



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:05 AM UTC

PDB ID : 9IVP / pdb_00009ivp
EMDB ID : EMD-60931
Title : 24-mer DARPin-apoferritin scaffold in complex with the maltose binding protein
Authors : Lu, X.; Yan, M.; Zhang, H.M.; Hao, Q.
Deposited on : 2024-07-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

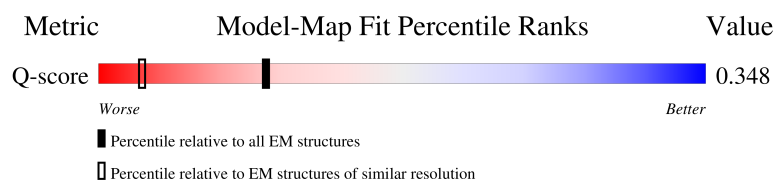
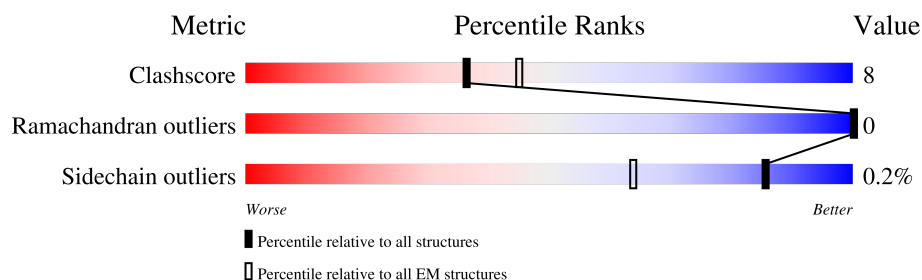
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



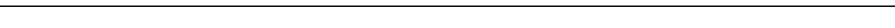
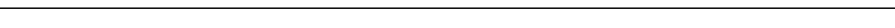
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	370	
1	BA	370	
1	C	370	
1	DA	370	

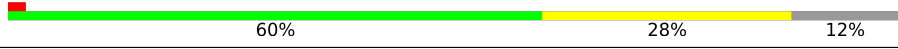
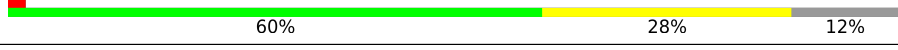
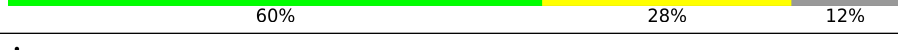
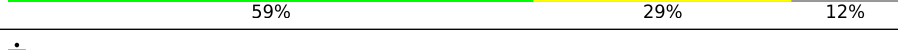
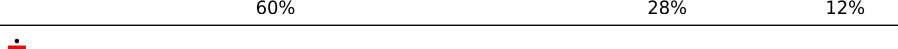
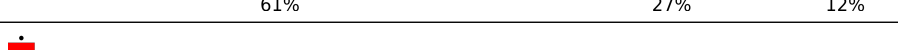
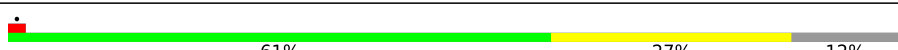
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Mol	Chain	Length	Quality of chain
1	E	370	
1	FA	370	
1	G	370	
1	HA	370	
1	I	370	
1	JA	370	
1	K	370	
1	LA	370	
1	M	370	
1	NA	370	
1	O	370	
1	PA	370	
1	Q	370	
1	RA	370	
1	S	370	
1	TA	370	
1	V	370	
1	VA	370	
1	X	370	
1	Z	370	
2	AA	416	
2	B	416	
2	CA	416	
2	D	416	
2	EA	416	

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Mol	Chain	Length	Quality of chain
2	F	416	
2	GA	416	
2	H	416	
2	IA	416	
2	J	416	
2	KA	416	
2	L	416	
2	MA	416	
2	N	416	
2	OA	416	
2	P	416	
2	QA	416	
2	R	416	
2	SA	416	
2	T	416	
2	UA	416	
2	W	416	
2	WA	416	
2	Y	416	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 128520 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 DARPin,Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	C	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	E	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	G	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	I	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	K	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	M	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	O	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	Q	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	S	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	V	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	X	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	Z	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	BA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	DA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	FA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	HA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	LA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	NA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	PA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	RA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	TA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		
1	VA	316	Total	C	N	O	S	0	0
			2485	1568	424	483	10		

There are 552 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ALA	ARG	conflict	UNP P02794
A	255	SER	PHE	conflict	UNP P02794
A	298	CYS	LYS	conflict	UNP P02794
A	351	SER	-	expression tag	UNP P02794
A	352	GLY	-	expression tag	UNP P02794
A	353	SER	-	expression tag	UNP P02794
A	354	GLY	-	expression tag	UNP P02794
A	355	ALA	-	expression tag	UNP P02794
A	356	GLU	-	expression tag	UNP P02794
A	357	ILE	-	expression tag	UNP P02794
A	358	GLU	-	expression tag	UNP P02794
A	359	GLN	-	expression tag	UNP P02794
A	360	ALA	-	expression tag	UNP P02794
A	361	LYS	-	expression tag	UNP P02794
A	362	LYS	-	expression tag	UNP P02794
A	363	GLU	-	expression tag	UNP P02794
A	364	ILE	-	expression tag	UNP P02794
A	365	ALA	-	expression tag	UNP P02794
A	366	TYR	-	expression tag	UNP P02794
A	367	LEU	-	expression tag	UNP P02794
A	368	ILE	-	expression tag	UNP P02794
A	369	LYS	-	expression tag	UNP P02794
A	370	LYS	-	expression tag	UNP P02794
C	253	ALA	ARG	conflict	UNP P02794
C	255	SER	PHE	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
C	298	CYS	LYS	conflict	UNP P02794
C	351	SER	-	expression tag	UNP P02794
C	352	GLY	-	expression tag	UNP P02794
C	353	SER	-	expression tag	UNP P02794
C	354	GLY	-	expression tag	UNP P02794
C	355	ALA	-	expression tag	UNP P02794
C	356	GLU	-	expression tag	UNP P02794
C	357	ILE	-	expression tag	UNP P02794
C	358	GLU	-	expression tag	UNP P02794
C	359	GLN	-	expression tag	UNP P02794
C	360	ALA	-	expression tag	UNP P02794
C	361	LYS	-	expression tag	UNP P02794
C	362	LYS	-	expression tag	UNP P02794
C	363	GLU	-	expression tag	UNP P02794
C	364	ILE	-	expression tag	UNP P02794
C	365	ALA	-	expression tag	UNP P02794
C	366	TYR	-	expression tag	UNP P02794
C	367	LEU	-	expression tag	UNP P02794
C	368	ILE	-	expression tag	UNP P02794
C	369	LYS	-	expression tag	UNP P02794
C	370	LYS	-	expression tag	UNP P02794
E	253	ALA	ARG	conflict	UNP P02794
E	255	SER	PHE	conflict	UNP P02794
E	298	CYS	LYS	conflict	UNP P02794
E	351	SER	-	expression tag	UNP P02794
E	352	GLY	-	expression tag	UNP P02794
E	353	SER	-	expression tag	UNP P02794
E	354	GLY	-	expression tag	UNP P02794
E	355	ALA	-	expression tag	UNP P02794
E	356	GLU	-	expression tag	UNP P02794
E	357	ILE	-	expression tag	UNP P02794
E	358	GLU	-	expression tag	UNP P02794
E	359	GLN	-	expression tag	UNP P02794
E	360	ALA	-	expression tag	UNP P02794
E	361	LYS	-	expression tag	UNP P02794
E	362	LYS	-	expression tag	UNP P02794
E	363	GLU	-	expression tag	UNP P02794
E	364	ILE	-	expression tag	UNP P02794
E	365	ALA	-	expression tag	UNP P02794
E	366	TYR	-	expression tag	UNP P02794
E	367	LEU	-	expression tag	UNP P02794
E	368	ILE	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
E	369	LYS	-	expression tag	UNP P02794
E	370	LYS	-	expression tag	UNP P02794
G	253	ALA	ARG	conflict	UNP P02794
G	255	SER	PHE	conflict	UNP P02794
G	298	CYS	LYS	conflict	UNP P02794
G	351	SER	-	expression tag	UNP P02794
G	352	GLY	-	expression tag	UNP P02794
G	353	SER	-	expression tag	UNP P02794
G	354	GLY	-	expression tag	UNP P02794
G	355	ALA	-	expression tag	UNP P02794
G	356	GLU	-	expression tag	UNP P02794
G	357	ILE	-	expression tag	UNP P02794
G	358	GLU	-	expression tag	UNP P02794
G	359	GLN	-	expression tag	UNP P02794
G	360	ALA	-	expression tag	UNP P02794
G	361	LYS	-	expression tag	UNP P02794
G	362	LYS	-	expression tag	UNP P02794
G	363	GLU	-	expression tag	UNP P02794
G	364	ILE	-	expression tag	UNP P02794
G	365	ALA	-	expression tag	UNP P02794
G	366	TYR	-	expression tag	UNP P02794
G	367	LEU	-	expression tag	UNP P02794
G	368	ILE	-	expression tag	UNP P02794
G	369	LYS	-	expression tag	UNP P02794
G	370	LYS	-	expression tag	UNP P02794
I	253	ALA	ARG	conflict	UNP P02794
I	255	SER	PHE	conflict	UNP P02794
I	298	CYS	LYS	conflict	UNP P02794
I	351	SER	-	expression tag	UNP P02794
I	352	GLY	-	expression tag	UNP P02794
I	353	SER	-	expression tag	UNP P02794
I	354	GLY	-	expression tag	UNP P02794
I	355	ALA	-	expression tag	UNP P02794
I	356	GLU	-	expression tag	UNP P02794
I	357	ILE	-	expression tag	UNP P02794
I	358	GLU	-	expression tag	UNP P02794
I	359	GLN	-	expression tag	UNP P02794
I	360	ALA	-	expression tag	UNP P02794
I	361	LYS	-	expression tag	UNP P02794
I	362	LYS	-	expression tag	UNP P02794
I	363	GLU	-	expression tag	UNP P02794
I	364	ILE	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
I	365	ALA	-	expression tag	UNP P02794
I	366	TYR	-	expression tag	UNP P02794
I	367	LEU	-	expression tag	UNP P02794
I	368	ILE	-	expression tag	UNP P02794
I	369	LYS	-	expression tag	UNP P02794
I	370	LYS	-	expression tag	UNP P02794
K	253	ALA	ARG	conflict	UNP P02794
K	255	SER	PHE	conflict	UNP P02794
K	298	CYS	LYS	conflict	UNP P02794
K	351	SER	-	expression tag	UNP P02794
K	352	GLY	-	expression tag	UNP P02794
K	353	SER	-	expression tag	UNP P02794
K	354	GLY	-	expression tag	UNP P02794
K	355	ALA	-	expression tag	UNP P02794
K	356	GLU	-	expression tag	UNP P02794
K	357	ILE	-	expression tag	UNP P02794
K	358	GLU	-	expression tag	UNP P02794
K	359	GLN	-	expression tag	UNP P02794
K	360	ALA	-	expression tag	UNP P02794
K	361	LYS	-	expression tag	UNP P02794
K	362	LYS	-	expression tag	UNP P02794
K	363	GLU	-	expression tag	UNP P02794
K	364	ILE	-	expression tag	UNP P02794
K	365	ALA	-	expression tag	UNP P02794
K	366	TYR	-	expression tag	UNP P02794
K	367	LEU	-	expression tag	UNP P02794
K	368	ILE	-	expression tag	UNP P02794
K	369	LYS	-	expression tag	UNP P02794
K	370	LYS	-	expression tag	UNP P02794
M	253	ALA	ARG	conflict	UNP P02794
M	255	SER	PHE	conflict	UNP P02794
M	298	CYS	LYS	conflict	UNP P02794
M	351	SER	-	expression tag	UNP P02794
M	352	GLY	-	expression tag	UNP P02794
M	353	SER	-	expression tag	UNP P02794
M	354	GLY	-	expression tag	UNP P02794
M	355	ALA	-	expression tag	UNP P02794
M	356	GLU	-	expression tag	UNP P02794
M	357	ILE	-	expression tag	UNP P02794
M	358	GLU	-	expression tag	UNP P02794
M	359	GLN	-	expression tag	UNP P02794
M	360	ALA	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
M	361	LYS	-	expression tag	UNP P02794
M	362	LYS	-	expression tag	UNP P02794
M	363	GLU	-	expression tag	UNP P02794
M	364	ILE	-	expression tag	UNP P02794
M	365	ALA	-	expression tag	UNP P02794
M	366	TYR	-	expression tag	UNP P02794
M	367	LEU	-	expression tag	UNP P02794
M	368	ILE	-	expression tag	UNP P02794
M	369	LYS	-	expression tag	UNP P02794
M	370	LYS	-	expression tag	UNP P02794
O	253	ALA	ARG	conflict	UNP P02794
O	255	SER	PHE	conflict	UNP P02794
O	298	CYS	LYS	conflict	UNP P02794
O	351	SER	-	expression tag	UNP P02794
O	352	GLY	-	expression tag	UNP P02794
O	353	SER	-	expression tag	UNP P02794
O	354	GLY	-	expression tag	UNP P02794
O	355	ALA	-	expression tag	UNP P02794
O	356	GLU	-	expression tag	UNP P02794
O	357	ILE	-	expression tag	UNP P02794
O	358	GLU	-	expression tag	UNP P02794
O	359	GLN	-	expression tag	UNP P02794
O	360	ALA	-	expression tag	UNP P02794
O	361	LYS	-	expression tag	UNP P02794
O	362	LYS	-	expression tag	UNP P02794
O	363	GLU	-	expression tag	UNP P02794
O	364	ILE	-	expression tag	UNP P02794
O	365	ALA	-	expression tag	UNP P02794
O	366	TYR	-	expression tag	UNP P02794
O	367	LEU	-	expression tag	UNP P02794
O	368	ILE	-	expression tag	UNP P02794
O	369	LYS	-	expression tag	UNP P02794
O	370	LYS	-	expression tag	UNP P02794
Q	253	ALA	ARG	conflict	UNP P02794
Q	255	SER	PHE	conflict	UNP P02794
Q	298	CYS	LYS	conflict	UNP P02794
Q	351	SER	-	expression tag	UNP P02794
Q	352	GLY	-	expression tag	UNP P02794
Q	353	SER	-	expression tag	UNP P02794
Q	354	GLY	-	expression tag	UNP P02794
Q	355	ALA	-	expression tag	UNP P02794
Q	356	GLU	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	357	ILE	-	expression tag	UNP P02794
Q	358	GLU	-	expression tag	UNP P02794
Q	359	GLN	-	expression tag	UNP P02794
Q	360	ALA	-	expression tag	UNP P02794
Q	361	LYS	-	expression tag	UNP P02794
Q	362	LYS	-	expression tag	UNP P02794
Q	363	GLU	-	expression tag	UNP P02794
Q	364	ILE	-	expression tag	UNP P02794
Q	365	ALA	-	expression tag	UNP P02794
Q	366	TYR	-	expression tag	UNP P02794
Q	367	LEU	-	expression tag	UNP P02794
Q	368	ILE	-	expression tag	UNP P02794
Q	369	LYS	-	expression tag	UNP P02794
Q	370	LYS	-	expression tag	UNP P02794
S	253	ALA	ARG	conflict	UNP P02794
S	255	SER	PHE	conflict	UNP P02794
S	298	CYS	LYS	conflict	UNP P02794
S	351	SER	-	expression tag	UNP P02794
S	352	GLY	-	expression tag	UNP P02794
S	353	SER	-	expression tag	UNP P02794
S	354	GLY	-	expression tag	UNP P02794
S	355	ALA	-	expression tag	UNP P02794
S	356	GLU	-	expression tag	UNP P02794
S	357	ILE	-	expression tag	UNP P02794
S	358	GLU	-	expression tag	UNP P02794
S	359	GLN	-	expression tag	UNP P02794
S	360	ALA	-	expression tag	UNP P02794
S	361	LYS	-	expression tag	UNP P02794
S	362	LYS	-	expression tag	UNP P02794
S	363	GLU	-	expression tag	UNP P02794
S	364	ILE	-	expression tag	UNP P02794
S	365	ALA	-	expression tag	UNP P02794
S	366	TYR	-	expression tag	UNP P02794
S	367	LEU	-	expression tag	UNP P02794
S	368	ILE	-	expression tag	UNP P02794
S	369	LYS	-	expression tag	UNP P02794
S	370	LYS	-	expression tag	UNP P02794
V	253	ALA	ARG	conflict	UNP P02794
V	255	SER	PHE	conflict	UNP P02794
V	298	CYS	LYS	conflict	UNP P02794
V	351	SER	-	expression tag	UNP P02794
V	352	GLY	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
V	353	SER	-	expression tag	UNP P02794
V	354	GLY	-	expression tag	UNP P02794
V	355	ALA	-	expression tag	UNP P02794
V	356	GLU	-	expression tag	UNP P02794
V	357	ILE	-	expression tag	UNP P02794
V	358	GLU	-	expression tag	UNP P02794
V	359	GLN	-	expression tag	UNP P02794
V	360	ALA	-	expression tag	UNP P02794
V	361	LYS	-	expression tag	UNP P02794
V	362	LYS	-	expression tag	UNP P02794
V	363	GLU	-	expression tag	UNP P02794
V	364	ILE	-	expression tag	UNP P02794
V	365	ALA	-	expression tag	UNP P02794
V	366	TYR	-	expression tag	UNP P02794
V	367	LEU	-	expression tag	UNP P02794
V	368	ILE	-	expression tag	UNP P02794
V	369	LYS	-	expression tag	UNP P02794
V	370	LYS	-	expression tag	UNP P02794
X	253	ALA	ARG	conflict	UNP P02794
X	255	SER	PHE	conflict	UNP P02794
X	298	CYS	LYS	conflict	UNP P02794
X	351	SER	-	expression tag	UNP P02794
X	352	GLY	-	expression tag	UNP P02794
X	353	SER	-	expression tag	UNP P02794
X	354	GLY	-	expression tag	UNP P02794
X	355	ALA	-	expression tag	UNP P02794
X	356	GLU	-	expression tag	UNP P02794
X	357	ILE	-	expression tag	UNP P02794
X	358	GLU	-	expression tag	UNP P02794
X	359	GLN	-	expression tag	UNP P02794
X	360	ALA	-	expression tag	UNP P02794
X	361	LYS	-	expression tag	UNP P02794
X	362	LYS	-	expression tag	UNP P02794
X	363	GLU	-	expression tag	UNP P02794
X	364	ILE	-	expression tag	UNP P02794
X	365	ALA	-	expression tag	UNP P02794
X	366	TYR	-	expression tag	UNP P02794
X	367	LEU	-	expression tag	UNP P02794
X	368	ILE	-	expression tag	UNP P02794
X	369	LYS	-	expression tag	UNP P02794
X	370	LYS	-	expression tag	UNP P02794
Z	253	ALA	ARG	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	255	SER	PHE	conflict	UNP P02794
Z	298	CYS	LYS	conflict	UNP P02794
Z	351	SER	-	expression tag	UNP P02794
Z	352	GLY	-	expression tag	UNP P02794
Z	353	SER	-	expression tag	UNP P02794
Z	354	GLY	-	expression tag	UNP P02794
Z	355	ALA	-	expression tag	UNP P02794
Z	356	GLU	-	expression tag	UNP P02794
Z	357	ILE	-	expression tag	UNP P02794
Z	358	GLU	-	expression tag	UNP P02794
Z	359	GLN	-	expression tag	UNP P02794
Z	360	ALA	-	expression tag	UNP P02794
Z	361	LYS	-	expression tag	UNP P02794
Z	362	LYS	-	expression tag	UNP P02794
Z	363	GLU	-	expression tag	UNP P02794
Z	364	ILE	-	expression tag	UNP P02794
Z	365	ALA	-	expression tag	UNP P02794
Z	366	TYR	-	expression tag	UNP P02794
Z	367	LEU	-	expression tag	UNP P02794
Z	368	ILE	-	expression tag	UNP P02794
Z	369	LYS	-	expression tag	UNP P02794
Z	370	LYS	-	expression tag	UNP P02794
BA	253	ALA	ARG	conflict	UNP P02794
BA	255	SER	PHE	conflict	UNP P02794
BA	298	CYS	LYS	conflict	UNP P02794
BA	351	SER	-	expression tag	UNP P02794
BA	352	GLY	-	expression tag	UNP P02794
BA	353	SER	-	expression tag	UNP P02794
BA	354	GLY	-	expression tag	UNP P02794
BA	355	ALA	-	expression tag	UNP P02794
BA	356	GLU	-	expression tag	UNP P02794
BA	357	ILE	-	expression tag	UNP P02794
BA	358	GLU	-	expression tag	UNP P02794
BA	359	GLN	-	expression tag	UNP P02794
BA	360	ALA	-	expression tag	UNP P02794
BA	361	LYS	-	expression tag	UNP P02794
BA	362	LYS	-	expression tag	UNP P02794
BA	363	GLU	-	expression tag	UNP P02794
BA	364	ILE	-	expression tag	UNP P02794
BA	365	ALA	-	expression tag	UNP P02794
BA	366	TYR	-	expression tag	UNP P02794
BA	367	LEU	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	368	ILE	-	expression tag	UNP P02794
BA	369	LYS	-	expression tag	UNP P02794
BA	370	LYS	-	expression tag	UNP P02794
DA	253	ALA	ARG	conflict	UNP P02794
DA	255	SER	PHE	conflict	UNP P02794
DA	298	CYS	LYS	conflict	UNP P02794
DA	351	SER	-	expression tag	UNP P02794
DA	352	GLY	-	expression tag	UNP P02794
DA	353	SER	-	expression tag	UNP P02794
DA	354	GLY	-	expression tag	UNP P02794
DA	355	ALA	-	expression tag	UNP P02794
DA	356	GLU	-	expression tag	UNP P02794
DA	357	ILE	-	expression tag	UNP P02794
DA	358	GLU	-	expression tag	UNP P02794
DA	359	GLN	-	expression tag	UNP P02794
DA	360	ALA	-	expression tag	UNP P02794
DA	361	LYS	-	expression tag	UNP P02794
DA	362	LYS	-	expression tag	UNP P02794
DA	363	GLU	-	expression tag	UNP P02794
DA	364	ILE	-	expression tag	UNP P02794
DA	365	ALA	-	expression tag	UNP P02794
DA	366	TYR	-	expression tag	UNP P02794
DA	367	LEU	-	expression tag	UNP P02794
DA	368	ILE	-	expression tag	UNP P02794
DA	369	LYS	-	expression tag	UNP P02794
DA	370	LYS	-	expression tag	UNP P02794
FA	253	ALA	ARG	conflict	UNP P02794
FA	255	SER	PHE	conflict	UNP P02794
FA	298	CYS	LYS	conflict	UNP P02794
FA	351	SER	-	expression tag	UNP P02794
FA	352	GLY	-	expression tag	UNP P02794
FA	353	SER	-	expression tag	UNP P02794
FA	354	GLY	-	expression tag	UNP P02794
FA	355	ALA	-	expression tag	UNP P02794
FA	356	GLU	-	expression tag	UNP P02794
FA	357	ILE	-	expression tag	UNP P02794
FA	358	GLU	-	expression tag	UNP P02794
FA	359	GLN	-	expression tag	UNP P02794
FA	360	ALA	-	expression tag	UNP P02794
FA	361	LYS	-	expression tag	UNP P02794
FA	362	LYS	-	expression tag	UNP P02794
FA	363	GLU	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
FA	364	ILE	-	expression tag	UNP P02794
FA	365	ALA	-	expression tag	UNP P02794
FA	366	TYR	-	expression tag	UNP P02794
FA	367	LEU	-	expression tag	UNP P02794
FA	368	ILE	-	expression tag	UNP P02794
FA	369	LYS	-	expression tag	UNP P02794
FA	370	LYS	-	expression tag	UNP P02794
HA	253	ALA	ARG	conflict	UNP P02794
HA	255	SER	PHE	conflict	UNP P02794
HA	298	CYS	LYS	conflict	UNP P02794
HA	351	SER	-	expression tag	UNP P02794
HA	352	GLY	-	expression tag	UNP P02794
HA	353	SER	-	expression tag	UNP P02794
HA	354	GLY	-	expression tag	UNP P02794
HA	355	ALA	-	expression tag	UNP P02794
HA	356	GLU	-	expression tag	UNP P02794
HA	357	ILE	-	expression tag	UNP P02794
HA	358	GLU	-	expression tag	UNP P02794
HA	359	GLN	-	expression tag	UNP P02794
HA	360	ALA	-	expression tag	UNP P02794
HA	361	LYS	-	expression tag	UNP P02794
HA	362	LYS	-	expression tag	UNP P02794
HA	363	GLU	-	expression tag	UNP P02794
HA	364	ILE	-	expression tag	UNP P02794
HA	365	ALA	-	expression tag	UNP P02794
HA	366	TYR	-	expression tag	UNP P02794
HA	367	LEU	-	expression tag	UNP P02794
HA	368	ILE	-	expression tag	UNP P02794
HA	369	LYS	-	expression tag	UNP P02794
HA	370	LYS	-	expression tag	UNP P02794
JA	253	ALA	ARG	conflict	UNP P02794
JA	255	SER	PHE	conflict	UNP P02794
JA	298	CYS	LYS	conflict	UNP P02794
JA	351	SER	-	expression tag	UNP P02794
JA	352	GLY	-	expression tag	UNP P02794
JA	353	SER	-	expression tag	UNP P02794
JA	354	GLY	-	expression tag	UNP P02794
JA	355	ALA	-	expression tag	UNP P02794
JA	356	GLU	-	expression tag	UNP P02794
JA	357	ILE	-	expression tag	UNP P02794
JA	358	GLU	-	expression tag	UNP P02794
JA	359	GLN	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
JA	360	ALA	-	expression tag	UNP P02794
JA	361	LYS	-	expression tag	UNP P02794
JA	362	LYS	-	expression tag	UNP P02794
JA	363	GLU	-	expression tag	UNP P02794
JA	364	ILE	-	expression tag	UNP P02794
JA	365	ALA	-	expression tag	UNP P02794
JA	366	TYR	-	expression tag	UNP P02794
JA	367	LEU	-	expression tag	UNP P02794
JA	368	ILE	-	expression tag	UNP P02794
JA	369	LYS	-	expression tag	UNP P02794
JA	370	LYS	-	expression tag	UNP P02794
LA	253	ALA	ARG	conflict	UNP P02794
LA	255	SER	PHE	conflict	UNP P02794
LA	298	CYS	LYS	conflict	UNP P02794
LA	351	SER	-	expression tag	UNP P02794
LA	352	GLY	-	expression tag	UNP P02794
LA	353	SER	-	expression tag	UNP P02794
LA	354	GLY	-	expression tag	UNP P02794
LA	355	ALA	-	expression tag	UNP P02794
LA	356	GLU	-	expression tag	UNP P02794
LA	357	ILE	-	expression tag	UNP P02794
LA	358	GLU	-	expression tag	UNP P02794
LA	359	GLN	-	expression tag	UNP P02794
LA	360	ALA	-	expression tag	UNP P02794
LA	361	LYS	-	expression tag	UNP P02794
LA	362	LYS	-	expression tag	UNP P02794
LA	363	GLU	-	expression tag	UNP P02794
LA	364	ILE	-	expression tag	UNP P02794
LA	365	ALA	-	expression tag	UNP P02794
LA	366	TYR	-	expression tag	UNP P02794
LA	367	LEU	-	expression tag	UNP P02794
LA	368	ILE	-	expression tag	UNP P02794
LA	369	LYS	-	expression tag	UNP P02794
LA	370	LYS	-	expression tag	UNP P02794
NA	253	ALA	ARG	conflict	UNP P02794
NA	255	SER	PHE	conflict	UNP P02794
NA	298	CYS	LYS	conflict	UNP P02794
NA	351	SER	-	expression tag	UNP P02794
NA	352	GLY	-	expression tag	UNP P02794
NA	353	SER	-	expression tag	UNP P02794
NA	354	GLY	-	expression tag	UNP P02794
NA	355	ALA	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
NA	356	GLU	-	expression tag	UNP P02794
NA	357	ILE	-	expression tag	UNP P02794
NA	358	GLU	-	expression tag	UNP P02794
NA	359	GLN	-	expression tag	UNP P02794
NA	360	ALA	-	expression tag	UNP P02794
NA	361	LYS	-	expression tag	UNP P02794
NA	362	LYS	-	expression tag	UNP P02794
NA	363	GLU	-	expression tag	UNP P02794
NA	364	ILE	-	expression tag	UNP P02794
NA	365	ALA	-	expression tag	UNP P02794
NA	366	TYR	-	expression tag	UNP P02794
NA	367	LEU	-	expression tag	UNP P02794
NA	368	ILE	-	expression tag	UNP P02794
NA	369	LYS	-	expression tag	UNP P02794
NA	370	LYS	-	expression tag	UNP P02794
PA	253	ALA	ARG	conflict	UNP P02794
PA	255	SER	PHE	conflict	UNP P02794
PA	298	CYS	LYS	conflict	UNP P02794
PA	351	SER	-	expression tag	UNP P02794
PA	352	GLY	-	expression tag	UNP P02794
PA	353	SER	-	expression tag	UNP P02794
PA	354	GLY	-	expression tag	UNP P02794
PA	355	ALA	-	expression tag	UNP P02794
PA	356	GLU	-	expression tag	UNP P02794
PA	357	ILE	-	expression tag	UNP P02794
PA	358	GLU	-	expression tag	UNP P02794
PA	359	GLN	-	expression tag	UNP P02794
PA	360	ALA	-	expression tag	UNP P02794
PA	361	LYS	-	expression tag	UNP P02794
PA	362	LYS	-	expression tag	UNP P02794
PA	363	GLU	-	expression tag	UNP P02794
PA	364	ILE	-	expression tag	UNP P02794
PA	365	ALA	-	expression tag	UNP P02794
PA	366	TYR	-	expression tag	UNP P02794
PA	367	LEU	-	expression tag	UNP P02794
PA	368	ILE	-	expression tag	UNP P02794
PA	369	LYS	-	expression tag	UNP P02794
PA	370	LYS	-	expression tag	UNP P02794
RA	253	ALA	ARG	conflict	UNP P02794
RA	255	SER	PHE	conflict	UNP P02794
RA	298	CYS	LYS	conflict	UNP P02794
RA	351	SER	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
RA	352	GLY	-	expression tag	UNP P02794
RA	353	SER	-	expression tag	UNP P02794
RA	354	GLY	-	expression tag	UNP P02794
RA	355	ALA	-	expression tag	UNP P02794
RA	356	GLU	-	expression tag	UNP P02794
RA	357	ILE	-	expression tag	UNP P02794
RA	358	GLU	-	expression tag	UNP P02794
RA	359	GLN	-	expression tag	UNP P02794
RA	360	ALA	-	expression tag	UNP P02794
RA	361	LYS	-	expression tag	UNP P02794
RA	362	LYS	-	expression tag	UNP P02794
RA	363	GLU	-	expression tag	UNP P02794
RA	364	ILE	-	expression tag	UNP P02794
RA	365	ALA	-	expression tag	UNP P02794
RA	366	TYR	-	expression tag	UNP P02794
RA	367	LEU	-	expression tag	UNP P02794
RA	368	ILE	-	expression tag	UNP P02794
RA	369	LYS	-	expression tag	UNP P02794
RA	370	LYS	-	expression tag	UNP P02794
TA	253	ALA	ARG	conflict	UNP P02794
TA	255	SER	PHE	conflict	UNP P02794
TA	298	CYS	LYS	conflict	UNP P02794
TA	351	SER	-	expression tag	UNP P02794
TA	352	GLY	-	expression tag	UNP P02794
TA	353	SER	-	expression tag	UNP P02794
TA	354	GLY	-	expression tag	UNP P02794
TA	355	ALA	-	expression tag	UNP P02794
TA	356	GLU	-	expression tag	UNP P02794
TA	357	ILE	-	expression tag	UNP P02794
TA	358	GLU	-	expression tag	UNP P02794
TA	359	GLN	-	expression tag	UNP P02794
TA	360	ALA	-	expression tag	UNP P02794
TA	361	LYS	-	expression tag	UNP P02794
TA	362	LYS	-	expression tag	UNP P02794
TA	363	GLU	-	expression tag	UNP P02794
TA	364	ILE	-	expression tag	UNP P02794
TA	365	ALA	-	expression tag	UNP P02794
TA	366	TYR	-	expression tag	UNP P02794
TA	367	LEU	-	expression tag	UNP P02794
TA	368	ILE	-	expression tag	UNP P02794
TA	369	LYS	-	expression tag	UNP P02794
TA	370	LYS	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
VA	253	ALA	ARG	conflict	UNP P02794
VA	255	SER	PHE	conflict	UNP P02794
VA	298	CYS	LYS	conflict	UNP P02794
VA	351	SER	-	expression tag	UNP P02794
VA	352	GLY	-	expression tag	UNP P02794
VA	353	SER	-	expression tag	UNP P02794
VA	354	GLY	-	expression tag	UNP P02794
VA	355	ALA	-	expression tag	UNP P02794
VA	356	GLU	-	expression tag	UNP P02794
VA	357	ILE	-	expression tag	UNP P02794
VA	358	GLU	-	expression tag	UNP P02794
VA	359	GLN	-	expression tag	UNP P02794
VA	360	ALA	-	expression tag	UNP P02794
VA	361	LYS	-	expression tag	UNP P02794
VA	362	LYS	-	expression tag	UNP P02794
VA	363	GLU	-	expression tag	UNP P02794
VA	364	ILE	-	expression tag	UNP P02794
VA	365	ALA	-	expression tag	UNP P02794
VA	366	TYR	-	expression tag	UNP P02794
VA	367	LEU	-	expression tag	UNP P02794
VA	368	ILE	-	expression tag	UNP P02794
VA	369	LYS	-	expression tag	UNP P02794
VA	370	LYS	-	expression tag	UNP P02794

- Molecule 2 is a protein called Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	D	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	F	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	H	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	J	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	L	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	N	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	P	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	T	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	W	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	Y	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	AA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	CA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	EA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	GA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	IA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	KA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	MA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	OA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	QA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	SA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	UA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		
2	WA	366	Total	C	N	O	S	6	0
			2870	1850	461	552	7		

There are 1200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP C3SHQ8
B	2	GLY	-	expression tag	UNP C3SHQ8
B	3	SER	-	expression tag	UNP C3SHQ8
B	4	SER	-	expression tag	UNP C3SHQ8
B	5	HIS	-	expression tag	UNP C3SHQ8
B	6	HIS	-	expression tag	UNP C3SHQ8
B	7	HIS	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	HIS	-	expression tag	UNP C3SHQ8
B	9	HIS	-	expression tag	UNP C3SHQ8
B	10	HIS	-	expression tag	UNP C3SHQ8
B	11	SER	-	expression tag	UNP C3SHQ8
B	12	SER	-	expression tag	UNP C3SHQ8
B	13	GLY	-	expression tag	UNP C3SHQ8
B	14	LEU	-	expression tag	UNP C3SHQ8
B	15	VAL	-	expression tag	UNP C3SHQ8
B	16	PRO	-	expression tag	UNP C3SHQ8
B	17	ARG	-	expression tag	UNP C3SHQ8
B	18	GLY	-	expression tag	UNP C3SHQ8
B	19	SER	-	expression tag	UNP C3SHQ8
B	20	HIS	-	expression tag	UNP C3SHQ8
B	21	MET	-	expression tag	UNP C3SHQ8
B	388	ASN	-	expression tag	UNP C3SHQ8
B	389	SER	-	expression tag	UNP C3SHQ8
B	390	SER	-	expression tag	UNP C3SHQ8
B	391	SER	-	expression tag	UNP C3SHQ8
B	392	ASN	-	expression tag	UNP C3SHQ8
B	393	ASN	-	expression tag	UNP C3SHQ8
B	394	ASN	-	expression tag	UNP C3SHQ8
B	395	ASN	-	expression tag	UNP C3SHQ8
B	396	ASN	-	expression tag	UNP C3SHQ8
B	397	ASN	-	expression tag	UNP C3SHQ8
B	398	ASN	-	expression tag	UNP C3SHQ8
B	399	ASN	-	expression tag	UNP C3SHQ8
B	400	ASN	-	expression tag	UNP C3SHQ8
B	401	ASN	-	expression tag	UNP C3SHQ8
B	402	LEU	-	expression tag	UNP C3SHQ8
B	403	GLY	-	expression tag	UNP C3SHQ8
B	404	ILE	-	expression tag	UNP C3SHQ8
B	405	GLU	-	expression tag	UNP C3SHQ8
B	406	GLY	-	expression tag	UNP C3SHQ8
B	407	ARG	-	expression tag	UNP C3SHQ8
B	408	GLU	-	expression tag	UNP C3SHQ8
B	409	ASN	-	expression tag	UNP C3SHQ8
B	410	LEU	-	expression tag	UNP C3SHQ8
B	411	TYR	-	expression tag	UNP C3SHQ8
B	412	PHE	-	expression tag	UNP C3SHQ8
B	413	GLN	-	expression tag	UNP C3SHQ8
B	414	GLY	-	expression tag	UNP C3SHQ8
B	415	GLY	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	416	SER	-	expression tag	UNP C3SHQ8
D	1	MET	-	initiating methionine	UNP C3SHQ8
D	2	GLY	-	expression tag	UNP C3SHQ8
D	3	SER	-	expression tag	UNP C3SHQ8
D	4	SER	-	expression tag	UNP C3SHQ8
D	5	HIS	-	expression tag	UNP C3SHQ8
D	6	HIS	-	expression tag	UNP C3SHQ8
D	7	HIS	-	expression tag	UNP C3SHQ8
D	8	HIS	-	expression tag	UNP C3SHQ8
D	9	HIS	-	expression tag	UNP C3SHQ8
D	10	HIS	-	expression tag	UNP C3SHQ8
D	11	SER	-	expression tag	UNP C3SHQ8
D	12	SER	-	expression tag	UNP C3SHQ8
D	13	GLY	-	expression tag	UNP C3SHQ8
D	14	LEU	-	expression tag	UNP C3SHQ8
D	15	VAL	-	expression tag	UNP C3SHQ8
D	16	PRO	-	expression tag	UNP C3SHQ8
D	17	ARG	-	expression tag	UNP C3SHQ8
D	18	GLY	-	expression tag	UNP C3SHQ8
D	19	SER	-	expression tag	UNP C3SHQ8
D	20	HIS	-	expression tag	UNP C3SHQ8
D	21	MET	-	expression tag	UNP C3SHQ8
D	388	ASN	-	expression tag	UNP C3SHQ8
D	389	SER	-	expression tag	UNP C3SHQ8
D	390	SER	-	expression tag	UNP C3SHQ8
D	391	SER	-	expression tag	UNP C3SHQ8
D	392	ASN	-	expression tag	UNP C3SHQ8
D	393	ASN	-	expression tag	UNP C3SHQ8
D	394	ASN	-	expression tag	UNP C3SHQ8
D	395	ASN	-	expression tag	UNP C3SHQ8
D	396	ASN	-	expression tag	UNP C3SHQ8
D	397	ASN	-	expression tag	UNP C3SHQ8
D	398	ASN	-	expression tag	UNP C3SHQ8
D	399	ASN	-	expression tag	UNP C3SHQ8
D	400	ASN	-	expression tag	UNP C3SHQ8
D	401	ASN	-	expression tag	UNP C3SHQ8
D	402	LEU	-	expression tag	UNP C3SHQ8
D	403	GLY	-	expression tag	UNP C3SHQ8
D	404	ILE	-	expression tag	UNP C3SHQ8
D	405	GLU	-	expression tag	UNP C3SHQ8
D	406	GLY	-	expression tag	UNP C3SHQ8
D	407	ARG	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	408	GLU	-	expression tag	UNP C3SHQ8
D	409	ASN	-	expression tag	UNP C3SHQ8
D	410	LEU	-	expression tag	UNP C3SHQ8
D	411	TYR	-	expression tag	UNP C3SHQ8
D	412	PHE	-	expression tag	UNP C3SHQ8
D	413	GLN	-	expression tag	UNP C3SHQ8
D	414	GLY	-	expression tag	UNP C3SHQ8
D	415	GLY	-	expression tag	UNP C3SHQ8
D	416	SER	-	expression tag	UNP C3SHQ8
F	1	MET	-	initiating methionine	UNP C3SHQ8
F	2	GLY	-	expression tag	UNP C3SHQ8
F	3	SER	-	expression tag	UNP C3SHQ8
F	4	SER	-	expression tag	UNP C3SHQ8
F	5	HIS	-	expression tag	UNP C3SHQ8
F	6	HIS	-	expression tag	UNP C3SHQ8
F	7	HIS	-	expression tag	UNP C3SHQ8
F	8	HIS	-	expression tag	UNP C3SHQ8
F	9	HIS	-	expression tag	UNP C3SHQ8
F	10	HIS	-	expression tag	UNP C3SHQ8
F	11	SER	-	expression tag	UNP C3SHQ8
F	12	SER	-	expression tag	UNP C3SHQ8
F	13	GLY	-	expression tag	UNP C3SHQ8
F	14	LEU	-	expression tag	UNP C3SHQ8
F	15	VAL	-	expression tag	UNP C3SHQ8
F	16	PRO	-	expression tag	UNP C3SHQ8
F	17	ARG	-	expression tag	UNP C3SHQ8
F	18	GLY	-	expression tag	UNP C3SHQ8
F	19	SER	-	expression tag	UNP C3SHQ8
F	20	HIS	-	expression tag	UNP C3SHQ8
F	21	MET	-	expression tag	UNP C3SHQ8
F	388	ASN	-	expression tag	UNP C3SHQ8
F	389	SER	-	expression tag	UNP C3SHQ8
F	390	SER	-	expression tag	UNP C3SHQ8
F	391	SER	-	expression tag	UNP C3SHQ8
F	392	ASN	-	expression tag	UNP C3SHQ8
F	393	ASN	-	expression tag	UNP C3SHQ8
F	394	ASN	-	expression tag	UNP C3SHQ8
F	395	ASN	-	expression tag	UNP C3SHQ8
F	396	ASN	-	expression tag	UNP C3SHQ8
F	397	ASN	-	expression tag	UNP C3SHQ8
F	398	ASN	-	expression tag	UNP C3SHQ8
F	399	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	400	ASN	-	expression tag	UNP C3SHQ8
F	401	ASN	-	expression tag	UNP C3SHQ8
F	402	LEU	-	expression tag	UNP C3SHQ8
F	403	GLY	-	expression tag	UNP C3SHQ8
F	404	ILE	-	expression tag	UNP C3SHQ8
F	405	GLU	-	expression tag	UNP C3SHQ8
F	406	GLY	-	expression tag	UNP C3SHQ8
F	407	ARG	-	expression tag	UNP C3SHQ8
F	408	GLU	-	expression tag	UNP C3SHQ8
F	409	ASN	-	expression tag	UNP C3SHQ8
F	410	LEU	-	expression tag	UNP C3SHQ8
F	411	TYR	-	expression tag	UNP C3SHQ8
F	412	PHE	-	expression tag	UNP C3SHQ8
F	413	GLN	-	expression tag	UNP C3SHQ8
F	414	GLY	-	expression tag	UNP C3SHQ8
F	415	GLY	-	expression tag	UNP C3SHQ8
F	416	SER	-	expression tag	UNP C3SHQ8
H	1	MET	-	initiating methionine	UNP C3SHQ8
H	2	GLY	-	expression tag	UNP C3SHQ8
H	3	SER	-	expression tag	UNP C3SHQ8
H	4	SER	-	expression tag	UNP C3SHQ8
H	5	HIS	-	expression tag	UNP C3SHQ8
H	6	HIS	-	expression tag	UNP C3SHQ8
H	7	HIS	-	expression tag	UNP C3SHQ8
H	8	HIS	-	expression tag	UNP C3SHQ8
H	9	HIS	-	expression tag	UNP C3SHQ8
H	10	HIS	-	expression tag	UNP C3SHQ8
H	11	SER	-	expression tag	UNP C3SHQ8
H	12	SER	-	expression tag	UNP C3SHQ8
H	13	GLY	-	expression tag	UNP C3SHQ8
H	14	LEU	-	expression tag	UNP C3SHQ8
H	15	VAL	-	expression tag	UNP C3SHQ8
H	16	PRO	-	expression tag	UNP C3SHQ8
H	17	ARG	-	expression tag	UNP C3SHQ8
H	18	GLY	-	expression tag	UNP C3SHQ8
H	19	SER	-	expression tag	UNP C3SHQ8
H	20	HIS	-	expression tag	UNP C3SHQ8
H	21	MET	-	expression tag	UNP C3SHQ8
H	388	ASN	-	expression tag	UNP C3SHQ8
H	389	SER	-	expression tag	UNP C3SHQ8
H	390	SER	-	expression tag	UNP C3SHQ8
H	391	SER	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	392	ASN	-	expression tag	UNP C3SHQ8
H	393	ASN	-	expression tag	UNP C3SHQ8
H	394	ASN	-	expression tag	UNP C3SHQ8
H	395	ASN	-	expression tag	UNP C3SHQ8
H	396	ASN	-	expression tag	UNP C3SHQ8
H	397	ASN	-	expression tag	UNP C3SHQ8
H	398	ASN	-	expression tag	UNP C3SHQ8
H	399	ASN	-	expression tag	UNP C3SHQ8
H	400	ASN	-	expression tag	UNP C3SHQ8
H	401	ASN	-	expression tag	UNP C3SHQ8
H	402	LEU	-	expression tag	UNP C3SHQ8
H	403	GLY	-	expression tag	UNP C3SHQ8
H	404	ILE	-	expression tag	UNP C3SHQ8
H	405	GLU	-	expression tag	UNP C3SHQ8
H	406	GLY	-	expression tag	UNP C3SHQ8
H	407	ARG	-	expression tag	UNP C3SHQ8
H	408	GLU	-	expression tag	UNP C3SHQ8
H	409	ASN	-	expression tag	UNP C3SHQ8
H	410	LEU	-	expression tag	UNP C3SHQ8
H	411	TYR	-	expression tag	UNP C3SHQ8
H	412	PHE	-	expression tag	UNP C3SHQ8
H	413	GLN	-	expression tag	UNP C3SHQ8
H	414	GLY	-	expression tag	UNP C3SHQ8
H	415	GLY	-	expression tag	UNP C3SHQ8
H	416	SER	-	expression tag	UNP C3SHQ8
J	1	MET	-	initiating methionine	UNP C3SHQ8
J	2	GLY	-	expression tag	UNP C3SHQ8
J	3	SER	-	expression tag	UNP C3SHQ8
J	4	SER	-	expression tag	UNP C3SHQ8
J	5	HIS	-	expression tag	UNP C3SHQ8
J	6	HIS	-	expression tag	UNP C3SHQ8
J	7	HIS	-	expression tag	UNP C3SHQ8
J	8	HIS	-	expression tag	UNP C3SHQ8
J	9	HIS	-	expression tag	UNP C3SHQ8
J	10	HIS	-	expression tag	UNP C3SHQ8
J	11	SER	-	expression tag	UNP C3SHQ8
J	12	SER	-	expression tag	UNP C3SHQ8
J	13	GLY	-	expression tag	UNP C3SHQ8
J	14	LEU	-	expression tag	UNP C3SHQ8
J	15	VAL	-	expression tag	UNP C3SHQ8
J	16	PRO	-	expression tag	UNP C3SHQ8
J	17	ARG	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	18	GLY	-	expression tag	UNP C3SHQ8
J	19	SER	-	expression tag	UNP C3SHQ8
J	20	HIS	-	expression tag	UNP C3SHQ8
J	21	MET	-	expression tag	UNP C3SHQ8
J	388	ASN	-	expression tag	UNP C3SHQ8
J	389	SER	-	expression tag	UNP C3SHQ8
J	390	SER	-	expression tag	UNP C3SHQ8
J	391	SER	-	expression tag	UNP C3SHQ8
J	392	ASN	-	expression tag	UNP C3SHQ8
J	393	ASN	-	expression tag	UNP C3SHQ8
J	394	ASN	-	expression tag	UNP C3SHQ8
J	395	ASN	-	expression tag	UNP C3SHQ8
J	396	ASN	-	expression tag	UNP C3SHQ8
J	397	ASN	-	expression tag	UNP C3SHQ8
J	398	ASN	-	expression tag	UNP C3SHQ8
J	399	ASN	-	expression tag	UNP C3SHQ8
J	400	ASN	-	expression tag	UNP C3SHQ8
J	401	ASN	-	expression tag	UNP C3SHQ8
J	402	LEU	-	expression tag	UNP C3SHQ8
J	403	GLY	-	expression tag	UNP C3SHQ8
J	404	ILE	-	expression tag	UNP C3SHQ8
J	405	GLU	-	expression tag	UNP C3SHQ8
J	406	GLY	-	expression tag	UNP C3SHQ8
J	407	ARG	-	expression tag	UNP C3SHQ8
J	408	GLU	-	expression tag	UNP C3SHQ8
J	409	ASN	-	expression tag	UNP C3SHQ8
J	410	LEU	-	expression tag	UNP C3SHQ8
J	411	TYR	-	expression tag	UNP C3SHQ8
J	412	PHE	-	expression tag	UNP C3SHQ8
J	413	GLN	-	expression tag	UNP C3SHQ8
J	414	GLY	-	expression tag	UNP C3SHQ8
J	415	GLY	-	expression tag	UNP C3SHQ8
J	416	SER	-	expression tag	UNP C3SHQ8
L	1	MET	-	initiating methionine	UNP C3SHQ8
L	2	GLY	-	expression tag	UNP C3SHQ8
L	3	SER	-	expression tag	UNP C3SHQ8
L	4	SER	-	expression tag	UNP C3SHQ8
L	5	HIS	-	expression tag	UNP C3SHQ8
L	6	HIS	-	expression tag	UNP C3SHQ8
L	7	HIS	-	expression tag	UNP C3SHQ8
L	8	HIS	-	expression tag	UNP C3SHQ8
L	9	HIS	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	10	HIS	-	expression tag	UNP C3SHQ8
L	11	SER	-	expression tag	UNP C3SHQ8
L	12	SER	-	expression tag	UNP C3SHQ8
L	13	GLY	-	expression tag	UNP C3SHQ8
L	14	LEU	-	expression tag	UNP C3SHQ8
L	15	VAL	-	expression tag	UNP C3SHQ8
L	16	PRO	-	expression tag	UNP C3SHQ8
L	17	ARG	-	expression tag	UNP C3SHQ8
L	18	GLY	-	expression tag	UNP C3SHQ8
L	19	SER	-	expression tag	UNP C3SHQ8
L	20	HIS	-	expression tag	UNP C3SHQ8
L	21	MET	-	expression tag	UNP C3SHQ8
L	388	ASN	-	expression tag	UNP C3SHQ8
L	389	SER	-	expression tag	UNP C3SHQ8
L	390	SER	-	expression tag	UNP C3SHQ8
L	391	SER	-	expression tag	UNP C3SHQ8
L	392	ASN	-	expression tag	UNP C3SHQ8
L	393	ASN	-	expression tag	UNP C3SHQ8
L	394	ASN	-	expression tag	UNP C3SHQ8
L	395	ASN	-	expression tag	UNP C3SHQ8
L	396	ASN	-	expression tag	UNP C3SHQ8
L	397	ASN	-	expression tag	UNP C3SHQ8
L	398	ASN	-	expression tag	UNP C3SHQ8
L	399	ASN	-	expression tag	UNP C3SHQ8
L	400	ASN	-	expression tag	UNP C3SHQ8
L	401	ASN	-	expression tag	UNP C3SHQ8
L	402	LEU	-	expression tag	UNP C3SHQ8
L	403	GLY	-	expression tag	UNP C3SHQ8
L	404	ILE	-	expression tag	UNP C3SHQ8
L	405	GLU	-	expression tag	UNP C3SHQ8
L	406	GLY	-	expression tag	UNP C3SHQ8
L	407	ARG	-	expression tag	UNP C3SHQ8
L	408	GLU	-	expression tag	UNP C3SHQ8
L	409	ASN	-	expression tag	UNP C3SHQ8
L	410	LEU	-	expression tag	UNP C3SHQ8
L	411	TYR	-	expression tag	UNP C3SHQ8
L	412	PHE	-	expression tag	UNP C3SHQ8
L	413	GLN	-	expression tag	UNP C3SHQ8
L	414	GLY	-	expression tag	UNP C3SHQ8
L	415	GLY	-	expression tag	UNP C3SHQ8
L	416	SER	-	expression tag	UNP C3SHQ8
N	1	MET	-	initiating methionine	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	2	GLY	-	expression tag	UNP C3SHQ8
N	3	SER	-	expression tag	UNP C3SHQ8
N	4	SER	-	expression tag	UNP C3SHQ8
N	5	HIS	-	expression tag	UNP C3SHQ8
N	6	HIS	-	expression tag	UNP C3SHQ8
N	7	HIS	-	expression tag	UNP C3SHQ8
N	8	HIS	-	expression tag	UNP C3SHQ8
N	9	HIS	-	expression tag	UNP C3SHQ8
N	10	HIS	-	expression tag	UNP C3SHQ8
N	11	SER	-	expression tag	UNP C3SHQ8
N	12	SER	-	expression tag	UNP C3SHQ8
N	13	GLY	-	expression tag	UNP C3SHQ8
N	14	LEU	-	expression tag	UNP C3SHQ8
N	15	VAL	-	expression tag	UNP C3SHQ8
N	16	PRO	-	expression tag	UNP C3SHQ8
N	17	ARG	-	expression tag	UNP C3SHQ8
N	18	GLY	-	expression tag	UNP C3SHQ8
N	19	SER	-	expression tag	UNP C3SHQ8
N	20	HIS	-	expression tag	UNP C3SHQ8
N	21	MET	-	expression tag	UNP C3SHQ8
N	388	ASN	-	expression tag	UNP C3SHQ8
N	389	SER	-	expression tag	UNP C3SHQ8
N	390	SER	-	expression tag	UNP C3SHQ8
N	391	SER	-	expression tag	UNP C3SHQ8
N	392	ASN	-	expression tag	UNP C3SHQ8
N	393	ASN	-	expression tag	UNP C3SHQ8
N	394	ASN	-	expression tag	UNP C3SHQ8
N	395	ASN	-	expression tag	UNP C3SHQ8
N	396	ASN	-	expression tag	UNP C3SHQ8
N	397	ASN	-	expression tag	UNP C3SHQ8
N	398	ASN	-	expression tag	UNP C3SHQ8
N	399	ASN	-	expression tag	UNP C3SHQ8
N	400	ASN	-	expression tag	UNP C3SHQ8
N	401	ASN	-	expression tag	UNP C3SHQ8
N	402	LEU	-	expression tag	UNP C3SHQ8
N	403	GLY	-	expression tag	UNP C3SHQ8
N	404	ILE	-	expression tag	UNP C3SHQ8
N	405	GLU	-	expression tag	UNP C3SHQ8
N	406	GLY	-	expression tag	UNP C3SHQ8
N	407	ARG	-	expression tag	UNP C3SHQ8
N	408	GLU	-	expression tag	UNP C3SHQ8
N	409	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	410	LEU	-	expression tag	UNP C3SHQ8
N	411	TYR	-	expression tag	UNP C3SHQ8
N	412	PHE	-	expression tag	UNP C3SHQ8
N	413	GLN	-	expression tag	UNP C3SHQ8
N	414	GLY	-	expression tag	UNP C3SHQ8
N	415	GLY	-	expression tag	UNP C3SHQ8
N	416	SER	-	expression tag	UNP C3SHQ8
P	1	MET	-	initiating methionine	UNP C3SHQ8
P	2	GLY	-	expression tag	UNP C3SHQ8
P	3	SER	-	expression tag	UNP C3SHQ8
P	4	SER	-	expression tag	UNP C3SHQ8
P	5	HIS	-	expression tag	UNP C3SHQ8
P	6	HIS	-	expression tag	UNP C3SHQ8
P	7	HIS	-	expression tag	UNP C3SHQ8
P	8	HIS	-	expression tag	UNP C3SHQ8
P	9	HIS	-	expression tag	UNP C3SHQ8
P	10	HIS	-	expression tag	UNP C3SHQ8
P	11	SER	-	expression tag	UNP C3SHQ8
P	12	SER	-	expression tag	UNP C3SHQ8
P	13	GLY	-	expression tag	UNP C3SHQ8
P	14	LEU	-	expression tag	UNP C3SHQ8
P	15	VAL	-	expression tag	UNP C3SHQ8
P	16	PRO	-	expression tag	UNP C3SHQ8
P	17	ARG	-	expression tag	UNP C3SHQ8
P	18	GLY	-	expression tag	UNP C3SHQ8
P	19	SER	-	expression tag	UNP C3SHQ8
P	20	HIS	-	expression tag	UNP C3SHQ8
P	21	MET	-	expression tag	UNP C3SHQ8
P	388	ASN	-	expression tag	UNP C3SHQ8
P	389	SER	-	expression tag	UNP C3SHQ8
P	390	SER	-	expression tag	UNP C3SHQ8
P	391	SER	-	expression tag	UNP C3SHQ8
P	392	ASN	-	expression tag	UNP C3SHQ8
P	393	ASN	-	expression tag	UNP C3SHQ8
P	394	ASN	-	expression tag	UNP C3SHQ8
P	395	ASN	-	expression tag	UNP C3SHQ8
P	396	ASN	-	expression tag	UNP C3SHQ8
P	397	ASN	-	expression tag	UNP C3SHQ8
P	398	ASN	-	expression tag	UNP C3SHQ8
P	399	ASN	-	expression tag	UNP C3SHQ8
P	400	ASN	-	expression tag	UNP C3SHQ8
P	401	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	402	LEU	-	expression tag	UNP C3SHQ8
P	403	GLY	-	expression tag	UNP C3SHQ8
P	404	ILE	-	expression tag	UNP C3SHQ8
P	405	GLU	-	expression tag	UNP C3SHQ8
P	406	GLY	-	expression tag	UNP C3SHQ8
P	407	ARG	-	expression tag	UNP C3SHQ8
P	408	GLU	-	expression tag	UNP C3SHQ8
P	409	ASN	-	expression tag	UNP C3SHQ8
P	410	LEU	-	expression tag	UNP C3SHQ8
P	411	TYR	-	expression tag	UNP C3SHQ8
P	412	PHE	-	expression tag	UNP C3SHQ8
P	413	GLN	-	expression tag	UNP C3SHQ8
P	414	GLY	-	expression tag	UNP C3SHQ8
P	415	GLY	-	expression tag	UNP C3SHQ8
P	416	SER	-	expression tag	UNP C3SHQ8
R	1	MET	-	initiating methionine	UNP C3SHQ8
R	2	GLY	-	expression tag	UNP C3SHQ8
R	3	SER	-	expression tag	UNP C3SHQ8
R	4	SER	-	expression tag	UNP C3SHQ8
R	5	HIS	-	expression tag	UNP C3SHQ8
R	6	HIS	-	expression tag	UNP C3SHQ8
R	7	HIS	-	expression tag	UNP C3SHQ8
R	8	HIS	-	expression tag	UNP C3SHQ8
R	9	HIS	-	expression tag	UNP C3SHQ8
R	10	HIS	-	expression tag	UNP C3SHQ8
R	11	SER	-	expression tag	UNP C3SHQ8
R	12	SER	-	expression tag	UNP C3SHQ8
R	13	GLY	-	expression tag	UNP C3SHQ8
R	14	LEU	-	expression tag	UNP C3SHQ8
R	15	VAL	-	expression tag	UNP C3SHQ8
R	16	PRO	-	expression tag	UNP C3SHQ8
R	17	ARG	-	expression tag	UNP C3SHQ8
R	18	GLY	-	expression tag	UNP C3SHQ8
R	19	SER	-	expression tag	UNP C3SHQ8
R	20	HIS	-	expression tag	UNP C3SHQ8
R	21	MET	-	expression tag	UNP C3SHQ8
R	388	ASN	-	expression tag	UNP C3SHQ8
R	389	SER	-	expression tag	UNP C3SHQ8
R	390	SER	-	expression tag	UNP C3SHQ8
R	391	SER	-	expression tag	UNP C3SHQ8
R	392	ASN	-	expression tag	UNP C3SHQ8
R	393	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
R	394	ASN	-	expression tag	UNP C3SHQ8
R	395	ASN	-	expression tag	UNP C3SHQ8
R	396	ASN	-	expression tag	UNP C3SHQ8
R	397	ASN	-	expression tag	UNP C3SHQ8
R	398	ASN	-	expression tag	UNP C3SHQ8
R	399	ASN	-	expression tag	UNP C3SHQ8
R	400	ASN	-	expression tag	UNP C3SHQ8
R	401	ASN	-	expression tag	UNP C3SHQ8
R	402	LEU	-	expression tag	UNP C3SHQ8
R	403	GLY	-	expression tag	UNP C3SHQ8
R	404	ILE	-	expression tag	UNP C3SHQ8
R	405	GLU	-	expression tag	UNP C3SHQ8
R	406	GLY	-	expression tag	UNP C3SHQ8
R	407	ARG	-	expression tag	UNP C3SHQ8
R	408	GLU	-	expression tag	UNP C3SHQ8
R	409	ASN	-	expression tag	UNP C3SHQ8
R	410	LEU	-	expression tag	UNP C3SHQ8
R	411	TYR	-	expression tag	UNP C3SHQ8
R	412	PHE	-	expression tag	UNP C3SHQ8
R	413	GLN	-	expression tag	UNP C3SHQ8
R	414	GLY	-	expression tag	UNP C3SHQ8
R	415	GLY	-	expression tag	UNP C3SHQ8
R	416	SER	-	expression tag	UNP C3SHQ8
T	1	MET	-	initiating methionine	UNP C3SHQ8
T	2	GLY	-	expression tag	UNP C3SHQ8
T	3	SER	-	expression tag	UNP C3SHQ8
T	4	SER	-	expression tag	UNP C3SHQ8
T	5	HIS	-	expression tag	UNP C3SHQ8
T	6	HIS	-	expression tag	UNP C3SHQ8
T	7	HIS	-	expression tag	UNP C3SHQ8
T	8	HIS	-	expression tag	UNP C3SHQ8
T	9	HIS	-	expression tag	UNP C3SHQ8
T	10	HIS	-	expression tag	UNP C3SHQ8
T	11	SER	-	expression tag	UNP C3SHQ8
T	12	SER	-	expression tag	UNP C3SHQ8
T	13	GLY	-	expression tag	UNP C3SHQ8
T	14	LEU	-	expression tag	UNP C3SHQ8
T	15	VAL	-	expression tag	UNP C3SHQ8
T	16	PRO	-	expression tag	UNP C3SHQ8
T	17	ARG	-	expression tag	UNP C3SHQ8
T	18	GLY	-	expression tag	UNP C3SHQ8
T	19	SER	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
T	20	HIS	-	expression tag	UNP C3SHQ8
T	21	MET	-	expression tag	UNP C3SHQ8
T	388	ASN	-	expression tag	UNP C3SHQ8
T	389	SER	-	expression tag	UNP C3SHQ8
T	390	SER	-	expression tag	UNP C3SHQ8
T	391	SER	-	expression tag	UNP C3SHQ8
T	392	ASN	-	expression tag	UNP C3SHQ8
T	393	ASN	-	expression tag	UNP C3SHQ8
T	394	ASN	-	expression tag	UNP C3SHQ8
T	395	ASN	-	expression tag	UNP C3SHQ8
T	396	ASN	-	expression tag	UNP C3SHQ8
T	397	ASN	-	expression tag	UNP C3SHQ8
T	398	ASN	-	expression tag	UNP C3SHQ8
T	399	ASN	-	expression tag	UNP C3SHQ8
T	400	ASN	-	expression tag	UNP C3SHQ8
T	401	ASN	-	expression tag	UNP C3SHQ8
T	402	LEU	-	expression tag	UNP C3SHQ8
T	403	GLY	-	expression tag	UNP C3SHQ8
T	404	ILE	-	expression tag	UNP C3SHQ8
T	405	GLU	-	expression tag	UNP C3SHQ8
T	406	GLY	-	expression tag	UNP C3SHQ8
T	407	ARG	-	expression tag	UNP C3SHQ8
T	408	GLU	-	expression tag	UNP C3SHQ8
T	409	ASN	-	expression tag	UNP C3SHQ8
T	410	LEU	-	expression tag	UNP C3SHQ8
T	411	TYR	-	expression tag	UNP C3SHQ8
T	412	PHE	-	expression tag	UNP C3SHQ8
T	413	GLN	-	expression tag	UNP C3SHQ8
T	414	GLY	-	expression tag	UNP C3SHQ8
T	415	GLY	-	expression tag	UNP C3SHQ8
T	416	SER	-	expression tag	UNP C3SHQ8
W	1	MET	-	initiating methionine	UNP C3SHQ8
W	2	GLY	-	expression tag	UNP C3SHQ8
W	3	SER	-	expression tag	UNP C3SHQ8
W	4	SER	-	expression tag	UNP C3SHQ8
W	5	HIS	-	expression tag	UNP C3SHQ8
W	6	HIS	-	expression tag	UNP C3SHQ8
W	7	HIS	-	expression tag	UNP C3SHQ8
W	8	HIS	-	expression tag	UNP C3SHQ8
W	9	HIS	-	expression tag	UNP C3SHQ8
W	10	HIS	-	expression tag	UNP C3SHQ8
W	11	SER	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
W	12	SER	-	expression tag	UNP C3SHQ8
W	13	GLY	-	expression tag	UNP C3SHQ8
W	14	LEU	-	expression tag	UNP C3SHQ8
W	15	VAL	-	expression tag	UNP C3SHQ8
W	16	PRO	-	expression tag	UNP C3SHQ8
W	17	ARG	-	expression tag	UNP C3SHQ8
W	18	GLY	-	expression tag	UNP C3SHQ8
W	19	SER	-	expression tag	UNP C3SHQ8
W	20	HIS	-	expression tag	UNP C3SHQ8
W	21	MET	-	expression tag	UNP C3SHQ8
W	388	ASN	-	expression tag	UNP C3SHQ8
W	389	SER	-	expression tag	UNP C3SHQ8
W	390	SER	-	expression tag	UNP C3SHQ8
W	391	SER	-	expression tag	UNP C3SHQ8
W	392	ASN	-	expression tag	UNP C3SHQ8
W	393	ASN	-	expression tag	UNP C3SHQ8
W	394	ASN	-	expression tag	UNP C3SHQ8
W	395	ASN	-	expression tag	UNP C3SHQ8
W	396	ASN	-	expression tag	UNP C3SHQ8
W	397	ASN	-	expression tag	UNP C3SHQ8
W	398	ASN	-	expression tag	UNP C3SHQ8
W	399	ASN	-	expression tag	UNP C3SHQ8
W	400	ASN	-	expression tag	UNP C3SHQ8
W	401	ASN	-	expression tag	UNP C3SHQ8
W	402	LEU	-	expression tag	UNP C3SHQ8
W	403	GLY	-	expression tag	UNP C3SHQ8
W	404	ILE	-	expression tag	UNP C3SHQ8
W	405	GLU	-	expression tag	UNP C3SHQ8
W	406	GLY	-	expression tag	UNP C3SHQ8
W	407	ARG	-	expression tag	UNP C3SHQ8
W	408	GLU	-	expression tag	UNP C3SHQ8
W	409	ASN	-	expression tag	UNP C3SHQ8
W	410	LEU	-	expression tag	UNP C3SHQ8
W	411	TYR	-	expression tag	UNP C3SHQ8
W	412	PHE	-	expression tag	UNP C3SHQ8
W	413	GLN	-	expression tag	UNP C3SHQ8
W	414	GLY	-	expression tag	UNP C3SHQ8
W	415	GLY	-	expression tag	UNP C3SHQ8
W	416	SER	-	expression tag	UNP C3SHQ8
Y	1	MET	-	initiating methionine	UNP C3SHQ8
Y	2	GLY	-	expression tag	UNP C3SHQ8
Y	3	SER	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	4	SER	-	expression tag	UNP C3SHQ8
Y	5	HIS	-	expression tag	UNP C3SHQ8
Y	6	HIS	-	expression tag	UNP C3SHQ8
Y	7	HIS	-	expression tag	UNP C3SHQ8
Y	8	HIS	-	expression tag	UNP C3SHQ8
Y	9	HIS	-	expression tag	UNP C3SHQ8
Y	10	HIS	-	expression tag	UNP C3SHQ8
Y	11	SER	-	expression tag	UNP C3SHQ8
Y	12	SER	-	expression tag	UNP C3SHQ8
Y	13	GLY	-	expression tag	UNP C3SHQ8
Y	14	LEU	-	expression tag	UNP C3SHQ8
Y	15	VAL	-	expression tag	UNP C3SHQ8
Y	16	PRO	-	expression tag	UNP C3SHQ8
Y	17	ARG	-	expression tag	UNP C3SHQ8
Y	18	GLY	-	expression tag	UNP C3SHQ8
Y	19	SER	-	expression tag	UNP C3SHQ8
Y	20	HIS	-	expression tag	UNP C3SHQ8
Y	21	MET	-	expression tag	UNP C3SHQ8
Y	388	ASN	-	expression tag	UNP C3SHQ8
Y	389	SER	-	expression tag	UNP C3SHQ8
Y	390	SER	-	expression tag	UNP C3SHQ8
Y	391	SER	-	expression tag	UNP C3SHQ8
Y	392	ASN	-	expression tag	UNP C3SHQ8
Y	393	ASN	-	expression tag	UNP C3SHQ8
Y	394	ASN	-	expression tag	UNP C3SHQ8
Y	395	ASN	-	expression tag	UNP C3SHQ8
Y	396	ASN	-	expression tag	UNP C3SHQ8
Y	397	ASN	-	expression tag	UNP C3SHQ8
Y	398	ASN	-	expression tag	UNP C3SHQ8
Y	399	ASN	-	expression tag	UNP C3SHQ8
Y	400	ASN	-	expression tag	UNP C3SHQ8
Y	401	ASN	-	expression tag	UNP C3SHQ8
Y	402	LEU	-	expression tag	UNP C3SHQ8
Y	403	GLY	-	expression tag	UNP C3SHQ8
Y	404	ILE	-	expression tag	UNP C3SHQ8
Y	405	GLU	-	expression tag	UNP C3SHQ8
Y	406	GLY	-	expression tag	UNP C3SHQ8
Y	407	ARG	-	expression tag	UNP C3SHQ8
Y	408	GLU	-	expression tag	UNP C3SHQ8
Y	409	ASN	-	expression tag	UNP C3SHQ8
Y	410	LEU	-	expression tag	UNP C3SHQ8
Y	411	TYR	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	412	PHE	-	expression tag	UNP C3SHQ8
Y	413	GLN	-	expression tag	UNP C3SHQ8
Y	414	GLY	-	expression tag	UNP C3SHQ8
Y	415	GLY	-	expression tag	UNP C3SHQ8
Y	416	SER	-	expression tag	UNP C3SHQ8
AA	1	MET	-	initiating methionine	UNP C3SHQ8
AA	2	GLY	-	expression tag	UNP C3SHQ8
AA	3	SER	-	expression tag	UNP C3SHQ8
AA	4	SER	-	expression tag	UNP C3SHQ8
AA	5	HIS	-	expression tag	UNP C3SHQ8
AA	6	HIS	-	expression tag	UNP C3SHQ8
AA	7	HIS	-	expression tag	UNP C3SHQ8
AA	8	HIS	-	expression tag	UNP C3SHQ8
AA	9	HIS	-	expression tag	UNP C3SHQ8
AA	10	HIS	-	expression tag	UNP C3SHQ8
AA	11	SER	-	expression tag	UNP C3SHQ8
AA	12	SER	-	expression tag	UNP C3SHQ8
AA	13	GLY	-	expression tag	UNP C3SHQ8
AA	14	LEU	-	expression tag	UNP C3SHQ8
AA	15	VAL	-	expression tag	UNP C3SHQ8
AA	16	PRO	-	expression tag	UNP C3SHQ8
AA	17	ARG	-	expression tag	UNP C3SHQ8
AA	18	GLY	-	expression tag	UNP C3SHQ8
AA	19	SER	-	expression tag	UNP C3SHQ8
AA	20	HIS	-	expression tag	UNP C3SHQ8
AA	21	MET	-	expression tag	UNP C3SHQ8
AA	388	ASN	-	expression tag	UNP C3SHQ8
AA	389	SER	-	expression tag	UNP C3SHQ8
AA	390	SER	-	expression tag	UNP C3SHQ8
AA	391	SER	-	expression tag	UNP C3SHQ8
AA	392	ASN	-	expression tag	UNP C3SHQ8
AA	393	ASN	-	expression tag	UNP C3SHQ8
AA	394	ASN	-	expression tag	UNP C3SHQ8
AA	395	ASN	-	expression tag	UNP C3SHQ8
AA	396	ASN	-	expression tag	UNP C3SHQ8
AA	397	ASN	-	expression tag	UNP C3SHQ8
AA	398	ASN	-	expression tag	UNP C3SHQ8
AA	399	ASN	-	expression tag	UNP C3SHQ8
AA	400	ASN	-	expression tag	UNP C3SHQ8
AA	401	ASN	-	expression tag	UNP C3SHQ8
AA	402	LEU	-	expression tag	UNP C3SHQ8
AA	403	GLY	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
AA	404	ILE	-	expression tag	UNP C3SHQ8
AA	405	GLU	-	expression tag	UNP C3SHQ8
AA	406	GLY	-	expression tag	UNP C3SHQ8
AA	407	ARG	-	expression tag	UNP C3SHQ8
AA	408	GLU	-	expression tag	UNP C3SHQ8
AA	409	ASN	-	expression tag	UNP C3SHQ8
AA	410	LEU	-	expression tag	UNP C3SHQ8
AA	411	TYR	-	expression tag	UNP C3SHQ8
AA	412	PHE	-	expression tag	UNP C3SHQ8
AA	413	GLN	-	expression tag	UNP C3SHQ8
AA	414	GLY	-	expression tag	UNP C3SHQ8
AA	415	GLY	-	expression tag	UNP C3SHQ8
AA	416	SER	-	expression tag	UNP C3SHQ8
CA	1	MET	-	initiating methionine	UNP C3SHQ8
CA	2	GLY	-	expression tag	UNP C3SHQ8
CA	3	SER	-	expression tag	UNP C3SHQ8
CA	4	SER	-	expression tag	UNP C3SHQ8
CA	5	HIS	-	expression tag	UNP C3SHQ8
CA	6	HIS	-	expression tag	UNP C3SHQ8
CA	7	HIS	-	expression tag	UNP C3SHQ8
CA	8	HIS	-	expression tag	UNP C3SHQ8
CA	9	HIS	-	expression tag	UNP C3SHQ8
CA	10	HIS	-	expression tag	UNP C3SHQ8
CA	11	SER	-	expression tag	UNP C3SHQ8
CA	12	SER	-	expression tag	UNP C3SHQ8
CA	13	GLY	-	expression tag	UNP C3SHQ8
CA	14	LEU	-	expression tag	UNP C3SHQ8
CA	15	VAL	-	expression tag	UNP C3SHQ8
CA	16	PRO	-	expression tag	UNP C3SHQ8
CA	17	ARG	-	expression tag	UNP C3SHQ8
CA	18	GLY	-	expression tag	UNP C3SHQ8
CA	19	SER	-	expression tag	UNP C3SHQ8
CA	20	HIS	-	expression tag	UNP C3SHQ8
CA	21	MET	-	expression tag	UNP C3SHQ8
CA	388	ASN	-	expression tag	UNP C3SHQ8
CA	389	SER	-	expression tag	UNP C3SHQ8
CA	390	SER	-	expression tag	UNP C3SHQ8
CA	391	SER	-	expression tag	UNP C3SHQ8
CA	392	ASN	-	expression tag	UNP C3SHQ8
CA	393	ASN	-	expression tag	UNP C3SHQ8
CA	394	ASN	-	expression tag	UNP C3SHQ8
CA	395	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
CA	396	ASN	-	expression tag	UNP C3SHQ8
CA	397	ASN	-	expression tag	UNP C3SHQ8
CA	398	ASN	-	expression tag	UNP C3SHQ8
CA	399	ASN	-	expression tag	UNP C3SHQ8
CA	400	ASN	-	expression tag	UNP C3SHQ8
CA	401	ASN	-	expression tag	UNP C3SHQ8
CA	402	LEU	-	expression tag	UNP C3SHQ8
CA	403	GLY	-	expression tag	UNP C3SHQ8
CA	404	ILE	-	expression tag	UNP C3SHQ8
CA	405	GLU	-	expression tag	UNP C3SHQ8
CA	406	GLY	-	expression tag	UNP C3SHQ8
CA	407	ARG	-	expression tag	UNP C3SHQ8
CA	408	GLU	-	expression tag	UNP C3SHQ8
CA	409	ASN	-	expression tag	UNP C3SHQ8
CA	410	LEU	-	expression tag	UNP C3SHQ8
CA	411	TYR	-	expression tag	UNP C3SHQ8
CA	412	PHE	-	expression tag	UNP C3SHQ8
CA	413	GLN	-	expression tag	UNP C3SHQ8
CA	414	GLY	-	expression tag	UNP C3SHQ8
CA	415	GLY	-	expression tag	UNP C3SHQ8
CA	416	SER	-	expression tag	UNP C3SHQ8
EA	1	MET	-	initiating methionine	UNP C3SHQ8
EA	2	GLY	-	expression tag	UNP C3SHQ8
EA	3	SER	-	expression tag	UNP C3SHQ8
EA	4	SER	-	expression tag	UNP C3SHQ8
EA	5	HIS	-	expression tag	UNP C3SHQ8
EA	6	HIS	-	expression tag	UNP C3SHQ8
EA	7	HIS	-	expression tag	UNP C3SHQ8
EA	8	HIS	-	expression tag	UNP C3SHQ8
EA	9	HIS	-	expression tag	UNP C3SHQ8
EA	10	HIS	-	expression tag	UNP C3SHQ8
EA	11	SER	-	expression tag	UNP C3SHQ8
EA	12	SER	-	expression tag	UNP C3SHQ8
EA	13	GLY	-	expression tag	UNP C3SHQ8
EA	14	LEU	-	expression tag	UNP C3SHQ8
EA	15	VAL	-	expression tag	UNP C3SHQ8
EA	16	PRO	-	expression tag	UNP C3SHQ8
EA	17	ARG	-	expression tag	UNP C3SHQ8
EA	18	GLY	-	expression tag	UNP C3SHQ8
EA	19	SER	-	expression tag	UNP C3SHQ8
EA	20	HIS	-	expression tag	UNP C3SHQ8
EA	21	MET	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
EA	388	ASN	-	expression tag	UNP C3SHQ8
EA	389	SER	-	expression tag	UNP C3SHQ8
EA	390	SER	-	expression tag	UNP C3SHQ8
EA	391	SER	-	expression tag	UNP C3SHQ8
EA	392	ASN	-	expression tag	UNP C3SHQ8
EA	393	ASN	-	expression tag	UNP C3SHQ8
EA	394	ASN	-	expression tag	UNP C3SHQ8
EA	395	ASN	-	expression tag	UNP C3SHQ8
EA	396	ASN	-	expression tag	UNP C3SHQ8
EA	397	ASN	-	expression tag	UNP C3SHQ8
EA	398	ASN	-	expression tag	UNP C3SHQ8
EA	399	ASN	-	expression tag	UNP C3SHQ8
EA	400	ASN	-	expression tag	UNP C3SHQ8
EA	401	ASN	-	expression tag	UNP C3SHQ8
EA	402	LEU	-	expression tag	UNP C3SHQ8
EA	403	GLY	-	expression tag	UNP C3SHQ8
EA	404	ILE	-	expression tag	UNP C3SHQ8
EA	405	GLU	-	expression tag	UNP C3SHQ8
EA	406	GLY	-	expression tag	UNP C3SHQ8
EA	407	ARG	-	expression tag	UNP C3SHQ8
EA	408	GLU	-	expression tag	UNP C3SHQ8
EA	409	ASN	-	expression tag	UNP C3SHQ8
EA	410	LEU	-	expression tag	UNP C3SHQ8
EA	411	TYR	-	expression tag	UNP C3SHQ8
EA	412	PHE	-	expression tag	UNP C3SHQ8
EA	413	GLN	-	expression tag	UNP C3SHQ8
EA	414	GLY	-	expression tag	UNP C3SHQ8
EA	415	GLY	-	expression tag	UNP C3SHQ8
EA	416	SER	-	expression tag	UNP C3SHQ8
GA	1	MET	-	initiating methionine	UNP C3SHQ8
GA	2	GLY	-	expression tag	UNP C3SHQ8
GA	3	SER	-	expression tag	UNP C3SHQ8
GA	4	SER	-	expression tag	UNP C3SHQ8
GA	5	HIS	-	expression tag	UNP C3SHQ8
GA	6	HIS	-	expression tag	UNP C3SHQ8
GA	7	HIS	-	expression tag	UNP C3SHQ8
GA	8	HIS	-	expression tag	UNP C3SHQ8
GA	9	HIS	-	expression tag	UNP C3SHQ8
GA	10	HIS	-	expression tag	UNP C3SHQ8
GA	11	SER	-	expression tag	UNP C3SHQ8
GA	12	SER	-	expression tag	UNP C3SHQ8
GA	13	GLY	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
GA	14	LEU	-	expression tag	UNP C3SHQ8
GA	15	VAL	-	expression tag	UNP C3SHQ8
GA	16	PRO	-	expression tag	UNP C3SHQ8
GA	17	ARG	-	expression tag	UNP C3SHQ8
GA	18	GLY	-	expression tag	UNP C3SHQ8
GA	19	SER	-	expression tag	UNP C3SHQ8
GA	20	HIS	-	expression tag	UNP C3SHQ8
GA	21	MET	-	expression tag	UNP C3SHQ8
GA	388	ASN	-	expression tag	UNP C3SHQ8
GA	389	SER	-	expression tag	UNP C3SHQ8
GA	390	SER	-	expression tag	UNP C3SHQ8
GA	391	SER	-	expression tag	UNP C3SHQ8
GA	392	ASN	-	expression tag	UNP C3SHQ8
GA	393	ASN	-	expression tag	UNP C3SHQ8
GA	394	ASN	-	expression tag	UNP C3SHQ8
GA	395	ASN	-	expression tag	UNP C3SHQ8
GA	396	ASN	-	expression tag	UNP C3SHQ8
GA	397	ASN	-	expression tag	UNP C3SHQ8
GA	398	ASN	-	expression tag	UNP C3SHQ8
GA	399	ASN	-	expression tag	UNP C3SHQ8
GA	400	ASN	-	expression tag	UNP C3SHQ8
GA	401	ASN	-	expression tag	UNP C3SHQ8
GA	402	LEU	-	expression tag	UNP C3SHQ8
GA	403	GLY	-	expression tag	UNP C3SHQ8
GA	404	ILE	-	expression tag	UNP C3SHQ8
GA	405	GLU	-	expression tag	UNP C3SHQ8
GA	406	GLY	-	expression tag	UNP C3SHQ8
GA	407	ARG	-	expression tag	UNP C3SHQ8
GA	408	GLU	-	expression tag	UNP C3SHQ8
GA	409	ASN	-	expression tag	UNP C3SHQ8
GA	410	LEU	-	expression tag	UNP C3SHQ8
GA	411	TYR	-	expression tag	UNP C3SHQ8
GA	412	PHE	-	expression tag	UNP C3SHQ8
GA	413	GLN	-	expression tag	UNP C3SHQ8
GA	414	GLY	-	expression tag	UNP C3SHQ8
GA	415	GLY	-	expression tag	UNP C3SHQ8
GA	416	SER	-	expression tag	UNP C3SHQ8
IA	1	MET	-	initiating methionine	UNP C3SHQ8
IA	2	GLY	-	expression tag	UNP C3SHQ8
IA	3	SER	-	expression tag	UNP C3SHQ8
IA	4	SER	-	expression tag	UNP C3SHQ8
IA	5	HIS	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	6	HIS	-	expression tag	UNP C3SHQ8
IA	7	HIS	-	expression tag	UNP C3SHQ8
IA	8	HIS	-	expression tag	UNP C3SHQ8
IA	9	HIS	-	expression tag	UNP C3SHQ8
IA	10	HIS	-	expression tag	UNP C3SHQ8
IA	11	SER	-	expression tag	UNP C3SHQ8
IA	12	SER	-	expression tag	UNP C3SHQ8
IA	13	GLY	-	expression tag	UNP C3SHQ8
IA	14	LEU	-	expression tag	UNP C3SHQ8
IA	15	VAL	-	expression tag	UNP C3SHQ8
IA	16	PRO	-	expression tag	UNP C3SHQ8
IA	17	ARG	-	expression tag	UNP C3SHQ8
IA	18	GLY	-	expression tag	UNP C3SHQ8
IA	19	SER	-	expression tag	UNP C3SHQ8
IA	20	HIS	-	expression tag	UNP C3SHQ8
IA	21	MET	-	expression tag	UNP C3SHQ8
IA	388	ASN	-	expression tag	UNP C3SHQ8
IA	389	SER	-	expression tag	UNP C3SHQ8
IA	390	SER	-	expression tag	UNP C3SHQ8
IA	391	SER	-	expression tag	UNP C3SHQ8
IA	392	ASN	-	expression tag	UNP C3SHQ8
IA	393	ASN	-	expression tag	UNP C3SHQ8
IA	394	ASN	-	expression tag	UNP C3SHQ8
IA	395	ASN	-	expression tag	UNP C3SHQ8
IA	396	ASN	-	expression tag	UNP C3SHQ8
IA	397	ASN	-	expression tag	UNP C3SHQ8
IA	398	ASN	-	expression tag	UNP C3SHQ8
IA	399	ASN	-	expression tag	UNP C3SHQ8
IA	400	ASN	-	expression tag	UNP C3SHQ8
IA	401	ASN	-	expression tag	UNP C3SHQ8
IA	402	LEU	-	expression tag	UNP C3SHQ8
IA	403	GLY	-	expression tag	UNP C3SHQ8
IA	404	ILE	-	expression tag	UNP C3SHQ8
IA	405	GLU	-	expression tag	UNP C3SHQ8
IA	406	GLY	-	expression tag	UNP C3SHQ8
IA	407	ARG	-	expression tag	UNP C3SHQ8
IA	408	GLU	-	expression tag	UNP C3SHQ8
IA	409	ASN	-	expression tag	UNP C3SHQ8
IA	410	LEU	-	expression tag	UNP C3SHQ8
IA	411	TYR	-	expression tag	UNP C3SHQ8
IA	412	PHE	-	expression tag	UNP C3SHQ8
IA	413	GLN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
IA	414	GLY	-	expression tag	UNP C3SHQ8
IA	415	GLY	-	expression tag	UNP C3SHQ8
IA	416	SER	-	expression tag	UNP C3SHQ8
KA	1	MET	-	initiating methionine	UNP C3SHQ8
KA	2	GLY	-	expression tag	UNP C3SHQ8
KA	3	SER	-	expression tag	UNP C3SHQ8
KA	4	SER	-	expression tag	UNP C3SHQ8
KA	5	HIS	-	expression tag	UNP C3SHQ8
KA	6	HIS	-	expression tag	UNP C3SHQ8
KA	7	HIS	-	expression tag	UNP C3SHQ8
KA	8	HIS	-	expression tag	UNP C3SHQ8
KA	9	HIS	-	expression tag	UNP C3SHQ8
KA	10	HIS	-	expression tag	UNP C3SHQ8
KA	11	SER	-	expression tag	UNP C3SHQ8
KA	12	SER	-	expression tag	UNP C3SHQ8
KA	13	GLY	-	expression tag	UNP C3SHQ8
KA	14	LEU	-	expression tag	UNP C3SHQ8
KA	15	VAL	-	expression tag	UNP C3SHQ8
KA	16	PRO	-	expression tag	UNP C3SHQ8
KA	17	ARG	-	expression tag	UNP C3SHQ8
KA	18	GLY	-	expression tag	UNP C3SHQ8
KA	19	SER	-	expression tag	UNP C3SHQ8
KA	20	HIS	-	expression tag	UNP C3SHQ8
KA	21	MET	-	expression tag	UNP C3SHQ8
KA	388	ASN	-	expression tag	UNP C3SHQ8
KA	389	SER	-	expression tag	UNP C3SHQ8
KA	390	SER	-	expression tag	UNP C3SHQ8
KA	391	SER	-	expression tag	UNP C3SHQ8
KA	392	ASN	-	expression tag	UNP C3SHQ8
KA	393	ASN	-	expression tag	UNP C3SHQ8
KA	394	ASN	-	expression tag	UNP C3SHQ8
KA	395	ASN	-	expression tag	UNP C3SHQ8
KA	396	ASN	-	expression tag	UNP C3SHQ8
KA	397	ASN	-	expression tag	UNP C3SHQ8
KA	398	ASN	-	expression tag	UNP C3SHQ8
KA	399	ASN	-	expression tag	UNP C3SHQ8
KA	400	ASN	-	expression tag	UNP C3SHQ8
KA	401	ASN	-	expression tag	UNP C3SHQ8
KA	402	LEU	-	expression tag	UNP C3SHQ8
KA	403	GLY	-	expression tag	UNP C3SHQ8
KA	404	ILE	-	expression tag	UNP C3SHQ8
KA	405	GLU	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
KA	406	GLY	-	expression tag	UNP C3SHQ8
KA	407	ARG	-	expression tag	UNP C3SHQ8
KA	408	GLU	-	expression tag	UNP C3SHQ8
KA	409	ASN	-	expression tag	UNP C3SHQ8
KA	410	LEU	-	expression tag	UNP C3SHQ8
KA	411	TYR	-	expression tag	UNP C3SHQ8
KA	412	PHE	-	expression tag	UNP C3SHQ8
KA	413	GLN	-	expression tag	UNP C3SHQ8
KA	414	GLY	-	expression tag	UNP C3SHQ8
KA	415	GLY	-	expression tag	UNP C3SHQ8
KA	416	SER	-	expression tag	UNP C3SHQ8
MA	1	MET	-	initiating methionine	UNP C3SHQ8
MA	2	GLY	-	expression tag	UNP C3SHQ8
MA	3	SER	-	expression tag	UNP C3SHQ8
MA	4	SER	-	expression tag	UNP C3SHQ8
MA	5	HIS	-	expression tag	UNP C3SHQ8
MA	6	HIS	-	expression tag	UNP C3SHQ8
MA	7	HIS	-	expression tag	UNP C3SHQ8
MA	8	HIS	-	expression tag	UNP C3SHQ8
MA	9	HIS	-	expression tag	UNP C3SHQ8
MA	10	HIS	-	expression tag	UNP C3SHQ8
MA	11	SER	-	expression tag	UNP C3SHQ8
MA	12	SER	-	expression tag	UNP C3SHQ8
MA	13	GLY	-	expression tag	UNP C3SHQ8
MA	14	LEU	-	expression tag	UNP C3SHQ8
MA	15	VAL	-	expression tag	UNP C3SHQ8
MA	16	PRO	-	expression tag	UNP C3SHQ8
MA	17	ARG	-	expression tag	UNP C3SHQ8
MA	18	GLY	-	expression tag	UNP C3SHQ8
MA	19	SER	-	expression tag	UNP C3SHQ8
MA	20	HIS	-	expression tag	UNP C3SHQ8
MA	21	MET	-	expression tag	UNP C3SHQ8
MA	388	ASN	-	expression tag	UNP C3SHQ8
MA	389	SER	-	expression tag	UNP C3SHQ8
MA	390	SER	-	expression tag	UNP C3SHQ8
MA	391	SER	-	expression tag	UNP C3SHQ8
MA	392	ASN	-	expression tag	UNP C3SHQ8
MA	393	ASN	-	expression tag	UNP C3SHQ8
MA	394	ASN	-	expression tag	UNP C3SHQ8
MA	395	ASN	-	expression tag	UNP C3SHQ8
MA	396	ASN	-	expression tag	UNP C3SHQ8
MA	397	ASN	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	398	ASN	-	expression tag	UNP C3SHQ8
MA	399	ASN	-	expression tag	UNP C3SHQ8
MA	400	ASN	-	expression tag	UNP C3SHQ8
MA	401	ASN	-	expression tag	UNP C3SHQ8
MA	402	LEU	-	expression tag	UNP C3SHQ8
MA	403	GLY	-	expression tag	UNP C3SHQ8
MA	404	ILE	-	expression tag	UNP C3SHQ8
MA	405	GLU	-	expression tag	UNP C3SHQ8
MA	406	GLY	-	expression tag	UNP C3SHQ8
MA	407	ARG	-	expression tag	UNP C3SHQ8
MA	408	GLU	-	expression tag	UNP C3SHQ8
MA	409	ASN	-	expression tag	UNP C3SHQ8
MA	410	LEU	-	expression tag	UNP C3SHQ8
MA	411	TYR	-	expression tag	UNP C3SHQ8
MA	412	PHE	-	expression tag	UNP C3SHQ8
MA	413	GLN	-	expression tag	UNP C3SHQ8
MA	414	GLY	-	expression tag	UNP C3SHQ8
MA	415	GLY	-	expression tag	UNP C3SHQ8
MA	416	SER	-	expression tag	UNP C3SHQ8
OA	1	MET	-	initiating methionine	UNP C3SHQ8
OA	2	GLY	-	expression tag	UNP C3SHQ8
OA	3	SER	-	expression tag	UNP C3SHQ8
OA	4	SER	-	expression tag	UNP C3SHQ8
OA	5	HIS	-	expression tag	UNP C3SHQ8
OA	6	HIS	-	expression tag	UNP C3SHQ8
OA	7	HIS	-	expression tag	UNP C3SHQ8
OA	8	HIS	-	expression tag	UNP C3SHQ8
OA	9	HIS	-	expression tag	UNP C3SHQ8
OA	10	HIS	-	expression tag	UNP C3SHQ8
OA	11	SER	-	expression tag	UNP C3SHQ8
OA	12	SER	-	expression tag	UNP C3SHQ8
OA	13	GLY	-	expression tag	UNP C3SHQ8
OA	14	LEU	-	expression tag	UNP C3SHQ8
OA	15	VAL	-	expression tag	UNP C3SHQ8
OA	16	PRO	-	expression tag	UNP C3SHQ8
OA	17	ARG	-	expression tag	UNP C3SHQ8
OA	18	GLY	-	expression tag	UNP C3SHQ8
OA	19	SER	-	expression tag	UNP C3SHQ8
OA	20	HIS	-	expression tag	UNP C3SHQ8
OA	21	MET	-	expression tag	UNP C3SHQ8
OA	388	ASN	-	expression tag	UNP C3SHQ8
OA	389	SER	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
OA	390	SER	-	expression tag	UNP C3SHQ8
OA	391	SER	-	expression tag	UNP C3SHQ8
OA	392	ASN	-	expression tag	UNP C3SHQ8
OA	393	ASN	-	expression tag	UNP C3SHQ8
OA	394	ASN	-	expression tag	UNP C3SHQ8
OA	395	ASN	-	expression tag	UNP C3SHQ8
OA	396	ASN	-	expression tag	UNP C3SHQ8
OA	397	ASN	-	expression tag	UNP C3SHQ8
OA	398	ASN	-	expression tag	UNP C3SHQ8
OA	399	ASN	-	expression tag	UNP C3SHQ8
OA	400	ASN	-	expression tag	UNP C3SHQ8
OA	401	ASN	-	expression tag	UNP C3SHQ8
OA	402	LEU	-	expression tag	UNP C3SHQ8
OA	403	GLY	-	expression tag	UNP C3SHQ8
OA	404	ILE	-	expression tag	UNP C3SHQ8
OA	405	GLU	-	expression tag	UNP C3SHQ8
OA	406	GLY	-	expression tag	UNP C3SHQ8
OA	407	ARG	-	expression tag	UNP C3SHQ8
OA	408	GLU	-	expression tag	UNP C3SHQ8
OA	409	ASN	-	expression tag	UNP C3SHQ8
OA	410	LEU	-	expression tag	UNP C3SHQ8
OA	411	TYR	-	expression tag	UNP C3SHQ8
OA	412	PHE	-	expression tag	UNP C3SHQ8
OA	413	GLN	-	expression tag	UNP C3SHQ8
OA	414	GLY	-	expression tag	UNP C3SHQ8
OA	415	GLY	-	expression tag	UNP C3SHQ8
OA	416	SER	-	expression tag	UNP C3SHQ8
QA	1	MET	-	initiating methionine	UNP C3SHQ8
QA	2	GLY	-	expression tag	UNP C3SHQ8
QA	3	SER	-	expression tag	UNP C3SHQ8
QA	4	SER	-	expression tag	UNP C3SHQ8
QA	5	HIS	-	expression tag	UNP C3SHQ8
QA	6	HIS	-	expression tag	UNP C3SHQ8
QA	7	HIS	-	expression tag	UNP C3SHQ8
QA	8	HIS	-	expression tag	UNP C3SHQ8
QA	9	HIS	-	expression tag	UNP C3SHQ8
QA	10	HIS	-	expression tag	UNP C3SHQ8
QA	11	SER	-	expression tag	UNP C3SHQ8
QA	12	SER	-	expression tag	UNP C3SHQ8
QA	13	GLY	-	expression tag	UNP C3SHQ8
QA	14	LEU	-	expression tag	UNP C3SHQ8
QA	15	VAL	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
QA	16	PRO	-	expression tag	UNP C3SHQ8
QA	17	ARG	-	expression tag	UNP C3SHQ8
QA	18	GLY	-	expression tag	UNP C3SHQ8
QA	19	SER	-	expression tag	UNP C3SHQ8
QA	20	HIS	-	expression tag	UNP C3SHQ8
QA	21	MET	-	expression tag	UNP C3SHQ8
QA	388	ASN	-	expression tag	UNP C3SHQ8
QA	389	SER	-	expression tag	UNP C3SHQ8
QA	390	SER	-	expression tag	UNP C3SHQ8
QA	391	SER	-	expression tag	UNP C3SHQ8
QA	392	ASN	-	expression tag	UNP C3SHQ8
QA	393	ASN	-	expression tag	UNP C3SHQ8
QA	394	ASN	-	expression tag	UNP C3SHQ8
QA	395	ASN	-	expression tag	UNP C3SHQ8
QA	396	ASN	-	expression tag	UNP C3SHQ8
QA	397	ASN	-	expression tag	UNP C3SHQ8
QA	398	ASN	-	expression tag	UNP C3SHQ8
QA	399	ASN	-	expression tag	UNP C3SHQ8
QA	400	ASN	-	expression tag	UNP C3SHQ8
QA	401	ASN	-	expression tag	UNP C3SHQ8
QA	402	LEU	-	expression tag	UNP C3SHQ8
QA	403	GLY	-	expression tag	UNP C3SHQ8
QA	404	ILE	-	expression tag	UNP C3SHQ8
QA	405	GLU	-	expression tag	UNP C3SHQ8
QA	406	GLY	-	expression tag	UNP C3SHQ8
QA	407	ARG	-	expression tag	UNP C3SHQ8
QA	408	GLU	-	expression tag	UNP C3SHQ8
QA	409	ASN	-	expression tag	UNP C3SHQ8
QA	410	LEU	-	expression tag	UNP C3SHQ8
QA	411	TYR	-	expression tag	UNP C3SHQ8
QA	412	PHE	-	expression tag	UNP C3SHQ8
QA	413	GLN	-	expression tag	UNP C3SHQ8
QA	414	GLY	-	expression tag	UNP C3SHQ8
QA	415	GLY	-	expression tag	UNP C3SHQ8
QA	416	SER	-	expression tag	UNP C3SHQ8
SA	1	MET	-	initiating methionine	UNP C3SHQ8
SA	2	GLY	-	expression tag	UNP C3SHQ8
SA	3	SER	-	expression tag	UNP C3SHQ8
SA	4	SER	-	expression tag	UNP C3SHQ8
SA	5	HIS	-	expression tag	UNP C3SHQ8
SA	6	HIS	-	expression tag	UNP C3SHQ8
SA	7	HIS	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
SA	8	HIS	-	expression tag	UNP C3SHQ8
SA	9	HIS	-	expression tag	UNP C3SHQ8
SA	10	HIS	-	expression tag	UNP C3SHQ8
SA	11	SER	-	expression tag	UNP C3SHQ8
SA	12	SER	-	expression tag	UNP C3SHQ8
SA	13	GLY	-	expression tag	UNP C3SHQ8
SA	14	LEU	-	expression tag	UNP C3SHQ8
SA	15	VAL	-	expression tag	UNP C3SHQ8
SA	16	PRO	-	expression tag	UNP C3SHQ8
SA	17	ARG	-	expression tag	UNP C3SHQ8
SA	18	GLY	-	expression tag	UNP C3SHQ8
SA	19	SER	-	expression tag	UNP C3SHQ8
SA	20	HIS	-	expression tag	UNP C3SHQ8
SA	21	MET	-	expression tag	UNP C3SHQ8
SA	388	ASN	-	expression tag	UNP C3SHQ8
SA	389	SER	-	expression tag	UNP C3SHQ8
SA	390	SER	-	expression tag	UNP C3SHQ8
SA	391	SER	-	expression tag	UNP C3SHQ8
SA	392	ASN	-	expression tag	UNP C3SHQ8
SA	393	ASN	-	expression tag	UNP C3SHQ8
SA	394	ASN	-	expression tag	UNP C3SHQ8
SA	395	ASN	-	expression tag	UNP C3SHQ8
SA	396	ASN	-	expression tag	UNP C3SHQ8
SA	397	ASN	-	expression tag	UNP C3SHQ8
SA	398	ASN	-	expression tag	UNP C3SHQ8
SA	399	ASN	-	expression tag	UNP C3SHQ8
SA	400	ASN	-	expression tag	UNP C3SHQ8
SA	401	ASN	-	expression tag	UNP C3SHQ8
SA	402	LEU	-	expression tag	UNP C3SHQ8
SA	403	GLY	-	expression tag	UNP C3SHQ8
SA	404	ILE	-	expression tag	UNP C3SHQ8
SA	405	GLU	-	expression tag	UNP C3SHQ8
SA	406	GLY	-	expression tag	UNP C3SHQ8
SA	407	ARG	-	expression tag	UNP C3SHQ8
SA	408	GLU	-	expression tag	UNP C3SHQ8
SA	409	ASN	-	expression tag	UNP C3SHQ8
SA	410	LEU	-	expression tag	UNP C3SHQ8
SA	411	TYR	-	expression tag	UNP C3SHQ8
SA	412	PHE	-	expression tag	UNP C3SHQ8
SA	413	GLN	-	expression tag	UNP C3SHQ8
SA	414	GLY	-	expression tag	UNP C3SHQ8
SA	415	GLY	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
SA	416	SER	-	expression tag	UNP C3SHQ8
UA	1	MET	-	initiating methionine	UNP C3SHQ8
UA	2	GLY	-	expression tag	UNP C3SHQ8
UA	3	SER	-	expression tag	UNP C3SHQ8
UA	4	SER	-	expression tag	UNP C3SHQ8
UA	5	HIS	-	expression tag	UNP C3SHQ8
UA	6	HIS	-	expression tag	UNP C3SHQ8
UA	7	HIS	-	expression tag	UNP C3SHQ8
UA	8	HIS	-	expression tag	UNP C3SHQ8
UA	9	HIS	-	expression tag	UNP C3SHQ8
UA	10	HIS	-	expression tag	UNP C3SHQ8
UA	11	SER	-	expression tag	UNP C3SHQ8
UA	12	SER	-	expression tag	UNP C3SHQ8
UA	13	GLY	-	expression tag	UNP C3SHQ8
UA	14	LEU	-	expression tag	UNP C3SHQ8
UA	15	VAL	-	expression tag	UNP C3SHQ8
UA	16	PRO	-	expression tag	UNP C3SHQ8
UA	17	ARG	-	expression tag	UNP C3SHQ8
UA	18	GLY	-	expression tag	UNP C3SHQ8
UA	19	SER	-	expression tag	UNP C3SHQ8
UA	20	HIS	-	expression tag	UNP C3SHQ8
UA	21	MET	-	expression tag	UNP C3SHQ8
UA	388	ASN	-	expression tag	UNP C3SHQ8
UA	389	SER	-	expression tag	UNP C3SHQ8
UA	390	SER	-	expression tag	UNP C3SHQ8
UA	391	SER	-	expression tag	UNP C3SHQ8
UA	392	ASN	-	expression tag	UNP C3SHQ8
UA	393	ASN	-	expression tag	UNP C3SHQ8
UA	394	ASN	-	expression tag	UNP C3SHQ8
UA	395	ASN	-	expression tag	UNP C3SHQ8
UA	396	ASN	-	expression tag	UNP C3SHQ8
UA	397	ASN	-	expression tag	UNP C3SHQ8
UA	398	ASN	-	expression tag	UNP C3SHQ8
UA	399	ASN	-	expression tag	UNP C3SHQ8
UA	400	ASN	-	expression tag	UNP C3SHQ8
UA	401	ASN	-	expression tag	UNP C3SHQ8
UA	402	LEU	-	expression tag	UNP C3SHQ8
UA	403	GLY	-	expression tag	UNP C3SHQ8
UA	404	ILE	-	expression tag	UNP C3SHQ8
UA	405	GLU	-	expression tag	UNP C3SHQ8
UA	406	GLY	-	expression tag	UNP C3SHQ8
UA	407	ARG	-	expression tag	UNP C3SHQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
UA	408	GLU	-	expression tag	UNP C3SHQ8
UA	409	ASN	-	expression tag	UNP C3SHQ8
UA	410	LEU	-	expression tag	UNP C3SHQ8
UA	411	TYR	-	expression tag	UNP C3SHQ8
UA	412	PHE	-	expression tag	UNP C3SHQ8
UA	413	GLN	-	expression tag	UNP C3SHQ8
UA	414	GLY	-	expression tag	UNP C3SHQ8
UA	415	GLY	-	expression tag	UNP C3SHQ8
UA	416	SER	-	expression tag	UNP C3SHQ8
WA	1	MET	-	initiating methionine	UNP C3SHQ8
WA	2	GLY	-	expression tag	UNP C3SHQ8
WA	3	SER	-	expression tag	UNP C3SHQ8
WA	4	SER	-	expression tag	UNP C3SHQ8
WA	5	HIS	-	expression tag	UNP C3SHQ8
WA	6	HIS	-	expression tag	UNP C3SHQ8
WA	7	HIS	-	expression tag	UNP C3SHQ8
WA	8	HIS	-	expression tag	UNP C3SHQ8
WA	9	HIS	-	expression tag	UNP C3SHQ8
WA	10	HIS	-	expression tag	UNP C3SHQ8
WA	11	SER	-	expression tag	UNP C3SHQ8
WA	12	SER	-	expression tag	UNP C3SHQ8
WA	13	GLY	-	expression tag	UNP C3SHQ8
WA	14	LEU	-	expression tag	UNP C3SHQ8
WA	15	VAL	-	expression tag	UNP C3SHQ8
WA	16	PRO	-	expression tag	UNP C3SHQ8
WA	17	ARG	-	expression tag	UNP C3SHQ8
WA	18	GLY	-	expression tag	UNP C3SHQ8
WA	19	SER	-	expression tag	UNP C3SHQ8
WA	20	HIS	-	expression tag	UNP C3SHQ8
WA	21	MET	-	expression tag	UNP C3SHQ8
WA	388	ASN	-	expression tag	UNP C3SHQ8
WA	389	SER	-	expression tag	UNP C3SHQ8
WA	390	SER	-	expression tag	UNP C3SHQ8
WA	391	SER	-	expression tag	UNP C3SHQ8
WA	392	ASN	-	expression tag	UNP C3SHQ8
WA	393	ASN	-	expression tag	UNP C3SHQ8
WA	394	ASN	-	expression tag	UNP C3SHQ8
WA	395	ASN	-	expression tag	UNP C3SHQ8
WA	396	ASN	-	expression tag	UNP C3SHQ8
WA	397	ASN	-	expression tag	UNP C3SHQ8
WA	398	ASN	-	expression tag	UNP C3SHQ8
WA	399	ASN	-	expression tag	UNP C3SHQ8

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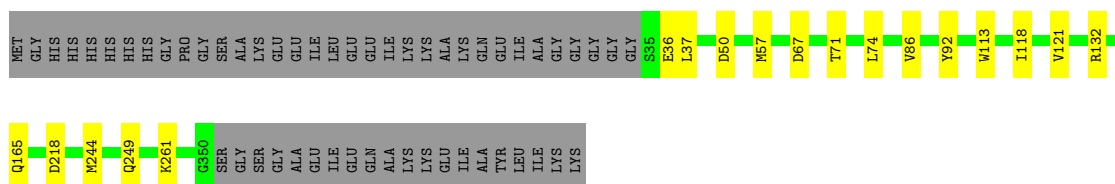
Chain	Residue	Modelled	Actual	Comment	Reference
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WA	402	LEU	-	expression tag	UNP C3SHQ8
WA	403	GLY	-	expression tag	UNP C3SHQ8
WA	404	ILE	-	expression tag	UNP C3SHQ8
WA	405	GLU	-	expression tag	UNP C3SHQ8
WA	406	GLY	-	expression tag	UNP C3SHQ8
WA	407	ARG	-	expression tag	UNP C3SHQ8
WA	408	GLU	-	expression tag	UNP C3SHQ8
WA	409	ASN	-	expression tag	UNP C3SHQ8
WA	410	LEU	-	expression tag	UNP C3SHQ8
WA	411	TYR	-	expression tag	UNP C3SHQ8
WA	412	PHE	-	expression tag	UNP C3SHQ8
WA	413	GLN	-	expression tag	UNP C3SHQ8
WA	414	GLY	-	expression tag	UNP C3SHQ8
WA	415	GLY	-	expression tag	UNP C3SHQ8
WA	416	SER	-	expression tag	UNP C3SHQ8

3 Residue-property plots [i](#)

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

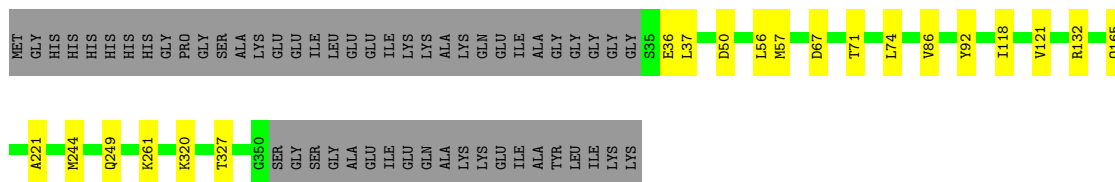
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain A: 



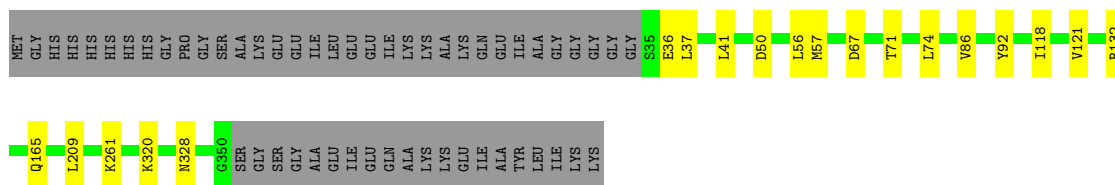
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain C: 



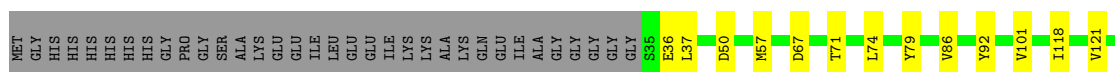
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

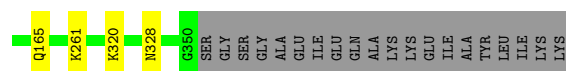
Chain E: 



- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

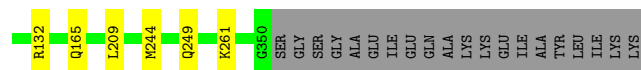
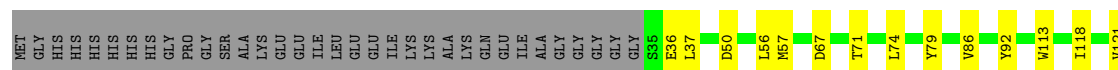
Chain G: 





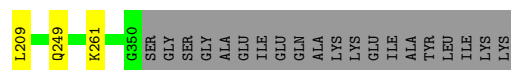
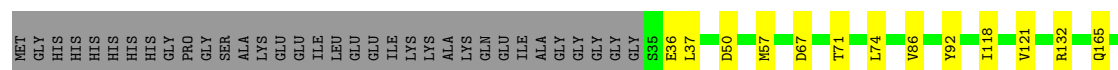
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain S: 80% 5% 15%



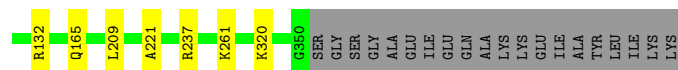
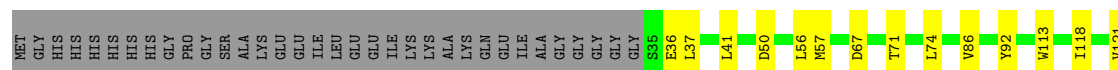
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain V: 81% 15%



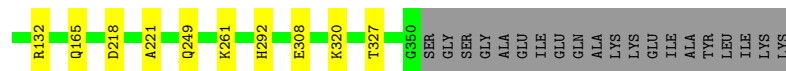
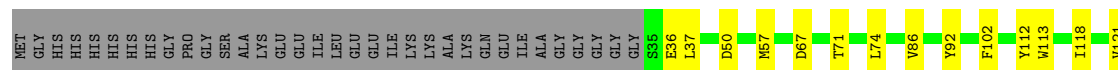
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain X: 80% 6% 15%



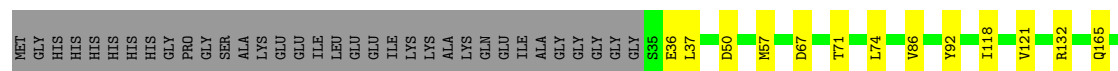
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

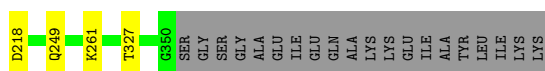
Chain Z: 79% 6% 15%



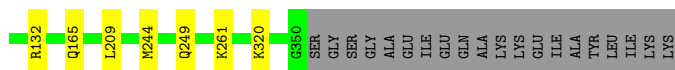
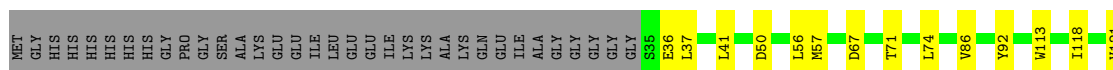
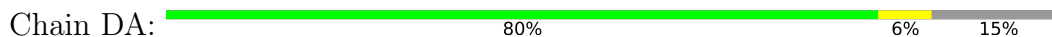
- Molecule 1: DARPin,Ferritin heavy chain, N-terminally processed

Chain BA: 81% 5% 15%

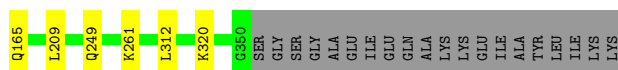
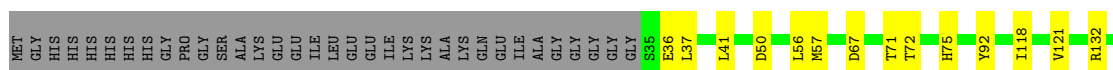
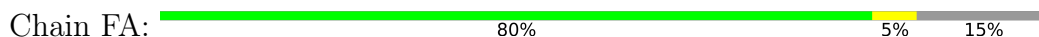




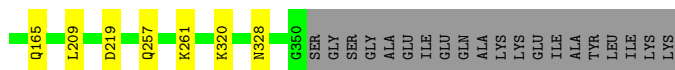
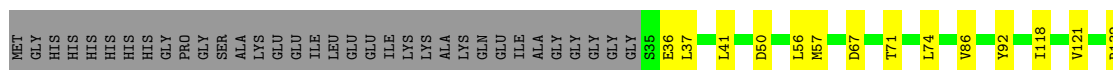
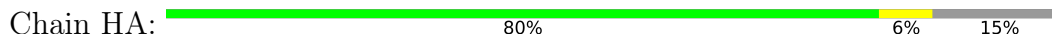
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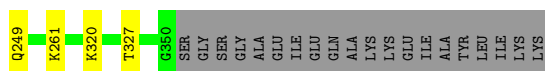
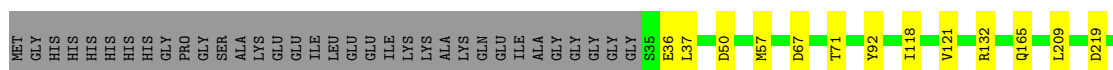
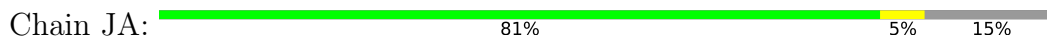
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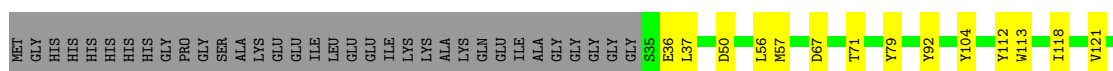
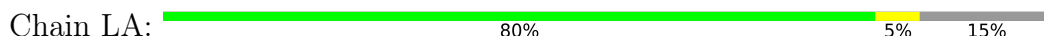
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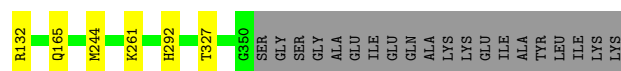


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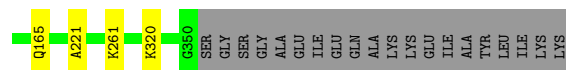
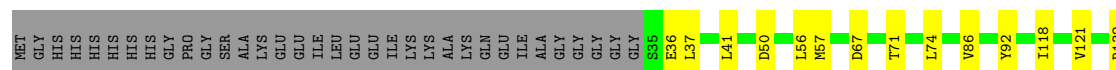
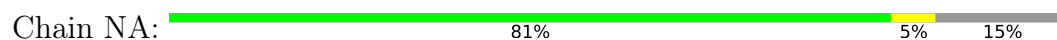


- Molecule 1: DARPin, Ferritin heavy chain, N-terminally processed

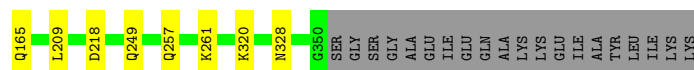
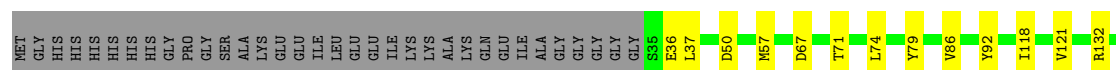
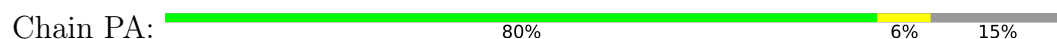




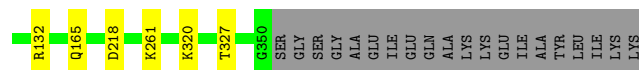
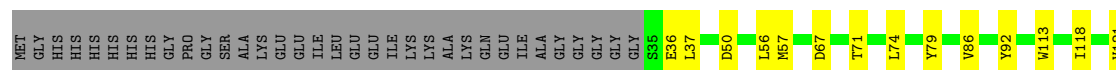
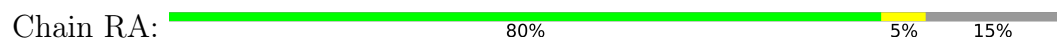
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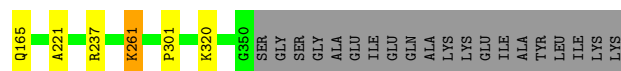
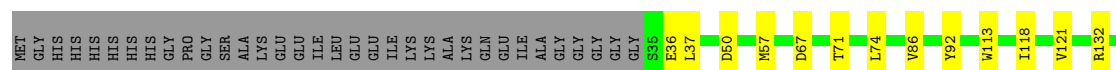
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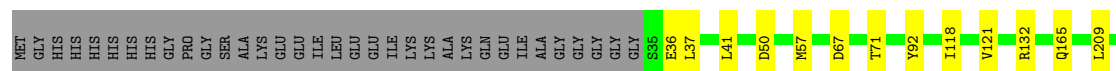
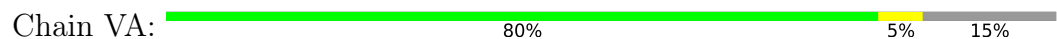
- Molecule 1: DARPin, Ferritin heavy chain, N-terminally processed

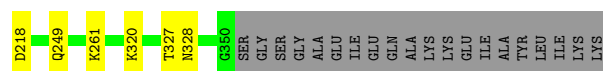


- Molecule 1: DARPin, Ferritin heavy chain, N-terminally processed

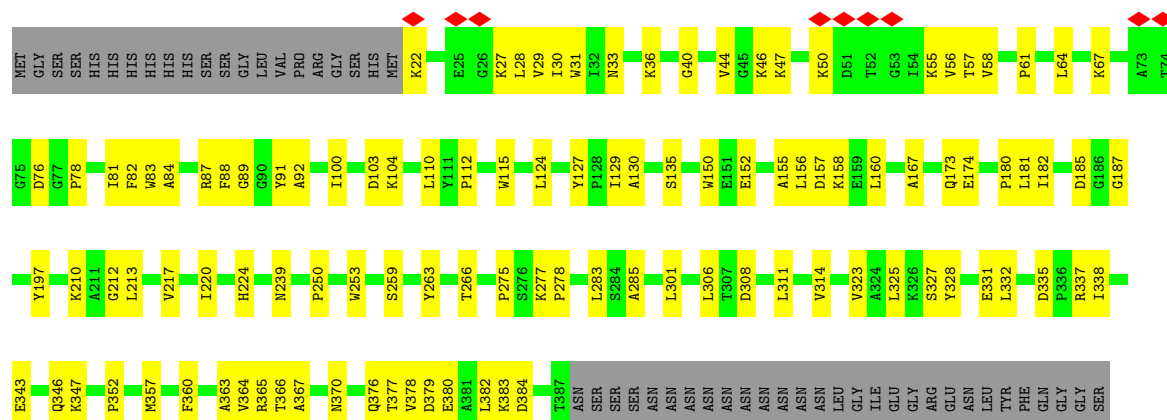


- Molecule 1: DARPin, Ferritin heavy chain, N-terminally processed

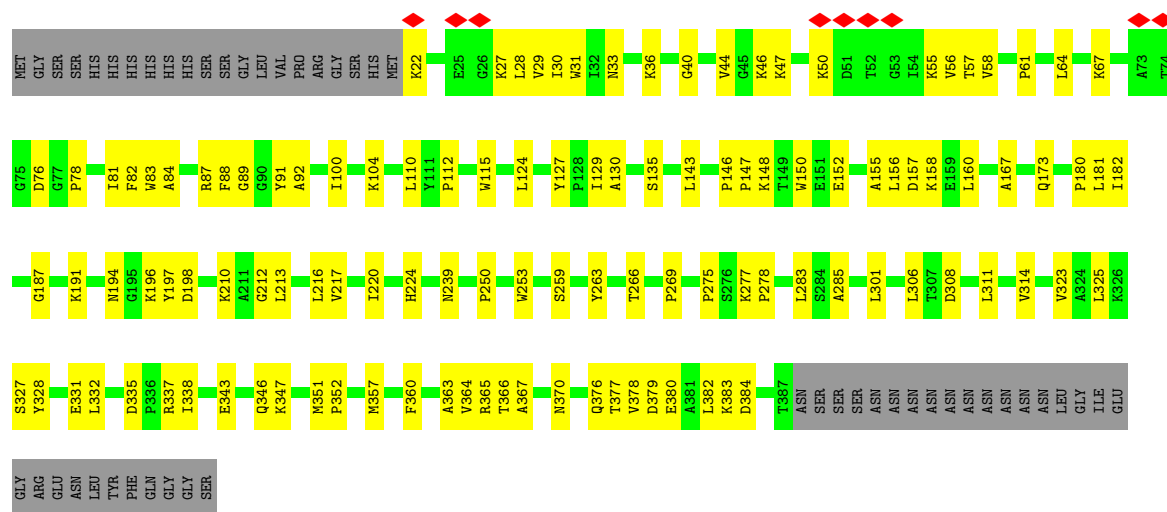




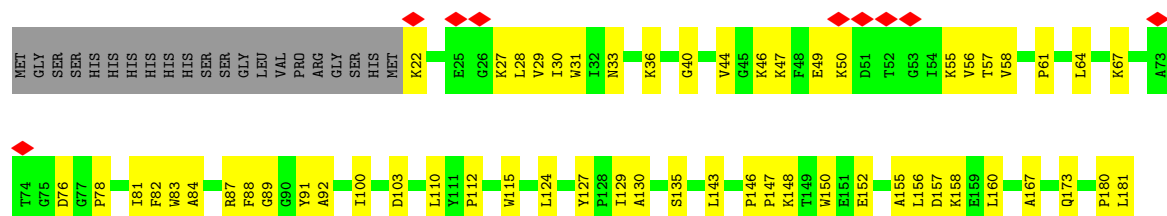
• Molecule 2: Maltodextrin-binding protein



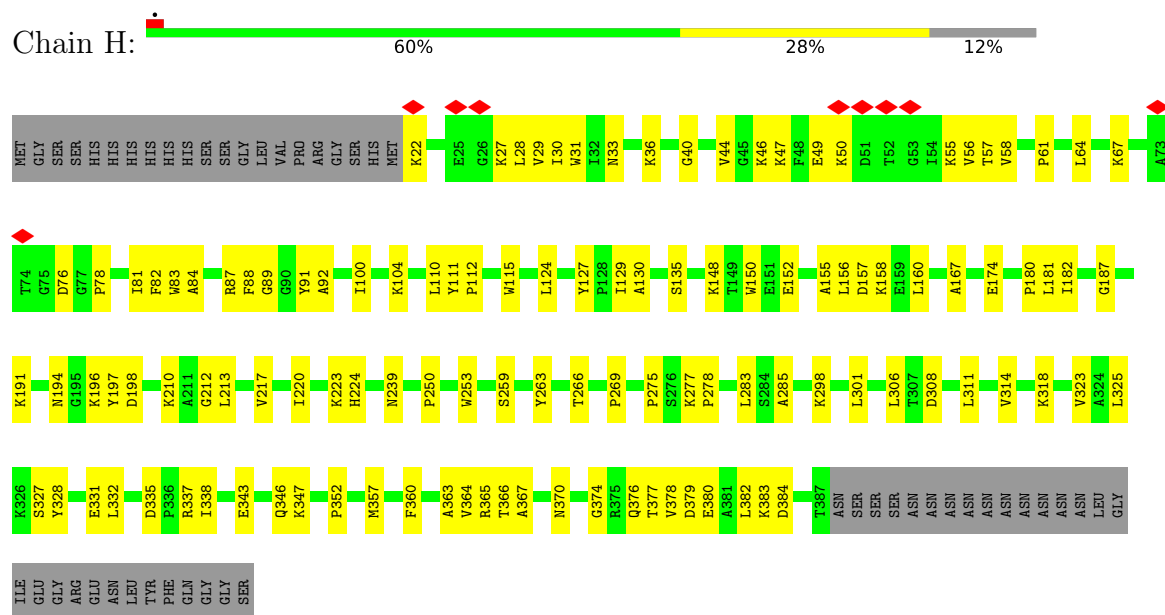
• Molecule 2: Maltodextrin-binding protein



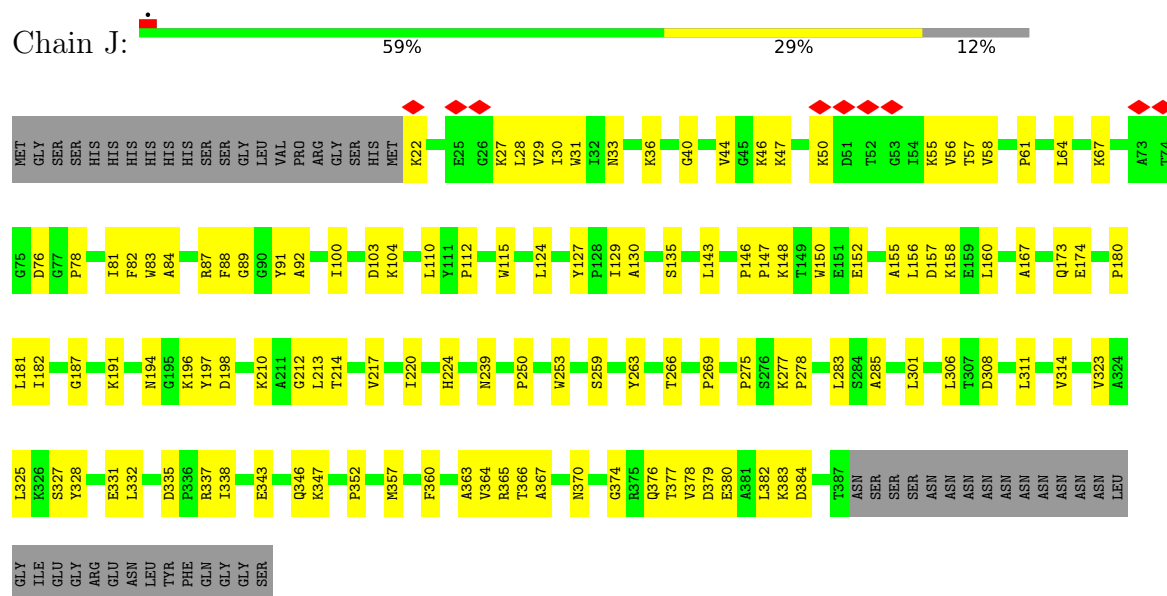
• Molecule 2: Maltodextrin-binding protein



- Molecule 2: Maltodextrin-binding protein



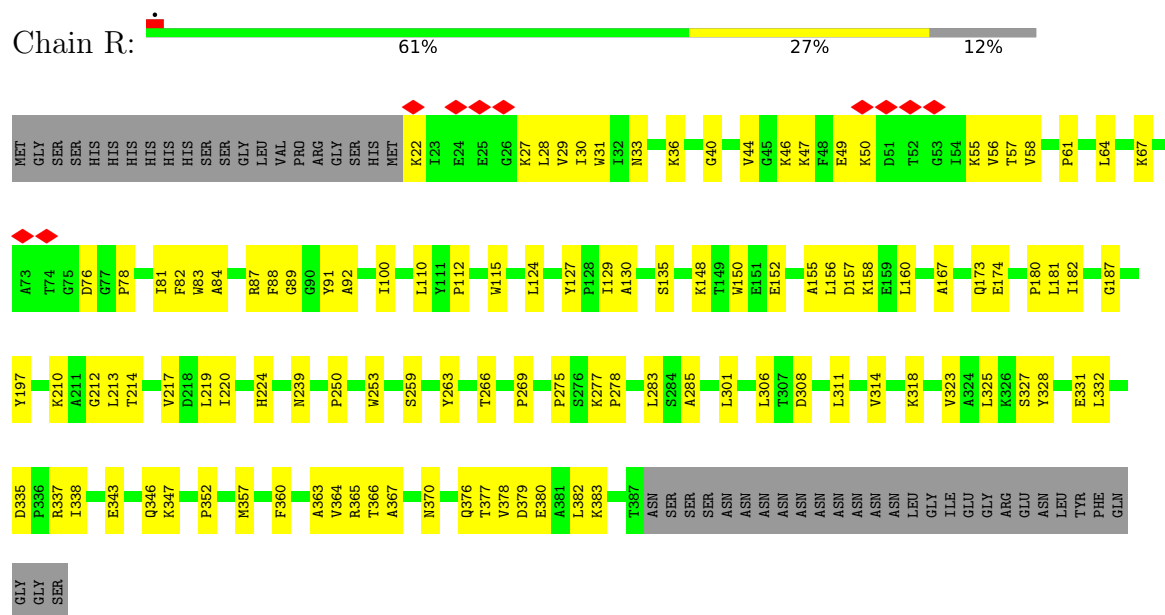
- Molecule 2: Maltodextrin-binding protein



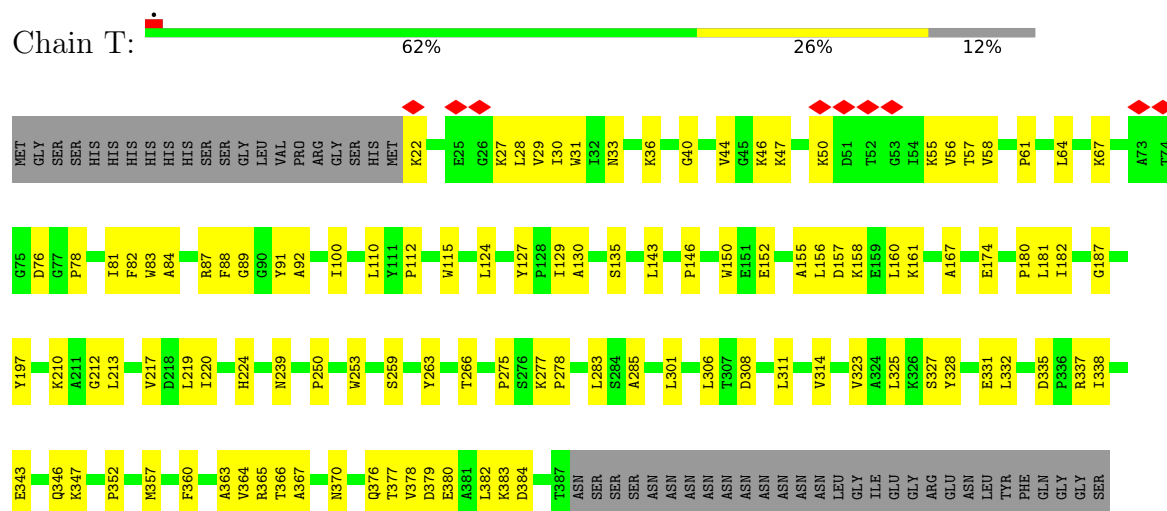
- Molecule 2: Maltodextrin-binding protein



- Molecule 2: Maltodextrin-binding protein

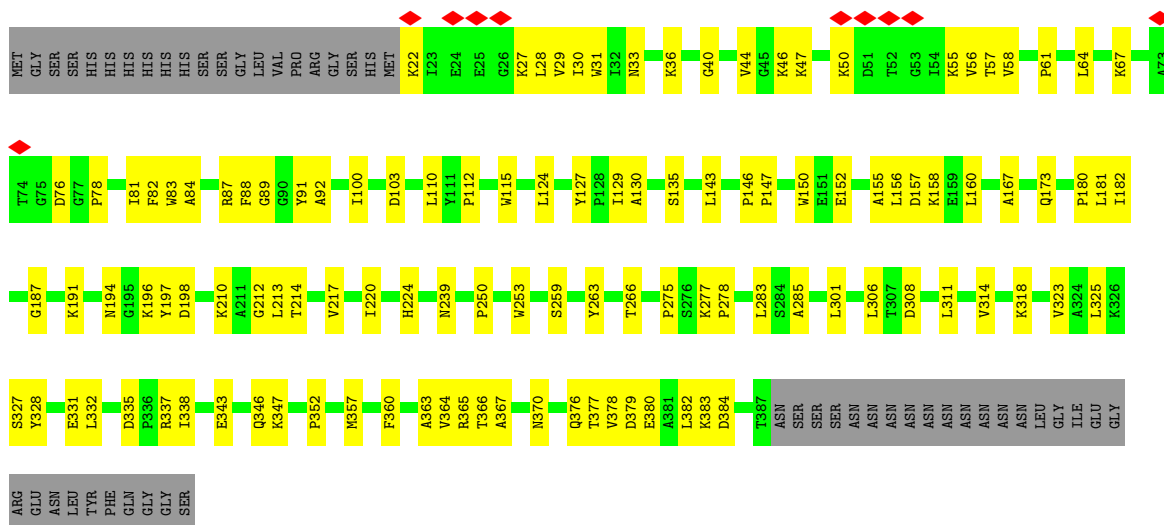


- Molecule 2: Maltodextrin-binding protein

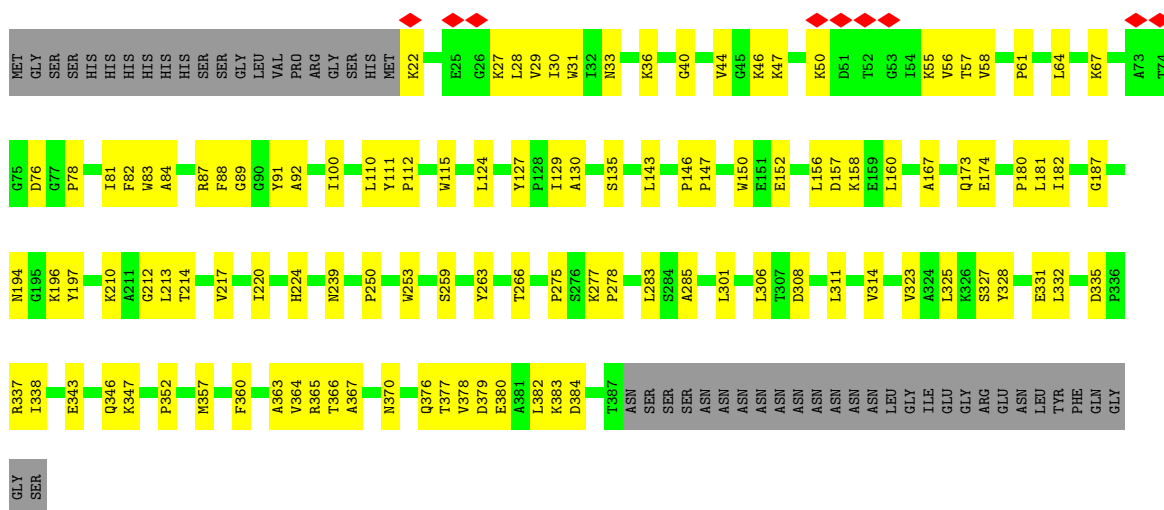


- Molecule 2: Maltodextrin-binding protein

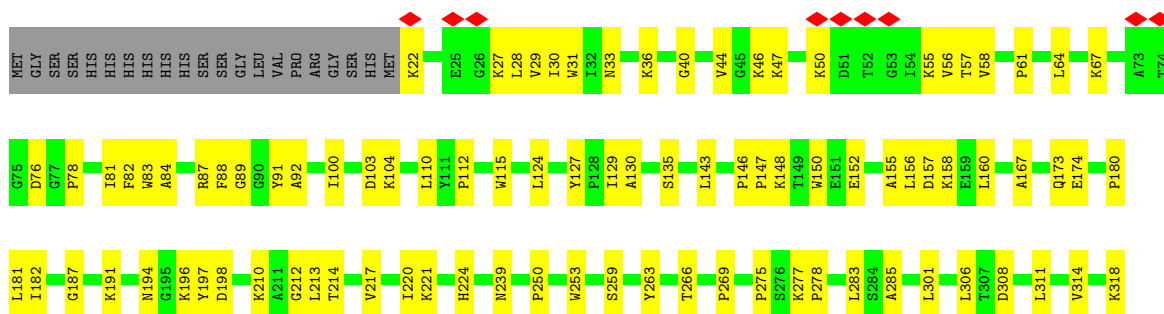


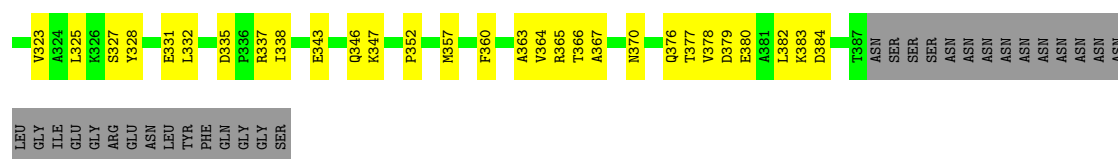


- Molecule 2: Maltodextrin-binding protein

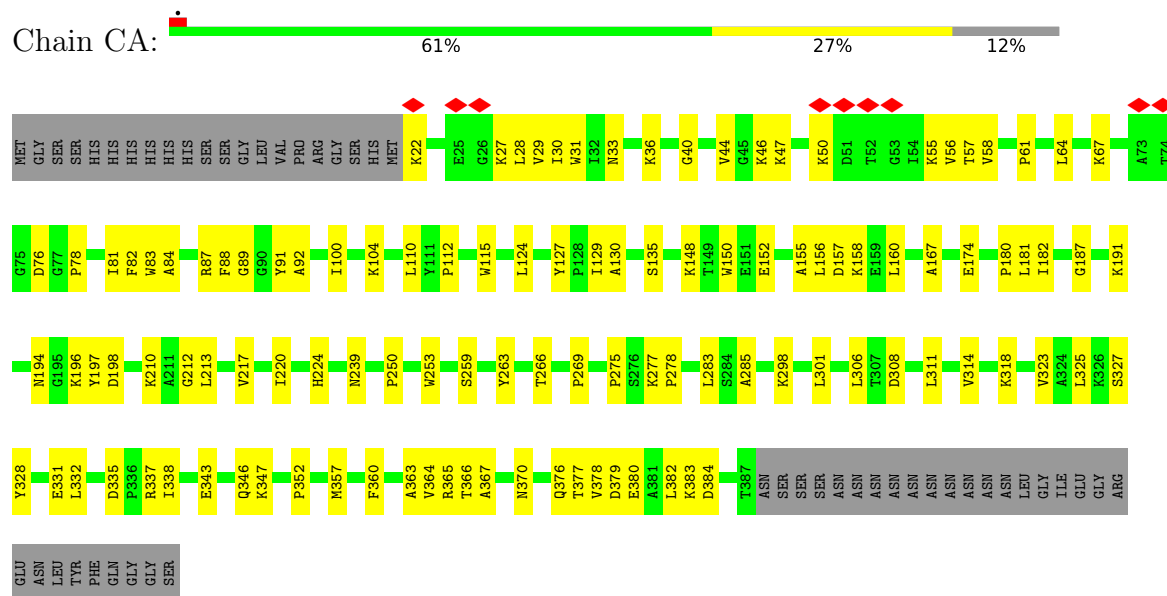


- Molecule 2: Maltodextrin-binding protein

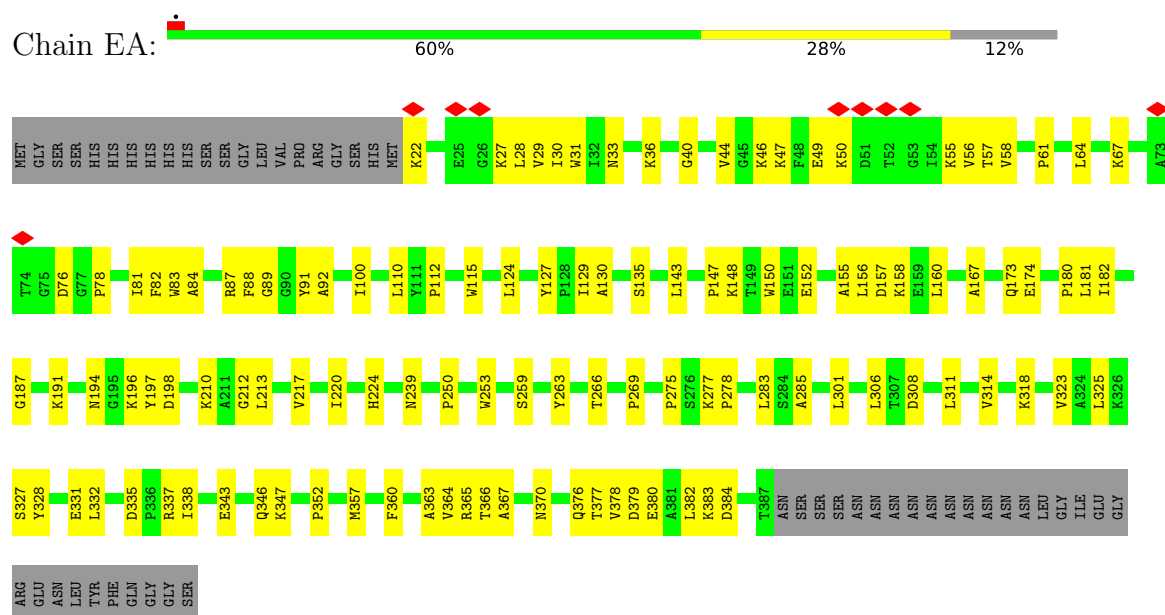




• Molecule 2: Maltodextrin-binding protein

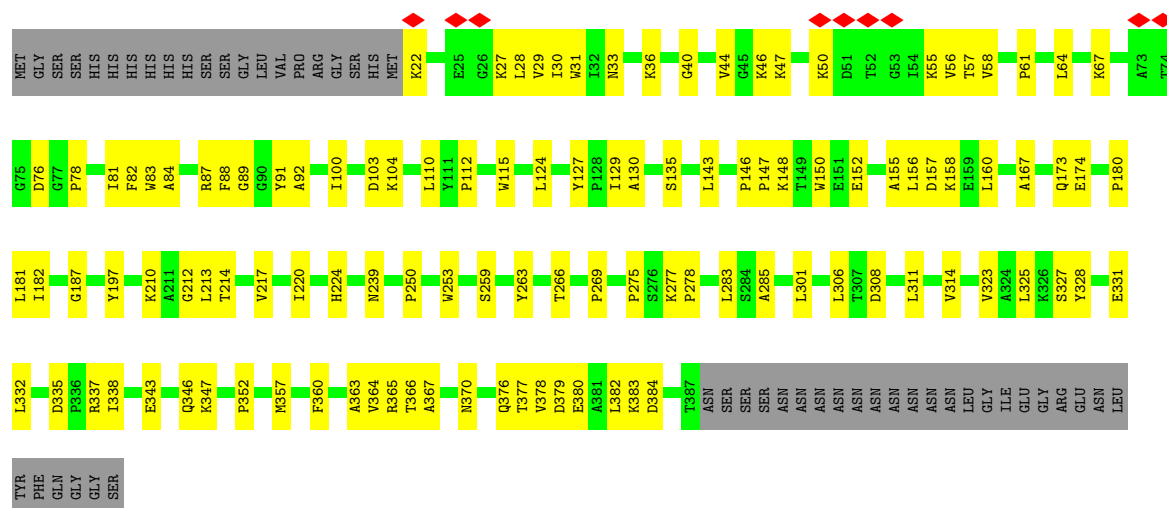


• Molecule 2: Maltodextrin-binding protein

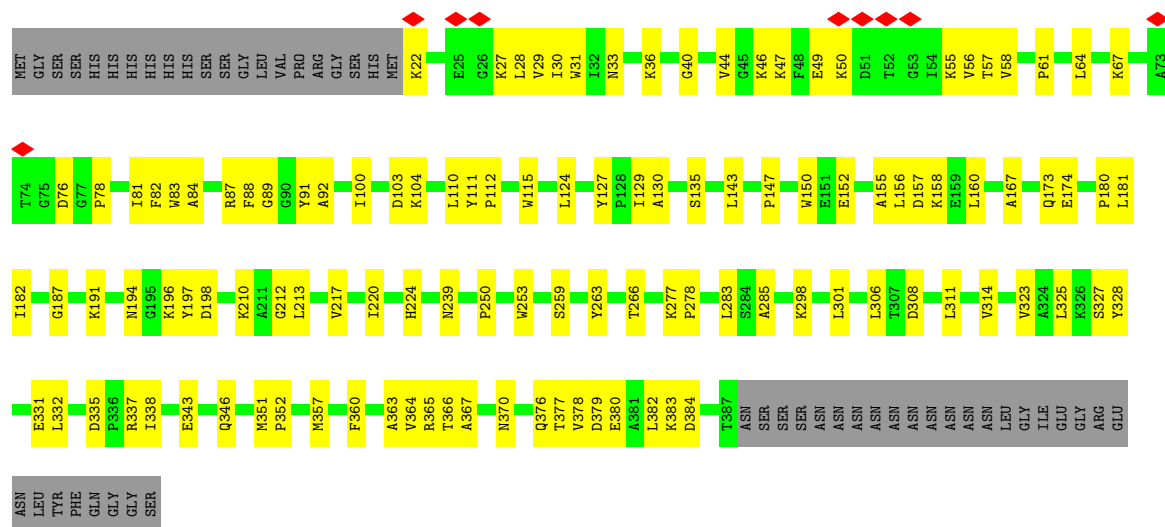


• Molecule 2: Maltodextrin-binding protein

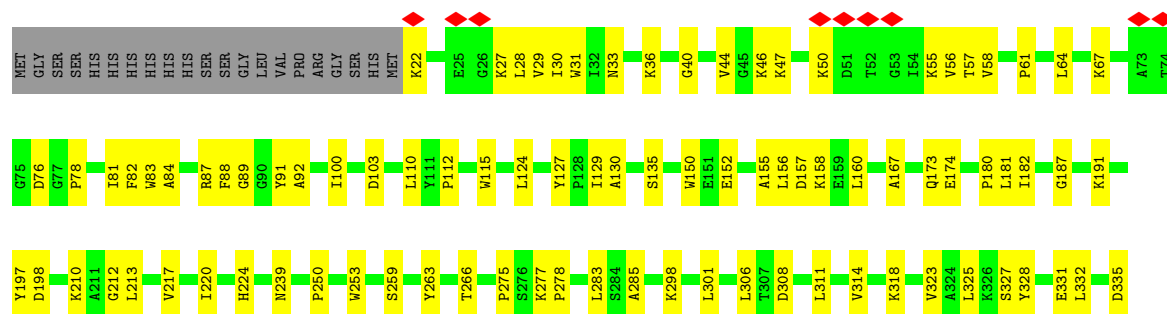


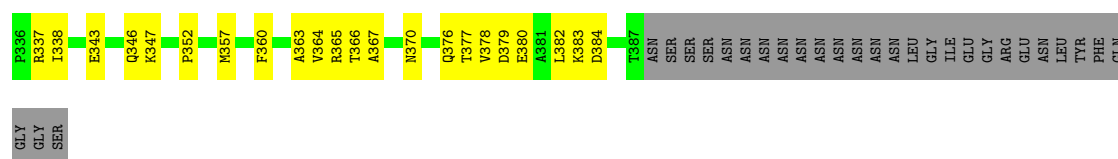


• Molecule 2: Maltodextrin-binding protein



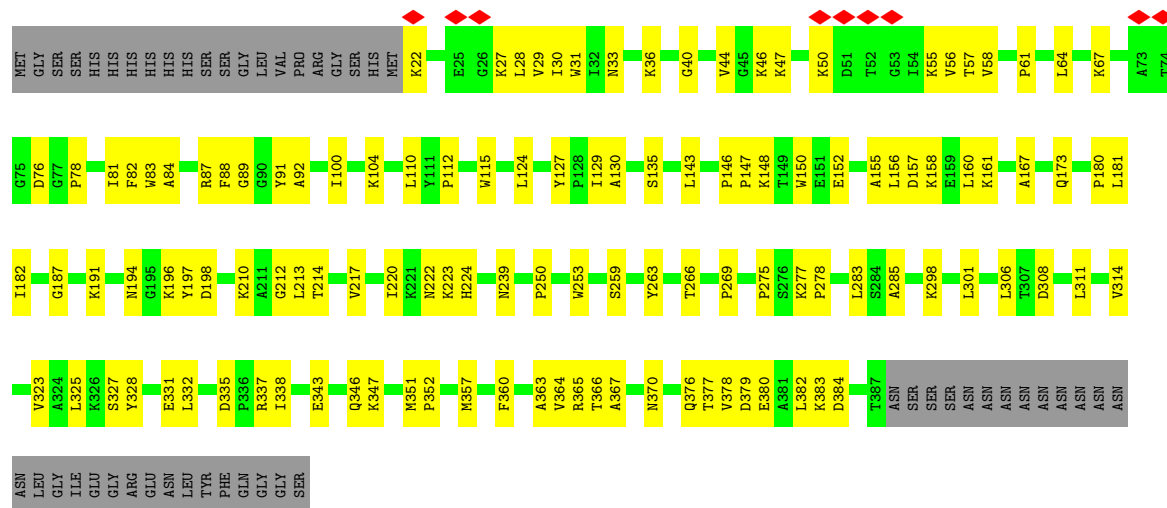
• Molecule 2: Maltodextrin-binding protein





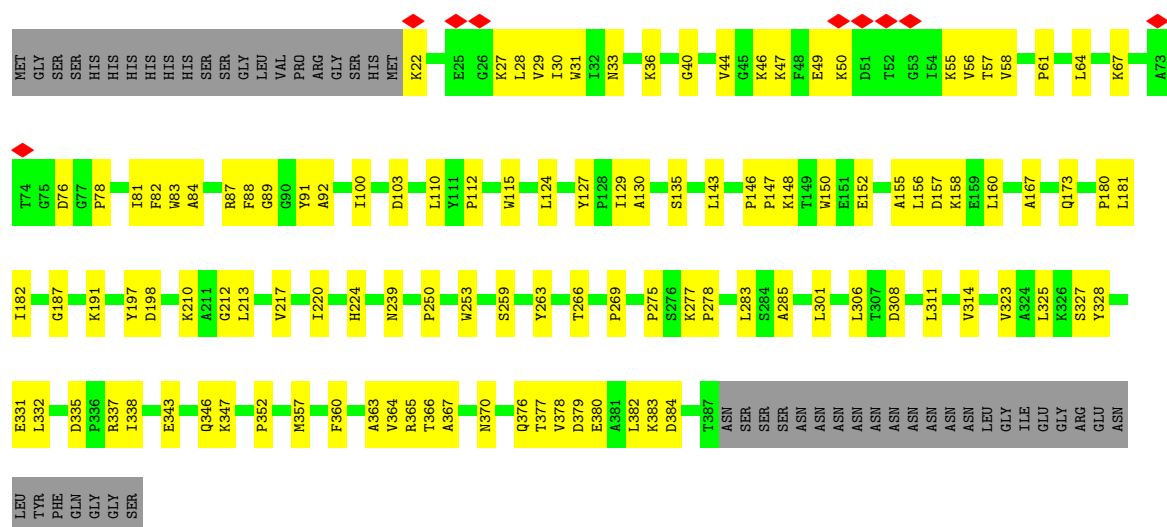
• Molecule 2: Maltodextrin-binding protein

Chain MA: 59% 29% 12%



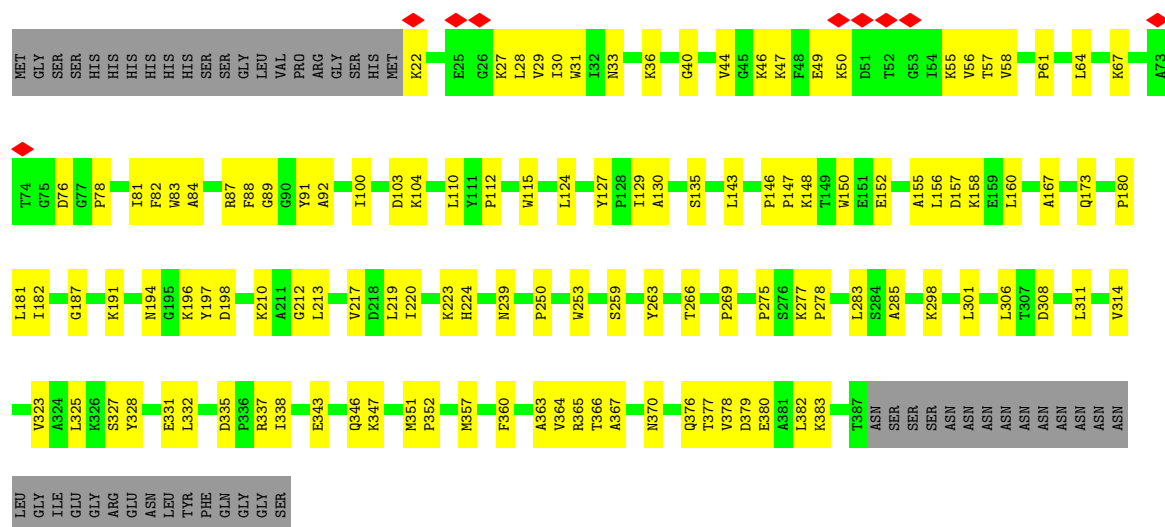
• Molecule 2: Maltodextrin-binding protein

Chain OA: 61% 27% 12%

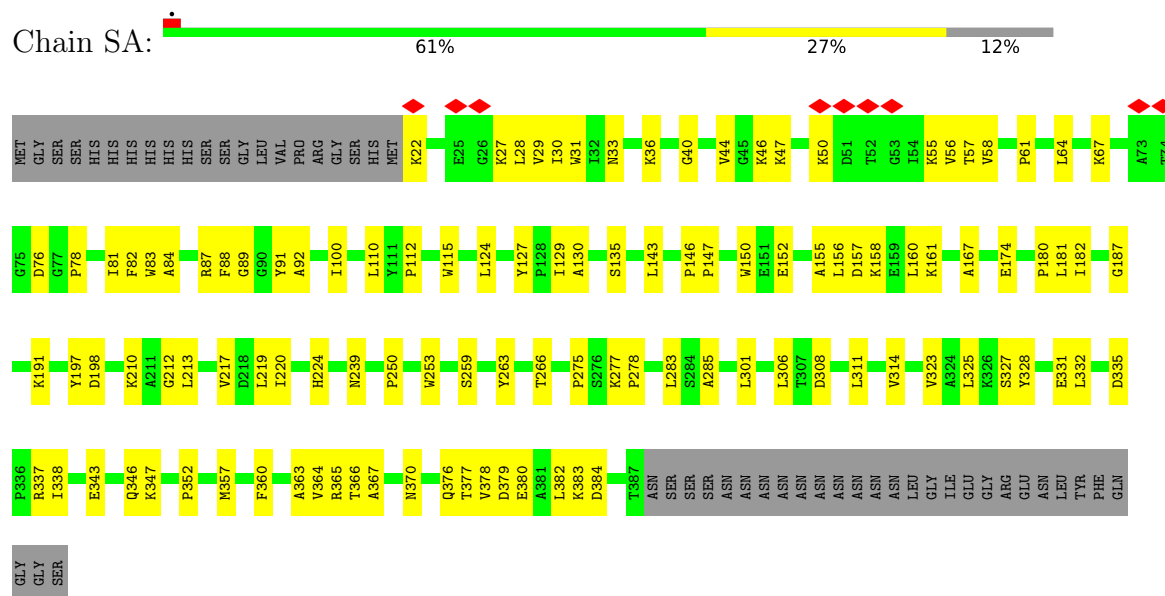


• Molecule 2: Maltodextrin-binding protein

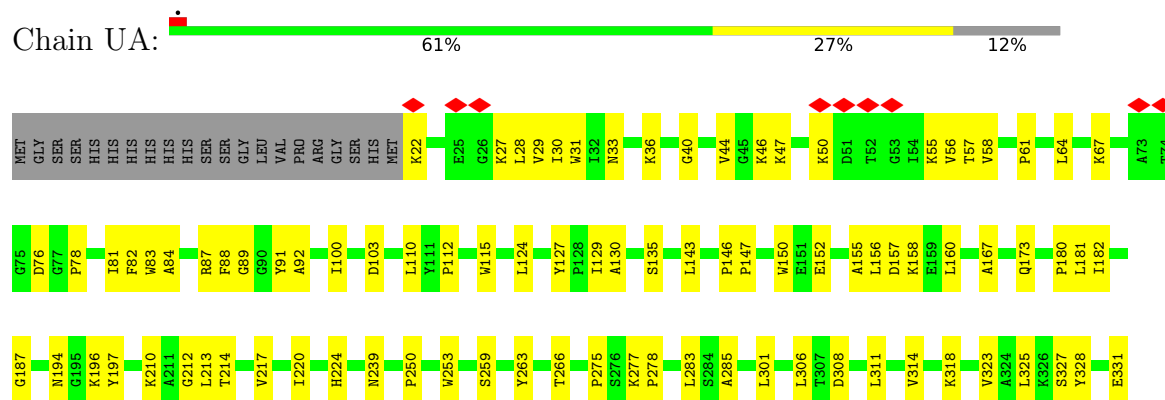
Chain QA: 59% 29% 12%



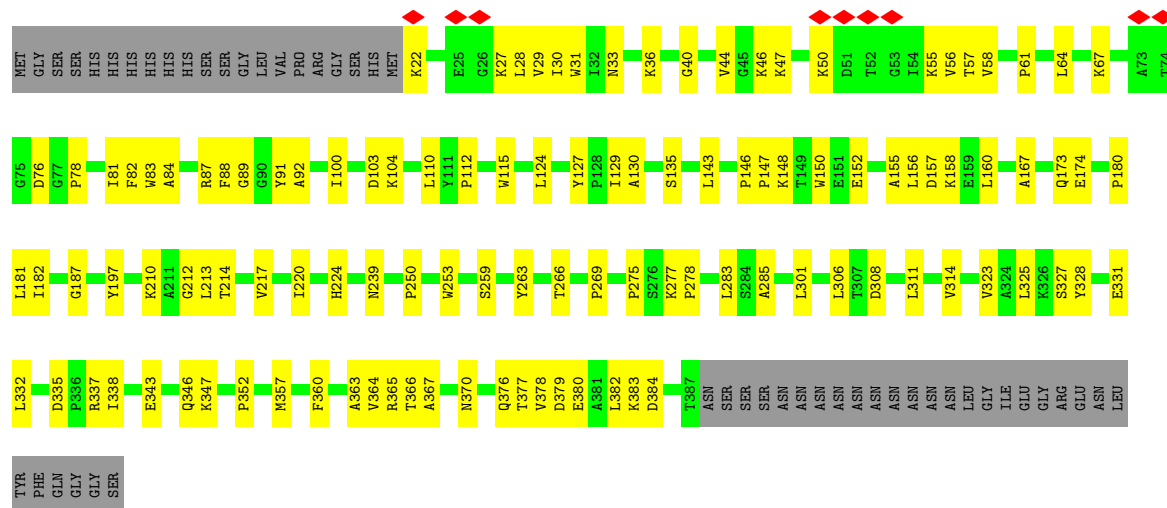
- Molecule 2: Maltodextrin-binding protein



- Molecule 2: Maltodextrin-binding protein



- Molecule 2: Maltodextrin-binding protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91926	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.127	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	344.32, 344.32, 344.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	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	0.33	0/2533	0.44	0/3431
1	BA	0.33	0/2533	0.44	0/3431
1	C	0.33	0/2533	0.44	0/3431
1	DA	0.33	0/2533	0.44	0/3431
1	E	0.33	0/2533	0.45	0/3431
1	FA	0.33	0/2533	0.44	0/3431
1	G	0.33	0/2533	0.45	0/3431
1	HA	0.33	0/2533	0.44	0/3431
1	I	0.33	0/2533	0.44	0/3431
1	JA	0.33	0/2533	0.44	0/3431
1	K	0.33	0/2533	0.44	0/3431
1	LA	0.33	0/2533	0.44	0/3431
1	M	0.33	0/2533	0.44	0/3431
1	NA	0.33	0/2533	0.44	0/3431
1	O	0.33	0/2533	0.44	0/3431
1	PA	0.33	0/2533	0.45	0/3431
1	Q	0.33	0/2533	0.45	0/3431
1	RA	0.33	0/2533	0.44	0/3431
1	S	0.33	0/2533	0.44	0/3431
1	TA	0.33	0/2533	0.44	0/3431
1	V	0.33	0/2533	0.44	0/3431
1	VA	0.33	0/2533	0.44	0/3431
1	X	0.33	0/2533	0.44	0/3431
1	Z	0.33	0/2533	0.44	0/3431
2	AA	0.17	0/2957	0.45	0/4014
2	B	0.17	0/2957	0.45	0/4014
2	CA	0.17	0/2957	0.45	0/4014
2	D	0.17	0/2957	0.45	0/4014
2	EA	0.17	0/2957	0.45	0/4014
2	F	0.17	0/2957	0.45	0/4014
2	GA	0.17	0/2957	0.45	0/4014
2	H	0.17	0/2957	0.45	0/4014
2	IA	0.17	0/2957	0.45	0/4014
2	J	0.17	0/2957	0.45	0/4014

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	KA	0.17	0/2957	0.45	0/4014
2	L	0.17	0/2957	0.45	0/4014
2	MA	0.17	0/2957	0.45	0/4014
2	N	0.17	0/2957	0.45	0/4014
2	OA	0.17	0/2957	0.45	0/4014
2	P	0.17	0/2957	0.45	0/4014
2	QA	0.17	0/2957	0.45	0/4014
2	R	0.17	0/2957	0.45	0/4014
2	SA	0.17	0/2957	0.45	0/4014
2	T	0.17	0/2957	0.45	0/4014
2	UA	0.17	0/2957	0.45	0/4014
2	W	0.17	0/2957	0.45	0/4014
2	WA	0.17	0/2957	0.45	0/4014
2	Y	0.17	0/2957	0.45	0/4014
All	All	0.26	0/131760	0.45	0/178680

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	2485	0	2414	12	0
1	BA	2485	0	2414	11	0
1	C	2485	0	2414	16	0
1	DA	2485	0	2414	14	0
1	E	2485	0	2414	15	0
1	FA	2485	0	2414	13	0
1	G	2485	0	2414	17	0
1	HA	2485	0	2414	16	0
1	I	2485	0	2414	13	0
1	JA	2485	0	2414	11	0
1	K	2485	0	2414	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	2485	0	2414	18	0
1	M	2485	0	2414	14	0
1	NA	2485	0	2414	14	0
1	O	2485	0	2414	13	0
1	PA	2485	0	2414	17	0
1	Q	2485	0	2414	12	0
1	RA	2485	0	2414	15	0
1	S	2485	0	2414	13	0
1	TA	2485	0	2414	14	0
1	V	2485	0	2414	9	0
1	VA	2485	0	2414	15	0
1	X	2485	0	2414	17	0
1	Z	2485	0	2414	20	0
2	AA	2870	0	2847	78	0
2	B	2870	0	2847	69	0
2	CA	2870	0	2847	69	0
2	D	2870	0	2847	72	0
2	EA	2870	0	2847	71	0
2	F	2870	0	2847	71	0
2	GA	2870	0	2847	71	0
2	H	2870	0	2847	73	0
2	IA	2870	0	2847	72	0
2	J	2870	0	2847	74	0
2	KA	2870	0	2847	68	0
2	L	2870	0	2847	71	0
2	MA	2870	0	2847	80	0
2	N	2870	0	2847	69	0
2	OA	2870	0	2847	70	0
2	P	2870	0	2847	72	0
2	QA	2870	0	2847	73	0
2	R	2870	0	2847	67	0
2	SA	2870	0	2847	71	0
2	T	2870	0	2847	67	0
2	UA	2870	0	2847	72	0
2	W	2870	0	2847	70	0
2	WA	2870	0	2847	71	0
2	Y	2870	0	2847	71	0
All	All	128520	0	126264	1969	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 8.

All (1969) 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:LA:79:TYR:OH	2:MA:161:LYS:NZ	1.96	0.99
1:G:327:THR:HG21	1:Z:218:ASP:O	1.62	0.99
1:G:218:ASP:O	1:I:327:THR:HG21	1.66	0.96
1:RA:79:TYR:OH	2:SA:161:LYS:NZ	2.09	0.84
1:LA:113:TRP:HZ3	2:MA:158:LYS:HA	1.51	0.76
1:M:327:THR:HG21	1:RA:218:ASP:O	1.88	0.73
1:E:320:LYS:HD3	1:VA:249:GLN:HA	1.72	0.69
1:K:320:LYS:HD3	1:PA:249:GLN:HA	1.75	0.68
1:G:249:GLN:HA	1:FA:320:LYS:HD3	1.75	0.68
1:K:327:THR:HG21	1:M:218:ASP:O	1.94	0.67
2:J:357:MET:O	2:J:360:PHE:HB3	1.95	0.67
2:W:352:PRO:HG2	2:W:357:MET:HE3	1.77	0.67
2:AA:357:MET:O	2:AA:360:PHE:HB3	1.95	0.67
2:D:352:PRO:HG2	2:D:357:MET:HE3	1.77	0.67
2:EA:357:MET:O	2:EA:360:PHE:HB3	1.95	0.67
2:UA:352:PRO:HG2	2:UA:357:MET:HE3	1.77	0.67
2:GA:352:PRO:HG2	2:GA:357:MET:HE3	1.77	0.66
2:MA:352:PRO:HG2	2:MA:357:MET:HE3	1.77	0.66
2:WA:357:MET:O	2:WA:360:PHE:HB3	1.95	0.66
2:R:357:MET:O	2:R:360:PHE:HB3	1.95	0.66
2:WA:352:PRO:HG2	2:WA:357:MET:HE3	1.77	0.66
2:GA:357:MET:O	2:GA:360:PHE:HB3	1.95	0.66
1:NA:221:ALA:HB3	1:PA:328:ASN:ND2	2.10	0.66
2:P:357:MET:O	2:P:360:PHE:HB3	1.95	0.66
2:T:352:PRO:HG2	2:T:357:MET:HE3	1.77	0.66
1:M:249:GLN:HA	1:JA:320:LYS:HD3	1.77	0.66
2:N:357:MET:O	2:N:360:PHE:HB3	1.95	0.66
2:T:357:MET:O	2:T:360:PHE:HB3	1.95	0.66
2:QA:352:PRO:HG2	2:QA:357:MET:HE3	1.77	0.66
2:SA:352:PRO:HG2	2:SA:357:MET:HE3	1.77	0.66
2:H:352:PRO:HG2	2:H:357:MET:HE3	1.77	0.66
2:MA:357:MET:O	2:MA:360:PHE:HB3	1.95	0.66
2:SA:357:MET:O	2:SA:360:PHE:HB3	1.95	0.66
2:F:352:PRO:HG2	2:F:357:MET:HE3	1.77	0.66
2:L:357:MET:O	2:L:360:PHE:HB3	1.95	0.66
2:T:217:VAL:HA	2:T:220:ILE:HG22	1.78	0.66
2:F:217:VAL:HA	2:F:220:ILE:HG22	1.78	0.66
2:L:352:PRO:HG2	2:L:357:MET:HE3	1.77	0.66
2:W:357:MET:O	2:W:360:PHE:HB3	1.95	0.66
2:EA:217:VAL:HA	2:EA:220:ILE:HG22	1.78	0.66
2:OA:217:VAL:HA	2:OA:220:ILE:HG22	1.78	0.66
2:OA:352:PRO:HG2	2:OA:357:MET:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:MET:O	2:B:360:PHE:HB3	1.95	0.66
2:Y:357:MET:O	2:Y:360:PHE:HB3	1.95	0.66
2:CA:352:PRO:HG2	2:CA:357:MET:HE3	1.77	0.66
2:IA:357:MET:O	2:IA:360:PHE:HB3	1.95	0.66
2:SA:217:VAL:HA	2:SA:220:ILE:HG22	1.78	0.66
2:D:217:VAL:HA	2:D:220:ILE:HG22	1.78	0.65
2:KA:352:PRO:HG2	2:KA:357:MET:HE3	1.77	0.65
2:QA:357:MET:O	2:QA:360:PHE:HB3	1.95	0.65
2:UA:357:MET:O	2:UA:360:PHE:HB3	1.95	0.65
2:B:352:PRO:HG2	2:B:357:MET:HE3	1.77	0.65
2:D:357:MET:O	2:D:360:PHE:HB3	1.95	0.65
2:N:352:PRO:HG2	2:N:357:MET:HE3	1.77	0.65
2:IA:352:PRO:HG2	2:IA:357:MET:HE3	1.77	0.65
2:KA:357:MET:O	2:KA:360:PHE:HB3	1.95	0.65
2:P:352:PRO:HG2	2:P:357:MET:HE3	1.77	0.65
2:GA:217:VAL:HA	2:GA:220:ILE:HG22	1.78	0.65
2:R:217:VAL:HA	2:R:220:ILE:HG22	1.78	0.65
2:EA:352:PRO:HG2	2:EA:357:MET:HE3	1.77	0.65
2:F:357:MET:O	2:F:360:PHE:HB3	1.95	0.65
1:I:249:GLN:HA	1:O:320:LYS:HD3	1.79	0.65
2:OA:357:MET:O	2:OA:360:PHE:HB3	1.95	0.65
2:WA:217:VAL:HA	2:WA:220:ILE:HG22	1.78	0.65
2:J:352:PRO:HG2	2:J:357:MET:HE3	1.77	0.65
2:L:27:LYS:HZ3	2:L:55:LYS:HG3	1.62	0.65
2:IA:27:LYS:HZ3	2:IA:55:LYS:HG3	1.62	0.65
2:MA:217:VAL:HA	2:MA:220:ILE:HG22	1.78	0.65
2:QA:217:VAL:HA	2:QA:220:ILE:HG22	1.78	0.65
2:H:357:MET:O	2:H:360:PHE:HB3	1.95	0.65
2:J:217:VAL:HA	2:J:220:ILE:HG22	1.78	0.65
2:AA:352:PRO:HG2	2:AA:357:MET:HE3	1.77	0.65
2:CA:217:VAL:HA	2:CA:220:ILE:HG22	1.78	0.65
2:R:352:PRO:HG2	2:R:357:MET:HE3	1.77	0.65
2:Y:217:VAL:HA	2:Y:220:ILE:HG22	1.78	0.65
2:Y:352:PRO:HG2	2:Y:357:MET:HE3	1.77	0.65
2:H:217:VAL:HA	2:H:220:ILE:HG22	1.78	0.64
2:AA:217:VAL:HA	2:AA:220:ILE:HG22	1.78	0.64
2:CA:357:MET:O	2:CA:360:PHE:HB3	1.95	0.64
2:H:152:GLU:HG3	2:H:156:LEU:HD23	1.80	0.64
2:P:217:VAL:HA	2:P:220:ILE:HG22	1.78	0.64
1:BA:249:GLN:HA	1:VA:320:LYS:HD3	1.79	0.64
2:L:152:GLU:HG3	2:L:156:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:217:VAL:HA	2:N:220:ILE:HG22	1.78	0.64
2:CA:152:GLU:HG3	2:CA:156:LEU:HD23	1.80	0.64
2:IA:152:GLU:HG3	2:IA:156:LEU:HD23	1.80	0.64
2:KA:217:VAL:HA	2:KA:220:ILE:HG22	1.78	0.64
2:UA:152:GLU:HG3	2:UA:156:LEU:HD23	1.80	0.64
2:N:152:GLU:HG3	2:N:156:LEU:HD23	1.80	0.64
2:WA:152:GLU:HG3	2:WA:156:LEU:HD23	1.80	0.64
2:B:217:VAL:HA	2:B:220:ILE:HG22	1.78	0.64
2:L:217:VAL:HA	2:L:220:ILE:HG22	1.78	0.64
2:W:152:GLU:HG3	2:W:156:LEU:HD23	1.80	0.64
2:W:217:VAL:HA	2:W:220:ILE:HG22	1.78	0.64
2:D:152:GLU:HG3	2:D:156:LEU:HD23	1.80	0.64
2:GA:152:GLU:HG3	2:GA:156:LEU:HD23	1.80	0.64
2:IA:217:VAL:HA	2:IA:220:ILE:HG22	1.78	0.64
2:MA:152:GLU:HG3	2:MA:156:LEU:HD23	1.80	0.64
2:B:152:GLU:HG3	2:B:156:LEU:HD23	1.80	0.64
2:R:152:GLU:HG3	2:R:156:LEU:HD23	1.80	0.64
2:Y:152:GLU:HG3	2:Y:156:LEU:HD23	1.80	0.63
1:Z:327:THR:HG21	1:BA:218:ASP:O	1.98	0.63
1:I:218:ASP:O	1:BA:327:THR:HG21	1.98	0.63
2:P:152:GLU:HG3	2:P:156:LEU:HD23	1.80	0.63
2:EA:152:GLU:HG3	2:EA:156:LEU:HD23	1.80	0.63
1:LA:113:TRP:CZ3	2:MA:158:LYS:HA	2.32	0.63
2:SA:187:GLY:O	2:SA:277:LYS:NZ	2.30	0.63
1:C:221:ALA:HB3	1:E:328:ASN:ND2	2.13	0.63
2:T:187:GLY:O	2:T:277:LYS:NZ	2.30	0.63
2:CA:27:LYS:HZ1	2:CA:57:THR:HG23	1.64	0.63
2:KA:152:GLU:HG3	2:KA:156:LEU:HD23	1.80	0.63
2:H:27:LYS:HZ1	2:H:57:THR:HG23	1.64	0.63
2:UA:217:VAL:HA	2:UA:220:ILE:HG22	1.78	0.63
2:F:187:GLY:O	2:F:277:LYS:NZ	2.30	0.63
2:AA:152:GLU:HG3	2:AA:156:LEU:HD23	1.80	0.63
2:N:380:GLU:HA	2:N:383:LYS:HE2	1.81	0.63
2:T:152:GLU:HG3	2:T:156:LEU:HD23	1.80	0.63
2:SA:152:GLU:HG3	2:SA:156:LEU:HD23	1.80	0.63
2:J:152:GLU:HG3	2:J:156:LEU:HD23	1.80	0.63
2:OA:187:GLY:O	2:OA:277:LYS:NZ	2.30	0.63
2:D:187:GLY:O	2:D:277:LYS:NZ	2.30	0.62
2:Y:380:GLU:HA	2:Y:383:LYS:HE2	1.81	0.62
2:QA:152:GLU:HG3	2:QA:156:LEU:HD23	1.80	0.62
1:M:244:MET:HE1	1:PA:209:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:187:GLY:O	2:AA:277:LYS:NZ	2.30	0.62
2:W:380:GLU:HA	2:W:383:LYS:HE2	1.81	0.62
2:KA:380:GLU:HA	2:KA:383:LYS:HE2	1.81	0.62
2:UA:380:GLU:HA	2:UA:383:LYS:HE2	1.81	0.62
2:F:152:GLU:HG3	2:F:156:LEU:HD23	1.80	0.62
2:QA:380:GLU:HA	2:QA:383:LYS:HE2	1.81	0.62
2:J:187:GLY:O	2:J:277:LYS:NZ	2.30	0.62
2:P:380:GLU:HA	2:P:383:LYS:HE2	1.81	0.62
2:MA:187:GLY:O	2:MA:277:LYS:NZ	2.30	0.62
2:OA:152:GLU:HG3	2:OA:156:LEU:HD23	1.80	0.62
2:B:380:GLU:HA	2:B:383:LYS:HE2	1.81	0.62
2:L:380:GLU:HA	2:L:383:LYS:HE2	1.81	0.62
2:CA:187:GLY:O	2:CA:277:LYS:NZ	2.30	0.62
2:IA:380:GLU:HA	2:IA:383:LYS:HE2	1.81	0.62
2:H:187:GLY:O	2:H:277:LYS:NZ	2.30	0.62
1:G:327:THR:CG2	1:Z:218:ASP:O	2.43	0.62
2:T:380:GLU:HA	2:T:383:LYS:HE2	1.81	0.62
2:MA:27:LYS:HZ1	2:MA:57:THR:HG23	1.64	0.62
2:SA:380:GLU:HA	2:SA:383:LYS:HE2	1.81	0.62
2:AA:380:GLU:HA	2:AA:383:LYS:HE2	1.81	0.62
2:J:380:GLU:HA	2:J:383:LYS:HE2	1.81	0.62
2:N:187:GLY:O	2:N:277:LYS:NZ	2.30	0.62
2:N:27:LYS:HZ3	2:N:55:LYS:HG3	1.64	0.61
2:H:380:GLU:HA	2:H:383:LYS:HE2	1.81	0.61
2:F:380:GLU:HA	2:F:383:LYS:HE2	1.81	0.61
2:WA:380:GLU:HA	2:WA:383:LYS:HE2	1.81	0.61
2:CA:380:GLU:HA	2:CA:383:LYS:HE2	1.81	0.61
2:OA:380:GLU:HA	2:OA:383:LYS:HE2	1.81	0.61
2:B:187:GLY:O	2:B:277:LYS:NZ	2.30	0.61
2:Y:187:GLY:O	2:Y:277:LYS:NZ	2.30	0.61
2:GA:30:ILE:HB	2:GA:58:VAL:HG12	1.83	0.61
2:WA:30:ILE:HB	2:WA:58:VAL:HG12	1.83	0.61
1:S:249:GLN:HA	1:TA:320:LYS:HD3	1.83	0.61
2:T:30:ILE:HB	2:T:58:VAL:HG12	1.83	0.61
2:P:30:ILE:HB	2:P:58:VAL:HG12	1.83	0.61
2:R:380:GLU:HA	2:R:383:LYS:HE2	1.81	0.61
2:EA:27:LYS:HZ1	2:EA:57:THR:HG23	1.66	0.61
2:GA:380:GLU:HA	2:GA:383:LYS:HE2	1.81	0.61
2:SA:30:ILE:HB	2:SA:58:VAL:HG12	1.83	0.61
2:OA:27:LYS:HZ3	2:OA:55:LYS:HG3	1.66	0.61
2:SA:27:LYS:HZ3	2:SA:55:LYS:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:LYS:HZ3	2:F:55:LYS:HG3	1.66	0.61
1:G:244:MET:HE1	1:HA:209:LEU:HD21	1.83	0.61
2:MA:30:ILE:HB	2:MA:58:VAL:HG12	1.83	0.61
2:MA:380:GLU:HA	2:MA:383:LYS:HE2	1.81	0.61
2:QA:30:ILE:HB	2:QA:58:VAL:HG12	1.83	0.61
2:D:27:LYS:HZ1	2:D:57:THR:HG23	1.65	0.60
2:D:380:GLU:HA	2:D:383:LYS:HE2	1.81	0.60
2:F:30:ILE:HB	2:F:58:VAL:HG12	1.83	0.60
2:J:30:ILE:HB	2:J:58:VAL:HG12	1.83	0.60
2:P:27:LYS:HZ1	2:P:57:THR:HG23	1.66	0.60
2:T:27:LYS:HZ3	2:T:55:LYS:HG3	1.65	0.60
2:Y:27:LYS:HZ3	2:Y:55:LYS:HG3	1.65	0.60
2:AA:27:LYS:HZ3	2:AA:55:LYS:HG3	1.65	0.60
2:AA:30:ILE:HB	2:AA:58:VAL:HG12	1.83	0.60
2:EA:380:GLU:HA	2:EA:383:LYS:HE2	1.81	0.60
2:QA:187:GLY:O	2:QA:277:LYS:NZ	2.30	0.60
2:WA:187:GLY:O	2:WA:277:LYS:NZ	2.30	0.60
2:D:30:ILE:HB	2:D:58:VAL:HG12	1.83	0.60
2:R:27:LYS:HZ1	2:R:57:THR:HG23	1.66	0.60
2:W:30:ILE:HB	2:W:58:VAL:HG12	1.83	0.60
2:GA:187:GLY:O	2:GA:277:LYS:NZ	2.30	0.60
2:OA:30:ILE:HB	2:OA:58:VAL:HG12	1.83	0.60
2:QA:27:LYS:HZ3	2:QA:55:LYS:HG3	1.66	0.60
2:UA:27:LYS:HZ3	2:UA:55:LYS:HG3	1.66	0.60
1:G:206:TYR:OH	1:HA:257:GLN:O	2.15	0.60
2:N:30:ILE:HB	2:N:58:VAL:HG12	1.83	0.60
2:P:187:GLY:O	2:P:277:LYS:NZ	2.30	0.60
2:EA:30:ILE:HB	2:EA:58:VAL:HG12	1.83	0.60
2:B:27:LYS:HZ3	2:B:55:LYS:HG3	1.66	0.60
2:J:27:LYS:HZ3	2:J:55:LYS:HG3	1.66	0.60
2:R:30:ILE:HB	2:R:58:VAL:HG12	1.83	0.60
2:UA:30:ILE:HB	2:UA:58:VAL:HG12	1.83	0.60
2:CA:30:ILE:HB	2:CA:58:VAL:HG12	1.83	0.60
2:B:30:ILE:HB	2:B:58:VAL:HG12	1.83	0.60
2:EA:187:GLY:O	2:EA:277:LYS:NZ	2.30	0.60
2:GA:27:LYS:HZ3	2:GA:55:LYS:HG3	1.66	0.60
2:KA:27:LYS:HZ3	2:KA:55:LYS:HG3	1.66	0.60
2:H:30:ILE:HB	2:H:58:VAL:HG12	1.83	0.60
2:R:187:GLY:O	2:R:277:LYS:NZ	2.30	0.60
2:Y:30:ILE:HB	2:Y:58:VAL:HG12	1.83	0.60
2:KA:30:ILE:HB	2:KA:58:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:LYS:HZ1	2:B:57:THR:HG23	1.67	0.60
2:J:27:LYS:HZ1	2:J:57:THR:HG23	1.67	0.60
2:R:27:LYS:HZ3	2:R:55:LYS:HG3	1.66	0.60
2:SA:27:LYS:HZ1	2:SA:57:THR:HG23	1.67	0.60
2:F:27:LYS:HZ1	2:F:57:THR:HG23	1.66	0.60
2:T:27:LYS:HZ1	2:T:57:THR:HG23	1.67	0.60
2:IA:187:GLY:O	2:IA:277:LYS:NZ	2.30	0.60
2:OA:27:LYS:HZ1	2:OA:57:THR:HG23	1.66	0.60
2:WA:27:LYS:HZ1	2:WA:57:THR:HG23	1.65	0.60
2:L:187:GLY:O	2:L:277:LYS:NZ	2.30	0.59
2:P:27:LYS:HZ3	2:P:55:LYS:HG3	1.66	0.59
2:W:27:LYS:HZ3	2:W:55:LYS:HG3	1.66	0.59
2:KA:187:GLY:O	2:KA:277:LYS:NZ	2.30	0.59
2:AA:27:LYS:HZ1	2:AA:57:THR:HG23	1.67	0.59
2:KA:27:LYS:HZ1	2:KA:57:THR:HG23	1.67	0.59
1:RA:113:TRP:HZ3	2:SA:158:LYS:HA	1.68	0.59
2:W:187:GLY:O	2:W:277:LYS:NZ	2.30	0.59
2:EA:27:LYS:HZ3	2:EA:55:LYS:HG3	1.66	0.59
2:IA:30:ILE:HB	2:IA:58:VAL:HG12	1.83	0.59
2:UA:187:GLY:O	2:UA:277:LYS:NZ	2.30	0.59
2:QA:27:LYS:HZ1	2:QA:57:THR:HG23	1.67	0.59
2:L:30:ILE:HB	2:L:58:VAL:HG12	1.83	0.59
2:W:27:LYS:HZ1	2:W:57:THR:HG23	1.66	0.59
2:GA:27:LYS:HZ1	2:GA:57:THR:HG23	1.66	0.59
2:D:135:SER:OG	2:D:266:THR:O	2.21	0.58
2:N:27:LYS:HZ1	2:N:57:THR:HG23	1.68	0.58
2:MA:135:SER:OG	2:MA:266:THR:O	2.21	0.58
1:NA:221:ALA:HB3	1:PA:328:ASN:HD21	1.69	0.58
2:UA:27:LYS:HZ1	2:UA:57:THR:HG23	1.67	0.58
2:WA:27:LYS:HZ3	2:WA:55:LYS:HG3	1.68	0.58
1:E:209:LEU:HD21	1:I:244:MET:HE1	1.84	0.58
2:B:135:SER:OG	2:B:266:THR:O	2.21	0.58
1:Z:249:GLN:HA	1:PA:320:LYS:HD3	1.84	0.58
2:D:27:LYS:HZ3	2:D:55:LYS:HG3	1.69	0.58
2:N:370:ASN:HB3	2:N:376:GLN:HB2	1.86	0.58
2:CA:135:SER:OG	2:CA:266:THR:O	2.21	0.58
2:GA:135:SER:OG	2:GA:266:THR:O	2.22	0.58
2:GA:370:ASN:HB3	2:GA:376:GLN:HB2	1.85	0.58
2:H:135:SER:OG	2:H:266:THR:O	2.21	0.58
2:J:370:ASN:HB3	2:J:376:GLN:HB2	1.86	0.58
2:Y:27:LYS:HZ1	2:Y:57:THR:HG23	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EA:370:ASN:HB3	2:EA:376:GLN:HB2	1.86	0.58
2:KA:135:SER:OG	2:KA:266:THR:O	2.21	0.58
2:P:370:ASN:HB3	2:P:376:GLN:HB2	1.86	0.58
2:R:370:ASN:HB3	2:R:376:GLN:HB2	1.86	0.58
2:AA:370:ASN:HB3	2:AA:376:GLN:HB2	1.86	0.58
2:WA:135:SER:OG	2:WA:266:THR:O	2.21	0.58
2:WA:370:ASN:HB3	2:WA:376:GLN:HB2	1.86	0.58
2:T:157:ASP:OD2	2:T:224:HIS:ND1	2.34	0.58
2:W:370:ASN:HB3	2:W:376:GLN:HB2	1.86	0.58
2:Y:370:ASN:HB3	2:Y:376:GLN:HB2	1.86	0.58
2:SA:157:ASP:OD2	2:SA:224:HIS:ND1	2.34	0.58
2:SA:370:ASN:HB3	2:SA:376:GLN:HB2	1.86	0.58
2:UA:370:ASN:HB3	2:UA:376:GLN:HB2	1.86	0.58
2:R:135:SER:OG	2:R:266:THR:O	2.21	0.58
2:W:33:ASN:HB3	2:W:36:LYS:HE3	1.86	0.58
2:MA:370:ASN:HB3	2:MA:376:GLN:HB2	1.86	0.58
1:A:249:GLN:HA	1:DA:320:LYS:HD3	1.85	0.57
2:D:370:ASN:HB3	2:D:376:GLN:HB2	1.86	0.57
2:R:33:ASN:HB3	2:R:36:LYS:HE3	1.86	0.57
2:T:370:ASN:HB3	2:T:376:GLN:HB2	1.86	0.57
2:QA:370:ASN:HB3	2:QA:376:GLN:HB2	1.86	0.57
2:H:370:ASN:HB3	2:H:376:GLN:HB2	1.86	0.57
2:CA:370:ASN:HB3	2:CA:376:GLN:HB2	1.86	0.57
2:EA:135:SER:OG	2:EA:266:THR:O	2.22	0.57
2:UA:33:ASN:HB3	2:UA:36:LYS:HE3	1.86	0.57
2:EA:33:ASN:HB3	2:EA:36:LYS:HE3	1.86	0.57
2:EA:157:ASP:OD2	2:EA:224:HIS:ND1	2.34	0.57
2:T:33:ASN:HB3	2:T:36:LYS:HE3	1.86	0.57
2:T:135:SER:OG	2:T:266:THR:O	2.22	0.57
2:MA:27:LYS:HZ3	2:MA:55:LYS:HG3	1.69	0.57
2:QA:135:SER:OG	2:QA:266:THR:O	2.21	0.57
2:SA:33:ASN:HB3	2:SA:36:LYS:HE3	1.86	0.57
2:IA:135:SER:OG	2:IA:266:THR:O	2.22	0.57
2:SA:112:PRO:HA	2:SA:115:TRP:HD1	1.70	0.57
2:SA:135:SER:OG	2:SA:266:THR:O	2.22	0.57
2:J:112:PRO:HA	2:J:115:TRP:HD1	1.70	0.57
2:L:135:SER:OG	2:L:266:THR:O	2.22	0.57
2:P:135:SER:OG	2:P:266:THR:O	2.22	0.57
2:T:112:PRO:HA	2:T:115:TRP:HD1	1.70	0.57
2:D:213:LEU:HD23	2:D:378:VAL:HG13	1.87	0.57
2:R:112:PRO:HA	2:R:115:TRP:HD1	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CA:213:LEU:HD23	2:CA:378:VAL:HG13	1.87	0.57
2:KA:370:ASN:HB3	2:KA:376:GLN:HB2	1.85	0.57
2:MA:213:LEU:HD23	2:MA:378:VAL:HG13	1.87	0.57
2:OA:33:ASN:HB3	2:OA:36:LYS:HE3	1.86	0.57
2:UA:135:SER:OG	2:UA:266:THR:O	2.21	0.57
2:UA:325:LEU:HD23	2:UA:328:TYR:HB2	1.87	0.57
1:A:244:MET:HE1	1:V:209:LEU:HD21	1.86	0.57
2:B:370:ASN:HB3	2:B:376:GLN:HB2	1.86	0.57
2:F:33:ASN:HB3	2:F:36:LYS:HE3	1.87	0.57
2:H:33:ASN:HB3	2:H:36:LYS:HE3	1.86	0.57
2:H:213:LEU:HD23	2:H:378:VAL:HG13	1.87	0.57
2:J:325:LEU:HD23	2:J:328:TYR:HB2	1.87	0.57
2:W:135:SER:OG	2:W:266:THR:O	2.22	0.57
2:AA:112:PRO:HA	2:AA:115:TRP:HD1	1.70	0.57
2:AA:325:LEU:HD23	2:AA:328:TYR:HB2	1.87	0.57
2:GA:213:LEU:HD23	2:GA:378:VAL:HG13	1.87	0.57
2:OA:370:ASN:HB3	2:OA:376:GLN:HB2	1.86	0.57
2:SA:332:LEU:HB3	2:SA:338:ILE:HG21	1.87	0.57
2:UA:213:LEU:HD23	2:UA:378:VAL:HG13	1.87	0.57
2:WA:213:LEU:HD23	2:WA:378:VAL:HG13	1.87	0.57
2:F:370:ASN:HB3	2:F:376:GLN:HB2	1.86	0.57
2:L:213:LEU:HD23	2:L:378:VAL:HG13	1.87	0.57
2:L:370:ASN:HB3	2:L:376:GLN:HB2	1.86	0.57
2:T:332:LEU:HB3	2:T:338:ILE:HG21	1.87	0.57
2:W:325:LEU:HD23	2:W:328:TYR:HB2	1.87	0.57
2:CA:33:ASN:HB3	2:CA:36:LYS:HE3	1.86	0.57
2:GA:33:ASN:HB3	2:GA:36:LYS:HE3	1.86	0.57
2:IA:213:LEU:HD23	2:IA:378:VAL:HG13	1.87	0.57
2:IA:370:ASN:HB3	2:IA:376:GLN:HB2	1.86	0.57
2:SA:213:LEU:HD23	2:SA:378:VAL:HG13	1.87	0.57
2:WA:112:PRO:HA	2:WA:115:TRP:HD1	1.70	0.57
2:B:213:LEU:HD23	2:B:378:VAL:HG13	1.87	0.57
2:B:332:LEU:HB3	2:B:338:ILE:HG21	1.87	0.57
2:L:112:PRO:HA	2:L:115:TRP:HD1	1.70	0.57
2:L:332:LEU:HB3	2:L:338:ILE:HG21	1.87	0.57
2:W:213:LEU:HD23	2:W:378:VAL:HG13	1.87	0.57
2:Y:135:SER:OG	2:Y:266:THR:O	2.21	0.57
2:GA:112:PRO:HA	2:GA:115:TRP:HD1	1.70	0.57
2:IA:112:PRO:HA	2:IA:115:TRP:HD1	1.70	0.57
2:IA:332:LEU:HB3	2:IA:338:ILE:HG21	1.87	0.57
2:KA:213:LEU:HD23	2:KA:378:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KA:332:LEU:HB3	2:KA:338:ILE:HG21	1.87	0.57
2:QA:33:ASN:HB3	2:QA:36:LYS:HE3	1.86	0.57
2:B:157:ASP:OD2	2:B:224:HIS:ND1	2.34	0.56
2:D:33:ASN:HB3	2:D:36:LYS:HE3	1.87	0.56
2:D:112:PRO:HA	2:D:115:TRP:HD1	1.70	0.56
2:F:135:SER:OG	2:F:266:THR:O	2.21	0.56
2:F:213:LEU:HD23	2:F:378:VAL:HG13	1.87	0.56
2:H:112:PRO:HA	2:H:115:TRP:HD1	1.70	0.56
2:J:135:SER:OG	2:J:266:THR:O	2.21	0.56
2:N:213:LEU:HD23	2:N:378:VAL:HG13	1.87	0.56
2:N:325:LEU:HD23	2:N:328:TYR:HB2	1.87	0.56
2:P:332:LEU:HB3	2:P:338:ILE:HG21	1.87	0.56
2:R:332:LEU:HB3	2:R:338:ILE:HG21	1.87	0.56
2:T:213:LEU:HD23	2:T:378:VAL:HG13	1.87	0.56
2:Y:33:ASN:HB3	2:Y:36:LYS:HE3	1.87	0.56
2:AA:135:SER:OG	2:AA:266:THR:O	2.21	0.56
2:EA:112:PRO:HA	2:EA:115:TRP:HD1	1.70	0.56
2:MA:112:PRO:HA	2:MA:115:TRP:HD1	1.70	0.56
2:OA:135:SER:OG	2:OA:266:THR:O	2.22	0.56
2:WA:33:ASN:HB3	2:WA:36:LYS:HE3	1.86	0.56
2:WA:325:LEU:HD23	2:WA:328:TYR:HB2	1.87	0.56
2:H:27:LYS:HZ3	2:H:55:LYS:HG3	1.71	0.56
2:J:33:ASN:HB3	2:J:36:LYS:HE3	1.87	0.56
2:J:332:LEU:HB3	2:J:338:ILE:HG21	1.87	0.56
2:N:135:SER:OG	2:N:266:THR:O	2.22	0.56
2:AA:33:ASN:HB3	2:AA:36:LYS:HE3	1.86	0.56
2:CA:27:LYS:HZ3	2:CA:55:LYS:HG3	1.70	0.56
2:EA:332:LEU:HB3	2:EA:338:ILE:HG21	1.87	0.56
2:F:112:PRO:HA	2:F:115:TRP:HD1	1.70	0.56
2:H:332:LEU:HB3	2:H:338:ILE:HG21	1.87	0.56
2:R:213:LEU:HD23	2:R:378:VAL:HG13	1.87	0.56
2:AA:332:LEU:HB3	2:AA:338:ILE:HG21	1.87	0.56
2:CA:112:PRO:HA	2:CA:115:TRP:HD1	1.70	0.56
2:CA:332:LEU:HB3	2:CA:338:ILE:HG21	1.87	0.56
2:GA:325:LEU:HD23	2:GA:328:TYR:HB2	1.87	0.56
2:MA:325:LEU:HD23	2:MA:328:TYR:HB2	1.87	0.56
2:OA:213:LEU:HD23	2:OA:378:VAL:HG13	1.87	0.56
2:QA:332:LEU:HB3	2:QA:338:ILE:HG21	1.87	0.56
2:B:112:PRO:HA	2:B:115:TRP:HD1	1.70	0.56
2:IA:325:LEU:HD23	2:IA:328:TYR:HB2	1.87	0.56
2:KA:33:ASN:HB3	2:KA:36:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KA:112:PRO:HA	2:KA:115:TRP:HD1	1.70	0.56
2:D:157:ASP:OD2	2:D:224:HIS:ND1	2.34	0.56
2:D:325:LEU:HD23	2:D:328:TYR:HB2	1.87	0.56
2:L:325:LEU:HD23	2:L:328:TYR:HB2	1.87	0.56
2:Y:325:LEU:HD23	2:Y:328:TYR:HB2	1.87	0.56
2:EA:213:LEU:HD23	2:EA:378:VAL:HG13	1.87	0.56
2:MA:33:ASN:HB3	2:MA:36:LYS:HE3	1.86	0.56
2:MA:332:LEU:HB3	2:MA:338:ILE:HG21	1.87	0.56
1:K:301:PRO:HB3	1:Z:292:HIS:CE1	2.40	0.56
2:P:33:ASN:HB3	2:P:36:LYS:HE3	1.86	0.56
2:W:364:VAL:O	2:W:367:ALA:HB3	2.06	0.56
2:Y:213:LEU:HD23	2:Y:378:VAL:HG13	1.87	0.56
2:D:332:LEU:HB3	2:D:338:ILE:HG21	1.87	0.56
2:J:213:LEU:HD23	2:J:378:VAL:HG13	1.87	0.56
2:P:325:LEU:HD23	2:P:328:TYR:HB2	1.87	0.56
2:OA:112:PRO:HA	2:OA:115:TRP:HD1	1.70	0.56
2:OA:332:LEU:HB3	2:OA:338:ILE:HG21	1.87	0.56
2:UA:332:LEU:HB3	2:UA:338:ILE:HG21	1.87	0.56
2:L:33:ASN:HB3	2:L:36:LYS:HE3	1.86	0.56
2:N:33:ASN:HB3	2:N:36:LYS:HE3	1.87	0.56
2:T:325:LEU:HD23	2:T:328:TYR:HB2	1.87	0.56
2:W:332:LEU:HB3	2:W:338:ILE:HG21	1.87	0.56
2:IA:33:ASN:HB3	2:IA:36:LYS:HE3	1.86	0.56
2:SA:325:LEU:HD23	2:SA:328:TYR:HB2	1.87	0.56
2:UA:364:VAL:O	2:UA:367:ALA:HB3	2.06	0.56
2:B:31:TRP:HB3	2:B:64:LEU:HD22	1.88	0.56
1:C:221:ALA:CB	1:E:328:ASN:HD21	2.18	0.56
2:F:332:LEU:HB3	2:F:338:ILE:HG21	1.87	0.56
2:R:325:LEU:HD23	2:R:328:TYR:HB2	1.87	0.56
2:AA:213:LEU:HD23	2:AA:378:VAL:HG13	1.87	0.56
2:KA:31:TRP:HB3	2:KA:64:LEU:HD22	1.88	0.56
2:H:325:LEU:HD23	2:H:328:TYR:HB2	1.87	0.56
2:L:31:TRP:HB3	2:L:64:LEU:HD22	1.88	0.56
2:L:364:VAL:O	2:L:367:ALA:HB3	2.06	0.56
2:N:112:PRO:HA	2:N:115:TRP:HD1	1.70	0.56
2:CA:325:LEU:HD23	2:CA:328:TYR:HB2	1.87	0.56
2:GA:364:VAL:O	2:GA:367:ALA:HB3	2.06	0.56
2:MA:31:TRP:HB3	2:MA:64:LEU:HD22	1.88	0.56
2:WA:364:VAL:O	2:WA:367:ALA:HB3	2.06	0.56
2:B:33:ASN:HB3	2:B:36:LYS:HE3	1.86	0.55
2:J:31:TRP:HB3	2:J:64:LEU:HD22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:31:TRP:HB3	2:P:64:LEU:HD22	1.88	0.55
2:Y:112:PRO:HA	2:Y:115:TRP:HD1	1.70	0.55
2:AA:31:TRP:HB3	2:AA:64:LEU:HD22	1.88	0.55
2:IA:31:TRP:HB3	2:IA:64:LEU:HD22	1.88	0.55
2:IA:364:VAL:O	2:IA:367:ALA:HB3	2.06	0.55
2:QA:31:TRP:HB3	2:QA:64:LEU:HD22	1.88	0.55
2:D:31:TRP:HB3	2:D:64:LEU:HD22	1.88	0.55
2:QA:112:PRO:HA	2:QA:115:TRP:HD1	1.70	0.55
2:QA:213:LEU:HD23	2:QA:378:VAL:HG13	1.87	0.55
2:WA:332:LEU:HB3	2:WA:338:ILE:HG21	1.87	0.55
2:D:364:VAL:O	2:D:367:ALA:HB3	2.06	0.55
2:R:364:VAL:O	2:R:367:ALA:HB3	2.06	0.55
2:W:112:PRO:HA	2:W:115:TRP:HD1	1.70	0.55
2:W:157:ASP:OD2	2:W:224:HIS:ND1	2.34	0.55
2:GA:332:LEU:HB3	2:GA:338:ILE:HG21	1.87	0.55
2:QA:325:LEU:HD23	2:QA:328:TYR:HB2	1.87	0.55
1:K:249:GLN:HA	1:Z:320:LYS:HD3	1.87	0.55
2:L:27:LYS:HZ1	2:L:57:THR:HG23	1.70	0.55
2:P:112:PRO:HA	2:P:115:TRP:HD1	1.70	0.55
2:EA:325:LEU:HD23	2:EA:328:TYR:HB2	1.87	0.55
2:EA:364:VAL:O	2:EA:367:ALA:HB3	2.06	0.55
2:GA:182:ILE:HA	2:GA:212:GLY:HA3	1.89	0.55
2:B:364:VAL:O	2:B:367:ALA:HB3	2.06	0.55
2:H:364:VAL:O	2:H:367:ALA:HB3	2.06	0.55
2:N:332:LEU:HB3	2:N:338:ILE:HG21	1.87	0.55
2:P:364:VAL:O	2:P:367:ALA:HB3	2.06	0.55
2:CA:364:VAL:O	2:CA:367:ALA:HB3	2.06	0.55
2:IA:27:LYS:HZ1	2:IA:57:THR:HG23	1.70	0.55
2:MA:157:ASP:OD2	2:MA:224:HIS:ND1	2.34	0.55
2:MA:364:VAL:O	2:MA:367:ALA:HB3	2.06	0.55
2:B:325:LEU:HD23	2:B:328:TYR:HB2	1.87	0.55
2:N:157:ASP:OD2	2:N:224:HIS:ND1	2.34	0.55
2:Y:31:TRP:HB3	2:Y:64:LEU:HD22	1.88	0.55
2:KA:364:VAL:O	2:KA:367:ALA:HB3	2.06	0.55
2:OA:325:LEU:HD23	2:OA:328:TYR:HB2	1.87	0.55
2:UA:112:PRO:HA	2:UA:115:TRP:HD1	1.70	0.55
2:WA:182:ILE:HA	2:WA:212:GLY:HA3	1.89	0.55
2:KA:325:LEU:HD23	2:KA:328:TYR:HB2	1.87	0.55
2:SA:364:VAL:O	2:SA:367:ALA:HB3	2.06	0.55
2:F:325:LEU:HD23	2:F:328:TYR:HB2	1.87	0.55
1:O:249:GLN:HA	1:HA:320:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:213:LEU:HD23	2:P:378:VAL:HG13	1.87	0.55
2:R:31:TRP:HB3	2:R:64:LEU:HD22	1.88	0.55
2:R:182:ILE:HA	2:R:212:GLY:HA3	1.89	0.55
2:T:364:VAL:O	2:T:367:ALA:HB3	2.06	0.55
2:Y:364:VAL:O	2:Y:367:ALA:HB3	2.06	0.55
2:UA:157:ASP:OD2	2:UA:224:HIS:ND1	2.34	0.55
2:N:31:TRP:HB3	2:N:64:LEU:HD22	1.88	0.55
2:N:364:VAL:O	2:N:367:ALA:HB3	2.06	0.55
2:D:182:ILE:HA	2:D:212:GLY:HA3	1.89	0.55
2:Y:332:LEU:HB3	2:Y:338:ILE:HG21	1.87	0.55
2:EA:31:TRP:HB3	2:EA:64:LEU:HD22	1.88	0.55
2:QA:364:VAL:O	2:QA:367:ALA:HB3	2.06	0.55
2:H:31:TRP:HB3	2:H:64:LEU:HD22	1.88	0.54
2:W:31:TRP:HB3	2:W:64:LEU:HD22	1.88	0.54
2:MA:182:ILE:HA	2:MA:212:GLY:HA3	1.89	0.54
2:OA:31:TRP:HB3	2:OA:64:LEU:HD22	1.88	0.54
2:F:31:TRP:HB3	2:F:64:LEU:HD22	1.88	0.54
2:F:364:VAL:O	2:F:367:ALA:HB3	2.06	0.54
2:J:364:VAL:O	2:J:367:ALA:HB3	2.06	0.54
2:Y:363:ALA:O	2:Y:366:THR:OG1	2.25	0.54
2:AA:364:VAL:O	2:AA:367:ALA:HB3	2.06	0.54
2:CA:31:TRP:HB3	2:CA:64:LEU:HD22	1.88	0.54
2:EA:182:ILE:HA	2:EA:212:GLY:HA3	1.89	0.54
2:KA:182:ILE:HA	2:KA:212:GLY:HA3	1.89	0.54
2:B:182:ILE:HA	2:B:212:GLY:HA3	1.89	0.54
2:F:182:ILE:HA	2:F:212:GLY:HA3	1.89	0.54
2:T:182:ILE:HA	2:T:212:GLY:HA3	1.89	0.54
2:OA:182:ILE:HA	2:OA:212:GLY:HA3	1.89	0.54
2:OA:364:VAL:O	2:OA:367:ALA:HB3	2.06	0.54
2:SA:182:ILE:HA	2:SA:212:GLY:HA3	1.89	0.54
2:UA:31:TRP:HB3	2:UA:64:LEU:HD22	1.88	0.54
2:J:182:ILE:HA	2:J:212:GLY:HA3	1.89	0.54
2:W:182:ILE:HA	2:W:212:GLY:HA3	1.89	0.54
2:WA:31:TRP:HB3	2:WA:64:LEU:HD22	1.88	0.54
2:L:182:ILE:HA	2:L:212:GLY:HA3	1.89	0.54
2:EA:363:ALA:O	2:EA:366:THR:OG1	2.25	0.54
2:IA:182:ILE:HA	2:IA:212:GLY:HA3	1.89	0.54
1:A:218:ASP:O	1:C:327:THR:HG21	2.08	0.54
2:T:377:THR:OG1	2:T:379:ASP:OD1	2.26	0.54
2:Y:377:THR:OG1	2:Y:379:ASP:OD1	2.26	0.54
2:QA:182:ILE:HA	2:QA:212:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UA:182:ILE:HA	2:UA:212:GLY:HA3	1.89	0.54
2:AA:182:ILE:HA	2:AA:212:GLY:HA3	1.89	0.54
2:GA:31:TRP:HB3	2:GA:64:LEU:HD22	1.88	0.54
2:KA:157:ASP:OD2	2:KA:224:HIS:ND1	2.34	0.54
2:SA:377:THR:OG1	2:SA:379:ASP:OD1	2.26	0.54
2:D:61:PRO:HG2	2:D:67:LYS:HE3	1.90	0.54
1:K:132:ARG:NH1	1:K:165:GLN:O	2.41	0.54
1:M:101:VAL:HG21	2:N:374:GLY:HA3	1.88	0.54
2:P:61:PRO:HG2	2:P:67:LYS:HE3	1.90	0.54
2:R:61:PRO:HG2	2:R:67:LYS:HE3	1.90	0.54
2:EA:61:PRO:HG2	2:EA:67:LYS:HE3	1.90	0.54
1:HA:132:ARG:NH1	1:HA:165:GLN:O	2.41	0.54
2:MA:61:PRO:HG2	2:MA:67:LYS:HE3	1.90	0.54
1:NA:221:ALA:CB	1:PA:328:ASN:HD21	2.21	0.54
2:OA:61:PRO:HG2	2:OA:67:LYS:HE3	1.90	0.54
1:C:132:ARG:NH1	1:C:165:GLN:O	2.41	0.54
2:F:61:PRO:HG2	2:F:67:LYS:HE3	1.90	0.54
1:I:132:ARG:NH1	1:I:165:GLN:O	2.41	0.54
1:X:132:ARG:NH1	1:X:165:GLN:O	2.41	0.54
2:CA:239:ASN:ND2	2:CA:259[B]:SER:OG	2.41	0.54
2:H:61:PRO:HG2	2:H:67:LYS:HE3	1.90	0.53
1:K:221:ALA:HB3	1:VA:328:ASN:ND2	2.23	0.53
2:R:363:ALA:O	2:R:366:THR:OG1	2.25	0.53
2:EA:377:THR:OG1	2:EA:379:ASP:OD1	2.26	0.53
2:GA:239:ASN:ND2	2:GA:259[B]:SER:OG	2.41	0.53
2:QA:61:PRO:HG2	2:QA:67:LYS:HE3	1.90	0.53
2:WA:239:ASN:ND2	2:WA:259[B]:SER:OG	2.41	0.53
1:I:101:VAL:HG21	2:J:374:GLY:HA3	1.89	0.53
2:N:377:THR:OG1	2:N:379:ASP:OD1	2.26	0.53
2:T:61:PRO:HG2	2:T:67:LYS:HE3	1.90	0.53
2:SA:61:PRO:HG2	2:SA:67:LYS:HE3	1.90	0.53
2:B:377:THR:OG1	2:B:379:ASP:OD1	2.26	0.53
1:E:132:ARG:NH1	1:E:165:GLN:O	2.41	0.53
2:T:31:TRP:HB3	2:T:64:LEU:HD22	1.88	0.53
2:CA:61:PRO:HG2	2:CA:67:LYS:HE3	1.90	0.53
2:H:182:ILE:HA	2:H:212:GLY:HA3	1.89	0.53
2:L:61:PRO:HG2	2:L:67:LYS:HE3	1.90	0.53
2:N:363:ALA:O	2:N:366:THR:OG1	2.25	0.53
1:Q:320:LYS:HD3	1:JA:249:GLN:HA	1.91	0.53
1:Z:132:ARG:NH1	1:Z:165:GLN:O	2.41	0.53
2:AA:377:THR:OG1	2:AA:379:ASP:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CA:182:ILE:HA	2:CA:212:GLY:HA3	1.89	0.53
2:KA:61:PRO:HG2	2:KA:67:LYS:HE3	1.90	0.53
1:NA:132:ARG:NH1	1:NA:165:GLN:O	2.41	0.53
2:SA:31:TRP:HB3	2:SA:64:LEU:HD22	1.88	0.53
2:P:182:ILE:HA	2:P:212:GLY:HA3	1.89	0.53
2:R:377:THR:OG1	2:R:379:ASP:OD1	2.26	0.53
2:J:377:THR:OG1	2:J:379:ASP:OD1	2.26	0.53
2:N:182:ILE:HA	2:N:212:GLY:HA3	1.89	0.53
2:Y:157:ASP:OD2	2:Y:224:HIS:ND1	2.34	0.53
2:Y:182:ILE:HA	2:Y:212:GLY:HA3	1.89	0.53
2:IA:61:PRO:HG2	2:IA:67:LYS:HE3	1.90	0.53
2:KA:377:THR:OG1	2:KA:379:ASP:OD1	2.26	0.53
2:MA:377:THR:OG1	2:MA:379:ASP:OD1	2.26	0.53
2:WA:363:ALA:O	2:WA:366:THR:OG1	2.25	0.53
2:D:377:THR:OG1	2:D:379:ASP:OD1	2.26	0.53
2:J:239:ASN:ND2	2:J:259[B]:SER:OG	2.41	0.53
2:AA:239:ASN:ND2	2:AA:259[B]:SER:OG	2.41	0.53
2:B:61:PRO:HG2	2:B:67:LYS:HE3	1.90	0.53
2:N:61:PRO:HG2	2:N:67:LYS:HE3	1.90	0.53
2:GA:363:ALA:O	2:GA:366:THR:OG1	2.25	0.53
2:H:377:THR:OG1	2:H:379:ASP:OD1	2.26	0.53
2:GA:308:ASP:N	2:GA:308:ASP:OD1	2.42	0.53
2:KA:191:LYS:NZ	2:KA:198:ASP:OD2	2.34	0.53
2:UA:377:THR:OG1	2:UA:379:ASP:OD1	2.26	0.53
2:WA:308:ASP:N	2:WA:308:ASP:OD1	2.42	0.53
2:W:377:THR:OG1	2:W:379:ASP:OD1	2.26	0.52
1:DA:132:ARG:NH1	1:DA:165:GLN:O	2.41	0.52
2:GA:377:THR:OG1	2:GA:379:ASP:OD1	2.26	0.52
2:QA:363:ALA:O	2:QA:366:THR:OG1	2.25	0.52
2:UA:61:PRO:HG2	2:UA:67:LYS:HE3	1.90	0.52
2:F:377:THR:OG1	2:F:379:ASP:OD1	2.26	0.52
2:N:239:ASN:ND2	2:N:259[B]:SER:OG	2.41	0.52
2:P:377:THR:OG1	2:P:379:ASP:OD1	2.26	0.52
2:CA:377:THR:OG1	2:CA:379:ASP:OD1	2.26	0.52
2:IA:377:THR:OG1	2:IA:379:ASP:OD1	2.26	0.52
1:Q:132:ARG:NH1	1:Q:165:GLN:O	2.41	0.52
2:W:61:PRO:HG2	2:W:67:LYS:HE3	1.90	0.52
2:Y:61:PRO:HG2	2:Y:67:LYS:HE3	1.90	0.52
2:AA:157:ASP:OD2	2:AA:224:HIS:ND1	2.34	0.52
2:IA:157:ASP:OD2	2:IA:224:HIS:ND1	2.34	0.52
1:TA:132:ARG:NH1	1:TA:165:GLN:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:ASP:OD2	2:F:224:HIS:ND1	2.34	0.52
2:L:377:THR:OG1	2:L:379:ASP:OD1	2.26	0.52
1:O:79:TYR:CE1	2:P:223:LYS:HB2	2.44	0.52
2:P:157:ASP:OD2	2:P:224:HIS:ND1	2.34	0.52
1:V:132:ARG:NH1	1:V:165:GLN:O	2.41	0.52
2:B:308:ASP:OD1	2:B:308:ASP:N	2.42	0.52
2:D:88:PHE:O	2:D:92:ALA:N	2.43	0.52
2:H:194:ASN:HB2	2:H:196:LYS:HZ2	1.75	0.52
2:N:46:LYS:O	2:N:50:LYS:HG3	2.10	0.52
2:R:308:ASP:OD1	2:R:308:ASP:N	2.42	0.52
2:Y:239:ASN:ND2	2:Y:259[B]:SER:OG	2.41	0.52
2:OA:157:ASP:OD2	2:OA:224:HIS:ND1	2.34	0.52
2:OA:377:THR:OG1	2:OA:379:ASP:OD1	2.26	0.52
2:QA:377:THR:OG1	2:QA:379:ASP:OD1	2.26	0.52
2:UA:308:ASP:OD1	2:UA:308:ASP:N	2.42	0.52
1:VA:67:ASP:OD1	1:VA:71:THR:N	2.41	0.52
2:WA:377:THR:OG1	2:WA:379:ASP:OD1	2.26	0.52
1:O:118:ILE:HA	1:O:121:VAL:HG22	1.92	0.52
2:Y:46:LYS:O	2:Y:50:LYS:HG3	2.10	0.52
1:BA:132:ARG:NH1	1:BA:165:GLN:O	2.41	0.52
2:GA:157:ASP:OD2	2:GA:224:HIS:ND1	2.34	0.52
1:PA:118:ILE:HA	1:PA:121:VAL:HG22	1.92	0.52
2:WA:157:ASP:OD2	2:WA:224:HIS:ND1	2.34	0.52
2:B:363:ALA:O	2:B:366:THR:OG1	2.25	0.52
2:D:239:ASN:ND2	2:D:259[B]:SER:OG	2.41	0.52
2:L:157:ASP:OD2	2:L:224:HIS:ND1	2.34	0.52
2:W:308:ASP:OD1	2:W:308:ASP:N	2.43	0.52
1:JA:118:ILE:HA	1:JA:121:VAL:HG22	1.92	0.52
2:KA:88:PHE:O	2:KA:92:ALA:N	2.43	0.52
2:KA:308:ASP:OD1	2:KA:308:ASP:N	2.43	0.52
2:QA:157:ASP:OD2	2:QA:224:HIS:ND1	2.34	0.52
1:RA:118:ILE:HA	1:RA:121:VAL:HG22	1.92	0.52
1:G:132:ARG:NH1	1:G:165:GLN:O	2.41	0.52
2:J:157:ASP:OD2	2:J:224:HIS:ND1	2.34	0.52
1:S:118:ILE:HA	1:S:121:VAL:HG22	1.92	0.52
1:FA:67:ASP:OD1	1:FA:71:THR:N	2.41	0.52
2:IA:88:PHE:O	2:IA:92:ALA:N	2.43	0.52
1:JA:132:ARG:NH1	1:JA:165:GLN:O	2.41	0.52
1:RA:132:ARG:NH1	1:RA:165:GLN:O	2.41	0.52
2:B:88:PHE:O	2:B:92:ALA:N	2.43	0.52
2:L:88:PHE:O	2:L:92:ALA:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:61:PRO:HG2	2:AA:67:LYS:HE3	1.90	0.52
1:BA:67:ASP:OD1	1:BA:71:THR:N	2.41	0.52
1:BA:118:ILE:HA	1:BA:121:VAL:HG22	1.92	0.52
2:GA:61:PRO:HG2	2:GA:67:LYS:HE3	1.90	0.52
2:MA:88:PHE:O	2:MA:92:ALA:N	2.43	0.52
1:A:113:TRP:HZ3	2:B:158:LYS:HA	1.75	0.52
1:A:118:ILE:HA	1:A:121:VAL:HG22	1.92	0.52
1:C:118:ILE:HA	1:C:121:VAL:HG22	1.92	0.52
2:F:46:LYS:O	2:F:50:LYS:HG3	2.10	0.52
1:G:67:ASP:OD1	1:G:71:THR:N	2.41	0.52
1:G:118:ILE:HA	1:G:121:VAL:HG22	1.92	0.52
1:K:67:ASP:OD1	1:K:71:THR:N	2.41	0.52
2:T:88:PHE:O	2:T:92:ALA:N	2.43	0.52
2:GA:46:LYS:O	2:GA:50:LYS:HG3	2.10	0.52
1:HA:67:ASP:OD1	1:HA:71:THR:N	2.41	0.52
1:NA:67:ASP:OD1	1:NA:71:THR:N	2.41	0.52
2:UA:46:LYS:O	2:UA:50:LYS:HG3	2.10	0.52
2:WA:46:LYS:O	2:WA:50:LYS:HG3	2.10	0.52
1:E:67:ASP:OD1	1:E:71:THR:N	2.41	0.51
2:H:46:LYS:O	2:H:50:LYS:HG3	2.10	0.51
2:J:61:PRO:HG2	2:J:67:LYS:HE3	1.90	0.51
2:R:88:PHE:O	2:R:92:ALA:N	2.43	0.51
1:S:132:ARG:NH1	1:S:165:GLN:O	2.41	0.51
2:W:46:LYS:O	2:W:50:LYS:HG3	2.10	0.51
2:Y:88:PHE:O	2:Y:92:ALA:N	2.43	0.51
1:FA:132:ARG:NH1	1:FA:165:GLN:O	2.41	0.51
2:GA:88:PHE:O	2:GA:92:ALA:N	2.43	0.51
1:LA:118:ILE:HA	1:LA:121:VAL:HG22	1.92	0.51
2:OA:46:LYS:O	2:OA:50:LYS:HG3	2.10	0.51
2:OA:88:PHE:O	2:OA:92:ALA:N	2.43	0.51
2:WA:61:PRO:HG2	2:WA:67:LYS:HE3	1.90	0.51
1:A:132:ARG:NH1	1:A:165:GLN:O	2.41	0.51
1:E:118:ILE:HA	1:E:121:VAL:HG22	1.92	0.51
2:F:88:PHE:O	2:F:92:ALA:N	2.43	0.51
2:L:46:LYS:O	2:L:50:LYS:HG3	2.10	0.51
2:P:363:ALA:O	2:P:366:THR:OG1	2.25	0.51
2:W:239:ASN:ND2	2:W:259[B]:SER:OG	2.41	0.51
2:CA:46:LYS:O	2:CA:50:LYS:HG3	2.10	0.51
2:KA:363:ALA:O	2:KA:366:THR:OG1	2.25	0.51
2:QA:46:LYS:O	2:QA:50:LYS:HG3	2.10	0.51
2:SA:88:PHE:O	2:SA:92:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:WA:88:PHE:O	2:WA:92:ALA:N	2.43	0.51
1:C:221:ALA:CB	1:E:328:ASN:ND2	2.73	0.51
2:P:46:LYS:O	2:P:50:LYS:HG3	2.10	0.51
2:T:239:ASN:ND2	2:T:259[B]:SER:OG	2.41	0.51
2:EA:46:LYS:O	2:EA:50:LYS:HG3	2.10	0.51
2:IA:46:LYS:O	2:IA:50:LYS:HG3	2.10	0.51
2:UA:88:PHE:O	2:UA:92:ALA:N	2.43	0.51
2:H:88:PHE:O	2:H:92:ALA:N	2.43	0.51
2:L:308:ASP:N	2:L:308:ASP:OD1	2.42	0.51
2:P:88:PHE:O	2:P:92:ALA:N	2.43	0.51
2:R:46:LYS:O	2:R:50:LYS:HG3	2.10	0.51
2:AA:46:LYS:O	2:AA:50:LYS:HG3	2.10	0.51
2:IA:308:ASP:N	2:IA:308:ASP:OD1	2.42	0.51
2:SA:308:ASP:OD1	2:SA:308:ASP:N	2.43	0.51
2:N:87:ARG:NH2	2:N:91:TYR:OH	2.44	0.51
2:T:46:LYS:O	2:T:50:LYS:HG3	2.10	0.51
2:Y:87:ARG:NH2	2:Y:91:TYR:OH	2.44	0.51
2:CA:88:PHE:O	2:CA:92:ALA:N	2.43	0.51
2:KA:46:LYS:O	2:KA:50:LYS:HG3	2.10	0.51
2:MA:239:ASN:ND2	2:MA:259[B]:SER:OG	2.41	0.51
1:NA:118:ILE:HA	1:NA:121:VAL:HG22	1.92	0.51
2:SA:46:LYS:O	2:SA:50:LYS:HG3	2.10	0.51
2:SA:239:ASN:ND2	2:SA:259[B]:SER:OG	2.41	0.51
1:VA:132:ARG:NH1	1:VA:165:GLN:O	2.41	0.51
2:B:46:LYS:O	2:B:50:LYS:HG3	2.10	0.51
2:J:46:LYS:O	2:J:50:LYS:HG3	2.10	0.51
2:P:239:ASN:ND2	2:P:259[B]:SER:OG	2.41	0.51
2:Y:308:ASP:N	2:Y:308:ASP:OD1	2.42	0.51
2:EA:88:PHE:O	2:EA:92:ALA:N	2.43	0.51
2:IA:239:ASN:ND2	2:IA:259[B]:SER:OG	2.41	0.51
2:KA:87:ARG:NH2	2:KA:91:TYR:OH	2.44	0.51
2:MA:87:ARG:NH2	2:MA:91:TYR:OH	2.44	0.51
2:QA:87:ARG:NH2	2:QA:91:TYR:OH	2.44	0.51
2:SA:363:ALA:O	2:SA:366:THR:OG1	2.25	0.51
2:B:87:ARG:NH2	2:B:91:TYR:OH	2.44	0.51
2:D:87:ARG:NH2	2:D:91:TYR:OH	2.44	0.51
2:P:87:ARG:NH2	2:P:91:TYR:OH	2.44	0.51
1:S:113:TRP:HZ3	2:T:158:LYS:HA	1.75	0.51
2:T:363:ALA:O	2:T:366:THR:OG1	2.25	0.51
1:V:118:ILE:HA	1:V:121:VAL:HG22	1.92	0.51
2:OA:87:ARG:NH2	2:OA:91:TYR:OH	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LYS:O	2:D:50:LYS:HG3	2.10	0.51
2:L:239:ASN:ND2	2:L:259[B]:SER:OG	2.41	0.51
2:R:87:ARG:NH2	2:R:91:TYR:OH	2.44	0.51
2:W:88:PHE:O	2:W:92:ALA:N	2.43	0.51
2:EA:87:ARG:NH2	2:EA:91:TYR:OH	2.44	0.51
2:KA:239:ASN:ND2	2:KA:259[B]:SER:OG	2.41	0.51
1:LA:113:TRP:CZ3	2:MA:158:LYS:HG2	2.46	0.51
2:MA:46:LYS:O	2:MA:50:LYS:HG3	2.10	0.51
2:QA:239:ASN:ND2	2:QA:259[B]:SER:OG	2.41	0.51
1:TA:118:ILE:HA	1:TA:121:VAL:HG22	1.92	0.51
1:A:67:ASP:OD1	1:A:71:THR:N	2.41	0.51
2:F:87:ARG:NH2	2:F:91:TYR:OH	2.44	0.51
2:L:363:ALA:O	2:L:366:THR:OG1	2.25	0.51
2:P:40:GLY:HA3	2:P:314:VAL:HA	1.93	0.51
2:OA:363:ALA:O	2:OA:366:THR:OG1	2.25	0.51
2:F:363:ALA:O	2:F:366:THR:OG1	2.25	0.51
1:I:118:ILE:HA	1:I:121:VAL:HG22	1.92	0.51
2:J:88:PHE:O	2:J:92:ALA:N	2.43	0.51
2:N:88:PHE:O	2:N:92:ALA:N	2.43	0.51
2:T:87:ARG:NH2	2:T:91:TYR:OH	2.44	0.51
1:X:113:TRP:HZ3	2:Y:158:LYS:HA	1.75	0.51
1:X:118:ILE:HA	1:X:121:VAL:HG22	1.92	0.51
2:SA:87:ARG:NH2	2:SA:91:TYR:OH	2.44	0.51
2:UA:239:ASN:ND2	2:UA:259[B]:SER:OG	2.41	0.51
2:H:40:GLY:HA3	2:H:314:VAL:HA	1.93	0.50
2:H:87:ARG:NH2	2:H:91:TYR:OH	2.44	0.50
2:Y:40:GLY:HA3	2:Y:314:VAL:HA	1.93	0.50
2:CA:40:GLY:HA3	2:CA:314:VAL:HA	1.93	0.50
1:JA:67:ASP:OD1	1:JA:71:THR:N	2.41	0.50
2:QA:40:GLY:HA3	2:QA:314:VAL:HA	1.93	0.50
2:WA:87:ARG:NH2	2:WA:91:TYR:OH	2.44	0.50
2:B:239:ASN:ND2	2:B:259[B]:SER:OG	2.41	0.50
1:K:118:ILE:HA	1:K:121:VAL:HG22	1.92	0.50
1:M:67:ASP:OD1	1:M:71:THR:N	2.41	0.50
2:AA:88:PHE:O	2:AA:92:ALA:N	2.43	0.50
2:CA:87:ARG:NH2	2:CA:91:TYR:OH	2.44	0.50
1:FA:118:ILE:HA	1:FA:121:VAL:HG22	1.92	0.50
2:GA:87:ARG:NH2	2:GA:91:TYR:OH	2.44	0.50
2:UA:87:ARG:NH2	2:UA:91:TYR:OH	2.44	0.50
1:G:101:VAL:HG21	2:H:374:GLY:HA3	1.93	0.50
2:H:157:ASP:OD2	2:H:224:HIS:ND1	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:GLY:HA3	2:N:314:VAL:HA	1.94	0.50
2:W:87:ARG:NH2	2:W:91:TYR:OH	2.44	0.50
2:AA:87:ARG:NH2	2:AA:91:TYR:OH	2.44	0.50
1:DA:118:ILE:HA	1:DA:121:VAL:HG22	1.92	0.50
2:IA:363:ALA:O	2:IA:366:THR:OG1	2.25	0.50
2:J:87:ARG:NH2	2:J:91:TYR:OH	2.44	0.50
1:M:118:ILE:HA	1:M:121:VAL:HG22	1.92	0.50
1:Z:118:ILE:HA	1:Z:121:VAL:HG22	1.92	0.50
1:LA:67:ASP:OD1	1:LA:71:THR:N	2.41	0.50
2:QA:88:PHE:O	2:QA:92:ALA:N	2.43	0.50
1:VA:118:ILE:HA	1:VA:121:VAL:HG22	1.92	0.50
2:J:130:ALA:HB3	2:J:283:LEU:HB3	1.94	0.50
2:L:44:VAL:HA	2:L:47:LYS:HE2	1.94	0.50
2:P:130:ALA:HB3	2:P:283:LEU:HB3	1.94	0.50
2:W:130:ALA:HB3	2:W:283:LEU:HB3	1.94	0.50
1:X:221:ALA:HB3	1:HA:328:ASN:ND2	2.26	0.50
2:AA:130:ALA:HB3	2:AA:283:LEU:HB3	1.94	0.50
2:CA:157:ASP:OD2	2:CA:224:HIS:ND1	2.34	0.50
2:GA:44:VAL:HA	2:GA:47:LYS:HE2	1.94	0.50
2:IA:87:ARG:NH2	2:IA:91:TYR:OH	2.44	0.50
2:QA:308:ASP:N	2:QA:308:ASP:OD1	2.43	0.50
2:SA:130:ALA:HB3	2:SA:283:LEU:HB3	1.94	0.50
2:WA:44:VAL:HA	2:WA:47:LYS:HE2	1.94	0.50
2:L:130:ALA:HB3	2:L:283:LEU:HB3	1.94	0.50
2:N:130:ALA:HB3	2:N:283:LEU:HB3	1.94	0.50
1:Q:118:ILE:HA	1:Q:121:VAL:HG22	1.92	0.50
2:W:40:GLY:HA3	2:W:314:VAL:HA	1.93	0.50
2:Y:130:ALA:HB3	2:Y:283:LEU:HB3	1.94	0.50
2:GA:130:ALA:HB3	2:GA:283:LEU:HB3	1.94	0.50
1:HA:118:ILE:HA	1:HA:121:VAL:HG22	1.92	0.50
2:IA:44:VAL:HA	2:IA:47:LYS:HE2	1.94	0.50
2:UA:44:VAL:HA	2:UA:47:LYS:HE2	1.94	0.50
2:UA:130:ALA:HB3	2:UA:283:LEU:HB3	1.94	0.50
2:H:308:ASP:OD1	2:H:308:ASP:N	2.42	0.50
2:L:87:ARG:NH2	2:L:91:TYR:OH	2.44	0.50
1:S:244:MET:HE1	1:DA:209:LEU:HD21	1.92	0.50
2:T:130:ALA:HB3	2:T:283:LEU:HB3	1.94	0.50
2:W:44:VAL:HA	2:W:47:LYS:HE2	1.94	0.50
2:CA:44:VAL:HA	2:CA:47:LYS:HE2	1.94	0.50
2:CA:363:ALA:O	2:CA:366:THR:OG1	2.25	0.50
2:IA:130:ALA:HB3	2:IA:283:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:130:ALA:HB3	2:OA:283:LEU:HB3	1.94	0.50
2:QA:160:LEU:HD12	2:QA:167:ALA:HA	1.94	0.50
2:SA:160:LEU:HD12	2:SA:167:ALA:HA	1.94	0.50
2:F:130:ALA:HB3	2:F:283:LEU:HB3	1.94	0.50
2:F:160:LEU:HD12	2:F:167:ALA:HA	1.94	0.50
2:H:44:VAL:HA	2:H:47:LYS:HE2	1.94	0.50
2:J:40:GLY:HA3	2:J:314:VAL:HA	1.93	0.50
2:T:160:LEU:HD12	2:T:167:ALA:HA	1.94	0.50
1:X:67:ASP:OD1	1:X:71:THR:N	2.41	0.50
2:CA:308:ASP:OD1	2:CA:308:ASP:N	2.42	0.50
2:IA:40:GLY:HA3	2:IA:314:VAL:HA	1.93	0.50
2:OA:40:GLY:HA3	2:OA:314:VAL:HA	1.93	0.50
2:OA:160:LEU:HD12	2:OA:167:ALA:HA	1.94	0.50
2:J:311:LEU:HA	2:J:314:VAL:HG12	1.94	0.50
1:M:132:ARG:NH1	1:M:165:GLN:O	2.41	0.50
2:P:160:LEU:HD12	2:P:167:ALA:HA	1.94	0.50
2:EA:311:LEU:HA	2:EA:314:VAL:HG12	1.94	0.50
1:LA:104:TYR:HE2	2:MA:222:ASN:ND2	2.10	0.50
2:MA:363:ALA:O	2:MA:366:THR:OG1	2.25	0.50
2:QA:130:ALA:HB3	2:QA:283:LEU:HB3	1.94	0.50
2:WA:130:ALA:HB3	2:WA:283:LEU:HB3	1.94	0.50
2:D:44:VAL:HA	2:D:47:LYS:HE2	1.94	0.49
2:F:40:GLY:HA3	2:F:314:VAL:HA	1.94	0.49
2:L:40:GLY:HA3	2:L:314:VAL:HA	1.93	0.49
2:T:40:GLY:HA3	2:T:314:VAL:HA	1.93	0.49
2:AA:311:LEU:HA	2:AA:314:VAL:HG12	1.94	0.49
2:KA:40:GLY:HA3	2:KA:314:VAL:HA	1.93	0.49
1:LA:132:ARG:NH1	1:LA:165:GLN:O	2.41	0.49
2:QA:44:VAL:HA	2:QA:47:LYS:HE2	1.94	0.49
2:SA:40:GLY:HA3	2:SA:314:VAL:HA	1.93	0.49
2:UA:40:GLY:HA3	2:UA:314:VAL:HA	1.93	0.49
2:H:363:ALA:O	2:H:366:THR:OG1	2.25	0.49
2:P:308:ASP:OD1	2:P:308:ASP:N	2.43	0.49
1:Q:328:ASN:ND2	1:TA:221:ALA:HB3	2.28	0.49
2:R:239:ASN:ND2	2:R:259[B]:SER:OG	2.41	0.49
2:R:311:LEU:HA	2:R:314:VAL:HG12	1.94	0.49
2:AA:40:GLY:HA3	2:AA:314:VAL:HA	1.93	0.49
2:EA:130:ALA:HB3	2:EA:283:LEU:HB3	1.94	0.49
2:WA:40:GLY:HA3	2:WA:314:VAL:HA	1.93	0.49
2:B:40:GLY:HA3	2:B:314:VAL:HA	1.93	0.49
1:C:67:ASP:OD1	1:C:71:THR:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:ALA:HB3	2:H:283:LEU:HB3	1.94	0.49
2:H:160:LEU:HD12	2:H:167:ALA:HA	1.94	0.49
1:O:67:ASP:OD1	1:O:71:THR:N	2.41	0.49
2:R:44:VAL:HA	2:R:47:LYS:HE2	1.94	0.49
2:Y:311:LEU:HA	2:Y:314:VAL:HG12	1.94	0.49
2:AA:363:ALA:O	2:AA:366:THR:OG1	2.25	0.49
2:CA:160:LEU:HD12	2:CA:167:ALA:HA	1.94	0.49
2:KA:44:VAL:HA	2:KA:47:LYS:HE2	1.94	0.49
2:MA:308:ASP:OD1	2:MA:308:ASP:N	2.43	0.49
2:MA:311:LEU:HA	2:MA:314:VAL:HG12	1.94	0.49
2:SA:311:LEU:HA	2:SA:314:VAL:HG12	1.94	0.49
2:D:363:ALA:O	2:D:366:THR:OG1	2.25	0.49
2:J:363:ALA:O	2:J:366:THR:OG1	2.25	0.49
2:T:311:LEU:HA	2:T:314:VAL:HG12	1.94	0.49
2:CA:130:ALA:HB3	2:CA:283:LEU:HB3	1.94	0.49
2:EA:40:GLY:HA3	2:EA:314:VAL:HA	1.93	0.49
2:GA:160:LEU:HD12	2:GA:167:ALA:HA	1.94	0.49
2:B:311:LEU:HA	2:B:314:VAL:HG12	1.94	0.49
2:D:308:ASP:OD1	2:D:308:ASP:N	2.42	0.49
2:N:311:LEU:HA	2:N:314:VAL:HG12	1.94	0.49
2:AA:36:LYS:O	2:AA:318:LYS:NZ	2.43	0.49
2:MA:44:VAL:HA	2:MA:47:LYS:HE2	1.94	0.49
1:PA:67:ASP:OD1	1:PA:71:THR:N	2.41	0.49
1:PA:132:ARG:NH1	1:PA:165:GLN:O	2.41	0.49
2:WA:160:LEU:HD12	2:WA:167:ALA:HA	1.94	0.49
2:B:44:VAL:HA	2:B:47:LYS:HE2	1.94	0.49
2:D:130:ALA:HB3	2:D:283:LEU:HB3	1.94	0.49
2:J:44:VAL:HA	2:J:47:LYS:HE2	1.94	0.49
1:O:132:ARG:NH1	1:O:165:GLN:O	2.41	0.49
2:P:44:VAL:HA	2:P:47:LYS:HE2	1.94	0.49
2:EA:250:PRO:HA	2:EA:253:TRP:CE2	2.48	0.49
2:GA:40:GLY:HA3	2:GA:314:VAL:HA	1.93	0.49
2:MA:40:GLY:HA3	2:MA:314:VAL:HA	1.94	0.49
1:RA:327:THR:HG21	1:VA:218:ASP:O	2.13	0.49
2:J:160:LEU:HD12	2:J:167:ALA:HA	1.94	0.49
2:R:40:GLY:HA3	2:R:314:VAL:HA	1.93	0.49
2:R:250:PRO:HA	2:R:253:TRP:CE2	2.48	0.49
2:T:44:VAL:HA	2:T:47:LYS:HE2	1.94	0.49
2:W:311:LEU:HA	2:W:314:VAL:HG12	1.94	0.49
2:AA:44:VAL:HA	2:AA:47:LYS:HE2	1.94	0.49
2:EA:160:LEU:HD12	2:EA:167:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:311:LEU:HA	2:OA:314:VAL:HG12	1.94	0.49
2:SA:44:VAL:HA	2:SA:47:LYS:HE2	1.94	0.49
2:UA:250:PRO:HA	2:UA:253:TRP:CE2	2.48	0.49
2:WA:311:LEU:HA	2:WA:314:VAL:HG12	1.94	0.49
2:D:40:GLY:HA3	2:D:314:VAL:HA	1.94	0.49
2:D:311:LEU:HA	2:D:314:VAL:HG12	1.94	0.49
2:N:44:VAL:HA	2:N:47:LYS:HE2	1.94	0.49
2:R:160:LEU:HD12	2:R:167:ALA:HA	1.94	0.49
2:W:250:PRO:HA	2:W:253:TRP:CE2	2.48	0.49
2:KA:36:LYS:O	2:KA:318:LYS:NZ	2.43	0.49
2:UA:363:ALA:O	2:UA:366:THR:OG1	2.25	0.49
2:F:311:LEU:HA	2:F:314:VAL:HG12	1.94	0.49
1:K:218:ASP:O	1:VA:327:THR:HG21	2.13	0.49
2:Y:44:VAL:HA	2:Y:47:LYS:HE2	1.94	0.49
2:GA:311:LEU:HA	2:GA:314:VAL:HG12	1.94	0.49
2:IA:194:ASN:HB2	2:IA:196:LYS:HZ2	1.77	0.49
2:KA:250:PRO:HA	2:KA:253:TRP:CE2	2.48	0.49
1:LA:113:TRP:CE3	2:MA:158:LYS:HG2	2.48	0.49
2:WA:250:PRO:HA	2:WA:253:TRP:CE2	2.48	0.49
2:D:160:LEU:HD12	2:D:167:ALA:HA	1.94	0.49
2:F:44:VAL:HA	2:F:47:LYS:HE2	1.94	0.49
2:L:194:ASN:HB2	2:L:196:LYS:HZ2	1.77	0.49
2:R:130:ALA:HB3	2:R:283:LEU:HB3	1.94	0.49
2:EA:44:VAL:HA	2:EA:47:LYS:HE2	1.94	0.49
2:KA:311:LEU:HA	2:KA:314:VAL:HG12	1.94	0.49
2:OA:44:VAL:HA	2:OA:47:LYS:HE2	1.94	0.49
2:QA:250:PRO:HA	2:QA:253:TRP:CE2	2.48	0.49
2:UA:376:GLN:NE2	2:UA:384:ASP:OD2	2.42	0.49
2:F:129:ILE:HG13	2:F:306:LEU:HD21	1.95	0.48
2:F:191:LYS:NZ	2:F:198:ASP:OD2	2.34	0.48
2:H:250:PRO:HA	2:H:253:TRP:CE2	2.48	0.48
2:Y:160:LEU:HD12	2:Y:167:ALA:HA	1.94	0.48
2:Y:250:PRO:HA	2:Y:253:TRP:CE2	2.48	0.48
2:AA:160:LEU:HD12	2:AA:167:ALA:HA	1.94	0.48
2:EA:129:ILE:HG13	2:EA:306:LEU:HD21	1.95	0.48
2:EA:239:ASN:ND2	2:EA:259[B]:SER:OG	2.41	0.48
2:EA:376:GLN:NE2	2:EA:384:ASP:OD2	2.42	0.48
2:GA:250:PRO:HA	2:GA:253:TRP:CE2	2.48	0.48
2:KA:160:LEU:HD12	2:KA:167:ALA:HA	1.94	0.48
2:MA:250:PRO:HA	2:MA:253:TRP:CE2	2.48	0.48
2:OA:129:ILE:HG13	2:OA:306:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SA:129:ILE:HG13	2:SA:306:LEU:HD21	1.95	0.48
2:UA:160:LEU:HD12	2:UA:167:ALA:HA	1.94	0.48
2:UA:311:LEU:HA	2:UA:314:VAL:HG12	1.94	0.48
2:B:250:PRO:HA	2:B:253:TRP:CE2	2.48	0.48
2:D:250:PRO:HA	2:D:253:TRP:CE2	2.48	0.48
2:D:343:GLU:HA	2:D:346:GLN:HG2	1.96	0.48
2:H:82:PHE:HB3	2:H:283:LEU:HD21	1.96	0.48
1:K:305:ASP:CG	1:Z:308:GLU:HG3	2.38	0.48
2:L:250:PRO:HA	2:L:253:TRP:CE2	2.48	0.48
2:N:160:LEU:HD12	2:N:167:ALA:HA	1.94	0.48
2:T:129:ILE:HG13	2:T:306:LEU:HD21	1.95	0.48
2:CA:82:PHE:HB3	2:CA:283:LEU:HD21	1.96	0.48
2:IA:250:PRO:HA	2:IA:253:TRP:CE2	2.48	0.48
2:KA:130:ALA:HB3	2:KA:283:LEU:HB3	1.94	0.48
2:MA:130:ALA:HB3	2:MA:283:LEU:HB3	1.94	0.48
2:OA:191:LYS:NZ	2:OA:198:ASP:OD2	2.34	0.48
2:OA:250:PRO:HA	2:OA:253:TRP:CE2	2.48	0.48
2:OA:308:ASP:N	2:OA:308:ASP:OD1	2.42	0.48
2:B:130:ALA:HB3	2:B:283:LEU:HB3	1.94	0.48
2:B:160:LEU:HD12	2:B:167:ALA:HA	1.94	0.48
2:F:250:PRO:HA	2:F:253:TRP:CE2	2.48	0.48
2:F:308:ASP:N	2:F:308:ASP:OD1	2.43	0.48
2:J:250:PRO:HA	2:J:253:TRP:CE2	2.48	0.48
2:CA:250:PRO:HA	2:CA:253:TRP:CE2	2.48	0.48
1:DA:67:ASP:OD1	1:DA:71:THR:N	2.41	0.48
2:MA:343:GLU:HA	2:MA:346:GLN:HG2	1.95	0.48
2:H:311:LEU:HA	2:H:314:VAL:HG12	1.94	0.48
2:P:250:PRO:HA	2:P:253:TRP:CE2	2.48	0.48
2:P:311:LEU:HA	2:P:314:VAL:HG12	1.94	0.48
2:AA:250:PRO:HA	2:AA:253:TRP:CE2	2.48	0.48
2:CA:311:LEU:HA	2:CA:314:VAL:HG12	1.94	0.48
2:MA:160:LEU:HD12	2:MA:167:ALA:HA	1.94	0.48
2:QA:129:ILE:HG13	2:QA:306:LEU:HD21	1.95	0.48
2:SA:343:GLU:HA	2:SA:346:GLN:HG2	1.96	0.48
2:UA:129:ILE:HG13	2:UA:306:LEU:HD21	1.95	0.48
2:F:343:GLU:HA	2:F:346:GLN:HG2	1.96	0.48
2:P:129:ILE:HG13	2:P:306:LEU:HD21	1.95	0.48
2:T:82:PHE:HB3	2:T:283:LEU:HD21	1.96	0.48
2:T:343:GLU:HA	2:T:346:GLN:HG2	1.96	0.48
2:Y:82:PHE:HB3	2:Y:283:LEU:HD21	1.96	0.48
2:CA:36:LYS:O	2:CA:318:LYS:NZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GA:343:GLU:HA	2:GA:346:GLN:HG2	1.95	0.48
2:IA:160:LEU:HD12	2:IA:167:ALA:HA	1.94	0.48
2:MA:82:PHE:HB3	2:MA:283:LEU:HD21	1.95	0.48
2:OA:343:GLU:HA	2:OA:346:GLN:HG2	1.96	0.48
2:WA:343:GLU:HA	2:WA:346:GLN:HG2	1.95	0.48
2:D:82:PHE:HB3	2:D:283:LEU:HD21	1.96	0.48
2:D:210:LYS:HG2	2:D:382:LEU:HD21	1.96	0.48
2:L:160:LEU:HD12	2:L:167:ALA:HA	1.94	0.48
2:P:343:GLU:HA	2:P:346:GLN:HG2	1.95	0.48
2:W:129:ILE:HG13	2:W:306:LEU:HD21	1.95	0.48
1:FA:209:LEU:HD21	1:LA:244:MET:HE1	1.95	0.48
2:OA:239:ASN:ND2	2:OA:259[B]:SER:OG	2.41	0.48
2:QA:343:GLU:HA	2:QA:346:GLN:HG2	1.96	0.48
2:SA:250:PRO:HA	2:SA:253:TRP:CE2	2.48	0.48
2:B:82:PHE:HB3	2:B:283:LEU:HD21	1.96	0.48
2:B:210:LYS:HG2	2:B:382:LEU:HD21	1.96	0.48
1:C:50:ASP:OD1	1:C:50:ASP:N	2.47	0.48
2:F:82:PHE:HB3	2:F:283:LEU:HD21	1.96	0.48
2:F:239:ASN:ND2	2:F:259[B]:SER:OG	2.41	0.48
2:N:82:PHE:HB3	2:N:283:LEU:HD21	1.96	0.48
2:N:250:PRO:HA	2:N:253:TRP:CE2	2.48	0.48
2:R:129:ILE:HG13	2:R:306:LEU:HD21	1.95	0.48
2:T:250:PRO:HA	2:T:253:TRP:CE2	2.48	0.48
2:W:160:LEU:HD12	2:W:167:ALA:HA	1.94	0.48
2:W:363:ALA:O	2:W:366:THR:OG1	2.25	0.48
1:X:50:ASP:OD1	1:X:50:ASP:N	2.47	0.48
2:KA:343:GLU:HA	2:KA:346:GLN:HG2	1.95	0.48
2:OA:82:PHE:HB3	2:OA:283:LEU:HD21	1.96	0.48
2:SA:82:PHE:HB3	2:SA:283:LEU:HD21	1.96	0.48
2:UA:82:PHE:HB3	2:UA:283:LEU:HD21	1.96	0.48
2:B:343:GLU:HA	2:B:346:GLN:HG2	1.95	0.48
2:D:129:ILE:HG13	2:D:306:LEU:HD21	1.95	0.48
1:I:50:ASP:OD1	1:I:50:ASP:N	2.47	0.48
2:J:308:ASP:OD1	2:J:308:ASP:N	2.43	0.48
2:J:343:GLU:HA	2:J:346:GLN:HG2	1.96	0.48
1:Q:67:ASP:OD1	1:Q:71:THR:N	2.41	0.48
1:Z:50:ASP:OD1	1:Z:50:ASP:N	2.47	0.48
2:AA:376:GLN:NE2	2:AA:384:ASP:OD2	2.42	0.48
1:BA:50:ASP:OD1	1:BA:50:ASP:N	2.47	0.48
2:IA:311:LEU:HA	2:IA:314:VAL:HG12	1.94	0.48
2:KA:210:LYS:HG2	2:KA:382:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:50:ASP:OD1	1:LA:50:ASP:N	2.47	0.48
2:MA:210:LYS:HG2	2:MA:382:LEU:HD21	1.96	0.48
1:I:67:ASP:OD1	1:I:71:THR:N	2.41	0.48
2:L:311:LEU:HA	2:L:314:VAL:HG12	1.94	0.48
2:L:343:GLU:HA	2:L:346:GLN:HG2	1.95	0.48
2:N:308:ASP:N	2:N:308:ASP:OD1	2.43	0.48
2:P:61:PRO:HD2	2:P:64:LEU:HD21	1.96	0.48
2:R:157:ASP:OD2	2:R:224:HIS:ND1	2.34	0.48
2:AA:308:ASP:N	2:AA:308:ASP:OD1	2.42	0.48
2:AA:343:GLU:HA	2:AA:346:GLN:HG2	1.95	0.48
2:CA:61:PRO:HD2	2:CA:64:LEU:HD21	1.96	0.48
2:IA:343:GLU:HA	2:IA:346:GLN:HG2	1.95	0.48
1:JA:50:ASP:OD1	1:JA:50:ASP:N	2.47	0.48
2:QA:61:PRO:HD2	2:QA:64:LEU:HD21	1.96	0.48
2:UA:210:LYS:HG2	2:UA:382:LEU:HD21	1.96	0.48
1:G:50:ASP:OD1	1:G:50:ASP:N	2.47	0.48
2:H:61:PRO:HD2	2:H:64:LEU:HD21	1.96	0.48
2:L:210:LYS:HG2	2:L:382:LEU:HD21	1.96	0.48
1:V:50:ASP:OD1	1:V:50:ASP:N	2.47	0.48
2:W:82:PHE:HB3	2:W:283:LEU:HD21	1.96	0.48
2:Y:343:GLU:HA	2:Y:346:GLN:HG2	1.95	0.48
2:EA:36:LYS:O	2:EA:318:LYS:NZ	2.43	0.48
2:EA:210:LYS:HG2	2:EA:382:LEU:HD21	1.96	0.48
2:IA:82:PHE:HB3	2:IA:283:LEU:HD21	1.96	0.48
2:IA:210:LYS:HG2	2:IA:382:LEU:HD21	1.96	0.48
2:KA:82:PHE:HB3	2:KA:283:LEU:HD21	1.96	0.48
2:MA:191:LYS:NZ	2:MA:198:ASP:OD2	2.34	0.48
1:TA:50:ASP:OD1	1:TA:50:ASP:N	2.47	0.48
1:A:50:ASP:OD1	1:A:50:ASP:N	2.47	0.47
2:F:194:ASN:HB2	2:F:196:LYS:HZ2	1.79	0.47
2:R:210:LYS:HG2	2:R:382:LEU:HD21	1.96	0.47
2:W:210:LYS:HG2	2:W:382:LEU:HD21	1.96	0.47
2:Y:194:ASN:HB2	2:Y:196:LYS:HZ2	1.79	0.47
2:F:61:PRO:HD2	2:F:64:LEU:HD21	1.96	0.47
2:L:82:PHE:HB3	2:L:283:LEU:HD21	1.96	0.47
1:S:50:ASP:OD1	1:S:50:ASP:N	2.47	0.47
2:AA:129:ILE:HG13	2:AA:306:LEU:HD21	1.95	0.47
2:CA:210:LYS:HG2	2:CA:382:LEU:HD21	1.96	0.47
2:EA:343:GLU:HA	2:EA:346:GLN:HG2	1.96	0.47
1:NA:221:ALA:CB	1:PA:328:ASN:ND2	2.78	0.47
2:OA:61:PRO:HD2	2:OA:64:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QA:82:PHE:HB3	2:QA:283:LEU:HD21	1.95	0.47
1:RA:50:ASP:OD1	1:RA:50:ASP:N	2.47	0.47
1:C:320:LYS:HD3	1:V:249:GLN:HA	1.96	0.47
1:G:301:PRO:HB2	1:FA:312:LEU:CD1	2.44	0.47
2:H:210:LYS:HG2	2:H:382:LEU:HD21	1.96	0.47
2:J:129:ILE:HG13	2:J:306:LEU:HD21	1.95	0.47
2:L:61:PRO:HD2	2:L:64:LEU:HD21	1.96	0.47
1:M:50:ASP:N	1:M:50:ASP:OD1	2.47	0.47
2:R:61:PRO:HD2	2:R:64:LEU:HD21	1.96	0.47
2:Y:129:ILE:HG13	2:Y:306:LEU:HD21	1.95	0.47
2:GA:82:PHE:HB3	2:GA:283:LEU:HD21	1.95	0.47
2:MA:129:ILE:HG13	2:MA:306:LEU:HD21	1.95	0.47
2:QA:210:LYS:HG2	2:QA:382:LEU:HD21	1.96	0.47
2:UA:61:PRO:HD2	2:UA:64:LEU:HD21	1.96	0.47
2:P:82:PHE:HB3	2:P:283:LEU:HD21	1.95	0.47
2:QA:311:LEU:HA	2:QA:314:VAL:HG12	1.94	0.47
2:B:61:PRO:HD2	2:B:64:LEU:HD21	1.96	0.47
2:F:210:LYS:HG2	2:F:382:LEU:HD21	1.96	0.47
2:R:343:GLU:HA	2:R:346:GLN:HG2	1.95	0.47
2:W:61:PRO:HD2	2:W:64:LEU:HD21	1.96	0.47
2:Y:61:PRO:HD2	2:Y:64:LEU:HD21	1.96	0.47
1:Z:67:ASP:OD1	1:Z:71:THR:N	2.41	0.47
2:AA:210:LYS:HG2	2:AA:382:LEU:HD21	1.96	0.47
2:GA:129:ILE:HG13	2:GA:306:LEU:HD21	1.95	0.47
2:IA:61:PRO:HD2	2:IA:64:LEU:HD21	1.96	0.47
2:OA:210:LYS:HG2	2:OA:382:LEU:HD21	1.96	0.47
2:UA:36:LYS:O	2:UA:318:LYS:NZ	2.43	0.47
2:WA:82:PHE:HB3	2:WA:283:LEU:HD21	1.96	0.47
2:WA:129:ILE:HG13	2:WA:306:LEU:HD21	1.95	0.47
2:J:210:LYS:HG2	2:J:382:LEU:HD21	1.96	0.47
1:M:206:TYR:OH	1:PA:257:GLN:O	2.23	0.47
2:N:343:GLU:HA	2:N:346:GLN:HG2	1.95	0.47
2:B:129:ILE:HG13	2:B:306:LEU:HD21	1.95	0.47
2:H:239:ASN:ND2	2:H:259[B]:SER:OG	2.41	0.47
1:K:221:ALA:CB	1:VA:328:ASN:ND2	2.78	0.47
2:N:129:ILE:HG13	2:N:306:LEU:HD21	1.95	0.47
2:T:61:PRO:HD2	2:T:64:LEU:HD21	1.96	0.47
1:Z:113:TRP:HZ3	2:AA:158:LYS:HA	1.79	0.47
2:AA:47:LYS:HE3	2:AA:47:LYS:HB2	1.70	0.47
2:CA:129:ILE:HG13	2:CA:306:LEU:HD21	1.95	0.47
2:CA:194:ASN:HB2	2:CA:196:LYS:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CA:343:GLU:HA	2:CA:346:GLN:HG2	1.95	0.47
2:EA:308:ASP:OD1	2:EA:308:ASP:N	2.42	0.47
2:GA:210:LYS:HG2	2:GA:382:LEU:HD21	1.96	0.47
2:KA:129:ILE:HG13	2:KA:306:LEU:HD21	1.95	0.47
2:SA:210:LYS:HG2	2:SA:382:LEU:HD21	1.96	0.47
2:H:129:ILE:HG13	2:H:306:LEU:HD21	1.95	0.47
2:W:343:GLU:HA	2:W:346:GLN:HG2	1.96	0.47
1:Z:113:TRP:CZ3	2:AA:158:LYS:HG2	2.50	0.47
2:MA:61:PRO:HD2	2:MA:64:LEU:HD21	1.96	0.47
2:SA:61:PRO:HD2	2:SA:64:LEU:HD21	1.96	0.47
2:UA:343:GLU:HA	2:UA:346:GLN:HG2	1.96	0.47
2:H:343:GLU:HA	2:H:346:GLN:HG2	1.95	0.47
2:N:61:PRO:HD2	2:N:64:LEU:HD21	1.96	0.47
2:P:210:LYS:HG2	2:P:382:LEU:HD21	1.96	0.47
2:R:82:PHE:HB3	2:R:283:LEU:HD21	1.96	0.47
2:T:210:LYS:HG2	2:T:382:LEU:HD21	1.96	0.47
2:WA:210:LYS:HG2	2:WA:382:LEU:HD21	1.96	0.47
2:D:22:LYS:HE3	2:D:76:ASP:HB2	1.97	0.47
2:L:129:ILE:HG13	2:L:306:LEU:HD21	1.95	0.47
2:N:194:ASN:HB2	2:N:196:LYS:HZ2	1.80	0.47
2:R:376:GLN:HB3	2:R:380:GLU:HB2	1.97	0.47
2:AA:82:PHE:HB3	2:AA:283:LEU:HD21	1.96	0.47
2:EA:61:PRO:HD2	2:EA:64:LEU:HD21	1.96	0.47
2:IA:22:LYS:HE3	2:IA:76:ASP:HB2	1.97	0.47
2:IA:129:ILE:HG13	2:IA:306:LEU:HD21	1.95	0.47
2:MA:22:LYS:HE3	2:MA:76:ASP:HB2	1.97	0.47
1:TA:67:ASP:OD1	1:TA:71:THR:N	2.41	0.47
2:B:22:LYS:HE3	2:B:76:ASP:HB2	1.97	0.46
1:V:67:ASP:OD1	1:V:71:THR:N	2.41	0.46
2:EA:82:PHE:HB3	2:EA:283:LEU:HD21	1.96	0.46
2:EA:376:GLN:HB3	2:EA:380:GLU:HB2	1.98	0.46
2:KA:61:PRO:HD2	2:KA:64:LEU:HD21	1.96	0.46
1:RA:67:ASP:OD1	1:RA:71:THR:N	2.41	0.46
2:F:376:GLN:HB3	2:F:380:GLU:HB2	1.97	0.46
2:L:22:LYS:HE3	2:L:76:ASP:HB2	1.97	0.46
2:N:210:LYS:HG2	2:N:382:LEU:HD21	1.96	0.46
2:EA:22:LYS:HE3	2:EA:76:ASP:HB2	1.97	0.46
2:KA:22:LYS:HE3	2:KA:76:ASP:HB2	1.97	0.46
2:KA:376:GLN:HB3	2:KA:380:GLU:HB2	1.98	0.46
2:OA:376:GLN:HB3	2:OA:380:GLU:HB2	1.98	0.46
2:QA:376:GLN:HB3	2:QA:380:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:PRO:HD2	2:D:64:LEU:HD21	1.96	0.46
2:J:82:PHE:HB3	2:J:283:LEU:HD21	1.96	0.46
2:Y:376:GLN:HB3	2:Y:380:GLU:HB2	1.98	0.46
2:AA:61:PRO:HD2	2:AA:64:LEU:HD21	1.96	0.46
2:B:376:GLN:HB3	2:B:380:GLU:HB2	1.98	0.46
2:L:191:LYS:NZ	2:L:198:ASP:OD2	2.34	0.46
2:P:376:GLN:HB3	2:P:380:GLU:HB2	1.97	0.46
1:Q:50:ASP:OD1	1:Q:50:ASP:N	2.47	0.46
2:R:22:LYS:HE3	2:R:76:ASP:HB2	1.98	0.46
2:AA:191:LYS:NZ	2:AA:198:ASP:OD2	2.34	0.46
2:CA:376:GLN:HB3	2:CA:380:GLU:HB2	1.98	0.46
2:GA:22:LYS:HE3	2:GA:76:ASP:HB2	1.97	0.46
2:SA:376:GLN:HB3	2:SA:380:GLU:HB2	1.97	0.46
2:D:376:GLN:HB3	2:D:380:GLU:HB2	1.97	0.46
2:H:376:GLN:HB3	2:H:380:GLU:HB2	1.98	0.46
2:J:22:LYS:HE3	2:J:76:ASP:HB2	1.97	0.46
2:J:61:PRO:HD2	2:J:64:LEU:HD21	1.96	0.46
2:R:36:LYS:O	2:R:318:LYS:NZ	2.43	0.46
1:S:67:ASP:OD1	1:S:71:THR:N	2.41	0.46
2:T:376:GLN:HB3	2:T:380:GLU:HB2	1.97	0.46
2:W:36:LYS:O	2:W:318:LYS:NZ	2.43	0.46
2:W:191:LYS:NZ	2:W:198:ASP:OD2	2.34	0.46
2:IA:191:LYS:NZ	2:IA:198:ASP:OD2	2.34	0.46
1:C:221:ALA:HB3	1:E:328:ASN:HD21	1.75	0.46
2:J:191:LYS:NZ	2:J:198:ASP:OD2	2.34	0.46
2:N:376:GLN:HB3	2:N:380:GLU:HB2	1.97	0.46
2:N:376:GLN:NE2	2:N:384:ASP:OD2	2.42	0.46
2:Y:376:GLN:NE2	2:Y:384:ASP:OD2	2.42	0.46
2:AA:22:LYS:HE3	2:AA:76:ASP:HB2	1.97	0.46
1:DA:50:ASP:OD1	1:DA:50:ASP:N	2.47	0.46
2:F:22:LYS:HE3	2:F:76:ASP:HB2	1.97	0.46
1:K:221:ALA:CB	1:VA:328:ASN:HD21	2.28	0.46
2:OA:22:LYS:HE3	2:OA:76:ASP:HB2	1.97	0.46
2:WA:22:LYS:HE3	2:WA:76:ASP:HB2	1.97	0.46
2:WA:61:PRO:HD2	2:WA:64:LEU:HD21	1.96	0.46
2:D:191:LYS:NZ	2:D:198:ASP:OD2	2.34	0.46
2:L:376:GLN:HB3	2:L:380:GLU:HB2	1.98	0.46
2:Y:210:LYS:HG2	2:Y:382:LEU:HD21	1.96	0.46
1:DA:56:LEU:HD23	1:DA:56:LEU:HA	1.83	0.46
1:JA:209:LEU:HD13	1:TA:237:ARG:NH1	2.30	0.46
2:J:47:LYS:HE3	2:J:47:LYS:HB2	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GA:376:GLN:HB3	2:GA:380:GLU:HB2	1.98	0.46
2:D:376:GLN:NE2	2:D:384:ASP:OD2	2.42	0.46
1:K:50:ASP:OD1	1:K:50:ASP:N	2.47	0.46
2:EA:81:ILE:O	2:EA:285:ALA:HA	2.16	0.46
2:EA:191:LYS:NZ	2:EA:198:ASP:OD2	2.34	0.46
2:GA:61:PRO:HD2	2:GA:64:LEU:HD21	1.96	0.46
1:LA:112:TYR:CE1	2:MA:158:LYS:HE3	2.51	0.46
2:MA:376:GLN:HB3	2:MA:380:GLU:HB2	1.97	0.46
2:QA:22:LYS:HE3	2:QA:76:ASP:HB2	1.97	0.46
1:G:79:TYR:CE1	2:H:223:LYS:HB2	2.51	0.45
2:W:22:LYS:HE3	2:W:76:ASP:HB2	1.97	0.45
1:HA:50:ASP:OD1	1:HA:50:ASP:N	2.47	0.45
2:IA:376:GLN:HB3	2:IA:380:GLU:HB2	1.98	0.45
2:WA:376:GLN:HB3	2:WA:380:GLU:HB2	1.98	0.45
2:H:22:LYS:HE3	2:H:76:ASP:HB2	1.97	0.45
1:O:50:ASP:OD1	1:O:50:ASP:N	2.47	0.45
2:P:263:TYR:OH	2:P:337:ARG:NH2	2.50	0.45
2:R:81:ILE:O	2:R:285:ALA:HA	2.17	0.45
2:CA:22:LYS:HE3	2:CA:76:ASP:HB2	1.97	0.45
2:KA:263:TYR:OH	2:KA:337:ARG:NH2	2.50	0.45
2:UA:22:LYS:HE3	2:UA:76:ASP:HB2	1.97	0.45
2:B:263:TYR:OH	2:B:337:ARG:NH2	2.50	0.45
2:N:81:ILE:O	2:N:285:ALA:HA	2.17	0.45
2:EA:263:TYR:OH	2:EA:337:ARG:NH2	2.50	0.45
2:GA:263:TYR:OH	2:GA:337:ARG:NH2	2.50	0.45
2:B:81:ILE:O	2:B:285:ALA:HA	2.17	0.45
2:R:263:TYR:OH	2:R:337:ARG:NH2	2.50	0.45
2:T:308:ASP:N	2:T:308:ASP:OD1	2.42	0.45
2:Y:22:LYS:HE3	2:Y:76:ASP:HB2	1.97	0.45
1:Z:112:TYR:CE1	2:AA:158:LYS:HE3	2.51	0.45
2:AA:376:GLN:HB3	2:AA:380:GLU:HB2	1.97	0.45
2:IA:81:ILE:O	2:IA:285:ALA:HA	2.17	0.45
2:KA:81:ILE:O	2:KA:285:ALA:HA	2.17	0.45
2:OA:127:TYR:HB2	2:OA:301:LEU:HD23	1.99	0.45
1:PA:50:ASP:OD1	1:PA:50:ASP:N	2.47	0.45
2:QA:127:TYR:HB2	2:QA:301:LEU:HD23	1.99	0.45
2:UA:81:ILE:O	2:UA:285:ALA:HA	2.17	0.45
2:WA:263:TYR:OH	2:WA:337:ARG:NH2	2.50	0.45
2:D:127:TYR:HB2	2:D:301:LEU:HD23	1.99	0.45
2:H:81:ILE:O	2:H:285:ALA:HA	2.17	0.45
2:L:81:ILE:O	2:L:285:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:263:TYR:OH	2:L:337:ARG:NH2	2.50	0.45
2:P:22:LYS:HE3	2:P:76:ASP:HB2	1.97	0.45
2:W:81:ILE:O	2:W:285:ALA:HA	2.17	0.45
2:W:127:TYR:HB2	2:W:301:LEU:HD23	1.99	0.45
2:IA:263:TYR:OH	2:IA:337:ARG:NH2	2.50	0.45
2:KA:127:TYR:HB2	2:KA:301:LEU:HD23	1.99	0.45
2:MA:127:TYR:HB2	2:MA:301:LEU:HD23	1.99	0.45
2:QA:263:TYR:OH	2:QA:337:ARG:NH2	2.50	0.45
2:F:127:TYR:HB2	2:F:301:LEU:HD23	1.99	0.45
2:H:263:TYR:OH	2:H:337:ARG:NH2	2.50	0.45
2:P:127:TYR:HB2	2:P:301:LEU:HD23	1.99	0.45
2:CA:81:ILE:O	2:CA:285:ALA:HA	2.17	0.45
2:CA:263:TYR:OH	2:CA:337:ARG:NH2	2.50	0.45
2:UA:127:TYR:HB2	2:UA:301:LEU:HD23	1.99	0.45
2:B:127:TYR:HB2	2:B:301:LEU:HD23	1.99	0.45
1:Q:328:ASN:HD21	1:TA:221:ALA:HB3	1.82	0.45
2:W:376:GLN:HB3	2:W:380:GLU:HB2	1.98	0.45
2:Y:81:ILE:O	2:Y:285:ALA:HA	2.17	0.45
2:EA:83:TRP:CD1	2:EA:84:ALA:H	2.35	0.45
2:J:376:GLN:HB3	2:J:380:GLU:HB2	1.97	0.45
2:N:22:LYS:HE3	2:N:76:ASP:HB2	1.97	0.45
2:N:263:TYR:OH	2:N:337:ARG:NH2	2.50	0.45
2:P:81:ILE:O	2:P:285:ALA:HA	2.17	0.45
2:R:83:TRP:CD1	2:R:84:ALA:H	2.35	0.45
1:S:57:MET:HB3	1:S:92:TYR:CZ	2.52	0.45
1:HA:57:MET:HB3	1:HA:92:TYR:CZ	2.52	0.45
1:LA:71:THR:HG23	2:MA:223:LYS:HZ1	1.82	0.45
2:MA:376:GLN:NE2	2:MA:384:ASP:OD2	2.42	0.45
1:RA:57:MET:HB3	1:RA:92:TYR:CZ	2.52	0.45
2:SA:22:LYS:HE3	2:SA:76:ASP:HB2	1.97	0.45
2:SA:263:TYR:OH	2:SA:337:ARG:NH2	2.50	0.45
2:B:83:TRP:CD1	2:B:84:ALA:H	2.35	0.45
1:I:57:MET:HB3	1:I:92:TYR:CZ	2.52	0.45
2:J:83:TRP:CD1	2:J:84:ALA:H	2.35	0.45
1:O:57:MET:HB3	1:O:92:TYR:CZ	2.52	0.45
1:Q:56:LEU:HD23	1:Q:56:LEU:HA	1.83	0.45
2:T:263:TYR:OH	2:T:337:ARG:NH2	2.50	0.45
2:AA:81:ILE:O	2:AA:285:ALA:HA	2.17	0.45
2:AA:83:TRP:CD1	2:AA:84:ALA:H	2.35	0.45
2:KA:83:TRP:CD1	2:KA:84:ALA:H	2.35	0.45
1:PA:57:MET:HB3	1:PA:92:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:113:TRP:CE3	2:SA:158:LYS:HG2	2.52	0.45
1:A:57:MET:HB3	1:A:92:TYR:CZ	2.52	0.45
2:F:263:TYR:OH	2:F:337:ARG:NH2	2.50	0.45
1:K:57:MET:HB3	1:K:92:TYR:CZ	2.52	0.45
2:T:22:LYS:HE3	2:T:76:ASP:HB2	1.97	0.45
1:Z:57:MET:HB3	1:Z:92:TYR:CZ	2.52	0.45
1:DA:57:MET:HB3	1:DA:92:TYR:CZ	2.52	0.45
1:JA:57:MET:HB3	1:JA:92:TYR:CZ	2.52	0.45
2:WA:81:ILE:O	2:WA:285:ALA:HA	2.17	0.45
2:WA:83:TRP:CD1	2:WA:84:ALA:H	2.35	0.45
2:B:104:LYS:HA	2:B:104:LYS:HD3	1.81	0.44
2:J:81:ILE:O	2:J:285:ALA:HA	2.17	0.44
1:Q:57:MET:HB3	1:Q:92:TYR:CZ	2.52	0.44
2:R:327:SER:O	2:R:331:GLU:HG3	2.18	0.44
2:T:327:SER:O	2:T:331:GLU:HG3	2.18	0.44
2:T:376:GLN:NE2	2:T:384:ASP:OD2	2.42	0.44
2:W:160:LEU:HD23	2:W:160:LEU:HA	1.83	0.44
2:Y:263:TYR:OH	2:Y:337:ARG:NH2	2.50	0.44
2:AA:263:TYR:OH	2:AA:337:ARG:NH2	2.50	0.44
2:EA:327:SER:O	2:EA:331:GLU:HG3	2.17	0.44
2:GA:81:ILE:O	2:GA:285:ALA:HA	2.17	0.44
2:GA:83:TRP:CD1	2:GA:84:ALA:H	2.35	0.44
1:HA:41:LEU:HD23	1:HA:41:LEU:HA	1.89	0.44
1:NA:57:MET:HB3	1:NA:92:TYR:CZ	2.52	0.44
2:OA:263:TYR:OH	2:OA:337:ARG:NH2	2.50	0.44
2:SA:327:SER:O	2:SA:331:GLU:HG3	2.18	0.44
2:SA:376:GLN:NE2	2:SA:384:ASP:OD2	2.42	0.44
1:C:57:MET:HB3	1:C:92:TYR:CZ	2.52	0.44
2:D:81:ILE:O	2:D:285:ALA:HA	2.17	0.44
1:E:57:MET:HB3	1:E:92:TYR:CZ	2.52	0.44
2:H:100:ILE:HD11	2:H:124:LEU:HG	2.00	0.44
2:Y:83:TRP:CD1	2:Y:84:ALA:H	2.35	0.44
1:DA:113:TRP:HZ3	2:EA:158:LYS:HA	1.82	0.44
2:EA:47:LYS:HB2	2:EA:47:LYS:HE3	1.69	0.44
1:FA:50:ASP:OD1	1:FA:50:ASP:N	2.47	0.44
2:GA:47:LYS:HE3	2:GA:47:LYS:HB2	1.69	0.44
2:QA:81:ILE:O	2:QA:285:ALA:HA	2.17	0.44
2:T:81:ILE:O	2:T:285:ALA:HA	2.17	0.44
2:CA:100:ILE:HD11	2:CA:124:LEU:HG	2.00	0.44
2:GA:127:TYR:HB2	2:GA:301:LEU:HD23	1.99	0.44
2:QA:327:SER:O	2:QA:331:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UA:376:GLN:HB3	2:UA:380:GLU:HB2	1.97	0.44
2:D:263:TYR:OH	2:D:337:ARG:NH2	2.50	0.44
2:F:81:ILE:O	2:F:285:ALA:HA	2.17	0.44
2:J:263:TYR:OH	2:J:337:ARG:NH2	2.50	0.44
2:L:100:ILE:HD11	2:L:124:LEU:HG	2.00	0.44
2:L:104:LYS:HA	2:L:104:LYS:HD3	1.81	0.44
2:N:83:TRP:CD1	2:N:84:ALA:H	2.35	0.44
2:P:100:ILE:HD11	2:P:124:LEU:HG	2.00	0.44
2:P:327:SER:O	2:P:331:GLU:HG3	2.18	0.44
2:Y:327:SER:O	2:Y:331:GLU:HG3	2.18	0.44
2:AA:327:SER:O	2:AA:331:GLU:HG3	2.18	0.44
1:FA:56:LEU:HD23	1:FA:56:LEU:HA	1.83	0.44
2:KA:327:SER:O	2:KA:331:GLU:HG3	2.18	0.44
2:MA:81:ILE:O	2:MA:285:ALA:HA	2.17	0.44
2:QA:100:ILE:HD11	2:QA:124:LEU:HG	2.00	0.44
2:SA:81:ILE:O	2:SA:285:ALA:HA	2.17	0.44
2:B:100:ILE:HD11	2:B:124:LEU:HG	2.00	0.44
2:F:376:GLN:NE2	2:F:384:ASP:OD2	2.42	0.44
2:J:327:SER:O	2:J:331:GLU:HG3	2.18	0.44
2:IA:100:ILE:HD11	2:IA:124:LEU:HG	2.00	0.44
2:MA:83:TRP:CD1	2:MA:84:ALA:H	2.35	0.44
1:VA:50:ASP:OD1	1:VA:50:ASP:N	2.47	0.44
2:WA:47:LYS:HE3	2:WA:47:LYS:HB2	1.70	0.44
1:C:249:GLN:HA	1:RA:320:LYS:HD3	1.98	0.44
2:D:83:TRP:CD1	2:D:84:ALA:H	2.35	0.44
2:N:327:SER:O	2:N:331:GLU:HG3	2.18	0.44
1:Q:41:LEU:HD23	1:Q:41:LEU:HA	1.89	0.44
2:R:100:ILE:HD11	2:R:124:LEU:HG	2.00	0.44
2:T:83:TRP:CD1	2:T:84:ALA:H	2.35	0.44
2:W:327:SER:O	2:W:331:GLU:HG3	2.18	0.44
2:KA:100:ILE:HD11	2:KA:124:LEU:HG	2.00	0.44
1:LA:57:MET:HB3	1:LA:92:TYR:CZ	2.52	0.44
2:MA:327:SER:O	2:MA:331:GLU:HG3	2.18	0.44
1:NA:50:ASP:N	1:NA:50:ASP:OD1	2.47	0.44
2:OA:81:ILE:O	2:OA:285:ALA:HA	2.17	0.44
1:RA:113:TRP:CZ3	2:SA:158:LYS:HG2	2.53	0.44
2:SA:83:TRP:CD1	2:SA:84:ALA:H	2.35	0.44
2:UA:263:TYR:OH	2:UA:337:ARG:NH2	2.50	0.44
2:UA:327:SER:O	2:UA:331:GLU:HG3	2.18	0.44
2:WA:127:TYR:HB2	2:WA:301:LEU:HD23	1.99	0.44
2:B:327:SER:O	2:B:331:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:327:SER:O	2:F:331:GLU:HG3	2.18	0.44
2:J:100:ILE:HD11	2:J:124:LEU:HG	2.00	0.44
1:S:79:TYR:OH	2:T:161:LYS:NZ	2.21	0.44
2:W:83:TRP:CD1	2:W:84:ALA:H	2.35	0.44
1:X:221:ALA:HB3	1:HA:328:ASN:HD21	1.82	0.44
2:CA:83:TRP:CD1	2:CA:84:ALA:H	2.35	0.44
2:CA:127:TYR:HB2	2:CA:301:LEU:HD23	1.99	0.44
1:DA:41:LEU:HD23	1:DA:41:LEU:HA	1.89	0.44
2:GA:376:GLN:NE2	2:GA:384:ASP:OD2	2.42	0.44
2:IA:104:LYS:HA	2:IA:104:LYS:HD3	1.82	0.44
2:MA:47:LYS:HE3	2:MA:47:LYS:HB2	1.70	0.44
2:OA:327:SER:O	2:OA:331:GLU:HG3	2.18	0.44
1:TA:113:TRP:HZ3	2:UA:158:LYS:HA	1.82	0.44
2:D:104:LYS:HA	2:D:104:LYS:HD3	1.81	0.44
2:D:327:SER:O	2:D:331:GLU:HG3	2.18	0.44
2:F:100:ILE:HD11	2:F:124:LEU:HG	2.00	0.44
2:H:83:TRP:CD1	2:H:84:ALA:H	2.35	0.44
2:H:127:TYR:HB2	2:H:301:LEU:HD23	1.99	0.44
2:J:376:GLN:NE2	2:J:384:ASP:OD2	2.42	0.44
2:W:263:TYR:OH	2:W:337:ARG:NH2	2.50	0.44
2:AA:127:TYR:HB2	2:AA:301:LEU:HD23	1.99	0.44
2:IA:127:TYR:HB2	2:IA:301:LEU:HD23	1.99	0.44
2:IA:327:SER:O	2:IA:331:GLU:HG3	2.18	0.44
1:LA:56:LEU:HD23	1:LA:56:LEU:HA	1.83	0.44
2:MA:263:TYR:OH	2:MA:337:ARG:NH2	2.50	0.44
2:OA:100:ILE:HD11	2:OA:124:LEU:HG	2.00	0.44
2:QA:83:TRP:CD1	2:QA:84:ALA:H	2.35	0.44
2:UA:83:TRP:CD1	2:UA:84:ALA:H	2.35	0.44
1:VA:57:MET:HB3	1:VA:92:TYR:CZ	2.52	0.44
1:E:50:ASP:OD1	1:E:50:ASP:N	2.47	0.44
2:F:47:LYS:HB2	2:F:47:LYS:HE3	1.69	0.44
2:L:83:TRP:CD1	2:L:84:ALA:H	2.35	0.44
2:L:127:TYR:HB2	2:L:301:LEU:HD23	1.99	0.44
2:N:127:TYR:HB2	2:N:301:LEU:HD23	1.99	0.44
2:T:100:ILE:HD11	2:T:124:LEU:HG	2.00	0.44
2:T:127:TYR:HB2	2:T:301:LEU:HD23	1.99	0.44
1:BA:57:MET:HB3	1:BA:92:TYR:CZ	2.52	0.44
2:CA:327:SER:O	2:CA:331:GLU:HG3	2.18	0.44
1:FA:57:MET:HB3	1:FA:92:TYR:CZ	2.52	0.44
2:OA:376:GLN:NE2	2:OA:384:ASP:OD2	2.42	0.44
2:SA:100:ILE:HD11	2:SA:124:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UA:100:ILE:HD11	2:UA:124:LEU:HG	2.00	0.44
2:UA:160:LEU:HD23	2:UA:160:LEU:HA	1.83	0.44
2:D:100:ILE:HD11	2:D:124:LEU:HG	2.00	0.43
2:H:327:SER:O	2:H:331:GLU:HG3	2.18	0.43
2:L:327:SER:O	2:L:331:GLU:HG3	2.18	0.43
1:S:209:LEU:HD21	1:DA:244:MET:HE1	1.99	0.43
2:Y:100:ILE:HD11	2:Y:124:LEU:HG	2.00	0.43
2:Y:127:TYR:HB2	2:Y:301:LEU:HD23	1.99	0.43
2:AA:100:ILE:HD11	2:AA:124:LEU:HG	2.00	0.43
2:EA:150:TRP:CD2	2:EA:181:LEU:HD13	2.54	0.43
2:IA:83:TRP:CD1	2:IA:84:ALA:H	2.35	0.43
2:KA:298:LYS:HE2	2:KA:298:LYS:HB2	1.90	0.43
2:F:83:TRP:CD1	2:F:84:ALA:H	2.35	0.43
1:G:57:MET:HB3	1:G:92:TYR:CZ	2.52	0.43
2:J:127:TYR:HB2	2:J:301:LEU:HD23	1.99	0.43
1:M:57:MET:HB3	1:M:92:TYR:CZ	2.52	0.43
2:CA:150:TRP:CD2	2:CA:181:LEU:HD13	2.53	0.43
2:EA:100:ILE:HD11	2:EA:124:LEU:HG	2.00	0.43
2:IA:28:LEU:HD23	2:IA:56:VAL:HG22	2.00	0.43
2:OA:47:LYS:HB2	2:OA:47:LYS:HE3	1.70	0.43
1:TA:57:MET:HB3	1:TA:92:TYR:CZ	2.52	0.43
2:H:150:TRP:CD2	2:H:181:LEU:HD13	2.53	0.43
2:J:29:VAL:HG13	2:J:78:PRO:HA	2.01	0.43
2:L:150:TRP:CD2	2:L:181:LEU:HD13	2.53	0.43
2:P:83:TRP:CD1	2:P:84:ALA:H	2.35	0.43
2:R:150:TRP:CD2	2:R:181:LEU:HD13	2.53	0.43
2:T:29:VAL:HG13	2:T:78:PRO:HA	2.01	0.43
1:V:57:MET:HB3	1:V:92:TYR:CZ	2.52	0.43
2:W:100:ILE:HD11	2:W:124:LEU:HG	2.00	0.43
1:X:57:MET:HB3	1:X:92:TYR:CZ	2.52	0.43
2:AA:29:VAL:HG13	2:AA:78:PRO:HA	2.01	0.43
2:GA:100:ILE:HD11	2:GA:124:LEU:HG	2.00	0.43
2:GA:150:TRP:CD2	2:GA:181:LEU:HD13	2.53	0.43
2:IA:150:TRP:CD2	2:IA:181:LEU:HD13	2.53	0.43
2:OA:83:TRP:CD1	2:OA:84:ALA:H	2.35	0.43
2:SA:29:VAL:HG13	2:SA:78:PRO:HA	2.01	0.43
2:SA:47:LYS:HE3	2:SA:47:LYS:HB2	1.70	0.43
2:SA:127:TYR:HB2	2:SA:301:LEU:HD23	1.99	0.43
2:SA:150:TRP:CD2	2:SA:181:LEU:HD13	2.53	0.43
2:WA:150:TRP:CD2	2:WA:181:LEU:HD13	2.54	0.43
2:WA:376:GLN:NE2	2:WA:384:ASP:OD2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:150:TRP:CD2	2:J:181:LEU:HD13	2.53	0.43
2:L:28:LEU:HD23	2:L:56:VAL:HG22	2.01	0.43
2:T:150:TRP:CD2	2:T:181:LEU:HD13	2.53	0.43
2:GA:160:LEU:HD23	2:GA:160:LEU:HA	1.83	0.43
2:MA:100:ILE:HD11	2:MA:124:LEU:HG	2.00	0.43
2:MA:150:TRP:CD2	2:MA:181:LEU:HD13	2.53	0.43
2:WA:29:VAL:HG13	2:WA:78:PRO:HA	2.01	0.43
2:WA:100:ILE:HD11	2:WA:124:LEU:HG	2.00	0.43
2:N:100:ILE:HD11	2:N:124:LEU:HG	2.00	0.43
2:P:191:LYS:NZ	2:P:198:ASP:OD2	2.34	0.43
2:R:29:VAL:HG13	2:R:78:PRO:HA	2.01	0.43
2:AA:150:TRP:CD2	2:AA:181:LEU:HD13	2.53	0.43
2:CA:28:LEU:HD23	2:CA:56:VAL:HG22	2.00	0.43
2:EA:29:VAL:HG13	2:EA:78:PRO:HA	2.01	0.43
2:GA:29:VAL:HG13	2:GA:78:PRO:HA	2.01	0.43
2:MA:89:GLY:O	2:MA:92:ALA:HB3	2.19	0.43
2:D:89:GLY:O	2:D:92:ALA:HB3	2.19	0.43
2:N:89:GLY:O	2:N:92:ALA:HB3	2.19	0.43
2:R:89:GLY:O	2:R:92:ALA:HB3	2.19	0.43
2:Y:89:GLY:O	2:Y:92:ALA:HB3	2.19	0.43
2:B:89:GLY:O	2:B:92:ALA:HB3	2.19	0.43
2:D:150:TRP:CD2	2:D:181:LEU:HD13	2.54	0.43
2:F:29:VAL:HG13	2:F:78:PRO:HA	2.01	0.43
2:J:28:LEU:HD23	2:J:56:VAL:HG22	2.01	0.43
2:N:28:LEU:HD23	2:N:56:VAL:HG22	2.01	0.43
2:AA:28:LEU:HD23	2:AA:56:VAL:HG22	2.01	0.43
2:CA:47:LYS:HE3	2:CA:47:LYS:HB2	1.70	0.43
2:EA:89:GLY:O	2:EA:92:ALA:HB3	2.19	0.43
1:JA:219:ASP:HA	1:LA:327:THR:HG21	2.01	0.43
2:KA:89:GLY:O	2:KA:92:ALA:HB3	2.19	0.43
2:OA:150:TRP:CD2	2:OA:181:LEU:HD13	2.53	0.43
2:WA:160:LEU:HD23	2:WA:160:LEU:HA	1.83	0.43
2:WA:327:SER:O	2:WA:331:GLU:HG3	2.18	0.43
2:B:28:LEU:HD23	2:B:56:VAL:HG22	2.01	0.43
2:B:150:TRP:CD2	2:B:181:LEU:HD13	2.54	0.43
2:B:323:VAL:HG21	2:B:328:TYR:HD2	1.84	0.43
2:F:150:TRP:CD2	2:F:181:LEU:HD13	2.53	0.43
2:H:28:LEU:HD23	2:H:56:VAL:HG22	2.01	0.43
2:N:323:VAL:HG21	2:N:328:TYR:HD2	1.84	0.43
2:R:323:VAL:HG21	2:R:328:TYR:HD2	1.84	0.43
2:T:47:LYS:HE3	2:T:47:LYS:HB2	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:194:ASN:HB2	2:W:196:LYS:HZ2	1.83	0.43
2:EA:36:LYS:NZ	2:EA:82:PHE:O	2.52	0.43
2:EA:127:TYR:HB2	2:EA:301:LEU:HD23	1.99	0.43
2:KA:323:VAL:HG21	2:KA:328:TYR:HD2	1.84	0.43
2:OA:29:VAL:HG13	2:OA:78:PRO:HA	2.01	0.43
2:QA:150:TRP:CD2	2:QA:181:LEU:HD13	2.53	0.43
2:L:29:VAL:HG13	2:L:78:PRO:HA	2.01	0.43
2:N:150:TRP:CD2	2:N:181:LEU:HD13	2.53	0.43
2:P:89:GLY:O	2:P:92:ALA:HB3	2.19	0.43
2:P:323:VAL:HG21	2:P:328:TYR:HD2	1.84	0.43
2:R:28:LEU:HD23	2:R:56:VAL:HG22	2.01	0.43
2:R:127:TYR:HB2	2:R:301:LEU:HD23	1.99	0.43
2:T:323:VAL:HG21	2:T:328:TYR:HD2	1.84	0.43
2:W:36:LYS:NZ	2:W:82:PHE:O	2.52	0.43
2:QA:191:LYS:NZ	2:QA:198:ASP:OD2	2.34	0.43
2:UA:36:LYS:NZ	2:UA:82:PHE:O	2.52	0.43
2:F:160:LEU:HD23	2:F:160:LEU:HA	1.83	0.43
2:F:323:VAL:HG21	2:F:328:TYR:HD2	1.84	0.43
2:H:47:LYS:HE3	2:H:47:LYS:HB2	1.69	0.43
2:R:36:LYS:NZ	2:R:82:PHE:O	2.52	0.43
2:Y:28:LEU:HD23	2:Y:56:VAL:HG22	2.00	0.43
2:Y:29:VAL:HG13	2:Y:78:PRO:HA	2.01	0.43
2:Y:323:VAL:HG21	2:Y:328:TYR:HD2	1.84	0.43
2:GA:327:SER:O	2:GA:331:GLU:HG3	2.18	0.43
2:IA:29:VAL:HG13	2:IA:78:PRO:HA	2.01	0.43
2:IA:89:GLY:O	2:IA:92:ALA:HB3	2.19	0.43
2:KA:28:LEU:HD23	2:KA:56:VAL:HG22	2.01	0.43
2:MA:323:VAL:HG21	2:MA:328:TYR:HD2	1.84	0.43
2:OA:323:VAL:HG21	2:OA:328:TYR:HD2	1.84	0.43
2:QA:323:VAL:HG21	2:QA:328:TYR:HD2	1.84	0.43
2:SA:323:VAL:HG21	2:SA:328:TYR:HD2	1.84	0.43
1:TA:261:LYS:HB2	1:TA:261:LYS:HE3	1.48	0.43
2:D:29:VAL:HG13	2:D:78:PRO:HA	2.01	0.42
2:D:47:LYS:HE3	2:D:47:LYS:HB2	1.70	0.42
2:D:323:VAL:HG21	2:D:328:TYR:HD2	1.84	0.42
2:F:197:TYR:CZ	2:F:352:PRO:HA	2.54	0.42
2:H:36:LYS:NZ	2:H:82:PHE:O	2.52	0.42
2:J:89:GLY:O	2:J:92:ALA:HB3	2.19	0.42
1:K:36:GLU:HG2	1:K:37:LEU:HG	2.01	0.42
2:L:89:GLY:O	2:L:92:ALA:HB3	2.19	0.42
2:N:36:LYS:NZ	2:N:82:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:150:TRP:CD2	2:P:181:LEU:HD13	2.53	0.42
1:S:36:GLU:HG2	1:S:37:LEU:HG	2.01	0.42
2:T:197:TYR:CZ	2:T:352:PRO:HA	2.54	0.42
2:W:323:VAL:HG21	2:W:328:TYR:HD2	1.84	0.42
2:AA:89:GLY:O	2:AA:92:ALA:HB3	2.19	0.42
2:CA:29:VAL:HG13	2:CA:78:PRO:HA	2.01	0.42
2:CA:36:LYS:NZ	2:CA:82:PHE:O	2.52	0.42
2:CA:191:LYS:NZ	2:CA:198:ASP:OD2	2.34	0.42
1:RA:36:GLU:HG2	1:RA:37:LEU:HG	2.01	0.42
2:SA:28:LEU:HD23	2:SA:56:VAL:HG22	2.01	0.42
2:SA:36:LYS:NZ	2:SA:82:PHE:O	2.52	0.42
2:UA:323:VAL:HG21	2:UA:328:TYR:HD2	1.84	0.42
2:WA:89:GLY:O	2:WA:92:ALA:HB3	2.19	0.42
2:H:191:LYS:NZ	2:H:198:ASP:OD2	2.34	0.42
1:K:219:ASP:OD1	1:K:219:ASP:N	2.49	0.42
2:L:197:TYR:CZ	2:L:352:PRO:HA	2.55	0.42
2:L:323:VAL:HG21	2:L:328:TYR:HD2	1.84	0.42
2:N:29:VAL:HG13	2:N:78:PRO:HA	2.01	0.42
2:R:197:TYR:CZ	2:R:352:PRO:HA	2.55	0.42
2:T:36:LYS:NZ	2:T:82:PHE:O	2.52	0.42
2:W:28:LEU:HD23	2:W:56:VAL:HG22	2.01	0.42
2:Y:36:LYS:NZ	2:Y:82:PHE:O	2.52	0.42
1:FA:249:GLN:HA	1:NA:320:LYS:HD3	2.00	0.42
1:HA:36:GLU:HG2	1:HA:37:LEU:HG	2.01	0.42
2:IA:197:TYR:CZ	2:IA:352:PRO:HA	2.55	0.42
2:KA:150:TRP:CD2	2:KA:181:LEU:HD13	2.53	0.42
1:LA:36:GLU:HG2	1:LA:37:LEU:HG	2.01	0.42
2:SA:197:TYR:CZ	2:SA:352:PRO:HA	2.55	0.42
2:H:29:VAL:HG13	2:H:78:PRO:HA	2.01	0.42
2:H:197:TYR:CZ	2:H:352:PRO:HA	2.55	0.42
1:M:56:LEU:HD23	1:M:56:LEU:HA	1.83	0.42
2:P:28:LEU:HD23	2:P:56:VAL:HG22	2.00	0.42
2:T:28:LEU:HD23	2:T:56:VAL:HG22	2.01	0.42
2:W:150:TRP:CD2	2:W:181:LEU:HD13	2.53	0.42
2:CA:197:TYR:CZ	2:CA:352:PRO:HA	2.55	0.42
1:DA:36:GLU:HG2	1:DA:37:LEU:HG	2.01	0.42
2:EA:28:LEU:HD23	2:EA:56:VAL:HG22	2.01	0.42
2:EA:197:TYR:CZ	2:EA:352:PRO:HA	2.55	0.42
2:EA:323:VAL:HG21	2:EA:328:TYR:HD2	1.84	0.42
2:IA:323:VAL:HG21	2:IA:328:TYR:HD2	1.84	0.42
2:KA:376:GLN:NE2	2:KA:384:ASP:OD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:160:LEU:HD23	2:OA:160:LEU:HA	1.83	0.42
2:OA:197:TYR:CZ	2:OA:352:PRO:HA	2.55	0.42
2:B:36:LYS:NZ	2:B:82:PHE:O	2.52	0.42
2:B:376:GLN:NE2	2:B:384:ASP:OD2	2.42	0.42
1:C:36:GLU:HG2	1:C:37:LEU:HG	2.01	0.42
1:I:36:GLU:HG2	1:I:37:LEU:HG	2.01	0.42
2:J:104:LYS:HA	2:J:104:LYS:HD3	1.81	0.42
2:Y:180:PRO:HG3	2:Y:278:PRO:HA	2.02	0.42
1:Z:36:GLU:HG2	1:Z:37:LEU:HG	2.01	0.42
2:CA:298:LYS:HE2	2:CA:298:LYS:HB2	1.90	0.42
2:GA:89:GLY:O	2:GA:92:ALA:HB3	2.19	0.42
2:KA:36:LYS:NZ	2:KA:82:PHE:O	2.52	0.42
2:MA:29:VAL:HG13	2:MA:78:PRO:HA	2.01	0.42
2:QA:89:GLY:O	2:QA:92:ALA:HB3	2.19	0.42
2:UA:28:LEU:HD23	2:UA:56:VAL:HG22	2.01	0.42
2:WA:28:LEU:HD23	2:WA:56:VAL:HG22	2.01	0.42
2:WA:36:LYS:NZ	2:WA:82:PHE:O	2.52	0.42
2:F:180:PRO:HG3	2:F:278:PRO:HA	2.02	0.42
2:W:89:GLY:O	2:W:92:ALA:HB3	2.19	0.42
2:Y:150:TRP:CD2	2:Y:181:LEU:HD13	2.53	0.42
2:Y:197:TYR:CZ	2:Y:352:PRO:HA	2.55	0.42
2:AA:160:LEU:HD23	2:AA:160:LEU:HA	1.83	0.42
1:FA:36:GLU:HG2	1:FA:37:LEU:HG	2.01	0.42
2:GA:28:LEU:HD23	2:GA:56:VAL:HG22	2.01	0.42
2:GA:36:LYS:NZ	2:GA:82:PHE:O	2.52	0.42
1:HA:219:ASP:OD1	1:HA:219:ASP:N	2.49	0.42
1:LA:292:HIS:CE1	1:TA:301:PRO:HB3	2.55	0.42
1:NA:56:LEU:HD23	1:NA:56:LEU:HA	1.83	0.42
2:OA:180:PRO:HG3	2:OA:278:PRO:HA	2.02	0.42
2:B:180:PRO:HG3	2:B:278:PRO:HA	2.02	0.42
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.83	0.42
2:F:36:LYS:NZ	2:F:82:PHE:O	2.52	0.42
2:L:298:LYS:HE2	2:L:298:LYS:HB2	1.90	0.42
2:N:197:TYR:CZ	2:N:352:PRO:HA	2.55	0.42
2:P:197:TYR:CZ	2:P:352:PRO:HA	2.55	0.42
2:T:89:GLY:O	2:T:92:ALA:HB3	2.19	0.42
2:AA:104:LYS:HA	2:AA:104:LYS:HD3	1.82	0.42
2:AA:323:VAL:HG21	2:AA:328:TYR:HD2	1.84	0.42
1:BA:36:GLU:HG2	1:BA:37:LEU:HG	2.01	0.42
2:OA:36:LYS:NZ	2:OA:82:PHE:O	2.52	0.42
2:SA:89:GLY:O	2:SA:92:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:UA:89:GLY:O	2:UA:92:ALA:HB3	2.19	0.42
1:VA:41:LEU:HD23	1:VA:41:LEU:HA	1.89	0.42
2:B:47:LYS:HE3	2:B:47:LYS:HB2	1.70	0.42
2:B:335:ASP:HB3	2:B:338:ILE:HG12	2.02	0.42
1:G:36:GLU:HG2	1:G:37:LEU:HG	2.01	0.42
2:H:110:LEU:HD21	2:H:306:LEU:HD13	2.02	0.42
2:H:376:GLN:NE2	2:H:384:ASP:OD2	2.42	0.42
2:N:180:PRO:HG3	2:N:278:PRO:HA	2.02	0.42
2:W:29:VAL:HG13	2:W:78:PRO:HA	2.01	0.42
2:IA:376:GLN:NE2	2:IA:384:ASP:OD2	2.42	0.42
2:KA:180:PRO:HG3	2:KA:278:PRO:HA	2.02	0.42
2:KA:197:TYR:CZ	2:KA:352:PRO:HA	2.55	0.42
2:MA:36:LYS:NZ	2:MA:82:PHE:O	2.52	0.42
2:MA:180:PRO:HG3	2:MA:278:PRO:HA	2.02	0.42
2:OA:89:GLY:O	2:OA:92:ALA:HB3	2.19	0.42
2:QA:28:LEU:HD23	2:QA:56:VAL:HG22	2.01	0.42
2:QA:180:PRO:HG3	2:QA:278:PRO:HA	2.02	0.42
2:UA:180:PRO:HG3	2:UA:278:PRO:HA	2.02	0.42
1:VA:36:GLU:HG2	1:VA:37:LEU:HG	2.01	0.42
1:A:36:GLU:HG2	1:A:37:LEU:HG	2.01	0.42
2:D:36:LYS:NZ	2:D:82:PHE:O	2.52	0.42
2:D:180:PRO:HG3	2:D:278:PRO:HA	2.02	0.42
2:J:323:VAL:HG21	2:J:328:TYR:HD2	1.84	0.42
1:O:237:ARG:NH1	1:X:209:LEU:HD13	2.35	0.42
1:Q:36:GLU:HG2	1:Q:37:LEU:HG	2.01	0.42
2:AA:36:LYS:NZ	2:AA:82:PHE:O	2.52	0.42
2:AA:335:ASP:HB3	2:AA:338:ILE:HG12	2.02	0.42
2:CA:110:LEU:HD21	2:CA:306:LEU:HD13	2.02	0.42
2:GA:104:LYS:HA	2:GA:104:LYS:HD3	1.81	0.42
2:IA:298:LYS:HE2	2:IA:298:LYS:HB2	1.90	0.42
2:MA:28:LEU:HD23	2:MA:56:VAL:HG22	2.01	0.42
2:MA:335:ASP:HB3	2:MA:338:ILE:HG12	2.02	0.42
2:QA:351[B]:MET:HE2	2:QA:351[B]:MET:HB2	1.98	0.42
2:WA:155:ALA:O	2:WA:158:LYS:HB2	2.20	0.42
2:D:335:ASP:HB3	2:D:338:ILE:HG12	2.02	0.42
2:F:89:GLY:O	2:F:92:ALA:HB3	2.19	0.42
2:H:298:LYS:HE2	2:H:298:LYS:HB2	1.90	0.42
2:J:180:PRO:HG3	2:J:278:PRO:HA	2.02	0.42
2:J:335:ASP:HB3	2:J:338:ILE:HG12	2.02	0.42
2:L:376:GLN:NE2	2:L:384:ASP:OD2	2.42	0.42
2:P:36:LYS:NZ	2:P:82:PHE:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:219:LEU:HD23	2:T:219:LEU:HA	1.92	0.42
2:W:110:LEU:HD21	2:W:306:LEU:HD13	2.02	0.42
2:AA:180:PRO:HG3	2:AA:278:PRO:HA	2.02	0.42
2:EA:194:ASN:HB2	2:EA:196:LYS:HZ2	1.85	0.42
2:GA:197:TYR:CZ	2:GA:352:PRO:HA	2.55	0.42
1:JA:36:GLU:HG2	1:JA:37:LEU:HG	2.01	0.42
2:KA:335:ASP:HB3	2:KA:338:ILE:HG12	2.02	0.42
2:MA:104:LYS:HA	2:MA:104:LYS:HD3	1.81	0.42
2:MA:155:ALA:O	2:MA:158:LYS:HB2	2.20	0.42
2:MA:197:TYR:CZ	2:MA:352:PRO:HA	2.55	0.42
2:UA:29:VAL:HG13	2:UA:78:PRO:HA	2.01	0.42
2:UA:150:TRP:CD2	2:UA:181:LEU:HD13	2.53	0.42
2:UA:197:TYR:CZ	2:UA:352:PRO:HA	2.55	0.42
2:B:197:TYR:CZ	2:B:352:PRO:HA	2.55	0.42
2:D:110:LEU:HD21	2:D:306:LEU:HD13	2.02	0.42
2:D:155:ALA:O	2:D:158:LYS:HB2	2.20	0.42
2:J:36:LYS:NZ	2:J:82:PHE:O	2.52	0.42
2:L:335:ASP:HB3	2:L:338:ILE:HG12	2.02	0.42
2:W:180:PRO:HG3	2:W:278:PRO:HA	2.02	0.42
2:AA:194:ASN:HB2	2:AA:196:LYS:HZ2	1.85	0.42
2:CA:89:GLY:O	2:CA:92:ALA:HB3	2.19	0.42
2:CA:376:GLN:NE2	2:CA:384:ASP:OD2	2.42	0.42
2:GA:155:ALA:O	2:GA:158:LYS:HB2	2.20	0.42
2:QA:197:TYR:CZ	2:QA:352:PRO:HA	2.55	0.42
2:QA:335:ASP:HB3	2:QA:338:ILE:HG12	2.02	0.42
2:SA:219:LEU:HD23	2:SA:219:LEU:HA	1.92	0.42
2:UA:110:LEU:HD21	2:UA:306:LEU:HD13	2.02	0.42
2:WA:323:VAL:HG21	2:WA:328:TYR:HD2	1.84	0.42
2:B:29:VAL:HG13	2:B:78:PRO:HA	2.01	0.41
2:D:28:LEU:HD23	2:D:56:VAL:HG22	2.01	0.41
2:F:275:PRO:HB2	2:F:347:LYS:HD2	2.03	0.41
2:H:89:GLY:O	2:H:92:ALA:HB3	2.19	0.41
2:H:155:ALA:O	2:H:158:LYS:HB2	2.20	0.41
2:J:160:LEU:HD23	2:J:160:LEU:HA	1.83	0.41
2:P:29:VAL:HG13	2:P:78:PRO:HA	2.01	0.41
2:P:104:LYS:HA	2:P:104:LYS:HD3	1.81	0.41
2:P:180:PRO:HG3	2:P:278:PRO:HA	2.02	0.41
2:T:155:ALA:O	2:T:158:LYS:HB2	2.20	0.41
2:W:197:TYR:CZ	2:W:352:PRO:HA	2.55	0.41
2:GA:110:LEU:HD21	2:GA:306:LEU:HD13	2.02	0.41
2:MA:110:LEU:HD21	2:MA:306:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QA:29:VAL:HG13	2:QA:78:PRO:HA	2.01	0.41
2:SA:155:ALA:O	2:SA:158:LYS:HB2	2.20	0.41
2:UA:155:ALA:O	2:UA:158:LYS:HB2	2.20	0.41
2:UA:335:ASP:HB3	2:UA:338:ILE:HG12	2.02	0.41
2:WA:104:LYS:HA	2:WA:104:LYS:HD3	1.82	0.41
2:WA:197:TYR:CZ	2:WA:352:PRO:HA	2.55	0.41
2:D:197:TYR:CZ	2:D:352:PRO:HA	2.55	0.41
1:E:36:GLU:HG2	1:E:37:LEU:HG	2.01	0.41
1:E:56:LEU:HD23	1:E:56:LEU:HA	1.83	0.41
1:E:74:LEU:HD11	1:E:86:VAL:HG13	2.02	0.41
2:H:323:VAL:HG21	2:H:328:TYR:HD2	1.84	0.41
2:J:143:LEU:HD21	2:J:147:PRO:HD3	2.03	0.41
2:T:110:LEU:HD21	2:T:306:LEU:HD13	2.02	0.41
2:T:335:ASP:HB3	2:T:338:ILE:HG12	2.02	0.41
2:Y:275:PRO:HB2	2:Y:347:LYS:HD2	2.03	0.41
2:GA:323:VAL:HG21	2:GA:328:TYR:HD2	1.84	0.41
2:IA:335:ASP:HB3	2:IA:338:ILE:HG12	2.02	0.41
1:NA:36:GLU:HG2	1:NA:37:LEU:HG	2.01	0.41
1:NA:74:LEU:HD11	1:NA:86:VAL:HG13	2.02	0.41
2:OA:275:PRO:HB2	2:OA:347:LYS:HD2	2.03	0.41
2:QA:36:LYS:NZ	2:QA:82:PHE:O	2.52	0.41
2:SA:110:LEU:HD21	2:SA:306:LEU:HD13	2.02	0.41
2:WA:110:LEU:HD21	2:WA:306:LEU:HD13	2.02	0.41
2:B:155:ALA:O	2:B:158:LYS:HB2	2.20	0.41
2:D:194:ASN:HB2	2:D:196:LYS:HZ2	1.84	0.41
2:D:275:PRO:HB2	2:D:347:LYS:HD2	2.02	0.41
1:G:74:LEU:HD11	1:G:86:VAL:HG13	2.02	0.41
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.83	0.41
2:L:36:LYS:NZ	2:L:82:PHE:O	2.52	0.41
2:L:110:LEU:HD21	2:L:306:LEU:HD13	2.02	0.41
2:N:275:PRO:HB2	2:N:347:LYS:HD2	2.03	0.41
2:Y:160:LEU:HD23	2:Y:160:LEU:HA	1.83	0.41
2:AA:143:LEU:HD21	2:AA:147:PRO:HD3	2.03	0.41
2:CA:155:ALA:O	2:CA:158:LYS:HB2	2.20	0.41
2:GA:335:ASP:HB3	2:GA:338:ILE:HG12	2.02	0.41
2:IA:36:LYS:NZ	2:IA:82:PHE:O	2.52	0.41
2:MA:275:PRO:HB2	2:MA:347:LYS:HD2	2.03	0.41
2:MA:351[B]:MET:HE2	2:MA:351[B]:MET:HB2	1.98	0.41
2:WA:180:PRO:HG3	2:WA:278:PRO:HA	2.02	0.41
2:WA:335:ASP:HB3	2:WA:338:ILE:HG12	2.02	0.41
2:F:155:ALA:O	2:F:158:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:197:TYR:CZ	2:J:352:PRO:HA	2.55	0.41
1:K:74:LEU:HD12	1:K:74:LEU:HA	1.91	0.41
2:L:155:ALA:O	2:L:158:LYS:HB2	2.20	0.41
1:O:36:GLU:HG2	1:O:37:LEU:HG	2.01	0.41
1:O:74:LEU:HD11	1:O:86:VAL:HG13	2.03	0.41
1:S:74:LEU:HD11	1:S:86:VAL:HG13	2.02	0.41
2:W:143:LEU:HD21	2:W:147:PRO:HD3	2.03	0.41
2:W:155:ALA:O	2:W:158:LYS:HB2	2.20	0.41
2:W:275:PRO:HB2	2:W:347:LYS:HD2	2.03	0.41
2:CA:323:VAL:HG21	2:CA:328:TYR:HD2	1.84	0.41
1:PA:74:LEU:HD11	1:PA:86:VAL:HG13	2.02	0.41
2:SA:335:ASP:HB3	2:SA:338:ILE:HG12	2.02	0.41
1:TA:36:GLU:HG2	1:TA:37:LEU:HG	2.01	0.41
2:WA:143:LEU:HD21	2:WA:147:PRO:HD3	2.03	0.41
2:F:110:LEU:HD21	2:F:306:LEU:HD13	2.02	0.41
2:J:173:GLN:O	2:J:365:ARG:NH2	2.54	0.41
2:N:143:LEU:HD21	2:N:147:PRO:HD3	2.03	0.41
2:R:275:PRO:HB2	2:R:347:LYS:HD2	2.02	0.41
2:T:180:PRO:HG3	2:T:278:PRO:HA	2.02	0.41
1:V:36:GLU:HG2	1:V:37:LEU:HG	2.01	0.41
2:W:335:ASP:HB3	2:W:338:ILE:HG12	2.02	0.41
2:GA:180:PRO:HG3	2:GA:278:PRO:HA	2.02	0.41
2:IA:110:LEU:HD21	2:IA:306:LEU:HD13	2.02	0.41
2:IA:155:ALA:O	2:IA:158:LYS:HB2	2.20	0.41
2:KA:29:VAL:HG13	2:KA:78:PRO:HA	2.01	0.41
2:KA:155:ALA:O	2:KA:158:LYS:HB2	2.20	0.41
2:OA:110:LEU:HD21	2:OA:306:LEU:HD13	2.02	0.41
2:OA:155:ALA:O	2:OA:158:LYS:HB2	2.20	0.41
2:QA:155:ALA:O	2:QA:158:LYS:HB2	2.20	0.41
1:RA:74:LEU:HD11	1:RA:86:VAL:HG13	2.02	0.41
2:WA:275:PRO:HB2	2:WA:347:LYS:HD2	2.03	0.41
2:B:173:GLN:O	2:B:365:ARG:NH2	2.54	0.41
2:P:173:GLN:O	2:P:365:ARG:NH2	2.54	0.41
2:P:335:ASP:HB3	2:P:338:ILE:HG12	2.02	0.41
2:P:351[B]:MET:HE2	2:P:351[B]:MET:HB2	1.98	0.41
1:V:74:LEU:HD11	1:V:86:VAL:HG13	2.02	0.41
2:Y:110:LEU:HD21	2:Y:306:LEU:HD13	2.02	0.41
2:Y:111:TYR:HA	2:Y:112:PRO:HD3	1.95	0.41
2:AA:173:GLN:O	2:AA:365:ARG:NH2	2.54	0.41
2:AA:197:TYR:CZ	2:AA:352:PRO:HA	2.55	0.41
1:BA:74:LEU:HD11	1:BA:86:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:72:THR:OG1	1:FA:75:HIS:ND1	2.41	0.41
2:GA:143:LEU:HD21	2:GA:147:PRO:HD3	2.03	0.41
2:GA:275:PRO:HB2	2:GA:347:LYS:HD2	2.03	0.41
2:OA:28:LEU:HD23	2:OA:56:VAL:HG22	2.00	0.41
1:PA:36:GLU:HG2	1:PA:37:LEU:HG	2.01	0.41
2:QA:194:ASN:HB2	2:QA:196:LYS:HZ2	1.85	0.41
2:B:275:PRO:HB2	2:B:347:LYS:HD2	2.03	0.41
1:C:244:MET:HE1	1:VA:209:LEU:HD21	2.02	0.41
2:F:28:LEU:HD23	2:F:56:VAL:HG22	2.01	0.41
2:H:104:LYS:HA	2:H:104:LYS:HD3	1.81	0.41
2:H:335:ASP:HB3	2:H:338:ILE:HG12	2.02	0.41
2:J:143:LEU:HD21	2:J:146:PRO:HA	2.03	0.41
2:J:214:THR:HA	2:J:217:VAL:HG22	2.03	0.41
2:P:275:PRO:HB2	2:P:347:LYS:HD2	2.02	0.41
1:X:36:GLU:HG2	1:X:37:LEU:HG	2.01	0.41
2:AA:143:LEU:HD21	2:AA:146:PRO:HA	2.03	0.41
2:AA:214:THR:HA	2:AA:217:VAL:HG22	2.03	0.41
2:CA:335:ASP:HB3	2:CA:338:ILE:HG12	2.02	0.41
2:EA:155:ALA:O	2:EA:158:LYS:HB2	2.20	0.41
2:EA:275:PRO:HB2	2:EA:347:LYS:HD2	2.03	0.41
1:HA:74:LEU:HD12	1:HA:74:LEU:HA	1.91	0.41
1:JA:327:THR:HG21	1:PA:218:ASP:O	2.21	0.41
2:KA:47:LYS:HE3	2:KA:47:LYS:HB2	1.70	0.41
2:KA:173:GLN:O	2:KA:365:ARG:NH2	2.54	0.41
2:KA:275:PRO:HB2	2:KA:347:LYS:HD2	2.03	0.41
2:MA:298:LYS:HE2	2:MA:298:LYS:HB2	1.90	0.41
2:SA:143:LEU:HD21	2:SA:146:PRO:HA	2.03	0.41
1:TA:74:LEU:HD11	1:TA:86:VAL:HG13	2.03	0.41
2:UA:143:LEU:HD21	2:UA:147:PRO:HD3	2.03	0.41
2:UA:275:PRO:HB2	2:UA:347:LYS:HD2	2.03	0.41
2:F:143:LEU:HD21	2:F:147:PRO:HD3	2.03	0.41
2:H:36:LYS:O	2:H:318:LYS:NZ	2.43	0.41
1:M:36:GLU:HG2	1:M:37:LEU:HG	2.01	0.41
2:R:173:GLN:O	2:R:365:ARG:NH2	2.54	0.41
2:T:143:LEU:HD21	2:T:146:PRO:HA	2.03	0.41
2:W:173:GLN:O	2:W:365:ARG:NH2	2.54	0.41
1:X:74:LEU:HD11	1:X:86:VAL:HG13	2.02	0.41
2:Y:143:LEU:HD21	2:Y:146:PRO:HA	2.03	0.41
2:Y:335:ASP:HB3	2:Y:338:ILE:HG12	2.02	0.41
1:Z:102:PHE:HD2	2:AA:221:LYS:HG3	1.85	0.41
2:AA:155:ALA:O	2:AA:158:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IA:111:TYR:HA	2:IA:112:PRO:HD3	1.96	0.41
2:OA:143:LEU:HD21	2:OA:147:PRO:HD3	2.03	0.41
2:QA:219:LEU:HD23	2:QA:219:LEU:HA	1.92	0.41
2:QA:275:PRO:HB2	2:QA:347:LYS:HD2	2.03	0.41
2:SA:180:PRO:HG3	2:SA:278:PRO:HA	2.02	0.41
2:UA:173:GLN:O	2:UA:365:ARG:NH2	2.54	0.41
2:D:143:LEU:HD21	2:D:146:PRO:HA	2.03	0.41
2:D:143:LEU:HD21	2:D:147:PRO:HD3	2.03	0.41
2:D:216:LEU:HD23	2:D:216:LEU:HA	1.94	0.41
2:F:143:LEU:HD21	2:F:146:PRO:HA	2.03	0.41
2:F:148:LYS:C	2:F:269:PRO:HB3	2.46	0.41
2:F:335:ASP:HB3	2:F:338:ILE:HG12	2.02	0.41
1:G:328:ASN:ND2	1:Z:221:ALA:CB	2.84	0.41
2:H:275:PRO:HB2	2:H:347:LYS:HD2	2.03	0.41
1:I:74:LEU:HD11	1:I:86:VAL:HG13	2.02	0.41
2:J:155:ALA:O	2:J:158:LYS:HB2	2.20	0.41
2:J:194:ASN:HB2	2:J:196:LYS:HZ2	1.86	0.41
2:J:275:PRO:HB2	2:J:347:LYS:HD2	2.03	0.41
2:L:111:TYR:HA	2:L:112:PRO:HD3	1.96	0.41
2:L:173:GLN:O	2:L:365:ARG:NH2	2.54	0.41
1:M:74:LEU:HD11	1:M:86:VAL:HG13	2.02	0.41
2:N:110:LEU:HD21	2:N:306:LEU:HD13	2.02	0.41
2:P:155:ALA:O	2:P:158:LYS:HB2	2.20	0.41
2:P:298:LYS:HE2	2:P:298:LYS:HB2	1.90	0.41
2:R:155:ALA:O	2:R:158:LYS:HB2	2.20	0.41
2:R:335:ASP:HB3	2:R:338:ILE:HG12	2.02	0.41
2:W:214:THR:HA	2:W:217:VAL:HG22	2.03	0.41
2:W:376:GLN:NE2	2:W:384:ASP:OD2	2.42	0.41
1:X:113:TRP:CZ3	2:Y:158:LYS:HA	2.55	0.41
2:Y:143:LEU:HD21	2:Y:147:PRO:HD3	2.03	0.41
2:Y:214:THR:HA	2:Y:217:VAL:HG22	2.03	0.41
2:AA:275:PRO:HB2	2:AA:347:LYS:HD2	2.03	0.41
2:CA:275:PRO:HB2	2:CA:347:LYS:HD2	2.03	0.41
2:EA:173:GLN:O	2:EA:365:ARG:NH2	2.54	0.41
1:FA:41:LEU:HD23	1:FA:41:LEU:HA	1.89	0.41
1:HA:56:LEU:HD23	1:HA:56:LEU:HA	1.83	0.41
2:IA:143:LEU:HD21	2:IA:147:PRO:HD3	2.03	0.41
2:IA:173:GLN:O	2:IA:365:ARG:NH2	2.54	0.41
2:MA:143:LEU:HD21	2:MA:146:PRO:HA	2.03	0.41
2:MA:194:ASN:HB2	2:MA:196:LYS:HZ2	1.85	0.41
2:OA:148:LYS:C	2:OA:269:PRO:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PA:79:TYR:CE1	2:QA:223:LYS:HB2	2.56	0.41
2:QA:104:LYS:HA	2:QA:104:LYS:HD3	1.82	0.41
2:QA:143:LEU:HD21	2:QA:146:PRO:HA	2.03	0.41
2:QA:148:LYS:C	2:QA:269:PRO:HB3	2.46	0.41
2:QA:173:GLN:O	2:QA:365:ARG:NH2	2.54	0.41
2:UA:143:LEU:HD21	2:UA:146:PRO:HA	2.03	0.41
2:B:110:LEU:HD21	2:B:306:LEU:HD13	2.02	0.41
2:J:148:LYS:C	2:J:269:PRO:HB3	2.46	0.41
1:K:74:LEU:HD11	1:K:86:VAL:HG13	2.02	0.41
2:N:143:LEU:HD21	2:N:146:PRO:HA	2.03	0.41
2:N:335:ASP:HB3	2:N:338:ILE:HG12	2.02	0.41
1:O:209:LEU:HD13	1:X:237:ARG:NH1	2.35	0.41
2:P:110:LEU:HD21	2:P:306:LEU:HD13	2.02	0.41
2:P:376:GLN:NE2	2:P:384:ASP:OD2	2.42	0.41
2:W:143:LEU:HD21	2:W:146:PRO:HA	2.03	0.41
1:X:41:LEU:HD23	1:X:41:LEU:HA	1.89	0.41
1:X:320:LYS:HD3	1:DA:249:GLN:HA	2.02	0.41
2:Y:22:LYS:HE3	2:Y:22:LYS:HB2	1.86	0.41
1:Z:74:LEU:HD11	1:Z:86:VAL:HG13	2.03	0.41
2:AA:148:LYS:C	2:AA:269:PRO:HB3	2.46	0.41
1:BA:74:LEU:HD12	1:BA:74:LEU:HA	1.91	0.41
2:IA:174:GLU:CD	2:IA:365:ARG:HH22	2.29	0.41
2:MA:143:LEU:HD21	2:MA:147:PRO:HD3	2.03	0.41
2:OA:143:LEU:HD21	2:OA:146:PRO:HA	2.03	0.41
2:UA:214:THR:HA	2:UA:217:VAL:HG22	2.03	0.41
2:UA:351[B]:MET:HE2	2:UA:351[B]:MET:HB2	1.98	0.41
2:WA:173:GLN:O	2:WA:365:ARG:NH2	2.54	0.41
1:E:41:LEU:HD23	1:E:41:LEU:HA	1.89	0.40
2:H:180:PRO:HG3	2:H:278:PRO:HA	2.02	0.40
2:J:110:LEU:HD21	2:J:306:LEU:HD13	2.02	0.40
2:J:174:GLU:CD	2:J:365:ARG:HH22	2.30	0.40
2:L:143:LEU:HD21	2:L:147:PRO:HD3	2.03	0.40
2:L:174:GLU:CD	2:L:365:ARG:HH22	2.30	0.40
2:N:214:THR:HA	2:N:217:VAL:HG22	2.03	0.40
1:O:244:MET:HE1	1:X:209:LEU:HD21	2.03	0.40
2:AA:174:GLU:CD	2:AA:365:ARG:HH22	2.30	0.40
2:CA:180:PRO:HG3	2:CA:278:PRO:HA	2.02	0.40
2:EA:49:GLU:HG2	2:EA:55:LYS:HA	2.04	0.40
2:GA:173:GLN:O	2:GA:365:ARG:NH2	2.54	0.40
2:IA:180:PRO:HG3	2:IA:278:PRO:HA	2.02	0.40
2:OA:173:GLN:O	2:OA:365:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OA:335:ASP:HB3	2:OA:338:ILE:HG12	2.02	0.40
1:RA:56:LEU:HD23	1:RA:56:LEU:HA	1.83	0.40
2:UA:47:LYS:HB2	2:UA:47:LYS:HE3	1.69	0.40
2:WA:143:LEU:HD21	2:WA:146:PRO:HA	2.03	0.40
1:A:74:LEU:HD11	1:A:86:VAL:HG13	2.03	0.40
2:D:22:LYS:HE3	2:D:22:LYS:HB2	1.86	0.40
2:D:173:GLN:O	2:D:365:ARG:NH2	2.54	0.40
2:D:351[B]:MET:HE2	2:D:351[B]:MET:HB2	1.98	0.40
2:F:49:GLU:HG2	2:F:55:LYS:HA	2.04	0.40
1:I:56:LEU:HD23	1:I:56:LEU:HA	1.83	0.40
2:L:180:PRO:HG3	2:L:278:PRO:HA	2.02	0.40
2:P:143:LEU:HD21	2:P:146:PRO:HA	2.03	0.40
2:P:148:LYS:C	2:P:269:PRO:HB3	2.46	0.40
1:X:56:LEU:HD23	1:X:56:LEU:HA	1.83	0.40
1:DA:74:LEU:HD11	1:DA:86:VAL:HG13	2.02	0.40
2:EA:143:LEU:HD21	2:EA:147:PRO:HD3	2.03	0.40
2:EA:148:LYS:C	2:EA:269:PRO:HB3	2.46	0.40
2:IA:47:LYS:HE3	2:IA:47:LYS:HB2	1.70	0.40
2:KA:174:GLU:CD	2:KA:365:ARG:HH22	2.30	0.40
2:OA:49:GLU:HG2	2:OA:55:LYS:HA	2.04	0.40
2:QA:298:LYS:HE2	2:QA:298:LYS:HB2	1.90	0.40
2:WA:148:LYS:C	2:WA:269:PRO:HB3	2.46	0.40
2:WA:174:GLU:CD	2:WA:365:ARG:HH22	2.29	0.40
2:WA:214:THR:HA	2:WA:217:VAL:HG22	2.03	0.40
1:A:113:TRP:CZ3	2:B:158:LYS:HA	2.55	0.40
2:F:173:GLN:O	2:F:365:ARG:NH2	2.54	0.40
2:H:148:LYS:C	2:H:269:PRO:HB3	2.46	0.40
2:H:174:GLU:CD	2:H:365:ARG:HH22	2.30	0.40
2:P:49:GLU:HG2	2:P:55:LYS:HA	2.04	0.40
2:R:49:GLU:HG2	2:R:55:LYS:HA	2.04	0.40
2:R:148:LYS:C	2:R:269:PRO:HB3	2.46	0.40
2:R:174:GLU:CD	2:R:365:ARG:HH22	2.30	0.40
2:R:180:PRO:HG3	2:R:278:PRO:HA	2.02	0.40
2:R:219:LEU:HD23	2:R:219:LEU:HA	1.92	0.40
2:Y:173:GLN:O	2:Y:365:ARG:NH2	2.54	0.40
2:AA:110:LEU:HD21	2:AA:306:LEU:HD13	2.02	0.40
2:CA:174:GLU:CD	2:CA:365:ARG:HH22	2.30	0.40
2:EA:110:LEU:HD21	2:EA:306:LEU:HD13	2.02	0.40
2:EA:335:ASP:HB3	2:EA:338:ILE:HG12	2.02	0.40
2:GA:174:GLU:CD	2:GA:365:ARG:HH22	2.30	0.40
2:IA:351[B]:MET:HE2	2:IA:351[B]:MET:HB2	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:KA:110:LEU:HD21	2:KA:306:LEU:HD13	2.02	0.40
2:MA:214:THR:HA	2:MA:217:VAL:HG22	2.03	0.40
1:NA:41:LEU:HD23	1:NA:41:LEU:HA	1.89	0.40
2:QA:110:LEU:HD21	2:QA:306:LEU:HD13	2.02	0.40
2:SA:191:LYS:NZ	2:SA:198:ASP:OD2	2.34	0.40
2:D:148:LYS:C	2:D:269:PRO:HB3	2.46	0.40
2:L:47:LYS:HE3	2:L:47:LYS:HB2	1.70	0.40
2:L:49:GLU:HG2	2:L:55:LYS:HA	2.04	0.40
2:N:155:ALA:O	2:N:158:LYS:HB2	2.20	0.40
2:N:174:GLU:CD	2:N:365:ARG:HH22	2.30	0.40
2:P:143:LEU:HD21	2:P:147:PRO:HD3	2.03	0.40
1:Q:74:LEU:HD11	1:Q:86:VAL:HG13	2.02	0.40
2:R:214:THR:HA	2:R:217:VAL:HG22	2.03	0.40
2:T:275:PRO:HB2	2:T:347:LYS:HD2	2.03	0.40
2:EA:174:GLU:CD	2:EA:365:ARG:HH22	2.29	0.40
2:GA:143:LEU:HD21	2:GA:146:PRO:HA	2.03	0.40
2:GA:148:LYS:C	2:GA:269:PRO:HB3	2.46	0.40
2:GA:214:THR:HA	2:GA:217:VAL:HG22	2.03	0.40
2:IA:49:GLU:HG2	2:IA:55:LYS:HA	2.04	0.40
2:MA:148:LYS:C	2:MA:269:PRO:HB3	2.46	0.40
2:QA:49:GLU:HG2	2:QA:55:LYS:HA	2.04	0.40
2:QA:143:LEU:HD21	2:QA:147:PRO:HD3	2.03	0.40
2:SA:143:LEU:HD21	2:SA:147:PRO:HD3	2.03	0.40
2:SA:174:GLU:CD	2:SA:365:ARG:HH22	2.29	0.40
2:SA:275:PRO:HB2	2:SA:347:LYS:HD2	2.03	0.40
2:B:174:GLU:CD	2:B:365:ARG:HH22	2.30	0.40
2:B:185:ASP:OD1	2:B:185:ASP:N	2.54	0.40
1:C:74:LEU:HD11	1:C:86:VAL:HG13	2.02	0.40
2:H:49:GLU:HG2	2:H:55:LYS:HA	2.04	0.40
2:H:111:TYR:HA	2:H:112:PRO:HD3	1.96	0.40
1:K:305:ASP:OD1	1:Z:308:GLU:HG3	2.22	0.40
1:K:346:LYS:HA	1:K:346:LYS:HD3	1.98	0.40
2:N:148:LYS:C	2:N:269:PRO:HB3	2.47	0.40
2:N:298:LYS:HE2	2:N:298:LYS:HB2	1.90	0.40
2:R:110:LEU:HD21	2:R:306:LEU:HD13	2.02	0.40
1:S:56:LEU:HD23	1:S:56:LEU:HA	1.83	0.40
2:T:174:GLU:CD	2:T:365:ARG:HH22	2.29	0.40
2:Y:174:GLU:CD	2:Y:365:ARG:HH22	2.30	0.40
2:CA:104:LYS:HA	2:CA:104:LYS:HD3	1.82	0.40
2:CA:148:LYS:C	2:CA:269:PRO:HB3	2.46	0.40
2:EA:180:PRO:HG3	2:EA:278:PRO:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:74:LEU:HD11	1:HA:86:VAL:HG13	2.03	0.40
2:MA:173:GLN:O	2:MA:365:ARG:NH2	2.54	0.40
2:UA:194:ASN:HB2	2:UA:196:LYS:HZ2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	BA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	C	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	DA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	E	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	FA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	G	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	HA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	I	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	JA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	K	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	LA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	M	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	NA	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	O	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	PA	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	Q	314/370 (85%)	306 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RA	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	S	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	TA	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	V	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
1	VA	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	X	314/370 (85%)	306 (98%)	8 (2%)	0	100	100
1	Z	314/370 (85%)	307 (98%)	7 (2%)	0	100	100
2	AA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	B	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	CA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	D	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	EA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	F	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	GA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	H	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	IA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	J	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	KA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	L	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	MA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	N	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	OA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	P	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	QA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	R	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	SA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	T	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	UA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	W	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	WA	370/416 (89%)	354 (96%)	16 (4%)	0	100	100
2	Y	370/416 (89%)	354 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	16416/18864 (87%)	15857 (97%)	559 (3%)	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	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	BA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	C	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	DA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	E	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	FA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	G	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	HA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	I	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	JA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	K	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	LA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	M	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	NA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	O	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	PA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	Q	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	RA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	S	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	TA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	V	260/298 (87%)	259 (100%)	1 (0%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	VA	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	X	260/298 (87%)	259 (100%)	1 (0%)	84	90
1	Z	260/298 (87%)	259 (100%)	1 (0%)	84	90
2	AA	299/336 (89%)	299 (100%)	0	100	100
2	B	299/336 (89%)	299 (100%)	0	100	100
2	CA	299/336 (89%)	299 (100%)	0	100	100
2	D	299/336 (89%)	299 (100%)	0	100	100
2	EA	299/336 (89%)	299 (100%)	0	100	100
2	F	299/336 (89%)	299 (100%)	0	100	100
2	GA	299/336 (89%)	299 (100%)	0	100	100
2	H	299/336 (89%)	299 (100%)	0	100	100
2	IA	299/336 (89%)	299 (100%)	0	100	100
2	J	299/336 (89%)	299 (100%)	0	100	100
2	KA	299/336 (89%)	299 (100%)	0	100	100
2	L	299/336 (89%)	299 (100%)	0	100	100
2	MA	299/336 (89%)	299 (100%)	0	100	100
2	N	299/336 (89%)	299 (100%)	0	100	100
2	OA	299/336 (89%)	299 (100%)	0	100	100
2	P	299/336 (89%)	299 (100%)	0	100	100
2	QA	299/336 (89%)	299 (100%)	0	100	100
2	R	299/336 (89%)	299 (100%)	0	100	100
2	SA	299/336 (89%)	299 (100%)	0	100	100
2	T	299/336 (89%)	299 (100%)	0	100	100
2	UA	299/336 (89%)	299 (100%)	0	100	100
2	W	299/336 (89%)	299 (100%)	0	100	100
2	WA	299/336 (89%)	299 (100%)	0	100	100
2	Y	299/336 (89%)	299 (100%)	0	100	100
All	All	13416/15216 (88%)	13392 (100%)	24 (0%)	85	92

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LYS

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Mol	Chain	Res	Type
1	C	261	LYS
1	E	261	LYS
1	G	261	LYS
1	I	261	LYS
1	K	261	LYS
1	M	261	LYS
1	O	261	LYS
1	Q	261	LYS
1	S	261	LYS
1	V	261	LYS
1	X	261	LYS
1	Z	261	LYS
1	BA	261	LYS
1	DA	261	LYS
1	FA	261	LYS
1	HA	261	LYS
1	JA	261	LYS
1	LA	261	LYS
1	NA	261	LYS
1	PA	261	LYS
1	RA	261	LYS
1	TA	261	LYS
1	VA	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (230) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	179	ASN
1	A	257	GLN
1	A	285	ASN
1	A	292	HIS
1	A	325	HIS
2	B	39	ASN
2	B	222	ASN
2	B	370	ASN
2	B	386	GLN
1	C	108	HIS
1	C	179	ASN
1	C	257	GLN
1	C	285	ASN
1	C	292	HIS

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Mol	Chain	Res	Type
2	D	39	ASN
2	D	70	GLN
2	D	222	ASN
2	D	370	ASN
2	D	386	GLN
1	E	108	HIS
1	E	179	ASN
1	E	257	GLN
1	E	285	ASN
1	E	292	HIS
1	E	328	ASN
2	F	39	ASN
2	F	70	GLN
2	F	370	ASN
2	F	386	GLN
1	G	108	HIS
1	G	179	ASN
1	G	257	GLN
1	G	285	ASN
1	G	292	HIS
1	G	328	ASN
2	H	39	ASN
2	H	70	GLN
2	H	370	ASN
2	H	386	GLN
1	I	108	HIS
1	I	179	ASN
1	I	257	GLN
1	I	285	ASN
1	I	292	HIS
2	J	39	ASN
2	J	70	GLN
2	J	222	ASN
2	J	370	ASN
2	J	386	GLN
1	K	108	HIS
1	K	179	ASN
1	K	257	GLN
1	K	285	ASN
1	K	292	HIS
1	K	328	ASN
2	L	39	ASN

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Mol	Chain	Res	Type
2	L	370	ASN
2	L	386	GLN
1	M	108	HIS
1	M	179	ASN
1	M	257	GLN
1	M	285	ASN
1	M	302	HIS
2	N	39	ASN
2	N	222	ASN
2	N	370	ASN
2	N	386	GLN
1	O	108	HIS
1	O	179	ASN
1	O	257	GLN
1	O	285	ASN
1	O	292	HIS
1	O	328	ASN
2	P	39	ASN
2	P	370	ASN
2	P	386	GLN
1	Q	108	HIS
1	Q	179	ASN
1	Q	257	GLN
1	Q	285	ASN
1	Q	292	HIS
1	Q	302	HIS
1	Q	328	ASN
2	R	39	ASN
2	R	70	GLN
2	R	222	ASN
2	R	370	ASN
2	R	386	GLN
1	S	108	HIS
1	S	179	ASN
1	S	257	GLN
1	S	285	ASN
1	S	292	HIS
2	T	39	ASN
2	T	70	GLN
2	T	370	ASN
2	T	386	GLN
1	V	108	HIS

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Mol	Chain	Res	Type
1	V	179	ASN
1	V	285	ASN
1	V	292	HIS
1	V	302	HIS
2	W	39	ASN
2	W	370	ASN
2	W	386	GLN
1	X	108	HIS
1	X	179	ASN
1	X	257	GLN
1	X	285	ASN
1	X	292	HIS
2	Y	39	ASN
2	Y	70	GLN
2	Y	370	ASN
2	Y	386	GLN
1	Z	108	HIS
1	Z	179	ASN
1	Z	257	GLN
1	Z	285	ASN
1	Z	292	HIS
1	Z	328	ASN
2	AA	39	ASN
2	AA	70	GLN
2	AA	370	ASN
2	AA	386	GLN
1	BA	108	HIS
1	BA	179	ASN
1	BA	257	GLN
1	BA	285	ASN
1	BA	292	HIS
2	CA	39	ASN
2	CA	70	GLN
2	CA	370	ASN
2	CA	386	GLN
1	DA	108	HIS
1	DA	179	ASN
1	DA	257	GLN
1	DA	285	ASN
2	EA	39	ASN
2	EA	70	GLN
2	EA	370	ASN

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Mol	Chain	Res	Type
2	EA	386	GLN
1	FA	108	HIS
1	FA	179	ASN
1	FA	257	GLN
1	FA	285	ASN
1	FA	292	HIS
2	GA	39	ASN
2	GA	222	ASN
2	GA	370	ASN
2	GA	386	GLN
1	HA	108	HIS
1	HA	179	ASN
1	HA	257	GLN
1	HA	285	ASN
1	HA	292	HIS
1	HA	328	ASN
2	IA	39	ASN
2	IA	222	ASN
2	IA	370	ASN
2	IA	386	GLN
1	JA	108	HIS
1	JA	179	ASN
1	JA	257	GLN
1	JA	285	ASN
1	JA	328	ASN
2	KA	39	ASN
2	KA	370	ASN
2	KA	386	GLN
1	LA	108	HIS
1	LA	179	ASN
1	LA	257	GLN
1	LA	285	ASN
1	LA	292	HIS
1	LA	310	HIS
1	LA	328	ASN
2	MA	39	ASN
2	MA	222	ASN
2	MA	370	ASN
2	MA	386	GLN
1	NA	108	HIS
1	NA	179	ASN
1	NA	257	GLN

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Mol	Chain	Res	Type
1	NA	285	ASN
1	NA	292	HIS
1	NA	328	ASN
2	OA	39	ASN
2	OA	70	GLN
2	OA	222	ASN
2	OA	370	ASN
2	OA	386	GLN
1	PA	108	HIS
1	PA	179	ASN
1	PA	257	GLN
1	PA	285	ASN
1	PA	292	HIS
1	PA	328	ASN
2	QA	39	ASN
2	QA	70	GLN
2	QA	370	ASN
2	QA	386	GLN
1	RA	108	HIS
1	RA	179	ASN
1	RA	257	GLN
1	RA	285	ASN
1	RA	292	HIS
1	RA	328	ASN
2	SA	39	ASN
2	SA	70	GLN
2	SA	370	ASN
2	SA	386	GLN
1	TA	108	HIS
1	TA	179	ASN
1	TA	257	GLN
1	TA	285	ASN
1	TA	328	ASN
2	UA	39	ASN
2	UA	222	ASN
2	UA	370	ASN
2	UA	386	GLN
1	VA	108	HIS
1	VA	179	ASN
1	VA	257	GLN
1	VA	285	ASN
1	VA	292	HIS

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Mol	Chain	Res	Type
1	VA	328	ASN
2	WA	39	ASN
2	WA	70	GLN
2	WA	370	ASN
2	WA	386	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

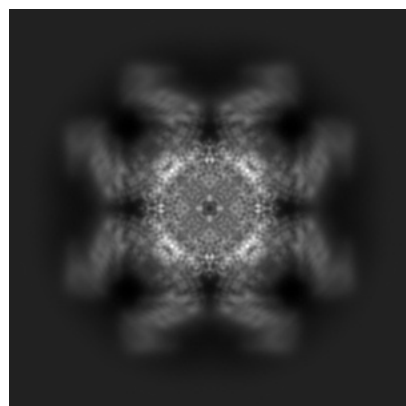
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60931. These allow visual inspection of the internal detail of the map and identification of artifacts.

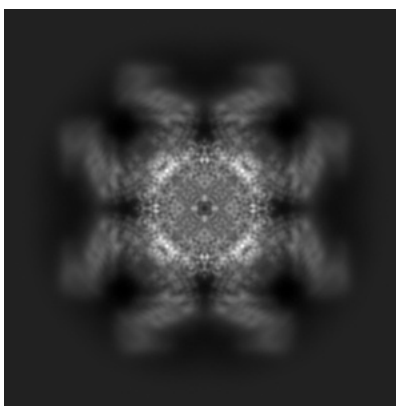
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

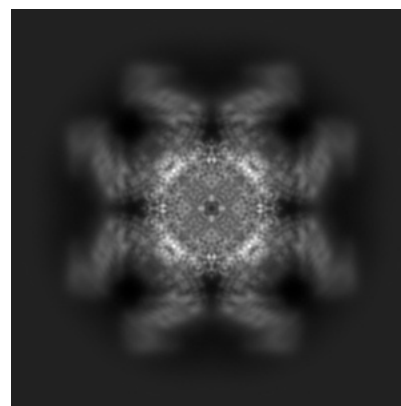
6.1.1 Primary map



X

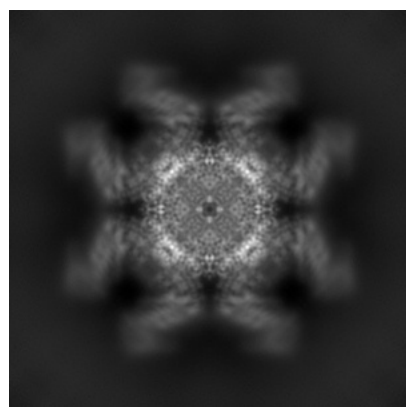


Y

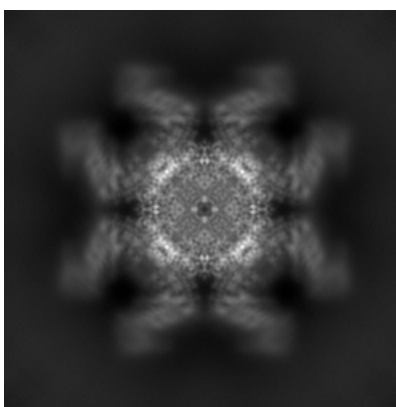


Z

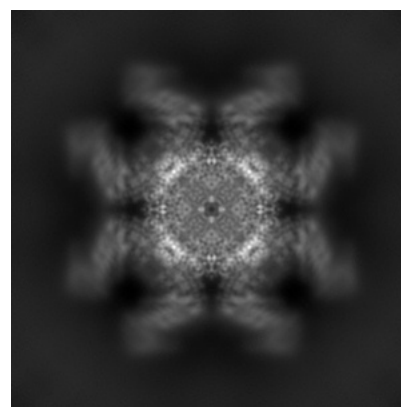
6.1.2 Raw map



X



Y

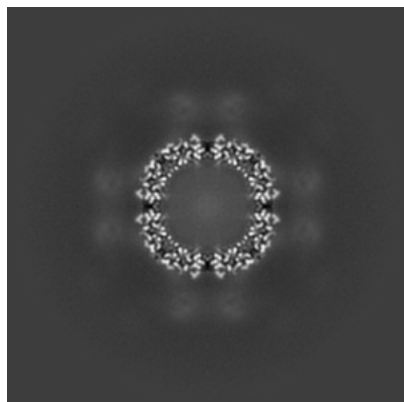


Z

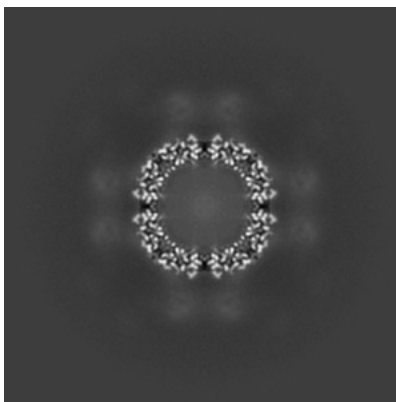
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

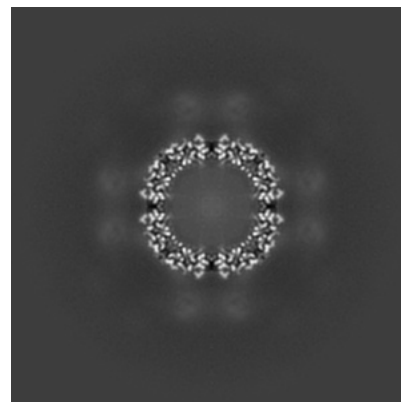
6.2.1 Primary map



X Index: 160

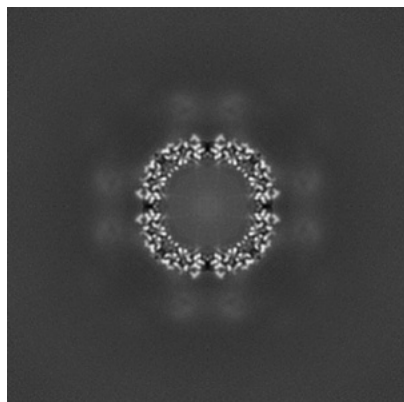


Y Index: 160

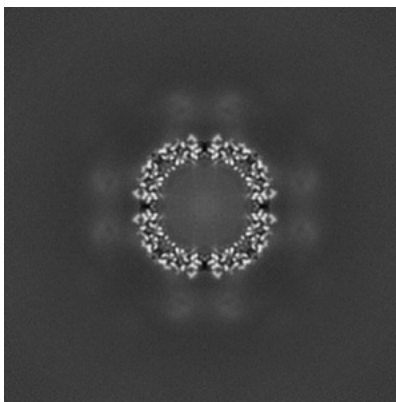


Z Index: 160

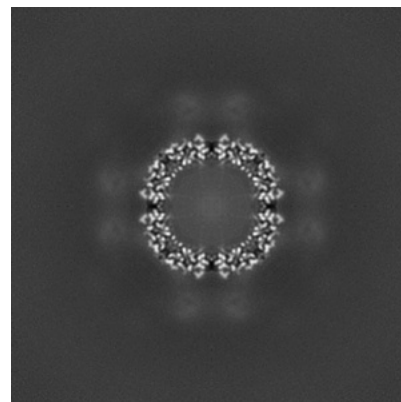
6.2.2 Raw map



X Index: 160



Y Index: 160

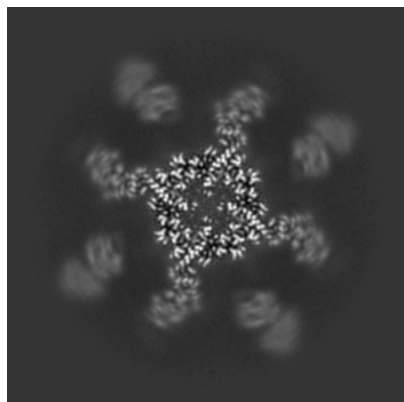


Z Index: 160

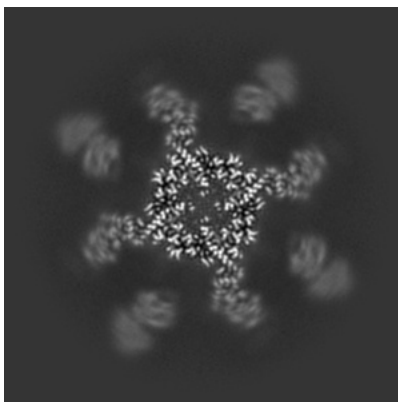
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

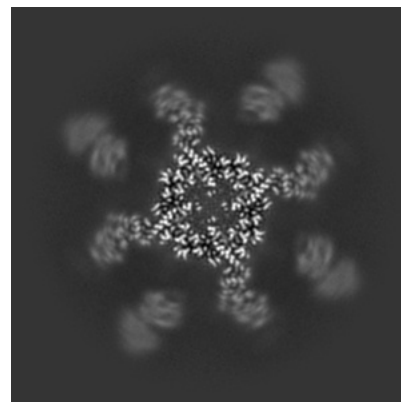
6.3.1 Primary map



X Index: 124

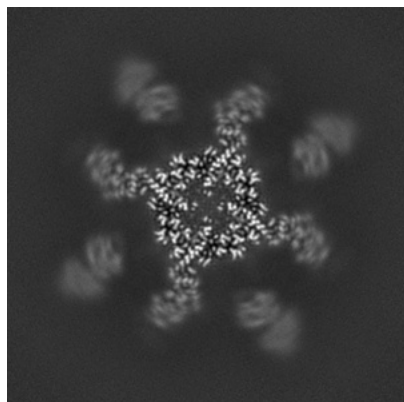


Y Index: 196

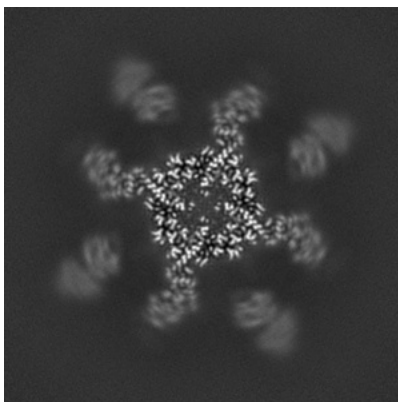


Z Index: 196

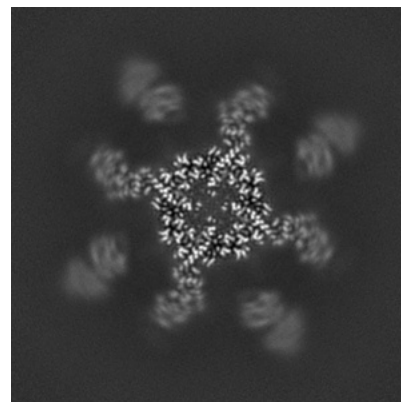
6.3.2 Raw map



X Index: 124



Y Index: 124

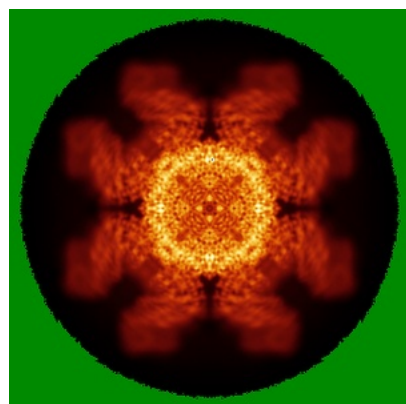


Z Index: 124

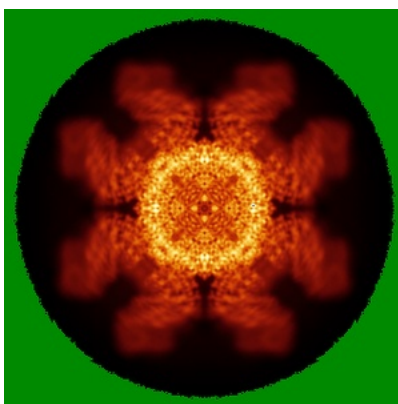
The images above show the largest variance slices of the map in three orthogonal directions.

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

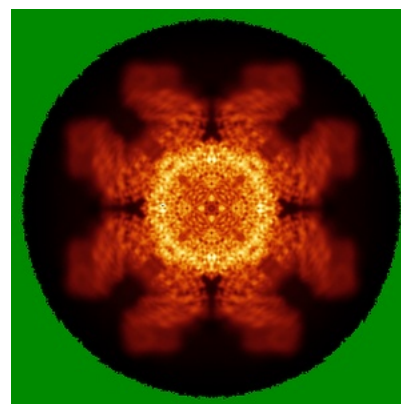
6.4.1 Primary map



X

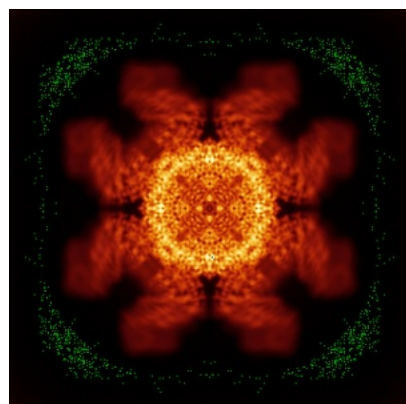


Y

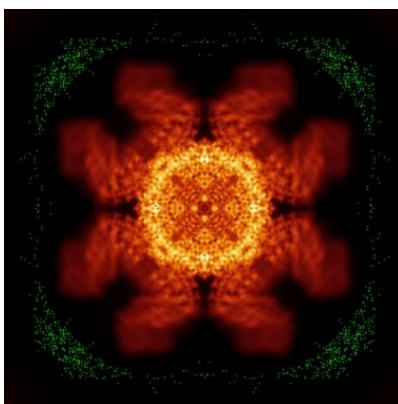


Z

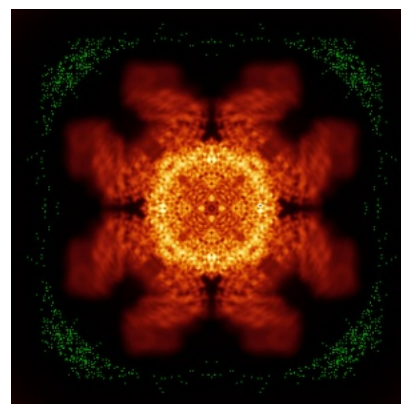
6.4.2 Raw map



X



Y

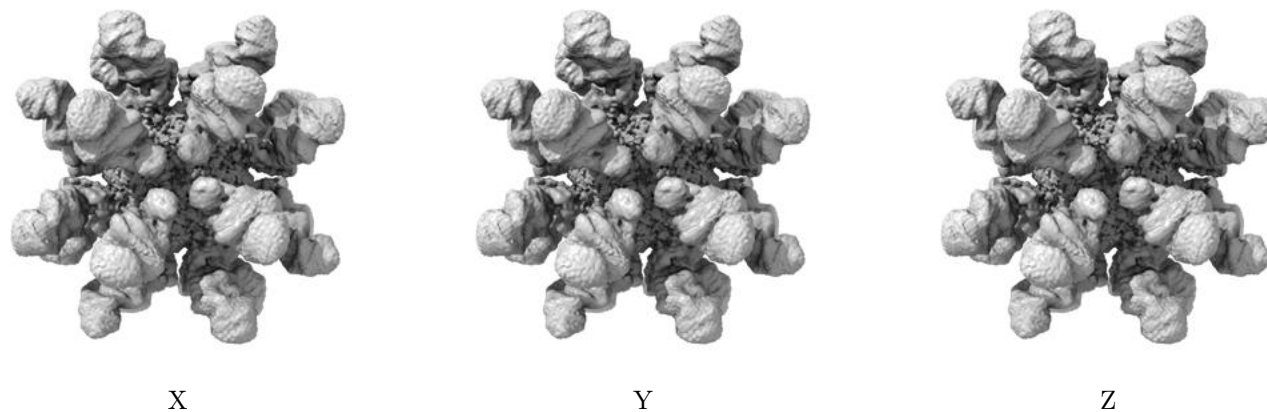


Z

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

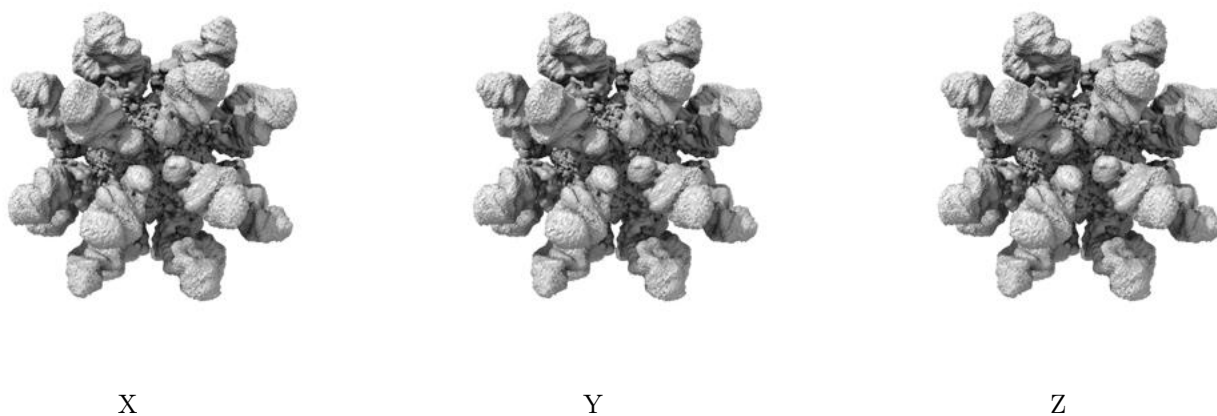
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

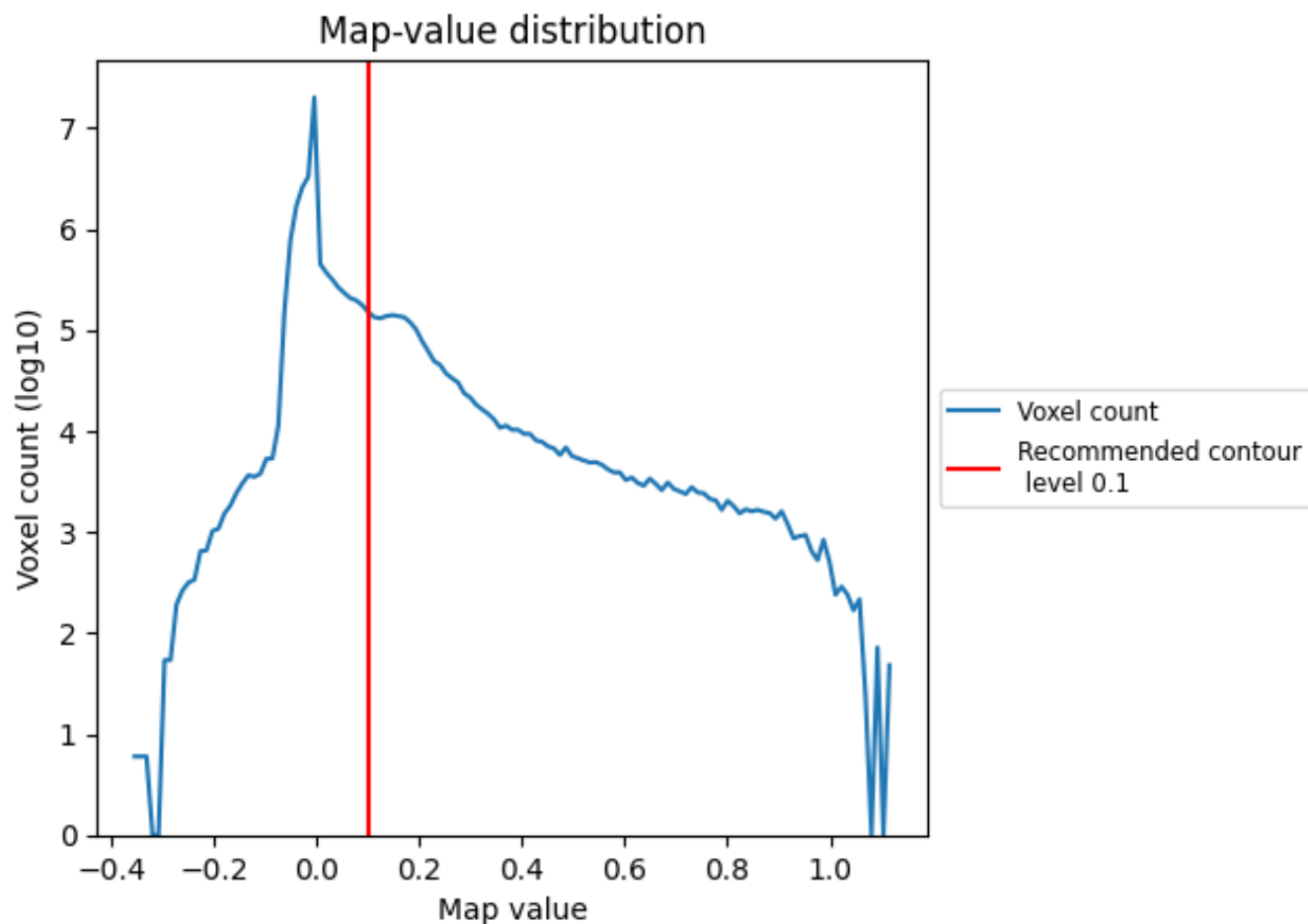
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

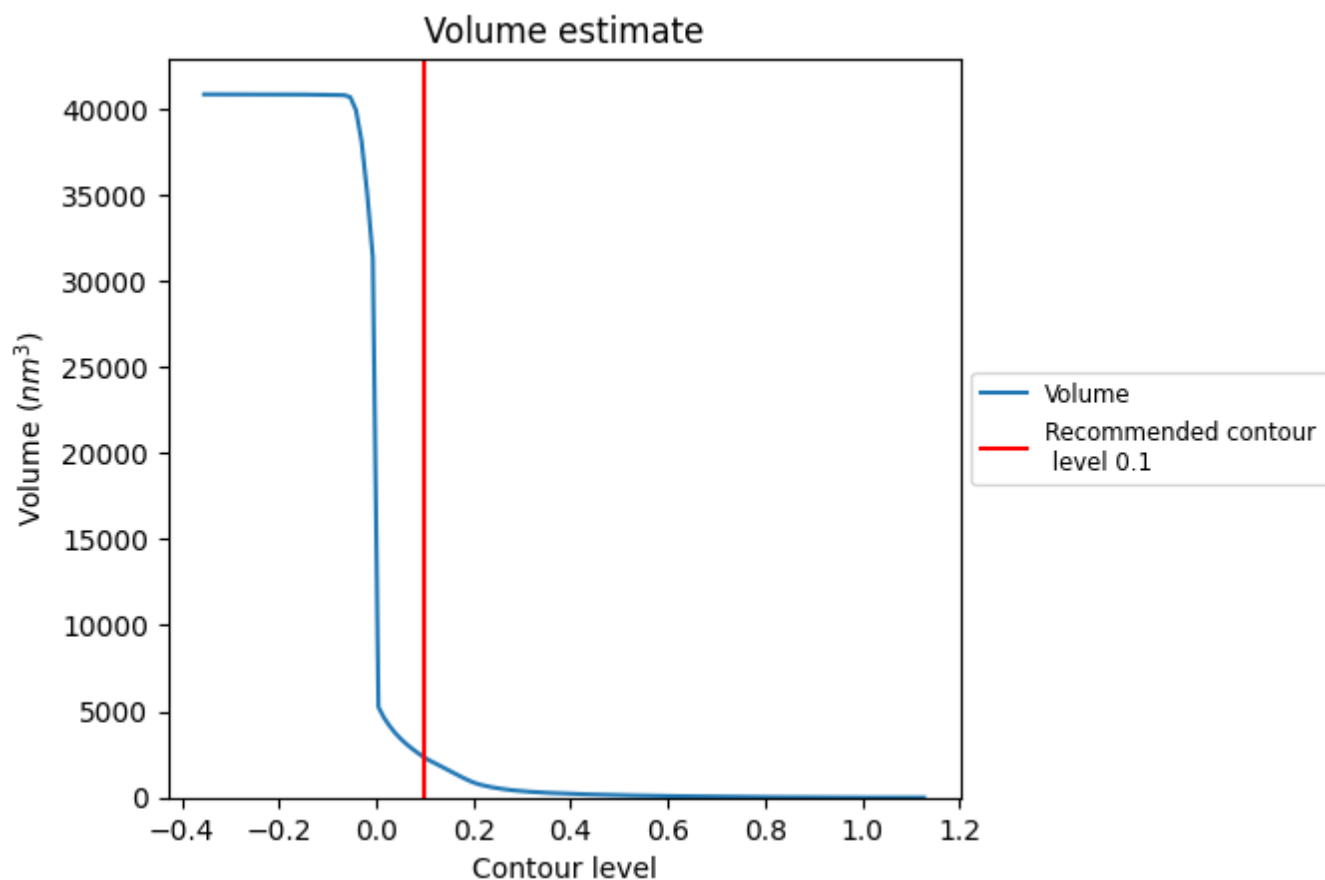
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

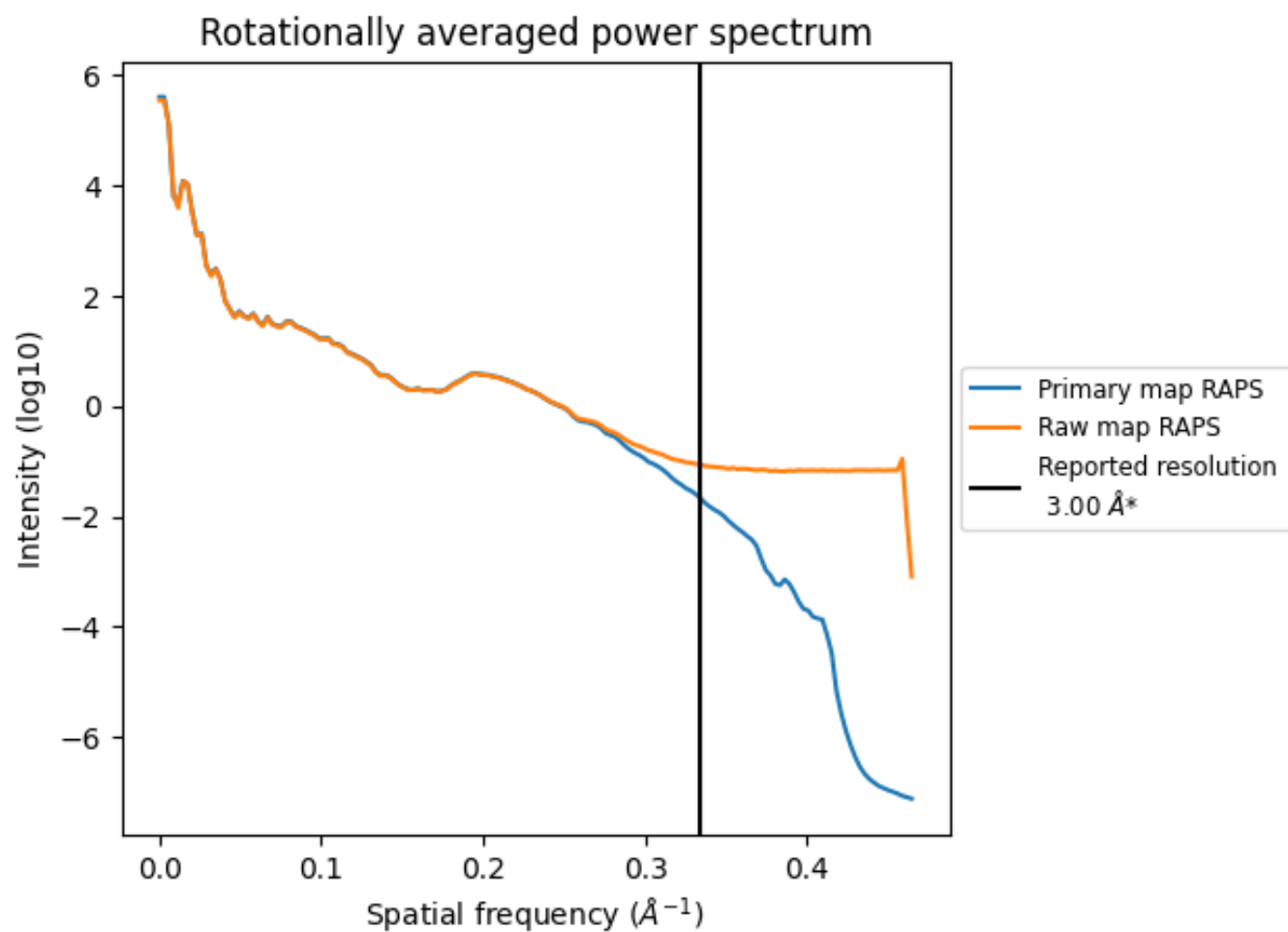
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2319 nm³; this corresponds to an approximate mass of 2095 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 ⓘ

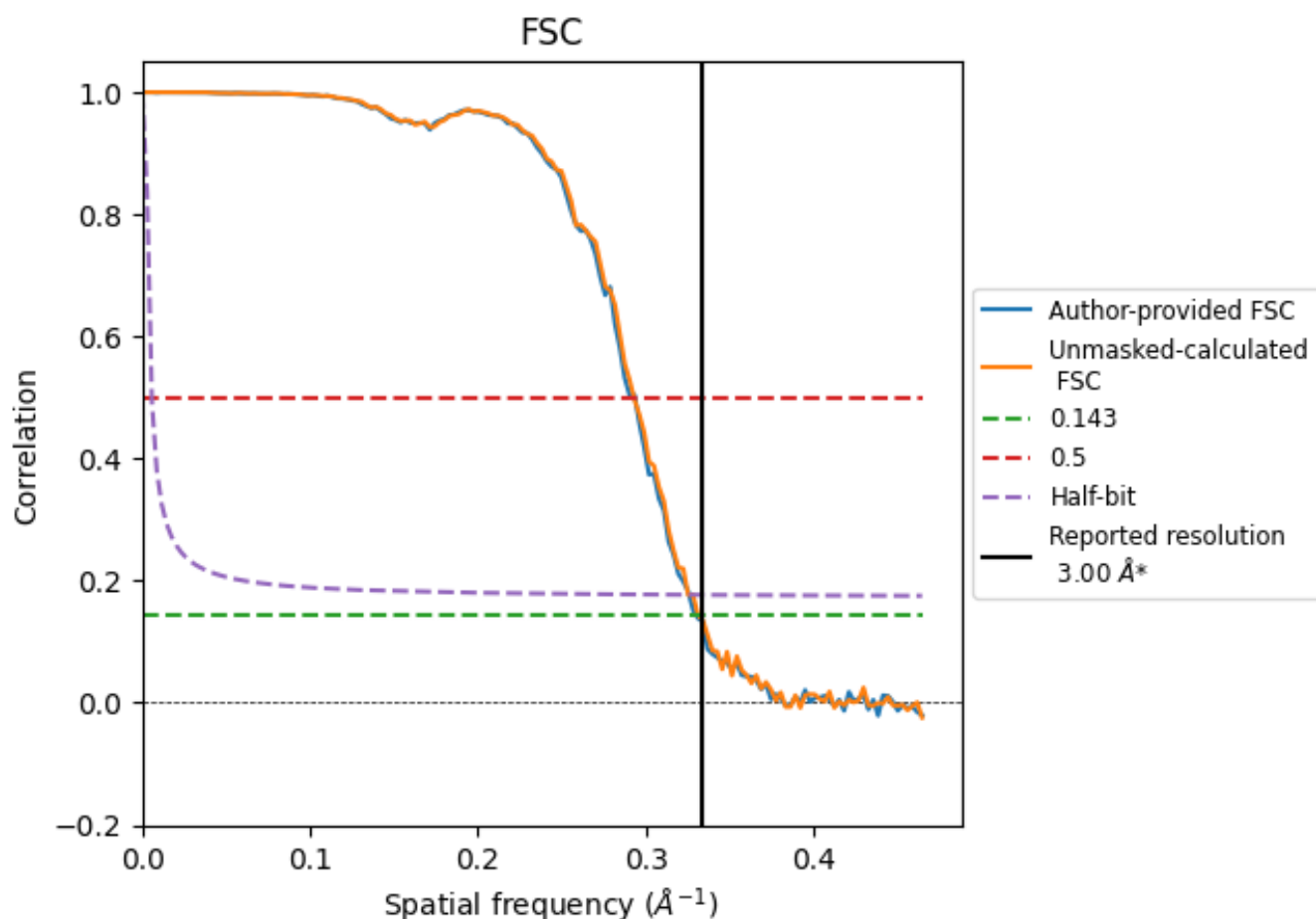


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

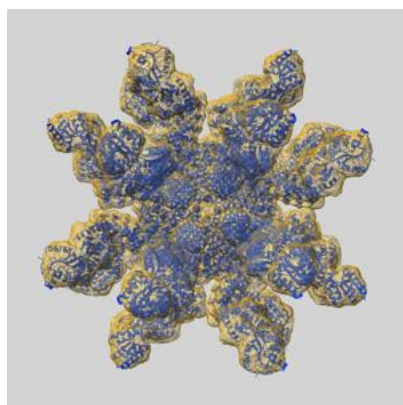
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.41	3.07
Unmasked-calculated*	3.02	3.41	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

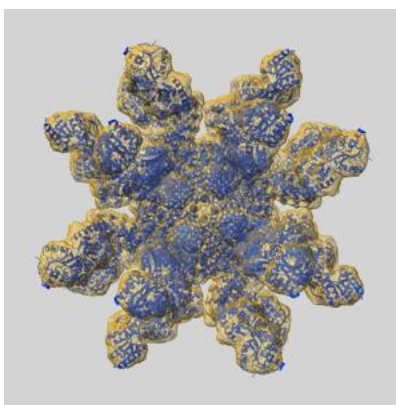
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60931 and PDB model 9IVP. Per-residue inclusion information can be found in section [3](#) on page [50](#).

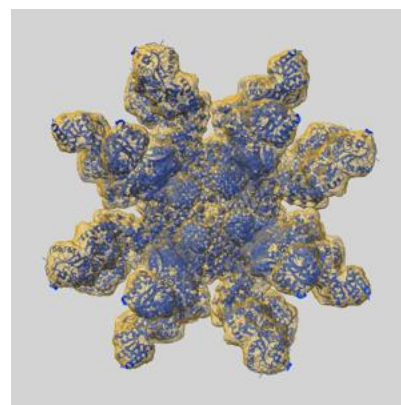
9.1 Map-model overlay [i](#)



X



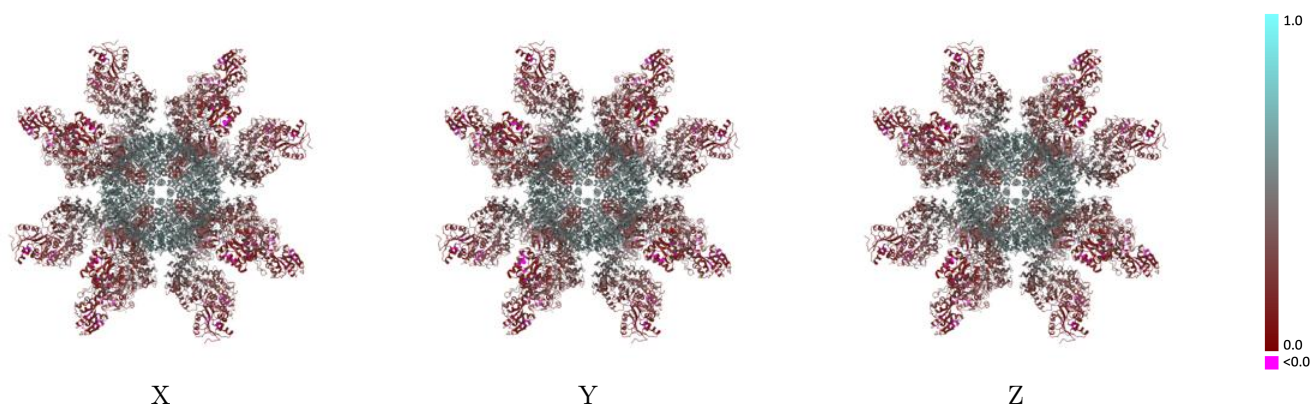
Y



Z

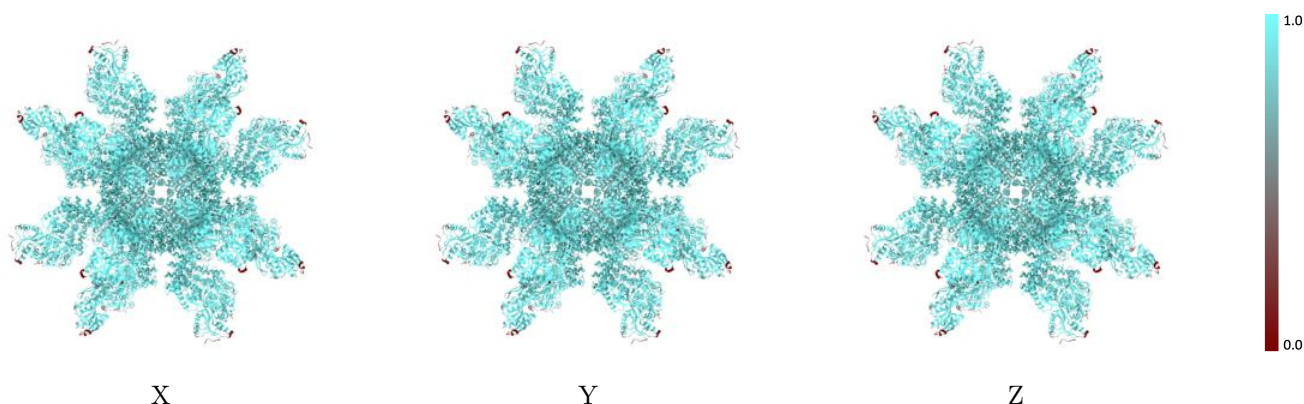
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



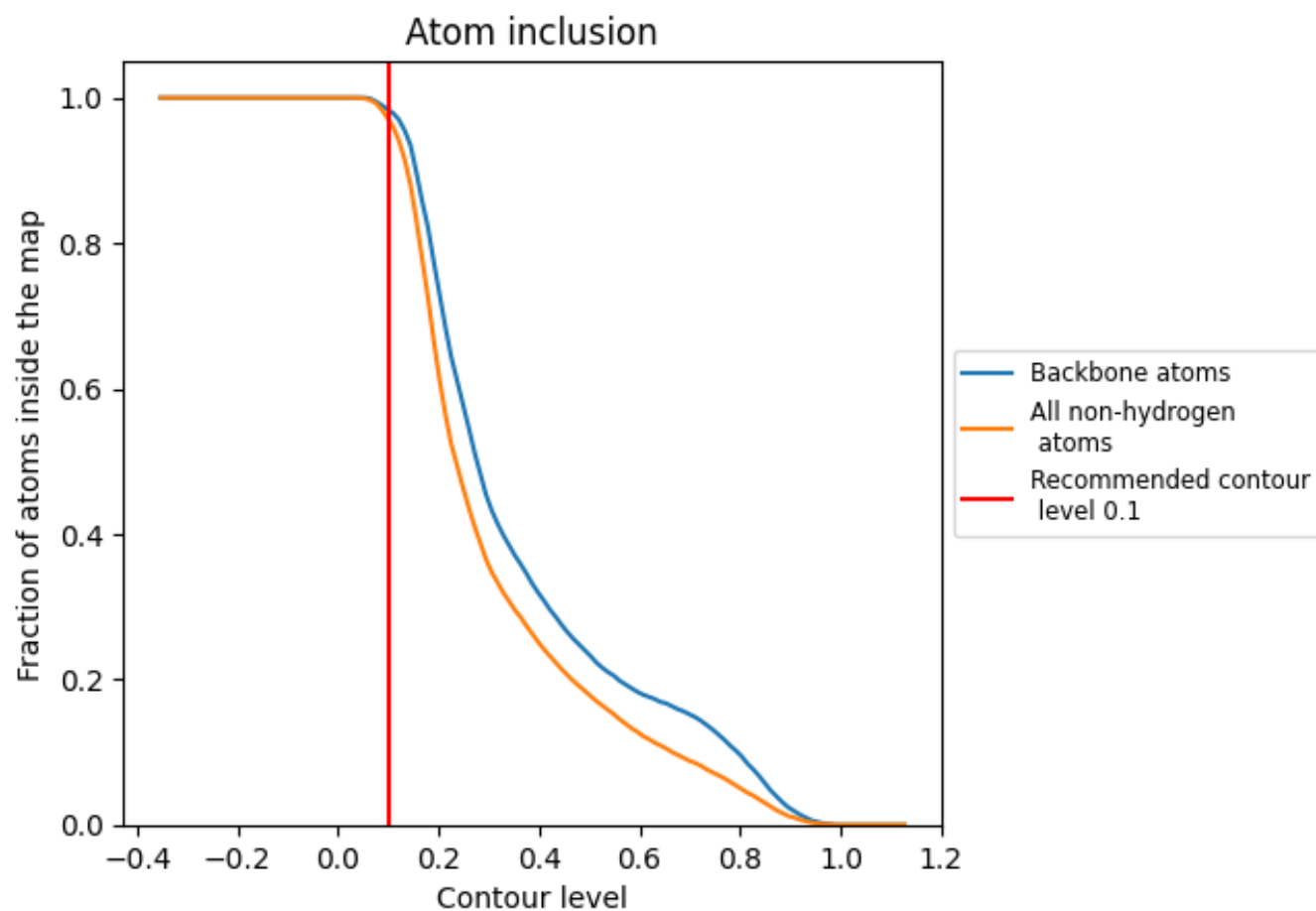
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.3480
A	 0.9960	 0.4840
AA	 0.9500	 0.2280
B	 0.9490	 0.2250
BA	 0.9950	 0.4860
C	 0.9950	 0.4870
CA	 0.9490	 0.2290
D	 0.9490	 0.2280
DA	 0.9960	 0.4910
E	 0.9950	 0.4860
EA	 0.9500	 0.2250
F	 0.9500	 0.2260
FA	 0.9950	 0.4880
G	 0.9940	 0.4720
GA	 0.9500	 0.2350
H	 0.9500	 0.2260
HA	 0.9940	 0.4920
I	 0.9950	 0.4740
IA	 0.9490	 0.2260
J	 0.9480	 0.2310
JA	 0.9940	 0.4930
K	 0.9940	 0.4920
KA	 0.9480	 0.2270
L	 0.9500	 0.2270
LA	 0.9930	 0.4710
M	 0.9950	 0.4700
MA	 0.9490	 0.2250
N	 0.9480	 0.2290
NA	 0.9950	 0.4850
O	 0.9950	 0.4900
OA	 0.9500	 0.2280
P	 0.9470	 0.2310
PA	 0.9950	 0.4850
Q	 0.9940	 0.4890
QA	 0.9500	 0.2240



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Chain	Atom inclusion	Q-score
R	 0.9480	 0.2330
RA	 0.9940	 0.4840
S	 0.9960	 0.4870
SA	 0.9490	 0.2280
T	 0.9500	 0.2240
TA	 0.9950	 0.4900
UA	 0.9490	 0.2260
V	 0.9940	 0.4880
VA	 0.9940	 0.4920
W	 0.9480	 0.2350
WA	 0.9500	 0.2270
X	 0.9950	 0.4890
Y	 0.9490	 0.2270
Z	 0.9930	 0.4800