:HB3	1:YA:12:THR:HG22	1.70	0.72
1:C:12:THR:HG22	1:FA:2:ASN:HB3	1.71	0.72
1:K:12:THR:HG22	1:XA:2:ASN:HB3	1.70	0.72
1:KA:2:ASN:HB3	1:R:12:THR:HG22	1.70	0.72
1:AA:2:ASN:HB3	1:M:12:THR:HG22	1.70	0.72
1:CA:12:THR:HG22	1:PA:2:ASN:HB3	1.71	0.72
1:FB:12:THR:HG22	1:LA:2:ASN:HB3	1.70	0.72
1:X:12:THR:HG22	1:ZA:2:ASN:HB3	1.71	0.72
1:GA:2:ASN:HB3	1:VA:12:THR:HG22	1.71	0.72
1:M:2:ASN:HB3	1:S:12:THR:HG22	1.70	0.72
1:O:12:THR:HG22	1:OA:2:ASN:HB3	1.70	0.72
1:OA:12:THR:HG22	1:YA:2:ASN:HB3	1.70	0.72
1:AB:2:ASN:HB3	1:G:12:THR:HG22	1.70	0.71
1:H:12:THR:HG22	1:V:2:ASN:HB3	1.71	0.71
1:IB:2:ASN:HB3	1:JA:12:THR:HG22	1.70	0.71
1:J:12:THR:HG22	1:JA:2:ASN:HB3	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:THR:HG22	1:H:2:ASN:HB3	1.71	0.71
1:L:12:THR:HG22	1:QA:2:ASN:HB3	1.70	0.71
1:RA:2:ASN:HB3	1:XA:12:THR:HG22	1.71	0.71
1:AA:12:THR:HG22	1:S:2:ASN:HB3	1.70	0.71
1:BB:2:ASN:HB3	1:HB:12:THR:HG22	1.70	0.71
1:D:2:ASN:HB3	1:V:12:THR:HG22	1.70	0.71
1:N:12:THR:HG22	1:R:2:ASN:HB3	1.71	0.70
1:C:2:ASN:HB3	1:I:12:THR:HG22	1.71	0.70
1:AB:223:ASP:OD2	1:AB:225:GLN:NE2	2.27	0.68
1:BB:223:ASP:OD2	1:BB:225:GLN:NE2	2.27	0.68
1:GA:223:ASP:OD2	1:GA:225:GLN:NE2	2.27	0.68
1:LA:223:ASP:OD2	1:LA:225:GLN:NE2	2.27	0.68
1:QA:223:ASP:OD2	1:QA:225:GLN:NE2	2.27	0.68
1:N:223:ASP:OD2	1:N:225:GLN:NE2	2.27	0.68
1:RA:223:ASP:OD2	1:RA:225:GLN:NE2	2.27	0.68
1:UA:223:ASP:OD2	1:UA:225:GLN:NE2	2.27	0.68
1:AA:223:ASP:OD2	1:AA:225:GLN:NE2	2.27	0.68
1:C:223:ASP:OD2	1:C:225:GLN:NE2	2.27	0.68
1:EB:223:ASP:OD2	1:EB:225:GLN:NE2	2.27	0.68
1:I:223:ASP:OD2	1:I:225:GLN:NE2	2.27	0.68
1:KA:223:ASP:OD2	1:KA:225:GLN:NE2	2.27	0.68
1:R:223:ASP:OD2	1:R:225:GLN:NE2	2.27	0.68
1:DB:223:ASP:OD2	1:DB:225:GLN:NE2	2.27	0.68
1:E:223:ASP:OD2	1:E:225:GLN:NE2	2.27	0.68
1:EA:223:ASP:OD2	1:EA:225:GLN:NE2	2.27	0.68
1:FA:223:ASP:OD2	1:FA:225:GLN:NE2	2.27	0.68
1:K:223:ASP:OD2	1:K:225:GLN:NE2	2.27	0.68
1:Q:223:ASP:OD2	1:Q:225:GLN:NE2	2.27	0.68
1:TA:223:ASP:OD2	1:TA:225:GLN:NE2	2.27	0.68
1:V:223:ASP:OD2	1:V:225:GLN:NE2	2.27	0.68
1:B:223:ASP:OD2	1:B:225:GLN:NE2	2.27	0.67
1:F:223:ASP:OD2	1:F:225:GLN:NE2	2.27	0.67
1:G:223:ASP:OD2	1:G:225:GLN:NE2	2.27	0.67
1:L:223:ASP:OD2	1:L:225:GLN:NE2	2.27	0.67
1:T:223:ASP:OD2	1:T:225:GLN:NE2	2.27	0.67
1:YA:223:ASP:OD2	1:YA:225:GLN:NE2	2.27	0.67
1:Z:223:ASP:OD2	1:Z:225:GLN:NE2	2.27	0.67
1:DA:223:ASP:OD2	1:DA:225:GLN:NE2	2.27	0.67
1:IB:223:ASP:OD2	1:IB:225:GLN:NE2	2.27	0.67
1:OA:223:ASP:OD2	1:OA:225:GLN:NE2	2.27	0.67
1:Y:223:ASP:OD2	1:Y:225:GLN:NE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:223:ASP:OD2	1:ZA:225:GLN:NE2	2.27	0.67
1:H:223:ASP:OD2	1:H:225:GLN:NE2	2.27	0.67
1:HA:223:ASP:OD2	1:HA:225:GLN:NE2	2.27	0.67
1:JA:223:ASP:OD2	1:JA:225:GLN:NE2	2.27	0.67
1:MA:223:ASP:OD2	1:MA:225:GLN:NE2	2.27	0.67
1:NA:223:ASP:OD2	1:NA:225:GLN:NE2	2.27	0.67
1:BA:223:ASP:OD2	1:BA:225:GLN:NE2	2.27	0.67
1:IA:223:ASP:OD2	1:IA:225:GLN:NE2	2.27	0.67
1:M:223:ASP:OD2	1:M:225:GLN:NE2	2.27	0.67
1:PA:223:ASP:OD2	1:PA:225:GLN:NE2	2.27	0.67
1:X:223:ASP:OD2	1:X:225:GLN:NE2	2.27	0.67
1:CA:223:ASP:OD2	1:CA:225:GLN:NE2	2.27	0.67
1:GB:223:ASP:OD2	1:GB:225:GLN:NE2	2.27	0.67
1:W:223:ASP:OD2	1:W:225:GLN:NE2	2.27	0.67
1:A:223:ASP:OD2	1:A:225:GLN:NE2	2.27	0.67
1:FB:223:ASP:OD2	1:FB:225:GLN:NE2	2.27	0.67
1:VA:223:ASP:OD2	1:VA:225:GLN:NE2	2.27	0.67
1:P:223:ASP:OD2	1:P:225:GLN:NE2	2.27	0.67
1:WA:223:ASP:OD2	1:WA:225:GLN:NE2	2.27	0.67
1:XA:223:ASP:OD2	1:XA:225:GLN:NE2	2.27	0.67
1:CB:223:ASP:OD2	1:CB:225:GLN:NE2	2.27	0.67
1:HB:223:ASP:OD2	1:HB:225:GLN:NE2	2.27	0.67
1:J:223:ASP:OD2	1:J:225:GLN:NE2	2.27	0.67
1:O:223:ASP:OD2	1:O:225:GLN:NE2	2.27	0.67
1:SA:223:ASP:OD2	1:SA:225:GLN:NE2	2.27	0.66
1:D:223:ASP:OD2	1:D:225:GLN:NE2	2.27	0.66
1:S:223:ASP:OD2	1:S:225:GLN:NE2	2.27	0.66
1:B:2:ASN:HB3	1:GA:12:THR:CG2	2.26	0.66
1:LA:12:THR:CG2	1:Q:2:ASN:HB3	2.26	0.66
1:B:12:THR:CG2	1:VA:2:ASN:HB3	2.26	0.66
1:FB:2:ASN:HB3	1:Q:12:THR:CG2	2.26	0.66
1:IB:2:ASN:HB3	1:JA:12:THR:CG2	2.26	0.66
1:OA:12:THR:CG2	1:YA:2:ASN:HB3	2.26	0.66
1:M:2:ASN:HB3	1:S:12:THR:CG2	2.27	0.65
1:AA:12:THR:CG2	1:S:2:ASN:HB3	2.26	0.65
1:D:12:THR:CG2	1:H:2:ASN:HB3	2.27	0.65
1:E:12:THR:CG2	1:Z:2:ASN:HB3	2.26	0.65
1:EA:2:ASN:HB3	1:T:12:THR:CG2	2.26	0.65
1:FA:12:THR:CG2	1:I:2:ASN:HB3	2.26	0.65
1:FB:12:THR:CG2	1:LA:2:ASN:HB3	2.26	0.65
1:GA:2:ASN:HB3	1:VA:12:THR:CG2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:HB3	1:V:12:THR:CG2	2.26	0.65
1:F:12:THR:CG2	1:HB:2:ASN:HB3	2.26	0.65
1:RA:2:ASN:HB3	1:XA:12:THR:CG2	2.27	0.65
1:A:2:ASN:HB3	1:WA:12:THR:CG2	2.27	0.65
1:BB:2:ASN:HB3	1:HB:12:THR:CG2	2.27	0.65
1:CA:2:ASN:HB3	1:Y:12:THR:CG2	2.27	0.65
1:K:12:THR:CG2	1:XA:2:ASN:HB3	2.26	0.65
1:KA:12:THR:CG2	1:N:2:ASN:HB3	2.26	0.65
1:X:12:THR:CG2	1:ZA:2:ASN:HB3	2.27	0.65
1:CA:12:THR:CG2	1:PA:2:ASN:HB3	2.27	0.65
1:DA:12:THR:CG2	1:X:2:ASN:HB3	2.27	0.65
1:GB:12:THR:CG2	1:P:2:ASN:HB3	2.27	0.65
1:B:51:SER:OG	1:WA:48:ALA:HB2	1.97	0.65
1:GB:48:ALA:HB2	1:Q:51:SER:OG	1.97	0.65
1:HA:2:ASN:HB3	1:NA:12:THR:CG2	2.27	0.65
1:K:2:ASN:HB3	1:RA:12:THR:CG2	2.27	0.65
1:BA:2:ASN:HB3	1:QA:12:THR:CG2	2.26	0.65
1:EB:2:ASN:HB3	1:MA:12:THR:CG2	2.27	0.65
1:KA:48:ALA:HB2	1:O:51:SER:OG	1.97	0.65
1:AA:48:ALA:HB2	1:T:51:SER:OG	1.97	0.65
1:BB:12:THR:CG2	1:F:2:ASN:HB3	2.27	0.65
1:EA:48:ALA:HB2	1:ZA:51:SER:OG	1.97	0.65
1:FA:48:ALA:HB2	1:J:51:SER:OG	1.97	0.65
1:IA:12:THR:CG2	1:MA:2:ASN:HB3	2.27	0.65
1:K:48:ALA:HB2	1:YA:51:SER:OG	1.97	0.65
1:KA:2:ASN:HB3	1:R:12:THR:CG2	2.26	0.65
1:C:12:THR:CG2	1:FA:2:ASN:HB3	2.27	0.65
1:E:51:SER:OG	1:V:48:ALA:HB2	1.97	0.65
1:F:48:ALA:HB2	1:IB:51:SER:OG	1.97	0.65
1:HA:12:THR:CG2	1:UA:2:ASN:HB3	2.27	0.65
1:AB:12:THR:CG2	1:W:2:ASN:HB3	2.26	0.64
1:HA:51:SER:OG	1:VA:48:ALA:HB2	1.97	0.64
1:N:48:ALA:HB2	1:S:51:SER:OG	1.98	0.64
1:OA:51:SER:OG	1:UA:48:ALA:HB2	1.97	0.64
1:PA:51:SER:OG	1:Z:48:ALA:HB2	1.97	0.64
1:BB:48:ALA:HB2	1:G:51:SER:OG	1.97	0.64
1:D:51:SER:OG	1:I:48:ALA:HB2	1.98	0.64
1:DB:2:ASN:HB3	1:EA:12:THR:CG2	2.26	0.64
1:EB:12:THR:CG2	1:IA:2:ASN:HB3	2.26	0.64
1:EB:48:ALA:HB2	1:JA:51:SER:OG	1.97	0.64
1:FB:48:ALA:HB2	1:MA:51:SER:OG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:48:ALA:HB2	1:VA:51:SER:OG	1.97	0.64
1:N:51:SER:OG	1:S:48:ALA:HB2	1.97	0.64
1:NA:2:ASN:HB3	1:UA:12:THR:CG2	2.26	0.64
1:O:12:THR:CG2	1:OA:2:ASN:HB3	2.26	0.64
1:BA:48:ALA:HB2	1:M:51:SER:OG	1.97	0.64
1:D:48:ALA:HB2	1:I:51:SER:OG	1.98	0.64
1:E:2:ASN:HB3	1:TA:12:THR:CG2	2.26	0.64
1:J:12:THR:CG2	1:JA:2:ASN:HB3	2.26	0.64
1:L:51:SER:OG	1:RA:48:ALA:HB2	1.97	0.64
1:SA:51:SER:OG	1:XA:48:ALA:HB2	1.97	0.64
1:AA:51:SER:OG	1:T:48:ALA:HB2	1.97	0.64
1:AB:2:ASN:HB3	1:G:12:THR:CG2	2.26	0.64
1:CB:12:THR:CG2	1:GB:2:ASN:HB3	2.27	0.64
1:CB:51:SER:OG	1:HB:48:ALA:HB2	1.98	0.64
1:DB:12:THR:CG2	1:T:2:ASN:HB3	2.26	0.64
1:FB:51:SER:OG	1:MA:48:ALA:HB2	1.97	0.64
1:H:51:SER:OG	1:W:48:ALA:HB2	1.97	0.64
1:SA:12:THR:CG2	1:WA:2:ASN:HB3	2.27	0.64
1:CA:48:ALA:HB2	1:QA:51:SER:OG	1.97	0.64
1:DB:51:SER:OG	1:P:48:ALA:HB2	1.97	0.64
1:E:48:ALA:HB2	1:V:51:SER:OG	1.97	0.64
1:TA:2:ASN:HB3	1:Z:12:THR:CG2	2.27	0.64
1:A:12:THR:CG2	1:SA:2:ASN:HB3	2.26	0.64
1:AB:51:SER:OG	1:X:48:ALA:HB2	1.97	0.64
1:CB:2:ASN:HB3	1:P:12:THR:CG2	2.26	0.64
1:DA:2:ASN:HB3	1:ZA:12:THR:CG2	2.26	0.64
1:L:12:THR:CG2	1:QA:2:ASN:HB3	2.26	0.64
1:PA:12:THR:CG2	1:Y:2:ASN:HB3	2.26	0.64
1:A:48:ALA:HB2	1:TA:51:SER:OG	1.97	0.64
1:AA:2:ASN:HB3	1:M:12:THR:CG2	2.27	0.64
1:BA:12:THR:CG2	1:L:2:ASN:HB3	2.26	0.64
1:H:12:THR:CG2	1:V:2:ASN:HB3	2.27	0.64
1:IA:48:ALA:HB2	1:NA:51:SER:OG	1.98	0.64
1:IA:51:SER:OG	1:NA:48:ALA:HB2	1.97	0.64
1:O:2:ASN:HB3	1:YA:12:THR:CG2	2.26	0.64
1:B:48:ALA:HB2	1:WA:51:SER:OG	1.97	0.64
1:G:2:ASN:HB3	1:W:12:THR:CG2	2.26	0.64
1:GB:51:SER:OG	1:Q:48:ALA:HB2	1.97	0.64
1:IB:12:THR:CG2	1:J:2:ASN:HB3	2.26	0.64
1:KA:51:SER:OG	1:O:48:ALA:HB2	1.97	0.64
1:BA:51:SER:OG	1:M:48:ALA:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:51:SER:OG	1:J:48:ALA:HB2	1.97	0.64
1:H:48:ALA:HB2	1:W:51:SER:OG	1.97	0.64
1:LA:51:SER:OG	1:R:48:ALA:HB2	1.97	0.64
1:C:48:ALA:HB2	1:GA:51:SER:OG	1.97	0.64
1:SA:48:ALA:HB2	1:XA:51:SER:OG	1.97	0.64
1:C:51:SER:OG	1:GA:48:ALA:HB2	1.97	0.63
1:DA:48:ALA:HB2	1:Y:51:SER:OG	1.97	0.63
1:DB:48:ALA:HB2	1:P:51:SER:OG	1.97	0.63
1:CA:51:SER:OG	1:QA:48:ALA:HB2	1.97	0.63
1:CB:48:ALA:HB2	1:HB:51:SER:OG	1.97	0.63
1:DA:51:SER:OG	1:Y:48:ALA:HB2	1.98	0.63
1:EA:51:SER:OG	1:ZA:48:ALA:HB2	1.97	0.63
1:LA:48:ALA:HB2	1:R:51:SER:OG	1.97	0.63
1:PA:48:ALA:HB2	1:Z:51:SER:OG	1.97	0.63
1:EB:51:SER:OG	1:JA:48:ALA:HB2	1.97	0.63
1:A:51:SER:OG	1:TA:48:ALA:HB2	1.97	0.63
1:F:51:SER:OG	1:IB:48:ALA:HB2	1.97	0.63
1:OA:48:ALA:HB2	1:UA:51:SER:OG	1.97	0.63
1:AB:48:ALA:HB2	1:X:51:SER:OG	1.97	0.63
1:K:51:SER:OG	1:YA:48:ALA:HB2	1.97	0.63
1:C:2:ASN:HB3	1:I:12:THR:CG2	2.27	0.63
1:N:12:THR:CG2	1:R:2:ASN:HB3	2.27	0.63
1:BB:93:GLU:OE2	1:F:3:ASN:HB2	1.99	0.62
1:BB:51:SER:OG	1:G:48:ALA:HB2	1.97	0.62
1:D:49:SER:HG	1:I:49:SER:HG	1.41	0.62
1:K:3:ASN:HB2	1:RA:93:GLU:OE2	2.00	0.62
1:L:48:ALA:HB2	1:RA:51:SER:OG	1.97	0.62
1:SA:93:GLU:OE2	1:WA:3:ASN:HB2	2.00	0.62
1:BA:93:GLU:OE2	1:L:3:ASN:HB2	2.00	0.62
1:CB:93:GLU:OE2	1:GB:3:ASN:HB2	2.00	0.62
1:D:93:GLU:OE2	1:H:3:ASN:HB2	2.00	0.62
1:J:93:GLU:OE2	1:JA:3:ASN:HB2	2.00	0.62
1:M:3:ASN:HB2	1:S:93:GLU:OE2	2.00	0.62
1:GB:93:GLU:OE2	1:P:3:ASN:HB2	2.00	0.62
1:NA:3:ASN:HB2	1:UA:93:GLU:OE2	2.00	0.62
1:O:93:GLU:OE2	1:OA:3:ASN:HB2	2.00	0.62
1:A:3:ASN:HB2	1:WA:93:GLU:OE2	2.00	0.62
1:B:93:GLU:OE2	1:VA:3:ASN:HB2	2.00	0.62
1:EB:93:GLU:OE2	1:IA:3:ASN:HB2	2.00	0.62
1:G:3:ASN:HB2	1:W:93:GLU:OE2	2.00	0.62
1:E:93:GLU:OE2	1:Z:3:ASN:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:3:ASN:HB2	1:T:93:GLU:OE2	2.00	0.62
1:FA:93:GLU:OE2	1:I:3:ASN:HB2	2.00	0.62
1:FB:3:ASN:HB2	1:Q:93:GLU:OE2	2.00	0.62
1:KA:93:GLU:OE2	1:N:3:ASN:HB2	2.00	0.62
1:CA:3:ASN:HB2	1:Y:93:GLU:OE2	2.00	0.62
1:DA:93:GLU:OE2	1:X:3:ASN:HB2	2.00	0.62
1:DA:3:ASN:HB2	1:ZA:93:GLU:OE2	2.00	0.62
1:DB:3:ASN:HB2	1:EA:93:GLU:OE2	2.00	0.62
1:GA:3:ASN:HB2	1:VA:93:GLU:OE2	2.00	0.62
1:PA:93:GLU:OE2	1:Y:3:ASN:HB2	2.00	0.62
1:BB:3:ASN:HB2	1:HB:93:GLU:OE2	2.00	0.61
1:FB:93:GLU:OE2	1:LA:3:ASN:HB2	2.00	0.61
1:RA:3:ASN:HB2	1:XA:93:GLU:OE2	2.00	0.61
1:TA:3:ASN:HB2	1:Z:93:GLU:OE2	2.00	0.61
1:AA:3:ASN:HB2	1:M:93:GLU:OE2	2.00	0.61
1:AB:3:ASN:HB2	1:G:93:GLU:OE2	2.00	0.61
1:H:93:GLU:OE2	1:V:3:ASN:HB2	2.00	0.61
1:L:93:GLU:OE2	1:QA:3:ASN:HB2	2.00	0.61
1:AB:93:GLU:OE2	1:W:3:ASN:HB2	2.00	0.61
1:BA:3:ASN:HB2	1:QA:93:GLU:OE2	2.00	0.61
1:C:3:ASN:HB2	1:I:93:GLU:OE2	2.00	0.61
1:F:93:GLU:OE2	1:HB:3:ASN:HB2	2.00	0.61
1:N:93:GLU:OE2	1:R:3:ASN:HB2	2.00	0.61
1:K:93:GLU:OE2	1:XA:3:ASN:HB2	2.00	0.61
1:EB:3:ASN:HB2	1:MA:93:GLU:OE2	2.00	0.61
1:HA:93:GLU:OE2	1:UA:3:ASN:HB2	2.00	0.61
1:LA:93:GLU:OE2	1:Q:3:ASN:HB2	2.00	0.61
1:IB:93:GLU:OE2	1:J:3:ASN:HB2	2.00	0.61
1:OA:93:GLU:OE2	1:YA:3:ASN:HB2	2.00	0.61
1:B:3:ASN:HB2	1:GA:93:GLU:OE2	2.00	0.61
1:CA:93:GLU:OE2	1:PA:3:ASN:HB2	1.99	0.61
1:IB:3:ASN:HB2	1:JA:93:GLU:OE2	2.00	0.61
1:X:93:GLU:OE2	1:ZA:3:ASN:HB2	2.00	0.61
1:O:3:ASN:HB2	1:YA:93:GLU:OE2	2.00	0.61
1:C:93:GLU:OE2	1:FA:3:ASN:HB2	2.00	0.61
1:D:3:ASN:HB2	1:V:93:GLU:OE2	2.00	0.61
1:IA:93:GLU:OE2	1:MA:3:ASN:HB2	2.00	0.60
1:AA:93:GLU:OE2	1:S:3:ASN:HB2	2.00	0.60
1:DB:93:GLU:OE2	1:T:3:ASN:HB2	2.00	0.60
1:KA:3:ASN:HB2	1:R:93:GLU:OE2	2.00	0.60
1:CB:3:ASN:HB2	1:P:93:GLU:OE2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ASN:HB2	1:TA:93:GLU:OE2	2.00	0.60
1:HA:3:ASN:HB2	1:NA:93:GLU:OE2	2.00	0.60
1:A:93:GLU:OE2	1:SA:3:ASN:HB2	2.00	0.60
1:BB:193:GLU:CD	1:IB:197:ARG:HH12	2.12	0.58
1:RA:193:GLU:CD	1:YA:197:ARG:HH12	2.12	0.58
1:D:197:ARG:HH12	1:FA:193:GLU:CD	2.12	0.58
1:KA:193:GLU:CD	1:S:197:ARG:HH12	2.12	0.58
1:Y:197:ARG:HH12	1:ZA:193:GLU:CD	2.12	0.57
1:B:197:ARG:HH12	1:SA:193:GLU:CD	2.12	0.57
1:A:193:GLU:CD	1:XA:197:ARG:HH12	2.12	0.57
1:CB:193:GLU:CD	1:Q:197:ARG:HH12	2.12	0.57
1:M:197:ARG:HH12	1:QA:193:GLU:CD	2.12	0.57
1:DA:197:ARG:HH12	1:PA:193:GLU:CD	2.12	0.57
1:N:123:TYR:OH	1:S:59:SER:O	2.23	0.57
1:AB:193:GLU:CD	1:H:197:ARG:HH12	2.12	0.57
1:D:59:SER:O	1:I:123:TYR:OH	2.23	0.57
1:EA:193:GLU:CD	1:P:197:ARG:HH12	2.12	0.57
1:HB:197:ARG:HH12	1:P:193:GLU:CD	2.12	0.57
1:A:197:ARG:HH12	1:Z:193:GLU:CD	2.13	0.57
1:IA:59:SER:O	1:NA:123:TYR:OH	2.23	0.57
1:IA:123:TYR:OH	1:NA:59:SER:O	2.23	0.57
1:C:59:SER:O	1:GA:123:TYR:OH	2.22	0.57
1:HA:123:TYR:OH	1:VA:59:SER:O	2.23	0.57
1:LA:123:TYR:OH	1:R:59:SER:O	2.22	0.57
1:AB:197:ARG:HH12	1:DA:193:GLU:CD	2.12	0.56
1:AB:59:SER:O	1:X:123:TYR:OH	2.23	0.56
1:QA:197:ARG:HH12	1:Y:193:GLU:CD	2.12	0.56
1:A:59:SER:O	1:TA:123:TYR:OH	2.22	0.56
1:EA:123:TYR:OH	1:ZA:59:SER:O	2.22	0.56
1:OA:123:TYR:OH	1:UA:59:SER:O	2.22	0.56
1:PA:59:SER:O	1:Z:123:TYR:OH	2.22	0.56
1:H:123:TYR:OH	1:W:59:SER:O	2.23	0.56
1:BA:59:SER:O	1:M:123:TYR:OH	2.23	0.56
1:K:197:ARG:HH12	1:OA:193:GLU:CD	2.13	0.56
1:KA:123:TYR:OH	1:O:59:SER:O	2.23	0.56
1:M:193:GLU:CD	1:T:197:ARG:HH12	2.12	0.56
1:FA:123:TYR:OH	1:J:59:SER:O	2.23	0.56
1:DB:197:ARG:HH12	1:GB:193:GLU:CD	2.12	0.56
1:E:197:ARG:HH12	1:H:193:GLU:CD	2.12	0.56
1:O:193:GLU:CD	1:UA:197:ARG:HH12	2.12	0.56
1:DA:59:SER:O	1:Y:123:TYR:OH	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:197:ARG:HH12	1:WA:193:GLU:CD	2.12	0.56
1:F:197:ARG:HH12	1:JA:193:GLU:CD	2.13	0.56
1:C:193:GLU:CD	1:J:197:ARG:HH12	2.12	0.55
1:BA:193:GLU:CD	1:RA:197:ARG:HH12	2.12	0.55
1:BB:197:ARG:HH12	1:W:193:GLU:CD	2.12	0.55
1:EB:197:ARG:HH12	1:J:193:GLU:CD	2.12	0.55
1:IA:197:ARG:HH12	1:UA:193:GLU:CD	2.12	0.55
1:FB:193:GLU:CD	1:R:197:ARG:HH12	2.12	0.55
1:JA:197:ARG:HH12	1:MA:193:GLU:CD	2.12	0.55
1:LA:197:ARG:HH12	1:N:193:GLU:CD	2.12	0.55
1:TA:193:GLU:CD	1:V:197:ARG:HH12	2.12	0.55
1:HA:193:GLU:CD	1:OA:197:ARG:HH12	2.12	0.55
1:C:197:ARG:HH12	1:VA:193:GLU:CD	2.12	0.55
1:EB:193:GLU:CD	1:NA:197:ARG:HH12	2.12	0.55
1:GA:197:ARG:HH12	1:I:193:GLU:CD	2.13	0.55
1:B:123:TYR:OH	1:WA:59:SER:O	2.22	0.54
1:BA:197:ARG:HH12	1:S:193:GLU:CD	2.12	0.54
1:D:123:TYR:OH	1:I:59:SER:O	2.23	0.54
1:FA:59:SER:O	1:J:123:TYR:OH	2.22	0.54
1:GB:123:TYR:OH	1:Q:59:SER:O	2.23	0.54
1:AA:197:ARG:HH12	1:DB:193:GLU:CD	2.12	0.54
1:B:59:SER:O	1:WA:123:TYR:OH	2.23	0.54
1:HA:49:SER:HG	1:VA:49:SER:HG	1.45	0.54
1:KA:59:SER:O	1:O:123:TYR:OH	2.22	0.54
1:N:59:SER:O	1:S:123:TYR:OH	2.23	0.54
1:K:59:SER:O	1:YA:123:TYR:OH	2.22	0.54
1:T:193:GLU:CD	1:ZA:197:ARG:HH12	2.12	0.54
1:AA:193:GLU:CD	1:N:197:ARG:HH12	2.12	0.54
1:GB:59:SER:O	1:Q:123:TYR:OH	2.22	0.54
1:SA:59:SER:O	1:XA:123:TYR:OH	2.23	0.54
1:CB:59:SER:O	1:HB:123:TYR:OH	2.23	0.54
1:NA:193:GLU:CD	1:VA:197:ARG:HH12	2.12	0.54
1:D:193:GLU:CD	1:W:197:ARG:HH12	2.12	0.54
1:F:59:SER:O	1:IB:123:TYR:OH	2.22	0.54
1:L:197:ARG:HH12	1:XA:193:GLU:CD	2.12	0.54
1:I:197:ARG:HH12	1:V:193:GLU:CD	2.12	0.54
1:AA:123:TYR:OH	1:T:59:SER:O	2.23	0.54
1:E:193:GLU:CD	1:PA:197:ARG:HH12	2.12	0.54
1:E:59:SER:O	1:V:123:TYR:OH	2.23	0.53
1:C:123:TYR:OH	1:GA:59:SER:O	2.23	0.53
1:FB:197:ARG:HH12	1:IA:193:GLU:CD	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:ARG:HH12	1:HB:193:GLU:CD	2.13	0.53
1:H:59:SER:O	1:W:123:TYR:OH	2.22	0.53
1:BB:59:SER:O	1:G:123:TYR:OH	2.22	0.53
1:CB:123:TYR:OH	1:HB:59:SER:O	2.23	0.53
1:SA:123:TYR:OH	1:XA:59:SER:O	2.23	0.53
1:BA:123:TYR:OH	1:M:59:SER:O	2.22	0.53
1:CA:59:SER:O	1:QA:123:TYR:OH	2.22	0.53
1:L:123:TYR:OH	1:RA:59:SER:O	2.22	0.53
1:AA:59:SER:O	1:T:123:TYR:OH	2.22	0.53
1:E:123:TYR:OH	1:V:59:SER:O	2.22	0.53
1:LA:59:SER:O	1:R:123:TYR:OH	2.23	0.53
1:AA:2:ASN:C	1:M:12:THR:HG22	2.34	0.53
1:O:12:THR:HG22	1:OA:2:ASN:C	2.34	0.53
1:PA:123:TYR:OH	1:Z:59:SER:O	2.23	0.53
1:AB:123:TYR:OH	1:X:59:SER:O	2.22	0.53
1:BA:12:THR:HG22	1:L:2:ASN:C	2.34	0.53
1:DA:12:THR:HG22	1:X:2:ASN:C	2.34	0.53
1:DB:123:TYR:OH	1:P:59:SER:O	2.22	0.53
1:EA:59:SER:O	1:ZA:123:TYR:OH	2.23	0.53
1:J:12:THR:HG22	1:JA:2:ASN:C	2.34	0.53
1:K:2:ASN:C	1:RA:12:THR:HG22	2.34	0.53
1:RA:2:ASN:C	1:XA:12:THR:HG22	2.34	0.53
1:AA:12:THR:HG22	1:S:2:ASN:C	2.34	0.53
1:BB:2:ASN:C	1:HB:12:THR:HG22	2.34	0.53
1:CA:2:ASN:C	1:Y:12:THR:HG22	2.34	0.53
1:CA:193:GLU:CD	1:Z:197:ARG:HH12	2.12	0.53
1:EA:197:ARG:HH12	1:X:193:GLU:CD	2.12	0.53
1:FA:197:ARG:HH12	1:IB:193:GLU:CD	2.13	0.53
1:FB:12:THR:HG22	1:LA:2:ASN:C	2.34	0.53
1:GA:2:ASN:C	1:VA:12:THR:HG22	2.34	0.53
1:H:12:THR:HG22	1:V:2:ASN:C	2.34	0.53
1:IB:2:ASN:C	1:JA:12:THR:HG22	2.34	0.53
1:K:12:THR:HG22	1:XA:2:ASN:C	2.34	0.53
1:KA:2:ASN:C	1:R:12:THR:HG22	2.34	0.53
1:NA:2:ASN:C	1:UA:12:THR:HG22	2.34	0.53
1:OA:12:THR:HG22	1:YA:2:ASN:C	2.34	0.53
1:BB:12:THR:HG22	1:F:2:ASN:C	2.34	0.53
1:C:12:THR:HG22	1:FA:2:ASN:C	2.34	0.53
1:CA:12:THR:HG22	1:PA:2:ASN:C	2.34	0.53
1:CA:197:ARG:HH12	1:L:193:GLU:CD	2.12	0.53
1:D:2:ASN:C	1:V:12:THR:HG22	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:2:ASN:C	1:EA:12:THR:HG22	2.34	0.53
1:DB:12:THR:HG22	1:T:2:ASN:C	2.34	0.53
1:E:2:ASN:C	1:TA:12:THR:HG22	2.34	0.53
1:EB:12:THR:HG22	1:IA:2:ASN:C	2.34	0.53
1:F:12:THR:HG22	1:HB:2:ASN:C	2.34	0.53
1:FB:123:TYR:OH	1:MA:59:SER:O	2.22	0.53
1:G:2:ASN:C	1:W:12:THR:HG22	2.34	0.53
1:X:12:THR:HG22	1:ZA:2:ASN:C	2.34	0.53
1:A:2:ASN:C	1:WA:12:THR:HG22	2.34	0.52
1:D:12:THR:HG22	1:H:2:ASN:C	2.34	0.52
1:G:193:GLU:CD	1:X:197:ARG:HH12	2.12	0.52
1:KA:197:ARG:HH12	1:YA:193:GLU:CD	2.12	0.52
1:M:2:ASN:C	1:S:12:THR:HG22	2.34	0.52
1:O:2:ASN:C	1:YA:12:THR:HG22	2.34	0.52
1:TA:2:ASN:C	1:Z:12:THR:HG22	2.34	0.52
1:B:2:ASN:C	1:GA:12:THR:HG22	2.34	0.52
1:BA:2:ASN:C	1:QA:12:THR:HG22	2.34	0.52
1:FA:12:THR:HG22	1:I:2:ASN:C	2.34	0.52
1:GB:12:THR:HG22	1:P:2:ASN:C	2.34	0.52
1:N:12:THR:HG22	1:R:2:ASN:C	2.34	0.52
1:PA:12:THR:HG22	1:Y:2:ASN:C	2.34	0.52
1:EB:2:ASN:C	1:MA:12:THR:HG22	2.34	0.52
1:HA:59:SER:O	1:VA:123:TYR:OH	2.22	0.52
1:KA:12:THR:HG22	1:N:2:ASN:C	2.34	0.52
1:LA:12:THR:HG22	1:Q:2:ASN:C	2.34	0.52
1:AB:12:THR:HG22	1:W:2:ASN:C	2.34	0.52
1:C:2:ASN:C	1:I:12:THR:HG22	2.34	0.52
1:DA:2:ASN:C	1:ZA:12:THR:HG22	2.34	0.52
1:SA:12:THR:HG22	1:WA:2:ASN:C	2.34	0.52
1:CB:12:THR:HG22	1:GB:2:ASN:C	2.34	0.52
1:E:12:THR:HG22	1:Z:2:ASN:C	2.34	0.52
1:EA:2:ASN:C	1:T:12:THR:HG22	2.34	0.52
1:HA:12:THR:HG22	1:UA:2:ASN:C	2.34	0.52
1:IB:12:THR:HG22	1:J:2:ASN:C	2.34	0.52
1:FB:2:ASN:C	1:Q:12:THR:HG22	2.34	0.52
1:B:12:THR:HG22	1:VA:2:ASN:C	2.34	0.52
1:HA:2:ASN:C	1:NA:12:THR:HG22	2.34	0.52
1:IA:12:THR:HG22	1:MA:2:ASN:C	2.34	0.52
1:A:12:THR:HG22	1:SA:2:ASN:C	2.34	0.52
1:CB:197:ARG:HH12	1:F:193:GLU:CD	2.12	0.51
1:K:193:GLU:CD	1:SA:197:ARG:HH12	2.12	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:2:ASN:C	1:P:12:THR:HG22	2.34	0.51
1:MA:197:ARG:HH12	1:Q:193:GLU:CD	2.12	0.51
1:AB:2:ASN:C	1:G:12:THR:HG22	2.34	0.51
1:L:12:THR:HG22	1:QA:2:ASN:C	2.34	0.51
1:OA:59:SER:O	1:UA:123:TYR:OH	2.23	0.51
1:EB:123:TYR:OH	1:JA:59:SER:O	2.23	0.51
1:CA:123:TYR:OH	1:QA:59:SER:O	2.23	0.51
1:TA:221:ASP:OD1	1:TA:256:THR:OG1	2.29	0.51
1:B:193:GLU:CD	1:HA:197:ARG:HH12	2.12	0.50
1:FB:59:SER:O	1:MA:123:TYR:OH	2.23	0.50
1:EB:59:SER:O	1:JA:123:TYR:OH	2.22	0.50
1:GB:224:LEU:HD11	1:GB:250:MET:HE2	1.94	0.50
1:WA:224:LEU:HD11	1:WA:250:MET:HE2	1.94	0.50
1:SA:224:LEU:HD11	1:SA:250:MET:HE2	1.94	0.50
1:DA:123:TYR:OH	1:Y:59:SER:O	2.23	0.50
1:F:224:LEU:HD11	1:F:250:MET:HE2	1.94	0.50
1:GA:193:GLU:CD	1:WA:197:ARG:HH12	2.12	0.50
1:GB:197:ARG:HH12	1:LA:193:GLU:CD	2.12	0.50
1:AA:224:LEU:HD11	1:AA:250:MET:HE2	1.94	0.50
1:CB:224:LEU:HD11	1:CB:250:MET:HE2	1.94	0.50
1:K:224:LEU:HD11	1:K:250:MET:HE2	1.94	0.50
1:A:123:TYR:OH	1:TA:59:SER:O	2.23	0.50
1:F:221:ASP:OD1	1:F:256:THR:OG1	2.29	0.50
1:K:221:ASP:OD1	1:K:256:THR:OG1	2.29	0.50
1:V:224:LEU:HD11	1:V:250:MET:HE2	1.94	0.50
1:HA:221:ASP:OD1	1:HA:256:THR:OG1	2.29	0.50
1:QA:224:LEU:HD11	1:QA:250:MET:HE2	1.94	0.50
1:YA:224:LEU:HD11	1:YA:250:MET:HE2	1.94	0.50
1:AB:224:LEU:HD11	1:AB:250:MET:HE2	1.94	0.50
1:BB:123:TYR:OH	1:G:59:SER:O	2.23	0.50
1:DB:59:SER:O	1:P:123:TYR:OH	2.23	0.50
1:DB:224:LEU:HD11	1:DB:250:MET:HE2	1.94	0.49
1:FA:224:LEU:HD11	1:FA:250:MET:HE2	1.94	0.49
1:IB:224:LEU:HD11	1:IB:250:MET:HE2	1.94	0.49
1:KA:224:LEU:HD11	1:KA:250:MET:HE2	1.94	0.49
1:L:59:SER:O	1:RA:123:TYR:OH	2.23	0.49
1:MA:221:ASP:OD1	1:MA:256:THR:OG1	2.29	0.49
1:TA:224:LEU:HD11	1:TA:250:MET:HE2	1.94	0.49
1:CB:221:ASP:OD1	1:CB:256:THR:OG1	2.29	0.49
1:IA:224:LEU:HD11	1:IA:250:MET:HE2	1.94	0.49
1:JA:224:LEU:HD11	1:JA:250:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:221:ASP:OD1	1:M:256:THR:OG1	2.29	0.49
1:SA:221:ASP:OD1	1:SA:256:THR:OG1	2.29	0.49
1:G:221:ASP:OD1	1:G:256:THR:OG1	2.29	0.49
1:L:221:ASP:OD1	1:L:256:THR:OG1	2.29	0.49
1:NA:224:LEU:HD11	1:NA:250:MET:HE2	1.94	0.49
1:PA:224:LEU:HD11	1:PA:250:MET:HE2	1.94	0.49
1:ZA:224:LEU:HD11	1:ZA:250:MET:HE2	1.94	0.49
1:H:221:ASP:OD1	1:H:256:THR:OG1	2.29	0.49
1:J:224:LEU:HD11	1:J:250:MET:HE2	1.93	0.49
1:OA:224:LEU:HD11	1:OA:250:MET:HE2	1.94	0.49
1:VA:224:LEU:HD11	1:VA:250:MET:HE2	1.94	0.49
1:CA:224:LEU:CD1	1:CA:250:MET:HE2	2.43	0.49
1:FB:224:LEU:HD11	1:FB:250:MET:HE2	1.94	0.49
1:IA:224:LEU:CD1	1:IA:250:MET:HE2	2.43	0.49
1:MA:224:LEU:CD1	1:MA:250:MET:HE2	2.43	0.49
1:X:224:LEU:CD1	1:X:250:MET:HE2	2.43	0.49
1:AA:224:LEU:CD1	1:AA:250:MET:HE2	2.43	0.49
1:BA:224:LEU:CD1	1:BA:250:MET:HE2	2.43	0.49
1:D:224:LEU:CD1	1:D:250:MET:HE2	2.43	0.49
1:DA:224:LEU:HD11	1:DA:250:MET:HE2	1.94	0.49
1:G:224:LEU:HD11	1:G:250:MET:HE2	1.94	0.49
1:GA:224:LEU:HD11	1:GA:250:MET:HE2	1.94	0.49
1:HA:224:LEU:CD1	1:HA:250:MET:HE2	2.43	0.49
1:HB:224:LEU:HD11	1:HB:250:MET:HE2	1.94	0.49
1:IB:224:LEU:CD1	1:IB:250:MET:HE2	2.43	0.49
1:PA:224:LEU:CD1	1:PA:250:MET:HE2	2.43	0.49
1:S:224:LEU:CD1	1:S:250:MET:HE2	2.43	0.49
1:V:224:LEU:CD1	1:V:250:MET:HE2	2.43	0.49
1:Y:224:LEU:HD11	1:Y:250:MET:HE2	1.94	0.49
1:ZA:224:LEU:CD1	1:ZA:250:MET:HE2	2.43	0.49
1:F:224:LEU:CD1	1:F:250:MET:HE2	2.43	0.49
1:GA:224:LEU:CD1	1:GA:250:MET:HE2	2.43	0.49
1:H:49:SER:HG	1:W:49:SER:HG	1.51	0.49
1:K:224:LEU:CD1	1:K:250:MET:HE2	2.43	0.49
1:LA:224:LEU:HD11	1:LA:250:MET:HE2	1.94	0.49
1:NA:224:LEU:CD1	1:NA:250:MET:HE2	2.43	0.49
1:UA:224:LEU:CD1	1:UA:250:MET:HE2	2.43	0.49
1:W:224:LEU:CD1	1:W:250:MET:HE2	2.43	0.49
1:WA:224:LEU:CD1	1:WA:250:MET:HE2	2.43	0.49
1:X:224:LEU:HD11	1:X:250:MET:HE2	1.94	0.49
1:XA:224:LEU:HD11	1:XA:250:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:YA:224:LEU:CD1	1:YA:250:MET:HE2	2.43	0.49
1:AB:224:LEU:CD1	1:AB:250:MET:HE2	2.43	0.49
1:BB:224:LEU:HD11	1:BB:250:MET:HE2	1.94	0.49
1:DA:224:LEU:CD1	1:DA:250:MET:HE2	2.43	0.49
1:EB:224:LEU:CD1	1:EB:250:MET:HE2	2.43	0.49
1:GB:224:LEU:CD1	1:GB:250:MET:HE2	2.43	0.49
1:H:224:LEU:CD1	1:H:250:MET:HE2	2.43	0.49
1:JA:221:ASP:OD1	1:JA:256:THR:OG1	2.29	0.49
1:L:224:LEU:HD11	1:L:250:MET:HE2	1.94	0.49
1:LA:224:LEU:CD1	1:LA:250:MET:HE2	2.43	0.49
1:M:224:LEU:CD1	1:M:250:MET:HE2	2.43	0.49
1:M:224:LEU:HD11	1:M:250:MET:HE2	1.94	0.49
1:O:224:LEU:HD11	1:O:250:MET:HE2	1.94	0.49
1:QA:224:LEU:CD1	1:QA:250:MET:HE2	2.43	0.49
1:CA:224:LEU:HD11	1:CA:250:MET:HE2	1.94	0.49
1:EA:224:LEU:CD1	1:EA:250:MET:HE2	2.43	0.49
1:FB:224:LEU:CD1	1:FB:250:MET:HE2	2.43	0.49
1:GB:221:ASP:OD1	1:GB:256:THR:OG1	2.29	0.49
1:H:224:LEU:HD11	1:H:250:MET:HE2	1.94	0.49
1:J:224:LEU:CD1	1:J:250:MET:HE2	2.43	0.49
1:O:197:ARG:HH12	1:R:193:GLU:CD	2.12	0.49
1:OA:221:ASP:OD1	1:OA:256:THR:OG1	2.29	0.49
1:P:224:LEU:CD1	1:P:250:MET:HE2	2.43	0.49
1:RA:224:LEU:HD11	1:RA:250:MET:HE2	1.94	0.49
1:UA:221:ASP:OD1	1:UA:256:THR:OG1	2.29	0.49
1:WA:221:ASP:OD1	1:WA:256:THR:OG1	2.29	0.49
1:Y:224:LEU:CD1	1:Y:250:MET:HE2	2.43	0.49
1:Z:224:LEU:CD1	1:Z:250:MET:HE2	2.43	0.49
1:A:224:LEU:CD1	1:A:250:MET:HE2	2.43	0.49
1:BA:224:LEU:HD11	1:BA:250:MET:HE2	1.94	0.49
1:G:224:LEU:CD1	1:G:250:MET:HE2	2.43	0.49
1:LA:221:ASP:OD1	1:LA:256:THR:OG1	2.29	0.49
1:O:224:LEU:CD1	1:O:250:MET:HE2	2.43	0.49
1:OA:224:LEU:CD1	1:OA:250:MET:HE2	2.43	0.49
1:B:224:LEU:HD11	1:B:250:MET:HE2	1.94	0.48
1:EB:224:LEU:HD11	1:EB:250:MET:HE2	1.94	0.48
1:JA:224:LEU:CD1	1:JA:250:MET:HE2	2.43	0.48
1:L:224:LEU:CD1	1:L:250:MET:HE2	2.43	0.48
1:MA:224:LEU:HD11	1:MA:250:MET:HE2	1.94	0.48
1:Q:224:LEU:HD11	1:Q:250:MET:HE2	1.94	0.48
1:S:221:ASP:OD1	1:S:256:THR:OG1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:224:LEU:CD1	1:TA:250:MET:HE2	2.43	0.48
1:VA:224:LEU:CD1	1:VA:250:MET:HE2	2.43	0.48
1:W:224:LEU:HD11	1:W:250:MET:HE2	1.94	0.48
1:A:224:LEU:HD11	1:A:250:MET:HE2	1.94	0.48
1:C:221:ASP:OD1	1:C:256:THR:OG1	2.29	0.48
1:DB:224:LEU:CD1	1:DB:250:MET:HE2	2.43	0.48
1:E:224:LEU:HD11	1:E:250:MET:HE2	1.94	0.48
1:GA:221:ASP:OD1	1:GA:256:THR:OG1	2.29	0.48
1:SA:224:LEU:CD1	1:SA:250:MET:HE2	2.43	0.48
1:UA:224:LEU:HD11	1:UA:250:MET:HE2	1.94	0.48
1:D:221:ASP:OD1	1:D:256:THR:OG1	2.29	0.48
1:HA:224:LEU:HD11	1:HA:250:MET:HE2	1.94	0.48
1:HB:224:LEU:CD1	1:HB:250:MET:HE2	2.43	0.48
1:N:224:LEU:CD1	1:N:250:MET:HE2	2.43	0.48
1:P:224:LEU:HD11	1:P:250:MET:HE2	1.94	0.48
1:R:221:ASP:OD1	1:R:256:THR:OG1	2.29	0.48
1:T:224:LEU:HD11	1:T:250:MET:HE2	1.94	0.48
1:BA:12:THR:CB	1:L:2:ASN:HB3	2.44	0.48
1:C:224:LEU:HD11	1:C:250:MET:HE2	1.94	0.48
1:CB:224:LEU:CD1	1:CB:250:MET:HE2	2.43	0.48
1:EA:224:LEU:HD11	1:EA:250:MET:HE2	1.94	0.48
1:I:224:LEU:CD1	1:I:250:MET:HE2	2.43	0.48
1:KA:221:ASP:OD1	1:KA:256:THR:OG1	2.29	0.48
1:R:224:LEU:HD11	1:R:250:MET:HE2	1.94	0.48
1:Z:224:LEU:HD11	1:Z:250:MET:HE2	1.94	0.48
1:A:2:ASN:HB3	1:WA:12:THR:CB	2.44	0.48
1:B:12:THR:CB	1:VA:2:ASN:HB3	2.44	0.48
1:F:123:TYR:OH	1:IB:59:SER:O	2.23	0.48
1:FB:2:ASN:HB3	1:Q:12:THR:CB	2.44	0.48
1:G:2:ASN:HB3	1:W:12:THR:CB	2.44	0.48
1:GB:12:THR:CB	1:P:2:ASN:HB3	2.44	0.48
1:KA:224:LEU:CD1	1:KA:250:MET:HE2	2.43	0.48
1:P:221:ASP:OD1	1:P:256:THR:OG1	2.29	0.48
1:A:221:ASP:OD1	1:A:256:THR:OG1	2.29	0.48
1:B:2:ASN:HB3	1:GA:12:THR:CB	2.44	0.48
1:BB:224:LEU:CD1	1:BB:250:MET:HE2	2.43	0.48
1:E:12:THR:CB	1:Z:2:ASN:HB3	2.44	0.48
1:EA:2:ASN:HB3	1:T:12:THR:CB	2.44	0.48
1:FA:224:LEU:CD1	1:FA:250:MET:HE2	2.43	0.48
1:FB:12:THR:CB	1:LA:2:ASN:HB3	2.44	0.48
1:GA:2:ASN:HB3	1:VA:12:THR:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LEU:HD11	1:I:250:MET:HE2	1.94	0.48
1:N:12:THR:CB	1:R:2:ASN:HB3	2.44	0.48
1:N:224:LEU:HD11	1:N:250:MET:HE2	1.94	0.48
1:RA:224:LEU:CD1	1:RA:250:MET:HE2	2.43	0.48
1:XA:224:LEU:CD1	1:XA:250:MET:HE2	2.43	0.48
1:AA:12:THR:CB	1:S:2:ASN:HB3	2.44	0.48
1:B:224:LEU:CD1	1:B:250:MET:HE2	2.43	0.48
1:C:2:ASN:HB3	1:I:12:THR:CB	2.44	0.48
1:C:224:LEU:CD1	1:C:250:MET:HE2	2.43	0.48
1:CB:2:ASN:HB3	1:P:12:THR:CB	2.44	0.48
1:DB:12:THR:CB	1:T:2:ASN:HB3	2.44	0.48
1:EB:221:ASP:OD1	1:EB:256:THR:OG1	2.29	0.48
1:FA:221:ASP:OD1	1:FA:256:THR:OG1	2.29	0.48
1:IA:221:ASP:OD1	1:IA:256:THR:OG1	2.29	0.48
1:IB:12:THR:CB	1:J:2:ASN:HB3	2.44	0.48
1:LA:12:THR:CB	1:Q:2:ASN:HB3	2.44	0.48
1:O:2:ASN:HB3	1:YA:12:THR:CB	2.44	0.48
1:OA:12:THR:CB	1:YA:2:ASN:HB3	2.44	0.48
1:BA:115:GLU:HG3	1:BA:250:MET:HE3	1.96	0.48
1:C:12:THR:CB	1:FA:2:ASN:HB3	2.44	0.48
1:CA:2:ASN:HB3	1:Y:12:THR:CB	2.44	0.48
1:DA:12:THR:CB	1:X:2:ASN:HB3	2.44	0.48
1:K:123:TYR:OH	1:YA:59:SER:O	2.23	0.48
1:KA:2:ASN:HB3	1:R:12:THR:CB	2.44	0.48
1:R:224:LEU:CD1	1:R:250:MET:HE2	2.43	0.48
1:T:224:LEU:CD1	1:T:250:MET:HE2	2.43	0.48
1:A:12:THR:CB	1:SA:2:ASN:HB3	2.44	0.48
1:D:2:ASN:HB3	1:V:12:THR:CB	2.44	0.48
1:E:2:ASN:HB3	1:TA:12:THR:CB	2.44	0.48
1:E:224:LEU:CD1	1:E:250:MET:HE2	2.43	0.48
1:FB:115:GLU:HG3	1:FB:250:MET:HE3	1.96	0.48
1:IB:2:ASN:HB3	1:JA:12:THR:CB	2.44	0.48
1:NA:221:ASP:OD1	1:NA:256:THR:OG1	2.29	0.48
1:O:115:GLU:HG3	1:O:250:MET:HE3	1.96	0.48
1:V:115:GLU:HG3	1:V:250:MET:HE3	1.96	0.48
1:AA:115:GLU:HG3	1:AA:250:MET:HE3	1.96	0.48
1:C:115:GLU:HG3	1:C:250:MET:HE3	1.96	0.48
1:D:115:GLU:HG3	1:D:250:MET:HE3	1.96	0.48
1:F:12:THR:CB	1:HB:2:ASN:HB3	2.44	0.48
1:FA:115:GLU:HG3	1:FA:250:MET:HE3	1.96	0.48
1:J:115:GLU:HG3	1:J:250:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:12:THR:CB	1:XA:2:ASN:HB3	2.44	0.48
1:N:221:ASP:OD1	1:N:256:THR:OG1	2.29	0.48
1:Q:224:LEU:CD1	1:Q:250:MET:HE2	2.43	0.48
1:R:115:GLU:HG3	1:R:250:MET:HE3	1.96	0.48
1:RA:115:GLU:HG3	1:RA:250:MET:HE3	1.96	0.48
1:S:115:GLU:HG3	1:S:250:MET:HE3	1.96	0.48
1:W:115:GLU:HG3	1:W:250:MET:HE3	1.96	0.48
1:AA:2:ASN:HB3	1:M:12:THR:CB	2.44	0.47
1:B:171:VAL:CG2	1:B:199:VAL:HG21	2.44	0.47
1:BB:115:GLU:HG3	1:BB:250:MET:HE3	1.96	0.47
1:BB:171:VAL:CG2	1:BB:199:VAL:HG21	2.44	0.47
1:DB:115:GLU:HG3	1:DB:250:MET:HE3	1.96	0.47
1:I:115:GLU:HG3	1:I:250:MET:HE3	1.96	0.47
1:N:115:GLU:HG3	1:N:250:MET:HE3	1.96	0.47
1:O:12:THR:CB	1:OA:2:ASN:HB3	2.44	0.47
1:Q:171:VAL:CG2	1:Q:199:VAL:HG21	2.44	0.47
1:S:224:LEU:HD11	1:S:250:MET:HE2	1.94	0.47
1:TA:115:GLU:HG3	1:TA:250:MET:HE3	1.96	0.47
1:VA:115:GLU:HG3	1:VA:250:MET:HE3	1.96	0.47
1:AA:221:ASP:OD1	1:AA:256:THR:OG1	2.29	0.47
1:AB:2:ASN:HB3	1:G:12:THR:CB	2.44	0.47
1:CA:115:GLU:HG3	1:CA:250:MET:HE3	1.96	0.47
1:DB:2:ASN:HB3	1:EA:12:THR:CB	2.44	0.47
1:GB:115:GLU:HG3	1:GB:250:MET:HE3	1.96	0.47
1:HA:2:ASN:HB3	1:NA:12:THR:CB	2.44	0.47
1:KA:115:GLU:HG3	1:KA:250:MET:HE3	1.96	0.47
1:L:12:THR:CB	1:QA:2:ASN:HB3	2.44	0.47
1:M:2:ASN:HB3	1:S:12:THR:CB	2.44	0.47
1:WA:171:VAL:CG2	1:WA:199:VAL:HG21	2.44	0.47
1:A:115:GLU:HG3	1:A:250:MET:HE3	1.96	0.47
1:AB:171:VAL:CG2	1:AB:199:VAL:HG21	2.44	0.47
1:CB:12:THR:CB	1:GB:2:ASN:HB3	2.44	0.47
1:D:12:THR:CB	1:H:2:ASN:HB3	2.44	0.47
1:D:224:LEU:HD11	1:D:250:MET:HE2	1.94	0.47
1:EA:171:VAL:CG2	1:EA:199:VAL:HG21	2.44	0.47
1:F:171:VAL:CG2	1:F:199:VAL:HG21	2.44	0.47
1:FA:171:VAL:CG2	1:FA:199:VAL:HG21	2.44	0.47
1:GB:171:VAL:CG2	1:GB:199:VAL:HG21	2.45	0.47
1:H:12:THR:CB	1:V:2:ASN:HB3	2.44	0.47
1:I:221:ASP:OD1	1:I:256:THR:OG1	2.29	0.47
1:IA:12:THR:CB	1:MA:2:ASN:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:171:VAL:CG2	1:IA:199:VAL:HG21	2.45	0.47
1:J:12:THR:CB	1:JA:2:ASN:HB3	2.44	0.47
1:K:171:VAL:CG2	1:K:199:VAL:HG21	2.44	0.47
1:KA:171:VAL:CG2	1:KA:199:VAL:HG21	2.44	0.47
1:NA:171:VAL:CG2	1:NA:199:VAL:HG21	2.44	0.47
1:P:115:GLU:HG3	1:P:250:MET:HE3	1.96	0.47
1:RA:171:VAL:CG2	1:RA:199:VAL:HG21	2.45	0.47
1:SA:12:THR:CB	1:WA:2:ASN:HB3	2.44	0.47
1:SA:171:VAL:CG2	1:SA:199:VAL:HG21	2.44	0.47
1:T:221:ASP:OD1	1:T:256:THR:OG1	2.29	0.47
1:WA:115:GLU:HG3	1:WA:250:MET:HE3	1.96	0.47
1:Z:171:VAL:CG2	1:Z:199:VAL:HG21	2.44	0.47
1:AB:115:GLU:HG3	1:AB:250:MET:HE3	1.96	0.47
1:E:115:GLU:HG3	1:E:250:MET:HE3	1.96	0.47
1:H:171:VAL:CG2	1:H:199:VAL:HG21	2.44	0.47
1:K:2:ASN:HB3	1:RA:12:THR:CB	2.44	0.47
1:O:171:VAL:CG2	1:O:199:VAL:HG21	2.45	0.47
1:RA:2:ASN:HB3	1:XA:12:THR:CB	2.44	0.47
1:V:221:ASP:OD1	1:V:256:THR:OG1	2.29	0.47
1:X:115:GLU:HG3	1:X:250:MET:HE3	1.96	0.47
1:BB:2:ASN:HB3	1:HB:12:THR:CB	2.44	0.47
1:CB:171:VAL:CG2	1:CB:199:VAL:HG21	2.45	0.47
1:FA:12:THR:CB	1:I:2:ASN:HB3	2.44	0.47
1:GA:171:VAL:CG2	1:GA:199:VAL:HG21	2.45	0.47
1:HA:12:THR:CB	1:UA:2:ASN:HB3	2.44	0.47
1:J:171:VAL:CG2	1:J:199:VAL:HG21	2.45	0.47
1:KA:12:THR:CB	1:N:2:ASN:HB3	2.44	0.47
1:LA:171:VAL:CG2	1:LA:199:VAL:HG21	2.45	0.47
1:M:171:VAL:CG2	1:M:199:VAL:HG21	2.45	0.47
1:QA:171:VAL:CG2	1:QA:199:VAL:HG21	2.45	0.47
1:T:115:GLU:HG3	1:T:250:MET:HE3	1.96	0.47
1:TA:2:ASN:HB3	1:Z:12:THR:CB	2.44	0.47
1:Y:115:GLU:HG3	1:Y:250:MET:HE3	1.96	0.47
1:YA:221:ASP:OD1	1:YA:256:THR:OG1	2.29	0.47
1:AA:171:VAL:CG2	1:AA:199:VAL:HG21	2.44	0.47
1:DA:115:GLU:HG3	1:DA:250:MET:HE3	1.96	0.47
1:E:221:ASP:OD1	1:E:256:THR:OG1	2.29	0.47
1:EB:2:ASN:HB3	1:MA:12:THR:CB	2.44	0.47
1:HB:115:GLU:HG3	1:HB:250:MET:HE3	1.96	0.47
1:PA:115:GLU:HG3	1:PA:250:MET:HE3	1.96	0.47
1:QA:115:GLU:HG3	1:QA:250:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:171:VAL:CG2	1:TA:199:VAL:HG21	2.45	0.47
1:A:171:VAL:CG2	1:A:199:VAL:HG21	2.44	0.47
1:BA:2:ASN:HB3	1:QA:12:THR:CB	2.44	0.47
1:BB:12:THR:CB	1:F:2:ASN:HB3	2.44	0.47
1:D:171:VAL:CG2	1:D:199:VAL:HG21	2.45	0.47
1:DB:171:VAL:CG2	1:DB:199:VAL:HG21	2.44	0.47
1:EA:221:ASP:OD1	1:EA:256:THR:OG1	2.29	0.47
1:G:171:VAL:CG2	1:G:199:VAL:HG21	2.44	0.47
1:IB:171:VAL:CG2	1:IB:199:VAL:HG21	2.44	0.47
1:IB:221:ASP:OD1	1:IB:256:THR:OG1	2.29	0.47
1:L:171:VAL:CG2	1:L:199:VAL:HG21	2.44	0.47
1:P:171:VAL:CG2	1:P:199:VAL:HG21	2.44	0.47
1:S:171:VAL:CG2	1:S:199:VAL:HG21	2.45	0.47
1:V:171:VAL:CG2	1:V:199:VAL:HG21	2.44	0.47
1:XA:115:GLU:HG3	1:XA:250:MET:HE3	1.96	0.47
1:YA:171:VAL:CG2	1:YA:199:VAL:HG21	2.45	0.47
1:ZA:115:GLU:HG3	1:ZA:250:MET:HE3	1.96	0.47
1:AB:12:THR:CB	1:W:2:ASN:HB3	2.44	0.47
1:CA:12:THR:CB	1:PA:2:ASN:HB3	2.44	0.47
1:FB:171:VAL:CG2	1:FB:199:VAL:HG21	2.44	0.47
1:G:115:GLU:HG3	1:G:250:MET:HE3	1.96	0.47
1:HA:115:GLU:HG3	1:HA:250:MET:HE3	1.96	0.47
1:I:171:VAL:CG2	1:I:199:VAL:HG21	2.44	0.47
1:N:171:VAL:CG2	1:N:199:VAL:HG21	2.44	0.47
1:NA:115:GLU:HG3	1:NA:250:MET:HE3	1.96	0.47
1:QA:221:ASP:OD1	1:QA:256:THR:OG1	2.29	0.47
1:RA:221:ASP:OD1	1:RA:256:THR:OG1	2.29	0.47
1:Z:221:ASP:OD1	1:Z:256:THR:OG1	2.29	0.47
1:BB:221:ASP:OD1	1:BB:256:THR:OG1	2.29	0.47
1:IA:115:GLU:HG3	1:IA:250:MET:HE3	1.96	0.47
1:L:115:GLU:HG3	1:L:250:MET:HE3	1.96	0.47
1:MA:115:GLU:HG3	1:MA:250:MET:HE3	1.96	0.47
1:NA:2:ASN:HB3	1:UA:12:THR:CB	2.44	0.47
1:R:171:VAL:CG2	1:R:199:VAL:HG21	2.45	0.47
1:VA:171:VAL:CG2	1:VA:199:VAL:HG21	2.45	0.47
1:Z:115:GLU:HG3	1:Z:250:MET:HE3	1.96	0.47
1:EB:12:THR:CB	1:IA:2:ASN:HB3	2.44	0.47
1:X:12:THR:CB	1:ZA:2:ASN:HB3	2.44	0.47
1:AB:221:ASP:OD1	1:AB:256:THR:OG1	2.29	0.46
1:C:171:VAL:CG2	1:C:199:VAL:HG21	2.45	0.46
1:JA:171:VAL:CG2	1:JA:199:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:171:VAL:CG2	1:PA:199:VAL:HG21	2.44	0.46
1:CA:171:VAL:CG2	1:CA:199:VAL:HG21	2.44	0.46
1:DA:2:ASN:HB3	1:ZA:12:THR:CB	2.44	0.46
1:EA:115:GLU:HG3	1:EA:250:MET:HE3	1.96	0.46
1:OA:171:VAL:CG2	1:OA:199:VAL:HG21	2.45	0.46
1:PA:12:THR:CB	1:Y:2:ASN:HB3	2.44	0.46
1:UA:171:VAL:CG2	1:UA:199:VAL:HG21	2.44	0.46
1:XA:171:VAL:CG2	1:XA:199:VAL:HG21	2.44	0.46
1:B:115:GLU:HG3	1:B:250:MET:HE3	1.96	0.46
1:B:221:ASP:OD1	1:B:256:THR:OG1	2.29	0.46
1:EB:171:VAL:CG2	1:EB:199:VAL:HG21	2.44	0.46
1:HB:171:VAL:CG2	1:HB:199:VAL:HG21	2.44	0.46
1:ZA:171:VAL:CG2	1:ZA:199:VAL:HG21	2.44	0.46
1:CB:115:GLU:HG3	1:CB:250:MET:HE3	1.96	0.46
1:IB:115:GLU:HG3	1:IB:250:MET:HE3	1.96	0.46
1:K:115:GLU:HG3	1:K:250:MET:HE3	1.96	0.46
1:Q:115:GLU:HG3	1:Q:250:MET:HE3	1.96	0.46
1:Q:221:ASP:OD1	1:Q:256:THR:OG1	2.29	0.46
1:SA:115:GLU:HG3	1:SA:250:MET:HE3	1.96	0.46
1:T:171:VAL:CG2	1:T:199:VAL:HG21	2.44	0.46
1:X:171:VAL:CG2	1:X:199:VAL:HG21	2.45	0.46
1:E:171:VAL:CG2	1:E:199:VAL:HG21	2.44	0.46
1:F:115:GLU:HG3	1:F:250:MET:HE3	1.96	0.46
1:GA:115:GLU:HG3	1:GA:250:MET:HE3	1.96	0.46
1:LA:115:GLU:HG3	1:LA:250:MET:HE3	1.96	0.46
1:M:115:GLU:HG3	1:M:250:MET:HE3	1.96	0.46
1:YA:115:GLU:HG3	1:YA:250:MET:HE3	1.96	0.46
1:BA:171:VAL:CG2	1:BA:199:VAL:HG21	2.45	0.46
1:CA:221:ASP:OD1	1:CA:256:THR:OG1	2.29	0.46
1:DA:171:VAL:CG2	1:DA:199:VAL:HG21	2.45	0.46
1:H:115:GLU:HG3	1:H:250:MET:HE3	1.96	0.46
1:MA:171:VAL:CG2	1:MA:199:VAL:HG21	2.45	0.46
1:Y:171:VAL:CG2	1:Y:199:VAL:HG21	2.44	0.46
1:JA:115:GLU:HG3	1:JA:250:MET:HE3	1.96	0.46
1:X:221:ASP:OD1	1:X:256:THR:OG1	2.29	0.46
1:Y:221:ASP:OD1	1:Y:256:THR:OG1	2.29	0.46
1:HA:171:VAL:CG2	1:HA:199:VAL:HG21	2.45	0.46
1:W:171:VAL:CG2	1:W:199:VAL:HG21	2.45	0.46
1:OA:115:GLU:HG3	1:OA:250:MET:HE3	1.96	0.46
1:UA:115:GLU:HG3	1:UA:250:MET:HE3	1.96	0.46
1:BB:151:ASP:N	1:BB:151:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:221:ASP:OD1	1:DA:256:THR:OG1	2.29	0.45
1:EB:115:GLU:HG3	1:EB:250:MET:HE3	1.96	0.45
1:GA:151:ASP:N	1:GA:151:ASP:OD1	2.49	0.45
1:IB:151:ASP:N	1:IB:151:ASP:OD1	2.49	0.45
1:LA:151:ASP:N	1:LA:151:ASP:OD1	2.49	0.45
1:RA:151:ASP:OD1	1:RA:151:ASP:N	2.49	0.45
1:B:151:ASP:N	1:B:151:ASP:OD1	2.49	0.45
1:C:151:ASP:OD1	1:C:151:ASP:N	2.49	0.45
1:HA:151:ASP:OD1	1:HA:151:ASP:N	2.49	0.45
1:MA:151:ASP:OD1	1:MA:151:ASP:N	2.49	0.45
1:Q:151:ASP:N	1:Q:151:ASP:OD1	2.49	0.45
1:YA:151:ASP:OD1	1:YA:151:ASP:N	2.49	0.45
1:DA:49:SER:HG	1:Y:49:SER:HG	1.51	0.45
1:R:151:ASP:OD1	1:R:151:ASP:N	2.49	0.45
1:UA:151:ASP:OD1	1:UA:151:ASP:N	2.49	0.45
1:A:151:ASP:OD1	1:A:151:ASP:N	2.49	0.45
1:EB:151:ASP:OD1	1:EB:151:ASP:N	2.49	0.45
1:F:151:ASP:OD1	1:F:151:ASP:N	2.49	0.45
1:K:151:ASP:OD1	1:K:151:ASP:N	2.49	0.45
1:I:151:ASP:OD1	1:I:151:ASP:N	2.49	0.45
1:P:151:ASP:OD1	1:P:151:ASP:N	2.49	0.45
1:XA:221:ASP:OD1	1:XA:256:THR:OG1	2.29	0.45
1:N:151:ASP:OD1	1:N:151:ASP:N	2.49	0.45
1:H:151:ASP:OD1	1:H:151:ASP:N	2.49	0.45
1:M:151:ASP:OD1	1:M:151:ASP:N	2.49	0.45
1:AA:151:ASP:OD1	1:AA:151:ASP:N	2.49	0.45
1:DB:221:ASP:OD1	1:DB:256:THR:OG1	2.29	0.45
1:HB:221:ASP:OD1	1:HB:256:THR:OG1	2.29	0.45
1:GB:151:ASP:OD1	1:GB:151:ASP:N	2.49	0.45
1:V:151:ASP:N	1:V:151:ASP:OD1	2.49	0.45
1:BA:2:ASN:HB3	1:QA:12:THR:HB	1.99	0.44
1:TA:151:ASP:OD1	1:TA:151:ASP:N	2.49	0.44
1:WA:151:ASP:OD1	1:WA:151:ASP:N	2.49	0.44
1:ZA:221:ASP:OD1	1:ZA:256:THR:OG1	2.29	0.44
1:AB:12:THR:HB	1:W:2:ASN:HB3	1.99	0.44
1:AB:151:ASP:OD1	1:AB:151:ASP:N	2.49	0.44
1:CA:151:ASP:OD1	1:CA:151:ASP:N	2.49	0.44
1:FA:12:THR:HB	1:I:2:ASN:HB3	2.00	0.44
1:KA:12:THR:HB	1:N:2:ASN:HB3	2.00	0.44
1:X:12:THR:HB	1:ZA:2:ASN:HB3	1.99	0.44
1:CA:2:ASN:HB3	1:Y:12:THR:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:12:THR:HB	1:PA:2:ASN:HB3	1.99	0.44
1:CB:2:ASN:HB3	1:P:12:THR:HB	1.99	0.44
1:DA:12:THR:HB	1:X:2:ASN:HB3	2.00	0.44
1:DB:151:ASP:N	1:DB:151:ASP:OD1	2.49	0.44
1:EA:151:ASP:N	1:EA:151:ASP:OD1	2.49	0.44
1:IB:2:ASN:HB3	1:JA:12:THR:HB	1.99	0.44
1:JA:151:ASP:OD1	1:JA:151:ASP:N	2.49	0.44
1:OA:12:THR:HB	1:YA:2:ASN:HB3	1.99	0.44
1:PA:221:ASP:OD1	1:PA:256:THR:OG1	2.29	0.44
1:BA:151:ASP:N	1:BA:151:ASP:OD1	2.49	0.44
1:HB:151:ASP:OD1	1:HB:151:ASP:N	2.49	0.44
1:O:12:THR:HB	1:OA:2:ASN:HB3	1.99	0.44
1:QA:151:ASP:N	1:QA:151:ASP:OD1	2.49	0.44
1:XA:151:ASP:N	1:XA:151:ASP:OD1	2.49	0.44
1:Z:151:ASP:OD1	1:Z:151:ASP:N	2.49	0.44
1:B:2:ASN:HB3	1:GA:12:THR:HB	1.99	0.44
1:DA:2:ASN:HB3	1:ZA:12:THR:HB	2.00	0.44
1:J:12:THR:HB	1:JA:2:ASN:HB3	1.99	0.44
1:OA:151:ASP:OD1	1:OA:151:ASP:N	2.49	0.44
1:W:151:ASP:OD1	1:W:151:ASP:N	2.49	0.44
1:X:151:ASP:N	1:X:151:ASP:OD1	2.49	0.44
1:A:12:THR:HB	1:SA:2:ASN:HB3	2.00	0.44
1:CB:151:ASP:OD1	1:CB:151:ASP:N	2.49	0.44
1:D:151:ASP:OD1	1:D:151:ASP:N	2.49	0.44
1:FB:2:ASN:HB3	1:Q:12:THR:HB	1.99	0.44
1:IA:151:ASP:OD1	1:IA:151:ASP:N	2.49	0.44
1:PA:12:THR:HB	1:Y:2:ASN:HB3	2.00	0.44
1:S:151:ASP:N	1:S:151:ASP:OD1	2.49	0.44
1:B:12:THR:HB	1:VA:2:ASN:HB3	1.99	0.44
1:C:12:THR:HB	1:FA:2:ASN:HB3	1.99	0.44
1:EB:12:THR:HB	1:IA:2:ASN:HB3	2.00	0.44
1:HA:12:THR:HB	1:UA:2:ASN:HB3	1.99	0.44
1:LA:12:THR:HB	1:Q:2:ASN:HB3	1.99	0.44
1:NA:2:ASN:HB3	1:UA:12:THR:HB	2.00	0.44
1:SA:151:ASP:N	1:SA:151:ASP:OD1	2.49	0.44
1:BA:12:THR:HB	1:L:2:ASN:HB3	1.99	0.44
1:EB:2:ASN:HB3	1:MA:12:THR:HB	2.00	0.44
1:NA:151:ASP:N	1:NA:151:ASP:OD1	2.50	0.44
1:A:2:ASN:HB3	1:WA:12:THR:HB	1.99	0.44
1:C:2:ASN:HB3	1:I:12:THR:HB	2.00	0.44
1:G:2:ASN:HB3	1:W:12:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:12:THR:HB	1:R:2:ASN:HB3	2.00	0.44
1:BB:2:ASN:HB3	1:HB:12:THR:HB	2.00	0.43
1:E:2:ASN:HB3	1:TA:12:THR:HB	1.99	0.43
1:J:151:ASP:N	1:J:151:ASP:OD1	2.49	0.43
1:KA:2:ASN:HB3	1:R:12:THR:HB	2.00	0.43
1:O:151:ASP:OD1	1:O:151:ASP:N	2.49	0.43
1:RA:2:ASN:HB3	1:XA:12:THR:HB	2.00	0.43
1:SA:12:THR:HB	1:WA:2:ASN:HB3	2.00	0.43
1:CB:12:THR:HB	1:GB:2:ASN:HB3	2.00	0.43
1:DB:12:THR:HB	1:T:2:ASN:HB3	1.99	0.43
1:HA:2:ASN:HB3	1:NA:12:THR:HB	2.00	0.43
1:WA:165:VAL:HG21	1:WA:258:GLU:O	2.19	0.43
1:Y:151:ASP:OD1	1:Y:151:ASP:N	2.49	0.43
1:ZA:165:VAL:HG21	1:ZA:258:GLU:O	2.19	0.43
1:FB:221:ASP:OD1	1:FB:256:THR:OG1	2.29	0.43
1:GB:12:THR:HB	1:P:2:ASN:HB3	2.00	0.43
1:GB:165:VAL:HG21	1:GB:258:GLU:O	2.19	0.43
1:IA:12:THR:HB	1:MA:2:ASN:HB3	2.00	0.43
1:K:12:THR:HB	1:XA:2:ASN:HB3	2.00	0.43
1:KA:151:ASP:OD1	1:KA:151:ASP:N	2.49	0.43
1:L:165:VAL:HG21	1:L:258:GLU:O	2.19	0.43
1:PA:165:VAL:HG21	1:PA:258:GLU:O	2.19	0.43
1:R:165:VAL:HG21	1:R:258:GLU:O	2.19	0.43
1:C:165:VAL:HG21	1:C:258:GLU:O	2.19	0.43
1:EA:2:ASN:HB3	1:T:12:THR:HB	1.99	0.43
1:EB:165:VAL:HG21	1:EB:258:GLU:O	2.19	0.43
1:F:12:THR:HB	1:HB:2:ASN:HB3	2.00	0.43
1:G:151:ASP:N	1:G:151:ASP:OD1	2.49	0.43
1:G:165:VAL:HG21	1:G:258:GLU:O	2.19	0.43
1:GA:2:ASN:HB3	1:VA:12:THR:HB	1.99	0.43
1:PA:151:ASP:OD1	1:PA:151:ASP:N	2.49	0.43
1:ZA:151:ASP:OD1	1:ZA:151:ASP:N	2.49	0.43
1:BA:221:ASP:OD1	1:BA:256:THR:OG1	2.29	0.43
1:CB:165:VAL:HG21	1:CB:258:GLU:O	2.19	0.43
1:DA:151:ASP:OD1	1:DA:151:ASP:N	2.49	0.43
1:FA:151:ASP:OD1	1:FA:151:ASP:N	2.49	0.43
1:FB:12:THR:HB	1:LA:2:ASN:HB3	1.99	0.43
1:HA:165:VAL:HG21	1:HA:258:GLU:O	2.19	0.43
1:JA:165:VAL:HG21	1:JA:258:GLU:O	2.19	0.43
1:MA:165:VAL:HG21	1:MA:258:GLU:O	2.19	0.43
1:OA:165:VAL:HG21	1:OA:258:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:165:VAL:HG21	1:SA:258:GLU:O	2.19	0.43
1:UA:165:VAL:HG21	1:UA:258:GLU:O	2.19	0.43
1:XA:165:VAL:HG21	1:XA:258:GLU:O	2.19	0.43
1:AA:2:ASN:HB3	1:M:12:THR:HB	1.99	0.43
1:E:12:THR:HB	1:Z:2:ASN:HB3	1.99	0.43
1:HB:165:VAL:HG21	1:HB:258:GLU:O	2.19	0.43
1:L:151:ASP:N	1:L:151:ASP:OD1	2.49	0.43
1:V:165:VAL:HG21	1:V:258:GLU:O	2.19	0.43
1:VA:151:ASP:N	1:VA:151:ASP:OD1	2.49	0.43
1:VA:221:ASP:OD1	1:VA:256:THR:OG1	2.29	0.43
1:AA:165:VAL:HG21	1:AA:258:GLU:O	2.19	0.43
1:DB:2:ASN:HB3	1:EA:12:THR:HB	1.99	0.43
1:FB:151:ASP:OD1	1:FB:151:ASP:N	2.49	0.43
1:H:12:THR:HB	1:V:2:ASN:HB3	1.99	0.43
1:L:12:THR:HB	1:QA:2:ASN:HB3	1.99	0.43
1:B:165:VAL:HG21	1:B:258:GLU:O	2.19	0.43
1:IB:12:THR:HB	1:J:2:ASN:HB3	1.99	0.43
1:O:2:ASN:HB3	1:YA:12:THR:HB	1.99	0.43
1:O:221:ASP:OD1	1:O:256:THR:OG1	2.29	0.43
1:Q:165:VAL:HG21	1:Q:258:GLU:O	2.19	0.43
1:T:165:VAL:HG21	1:T:258:GLU:O	2.19	0.43
1:AB:2:ASN:HB3	1:G:12:THR:HB	1.99	0.43
1:DB:165:VAL:HG21	1:DB:258:GLU:O	2.19	0.43
1:E:165:VAL:HG21	1:E:258:GLU:O	2.19	0.43
1:GA:165:VAL:HG21	1:GA:258:GLU:O	2.19	0.43
1:LA:165:VAL:HG21	1:LA:258:GLU:O	2.19	0.43
1:TA:165:VAL:HG21	1:TA:258:GLU:O	2.19	0.43
1:W:221:ASP:OD1	1:W:256:THR:OG1	2.29	0.43
1:K:2:ASN:HB3	1:RA:12:THR:HB	1.99	0.43
1:BA:165:VAL:HG21	1:BA:258:GLU:O	2.19	0.42
1:BB:12:THR:HB	1:F:2:ASN:HB3	2.00	0.42
1:O:165:VAL:HG21	1:O:258:GLU:O	2.19	0.42
1:QA:165:VAL:HG21	1:QA:258:GLU:O	2.19	0.42
1:TA:2:ASN:HB3	1:Z:12:THR:HB	2.00	0.42
1:W:165:VAL:HG21	1:W:258:GLU:O	2.19	0.42
1:BB:165:VAL:HG21	1:BB:258:GLU:O	2.19	0.42
1:I:165:VAL:HG21	1:I:258:GLU:O	2.19	0.42
1:J:165:VAL:HG21	1:J:258:GLU:O	2.19	0.42
1:K:165:VAL:HG21	1:K:258:GLU:O	2.19	0.42
1:KA:165:VAL:HG21	1:KA:258:GLU:O	2.19	0.42
1:N:165:VAL:HG21	1:N:258:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:VAL:HG21	1:A:258:GLU:O	2.19	0.42
1:AB:165:VAL:HG21	1:AB:258:GLU:O	2.19	0.42
1:F:165:VAL:HG21	1:F:258:GLU:O	2.19	0.42
1:J:221:ASP:OD1	1:J:256:THR:OG1	2.29	0.42
1:M:165:VAL:HG21	1:M:258:GLU:O	2.19	0.42
1:DA:165:VAL:HG21	1:DA:258:GLU:O	2.19	0.42
1:E:151:ASP:N	1:E:151:ASP:OD1	2.49	0.42
1:FA:165:VAL:HG21	1:FA:258:GLU:O	2.19	0.42
1:IA:165:VAL:HG21	1:IA:258:GLU:O	2.19	0.42
1:RA:165:VAL:HG21	1:RA:258:GLU:O	2.19	0.42
1:H:165:VAL:HG21	1:H:258:GLU:O	2.19	0.42
1:NA:165:VAL:HG21	1:NA:258:GLU:O	2.19	0.42
1:P:165:VAL:HG21	1:P:258:GLU:O	2.19	0.42
1:Y:165:VAL:HG21	1:Y:258:GLU:O	2.19	0.42
1:CA:165:VAL:HG21	1:CA:258:GLU:O	2.19	0.42
1:IB:165:VAL:HG21	1:IB:258:GLU:O	2.19	0.42
1:J:117:ARG:HE	1:J:117:ARG:HB3	1.77	0.42
1:O:117:ARG:HE	1:O:117:ARG:HB3	1.77	0.42
1:AA:12:THR:HB	1:S:2:ASN:HB3	2.00	0.42
1:T:151:ASP:OD1	1:T:151:ASP:N	2.49	0.42
1:YA:165:VAL:HG21	1:YA:258:GLU:O	2.19	0.42
1:Z:165:VAL:HG21	1:Z:258:GLU:O	2.19	0.42
1:D:2:ASN:HB3	1:V:12:THR:HB	2.00	0.42
1:D:12:THR:HB	1:H:2:ASN:HB3	2.00	0.42
1:FB:165:VAL:HG21	1:FB:258:GLU:O	2.19	0.42
1:S:165:VAL:HG21	1:S:258:GLU:O	2.19	0.42
1:VA:165:VAL:HG21	1:VA:258:GLU:O	2.19	0.42
1:D:165:VAL:HG21	1:D:258:GLU:O	2.19	0.42
1:EA:165:VAL:HG21	1:EA:258:GLU:O	2.19	0.42
1:M:2:ASN:HB3	1:S:12:THR:HB	2.00	0.42
1:X:165:VAL:HG21	1:X:258:GLU:O	2.19	0.42
1:FB:117:ARG:HE	1:FB:117:ARG:HB3	1.77	0.42
1:VA:117:ARG:HE	1:VA:117:ARG:HB3	1.77	0.41
1:AA:117:ARG:HE	1:AA:117:ARG:HB3	1.77	0.41
1:O:10:PRO:CA	1:OA:8:LEU:HD11	2.51	0.41
1:AB:8:LEU:HD11	1:G:10:PRO:CA	2.51	0.41
1:J:10:PRO:CA	1:JA:8:LEU:HD11	2.51	0.41
1:L:10:PRO:CA	1:QA:8:LEU:HD11	2.51	0.41
1:V:117:ARG:HE	1:V:117:ARG:HB3	1.77	0.41
1:B:8:LEU:HD11	1:GA:10:PRO:CA	2.51	0.41
1:FA:49:SER:HG	1:J:49:SER:HG	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:10:PRO:CA	1:LA:8:LEU:HD11	2.51	0.41
1:IB:10:PRO:CA	1:J:8:LEU:HD11	2.51	0.41
1:LA:10:PRO:CA	1:Q:8:LEU:HD11	2.51	0.41
1:O:8:LEU:HD11	1:YA:10:PRO:CA	2.51	0.41
1:BA:10:PRO:CA	1:L:8:LEU:HD11	2.51	0.41
1:DA:8:LEU:HD11	1:ZA:10:PRO:CA	2.51	0.41
1:G:8:LEU:HD11	1:W:10:PRO:CA	2.51	0.41
1:GA:8:LEU:HD11	1:VA:10:PRO:CA	2.51	0.41
1:IB:8:LEU:HD11	1:JA:10:PRO:CA	2.51	0.41
1:K:8:LEU:HD11	1:RA:10:PRO:CA	2.51	0.41
1:OA:10:PRO:CA	1:YA:8:LEU:HD11	2.51	0.41
1:PA:10:PRO:CA	1:Y:8:LEU:HD11	2.51	0.41
1:BB:10:PRO:CA	1:F:8:LEU:HD11	2.51	0.41
1:CA:10:PRO:CA	1:PA:8:LEU:HD11	2.51	0.41
1:NA:8:LEU:HD11	1:UA:10:PRO:CA	2.51	0.41
1:X:10:PRO:CA	1:ZA:8:LEU:HD11	2.51	0.41
1:CA:8:LEU:HD11	1:Y:10:PRO:CA	2.51	0.40
1:DA:10:PRO:CA	1:X:8:LEU:HD11	2.51	0.40
1:E:117:ARG:HE	1:E:117:ARG:HB3	1.77	0.40
1:EB:10:PRO:CA	1:IA:8:LEU:HD11	2.51	0.40
1:DB:10:PRO:CA	1:T:8:LEU:HD11	2.51	0.40
1:FA:10:PRO:CA	1:I:8:LEU:HD11	2.51	0.40
1:HA:8:LEU:HD11	1:NA:10:PRO:CA	2.51	0.40
1:KA:10:PRO:CA	1:N:8:LEU:HD11	2.51	0.40
1:N:10:PRO:CA	1:R:8:LEU:HD11	2.51	0.40
1:C:8:LEU:HD11	1:I:10:PRO:CA	2.52	0.40
1:F:10:PRO:CA	1:HB:8:LEU:HD11	2.51	0.40
1:IA:10:PRO:CA	1:MA:8:LEU:HD11	2.51	0.40
1:T:117:ARG:HE	1:T:117:ARG:HB3	1.77	0.40
1:E:8:LEU:HD11	1:TA:10:PRO:CA	2.51	0.40
1:EB:8:LEU:HD11	1:MA:10:PRO:CA	2.51	0.40
1:HA:10:PRO:CA	1:UA:8:LEU:HD11	2.51	0.40
1:K:10:PRO:CA	1:XA:8:LEU:HD11	2.51	0.40
1:XA:117:ARG:HE	1:XA:117:ARG:HB3	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	AA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	AB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	B	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	BA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	BB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	C	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	CA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	CB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	D	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	DA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	DB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	E	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	EA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	EB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	F	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	FA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	FB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	G	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	GA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	GB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	H	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	HA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	HB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	I	262/275 (95%)	261 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	IA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	IB	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	J	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	JA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	K	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	KA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	L	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	LA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	M	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	MA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	N	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	NA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	O	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	OA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	P	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	PA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	Q	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	QA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	R	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	RA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	S	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	SA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	T	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	TA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	UA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	V	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	VA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	W	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	WA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	X	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	XA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	YA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	Z	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
1	ZA	262/275 (95%)	261 (100%)	1 (0%)	0	100	100
All	All	15720/16500 (95%)	15660 (100%)	60 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/226 (95%)	215 (100%)	0	100	100
1	AA	215/226 (95%)	215 (100%)	0	100	100
1	AB	215/226 (95%)	215 (100%)	0	100	100
1	B	215/226 (95%)	215 (100%)	0	100	100
1	BA	215/226 (95%)	215 (100%)	0	100	100
1	BB	215/226 (95%)	215 (100%)	0	100	100
1	C	215/226 (95%)	215 (100%)	0	100	100
1	CA	215/226 (95%)	215 (100%)	0	100	100
1	CB	215/226 (95%)	215 (100%)	0	100	100
1	D	215/226 (95%)	215 (100%)	0	100	100
1	DA	215/226 (95%)	215 (100%)	0	100	100
1	DB	215/226 (95%)	215 (100%)	0	100	100
1	E	215/226 (95%)	215 (100%)	0	100	100
1	EA	215/226 (95%)	215 (100%)	0	100	100
1	EB	215/226 (95%)	215 (100%)	0	100	100
1	F	215/226 (95%)	215 (100%)	0	100	100
1	FA	215/226 (95%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FB	215/226 (95%)	215 (100%)	0	100	100
1	G	215/226 (95%)	215 (100%)	0	100	100
1	GA	215/226 (95%)	215 (100%)	0	100	100
1	GB	215/226 (95%)	215 (100%)	0	100	100
1	H	215/226 (95%)	215 (100%)	0	100	100
1	HA	215/226 (95%)	215 (100%)	0	100	100
1	HB	215/226 (95%)	215 (100%)	0	100	100
1	I	215/226 (95%)	215 (100%)	0	100	100
1	IA	215/226 (95%)	215 (100%)	0	100	100
1	IB	215/226 (95%)	215 (100%)	0	100	100
1	J	215/226 (95%)	215 (100%)	0	100	100
1	JA	215/226 (95%)	215 (100%)	0	100	100
1	K	215/226 (95%)	215 (100%)	0	100	100
1	KA	215/226 (95%)	215 (100%)	0	100	100
1	L	215/226 (95%)	215 (100%)	0	100	100
1	LA	215/226 (95%)	215 (100%)	0	100	100
1	M	215/226 (95%)	215 (100%)	0	100	100
1	MA	215/226 (95%)	215 (100%)	0	100	100
1	N	215/226 (95%)	215 (100%)	0	100	100
1	NA	215/226 (95%)	215 (100%)	0	100	100
1	O	215/226 (95%)	215 (100%)	0	100	100
1	OA	215/226 (95%)	215 (100%)	0	100	100
1	P	215/226 (95%)	215 (100%)	0	100	100
1	PA	215/226 (95%)	215 (100%)	0	100	100
1	Q	215/226 (95%)	215 (100%)	0	100	100
1	QA	215/226 (95%)	215 (100%)	0	100	100
1	R	215/226 (95%)	215 (100%)	0	100	100
1	RA	215/226 (95%)	215 (100%)	0	100	100
1	S	215/226 (95%)	215 (100%)	0	100	100
1	SA	215/226 (95%)	215 (100%)	0	100	100
1	T	215/226 (95%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	TA	215/226 (95%)	215 (100%)	0	100	100
1	UA	215/226 (95%)	215 (100%)	0	100	100
1	V	215/226 (95%)	215 (100%)	0	100	100
1	VA	215/226 (95%)	215 (100%)	0	100	100
1	W	215/226 (95%)	215 (100%)	0	100	100
1	WA	215/226 (95%)	215 (100%)	0	100	100
1	X	215/226 (95%)	215 (100%)	0	100	100
1	XA	215/226 (95%)	215 (100%)	0	100	100
1	Y	215/226 (95%)	215 (100%)	0	100	100
1	YA	215/226 (95%)	215 (100%)	0	100	100
1	Z	215/226 (95%)	215 (100%)	0	100	100
1	ZA	215/226 (95%)	215 (100%)	0	100	100
All	All	12900/13560 (95%)	12900 (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. There are no such sidechains identified.

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.

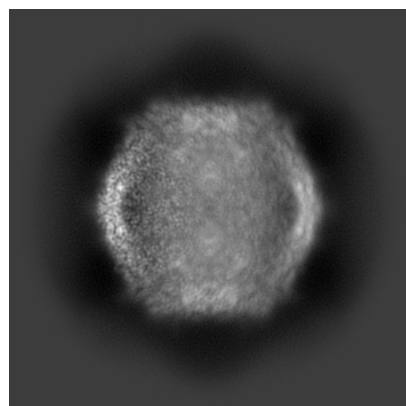
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50585. These allow visual inspection of the internal detail of the map and identification of artifacts.

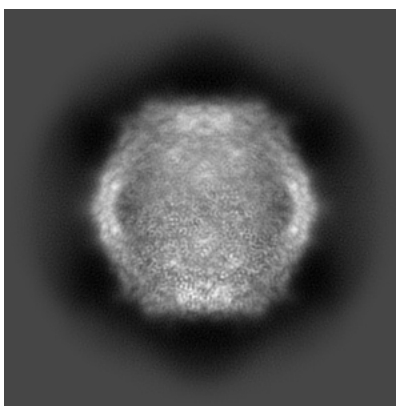
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

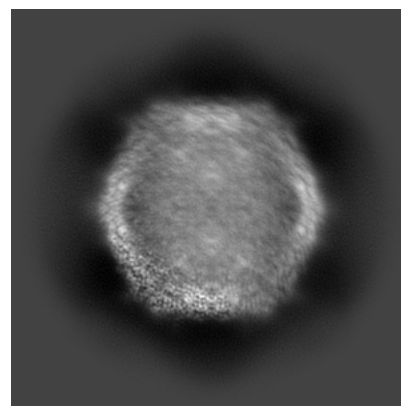
6.1.1 Primary map



X

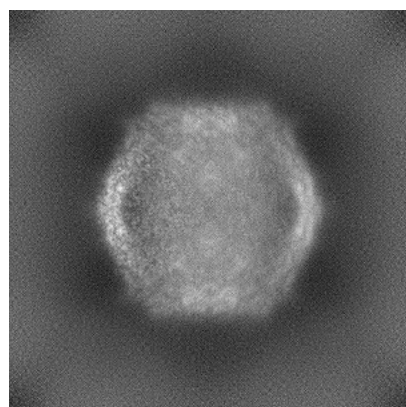


Y

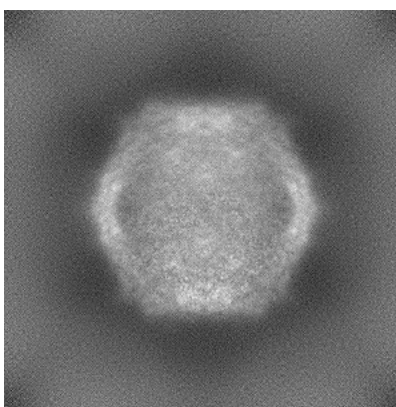


Z

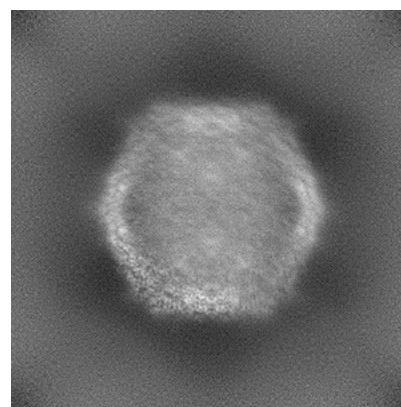
6.1.2 Raw map



X



Y

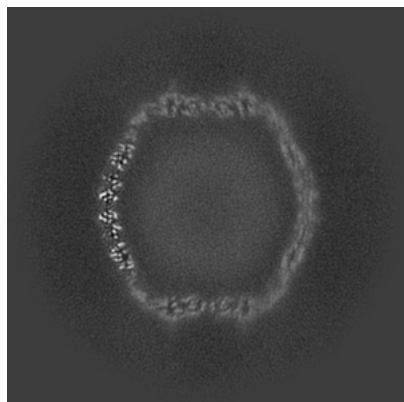


Z

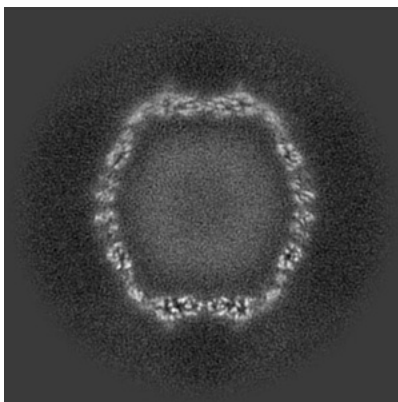
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

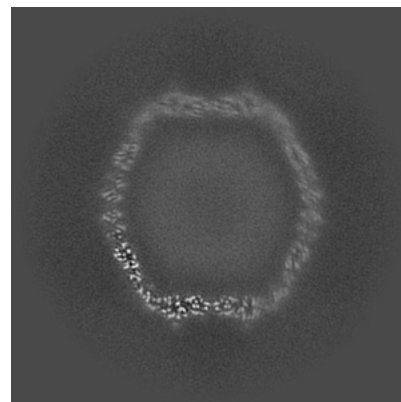
6.2.1 Primary map



X Index: 256

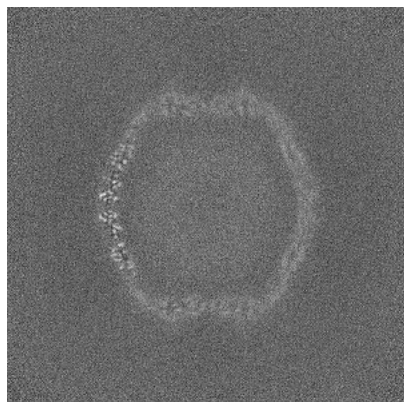


Y Index: 256

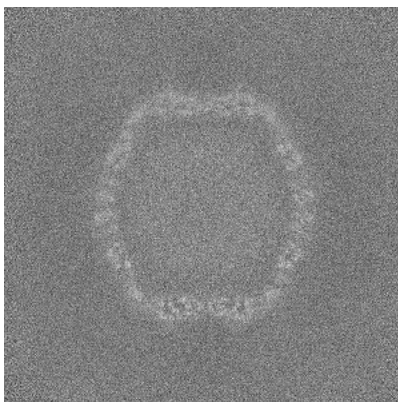


Z Index: 256

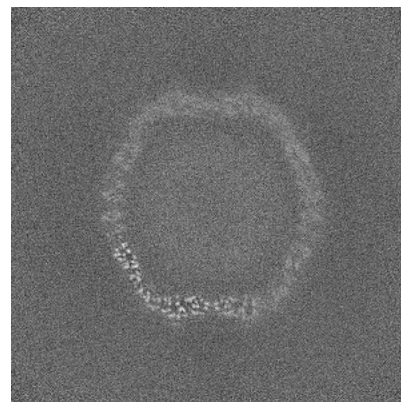
6.2.2 Raw map



X Index: 256



Y Index: 256

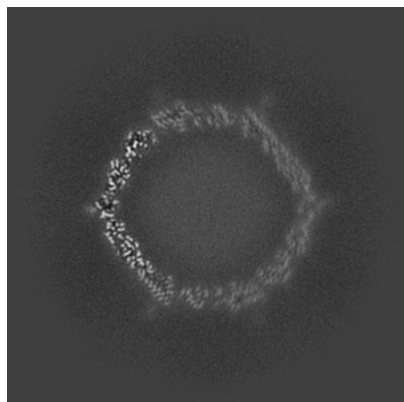


Z Index: 256

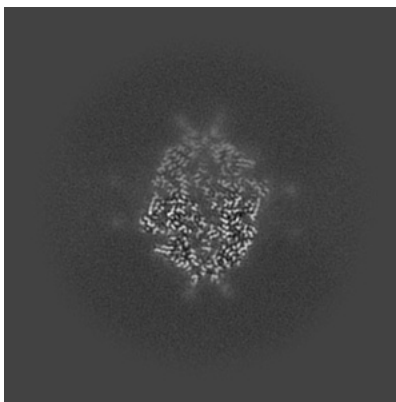
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

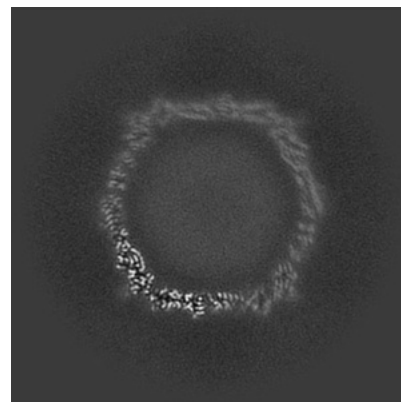
6.3.1 Primary map



X Index: 208

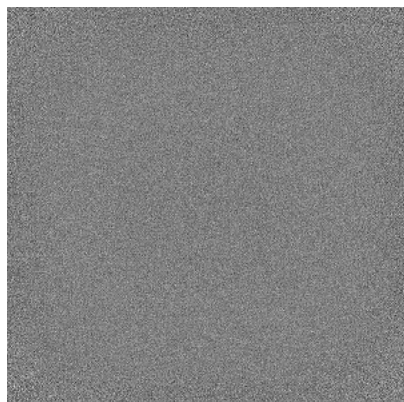


Y Index: 140

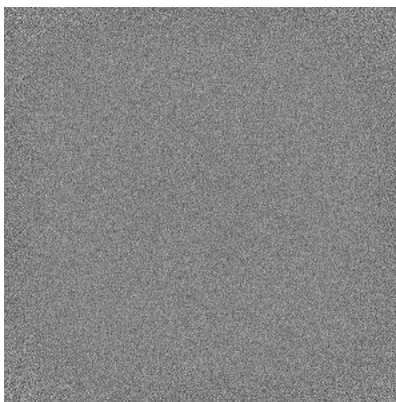


Z Index: 232

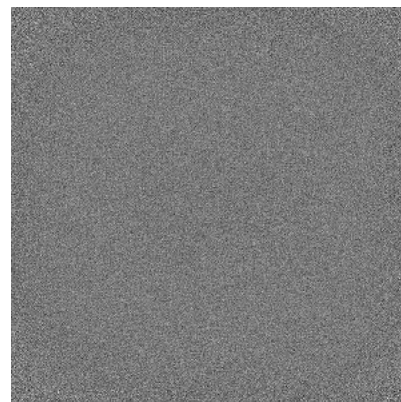
6.3.2 Raw map



X Index: 0



Y Index: 0

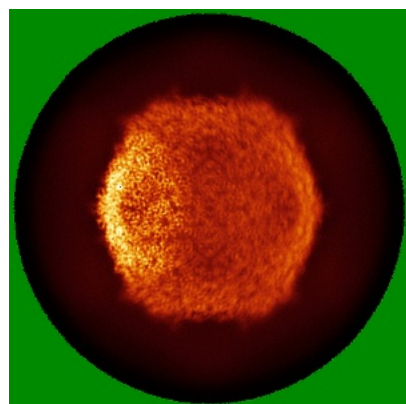


Z Index: 0

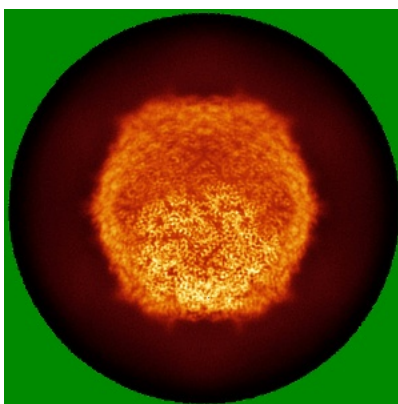
The images above show the largest variance slices of the map in three orthogonal directions.

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

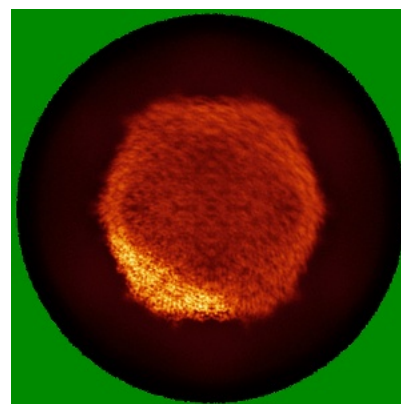
6.4.1 Primary map



X

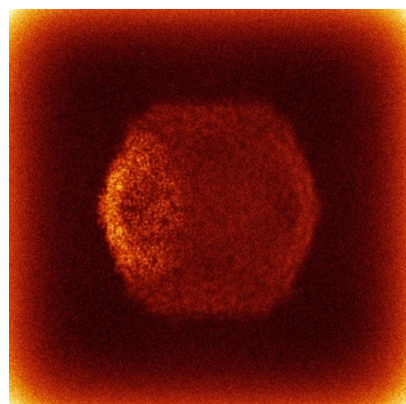


Y

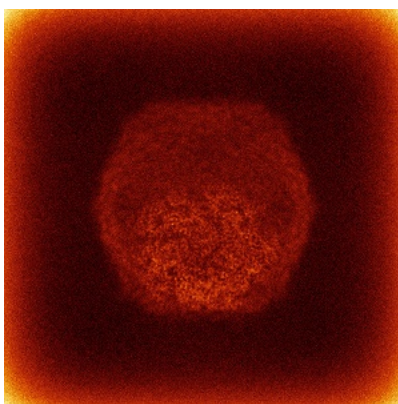


Z

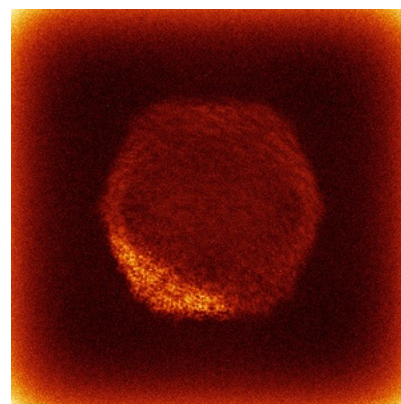
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



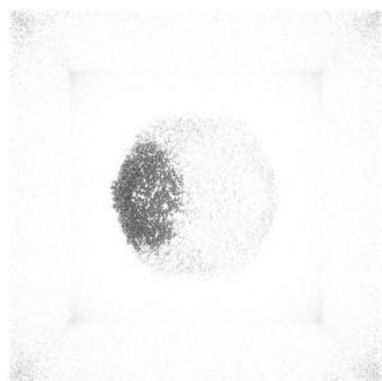
Y



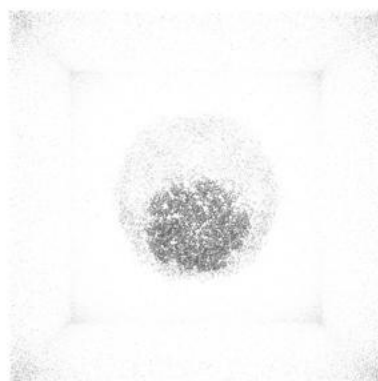
Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

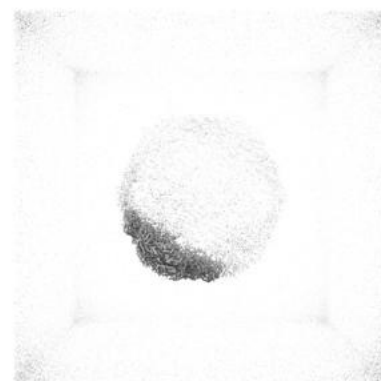
6.5.2 Raw map



X



Y



Z

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

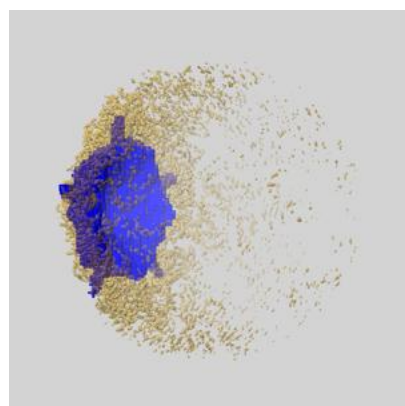
6.6 Mask visualisation [i](#)

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

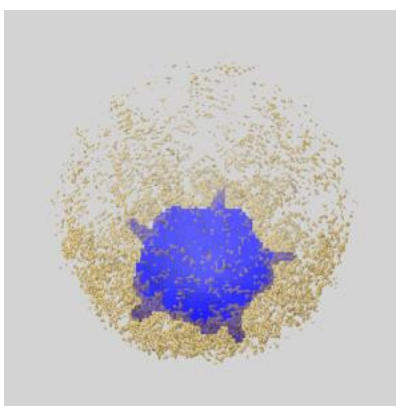
A mask typically either:

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

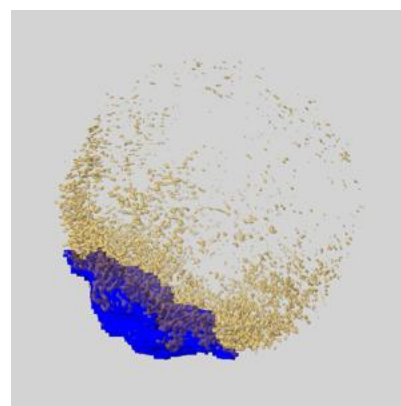
6.6.1 emd_50585_msk_1.map [i](#)



X



Y

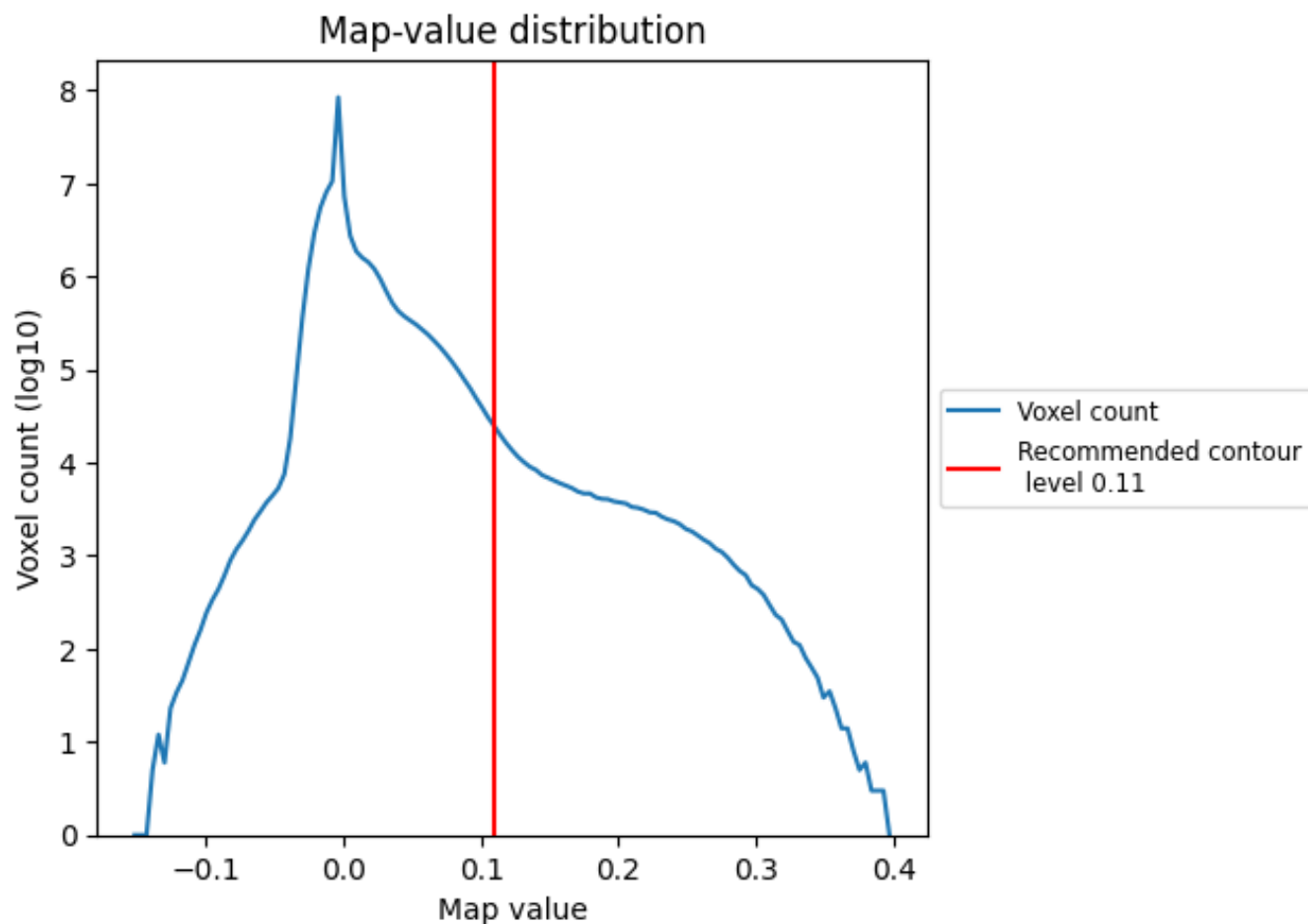


Z

7 Map analysis [i](#)

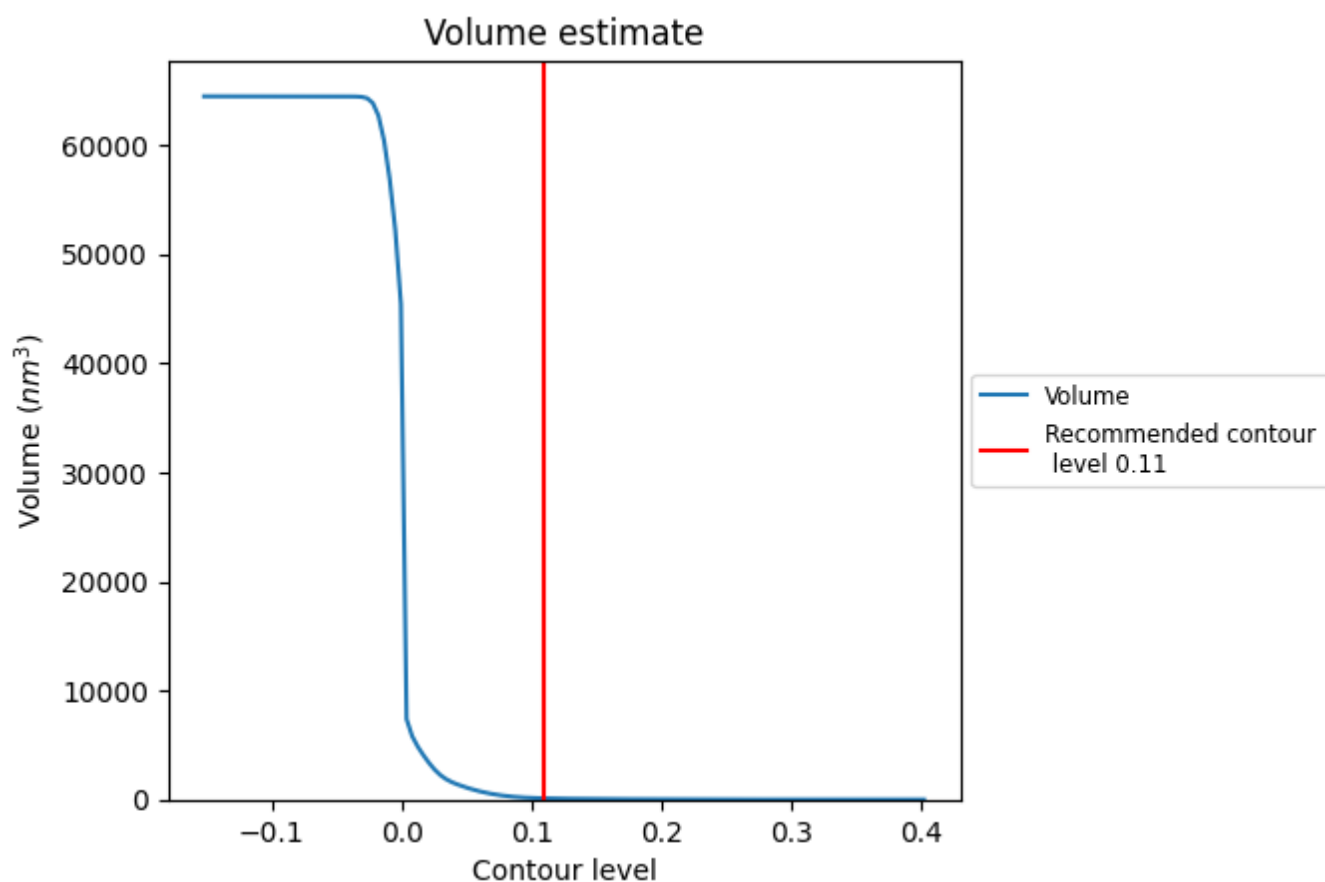
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

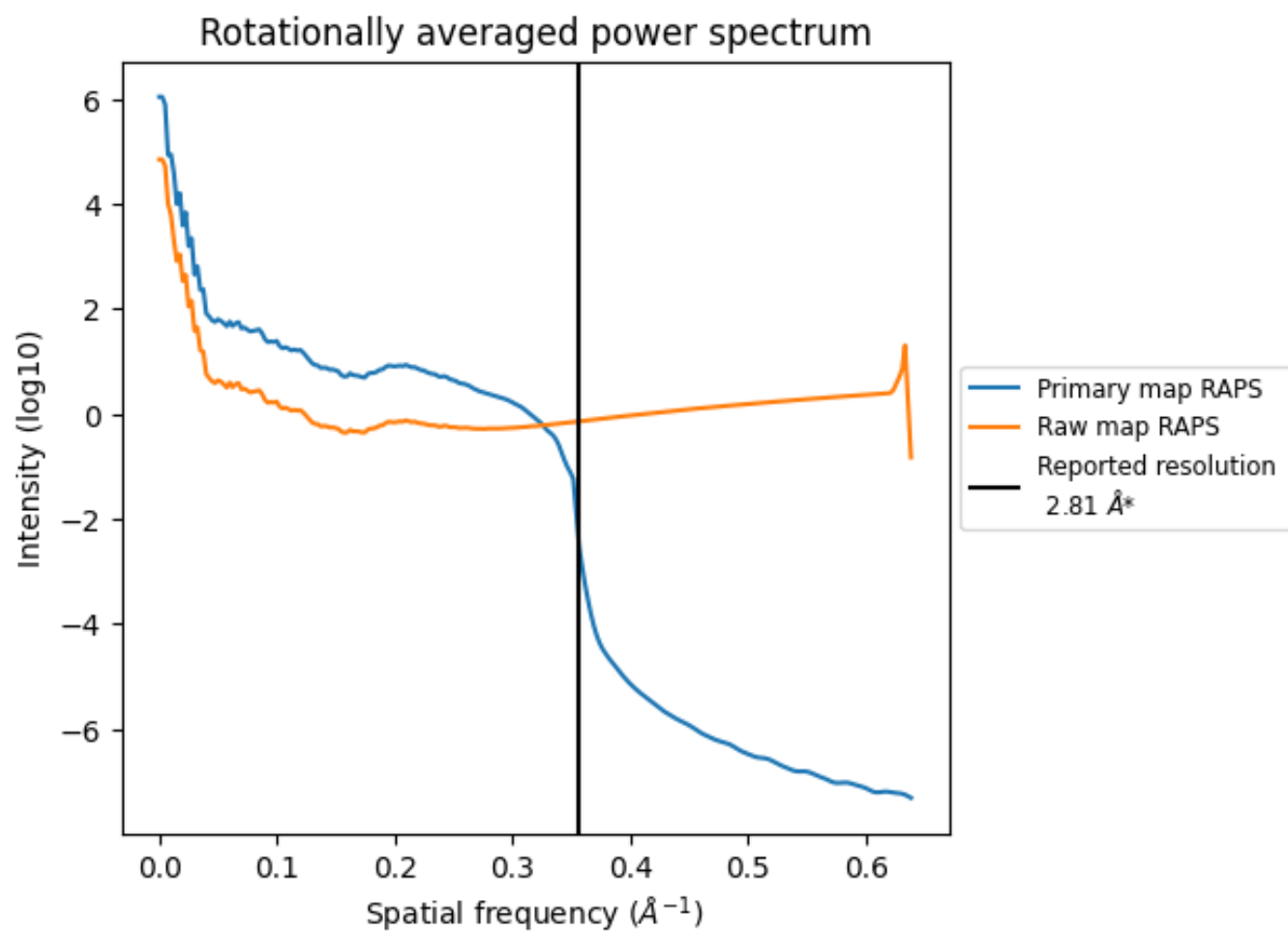
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm³; this corresponds to an approximate mass of 99 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 ⓘ

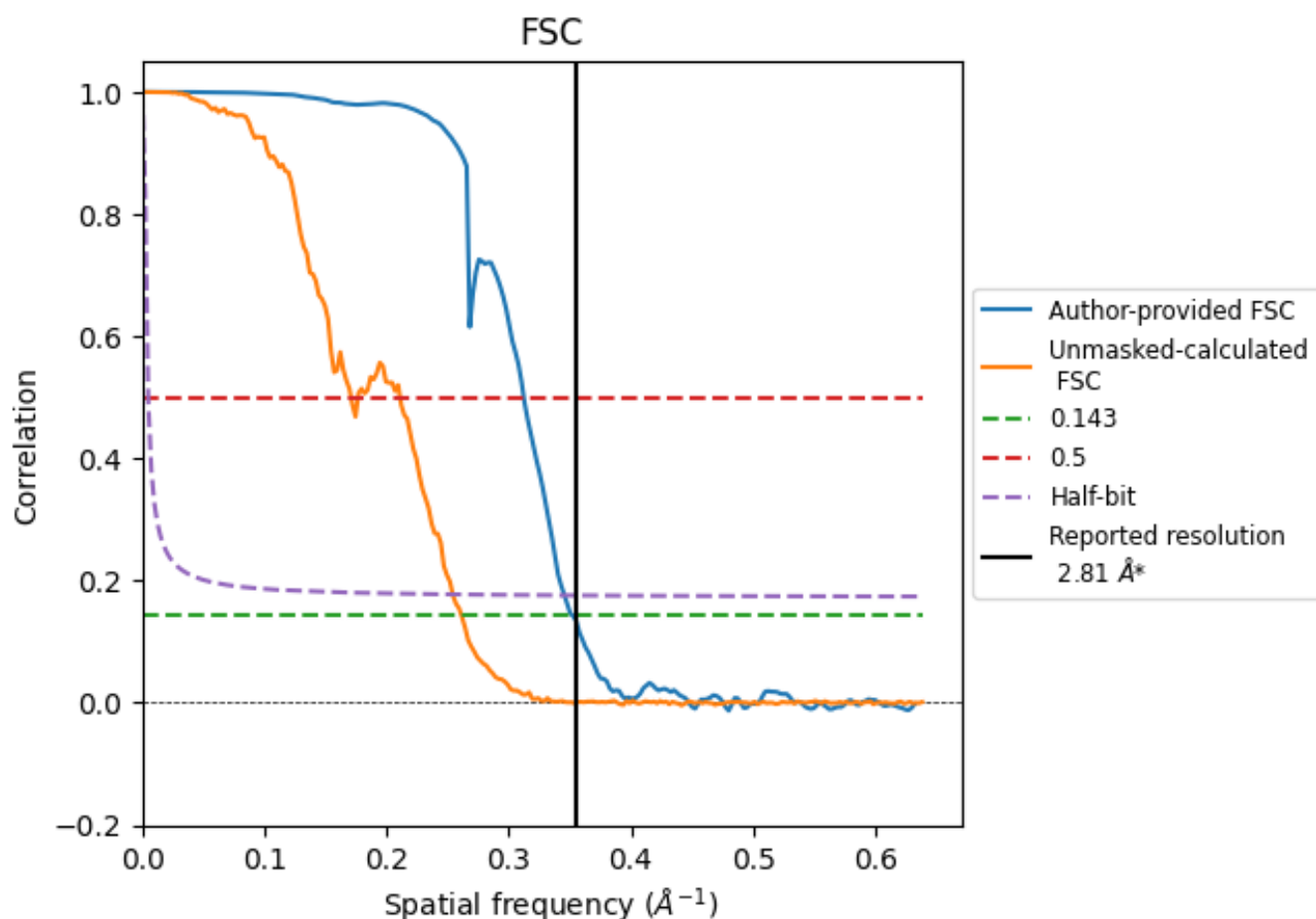


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.356 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

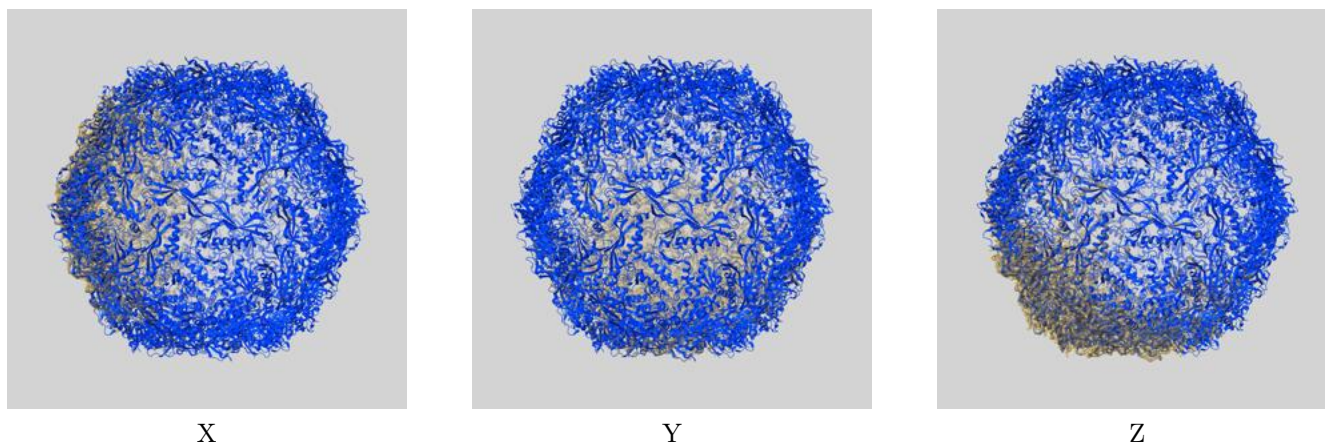
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.84	3.20	2.89
Unmasked-calculated*	3.83	5.85	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

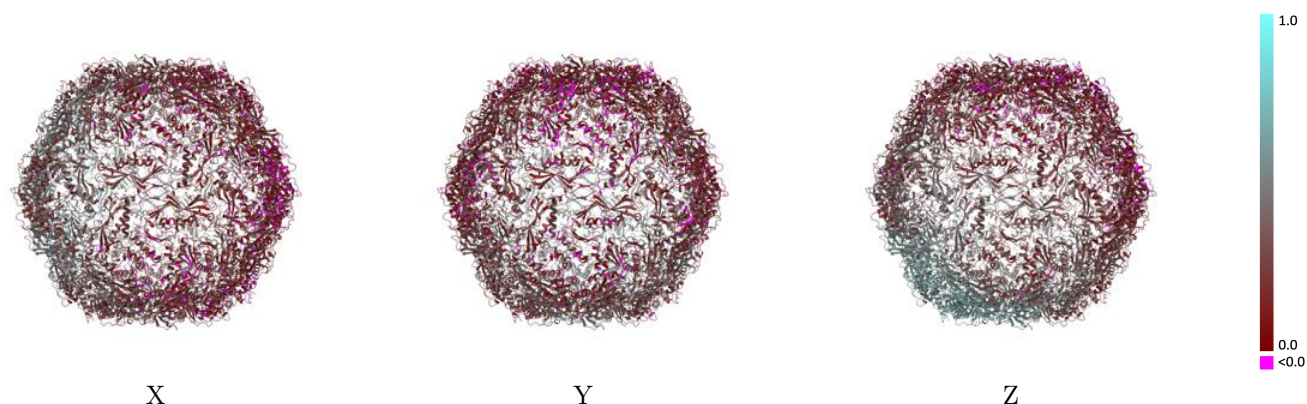
This section contains information regarding the fit between EMDB map EMD-50585 and PDB model 9FN9. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



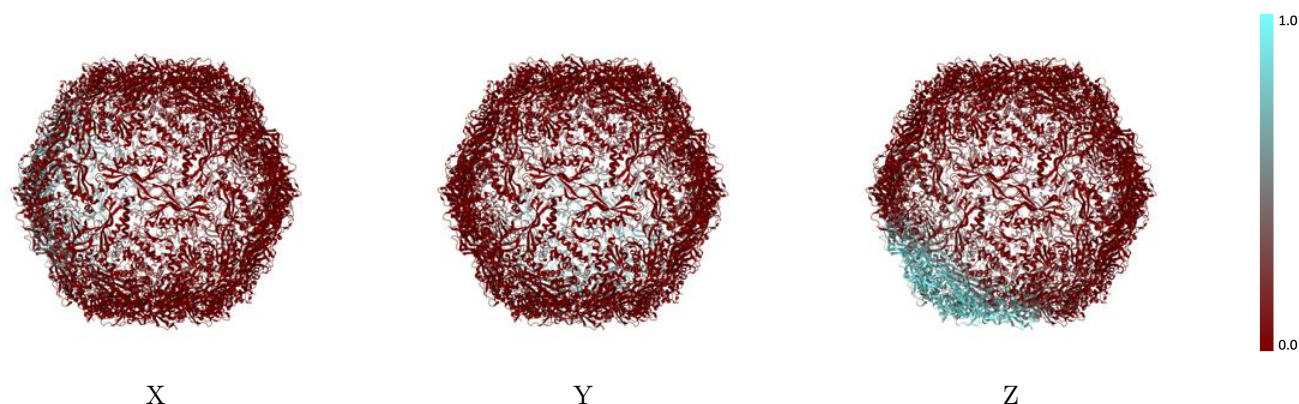
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



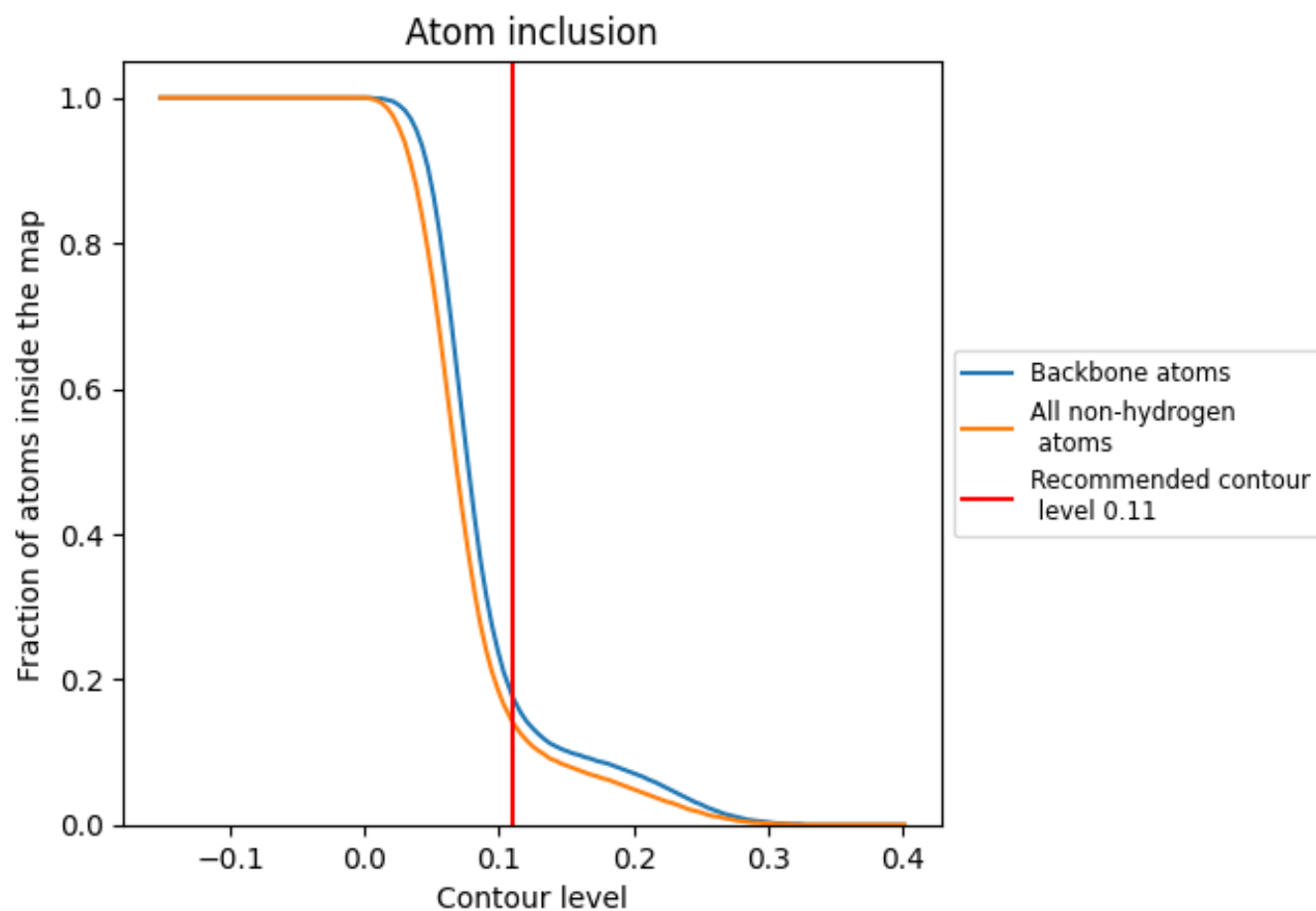
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 18% of all backbone atoms, 14% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1410	 0.3140
A	 0.8000	 0.5860
AA	 0.0080	 0.2570
AB	 0.0130	 0.3360
B	 0.0960	 0.3700
BA	 0.2780	 0.4320
BB	 0.0010	 0.1980
C	 0.0030	 0.2350
CA	 0.7780	 0.5770
CB	 0.0000	 0.1620
D	 0.0120	 0.2370
DA	 0.0900	 0.3830
DB	 0.0010	 0.2240
E	 0.2750	 0.4290
EA	 0.0020	 0.2330
EB	 0.0020	 0.1970
F	 0.0010	 0.1520
FA	 0.0000	 0.2190
FB	 0.0010	 0.1960
G	 0.0030	 0.2130
GA	 0.0530	 0.3360
GB	 0.0020	 0.2070
H	 0.0460	 0.3490
HA	 0.0140	 0.3170
HB	 0.0000	 0.2000
I	 0.0140	 0.3240
IA	 0.0010	 0.2030
IB	 0.0010	 0.1920
J	 0.0020	 0.2050
JA	 0.0010	 0.1570
K	 0.2780	 0.4180
KA	 0.0120	 0.3530
L	 0.7840	 0.5750
LA	 0.0010	 0.2060
M	 0.1020	 0.3810



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Chain	Atom inclusion	Q-score
MA	 0.0010	 0.1500
N	 0.0030	 0.2410
NA	 0.0010	 0.2100
O	 0.0110	 0.2570
OA	 0.0430	 0.3440
P	 0.0010	 0.2130
PA	 0.4640	 0.4550
Q	 0.0010	 0.1570
QA	 0.4540	 0.4500
R	 0.0000	 0.2250
RA	 0.4530	 0.4480
S	 0.0500	 0.3580
SA	 0.4520	 0.4410
T	 0.0100	 0.3330
TA	 0.4650	 0.4410
UA	 0.0020	 0.2240
V	 0.1010	 0.3720
VA	 0.0100	 0.2440
W	 0.0040	 0.2310
WA	 0.2780	 0.4170
X	 0.0090	 0.2580
XA	 0.7890	 0.5790
Y	 0.2700	 0.4320
YA	 0.1010	 0.3880
Z	 0.7900	 0.5750
ZA	 0.0470	 0.3570