



## Full wwPDB EM Validation Report ⓘ

May 27, 2025 – 04:06 PM JST

PDB ID : 9J48 / pdb\_00009j48  
EMDB ID : EMD-61130  
Title : GFP bound to 24-mer DARPin-apoferritin model 6c  
Authors : Lu, X.; Yan, M.; Zhang, H.M.; Hao, Q.  
Deposited on : 2024-08-09  
Resolution : 3.04 Å (reported)  
Based on initial model : 3AJ0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

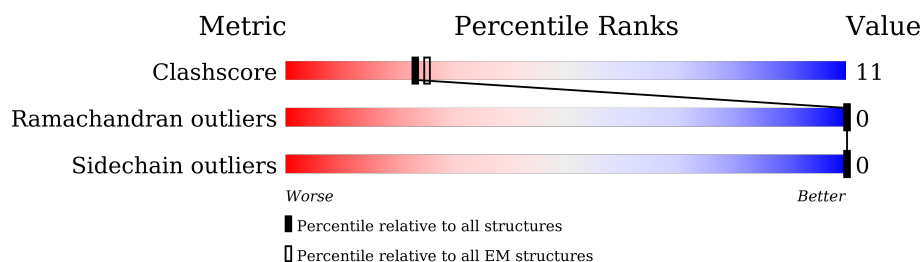
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.04 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.
















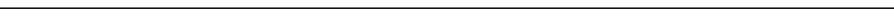











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	394	71% 11% 19%
1	B	394	70% 11% 19%
1	C	394	71% 11% 19%
1	D	394	70% 12% 19%
1	E	394	71% 11% 19%
1	F	394	70% 11% 19%
1	G	394	70% 11% 19%
1	H	394	71% 11% 19%

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Mol	Chain	Length	Quality of chain
1	I	394	
1	J	394	
1	K	394	
1	L	394	
1	M	394	
1	N	394	
1	O	394	
1	P	394	
1	Q	394	
1	R	394	
1	S	394	
1	T	394	
1	V	394	
1	W	394	
1	X	394	
1	Y	394	
2	a	234	
2	b	234	
2	c	234	
2	d	234	
2	e	234	
2	f	234	
2	g	234	
2	h	234	
2	i	234	

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Mol	Chain	Length	Quality of chain
2	j	234	
2	k	234	
2	l	234	
2	m	234	
2	n	234	
2	o	234	
2	p	234	
2	q	234	
2	r	234	
2	s	234	
2	t	234	
2	v	234	
2	w	234	
2	x	234	
2	y	234	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 103512 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 Designed ankyrin repeat proteins,Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	B	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	C	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	D	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	E	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	F	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	G	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	H	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	I	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	J	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	K	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	L	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	M	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	N	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	O	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	P	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	R	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	S	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	T	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	V	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	W	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	X	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		
1	Y	321	Total	C	N	O	S	0	0
			2485	1562	434	481	8		

There are 792 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	ALA	SER	conflict	UNP P02794
A	220	TYR	ARG	conflict	UNP P02794
A	277	GLU	ARG	conflict	UNP P02794
A	279	SER	PHE	conflict	UNP P02794
A	282	SER	ASP	conflict	UNP P02794
A	284	SER	LYS	conflict	UNP P02794
A	285	SER	LYS	conflict	UNP P02794
A	288	SER	CYS	conflict	UNP P02794
A	300	SER	CYS	conflict	UNP P02794
A	307	ALA	ASN	conflict	UNP P02794
A	310	ALA	GLN	conflict	UNP P02794
A	314	ARG	GLU	conflict	UNP P02794
A	322	CYS	LYS	conflict	UNP P02794
A	375	SER	-	expression tag	UNP P02794
A	376	GLY	-	expression tag	UNP P02794
A	377	SER	-	expression tag	UNP P02794
A	378	GLY	-	expression tag	UNP P02794
A	379	ALA	-	expression tag	UNP P02794
A	380	GLU	-	expression tag	UNP P02794
A	381	ILE	-	expression tag	UNP P02794
A	382	GLU	-	expression tag	UNP P02794
A	383	GLN	-	expression tag	UNP P02794
A	384	ALA	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LYS	-	expression tag	UNP P02794
A	386	LYS	-	expression tag	UNP P02794
A	387	GLU	-	expression tag	UNP P02794
A	388	ILE	-	expression tag	UNP P02794
A	389	ALA	-	expression tag	UNP P02794
A	390	TYR	-	expression tag	UNP P02794
A	391	LEU	-	expression tag	UNP P02794
A	392	ILE	-	expression tag	UNP P02794
A	393	LYS	-	expression tag	UNP P02794
A	394	LYS	-	expression tag	UNP P02794
B	214	ALA	SER	conflict	UNP P02794
B	220	TYR	ARG	conflict	UNP P02794
B	277	GLU	ARG	conflict	UNP P02794
B	279	SER	PHE	conflict	UNP P02794
B	282	SER	ASP	conflict	UNP P02794
B	284	SER	LYS	conflict	UNP P02794
B	285	SER	LYS	conflict	UNP P02794
B	288	SER	CYS	conflict	UNP P02794
B	300	SER	CYS	conflict	UNP P02794
B	307	ALA	ASN	conflict	UNP P02794
B	310	ALA	GLN	conflict	UNP P02794
B	314	ARG	GLU	conflict	UNP P02794
B	322	CYS	LYS	conflict	UNP P02794
B	375	SER	-	expression tag	UNP P02794
B	376	GLY	-	expression tag	UNP P02794
B	377	SER	-	expression tag	UNP P02794
B	378	GLY	-	expression tag	UNP P02794
B	379	ALA	-	expression tag	UNP P02794
B	380	GLU	-	expression tag	UNP P02794
B	381	ILE	-	expression tag	UNP P02794
B	382	GLU	-	expression tag	UNP P02794
B	383	GLN	-	expression tag	UNP P02794
B	384	ALA	-	expression tag	UNP P02794
B	385	LYS	-	expression tag	UNP P02794
B	386	LYS	-	expression tag	UNP P02794
B	387	GLU	-	expression tag	UNP P02794
B	388	ILE	-	expression tag	UNP P02794
B	389	ALA	-	expression tag	UNP P02794
B	390	TYR	-	expression tag	UNP P02794
B	391	LEU	-	expression tag	UNP P02794
B	392	ILE	-	expression tag	UNP P02794
B	393	LYS	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	LYS	-	expression tag	UNP P02794
C	214	ALA	SER	conflict	UNP P02794
C	220	TYR	ARG	conflict	UNP P02794
C	277	GLU	ARG	conflict	UNP P02794
C	279	SER	PHE	conflict	UNP P02794
C	282	SER	ASP	conflict	UNP P02794
C	284	SER	LYS	conflict	UNP P02794
C	285	SER	LYS	conflict	UNP P02794
C	288	SER	CYS	conflict	UNP P02794
C	300	SER	CYS	conflict	UNP P02794
C	307	ALA	ASN	conflict	UNP P02794
C	310	ALA	GLN	conflict	UNP P02794
C	314	ARG	GLU	conflict	UNP P02794
C	322	CYS	LYS	conflict	UNP P02794
C	375	SER	-	expression tag	UNP P02794
C	376	GLY	-	expression tag	UNP P02794
C	377	SER	-	expression tag	UNP P02794
C	378	GLY	-	expression tag	UNP P02794
C	379	ALA	-	expression tag	UNP P02794
C	380	GLU	-	expression tag	UNP P02794
C	381	ILE	-	expression tag	UNP P02794
C	382	GLU	-	expression tag	UNP P02794
C	383	GLN	-	expression tag	UNP P02794
C	384	ALA	-	expression tag	UNP P02794
C	385	LYS	-	expression tag	UNP P02794
C	386	LYS	-	expression tag	UNP P02794
C	387	GLU	-	expression tag	UNP P02794
C	388	ILE	-	expression tag	UNP P02794
C	389	ALA	-	expression tag	UNP P02794
C	390	TYR	-	expression tag	UNP P02794
C	391	LEU	-	expression tag	UNP P02794
C	392	ILE	-	expression tag	UNP P02794
C	393	LYS	-	expression tag	UNP P02794
C	394	LYS	-	expression tag	UNP P02794
D	214	ALA	SER	conflict	UNP P02794
D	220	TYR	ARG	conflict	UNP P02794
D	277	GLU	ARG	conflict	UNP P02794
D	279	SER	PHE	conflict	UNP P02794
D	282	SER	ASP	conflict	UNP P02794
D	284	SER	LYS	conflict	UNP P02794
D	285	SER	LYS	conflict	UNP P02794
D	288	SER	CYS	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
D	300	SER	CYS	conflict	UNP P02794
D	307	ALA	ASN	conflict	UNP P02794
D	310	ALA	GLN	conflict	UNP P02794
D	314	ARG	GLU	conflict	UNP P02794
D	322	CYS	LYS	conflict	UNP P02794
D	375	SER	-	expression tag	UNP P02794
D	376	GLY	-	expression tag	UNP P02794
D	377	SER	-	expression tag	UNP P02794
D	378	GLY	-	expression tag	UNP P02794
D	379	ALA	-	expression tag	UNP P02794
D	380	GLU	-	expression tag	UNP P02794
D	381	ILE	-	expression tag	UNP P02794
D	382	GLU	-	expression tag	UNP P02794
D	383	GLN	-	expression tag	UNP P02794
D	384	ALA	-	expression tag	UNP P02794
D	385	LYS	-	expression tag	UNP P02794
D	386	LYS	-	expression tag	UNP P02794
D	387	GLU	-	expression tag	UNP P02794
D	388	ILE	-	expression tag	UNP P02794
D	389	ALA	-	expression tag	UNP P02794
D	390	TYR	-	expression tag	UNP P02794
D	391	LEU	-	expression tag	UNP P02794
D	392	ILE	-	expression tag	UNP P02794
D	393	LYS	-	expression tag	UNP P02794
D	394	LYS	-	expression tag	UNP P02794
E	214	ALA	SER	conflict	UNP P02794
E	220	TYR	ARG	conflict	UNP P02794
E	277	GLU	ARG	conflict	UNP P02794
E	279	SER	PHE	conflict	UNP P02794
E	282	SER	ASP	conflict	UNP P02794
E	284	SER	LYS	conflict	UNP P02794
E	285	SER	LYS	conflict	UNP P02794
E	288	SER	CYS	conflict	UNP P02794
E	300	SER	CYS	conflict	UNP P02794
E	307	ALA	ASN	conflict	UNP P02794
E	310	ALA	GLN	conflict	UNP P02794
E	314	ARG	GLU	conflict	UNP P02794
E	322	CYS	LYS	conflict	UNP P02794
E	375	SER	-	expression tag	UNP P02794
E	376	GLY	-	expression tag	UNP P02794
E	377	SER	-	expression tag	UNP P02794
E	378	GLY	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
E	379	ALA	-	expression tag	UNP P02794
E	380	GLU	-	expression tag	UNP P02794
E	381	ILE	-	expression tag	UNP P02794
E	382	GLU	-	expression tag	UNP P02794
E	383	GLN	-	expression tag	UNP P02794
E	384	ALA	-	expression tag	UNP P02794
E	385	LYS	-	expression tag	UNP P02794
E	386	LYS	-	expression tag	UNP P02794
E	387	GLU	-	expression tag	UNP P02794
E	388	ILE	-	expression tag	UNP P02794
E	389	ALA	-	expression tag	UNP P02794
E	390	TYR	-	expression tag	UNP P02794
E	391	LEU	-	expression tag	UNP P02794
E	392	ILE	-	expression tag	UNP P02794
E	393	LYS	-	expression tag	UNP P02794
E	394	LYS	-	expression tag	UNP P02794
F	214	ALA	SER	conflict	UNP P02794
F	220	TYR	ARG	conflict	UNP P02794
F	277	GLU	ARG	conflict	UNP P02794
F	279	SER	PHE	conflict	UNP P02794
F	282	SER	ASP	conflict	UNP P02794
F	284	SER	LYS	conflict	UNP P02794
F	285	SER	LYS	conflict	UNP P02794
F	288	SER	CYS	conflict	UNP P02794
F	300	SER	CYS	conflict	UNP P02794
F	307	ALA	ASN	conflict	UNP P02794
F	310	ALA	GLN	conflict	UNP P02794
F	314	ARG	GLU	conflict	UNP P02794
F	322	CYS	LYS	conflict	UNP P02794
F	375	SER	-	expression tag	UNP P02794
F	376	GLY	-	expression tag	UNP P02794
F	377	SER	-	expression tag	UNP P02794
F	378	GLY	-	expression tag	UNP P02794
F	379	ALA	-	expression tag	UNP P02794
F	380	GLU	-	expression tag	UNP P02794
F	381	ILE	-	expression tag	UNP P02794
F	382	GLU	-	expression tag	UNP P02794
F	383	GLN	-	expression tag	UNP P02794
F	384	ALA	-	expression tag	UNP P02794
F	385	LYS	-	expression tag	UNP P02794
F	386	LYS	-	expression tag	UNP P02794
F	387	GLU	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
F	388	ILE	-	expression tag	UNP P02794
F	389	ALA	-	expression tag	UNP P02794
F	390	TYR	-	expression tag	UNP P02794
F	391	LEU	-	expression tag	UNP P02794
F	392	ILE	-	expression tag	UNP P02794
F	393	LYS	-	expression tag	UNP P02794
F	394	LYS	-	expression tag	UNP P02794
G	214	ALA	SER	conflict	UNP P02794
G	220	TYR	ARG	conflict	UNP P02794
G	277	GLU	ARG	conflict	UNP P02794
G	279	SER	PHE	conflict	UNP P02794
G	282	SER	ASP	conflict	UNP P02794
G	284	SER	LYS	conflict	UNP P02794
G	285	SER	LYS	conflict	UNP P02794
G	288	SER	CYS	conflict	UNP P02794
G	300	SER	CYS	conflict	UNP P02794
G	307	ALA	ASN	conflict	UNP P02794
G	310	ALA	GLN	conflict	UNP P02794
G	314	ARG	GLU	conflict	UNP P02794
G	322	CYS	LYS	conflict	UNP P02794
G	375	SER	-	expression tag	UNP P02794
G	376	GLY	-	expression tag	UNP P02794
G	377	SER	-	expression tag	UNP P02794
G	378	GLY	-	expression tag	UNP P02794
G	379	ALA	-	expression tag	UNP P02794
G	380	GLU	-	expression tag	UNP P02794
G	381	ILE	-	expression tag	UNP P02794
G	382	GLU	-	expression tag	UNP P02794
G	383	GLN	-	expression tag	UNP P02794
G	384	ALA	-	expression tag	UNP P02794
G	385	LYS	-	expression tag	UNP P02794
G	386	LYS	-	expression tag	UNP P02794
G	387	GLU	-	expression tag	UNP P02794
G	388	ILE	-	expression tag	UNP P02794
G	389	ALA	-	expression tag	UNP P02794
G	390	TYR	-	expression tag	UNP P02794
G	391	LEU	-	expression tag	UNP P02794
G	392	ILE	-	expression tag	UNP P02794
G	393	LYS	-	expression tag	UNP P02794
G	394	LYS	-	expression tag	UNP P02794
H	214	ALA	SER	conflict	UNP P02794
H	220	TYR	ARG	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
H	277	GLU	ARG	conflict	UNP P02794
H	279	SER	PHE	conflict	UNP P02794
H	282	SER	ASP	conflict	UNP P02794
H	284	SER	LYS	conflict	UNP P02794
H	285	SER	LYS	conflict	UNP P02794
H	288	SER	CYS	conflict	UNP P02794
H	300	SER	CYS	conflict	UNP P02794
H	307	ALA	ASN	conflict	UNP P02794
H	310	ALA	GLN	conflict	UNP P02794
H	314	ARG	GLU	conflict	UNP P02794
H	322	CYS	LYS	conflict	UNP P02794
H	375	SER	-	expression tag	UNP P02794
H	376	GLY	-	expression tag	UNP P02794
H	377	SER	-	expression tag	UNP P02794
H	378	GLY	-	expression tag	UNP P02794
H	379	ALA	-	expression tag	UNP P02794
H	380	GLU	-	expression tag	UNP P02794
H	381	ILE	-	expression tag	UNP P02794
H	382	GLU	-	expression tag	UNP P02794
H	383	GLN	-	expression tag	UNP P02794
H	384	ALA	-	expression tag	UNP P02794
H	385	LYS	-	expression tag	UNP P02794
H	386	LYS	-	expression tag	UNP P02794
H	387	GLU	-	expression tag	UNP P02794
H	388	ILE	-	expression tag	UNP P02794
H	389	ALA	-	expression tag	UNP P02794
H	390	TYR	-	expression tag	UNP P02794
H	391	LEU	-	expression tag	UNP P02794
H	392	ILE	-	expression tag	UNP P02794
H	393	LYS	-	expression tag	UNP P02794
H	394	LYS	-	expression tag	UNP P02794
I	214	ALA	SER	conflict	UNP P02794
I	220	TYR	ARG	conflict	UNP P02794
I	277	GLU	ARG	conflict	UNP P02794
I	279	SER	PHE	conflict	UNP P02794
I	282	SER	ASP	conflict	UNP P02794
I	284	SER	LYS	conflict	UNP P02794
I	285	SER	LYS	conflict	UNP P02794
I	288	SER	CYS	conflict	UNP P02794
I	300	SER	CYS	conflict	UNP P02794
I	307	ALA	ASN	conflict	UNP P02794
I	310	ALA	GLN	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
I	314	ARG	GLU	conflict	UNP P02794
I	322	CYS	LYS	conflict	UNP P02794
I	375	SER	-	expression tag	UNP P02794
I	376	GLY	-	expression tag	UNP P02794
I	377	SER	-	expression tag	UNP P02794
I	378	GLY	-	expression tag	UNP P02794
I	379	ALA	-	expression tag	UNP P02794
I	380	GLU	-	expression tag	UNP P02794
I	381	ILE	-	expression tag	UNP P02794
I	382	GLU	-	expression tag	UNP P02794
I	383	GLN	-	expression tag	UNP P02794
I	384	ALA	-	expression tag	UNP P02794
I	385	LYS	-	expression tag	UNP P02794
I	386	LYS	-	expression tag	UNP P02794
I	387	GLU	-	expression tag	UNP P02794
I	388	ILE	-	expression tag	UNP P02794
I	389	ALA	-	expression tag	UNP P02794
I	390	TYR	-	expression tag	UNP P02794
I	391	LEU	-	expression tag	UNP P02794
I	392	ILE	-	expression tag	UNP P02794
I	393	LYS	-	expression tag	UNP P02794
I	394	LYS	-	expression tag	UNP P02794
J	214	ALA	SER	conflict	UNP P02794
J	220	TYR	ARG	conflict	UNP P02794
J	277	GLU	ARG	conflict	UNP P02794
J	279	SER	PHE	conflict	UNP P02794
J	282	SER	ASP	conflict	UNP P02794
J	284	SER	LYS	conflict	UNP P02794
J	285	SER	LYS	conflict	UNP P02794
J	288	SER	CYS	conflict	UNP P02794
J	300	SER	CYS	conflict	UNP P02794
J	307	ALA	ASN	conflict	UNP P02794
J	310	ALA	GLN	conflict	UNP P02794
J	314	ARG	GLU	conflict	UNP P02794
J	322	CYS	LYS	conflict	UNP P02794
J	375	SER	-	expression tag	UNP P02794
J	376	GLY	-	expression tag	UNP P02794
J	377	SER	-	expression tag	UNP P02794
J	378	GLY	-	expression tag	UNP P02794
J	379	ALA	-	expression tag	UNP P02794
J	380	GLU	-	expression tag	UNP P02794
J	381	ILE	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
J	382	GLU	-	expression tag	UNP P02794
J	383	GLN	-	expression tag	UNP P02794
J	384	ALA	-	expression tag	UNP P02794
J	385	LYS	-	expression tag	UNP P02794
J	386	LYS	-	expression tag	UNP P02794
J	387	GLU	-	expression tag	UNP P02794
J	388	ILE	-	expression tag	UNP P02794
J	389	ALA	-	expression tag	UNP P02794
J	390	TYR	-	expression tag	UNP P02794
J	391	LEU	-	expression tag	UNP P02794
J	392	ILE	-	expression tag	UNP P02794
J	393	LYS	-	expression tag	UNP P02794
J	394	LYS	-	expression tag	UNP P02794
K	214	ALA	SER	conflict	UNP P02794
K	220	TYR	ARG	conflict	UNP P02794
K	277	GLU	ARG	conflict	UNP P02794
K	279	SER	PHE	conflict	UNP P02794
K	282	SER	ASP	conflict	UNP P02794
K	284	SER	LYS	conflict	UNP P02794
K	285	SER	LYS	conflict	UNP P02794
K	288	SER	CYS	conflict	UNP P02794
K	300	SER	CYS	conflict	UNP P02794
K	307	ALA	ASN	conflict	UNP P02794
K	310	ALA	GLN	conflict	UNP P02794
K	314	ARG	GLU	conflict	UNP P02794
K	322	CYS	LYS	conflict	UNP P02794
K	375	SER	-	expression tag	UNP P02794
K	376	GLY	-	expression tag	UNP P02794
K	377	SER	-	expression tag	UNP P02794
K	378	GLY	-	expression tag	UNP P02794
K	379	ALA	-	expression tag	UNP P02794
K	380	GLU	-	expression tag	UNP P02794
K	381	ILE	-	expression tag	UNP P02794
K	382	GLU	-	expression tag	UNP P02794
K	383	GLN	-	expression tag	UNP P02794
K	384	ALA	-	expression tag	UNP P02794
K	385	LYS	-	expression tag	UNP P02794
K	386	LYS	-	expression tag	UNP P02794
K	387	GLU	-	expression tag	UNP P02794
K	388	ILE	-	expression tag	UNP P02794
K	389	ALA	-	expression tag	UNP P02794
K	390	TYR	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
K	391	LEU	-	expression tag	UNP P02794
K	392	ILE	-	expression tag	UNP P02794
K	393	LYS	-	expression tag	UNP P02794
K	394	LYS	-	expression tag	UNP P02794
L	214	ALA	SER	conflict	UNP P02794
L	220	TYR	ARG	conflict	UNP P02794
L	277	GLU	ARG	conflict	UNP P02794
L	279	SER	PHE	conflict	UNP P02794
L	282	SER	ASP	conflict	UNP P02794
L	284	SER	LYS	conflict	UNP P02794
L	285	SER	LYS	conflict	UNP P02794
L	288	SER	CYS	conflict	UNP P02794
L	300	SER	CYS	conflict	UNP P02794
L	307	ALA	ASN	conflict	UNP P02794
L	310	ALA	GLN	conflict	UNP P02794
L	314	ARG	GLU	conflict	UNP P02794
L	322	CYS	LYS	conflict	UNP P02794
L	375	SER	-	expression tag	UNP P02794
L	376	GLY	-	expression tag	UNP P02794
L	377	SER	-	expression tag	UNP P02794
L	378	GLY	-	expression tag	UNP P02794
L	379	ALA	-	expression tag	UNP P02794
L	380	GLU	-	expression tag	UNP P02794
L	381	ILE	-	expression tag	UNP P02794
L	382	GLU	-	expression tag	UNP P02794
L	383	GLN	-	expression tag	UNP P02794
L	384	ALA	-	expression tag	UNP P02794
L	385	LYS	-	expression tag	UNP P02794
L	386	LYS	-	expression tag	UNP P02794
L	387	GLU	-	expression tag	UNP P02794
L	388	ILE	-	expression tag	UNP P02794
L	389	ALA	-	expression tag	UNP P02794
L	390	TYR	-	expression tag	UNP P02794
L	391	LEU	-	expression tag	UNP P02794
L	392	ILE	-	expression tag	UNP P02794
L	393	LYS	-	expression tag	UNP P02794
L	394	LYS	-	expression tag	UNP P02794
M	214	ALA	SER	conflict	UNP P02794
M	220	TYR	ARG	conflict	UNP P02794
M	277	GLU	ARG	conflict	UNP P02794
M	279	SER	PHE	conflict	UNP P02794
M	282	SER	ASP	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
M	284	SER	LYS	conflict	UNP P02794
M	285	SER	LYS	conflict	UNP P02794
M	288	SER	CYS	conflict	UNP P02794
M	300	SER	CYS	conflict	UNP P02794
M	307	ALA	ASN	conflict	UNP P02794
M	310	ALA	GLN	conflict	UNP P02794
M	314	ARG	GLU	conflict	UNP P02794
M	322	CYS	LYS	conflict	UNP P02794
M	375	SER	-	expression tag	UNP P02794
M	376	GLY	-	expression tag	UNP P02794
M	377	SER	-	expression tag	UNP P02794
M	378	GLY	-	expression tag	UNP P02794
M	379	ALA	-	expression tag	UNP P02794
M	380	GLU	-	expression tag	UNP P02794
M	381	ILE	-	expression tag	UNP P02794
M	382	GLU	-	expression tag	UNP P02794
M	383	GLN	-	expression tag	UNP P02794
M	384	ALA	-	expression tag	UNP P02794
M	385	LYS	-	expression tag	UNP P02794
M	386	LYS	-	expression tag	UNP P02794
M	387	GLU	-	expression tag	UNP P02794
M	388	ILE	-	expression tag	UNP P02794
M	389	ALA	-	expression tag	UNP P02794
M	390	TYR	-	expression tag	UNP P02794
M	391	LEU	-	expression tag	UNP P02794
M	392	ILE	-	expression tag	UNP P02794
M	393	LYS	-	expression tag	UNP P02794
M	394	LYS	-	expression tag	UNP P02794
N	214	ALA	SER	conflict	UNP P02794
N	220	TYR	ARG	conflict	UNP P02794
N	277	GLU	ARG	conflict	UNP P02794
N	279	SER	PHE	conflict	UNP P02794
N	282	SER	ASP	conflict	UNP P02794
N	284	SER	LYS	conflict	UNP P02794
N	285	SER	LYS	conflict	UNP P02794
N	288	SER	CYS	conflict	UNP P02794
N	300	SER	CYS	conflict	UNP P02794
N	307	ALA	ASN	conflict	UNP P02794
N	310	ALA	GLN	conflict	UNP P02794
N	314	ARG	GLU	conflict	UNP P02794
N	322	CYS	LYS	conflict	UNP P02794
N	375	SER	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
N	376	GLY	-	expression tag	UNP P02794
N	377	SER	-	expression tag	UNP P02794
N	378	GLY	-	expression tag	UNP P02794
N	379	ALA	-	expression tag	UNP P02794
N	380	GLU	-	expression tag	UNP P02794
N	381	ILE	-	expression tag	UNP P02794
N	382	GLU	-	expression tag	UNP P02794
N	383	GLN	-	expression tag	UNP P02794
N	384	ALA	-	expression tag	UNP P02794
N	385	LYS	-	expression tag	UNP P02794
N	386	LYS	-	expression tag	UNP P02794
N	387	GLU	-	expression tag	UNP P02794
N	388	ILE	-	expression tag	UNP P02794
N	389	ALA	-	expression tag	UNP P02794
N	390	TYR	-	expression tag	UNP P02794
N	391	LEU	-	expression tag	UNP P02794
N	392	ILE	-	expression tag	UNP P02794
N	393	LYS	-	expression tag	UNP P02794
N	394	LYS	-	expression tag	UNP P02794
O	214	ALA	SER	conflict	UNP P02794
O	220	TYR	ARG	conflict	UNP P02794
O	277	GLU	ARG	conflict	UNP P02794
O	279	SER	PHE	conflict	UNP P02794
O	282	SER	ASP	conflict	UNP P02794
O	284	SER	LYS	conflict	UNP P02794
O	285	SER	LYS	conflict	UNP P02794
O	288	SER	CYS	conflict	UNP P02794
O	300	SER	CYS	conflict	UNP P02794
O	307	ALA	ASN	conflict	UNP P02794
O	310	ALA	GLN	conflict	UNP P02794
O	314	ARG	GLU	conflict	UNP P02794
O	322	CYS	LYS	conflict	UNP P02794
O	375	SER	-	expression tag	UNP P02794
O	376	GLY	-	expression tag	UNP P02794
O	377	SER	-	expression tag	UNP P02794
O	378	GLY	-	expression tag	UNP P02794
O	379	ALA	-	expression tag	UNP P02794
O	380	GLU	-	expression tag	UNP P02794
O	381	ILE	-	expression tag	UNP P02794
O	382	GLU	-	expression tag	UNP P02794
O	383	GLN	-	expression tag	UNP P02794
O	384	ALA	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
O	385	LYS	-	expression tag	UNP P02794
O	386	LYS	-	expression tag	UNP P02794
O	387	GLU	-	expression tag	UNP P02794
O	388	ILE	-	expression tag	UNP P02794
O	389	ALA	-	expression tag	UNP P02794
O	390	TYR	-	expression tag	UNP P02794
O	391	LEU	-	expression tag	UNP P02794
O	392	ILE	-	expression tag	UNP P02794
O	393	LYS	-	expression tag	UNP P02794
O	394	LYS	-	expression tag	UNP P02794
P	214	ALA	SER	conflict	UNP P02794
P	220	TYR	ARG	conflict	UNP P02794
P	277	GLU	ARG	conflict	UNP P02794
P	279	SER	PHE	conflict	UNP P02794
P	282	SER	ASP	conflict	UNP P02794
P	284	SER	LYS	conflict	UNP P02794
P	285	SER	LYS	conflict	UNP P02794
P	288	SER	CYS	conflict	UNP P02794
P	300	SER	CYS	conflict	UNP P02794
P	307	ALA	ASN	conflict	UNP P02794
P	310	ALA	GLN	conflict	UNP P02794
P	314	ARG	GLU	conflict	UNP P02794
P	322	CYS	LYS	conflict	UNP P02794
P	375	SER	-	expression tag	UNP P02794
P	376	GLY	-	expression tag	UNP P02794
P	377	SER	-	expression tag	UNP P02794
P	378	GLY	-	expression tag	UNP P02794
P	379	ALA	-	expression tag	UNP P02794
P	380	GLU	-	expression tag	UNP P02794
P	381	ILE	-	expression tag	UNP P02794
P	382	GLU	-	expression tag	UNP P02794
P	383	GLN	-	expression tag	UNP P02794
P	384	ALA	-	expression tag	UNP P02794
P	385	LYS	-	expression tag	UNP P02794
P	386	LYS	-	expression tag	UNP P02794
P	387	GLU	-	expression tag	UNP P02794
P	388	ILE	-	expression tag	UNP P02794
P	389	ALA	-	expression tag	UNP P02794
P	390	TYR	-	expression tag	UNP P02794
P	391	LEU	-	expression tag	UNP P02794
P	392	ILE	-	expression tag	UNP P02794
P	393	LYS	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
P	394	LYS	-	expression tag	UNP P02794
Q	214	ALA	SER	conflict	UNP P02794
Q	220	TYR	ARG	conflict	UNP P02794
Q	277	GLU	ARG	conflict	UNP P02794
Q	279	SER	PHE	conflict	UNP P02794
Q	282	SER	ASP	conflict	UNP P02794
Q	284	SER	LYS	conflict	UNP P02794
Q	285	SER	LYS	conflict	UNP P02794
Q	288	SER	CYS	conflict	UNP P02794
Q	300	SER	CYS	conflict	UNP P02794
Q	307	ALA	ASN	conflict	UNP P02794
Q	310	ALA	GLN	conflict	UNP P02794
Q	314	ARG	GLU	conflict	UNP P02794
Q	322	CYS	LYS	conflict	UNP P02794
Q	375	SER	-	expression tag	UNP P02794
Q	376	GLY	-	expression tag	UNP P02794
Q	377	SER	-	expression tag	UNP P02794
Q	378	GLY	-	expression tag	UNP P02794
Q	379	ALA	-	expression tag	UNP P02794
Q	380	GLU	-	expression tag	UNP P02794
Q	381	ILE	-	expression tag	UNP P02794
Q	382	GLU	-	expression tag	UNP P02794
Q	383	GLN	-	expression tag	UNP P02794
Q	384	ALA	-	expression tag	UNP P02794
Q	385	LYS	-	expression tag	UNP P02794
Q	386	LYS	-	expression tag	UNP P02794
Q	387	GLU	-	expression tag	UNP P02794
Q	388	ILE	-	expression tag	UNP P02794
Q	389	ALA	-	expression tag	UNP P02794
Q	390	TYR	-	expression tag	UNP P02794
Q	391	LEU	-	expression tag	UNP P02794
Q	392	ILE	-	expression tag	UNP P02794
Q	393	LYS	-	expression tag	UNP P02794
Q	394	LYS	-	expression tag	UNP P02794
R	214	ALA	SER	conflict	UNP P02794
R	220	TYR	ARG	conflict	UNP P02794
R	277	GLU	ARG	conflict	UNP P02794
R	279	SER	PHE	conflict	UNP P02794
R	282	SER	ASP	conflict	UNP P02794
R	284	SER	LYS	conflict	UNP P02794
R	285	SER	LYS	conflict	UNP P02794
R	288	SER	CYS	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
R	300	SER	CYS	conflict	UNP P02794
R	307	ALA	ASN	conflict	UNP P02794
R	310	ALA	GLN	conflict	UNP P02794
R	314	ARG	GLU	conflict	UNP P02794
R	322	CYS	LYS	conflict	UNP P02794
R	375	SER	-	expression tag	UNP P02794
R	376	GLY	-	expression tag	UNP P02794
R	377	SER	-	expression tag	UNP P02794
R	378	GLY	-	expression tag	UNP P02794
R	379	ALA	-	expression tag	UNP P02794
R	380	GLU	-	expression tag	UNP P02794
R	381	ILE	-	expression tag	UNP P02794
R	382	GLU	-	expression tag	UNP P02794
R	383	GLN	-	expression tag	UNP P02794
R	384	ALA	-	expression tag	UNP P02794
R	385	LYS	-	expression tag	UNP P02794
R	386	LYS	-	expression tag	UNP P02794
R	387	GLU	-	expression tag	UNP P02794
R	388	ILE	-	expression tag	UNP P02794
R	389	ALA	-	expression tag	UNP P02794
R	390	TYR	-	expression tag	UNP P02794
R	391	LEU	-	expression tag	UNP P02794
R	392	ILE	-	expression tag	UNP P02794
R	393	LYS	-	expression tag	UNP P02794
R	394	LYS	-	expression tag	UNP P02794
S	214	ALA	SER	conflict	UNP P02794
S	220	TYR	ARG	conflict	UNP P02794
S	277	GLU	ARG	conflict	UNP P02794
S	279	SER	PHE	conflict	UNP P02794
S	282	SER	ASP	conflict	UNP P02794
S	284	SER	LYS	conflict	UNP P02794
S	285	SER	LYS	conflict	UNP P02794
S	288	SER	CYS	conflict	UNP P02794
S	300	SER	CYS	conflict	UNP P02794
S	307	ALA	ASN	conflict	UNP P02794
S	310	ALA	GLN	conflict	UNP P02794
S	314	ARG	GLU	conflict	UNP P02794
S	322	CYS	LYS	conflict	UNP P02794
S	375	SER	-	expression tag	UNP P02794
S	376	GLY	-	expression tag	UNP P02794
S	377	SER	-	expression tag	UNP P02794
S	378	GLY	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
S	379	ALA	-	expression tag	UNP P02794
S	380	GLU	-	expression tag	UNP P02794
S	381	ILE	-	expression tag	UNP P02794
S	382	GLU	-	expression tag	UNP P02794
S	383	GLN	-	expression tag	UNP P02794
S	384	ALA	-	expression tag	UNP P02794
S	385	LYS	-	expression tag	UNP P02794
S	386	LYS	-	expression tag	UNP P02794
S	387	GLU	-	expression tag	UNP P02794
S	388	ILE	-	expression tag	UNP P02794
S	389	ALA	-	expression tag	UNP P02794
S	390	TYR	-	expression tag	UNP P02794
S	391	LEU	-	expression tag	UNP P02794
S	392	ILE	-	expression tag	UNP P02794
S	393	LYS	-	expression tag	UNP P02794
S	394	LYS	-	expression tag	UNP P02794
T	214	ALA	SER	conflict	UNP P02794
T	220	TYR	ARG	conflict	UNP P02794
T	277	GLU	ARG	conflict	UNP P02794
T	279	SER	PHE	conflict	UNP P02794
T	282	SER	ASP	conflict	UNP P02794
T	284	SER	LYS	conflict	UNP P02794
T	285	SER	LYS	conflict	UNP P02794
T	288	SER	CYS	conflict	UNP P02794
T	300	SER	CYS	conflict	UNP P02794
T	307	ALA	ASN	conflict	UNP P02794
T	310	ALA	GLN	conflict	UNP P02794
T	314	ARG	GLU	conflict	UNP P02794
T	322	CYS	LYS	conflict	UNP P02794
T	375	SER	-	expression tag	UNP P02794
T	376	GLY	-	expression tag	UNP P02794
T	377	SER	-	expression tag	UNP P02794
T	378	GLY	-	expression tag	UNP P02794
T	379	ALA	-	expression tag	UNP P02794
T	380	GLU	-	expression tag	UNP P02794
T	381	ILE	-	expression tag	UNP P02794
T	382	GLU	-	expression tag	UNP P02794
T	383	GLN	-	expression tag	UNP P02794
T	384	ALA	-	expression tag	UNP P02794
T	385	LYS	-	expression tag	UNP P02794
T	386	LYS	-	expression tag	UNP P02794
T	387	GLU	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
T	388	ILE	-	expression tag	UNP P02794
T	389	ALA	-	expression tag	UNP P02794
T	390	TYR	-	expression tag	UNP P02794
T	391	LEU	-	expression tag	UNP P02794
T	392	ILE	-	expression tag	UNP P02794
T	393	LYS	-	expression tag	UNP P02794
T	394	LYS	-	expression tag	UNP P02794
V	214	ALA	SER	conflict	UNP P02794
V	220	TYR	ARG	conflict	UNP P02794
V	277	GLU	ARG	conflict	UNP P02794
V	279	SER	PHE	conflict	UNP P02794
V	282	SER	ASP	conflict	UNP P02794
V	284	SER	LYS	conflict	UNP P02794
V	285	SER	LYS	conflict	UNP P02794
V	288	SER	CYS	conflict	UNP P02794
V	300	SER	CYS	conflict	UNP P02794
V	307	ALA	ASN	conflict	UNP P02794
V	310	ALA	GLN	conflict	UNP P02794
V	314	ARG	GLU	conflict	UNP P02794
V	322	CYS	LYS	conflict	UNP P02794
V	375	SER	-	expression tag	UNP P02794
V	376	GLY	-	expression tag	UNP P02794
V	377	SER	-	expression tag	UNP P02794
V	378	GLY	-	expression tag	UNP P02794
V	379	ALA	-	expression tag	UNP P02794
V	380	GLU	-	expression tag	UNP P02794
V	381	ILE	-	expression tag	UNP P02794
V	382	GLU	-	expression tag	UNP P02794
V	383	GLN	-	expression tag	UNP P02794
V	384	ALA	-	expression tag	UNP P02794
V	385	LYS	-	expression tag	UNP P02794
V	386	LYS	-	expression tag	UNP P02794
V	387	GLU	-	expression tag	UNP P02794
V	388	ILE	-	expression tag	UNP P02794
V	389	ALA	-	expression tag	UNP P02794
V	390	TYR	-	expression tag	UNP P02794
V	391	LEU	-	expression tag	UNP P02794
V	392	ILE	-	expression tag	UNP P02794
V	393	LYS	-	expression tag	UNP P02794
V	394	LYS	-	expression tag	UNP P02794
W	214	ALA	SER	conflict	UNP P02794
W	220	TYR	ARG	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
W	277	GLU	ARG	conflict	UNP P02794
W	279	SER	PHE	conflict	UNP P02794
W	282	SER	ASP	conflict	UNP P02794
W	284	SER	LYS	conflict	UNP P02794
W	285	SER	LYS	conflict	UNP P02794
W	288	SER	CYS	conflict	UNP P02794
W	300	SER	CYS	conflict	UNP P02794
W	307	ALA	ASN	conflict	UNP P02794
W	310	ALA	GLN	conflict	UNP P02794
W	314	ARG	GLU	conflict	UNP P02794
W	322	CYS	LYS	conflict	UNP P02794
W	375	SER	-	expression tag	UNP P02794
W	376	GLY	-	expression tag	UNP P02794
W	377	SER	-	expression tag	UNP P02794
W	378	GLY	-	expression tag	UNP P02794
W	379	ALA	-	expression tag	UNP P02794
W	380	GLU	-	expression tag	UNP P02794
W	381	ILE	-	expression tag	UNP P02794
W	382	GLU	-	expression tag	UNP P02794
W	383	GLN	-	expression tag	UNP P02794
W	384	ALA	-	expression tag	UNP P02794
W	385	LYS	-	expression tag	UNP P02794
W	386	LYS	-	expression tag	UNP P02794
W	387	GLU	-	expression tag	UNP P02794
W	388	ILE	-	expression tag	UNP P02794
W	389	ALA	-	expression tag	UNP P02794
W	390	TYR	-	expression tag	UNP P02794
W	391	LEU	-	expression tag	UNP P02794
W	392	ILE	-	expression tag	UNP P02794
W	393	LYS	-	expression tag	UNP P02794
W	394	LYS	-	expression tag	UNP P02794
X	214	ALA	SER	conflict	UNP P02794
X	220	TYR	ARG	conflict	UNP P02794
X	277	GLU	ARG	conflict	UNP P02794
X	279	SER	PHE	conflict	UNP P02794
X	282	SER	ASP	conflict	UNP P02794
X	284	SER	LYS	conflict	UNP P02794
X	285	SER	LYS	conflict	UNP P02794
X	288	SER	CYS	conflict	UNP P02794
X	300	SER	CYS	conflict	UNP P02794
X	307	ALA	ASN	conflict	UNP P02794
X	310	ALA	GLN	conflict	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
X	314	ARG	GLU	conflict	UNP P02794
X	322	CYS	LYS	conflict	UNP P02794
X	375	SER	-	expression tag	UNP P02794
X	376	GLY	-	expression tag	UNP P02794
X	377	SER	-	expression tag	UNP P02794
X	378	GLY	-	expression tag	UNP P02794
X	379	ALA	-	expression tag	UNP P02794
X	380	GLU	-	expression tag	UNP P02794
X	381	ILE	-	expression tag	UNP P02794
X	382	GLU	-	expression tag	UNP P02794
X	383	GLN	-	expression tag	UNP P02794
X	384	ALA	-	expression tag	UNP P02794
X	385	LYS	-	expression tag	UNP P02794
X	386	LYS	-	expression tag	UNP P02794
X	387	GLU	-	expression tag	UNP P02794
X	388	ILE	-	expression tag	UNP P02794
X	389	ALA	-	expression tag	UNP P02794
X	390	TYR	-	expression tag	UNP P02794
X	391	LEU	-	expression tag	UNP P02794
X	392	ILE	-	expression tag	UNP P02794
X	393	LYS	-	expression tag	UNP P02794
X	394	LYS	-	expression tag	UNP P02794
Y	214	ALA	SER	conflict	UNP P02794
Y	220	TYR	ARG	conflict	UNP P02794
Y	277	GLU	ARG	conflict	UNP P02794
Y	279	SER	PHE	conflict	UNP P02794
Y	282	SER	ASP	conflict	UNP P02794
Y	284	SER	LYS	conflict	UNP P02794
Y	285	SER	LYS	conflict	UNP P02794
Y	288	SER	CYS	conflict	UNP P02794
Y	300	SER	CYS	conflict	UNP P02794
Y	307	ALA	ASN	conflict	UNP P02794
Y	310	ALA	GLN	conflict	UNP P02794
Y	314	ARG	GLU	conflict	UNP P02794
Y	322	CYS	LYS	conflict	UNP P02794
Y	375	SER	-	expression tag	UNP P02794
Y	376	GLY	-	expression tag	UNP P02794
Y	377	SER	-	expression tag	UNP P02794
Y	378	GLY	-	expression tag	UNP P02794
Y	379	ALA	-	expression tag	UNP P02794
Y	380	GLU	-	expression tag	UNP P02794
Y	381	ILE	-	expression tag	UNP P02794

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	382	GLU	-	expression tag	UNP P02794
Y	383	GLN	-	expression tag	UNP P02794
Y	384	ALA	-	expression tag	UNP P02794
Y	385	LYS	-	expression tag	UNP P02794
Y	386	LYS	-	expression tag	UNP P02794
Y	387	GLU	-	expression tag	UNP P02794
Y	388	ILE	-	expression tag	UNP P02794
Y	389	ALA	-	expression tag	UNP P02794
Y	390	TYR	-	expression tag	UNP P02794
Y	391	LEU	-	expression tag	UNP P02794
Y	392	ILE	-	expression tag	UNP P02794
Y	393	LYS	-	expression tag	UNP P02794
Y	394	LYS	-	expression tag	UNP P02794

- Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	b	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	c	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	d	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	e	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	f	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	g	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	h	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	i	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	j	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	k	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	l	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	m	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	o	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	p	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	q	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	r	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	s	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	t	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	v	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	w	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	x	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		
2	y	229	Total	C	N	O	S	0	0
			1828	1156	317	350	5		

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2	SER	ARG	conflict	UNP A0A059PIQ0
a	30	ARG	SER	conflict	UNP A0A059PIQ0
a	66	CRO	THR	chromophore	UNP A0A059PIQ0
a	66	CRO	TYR	chromophore	UNP A0A059PIQ0
a	66	CRO	GLY	chromophore	UNP A0A059PIQ0
a	72	SER	ALA	conflict	UNP A0A059PIQ0
a	80	ARG	GLN	conflict	UNP A0A059PIQ0
a	232	HIS	-	expression tag	UNP A0A059PIQ0
a	233	HIS	-	expression tag	UNP A0A059PIQ0
a	234	HIS	-	expression tag	UNP A0A059PIQ0
a	235	HIS	-	expression tag	UNP A0A059PIQ0
a	236	HIS	-	expression tag	UNP A0A059PIQ0
b	2	SER	ARG	conflict	UNP A0A059PIQ0
b	30	ARG	SER	conflict	UNP A0A059PIQ0
b	66	CRO	THR	chromophore	UNP A0A059PIQ0
b	66	CRO	TYR	chromophore	UNP A0A059PIQ0
b	66	CRO	GLY	chromophore	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
b	72	SER	ALA	conflict	UNP A0A059PIQ0
b	80	ARG	GLN	conflict	UNP A0A059PIQ0
b	232	HIS	-	expression tag	UNP A0A059PIQ0
b	233	HIS	-	expression tag	UNP A0A059PIQ0
b	234	HIS	-	expression tag	UNP A0A059PIQ0
b	235	HIS	-	expression tag	UNP A0A059PIQ0
b	236	HIS	-	expression tag	UNP A0A059PIQ0
c	2	SER	ARG	conflict	UNP A0A059PIQ0
c	30	ARG	SER	conflict	UNP A0A059PIQ0
c	66	CRO	THR	chromophore	UNP A0A059PIQ0
c	66	CRO	TYR	chromophore	UNP A0A059PIQ0
c	66	CRO	GLY	chromophore	UNP A0A059PIQ0
c	72	SER	ALA	conflict	UNP A0A059PIQ0
c	80	ARG	GLN	conflict	UNP A0A059PIQ0
c	232	HIS	-	expression tag	UNP A0A059PIQ0
c	233	HIS	-	expression tag	UNP A0A059PIQ0
c	234	HIS	-	expression tag	UNP A0A059PIQ0
c	235	HIS	-	expression tag	UNP A0A059PIQ0
c	236	HIS	-	expression tag	UNP A0A059PIQ0
d	2	SER	ARG	conflict	UNP A0A059PIQ0
d	30	ARG	SER	conflict	UNP A0A059PIQ0
d	66	CRO	THR	chromophore	UNP A0A059PIQ0
d	66	CRO	TYR	chromophore	UNP A0A059PIQ0
d	66	CRO	GLY	chromophore	UNP A0A059PIQ0
d	72	SER	ALA	conflict	UNP A0A059PIQ0
d	80	ARG	GLN	conflict	UNP A0A059PIQ0
d	232	HIS	-	expression tag	UNP A0A059PIQ0
d	233	HIS	-	expression tag	UNP A0A059PIQ0
d	234	HIS	-	expression tag	UNP A0A059PIQ0
d	235	HIS	-	expression tag	UNP A0A059PIQ0
d	236	HIS	-	expression tag	UNP A0A059PIQ0
e	2	SER	ARG	conflict	UNP A0A059PIQ0
e	30	ARG	SER	conflict	UNP A0A059PIQ0
e	66	CRO	THR	chromophore	UNP A0A059PIQ0
e	66	CRO	TYR	chromophore	UNP A0A059PIQ0
e	66	CRO	GLY	chromophore	UNP A0A059PIQ0
e	72	SER	ALA	conflict	UNP A0A059PIQ0
e	80	ARG	GLN	conflict	UNP A0A059PIQ0
e	232	HIS	-	expression tag	UNP A0A059PIQ0
e	233	HIS	-	expression tag	UNP A0A059PIQ0
e	234	HIS	-	expression tag	UNP A0A059PIQ0
e	235	HIS	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
e	236	HIS	-	expression tag	UNP A0A059PIQ0
f	2	SER	ARG	conflict	UNP A0A059PIQ0
f	30	ARG	SER	conflict	UNP A0A059PIQ0
f	66	CRO	THR	chromophore	UNP A0A059PIQ0
f	66	CRO	TYR	chromophore	UNP A0A059PIQ0
f	66	CRO	GLY	chromophore	UNP A0A059PIQ0
f	72	SER	ALA	conflict	UNP A0A059PIQ0
f	80	ARG	GLN	conflict	UNP A0A059PIQ0
f	232	HIS	-	expression tag	UNP A0A059PIQ0
f	233	HIS	-	expression tag	UNP A0A059PIQ0
f	234	HIS	-	expression tag	UNP A0A059PIQ0
f	235	HIS	-	expression tag	UNP A0A059PIQ0
f	236	HIS	-	expression tag	UNP A0A059PIQ0
g	2	SER	ARG	conflict	UNP A0A059PIQ0
g	30	ARG	SER	conflict	UNP A0A059PIQ0
g	66	CRO	THR	chromophore	UNP A0A059PIQ0
g	66	CRO	TYR	chromophore	UNP A0A059PIQ0
g	66	CRO	GLY	chromophore	UNP A0A059PIQ0
g	72	SER	ALA	conflict	UNP A0A059PIQ0
g	80	ARG	GLN	conflict	UNP A0A059PIQ0
g	232	HIS	-	expression tag	UNP A0A059PIQ0
g	233	HIS	-	expression tag	UNP A0A059PIQ0
g	234	HIS	-	expression tag	UNP A0A059PIQ0
g	235	HIS	-	expression tag	UNP A0A059PIQ0
g	236	HIS	-	expression tag	UNP A0A059PIQ0
h	2	SER	ARG	conflict	UNP A0A059PIQ0
h	30	ARG	SER	conflict	UNP A0A059PIQ0
h	66	CRO	THR	chromophore	UNP A0A059PIQ0
h	66	CRO	TYR	chromophore	UNP A0A059PIQ0
h	66	CRO	GLY	chromophore	UNP A0A059PIQ0
h	72	SER	ALA	conflict	UNP A0A059PIQ0
h	80	ARG	GLN	conflict	UNP A0A059PIQ0
h	232	HIS	-	expression tag	UNP A0A059PIQ0
h	233	HIS	-	expression tag	UNP A0A059PIQ0
h	234	HIS	-	expression tag	UNP A0A059PIQ0
h	235	HIS	-	expression tag	UNP A0A059PIQ0
h	236	HIS	-	expression tag	UNP A0A059PIQ0
i	2	SER	ARG	conflict	UNP A0A059PIQ0
i	30	ARG	SER	conflict	UNP A0A059PIQ0
i	66	CRO	THR	chromophore	UNP A0A059PIQ0
i	66	CRO	TYR	chromophore	UNP A0A059PIQ0
i	66	CRO	GLY	chromophore	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
i	72	SER	ALA	conflict	UNP A0A059PIQ0
i	80	ARG	GLN	conflict	UNP A0A059PIQ0
i	232	HIS	-	expression tag	UNP A0A059PIQ0
i	233	HIS	-	expression tag	UNP A0A059PIQ0
i	234	HIS	-	expression tag	UNP A0A059PIQ0
i	235	HIS	-	expression tag	UNP A0A059PIQ0
i	236	HIS	-	expression tag	UNP A0A059PIQ0
j	2	SER	ARG	conflict	UNP A0A059PIQ0
j	30	ARG	SER	conflict	UNP A0A059PIQ0
j	66	CRO	THR	chromophore	UNP A0A059PIQ0
j	66	CRO	TYR	chromophore	UNP A0A059PIQ0
j	66	CRO	GLY	chromophore	UNP A0A059PIQ0
j	72	SER	ALA	conflict	UNP A0A059PIQ0
j	80	ARG	GLN	conflict	UNP A0A059PIQ0
j	232	HIS	-	expression tag	UNP A0A059PIQ0
j	233	HIS	-	expression tag	UNP A0A059PIQ0
j	234	HIS	-	expression tag	UNP A0A059PIQ0
j	235	HIS	-	expression tag	UNP A0A059PIQ0
j	236	HIS	-	expression tag	UNP A0A059PIQ0
k	2	SER	ARG	conflict	UNP A0A059PIQ0
k	30	ARG	SER	conflict	UNP A0A059PIQ0
k	66	CRO	THR	chromophore	UNP A0A059PIQ0
k	66	CRO	TYR	chromophore	UNP A0A059PIQ0
k	66	CRO	GLY	chromophore	UNP A0A059PIQ0
k	72	SER	ALA	conflict	UNP A0A059PIQ0
k	80	ARG	GLN	conflict	UNP A0A059PIQ0
k	232	HIS	-	expression tag	UNP A0A059PIQ0
k	233	HIS	-	expression tag	UNP A0A059PIQ0
k	234	HIS	-	expression tag	UNP A0A059PIQ0
k	235	HIS	-	expression tag	UNP A0A059PIQ0
k	236	HIS	-	expression tag	UNP A0A059PIQ0
l	2	SER	ARG	conflict	UNP A0A059PIQ0
l	30	ARG	SER	conflict	UNP A0A059PIQ0
l	66	CRO	THR	chromophore	UNP A0A059PIQ0
l	66	CRO	TYR	chromophore	UNP A0A059PIQ0
l	66	CRO	GLY	chromophore	UNP A0A059PIQ0
l	72	SER	ALA	conflict	UNP A0A059PIQ0
l	80	ARG	GLN	conflict	UNP A0A059PIQ0
l	232	HIS	-	expression tag	UNP A0A059PIQ0
l	233	HIS	-	expression tag	UNP A0A059PIQ0
l	234	HIS	-	expression tag	UNP A0A059PIQ0
l	235	HIS	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
l	236	HIS	-	expression tag	UNP A0A059PIQ0
m	2	SER	ARG	conflict	UNP A0A059PIQ0
m	30	ARG	SER	conflict	UNP A0A059PIQ0
m	66	CRO	THR	chromophore	UNP A0A059PIQ0
m	66	CRO	TYR	chromophore	UNP A0A059PIQ0
m	66	CRO	GLY	chromophore	UNP A0A059PIQ0
m	72	SER	ALA	conflict	UNP A0A059PIQ0
m	80	ARG	GLN	conflict	UNP A0A059PIQ0
m	232	HIS	-	expression tag	UNP A0A059PIQ0
m	233	HIS	-	expression tag	UNP A0A059PIQ0
m	234	HIS	-	expression tag	UNP A0A059PIQ0
m	235	HIS	-	expression tag	UNP A0A059PIQ0
m	236	HIS	-	expression tag	UNP A0A059PIQ0
n	2	SER	ARG	conflict	UNP A0A059PIQ0
n	30	ARG	SER	conflict	UNP A0A059PIQ0
n	66	CRO	THR	chromophore	UNP A0A059PIQ0
n	66	CRO	TYR	chromophore	UNP A0A059PIQ0
n	66	CRO	GLY	chromophore	UNP A0A059PIQ0
n	72	SER	ALA	conflict	UNP A0A059PIQ0
n	80	ARG	GLN	conflict	UNP A0A059PIQ0
n	232	HIS	-	expression tag	UNP A0A059PIQ0
n	233	HIS	-	expression tag	UNP A0A059PIQ0
n	234	HIS	-	expression tag	UNP A0A059PIQ0
n	235	HIS	-	expression tag	UNP A0A059PIQ0
n	236	HIS	-	expression tag	UNP A0A059PIQ0
o	2	SER	ARG	conflict	UNP A0A059PIQ0
o	30	ARG	SER	conflict	UNP A0A059PIQ0
o	66	CRO	THR	chromophore	UNP A0A059PIQ0
o	66	CRO	TYR	chromophore	UNP A0A059PIQ0
o	66	CRO	GLY	chromophore	UNP A0A059PIQ0
o	72	SER	ALA	conflict	UNP A0A059PIQ0
o	80	ARG	GLN	conflict	UNP A0A059PIQ0
o	232	HIS	-	expression tag	UNP A0A059PIQ0
o	233	HIS	-	expression tag	UNP A0A059PIQ0
o	234	HIS	-	expression tag	UNP A0A059PIQ0
o	235	HIS	-	expression tag	UNP A0A059PIQ0
o	236	HIS	-	expression tag	UNP A0A059PIQ0
p	2	SER	ARG	conflict	UNP A0A059PIQ0
p	30	ARG	SER	conflict	UNP A0A059PIQ0
p	66	CRO	THR	chromophore	UNP A0A059PIQ0
p	66	CRO	TYR	chromophore	UNP A0A059PIQ0
p	66	CRO	GLY	chromophore	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
p	72	SER	ALA	conflict	UNP A0A059PIQ0
p	80	ARG	GLN	conflict	UNP A0A059PIQ0
p	232	HIS	-	expression tag	UNP A0A059PIQ0
p	233	HIS	-	expression tag	UNP A0A059PIQ0
p	234	HIS	-	expression tag	UNP A0A059PIQ0
p	235	HIS	-	expression tag	UNP A0A059PIQ0
p	236	HIS	-	expression tag	UNP A0A059PIQ0
q	2	SER	ARG	conflict	UNP A0A059PIQ0
q	30	ARG	SER	conflict	UNP A0A059PIQ0
q	66	CRO	THR	chromophore	UNP A0A059PIQ0
q	66	CRO	TYR	chromophore	UNP A0A059PIQ0
q	66	CRO	GLY	chromophore	UNP A0A059PIQ0
q	72	SER	ALA	conflict	UNP A0A059PIQ0
q	80	ARG	GLN	conflict	UNP A0A059PIQ0
q	232	HIS	-	expression tag	UNP A0A059PIQ0
q	233	HIS	-	expression tag	UNP A0A059PIQ0
q	234	HIS	-	expression tag	UNP A0A059PIQ0
q	235	HIS	-	expression tag	UNP A0A059PIQ0
q	236	HIS	-	expression tag	UNP A0A059PIQ0
r	2	SER	ARG	conflict	UNP A0A059PIQ0
r	30	ARG	SER	conflict	UNP A0A059PIQ0
r	66	CRO	THR	chromophore	UNP A0A059PIQ0
r	66	CRO	TYR	chromophore	UNP A0A059PIQ0
r	66	CRO	GLY	chromophore	UNP A0A059PIQ0
r	72	SER	ALA	conflict	UNP A0A059PIQ0
r	80	ARG	GLN	conflict	UNP A0A059PIQ0
r	232	HIS	-	expression tag	UNP A0A059PIQ0
r	233	HIS	-	expression tag	UNP A0A059PIQ0
r	234	HIS	-	expression tag	UNP A0A059PIQ0
r	235	HIS	-	expression tag	UNP A0A059PIQ0
r	236	HIS	-	expression tag	UNP A0A059PIQ0
s	2	SER	ARG	conflict	UNP A0A059PIQ0
s	30	ARG	SER	conflict	UNP A0A059PIQ0
s	66	CRO	THR	chromophore	UNP A0A059PIQ0
s	66	CRO	TYR	chromophore	UNP A0A059PIQ0
s	66	CRO	GLY	chromophore	UNP A0A059PIQ0
s	72	SER	ALA	conflict	UNP A0A059PIQ0
s	80	ARG	GLN	conflict	UNP A0A059PIQ0
s	232	HIS	-	expression tag	UNP A0A059PIQ0
s	233	HIS	-	expression tag	UNP A0A059PIQ0
s	234	HIS	-	expression tag	UNP A0A059PIQ0
s	235	HIS	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
s	236	HIS	-	expression tag	UNP A0A059PIQ0
t	2	SER	ARG	conflict	UNP A0A059PIQ0
t	30	ARG	SER	conflict	UNP A0A059PIQ0
t	66	CRO	THR	chromophore	UNP A0A059PIQ0
t	66	CRO	TYR	chromophore	UNP A0A059PIQ0
t	66	CRO	GLY	chromophore	UNP A0A059PIQ0
t	72	SER	ALA	conflict	UNP A0A059PIQ0
t	80	ARG	GLN	conflict	UNP A0A059PIQ0
t	232	HIS	-	expression tag	UNP A0A059PIQ0
t	233	HIS	-	expression tag	UNP A0A059PIQ0
t	234	HIS	-	expression tag	UNP A0A059PIQ0
t	235	HIS	-	expression tag	UNP A0A059PIQ0
t	236	HIS	-	expression tag	UNP A0A059PIQ0
v	2	SER	ARG	conflict	UNP A0A059PIQ0
v	30	ARG	SER	conflict	UNP A0A059PIQ0
v	66	CRO	THR	chromophore	UNP A0A059PIQ0
v	66	CRO	TYR	chromophore	UNP A0A059PIQ0
v	66	CRO	GLY	chromophore	UNP A0A059PIQ0
v	72	SER	ALA	conflict	UNP A0A059PIQ0
v	80	ARG	GLN	conflict	UNP A0A059PIQ0
v	232	HIS	-	expression tag	UNP A0A059PIQ0
v	233	HIS	-	expression tag	UNP A0A059PIQ0
v	234	HIS	-	expression tag	UNP A0A059PIQ0
v	235	HIS	-	expression tag	UNP A0A059PIQ0
v	236	HIS	-	expression tag	UNP A0A059PIQ0
w	2	SER	ARG	conflict	UNP A0A059PIQ0
w	30	ARG	SER	conflict	UNP A0A059PIQ0
w	66	CRO	THR	chromophore	UNP A0A059PIQ0
w	66	CRO	TYR	chromophore	UNP A0A059PIQ0
w	66	CRO	GLY	chromophore	UNP A0A059PIQ0
w	72	SER	ALA	conflict	UNP A0A059PIQ0
w	80	ARG	GLN	conflict	UNP A0A059PIQ0
w	232	HIS	-	expression tag	UNP A0A059PIQ0
w	233	HIS	-	expression tag	UNP A0A059PIQ0
w	234	HIS	-	expression tag	UNP A0A059PIQ0
w	235	HIS	-	expression tag	UNP A0A059PIQ0
w	236	HIS	-	expression tag	UNP A0A059PIQ0
x	2	SER	ARG	conflict	UNP A0A059PIQ0
x	30	ARG	SER	conflict	UNP A0A059PIQ0
x	66	CRO	THR	chromophore	UNP A0A059PIQ0
x	66	CRO	TYR	chromophore	UNP A0A059PIQ0
x	66	CRO	GLY	chromophore	UNP A0A059PIQ0

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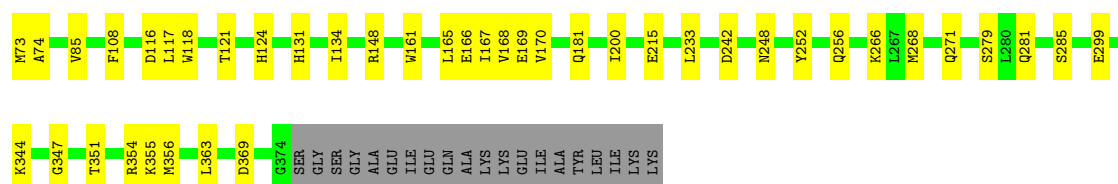


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Chain	Residue	Modelled	Actual	Comment	Reference
x	72	SER	ALA	conflict	UNP A0A059PIQ0
x	80	ARG	GLN	conflict	UNP A0A059PIQ0
x	232	HIS	-	expression tag	UNP A0A059PIQ0
x	233	HIS	-	expression tag	UNP A0A059PIQ0
x	234	HIS	-	expression tag	UNP A0A059PIQ0
x	235	HIS	-	expression tag	UNP A0A059PIQ0
x	236	HIS	-	expression tag	UNP A0A059PIQ0
y	2	SER	ARG	conflict	UNP A0A059PIQ0
y	30	ARG	SER	conflict	UNP A0A059PIQ0
y	66	CRO	THR	chromophore	UNP A0A059PIQ0
y	66	CRO	TYR	chromophore	UNP A0A059PIQ0
y	66	CRO	GLY	chromophore	UNP A0A059PIQ0
y	72	SER	ALA	conflict	UNP A0A059PIQ0
y	80	ARG	GLN	conflict	UNP A0A059PIQ0
y	232	HIS	-	expression tag	UNP A0A059PIQ0
y	233	HIS	-	expression tag	UNP A0A059PIQ0
y	234	HIS	-	expression tag	UNP A0A059PIQ0
y	235	HIS	-	expression tag	UNP A0A059PIQ0
y	236	HIS	-	expression tag	UNP A0A059PIQ0

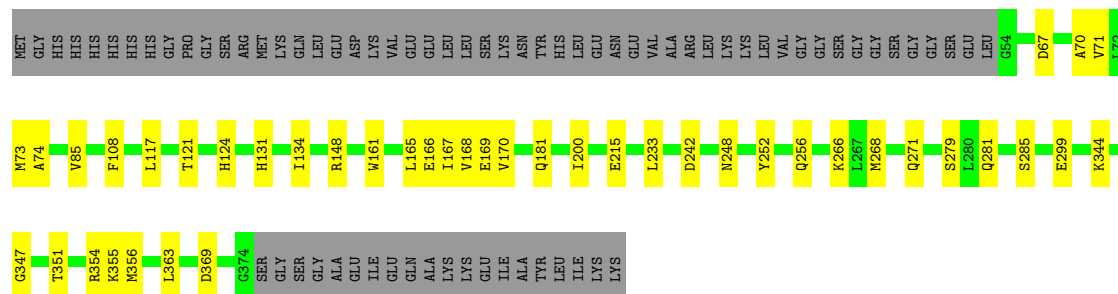






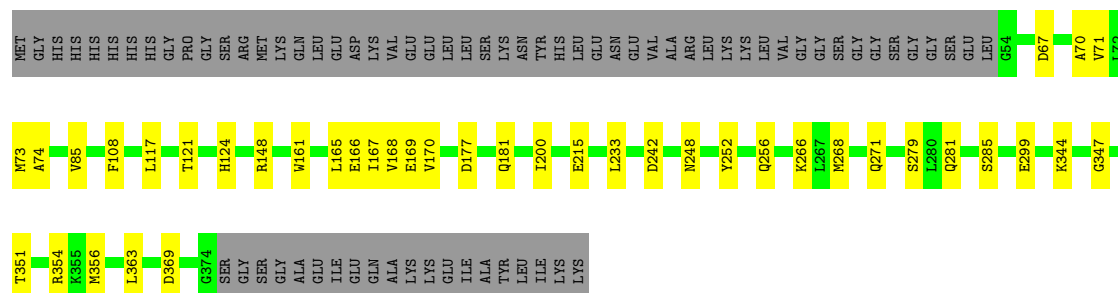
- Molecule 1: Designed ankyrin repeat proteins,Ferritin heavy chain, N-terminally processed

Chain H: 71% 11% 19%



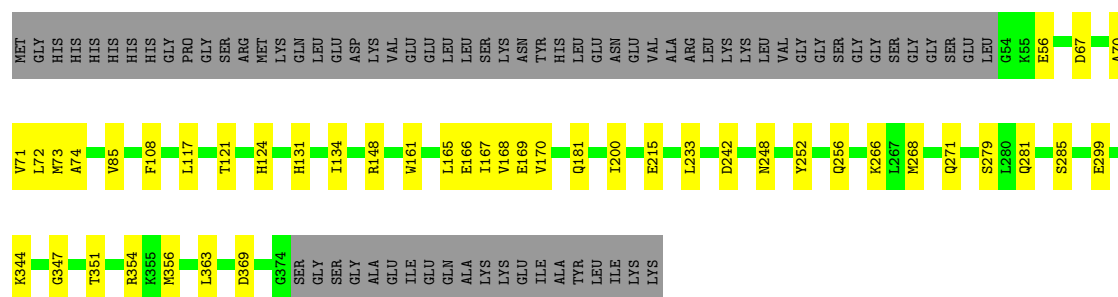
- Molecule 1: Designed ankyrin repeat proteins,Ferritin heavy chain, N-terminally processed

Chain I: 71% 10% 19%



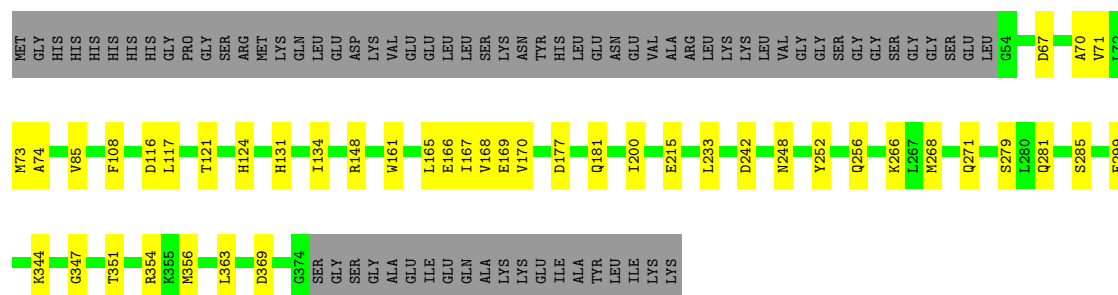
- Molecule 1: Designed ankyrin repeat proteins,Ferritin heavy chain, N-terminally processed

Chain J: 70% 11% 19%



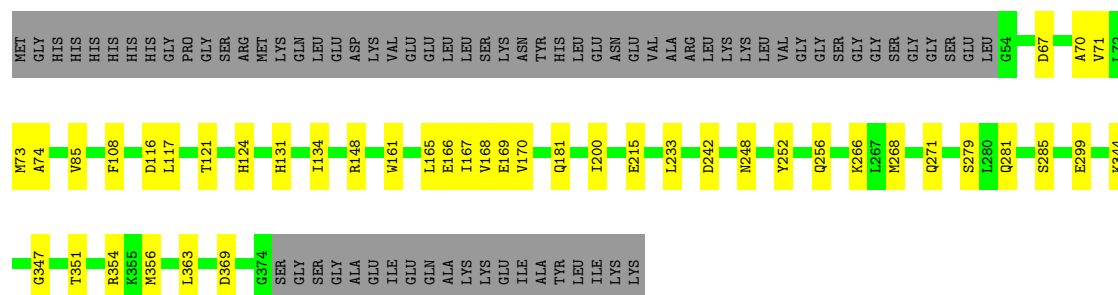
- Molecule 1: Designed ankyrin repeat proteins,Ferritin heavy chain, N-terminally processed

Chain K: 70% 11% 19%



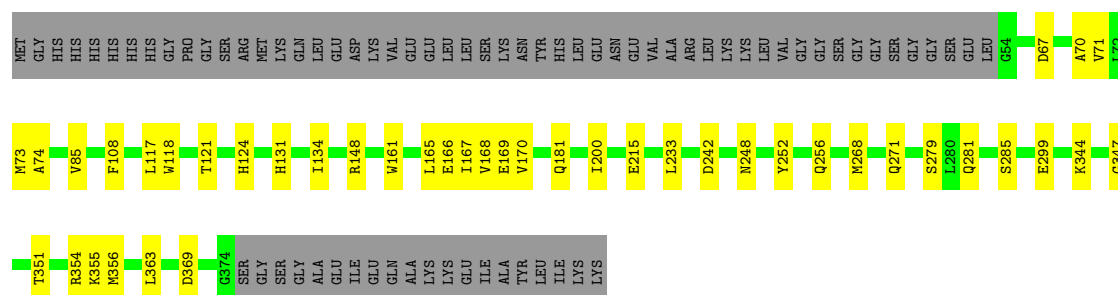
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain L: 71% 11% 19%



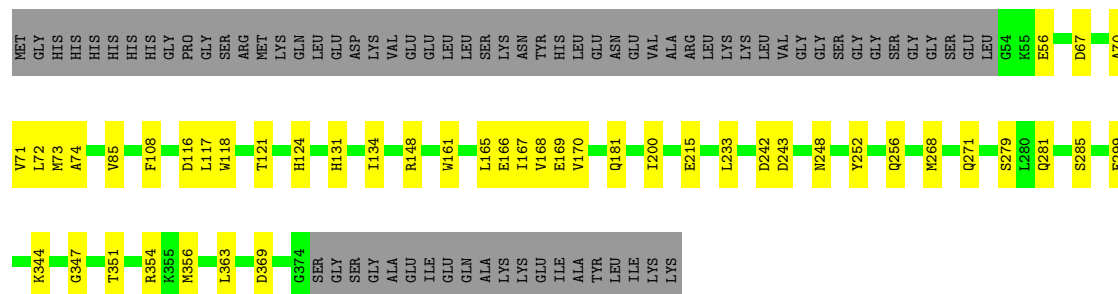
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain M: 71% 11% 19%



- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain N: 70% 12% 19%



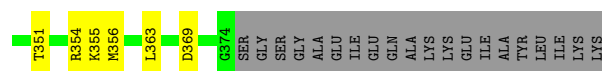
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

[illegible]

- |      |      |     |
|------|------|-----|
| G347 | M73  | MET |
| T351 | A74  | GLY |
| R354 | V85  | HIS |
| K385 | F108 | HIS |
| M356 | L117 | HIS |
| L363 | T121 | GLY |
| D369 | H124 | PRO |
| G374 | H131 | SER |
| SER  | I134 | ARG |
| GLY  | R148 | LYS |
| ALA  | W161 | GLN |
| GLU  | L165 | LEU |
| GLN  | E166 | ASP |
| ALA  | I167 | LYS |
| LYS  | V168 | GLU |
| LVS  | E169 | LEU |
| GLU  | V170 | SER |
| ILE  | D177 | ASN |
| ALA  | Q181 | TVR |
| TRR  | I200 | HIS |
| LEU  | E215 | LEU |
| ILE  | L233 | GLU |
| LVS  | D242 | ASN |
| LVS  | D243 | GLU |
|      | N248 | VAL |
|      | Y252 | ALA |
|      | Q256 | ARG |
|      | M268 | LEU |
|      | Q271 | LYS |
|      | S279 | LYS |
|      | L280 | LEU |
|      | Q281 | VAL |
|      | S285 | GLY |
|      | E299 | GLY |
|      | V314 | GLY |
|      |      | SER |
|      |      | GLY |
|      |      | GLU |
|      |      | LEU |
|      |      | G54 |
|      |      | D67 |
|      |      | A70 |
|      |      | V71 |
|      |      | L73 |

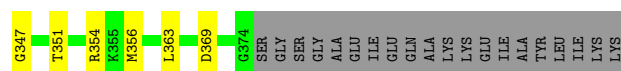
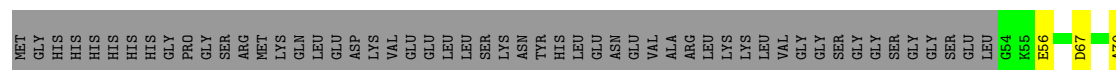
- [illegible]

- |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | GLY | HIS | HIS  | HIS  | HIS  | HIS  | HIS  | GLY  | PRO  | GLY  | SER  | ARG  | MET  | LYS  | GLN  | LEU  | GLU  | ASP  | VAL  | GLU  | GLY  | LEU  | SER  | LYS  | ASN  | TYR  | HIS  | LEU  | GLU  | ASN  | GLU  | VAL  | ALA  | ARG  | LEU | LYS | LYS | LEU | VAL | GLY | GLY | GLY | SER | GLY | SER | GLY | GLU | LEU | G64 | D67 | A70 | V71 | L72 |
| M73 | A74 | V85 | F108 | L117 | T121 | H124 | H131 | I134 | R148 | W161 | L165 | E166 | I167 | V168 | E169 | V170 | Q181 | I200 | E215 | L233 | D242 | D243 | N248 | Y252 | Q256 | M268 | Q271 | S279 | L280 | Q281 | S285 | E299 | K344 | P347 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |



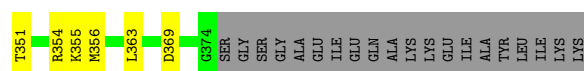
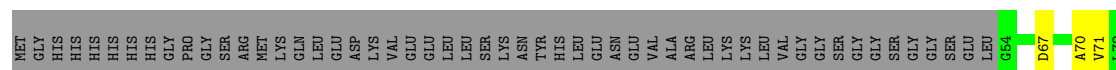
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain S: 71% 11% 19%



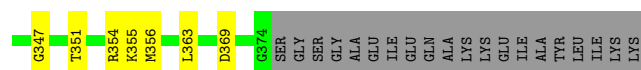
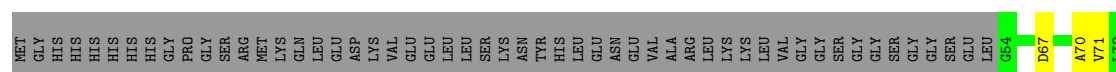
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain T: 71% 11% 19%



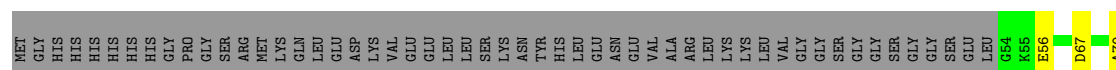
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain V: 70% 11% 19%



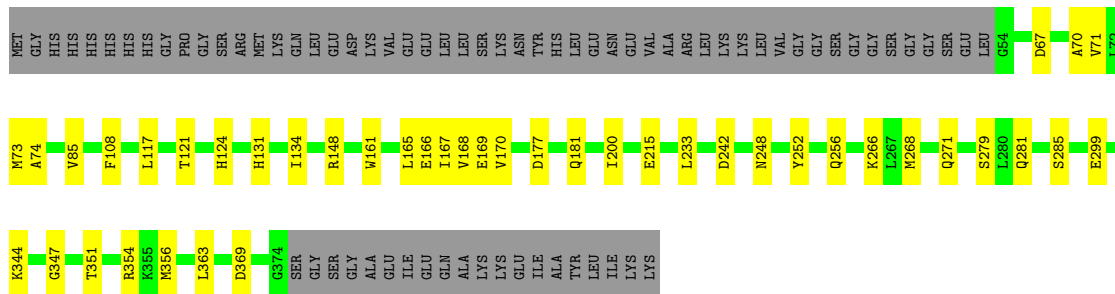
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain W: 70% 11% 19%



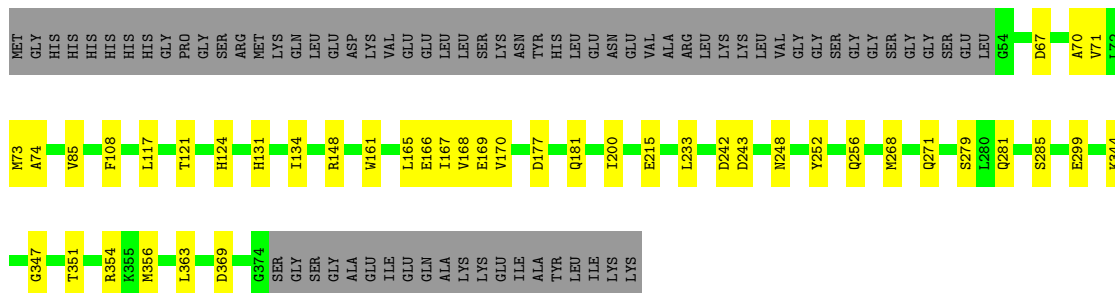
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain X:  71% 11% 19%



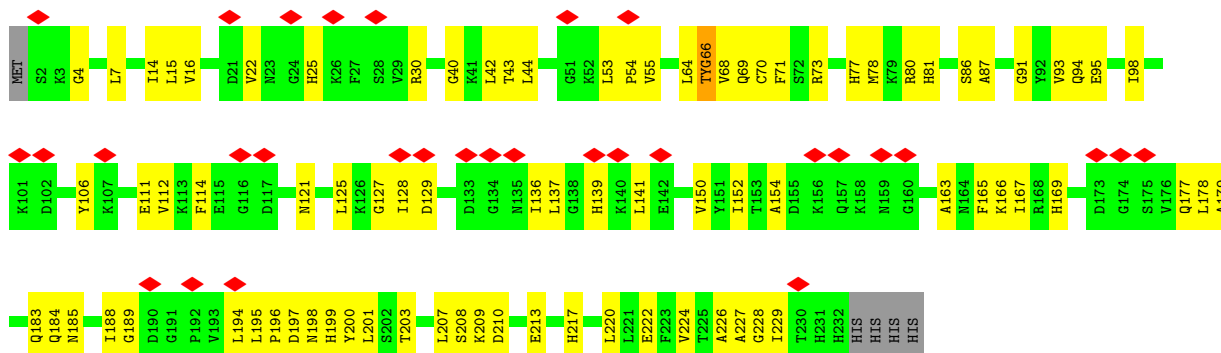
- Molecule 1: Designed ankyrin repeat proteins, Ferritin heavy chain, N-terminally processed

Chain Y: 



- Molecule 2: Green fluorescent protein

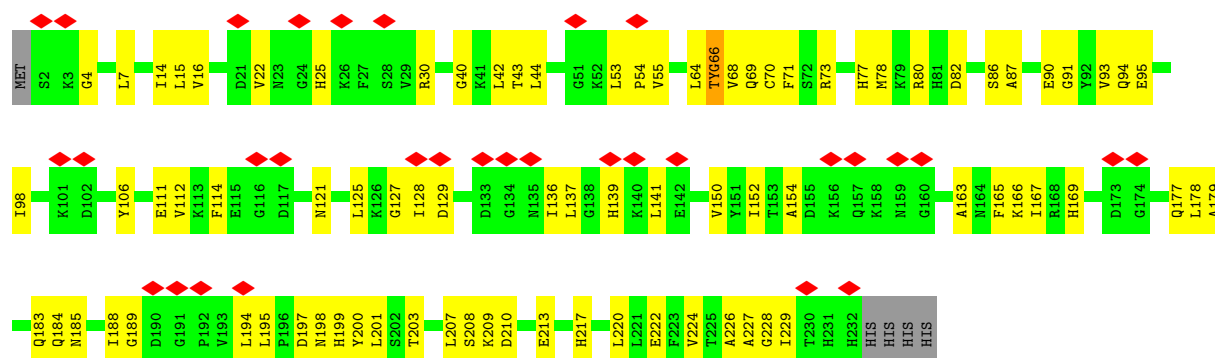
Chain a:  13% 62% 25%



- Molecule 2: Green fluorescent protein

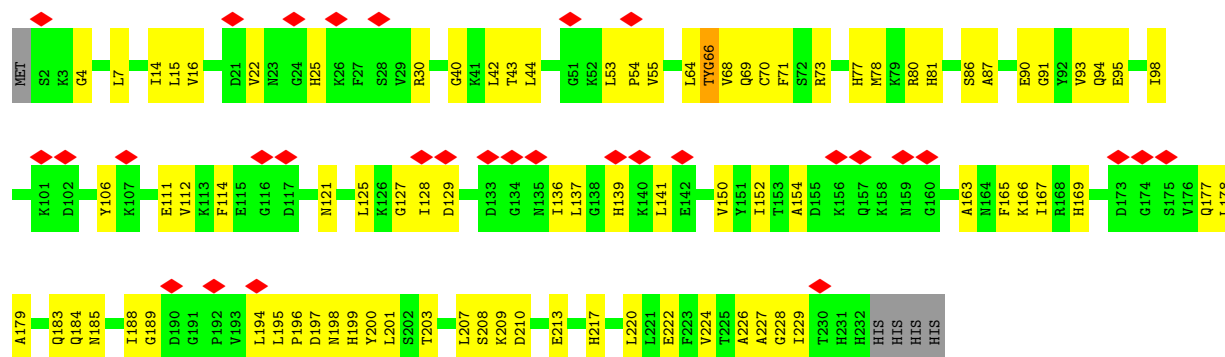


Chain b: 



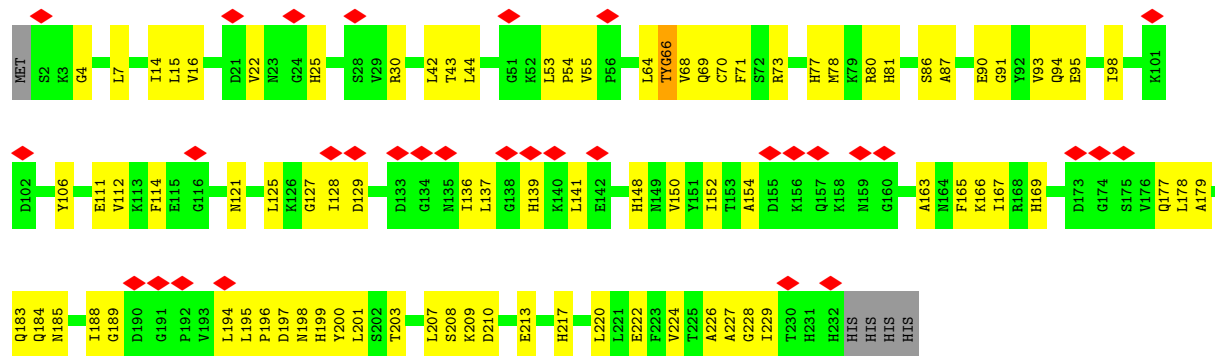
• Molecule 2: Green fluorescent protein

Chain c: 



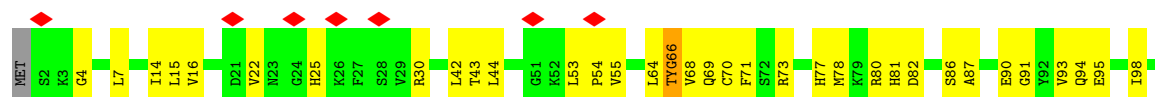
• Molecule 2: Green fluorescent protein

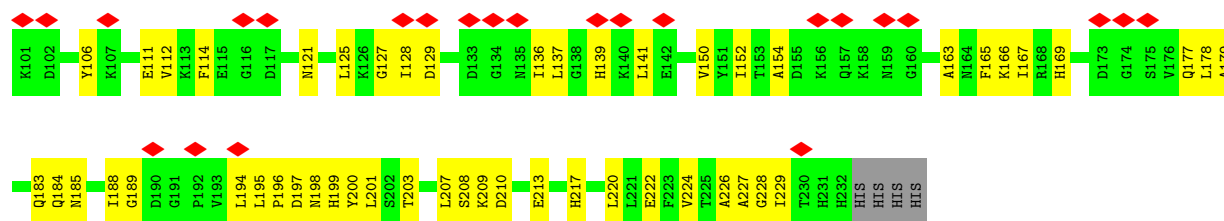
Chain d: 



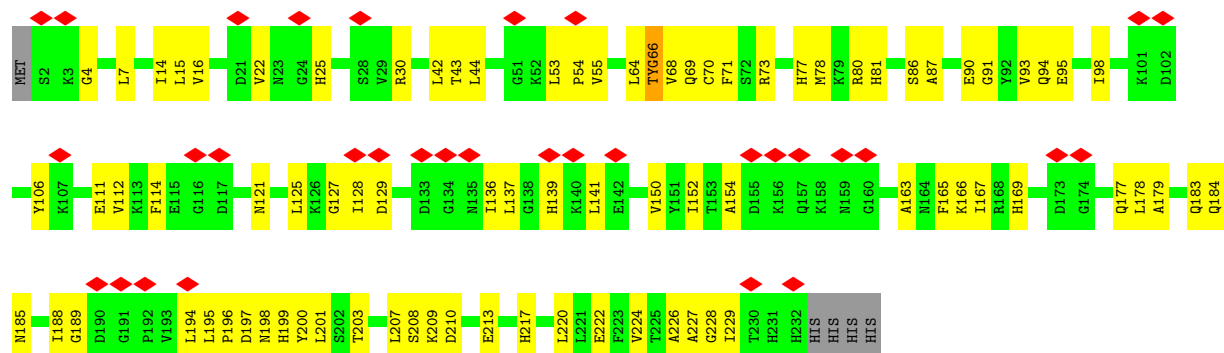
• Molecule 2: Green fluorescent protein

Chain e: 

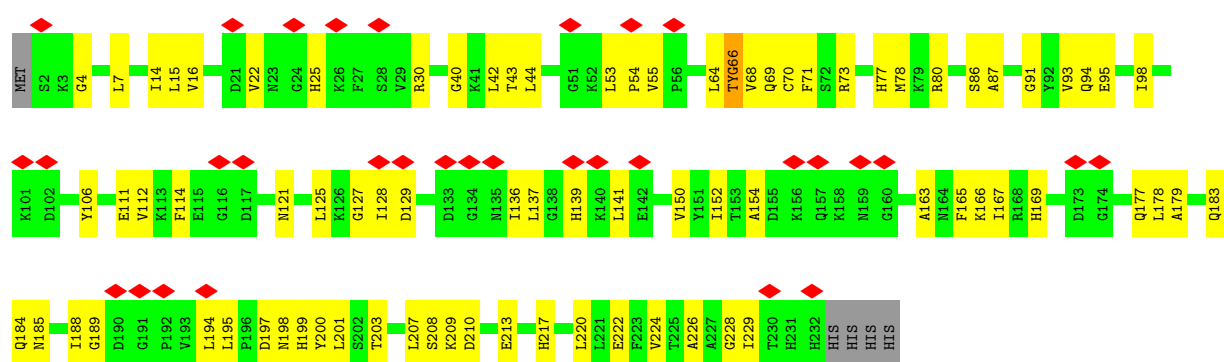




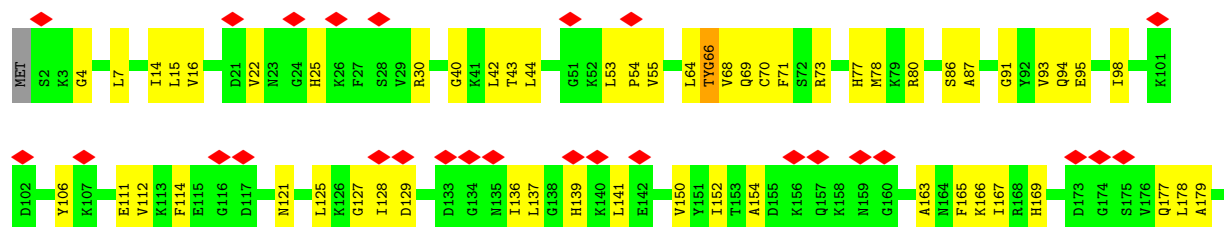
• Molecule 2: Green fluorescent protein

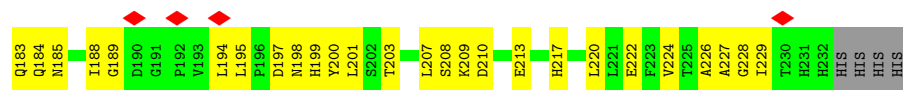


• Molecule 2: Green fluorescent protein

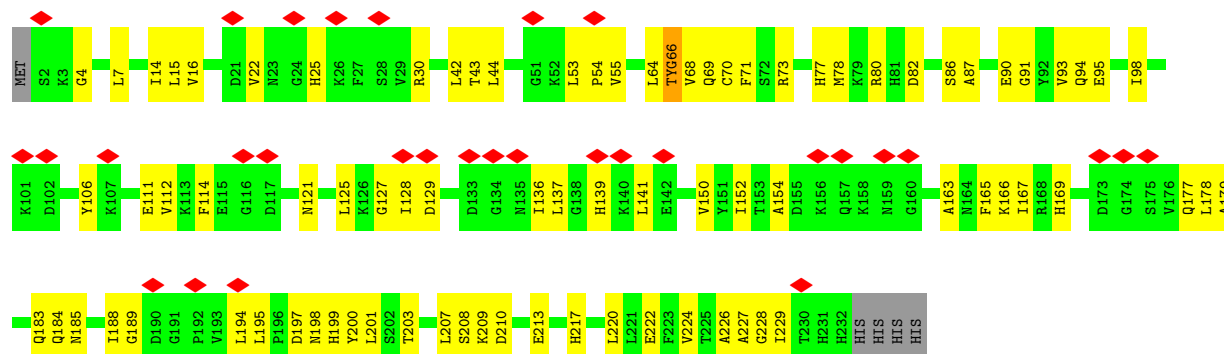


• Molecule 2: Green fluorescent protein

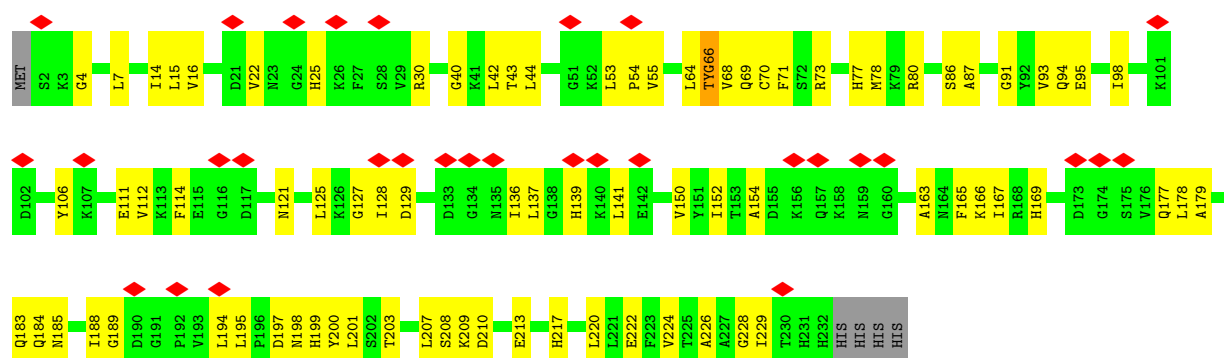




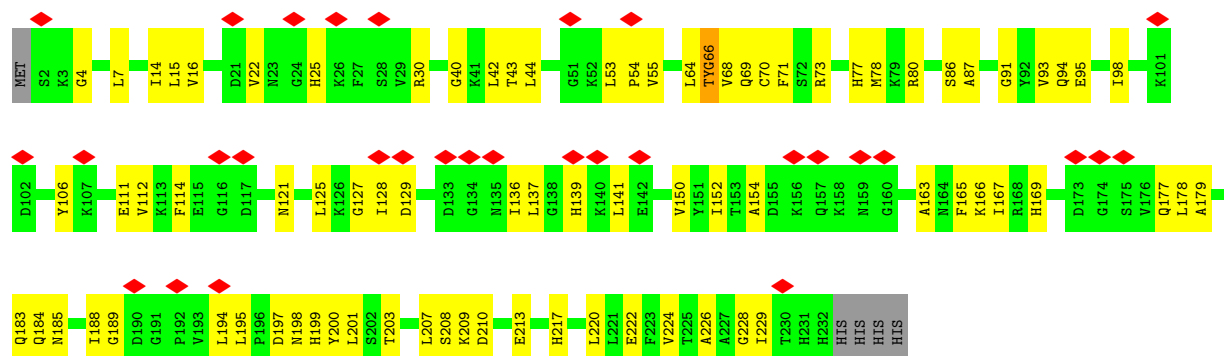
• Molecule 2: Green fluorescent protein



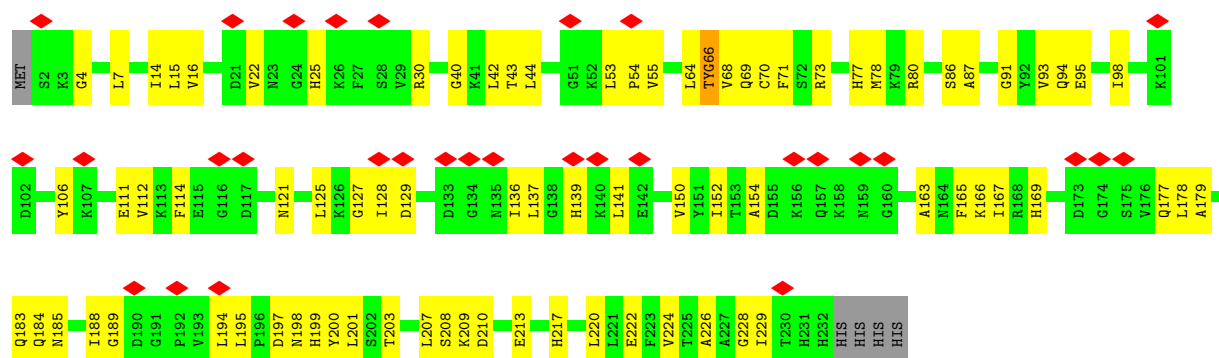
• Molecule 2: Green fluorescent protein



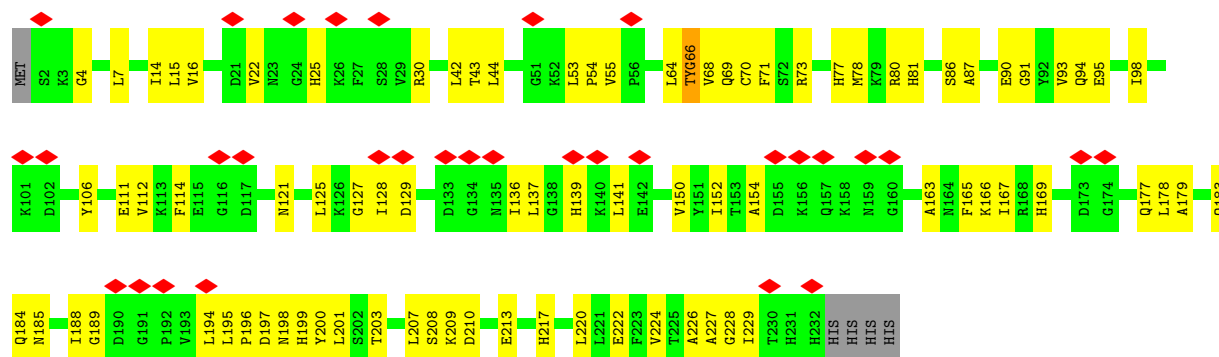
• Molecule 2: Green fluorescent protein



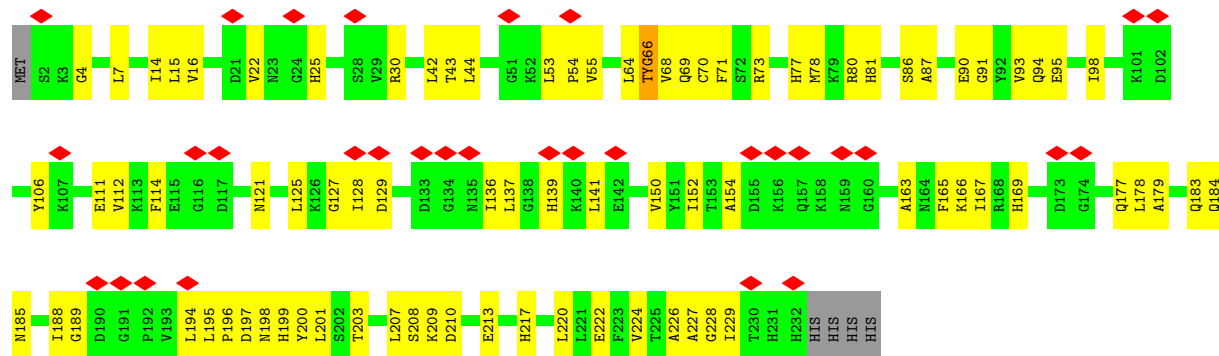
• Molecule 2: Green fluorescent protein



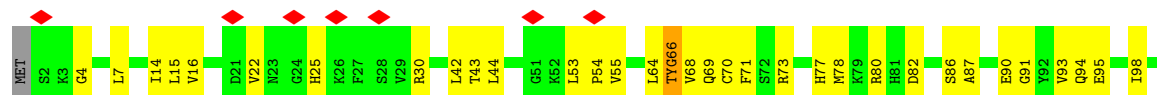
• Molecule 2: Green fluorescent protein

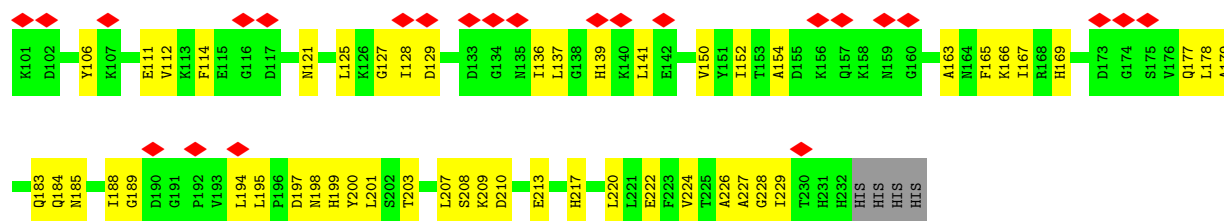


• Molecule 2: Green fluorescent protein

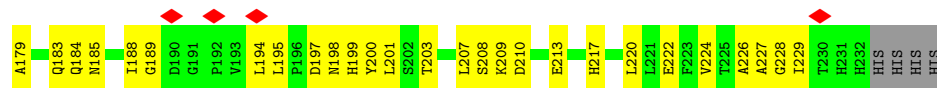
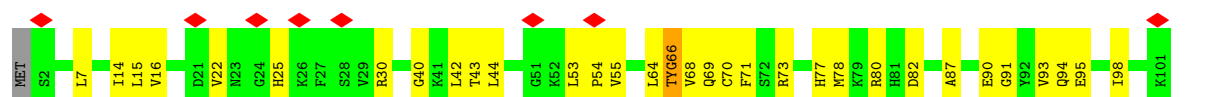


• Molecule 2: Green fluorescent protein

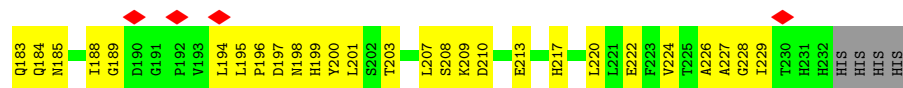
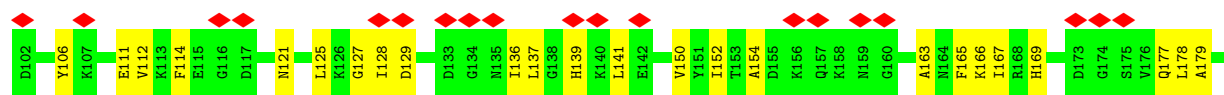
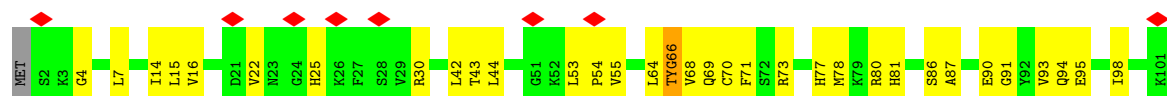




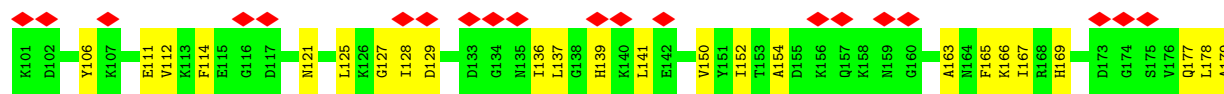
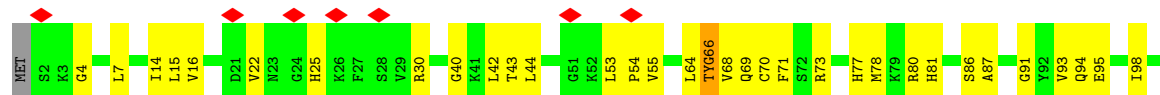
• Molecule 2: Green fluorescent protein

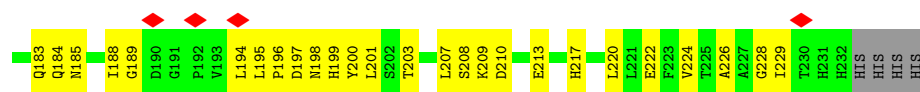


• Molecule 2: Green fluorescent protein

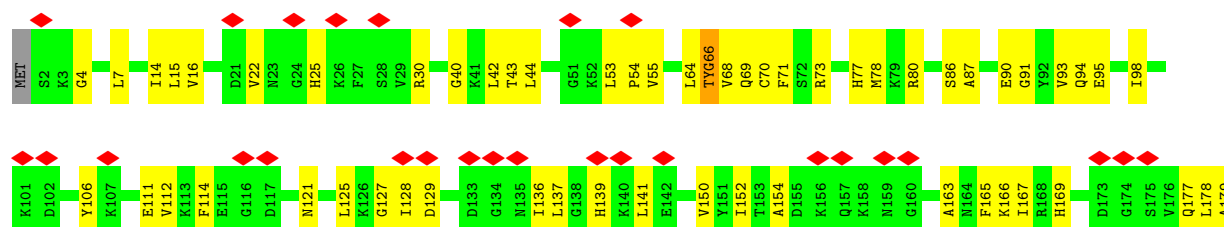


• Molecule 2: Green fluorescent protein

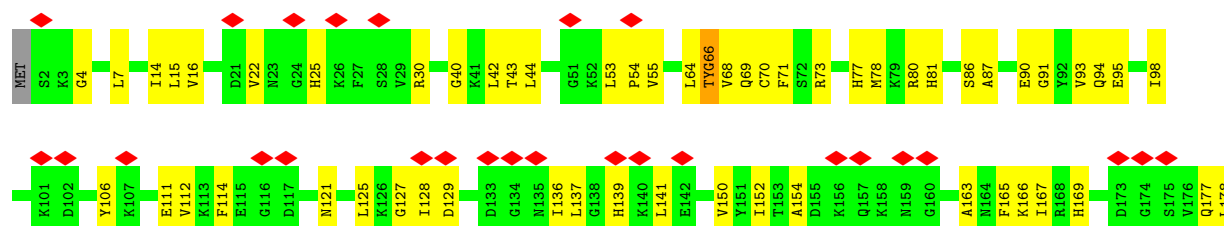




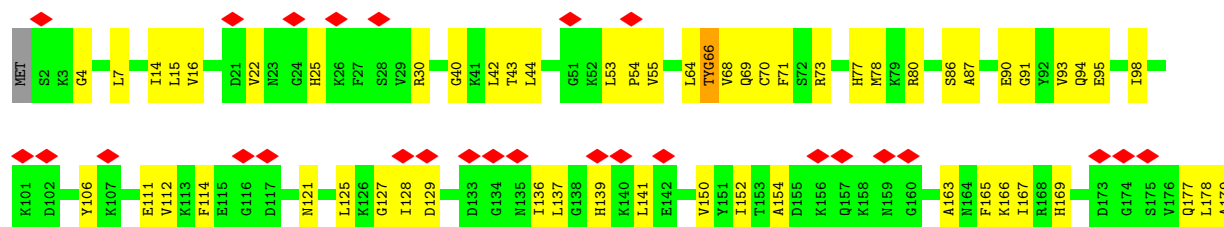
• Molecule 2: Green fluorescent protein



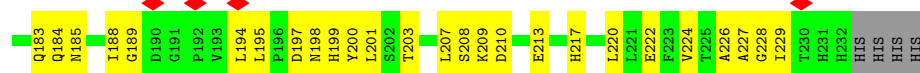
• Molecule 2: Green fluorescent protein

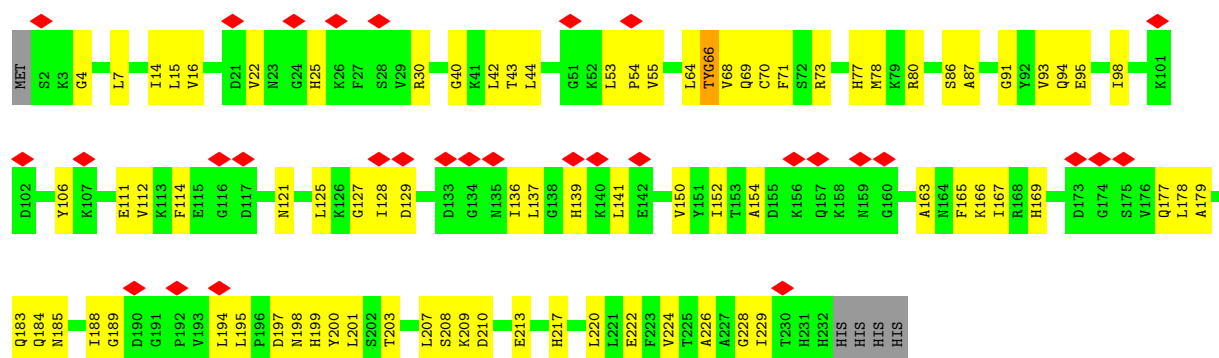


• Molecule 2: Green fluorescent protein

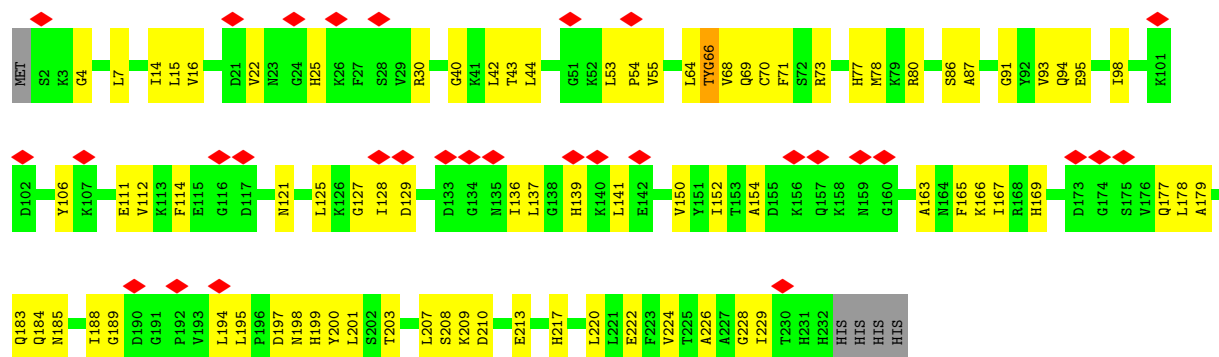


• Molecule 2: Green fluorescent protein

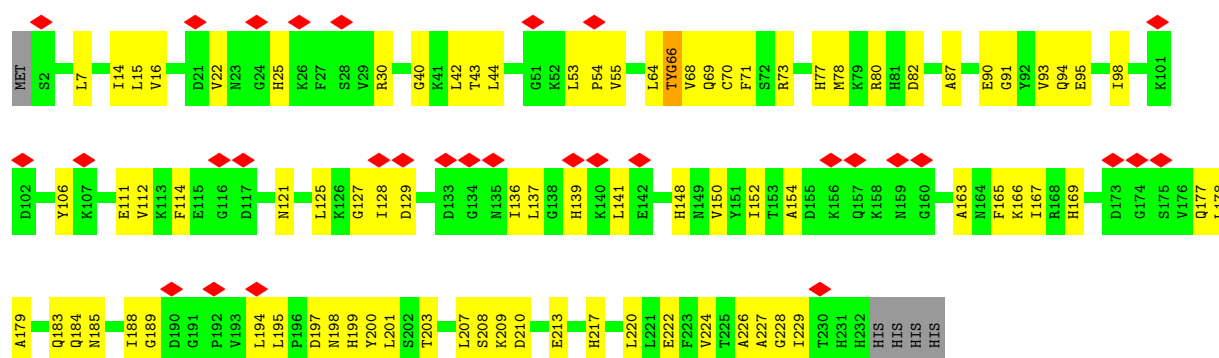




• Molecule 2: Green fluorescent protein



• Molecule 2: Green fluorescent protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	17397	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	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.541	Depositor
Minimum map value	-1.624	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.143	Depositor
Recommended contour level	0.3	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

Bond lengths and bond angles in the following residue types are not validated in this section: CRO

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	0/2532	0.51	0/3434
1	B	0.33	0/2532	0.51	0/3434
1	C	0.33	0/2532	0.51	0/3434
1	D	0.33	0/2532	0.51	0/3434
1	E	0.33	0/2532	0.51	0/3434
1	F	0.33	0/2532	0.51	0/3434
1	G	0.33	0/2532	0.51	0/3434
1	H	0.33	0/2532	0.51	0/3434
1	I	0.33	0/2532	0.51	0/3434
1	J	0.33	0/2532	0.51	0/3434
1	K	0.33	0/2532	0.51	0/3434
1	L	0.33	0/2532	0.51	0/3434
1	M	0.33	0/2532	0.51	0/3434
1	N	0.33	0/2532	0.51	0/3434
1	O	0.33	0/2532	0.51	0/3434
1	P	0.33	0/2532	0.51	0/3434
1	Q	0.33	0/2532	0.51	0/3434
1	R	0.34	0/2532	0.51	0/3434
1	S	0.33	0/2532	0.51	0/3434
1	T	0.33	0/2532	0.51	0/3434
1	V	0.33	0/2532	0.51	0/3434
1	W	0.33	0/2532	0.51	0/3434
1	X	0.33	0/2532	0.51	0/3434
1	Y	0.33	0/2532	0.51	0/3434
2	a	0.24	0/1846	0.54	0/2494
2	b	0.24	0/1846	0.54	0/2494
2	c	0.24	0/1846	0.54	0/2494
2	d	0.24	0/1846	0.54	0/2494
2	e	0.24	0/1846	0.54	0/2494
2	f	0.24	0/1846	0.54	0/2494
2	g	0.24	0/1846	0.54	0/2494
2	h	0.24	0/1846	0.54	0/2494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	i	0.24	0/1846	0.54	0/2494
2	j	0.24	0/1846	0.54	0/2494
2	k	0.24	0/1846	0.54	0/2494
2	l	0.24	0/1846	0.54	0/2494
2	m	0.24	0/1846	0.54	0/2494
2	n	0.24	0/1846	0.54	0/2494
2	o	0.24	0/1846	0.54	0/2494
2	p	0.24	0/1846	0.54	0/2494
2	q	0.24	0/1846	0.54	0/2494
2	r	0.24	0/1846	0.54	0/2494
2	s	0.24	0/1846	0.54	0/2494
2	t	0.24	0/1846	0.54	0/2494
2	v	0.24	0/1846	0.54	0/2494
2	w	0.24	0/1846	0.54	0/2494
2	x	0.24	0/1846	0.54	0/2494
2	y	0.24	0/1846	0.54	0/2494
All	All	0.30	0/105072	0.52	0/142272

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	2416	43	0
1	B	2485	0	2416	44	0
1	C	2485	0	2416	45	0
1	D	2485	0	2416	47	0
1	E	2485	0	2416	44	0
1	F	2485	0	2416	46	0
1	G	2485	0	2416	47	0
1	H	2485	0	2416	44	0
1	I	2485	0	2416	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2485	0	2416	44	0
1	K	2485	0	2416	45	0
1	L	2485	0	2416	45	0
1	M	2485	0	2416	44	0
1	N	2485	0	2416	46	0
1	O	2485	0	2416	43	0
1	P	2485	0	2416	44	0
1	Q	2485	0	2416	45	0
1	R	2485	0	2416	45	0
1	S	2485	0	2416	43	0
1	T	2485	0	2416	44	0
1	V	2485	0	2416	45	0
1	W	2485	0	2416	45	0
1	X	2485	0	2416	44	0
1	Y	2485	0	2416	44	0
2	a	1828	0	1776	63	0
2	b	1828	0	1776	63	0
2	c	1828	0	1776	64	0
2	d	1828	0	1776	65	0
2	e	1828	0	1776	64	0
2	f	1828	0	1776	63	0
2	g	1828	0	1776	62	0
2	h	1828	0	1776	62	0
2	i	1828	0	1776	62	0
2	j	1828	0	1776	61	0
2	k	1828	0	1776	61	0
2	l	1828	0	1776	61	0
2	m	1828	0	1776	64	0
2	n	1828	0	1776	63	0
2	o	1828	0	1776	62	0
2	p	1828	0	1776	64	0
2	q	1828	0	1776	62	0
2	r	1828	0	1776	62	0
2	s	1828	0	1776	62	0
2	t	1828	0	1776	64	0
2	v	1828	0	1776	63	0
2	w	1828	0	1776	61	0
2	x	1828	0	1776	61	0
2	y	1828	0	1776	64	0
All	All	103512	0	100608	2229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (2229) 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:J:71:VAL:HG12	1:N:67:ASP:O	1.75	0.87
1:A:67:ASP:O	1:M:71:VAL:HG12	1.75	0.87
1:D:67:ASP:O	1:W:71:VAL:HG12	1.75	0.87
1:S:67:ASP:O	1:Y:71:VAL:HG12	1.75	0.87
1:B:67:ASP:O	1:P:71:VAL:HG12	1.75	0.87
1:G:67:ASP:O	1:H:71:VAL:HG12	1.75	0.87
1:L:67:ASP:O	1:V:71:VAL:HG12	1.75	0.87
1:B:71:VAL:HG12	1:P:67:ASP:O	1.75	0.86
1:S:71:VAL:HG12	1:Y:67:ASP:O	1.75	0.86
1:G:71:VAL:HG12	1:H:67:ASP:O	1.75	0.86
1:L:71:VAL:HG12	1:V:67:ASP:O	1.75	0.86
2:x:98:ILE:HG12	2:x:106:TYR:HB2	1.57	0.86
2:y:98:ILE:HG12	2:y:106:TYR:HB2	1.57	0.86
2:k:98:ILE:HG12	2:k:106:TYR:HB2	1.57	0.86
2:p:98:ILE:HG12	2:p:106:TYR:HB2	1.57	0.86
1:F:67:ASP:O	1:O:71:VAL:HG12	1.75	0.86
2:a:98:ILE:HG12	2:a:106:TYR:HB2	1.57	0.86
2:b:98:ILE:HG12	2:b:106:TYR:HB2	1.57	0.86
2:f:98:ILE:HG12	2:f:106:TYR:HB2	1.57	0.86
1:I:71:VAL:HG12	1:Q:67:ASP:O	1.75	0.86
2:s:98:ILE:HG12	2:s:106:TYR:HB2	1.57	0.86
1:C:67:ASP:O	1:X:71:VAL:HG12	1.75	0.86
2:d:98:ILE:HG12	2:d:106:TYR:HB2	1.57	0.86
1:F:71:VAL:HG12	1:O:67:ASP:O	1.75	0.86
1:K:67:ASP:O	1:T:71:VAL:HG12	1.75	0.86
1:A:71:VAL:HG12	1:M:67:ASP:O	1.75	0.86
1:I:67:ASP:O	1:Q:71:VAL:HG12	1.75	0.86
2:n:98:ILE:HG12	2:n:106:TYR:HB2	1.57	0.86
2:q:98:ILE:HG12	2:q:106:TYR:HB2	1.57	0.86
2:r:98:ILE:HG12	2:r:106:TYR:HB2	1.57	0.86
1:C:71:VAL:HG12	1:X:67:ASP:O	1.75	0.86
1:K:71:VAL:HG12	1:T:67:ASP:O	1.75	0.86
1:J:67:ASP:O	1:N:71:VAL:HG12	1.75	0.86
1:D:71:VAL:HG12	1:W:67:ASP:O	1.75	0.85
2:v:98:ILE:HG12	2:v:106:TYR:HB2	1.57	0.85
2:m:98:ILE:HG12	2:m:106:TYR:HB2	1.57	0.85
2:o:98:ILE:HG12	2:o:106:TYR:HB2	1.57	0.85
2:g:98:ILE:HG12	2:g:106:TYR:HB2	1.57	0.85
2:h:98:ILE:HG12	2:h:106:TYR:HB2	1.57	0.84
2:l:98:ILE:HG12	2:l:106:TYR:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:98:ILE:HG12	2:e:106:TYR:HB2	1.57	0.84
2:i:98:ILE:HG12	2:i:106:TYR:HB2	1.57	0.84
2:c:98:ILE:HG12	2:c:106:TYR:HB2	1.57	0.84
2:j:98:ILE:HG12	2:j:106:TYR:HB2	1.57	0.84
2:t:98:ILE:HG12	2:t:106:TYR:HB2	1.57	0.84
2:w:98:ILE:HG12	2:w:106:TYR:HB2	1.57	0.84
1:E:67:ASP:O	1:R:71:VAL:HG12	1.77	0.83
1:E:71:VAL:HG12	1:R:67:ASP:O	1.78	0.83
1:H:233:LEU:HD21	1:I:268:MET:HE1	1.61	0.83
1:K:233:LEU:HD21	1:P:268:MET:HE1	1.61	0.83
1:O:268:MET:HE1	1:V:233:LEU:HD21	1.61	0.83
1:X:233:LEU:HD21	1:Y:268:MET:HE1	1.61	0.83
1:N:233:LEU:HD21	1:S:268:MET:HE1	1.61	0.83
1:B:268:MET:HE1	1:D:233:LEU:HD21	1.61	0.82
1:Q:233:LEU:HD21	1:R:268:MET:HE1	1.61	0.82
1:C:233:LEU:HD21	1:J:268:MET:HE1	1.61	0.82
1:C:268:MET:HE1	1:J:233:LEU:HD21	1.61	0.82
1:L:233:LEU:HD21	1:M:268:MET:HE1	1.61	0.82
1:T:233:LEU:HD21	1:W:268:MET:HE1	1.61	0.82
1:E:268:MET:HE1	1:G:233:LEU:HD21	1.61	0.82
1:T:268:MET:HE1	1:W:233:LEU:HD21	1.61	0.82
1:A:233:LEU:HD21	1:F:268:MET:HE1	1.61	0.82
1:A:268:MET:HE1	1:F:233:LEU:HD21	1.61	0.82
1:B:233:LEU:HD21	1:D:268:MET:HE1	1.61	0.82
1:L:268:MET:HE1	1:M:233:LEU:HD21	1.61	0.82
1:N:268:MET:HE1	1:S:233:LEU:HD21	1.61	0.82
1:E:233:LEU:HD21	1:G:268:MET:HE1	1.61	0.82
1:Q:268:MET:HE1	1:R:233:LEU:HD21	1.62	0.81
1:K:268:MET:HE1	1:P:233:LEU:HD21	1.61	0.81
2:b:68:VAL:HG12	2:b:121:ASN:HD21	1.46	0.81
2:s:68:VAL:HG12	2:s:121:ASN:HD21	1.46	0.81
1:X:268:MET:HE1	1:Y:233:LEU:HD21	1.61	0.81
1:O:233:LEU:HD21	1:V:268:MET:HE1	1.61	0.80
2:t:68:VAL:HG12	2:t:121:ASN:HD21	1.46	0.80
2:c:68:VAL:HG12	2:c:121:ASN:HD21	1.46	0.80
1:H:268:MET:HE1	1:I:233:LEU:HD21	1.61	0.80
2:n:68:VAL:HG12	2:n:121:ASN:HD21	1.46	0.80
2:q:68:VAL:HG12	2:q:121:ASN:HD21	1.46	0.80
2:r:68:VAL:HG12	2:r:121:ASN:HD21	1.46	0.80
2:d:68:VAL:HG12	2:d:121:ASN:HD21	1.46	0.80
2:f:68:VAL:HG12	2:f:121:ASN:HD21	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:68:VAL:HG12	2:a:121:ASN:HD21	1.46	0.80
2:x:68:VAL:HG12	2:x:121:ASN:HD21	1.46	0.80
2:k:68:VAL:HG12	2:k:121:ASN:HD21	1.46	0.80
2:p:68:VAL:HG12	2:p:121:ASN:HD21	1.46	0.80
2:y:68:VAL:HG12	2:y:121:ASN:HD21	1.46	0.79
2:v:68:VAL:HG12	2:v:121:ASN:HD21	1.46	0.79
2:j:68:VAL:HG12	2:j:121:ASN:HD21	1.46	0.79
2:o:68:VAL:HG12	2:o:121:ASN:HD21	1.46	0.79
2:h:68:VAL:HG12	2:h:121:ASN:HD21	1.46	0.79
2:w:68:VAL:HG12	2:w:121:ASN:HD21	1.46	0.79
2:i:68:VAL:HG12	2:i:121:ASN:HD21	1.46	0.79
2:l:68:VAL:HG12	2:l:121:ASN:HD21	1.46	0.79
2:g:68:VAL:HG12	2:g:121:ASN:HD21	1.46	0.79
2:e:68:VAL:HG12	2:e:121:ASN:HD21	1.46	0.79
2:m:68:VAL:HG12	2:m:121:ASN:HD21	1.46	0.78
2:y:209:LYS:NZ	2:y:217:HIS:O	2.17	0.77
2:p:209:LYS:NZ	2:p:217:HIS:O	2.17	0.77
2:c:209:LYS:NZ	2:c:217:HIS:O	2.17	0.76
2:m:209:LYS:NZ	2:m:217:HIS:O	2.17	0.76
2:t:209:LYS:NZ	2:t:217:HIS:O	2.17	0.76
2:e:209:LYS:NZ	2:e:217:HIS:O	2.17	0.76
2:q:209:LYS:NZ	2:q:217:HIS:O	2.17	0.75
2:h:209:LYS:NZ	2:h:217:HIS:O	2.17	0.75
2:v:209:LYS:NZ	2:v:217:HIS:O	2.17	0.75
2:f:209:LYS:NZ	2:f:217:HIS:O	2.17	0.75
2:r:209:LYS:NZ	2:r:217:HIS:O	2.17	0.74
2:a:209:LYS:NZ	2:a:217:HIS:O	2.17	0.74
2:d:209:LYS:NZ	2:d:217:HIS:O	2.17	0.74
2:k:209:LYS:NZ	2:k:217:HIS:O	2.17	0.74
2:o:209:LYS:NZ	2:o:217:HIS:O	2.17	0.73
2:x:209:LYS:NZ	2:x:217:HIS:O	2.17	0.73
2:i:209:LYS:NZ	2:i:217:HIS:O	2.17	0.73
1:E:70:ALA:HB1	1:R:74:ALA:HB2	1.71	0.72
2:w:209:LYS:NZ	2:w:217:HIS:O	2.17	0.72
2:j:209:LYS:NZ	2:j:217:HIS:O	2.17	0.72
2:l:209:LYS:NZ	2:l:217:HIS:O	2.17	0.72
2:g:209:LYS:NZ	2:g:217:HIS:O	2.17	0.72
2:n:209:LYS:NZ	2:n:217:HIS:O	2.17	0.70
1:G:74:ALA:HB2	1:H:70:ALA:HB1	1.75	0.69
1:L:74:ALA:HB2	1:V:70:ALA:HB1	1.75	0.69
1:K:74:ALA:HB2	1:T:70:ALA:HB1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB2	1:M:70:ALA:HB1	1.75	0.69
1:C:70:ALA:HB1	1:X:74:ALA:HB2	1.75	0.69
1:G:70:ALA:HB1	1:H:74:ALA:HB2	1.75	0.69
1:K:70:ALA:HB1	1:T:74:ALA:HB2	1.75	0.69
1:L:70:ALA:HB1	1:V:74:ALA:HB2	1.75	0.69
1:C:74:ALA:HB2	1:X:70:ALA:HB1	1.75	0.69
1:B:74:ALA:HB2	1:P:70:ALA:HB1	1.75	0.69
1:S:74:ALA:HB2	1:Y:70:ALA:HB1	1.75	0.69
2:b:209:LYS:NZ	2:b:217:HIS:O	2.17	0.69
1:A:70:ALA:HB1	1:M:74:ALA:HB2	1.75	0.69
1:B:70:ALA:HB1	1:P:74:ALA:HB2	1.75	0.68
1:E:70:ALA:CB	1:R:74:ALA:CB	2.71	0.68
1:S:70:ALA:HB1	1:Y:74:ALA:HB2	1.75	0.68
2:s:209:LYS:NZ	2:s:217:HIS:O	2.17	0.68
1:F:70:ALA:HB1	1:O:74:ALA:HB2	1.75	0.68
1:J:74:ALA:HB2	1:N:70:ALA:HB1	1.75	0.68
1:D:70:ALA:HB1	1:W:74:ALA:HB2	1.75	0.67
1:I:74:ALA:HB2	1:Q:70:ALA:HB1	1.75	0.67
1:D:74:ALA:HB2	1:W:70:ALA:HB1	1.75	0.67
1:J:70:ALA:HB1	1:N:74:ALA:HB2	1.75	0.67
1:E:74:ALA:HB2	1:R:70:ALA:HB1	1.76	0.67
1:B:74:ALA:CB	1:P:70:ALA:CB	2.73	0.67
1:D:74:ALA:CB	1:W:70:ALA:CB	2.73	0.67
1:S:74:ALA:CB	1:Y:70:ALA:CB	2.73	0.67
1:J:70:ALA:CB	1:N:74:ALA:CB	2.73	0.67
1:I:70:ALA:HB1	1:Q:74:ALA:HB2	1.75	0.67
1:D:70:ALA:CB	1:W:74:ALA:CB	2.73	0.66
1:J:74:ALA:CB	1:N:70:ALA:CB	2.73	0.66
1:C:70:ALA:CB	1:X:74:ALA:CB	2.73	0.66
1:C:74:ALA:CB	1:X:70:ALA:CB	2.73	0.66
1:E:70:ALA:HB1	1:R:74:ALA:CB	2.25	0.66
1:F:74:ALA:HB2	1:O:70:ALA:HB1	1.75	0.66
1:K:70:ALA:CB	1:T:74:ALA:CB	2.73	0.66
1:F:74:ALA:CB	1:O:70:ALA:CB	2.73	0.66
1:K:74:ALA:CB	1:T:70:ALA:CB	2.73	0.66
2:s:152:ILE:O	2:s:198:ASN:HA	1.96	0.66
1:A:70:ALA:CB	1:M:74:ALA:CB	2.73	0.66
2:b:152:ILE:O	2:b:198:ASN:HA	1.96	0.66
2:d:152:ILE:O	2:d:198:ASN:HA	1.96	0.66
1:I:70:ALA:CB	1:Q:74:ALA:CB	2.73	0.66
2:n:152:ILE:O	2:n:198:ASN:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:152:ILE:O	2:j:198:ASN:HA	1.96	0.66
1:G:70:ALA:CB	1:H:74:ALA:CB	2.73	0.66
1:L:70:ALA:CB	1:V:74:ALA:CB	2.73	0.66
2:w:152:ILE:O	2:w:198:ASN:HA	1.96	0.66
2:v:152:ILE:O	2:v:198:ASN:HA	1.96	0.66
1:B:70:ALA:CB	1:P:74:ALA:CB	2.73	0.66
2:h:152:ILE:O	2:h:198:ASN:HA	1.96	0.66
1:S:70:ALA:CB	1:Y:74:ALA:CB	2.73	0.66
2:t:152:ILE:O	2:t:198:ASN:HA	1.96	0.66
2:c:152:ILE:O	2:c:198:ASN:HA	1.96	0.66
1:F:70:ALA:CB	1:O:74:ALA:CB	2.73	0.66
1:I:74:ALA:CB	1:Q:70:ALA:CB	2.73	0.66
1:A:74:ALA:CB	1:M:70:ALA:CB	2.73	0.66
2:g:152:ILE:O	2:g:198:ASN:HA	1.96	0.66
2:x:152:ILE:O	2:x:198:ASN:HA	1.96	0.65
2:l:152:ILE:O	2:l:198:ASN:HA	1.96	0.65
2:k:152:ILE:O	2:k:198:ASN:HA	1.96	0.65
1:L:74:ALA:CB	1:V:70:ALA:CB	2.73	0.65
2:a:152:ILE:O	2:a:198:ASN:HA	1.96	0.65
1:G:74:ALA:CB	1:H:70:ALA:CB	2.73	0.65
2:o:152:ILE:O	2:o:198:ASN:HA	1.96	0.65
2:r:152:ILE:O	2:r:198:ASN:HA	1.96	0.65
2:i:152:ILE:O	2:i:198:ASN:HA	1.96	0.65
2:h:93:VAL:HG12	2:h:111:GLU:HG2	1.79	0.65
2:m:55:VAL:HG12	2:m:137:LEU:HD22	1.79	0.65
2:o:68:VAL:HG12	2:o:121:ASN:ND2	2.12	0.65
2:t:68:VAL:HG12	2:t:121:ASN:ND2	2.12	0.65
2:t:93:VAL:HG12	2:t:111:GLU:HG2	1.79	0.65
2:v:93:VAL:HG12	2:v:111:GLU:HG2	1.79	0.65
2:a:55:VAL:HG12	2:a:137:LEU:HD22	1.79	0.65
2:c:68:VAL:HG12	2:c:121:ASN:ND2	2.12	0.65
2:c:93:VAL:HG12	2:c:111:GLU:HG2	1.79	0.65
2:e:55:VAL:HG12	2:e:137:LEU:HD22	1.79	0.65
2:g:93:VAL:HG12	2:g:111:GLU:HG2	1.79	0.65
2:i:68:VAL:HG12	2:i:121:ASN:ND2	2.12	0.65
2:r:55:VAL:HG12	2:r:137:LEU:HD22	1.79	0.65
2:d:68:VAL:HG12	2:d:121:ASN:ND2	2.12	0.65
2:k:93:VAL:HG12	2:k:111:GLU:HG2	1.79	0.65
2:l:93:VAL:HG12	2:l:111:GLU:HG2	1.79	0.65
2:n:68:VAL:HG12	2:n:121:ASN:ND2	2.12	0.65
2:y:152:ILE:O	2:y:198:ASN:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:55:VAL:HG12	2:b:137:LEU:HD22	1.79	0.64
1:D:161:TRP:HE1	2:d:73:ARG:HD2	1.62	0.64
2:e:152:ILE:O	2:e:198:ASN:HA	1.96	0.64
2:l:68:VAL:HG12	2:l:121:ASN:ND2	2.12	0.64
2:x:93:VAL:HG12	2:x:111:GLU:HG2	1.79	0.64
2:b:68:VAL:HG12	2:b:121:ASN:ND2	2.12	0.64
1:E:74:ALA:CB	1:R:70:ALA:CB	2.75	0.64
2:f:55:VAL:HG12	2:f:137:LEU:HD22	1.79	0.64
2:g:68:VAL:HG12	2:g:121:ASN:ND2	2.12	0.64
2:i:55:VAL:HG12	2:i:137:LEU:HD22	1.79	0.64
2:m:152:ILE:O	2:m:198:ASN:HA	1.96	0.64
2:p:152:ILE:O	2:p:198:ASN:HA	1.96	0.64
2:s:68:VAL:HG12	2:s:121:ASN:ND2	2.12	0.64
2:q:55:VAL:HG12	2:q:137:LEU:HD22	1.79	0.64
2:s:55:VAL:HG12	2:s:137:LEU:HD22	1.79	0.64
2:m:128:ILE:HG22	2:m:129:ASP:H	1.63	0.64
2:o:55:VAL:HG12	2:o:137:LEU:HD22	1.79	0.64
2:a:128:ILE:HG22	2:a:129:ASP:H	1.63	0.64
2:f:152:ILE:O	2:f:198:ASN:HA	1.96	0.64
2:j:93:VAL:HG12	2:j:111:GLU:HG2	1.79	0.64
2:k:128:ILE:HG22	2:k:129:ASP:H	1.63	0.64
2:n:128:ILE:HG22	2:n:129:ASP:H	1.63	0.64
2:p:55:VAL:HG12	2:p:137:LEU:HD22	1.79	0.64
2:r:128:ILE:HG22	2:r:129:ASP:H	1.63	0.64
2:x:68:VAL:HG12	2:x:121:ASN:ND2	2.12	0.64
1:A:70:ALA:HB1	1:M:74:ALA:CB	2.28	0.64
1:C:70:ALA:HB1	1:X:74:ALA:CB	2.28	0.64
2:d:93:VAL:HG12	2:d:111:GLU:HG2	1.79	0.64
2:d:128:ILE:HG22	2:d:129:ASP:H	1.63	0.64
1:F:70:ALA:HB1	1:O:74:ALA:CB	2.28	0.64
2:f:128:ILE:HG22	2:f:129:ASP:H	1.63	0.64
1:I:74:ALA:CB	1:Q:70:ALA:HB1	2.28	0.64
1:K:74:ALA:CB	1:T:70:ALA:HB1	2.28	0.64
2:k:68:VAL:HG12	2:k:121:ASN:ND2	2.12	0.64
2:x:128:ILE:HG22	2:x:129:ASP:H	1.63	0.64
2:y:55:VAL:HG12	2:y:137:LEU:HD22	1.79	0.64
1:B:74:ALA:CB	1:P:70:ALA:HB1	2.28	0.64
1:D:74:ALA:CB	1:W:70:ALA:HB1	2.28	0.64
2:e:128:ILE:HG22	2:e:129:ASP:H	1.63	0.64
1:G:74:ALA:CB	1:H:70:ALA:HB1	2.28	0.64
2:q:152:ILE:O	2:q:198:ASN:HA	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:93:VAL:HG12	2:w:111:GLU:HG2	1.79	0.64
2:e:68:VAL:HG12	2:e:121:ASN:ND2	2.12	0.64
1:J:70:ALA:HB1	1:N:74:ALA:CB	2.28	0.64
1:L:74:ALA:CB	1:V:70:ALA:HB1	2.28	0.64
2:l:55:VAL:HG12	2:l:137:LEU:HD22	1.79	0.64
2:n:93:VAL:HG12	2:n:111:GLU:HG2	1.79	0.64
2:p:128:ILE:HG22	2:p:129:ASP:H	1.63	0.64
2:q:128:ILE:HG22	2:q:129:ASP:H	1.63	0.64
1:S:74:ALA:CB	1:Y:70:ALA:HB1	2.28	0.64
2:s:93:VAL:HG12	2:s:111:GLU:HG2	1.79	0.64
2:w:68:VAL:HG12	2:w:121:ASN:ND2	2.12	0.64
2:y:128:ILE:HG22	2:y:129:ASP:H	1.63	0.64
1:C:74:ALA:CB	1:X:70:ALA:HB1	2.28	0.64
1:I:121:THR:HB	1:I:124:HIS:HD2	1.63	0.64
2:j:68:VAL:HG12	2:j:121:ASN:ND2	2.12	0.64
2:h:68:VAL:HG12	2:h:121:ASN:ND2	2.12	0.64
1:I:70:ALA:HB1	1:Q:74:ALA:CB	2.28	0.64
1:K:70:ALA:HB1	1:T:74:ALA:CB	2.28	0.64
1:K:121:THR:HB	1:K:124:HIS:HD2	1.63	0.64
1:O:121:THR:HB	1:O:124:HIS:HD2	1.63	0.64
2:s:128:ILE:HG22	2:s:129:ASP:H	1.63	0.64
2:t:128:ILE:HG22	2:t:129:ASP:H	1.63	0.64
1:E:74:ALA:CB	1:R:70:ALA:HB1	2.28	0.63
1:F:74:ALA:CB	1:O:70:ALA:HB1	2.28	0.63
1:G:121:THR:HB	1:G:124:HIS:HD2	1.63	0.63
2:g:55:VAL:HG12	2:g:137:LEU:HD22	1.79	0.63
2:h:55:VAL:HG12	2:h:137:LEU:HD22	1.79	0.63
1:L:70:ALA:HB1	1:V:74:ALA:CB	2.28	0.63
1:L:121:THR:HB	1:L:124:HIS:HD2	1.63	0.63
2:m:68:VAL:HG12	2:m:121:ASN:ND2	2.12	0.63
1:X:121:THR:HB	1:X:124:HIS:HD2	1.63	0.63
2:b:93:VAL:HG12	2:b:111:GLU:HG2	1.79	0.63
2:b:128:ILE:HG22	2:b:129:ASP:H	1.63	0.63
2:c:128:ILE:HG22	2:c:129:ASP:H	1.63	0.63
1:G:70:ALA:HB1	1:H:74:ALA:CB	2.28	0.63
2:r:93:VAL:HG12	2:r:111:GLU:HG2	1.79	0.63
2:v:55:VAL:HG12	2:v:137:LEU:HD22	1.79	0.63
2:v:68:VAL:HG12	2:v:121:ASN:ND2	2.12	0.63
2:y:93:VAL:HG12	2:y:111:GLU:HG2	1.79	0.63
2:a:93:VAL:HG12	2:a:111:GLU:HG2	1.79	0.63
2:p:68:VAL:HG12	2:p:121:ASN:ND2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:128:ILE:HG22	2:h:129:ASP:H	1.63	0.63
2:p:93:VAL:HG12	2:p:111:GLU:HG2	1.79	0.63
2:y:68:VAL:HG12	2:y:121:ASN:ND2	2.12	0.63
2:a:68:VAL:HG12	2:a:121:ASN:ND2	2.12	0.63
2:m:93:VAL:HG12	2:m:111:GLU:HG2	1.79	0.63
1:N:121:THR:HB	1:N:124:HIS:HD2	1.63	0.63
1:T:121:THR:HB	1:T:124:HIS:HD2	1.63	0.63
2:t:55:VAL:HG12	2:t:137:LEU:HD22	1.79	0.63
1:V:121:THR:HB	1:V:124:HIS:HD2	1.63	0.63
1:A:74:ALA:CB	1:M:70:ALA:HB1	2.28	0.63
1:C:121:THR:HB	1:C:124:HIS:HD2	1.63	0.63
2:c:55:VAL:HG12	2:c:137:LEU:HD22	1.79	0.63
1:D:121:THR:HB	1:D:124:HIS:HD2	1.63	0.63
2:d:55:VAL:HG12	2:d:137:LEU:HD22	1.79	0.63
2:e:93:VAL:HG12	2:e:111:GLU:HG2	1.79	0.63
1:H:121:THR:HB	1:H:124:HIS:HD2	1.63	0.63
2:r:68:VAL:HG12	2:r:121:ASN:ND2	2.12	0.63
2:v:128:ILE:HG22	2:v:129:ASP:H	1.63	0.63
1:W:121:THR:HB	1:W:124:HIS:HD2	1.63	0.63
1:J:74:ALA:CB	1:N:70:ALA:HB1	2.28	0.63
2:j:55:VAL:HG12	2:j:137:LEU:HD22	1.79	0.63
2:k:55:VAL:HG12	2:k:137:LEU:HD22	1.79	0.63
2:x:55:VAL:HG12	2:x:137:LEU:HD22	1.79	0.63
1:B:70:ALA:HB1	1:P:74:ALA:CB	2.28	0.63
1:J:121:THR:HB	1:J:124:HIS:HD2	1.63	0.63
2:n:55:VAL:HG12	2:n:137:LEU:HD22	1.79	0.63
1:D:70:ALA:HB1	1:W:74:ALA:CB	2.28	0.63
1:J:299:GLU:OE2	1:J:354:ARG:NH2	2.32	0.63
1:W:299:GLU:OE2	1:W:354:ARG:NH2	2.32	0.63
2:w:55:VAL:HG12	2:w:137:LEU:HD22	1.79	0.63
1:D:299:GLU:OE2	1:D:354:ARG:NH2	2.32	0.62
1:K:299:GLU:OE2	1:K:354:ARG:NH2	2.32	0.62
1:N:299:GLU:OE2	1:N:354:ARG:NH2	2.32	0.62
2:q:68:VAL:HG12	2:q:121:ASN:ND2	2.12	0.62
1:S:70:ALA:HB1	1:Y:74:ALA:CB	2.28	0.62
1:V:299:GLU:OE2	1:V:354:ARG:NH2	2.32	0.62
1:Y:121:THR:HB	1:Y:124:HIS:HD2	1.63	0.62
1:Y:299:GLU:OE2	1:Y:354:ARG:NH2	2.32	0.62
1:A:299:GLU:OE2	1:A:354:ARG:NH2	2.32	0.62
1:E:299:GLU:OE2	1:E:354:ARG:NH2	2.32	0.62
2:f:93:VAL:HG12	2:f:111:GLU:HG2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:128:ILE:HG22	2:g:129:ASP:H	1.63	0.62
1:H:299:GLU:OE2	1:H:354:ARG:NH2	2.32	0.62
2:l:128:ILE:HG22	2:l:129:ASP:H	1.63	0.62
1:M:299:GLU:OE2	1:M:354:ARG:NH2	2.32	0.62
1:P:121:THR:HB	1:P:124:HIS:HD2	1.63	0.62
1:P:299:GLU:OE2	1:P:354:ARG:NH2	2.32	0.62
1:X:299:GLU:OE2	1:X:354:ARG:NH2	2.32	0.62
1:I:299:GLU:OE2	1:I:354:ARG:NH2	2.32	0.62
2:i:93:VAL:HG12	2:i:111:GLU:HG2	1.79	0.62
1:M:121:THR:HB	1:M:124:HIS:HD2	1.63	0.62
1:O:299:GLU:OE2	1:O:354:ARG:NH2	2.32	0.62
2:o:93:VAL:HG12	2:o:111:GLU:HG2	1.79	0.62
2:q:93:VAL:HG12	2:q:111:GLU:HG2	1.79	0.62
1:R:121:THR:HB	1:R:124:HIS:HD2	1.63	0.62
1:R:299:GLU:OE2	1:R:354:ARG:NH2	2.32	0.62
1:E:121:THR:HB	1:E:124:HIS:HD2	1.63	0.62
2:f:68:VAL:HG12	2:f:121:ASN:ND2	2.12	0.62
1:A:121:THR:HB	1:A:124:HIS:HD2	1.63	0.62
1:Q:299:GLU:OE2	1:Q:354:ARG:NH2	2.32	0.62
1:F:299:GLU:OE2	1:F:354:ARG:NH2	2.32	0.62
1:G:299:GLU:OE2	1:G:354:ARG:NH2	2.32	0.62
1:L:299:GLU:OE2	1:L:354:ARG:NH2	2.32	0.62
1:B:121:THR:HB	1:B:124:HIS:HD2	1.63	0.62
1:Q:121:THR:HB	1:Q:124:HIS:HD2	1.63	0.62
2:g:203:THR:HG23	2:g:224:VAL:HG22	1.82	0.62
2:l:203:THR:HG23	2:l:224:VAL:HG22	1.82	0.62
2:w:128:ILE:HG22	2:w:129:ASP:H	1.63	0.62
1:F:121:THR:HB	1:F:124:HIS:HD2	1.63	0.62
2:i:203:THR:HG23	2:i:224:VAL:HG22	1.82	0.62
2:o:203:THR:HG23	2:o:224:VAL:HG22	1.82	0.62
1:S:121:THR:HB	1:S:124:HIS:HD2	1.63	0.62
2:v:203:THR:HG23	2:v:224:VAL:HG22	1.82	0.62
2:h:203:THR:HG23	2:h:224:VAL:HG22	1.82	0.61
2:i:128:ILE:HG22	2:i:129:ASP:H	1.63	0.61
2:j:128:ILE:HG22	2:j:129:ASP:H	1.63	0.61
1:S:299:GLU:OE2	1:S:354:ARG:NH2	2.32	0.61
1:B:299:GLU:OE2	1:B:354:ARG:NH2	2.32	0.61
1:C:299:GLU:OE2	1:C:354:ARG:NH2	2.32	0.61
2:c:203:THR:HG23	2:c:224:VAL:HG22	1.82	0.61
2:n:203:THR:HG23	2:n:224:VAL:HG22	1.82	0.61
1:T:299:GLU:OE2	1:T:354:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:203:THR:HG23	2:d:224:VAL:HG22	1.82	0.61
2:f:203:THR:HG23	2:f:224:VAL:HG22	1.82	0.61
2:j:203:THR:HG23	2:j:224:VAL:HG22	1.82	0.61
2:o:128:ILE:HG22	2:o:129:ASP:H	1.63	0.61
2:q:203:THR:HG23	2:q:224:VAL:HG22	1.82	0.61
2:t:203:THR:HG23	2:t:224:VAL:HG22	1.82	0.61
2:a:203:THR:HG23	2:a:224:VAL:HG22	1.82	0.61
2:w:203:THR:HG23	2:w:224:VAL:HG22	1.82	0.61
2:r:203:THR:HG23	2:r:224:VAL:HG22	1.82	0.61
2:x:203:THR:HG23	2:x:224:VAL:HG22	1.82	0.61
2:e:203:THR:HG23	2:e:224:VAL:HG22	1.82	0.61
2:k:203:THR:HG23	2:k:224:VAL:HG22	1.82	0.61
2:y:203:THR:HG23	2:y:224:VAL:HG22	1.82	0.61
2:p:203:THR:HG23	2:p:224:VAL:HG22	1.82	0.61
2:m:203:THR:HG23	2:m:224:VAL:HG22	1.82	0.61
2:t:163:ALA:HB3	2:t:183:GLN:HG2	1.83	0.60
2:c:163:ALA:HB3	2:c:183:GLN:HG2	1.83	0.60
2:d:163:ALA:HB3	2:d:183:GLN:HG2	1.83	0.60
2:n:163:ALA:HB3	2:n:183:GLN:HG2	1.83	0.60
2:b:77:HIS:CD2	2:b:78:MET:HG3	2.37	0.60
2:d:68:VAL:CG1	2:d:121:ASN:ND2	2.65	0.60
2:l:163:ALA:HB3	2:l:183:GLN:HG2	1.83	0.60
2:n:68:VAL:CG1	2:n:121:ASN:ND2	2.65	0.60
2:g:163:ALA:HB3	2:g:183:GLN:HG2	1.83	0.60
2:i:68:VAL:CG1	2:i:121:ASN:ND2	2.65	0.60
2:i:163:ALA:HB3	2:i:183:GLN:HG2	1.83	0.60
2:o:68:VAL:CG1	2:o:121:ASN:ND2	2.65	0.60
2:o:163:ALA:HB3	2:o:183:GLN:HG2	1.83	0.60
2:s:77:HIS:CD2	2:s:78:MET:HG3	2.37	0.60
2:s:203:THR:HG23	2:s:224:VAL:HG22	1.82	0.60
2:a:68:VAL:CG1	2:a:121:ASN:ND2	2.65	0.60
2:c:68:VAL:CG1	2:c:121:ASN:ND2	2.65	0.60
2:h:68:VAL:CG1	2:h:121:ASN:ND2	2.65	0.60
2:k:77:HIS:CD2	2:k:78:MET:HG3	2.37	0.60
2:r:68:VAL:CG1	2:r:121:ASN:ND2	2.65	0.60
2:t:68:VAL:CG1	2:t:121:ASN:ND2	2.65	0.60
2:v:68:VAL:CG1	2:v:121:ASN:ND2	2.65	0.60
2:p:163:ALA:HB3	2:p:183:GLN:HG2	1.83	0.60
2:t:77:HIS:CD2	2:t:78:MET:HG3	2.37	0.60
2:w:7:LEU:HB3	2:w:114:PHE:HE2	1.67	0.60
2:w:68:VAL:CG1	2:w:121:ASN:ND2	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:77:HIS:CD2	2:x:78:MET:HG3	2.37	0.60
2:y:163:ALA:HB3	2:y:183:GLN:HG2	1.83	0.60
2:b:203:THR:HG23	2:b:224:VAL:HG22	1.82	0.60
2:c:7:LEU:HB3	2:c:114:PHE:HE2	1.67	0.60
2:c:77:HIS:CD2	2:c:78:MET:HG3	2.37	0.60
2:d:7:LEU:HB3	2:d:114:PHE:HE2	1.67	0.60
2:e:7:LEU:HB3	2:e:114:PHE:HE2	1.67	0.60
2:j:7:LEU:HB3	2:j:114:PHE:HE2	1.67	0.60
2:j:68:VAL:CG1	2:j:121:ASN:ND2	2.65	0.60
2:k:163:ALA:HB3	2:k:183:GLN:HG2	1.83	0.60
2:n:7:LEU:HB3	2:n:114:PHE:HE2	1.67	0.60
2:t:7:LEU:HB3	2:t:114:PHE:HE2	1.67	0.60
2:x:163:ALA:HB3	2:x:183:GLN:HG2	1.83	0.60
2:y:77:HIS:CD2	2:y:78:MET:HG3	2.37	0.60
2:m:68:VAL:CG1	2:m:121:ASN:ND2	2.65	0.59
2:m:163:ALA:HB3	2:m:183:GLN:HG2	1.83	0.59
2:p:77:HIS:CD2	2:p:78:MET:HG3	2.37	0.59
2:q:77:HIS:CD2	2:q:78:MET:HG3	2.37	0.59
2:a:77:HIS:CD2	2:a:78:MET:HG3	2.37	0.59
2:e:68:VAL:CG1	2:e:121:ASN:ND2	2.65	0.59
2:f:77:HIS:CD2	2:f:78:MET:HG3	2.37	0.59
2:m:7:LEU:HB3	2:m:114:PHE:HE2	1.67	0.59
2:q:68:VAL:CG1	2:q:121:ASN:ND2	2.65	0.59
2:r:77:HIS:CD2	2:r:78:MET:HG3	2.37	0.59
2:s:7:LEU:HB3	2:s:114:PHE:HE2	1.67	0.59
2:b:7:LEU:HB3	2:b:114:PHE:HE2	1.67	0.59
2:e:163:ALA:HB3	2:e:183:GLN:HG2	1.83	0.59
2:f:68:VAL:CG1	2:f:121:ASN:ND2	2.65	0.59
2:k:68:VAL:CG1	2:k:121:ASN:ND2	2.65	0.59
2:s:68:VAL:CG1	2:s:121:ASN:ND2	2.65	0.59
2:s:163:ALA:HB3	2:s:183:GLN:HG2	1.83	0.59
2:v:77:HIS:CD2	2:v:78:MET:HG3	2.37	0.59
2:w:163:ALA:HB3	2:w:183:GLN:HG2	1.83	0.59
2:b:68:VAL:CG1	2:b:121:ASN:ND2	2.65	0.59
2:b:163:ALA:HB3	2:b:183:GLN:HG2	1.83	0.59
2:g:68:VAL:CG1	2:g:121:ASN:ND2	2.65	0.59
2:l:68:VAL:CG1	2:l:121:ASN:ND2	2.65	0.59
2:x:7:LEU:HB3	2:x:114:PHE:HE2	1.67	0.59
2:e:77:HIS:CD2	2:e:78:MET:HG3	2.37	0.59
2:f:7:LEU:HB3	2:f:114:PHE:HE2	1.67	0.59
2:h:77:HIS:CD2	2:h:78:MET:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:7:LEU:HB3	2:i:114:PHE:HE2	1.67	0.59
2:j:77:HIS:CD2	2:j:78:MET:HG3	2.37	0.59
2:j:163:ALA:HB3	2:j:183:GLN:HG2	1.83	0.59
2:k:7:LEU:HB3	2:k:114:PHE:HE2	1.67	0.59
2:l:7:LEU:HB3	2:l:114:PHE:HE2	1.67	0.59
2:m:77:HIS:CD2	2:m:78:MET:HG3	2.37	0.59
2:o:7:LEU:HB3	2:o:114:PHE:HE2	1.67	0.59
2:q:7:LEU:HB3	2:q:114:PHE:HE2	1.67	0.59
2:w:77:HIS:CD2	2:w:78:MET:HG3	2.37	0.59
2:x:68:VAL:CG1	2:x:121:ASN:ND2	2.65	0.59
2:h:163:ALA:HB3	2:h:183:GLN:HG2	1.83	0.59
2:v:163:ALA:HB3	2:v:183:GLN:HG2	1.83	0.59
2:d:77:HIS:CD2	2:d:78:MET:HG3	2.37	0.59
2:g:7:LEU:HB3	2:g:114:PHE:HE2	1.67	0.59
2:n:77:HIS:CD2	2:n:78:MET:HG3	2.37	0.59
2:p:7:LEU:HB3	2:p:114:PHE:HE2	1.67	0.59
2:y:7:LEU:HB3	2:y:114:PHE:HE2	1.67	0.59
2:f:163:ALA:HB3	2:f:183:GLN:HG2	1.83	0.59
2:a:7:LEU:HB3	2:a:114:PHE:HE2	1.67	0.58
2:p:68:VAL:CG1	2:p:121:ASN:ND2	2.65	0.58
2:r:7:LEU:HB3	2:r:114:PHE:HE2	1.67	0.58
2:y:68:VAL:CG1	2:y:121:ASN:ND2	2.65	0.58
2:a:163:ALA:HB3	2:a:183:GLN:HG2	1.83	0.58
2:g:77:HIS:CD2	2:g:78:MET:HG3	2.37	0.58
2:i:77:HIS:CD2	2:i:78:MET:HG3	2.37	0.58
2:h:7:LEU:HB3	2:h:114:PHE:HE2	1.67	0.58
2:l:77:HIS:CD2	2:l:78:MET:HG3	2.37	0.58
2:o:77:HIS:CD2	2:o:78:MET:HG3	2.37	0.58
2:v:7:LEU:HB3	2:v:114:PHE:HE2	1.67	0.58
2:q:163:ALA:HB3	2:q:183:GLN:HG2	1.83	0.58
2:r:163:ALA:HB3	2:r:183:GLN:HG2	1.83	0.58
1:I:74:ALA:HB2	1:Q:70:ALA:CB	2.34	0.57
1:F:70:ALA:CB	1:O:74:ALA:HB2	2.34	0.57
1:L:74:ALA:HB2	1:V:70:ALA:CB	2.34	0.57
1:E:70:ALA:CB	1:R:74:ALA:HB2	2.32	0.57
1:L:70:ALA:CB	1:V:74:ALA:HB2	2.34	0.57
1:G:70:ALA:CB	1:H:74:ALA:HB2	2.34	0.57
2:m:87:ALA:O	2:m:91:GLY:N	2.37	0.57
1:B:70:ALA:CB	1:P:74:ALA:HB2	2.34	0.56
1:S:70:ALA:CB	1:Y:74:ALA:HB2	2.34	0.56
2:a:54:PRO:O	2:a:139:HIS:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ALA:CB	1:T:74:ALA:HB2	2.34	0.56
1:A:74:ALA:HB2	1:M:70:ALA:CB	2.34	0.56
1:B:74:ALA:HB2	1:P:70:ALA:CB	2.34	0.56
2:b:54:PRO:O	2:b:139:HIS:NE2	2.39	0.56
1:C:74:ALA:HB2	1:X:70:ALA:CB	2.34	0.56
1:D:74:ALA:HB2	1:W:70:ALA:CB	2.34	0.56
1:D:74:ALA:CB	1:W:70:ALA:HB2	2.36	0.56
2:e:87:ALA:O	2:e:91:GLY:N	2.37	0.56
1:J:70:ALA:HB2	1:N:74:ALA:CB	2.36	0.56
1:L:74:ALA:CB	1:V:70:ALA:HB2	2.36	0.56
2:r:54:PRO:O	2:r:139:HIS:NE2	2.39	0.56
1:S:74:ALA:HB2	1:Y:70:ALA:CB	2.34	0.56
2:s:54:PRO:O	2:s:139:HIS:NE2	2.39	0.56
1:G:70:ALA:HB2	1:H:74:ALA:CB	2.36	0.56
1:G:74:ALA:CB	1:H:70:ALA:HB2	2.36	0.56
1:L:70:ALA:HB2	1:V:74:ALA:CB	2.36	0.56
1:E:70:ALA:HB2	1:R:74:ALA:CB	2.34	0.56
1:J:70:ALA:CB	1:N:74:ALA:HB2	2.34	0.56
2:e:54:PRO:O	2:e:139:HIS:NE2	2.39	0.56
2:y:54:PRO:O	2:y:139:HIS:NE2	2.39	0.56
1:A:70:ALA:CB	1:M:74:ALA:HB2	2.34	0.56
1:B:70:ALA:HB2	1:P:74:ALA:CB	2.36	0.56
1:F:70:ALA:HB2	1:O:74:ALA:CB	2.36	0.56
2:g:54:PRO:O	2:g:139:HIS:NE2	2.39	0.56
2:h:177:GLN:HE22	2:h:179:ALA:HB2	1.71	0.56
1:I:74:ALA:CB	1:Q:70:ALA:HB2	2.36	0.56
2:k:177:GLN:HE22	2:k:179:ALA:HB2	1.71	0.56
2:m:54:PRO:O	2:m:139:HIS:NE2	2.39	0.56
2:p:54:PRO:O	2:p:139:HIS:NE2	2.39	0.56
2:v:177:GLN:HE22	2:v:179:ALA:HB2	1.71	0.56
2:x:177:GLN:HE22	2:x:179:ALA:HB2	1.71	0.56
2:c:54:PRO:O	2:c:139:HIS:NE2	2.39	0.56
2:d:177:GLN:HE22	2:d:179:ALA:HB2	1.71	0.56
1:S:70:ALA:HB2	1:Y:74:ALA:CB	2.36	0.56
2:l:54:PRO:O	2:l:139:HIS:NE2	2.39	0.56
2:n:177:GLN:HE22	2:n:179:ALA:HB2	1.71	0.56
2:t:54:PRO:O	2:t:139:HIS:NE2	2.39	0.56
1:B:74:ALA:CB	1:P:70:ALA:HB2	2.36	0.55
2:h:54:PRO:O	2:h:139:HIS:NE2	2.39	0.55
2:n:54:PRO:O	2:n:139:HIS:NE2	2.39	0.55
2:d:54:PRO:O	2:d:139:HIS:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:177:GLN:HE22	2:l:179:ALA:HB2	1.71	0.55
2:p:188:ILE:HG13	2:p:189:GLY:N	2.21	0.55
2:v:54:PRO:O	2:v:139:HIS:NE2	2.39	0.55
2:w:54:PRO:O	2:w:139:HIS:NE2	2.39	0.55
2:y:188:ILE:HG13	2:y:189:GLY:N	2.21	0.55
2:d:188:ILE:HG13	2:d:189:GLY:N	2.21	0.55
2:i:54:PRO:O	2:i:139:HIS:NE2	2.39	0.55
1:K:74:ALA:CB	1:T:70:ALA:HB2	2.36	0.55
2:k:54:PRO:O	2:k:139:HIS:NE2	2.39	0.55
2:k:188:ILE:HG13	2:k:189:GLY:N	2.21	0.55
2:n:188:ILE:HG13	2:n:189:GLY:N	2.21	0.55
1:S:74:ALA:CB	1:Y:70:ALA:HB2	2.36	0.55
2:w:177:GLN:HE22	2:w:179:ALA:HB2	1.71	0.55
2:x:54:PRO:O	2:x:139:HIS:NE2	2.39	0.55
1:A:70:ALA:HB2	1:M:74:ALA:CB	2.36	0.55
1:C:70:ALA:HB2	1:X:74:ALA:CB	2.36	0.55
2:c:177:GLN:HE22	2:c:179:ALA:HB2	1.71	0.55
2:f:54:PRO:O	2:f:139:HIS:NE2	2.39	0.55
2:j:54:PRO:O	2:j:139:HIS:NE2	2.39	0.55
2:j:177:GLN:HE22	2:j:179:ALA:HB2	1.71	0.55
2:o:54:PRO:O	2:o:139:HIS:NE2	2.39	0.55
2:x:188:ILE:HG13	2:x:189:GLY:N	2.21	0.55
1:D:70:ALA:CB	1:W:74:ALA:HB2	2.34	0.55
1:F:74:ALA:HB2	1:O:70:ALA:CB	2.34	0.55
1:F:74:ALA:CB	1:O:70:ALA:HB2	2.36	0.55
1:I:70:ALA:HB2	1:Q:74:ALA:CB	2.36	0.55
2:q:54:PRO:O	2:q:139:HIS:NE2	2.39	0.55
2:t:177:GLN:HE22	2:t:179:ALA:HB2	1.71	0.55
1:A:74:ALA:CB	1:M:70:ALA:HB2	2.36	0.55
1:C:74:ALA:CB	1:X:70:ALA:HB2	2.36	0.55
1:D:70:ALA:HB2	1:W:74:ALA:CB	2.36	0.55
1:J:74:ALA:CB	1:N:70:ALA:HB2	2.36	0.55
1:K:70:ALA:HB2	1:T:74:ALA:CB	2.36	0.55
2:q:87:ALA:O	2:q:91:GLY:N	2.37	0.55
2:r:177:GLN:HE22	2:r:179:ALA:HB2	1.71	0.55
2:v:188:ILE:HG13	2:v:189:GLY:N	2.21	0.55
2:y:177:GLN:HE22	2:y:179:ALA:HB2	1.71	0.55
2:f:87:ALA:O	2:f:91:GLY:N	2.37	0.55
2:g:177:GLN:HE22	2:g:179:ALA:HB2	1.71	0.55
2:h:188:ILE:HG13	2:h:189:GLY:N	2.21	0.55
1:I:70:ALA:CB	1:Q:74:ALA:HB2	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:ALA:HB2	1:N:70:ALA:CB	2.34	0.55
2:p:177:GLN:HE22	2:p:179:ALA:HB2	1.71	0.55
2:a:87:ALA:O	2:a:91:GLY:N	2.37	0.55
2:a:177:GLN:HE22	2:a:179:ALA:HB2	1.71	0.55
2:m:177:GLN:HE22	2:m:179:ALA:HB2	1.71	0.55
2:j:188:ILE:HG13	2:j:189:GLY:N	2.21	0.55
2:r:87:ALA:O	2:r:91:GLY:N	2.37	0.55
2:f:188:ILE:HG13	2:f:189:GLY:N	2.21	0.55
2:h:199:HIS:HB2	2:h:228:GLY:HA3	1.89	0.55
2:m:188:ILE:HG13	2:m:189:GLY:N	2.21	0.55
2:q:177:GLN:HE22	2:q:179:ALA:HB2	1.71	0.55
2:v:199:HIS:HB2	2:v:228:GLY:HA3	1.89	0.55
1:C:70:ALA:CB	1:X:74:ALA:HB2	2.34	0.54
2:q:199:HIS:HB2	2:q:228:GLY:HA3	1.89	0.54
2:w:188:ILE:HG13	2:w:189:GLY:N	2.21	0.54
2:b:199:HIS:HB2	2:b:228:GLY:HA3	1.89	0.54
2:d:199:HIS:HB2	2:d:228:GLY:HA3	1.89	0.54
2:f:199:HIS:HB2	2:f:228:GLY:HA3	1.89	0.54
2:i:199:HIS:HB2	2:i:228:GLY:HA3	1.89	0.54
2:l:188:ILE:HG13	2:l:189:GLY:N	2.21	0.54
2:o:199:HIS:HB2	2:o:228:GLY:HA3	1.89	0.54
2:t:188:ILE:HG13	2:t:189:GLY:N	2.21	0.54
2:b:177:GLN:HE22	2:b:179:ALA:HB2	1.71	0.54
2:c:87:ALA:O	2:c:91:GLY:N	2.37	0.54
2:e:177:GLN:HE22	2:e:179:ALA:HB2	1.71	0.54
2:q:188:ILE:HG13	2:q:189:GLY:N	2.21	0.54
2:r:199:HIS:HB2	2:r:228:GLY:HA3	1.89	0.54
2:s:188:ILE:HG13	2:s:189:GLY:N	2.21	0.54
2:s:199:HIS:HB2	2:s:228:GLY:HA3	1.89	0.54
2:t:199:HIS:HB2	2:t:228:GLY:HA3	1.89	0.54
2:a:199:HIS:HB2	2:a:228:GLY:HA3	1.89	0.54
2:c:188:ILE:HG13	2:c:189:GLY:N	2.21	0.54
2:c:199:HIS:HB2	2:c:228:GLY:HA3	1.89	0.54
2:f:177:GLN:HE22	2:f:179:ALA:HB2	1.71	0.54
2:g:188:ILE:HG13	2:g:189:GLY:N	2.21	0.54
2:i:177:GLN:HE22	2:i:179:ALA:HB2	1.71	0.54
1:K:74:ALA:HB2	1:T:70:ALA:CB	2.34	0.54
2:n:199:HIS:HB2	2:n:228:GLY:HA3	1.89	0.54
2:o:177:GLN:HE22	2:o:179:ALA:HB2	1.71	0.54
2:b:87:ALA:O	2:b:91:GLY:N	2.37	0.54
2:r:188:ILE:HG13	2:r:189:GLY:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:177:GLN:HE22	2:s:179:ALA:HB2	1.71	0.54
2:b:152:ILE:HD11	2:b:199:HIS:NE2	2.23	0.54
2:e:188:ILE:HG13	2:e:189:GLY:N	2.21	0.54
2:s:152:ILE:HD11	2:s:199:HIS:NE2	2.23	0.54
2:t:87:ALA:O	2:t:91:GLY:N	2.37	0.54
2:a:188:ILE:HG13	2:a:189:GLY:N	2.21	0.54
2:s:87:ALA:O	2:s:91:GLY:N	2.37	0.54
2:b:188:ILE:HG13	2:b:189:GLY:N	2.21	0.54
2:q:152:ILE:HD11	2:q:199:HIS:NE2	2.23	0.54
2:v:152:ILE:HD11	2:v:199:HIS:NE2	2.23	0.54
2:h:152:ILE:HD11	2:h:199:HIS:NE2	2.23	0.54
2:j:199:HIS:HB2	2:j:228:GLY:HA3	1.89	0.54
2:w:199:HIS:HB2	2:w:228:GLY:HA3	1.89	0.54
2:f:152:ILE:HD11	2:f:199:HIS:NE2	2.23	0.54
2:o:188:ILE:HG13	2:o:189:GLY:N	2.21	0.54
2:t:152:ILE:HD11	2:t:199:HIS:NE2	2.23	0.54
2:c:152:ILE:HD11	2:c:199:HIS:NE2	2.23	0.53
2:i:87:ALA:O	2:i:91:GLY:N	2.37	0.53
2:n:152:ILE:HD11	2:n:199:HIS:NE2	2.23	0.53
2:d:87:ALA:O	2:d:91:GLY:N	2.37	0.53
2:d:152:ILE:HD11	2:d:199:HIS:NE2	2.23	0.53
2:i:188:ILE:HG13	2:i:189:GLY:N	2.21	0.53
2:o:87:ALA:O	2:o:91:GLY:N	2.37	0.53
2:x:87:ALA:O	2:x:91:GLY:N	2.37	0.53
2:y:152:ILE:HD11	2:y:199:HIS:NE2	2.23	0.53
2:y:199:HIS:HB2	2:y:228:GLY:HA3	1.89	0.53
2:k:87:ALA:O	2:k:91:GLY:N	2.37	0.53
2:p:152:ILE:HD11	2:p:199:HIS:NE2	2.23	0.53
2:p:199:HIS:HB2	2:p:228:GLY:HA3	1.89	0.53
2:l:199:HIS:HB2	2:l:228:GLY:HA3	1.89	0.53
2:n:87:ALA:O	2:n:91:GLY:N	2.37	0.53
1:E:74:ALA:CB	1:R:70:ALA:HB2	2.38	0.53
2:e:152:ILE:HD11	2:e:199:HIS:NE2	2.23	0.53
2:g:87:ALA:O	2:g:91:GLY:N	2.37	0.53
2:g:199:HIS:HB2	2:g:228:GLY:HA3	1.89	0.53
2:i:152:ILE:HD11	2:i:199:HIS:NE2	2.23	0.53
2:m:152:ILE:HD11	2:m:199:HIS:NE2	2.23	0.53
2:o:152:ILE:HD11	2:o:199:HIS:NE2	2.23	0.53
2:k:152:ILE:HD11	2:k:199:HIS:NE2	2.23	0.53
2:p:87:ALA:O	2:p:91:GLY:N	2.37	0.53
2:x:152:ILE:HD11	2:x:199:HIS:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:199:HIS:HB2	2:x:228:GLY:HA3	1.89	0.53
2:k:199:HIS:HB2	2:k:228:GLY:HA3	1.89	0.53
2:l:87:ALA:O	2:l:91:GLY:N	2.37	0.53
2:l:152:ILE:HD11	2:l:199:HIS:NE2	2.23	0.53
2:a:152:ILE:HD11	2:a:199:HIS:NE2	2.23	0.53
1:K:344:LYS:HE2	1:R:242:ASP:HB3	1.91	0.53
2:e:199:HIS:HB2	2:e:228:GLY:HA3	1.89	0.53
2:g:152:ILE:HD11	2:g:199:HIS:NE2	2.23	0.53
2:j:152:ILE:HD11	2:j:199:HIS:NE2	2.23	0.53
2:y:87:ALA:O	2:y:91:GLY:N	2.37	0.53
2:r:152:ILE:HD11	2:r:199:HIS:NE2	2.23	0.52
2:w:152:ILE:HD11	2:w:199:HIS:NE2	2.23	0.52
1:E:74:ALA:HB2	1:R:70:ALA:CB	2.37	0.52
2:m:199:HIS:HB2	2:m:228:GLY:HA3	1.89	0.52
1:G:74:ALA:HB2	1:H:70:ALA:CB	2.34	0.52
1:D:118:TRP:CE2	2:d:43:THR:OG1	2.63	0.52
2:j:14:ILE:HG21	2:j:44:LEU:HD22	1.92	0.52
2:w:14:ILE:HG21	2:w:44:LEU:HD22	1.92	0.52
2:h:87:ALA:O	2:h:91:GLY:N	2.37	0.52
2:t:14:ILE:HG21	2:t:44:LEU:HD22	1.92	0.52
2:b:14:ILE:HG21	2:b:44:LEU:HD22	1.92	0.52
2:c:14:ILE:HG21	2:c:44:LEU:HD22	1.92	0.52
2:o:14:ILE:HG21	2:o:44:LEU:HD22	1.92	0.52
2:i:14:ILE:HG21	2:i:44:LEU:HD22	1.92	0.52
2:p:14:ILE:HG21	2:p:44:LEU:HD22	1.92	0.52
2:s:14:ILE:HG21	2:s:44:LEU:HD22	1.92	0.52
2:v:87:ALA:O	2:v:91:GLY:N	2.37	0.52
2:y:14:ILE:HG21	2:y:44:LEU:HD22	1.92	0.52
2:f:14:ILE:HG21	2:f:44:LEU:HD22	1.92	0.51
2:h:14:ILE:HG21	2:h:44:LEU:HD22	1.92	0.51
2:m:14:ILE:HG21	2:m:44:LEU:HD22	1.92	0.51
2:n:69:GLN:C	2:n:71:PHE:H	2.19	0.51
2:s:69:GLN:C	2:s:71:PHE:H	2.19	0.51
2:a:69:GLN:C	2:a:71:PHE:H	2.19	0.51
2:e:14:ILE:HG21	2:e:44:LEU:HD22	1.92	0.51
2:q:14:ILE:HG21	2:q:44:LEU:HD22	1.92	0.51
2:v:14:ILE:HG21	2:v:44:LEU:HD22	1.92	0.51
2:b:69:GLN:C	2:b:71:PHE:H	2.19	0.51
2:p:69:GLN:C	2:p:71:PHE:H	2.19	0.51
2:r:69:GLN:C	2:r:71:PHE:H	2.19	0.51
2:x:69:GLN:C	2:x:71:PHE:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LYS:HE2	1:K:242:ASP:HB3	1.93	0.51
1:F:344:LYS:HE2	1:I:242:ASP:HB3	1.93	0.51
2:k:69:GLN:C	2:k:71:PHE:H	2.19	0.51
2:m:69:GLN:C	2:m:71:PHE:H	2.19	0.51
2:n:14:ILE:HG21	2:n:44:LEU:HD22	1.92	0.51
1:O:242:ASP:HB3	1:Q:344:LYS:HE2	1.93	0.51
1:T:344:LYS:HE2	1:X:242:ASP:HB3	1.93	0.51
2:y:69:GLN:C	2:y:71:PHE:H	2.19	0.51
2:g:69:GLN:C	2:g:71:PHE:H	2.19	0.51
1:N:344:LYS:HE2	1:Q:242:ASP:HB3	1.93	0.51
1:D:344:LYS:HE2	1:F:242:ASP:HB3	1.93	0.51
1:I:344:LYS:HE2	1:J:242:ASP:HB3	1.93	0.51
2:c:69:GLN:C	2:c:71:PHE:H	2.19	0.51
2:d:14:ILE:HG21	2:d:44:LEU:HD22	1.92	0.51
2:e:69:GLN:C	2:e:71:PHE:H	2.19	0.51
2:j:87:ALA:O	2:j:91:GLY:N	2.37	0.51
2:l:69:GLN:C	2:l:71:PHE:H	2.19	0.51
1:O:344:LYS:HE2	1:W:242:ASP:HB3	1.93	0.51
2:r:14:ILE:HG21	2:r:44:LEU:HD22	1.92	0.51
2:t:69:GLN:C	2:t:71:PHE:H	2.19	0.51
2:w:87:ALA:O	2:w:91:GLY:N	2.37	0.51
1:A:242:ASP:HB3	1:X:344:LYS:HE2	1.93	0.51
1:D:242:ASP:HB3	1:J:344:LYS:HE2	1.93	0.51
2:g:14:ILE:HG21	2:g:44:LEU:HD22	1.92	0.51
1:H:344:LYS:HE2	1:Y:242:ASP:HB3	1.93	0.51
1:P:242:ASP:HB3	1:V:344:LYS:HE2	1.93	0.51
2:q:69:GLN:C	2:q:71:PHE:H	2.19	0.51
2:v:128:ILE:HG22	2:v:129:ASP:N	2.26	0.51
2:a:14:ILE:HG21	2:a:44:LEU:HD22	1.92	0.50
2:f:69:GLN:C	2:f:71:PHE:H	2.19	0.50
1:H:347:GLY:O	1:H:351:THR:HG23	2.12	0.50
2:h:128:ILE:HG22	2:h:129:ASP:N	2.26	0.50
2:i:69:GLN:C	2:i:71:PHE:H	2.19	0.50
1:N:242:ASP:HB3	1:W:344:LYS:HE2	1.93	0.50
1:V:347:GLY:O	1:V:351:THR:HG23	2.12	0.50
1:A:347:GLY:O	1:A:351:THR:HG23	2.12	0.50
2:i:128:ILE:HG22	2:i:129:ASP:N	2.26	0.50
2:p:128:ILE:HG22	2:p:129:ASP:N	2.26	0.50
1:R:347:GLY:O	1:R:351:THR:HG23	2.12	0.50
2:y:128:ILE:HG22	2:y:129:ASP:N	2.26	0.50
2:c:128:ILE:HG22	2:c:129:ASP:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:14:ILE:HG21	2:l:44:LEU:HD22	1.92	0.50
2:o:69:GLN:C	2:o:71:PHE:H	2.19	0.50
2:o:128:ILE:HG22	2:o:129:ASP:N	2.26	0.50
1:D:347:GLY:O	1:D:351:THR:HG23	2.12	0.50
1:G:242:ASP:HB3	1:S:344:LYS:HE2	1.93	0.50
1:J:347:GLY:O	1:J:351:THR:HG23	2.12	0.50
2:j:69:GLN:C	2:j:71:PHE:H	2.19	0.50
2:t:128:ILE:HG22	2:t:129:ASP:N	2.26	0.50
1:W:347:GLY:O	1:W:351:THR:HG23	2.12	0.50
1:B:344:LYS:HE2	1:L:242:ASP:HB3	1.93	0.50
2:d:69:GLN:C	2:d:71:PHE:H	2.18	0.50
2:k:201:LEU:HD12	2:k:226:ALA:HB2	1.94	0.50
2:m:69:GLN:C	2:m:71:PHE:N	2.70	0.50
1:N:347:GLY:O	1:N:351:THR:HG23	2.12	0.50
1:P:347:GLY:O	1:P:351:THR:HG23	2.12	0.50
2:x:201:LEU:HD12	2:x:226:ALA:HB2	1.94	0.50
1:Y:347:GLY:O	1:Y:351:THR:HG23	2.12	0.50
2:k:77:HIS:HD2	2:k:78:MET:HG3	1.77	0.50
2:p:201:LEU:HD12	2:p:226:ALA:HB2	1.94	0.50
1:S:347:GLY:O	1:S:351:THR:HG23	2.12	0.50
2:x:77:HIS:HD2	2:x:78:MET:HG3	1.77	0.50
2:y:201:LEU:HD12	2:y:226:ALA:HB2	1.94	0.50
1:B:242:ASP:HB3	1:G:344:LYS:HE2	1.93	0.50
1:B:347:GLY:O	1:B:351:THR:HG23	2.12	0.50
2:e:69:GLN:C	2:e:71:PHE:N	2.70	0.50
2:f:77:HIS:HD2	2:f:78:MET:HG3	1.77	0.50
1:L:344:LYS:HE2	1:S:242:ASP:HB3	1.93	0.50
2:n:77:HIS:HD2	2:n:78:MET:HG3	1.77	0.50
2:n:128:ILE:HG22	2:n:129:ASP:N	2.26	0.50
2:x:128:ILE:HG22	2:x:129:ASP:N	2.26	0.50
2:b:77:HIS:HD2	2:b:78:MET:HG3	1.77	0.50
2:b:201:LEU:HA	2:b:226:ALA:HA	1.94	0.50
2:d:69:GLN:C	2:d:71:PHE:N	2.70	0.50
2:d:77:HIS:HD2	2:d:78:MET:HG3	1.77	0.50
2:d:128:ILE:HG22	2:d:129:ASP:N	2.26	0.50
1:E:344:LYS:HE2	1:T:242:ASP:HB3	1.93	0.50
2:j:201:LEU:HD12	2:j:226:ALA:HB2	1.94	0.50
2:k:128:ILE:HG22	2:k:129:ASP:N	2.26	0.50
1:M:347:GLY:O	1:M:351:THR:HG23	2.12	0.50
2:n:200:TYR:CE1	2:n:228:GLY:HA2	2.47	0.50
2:r:201:LEU:HA	2:r:226:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:69:GLN:C	2:w:71:PHE:H	2.19	0.50
2:w:128:ILE:HG22	2:w:129:ASP:N	2.26	0.50
2:x:14:ILE:HG21	2:x:44:LEU:HD22	1.92	0.50
1:A:67:ASP:O	1:M:71:VAL:CG1	2.56	0.50
2:a:69:GLN:C	2:a:71:PHE:N	2.70	0.50
2:a:201:LEU:HA	2:a:226:ALA:HA	1.94	0.50
2:b:201:LEU:HD12	2:b:226:ALA:HB2	1.94	0.50
1:C:242:ASP:HB3	1:M:344:LYS:HE2	1.93	0.50
2:c:201:LEU:HA	2:c:226:ALA:HA	1.94	0.50
2:d:200:TYR:CE1	2:d:228:GLY:HA2	2.47	0.50
1:E:347:GLY:O	1:E:351:THR:HG23	2.12	0.50
2:e:200:TYR:CE1	2:e:228:GLY:HA2	2.47	0.50
2:f:201:LEU:HA	2:f:226:ALA:HA	1.94	0.50
2:g:201:LEU:HA	2:g:226:ALA:HA	1.94	0.50
2:h:200:TYR:CE1	2:h:228:GLY:HA2	2.47	0.50
2:i:201:LEU:HA	2:i:226:ALA:HA	1.94	0.50
2:j:69:GLN:C	2:j:71:PHE:N	2.70	0.50
2:m:200:TYR:CE1	2:m:228:GLY:HA2	2.47	0.50
2:n:69:GLN:C	2:n:71:PHE:N	2.70	0.50
2:o:201:LEU:HA	2:o:226:ALA:HA	1.94	0.50
2:q:69:GLN:C	2:q:71:PHE:N	2.70	0.50
2:r:69:GLN:C	2:r:71:PHE:N	2.70	0.50
2:s:201:LEU:HA	2:s:226:ALA:HA	1.94	0.50
2:s:201:LEU:HD12	2:s:226:ALA:HB2	1.94	0.50
2:v:200:TYR:CE1	2:v:228:GLY:HA2	2.47	0.50
2:w:69:GLN:C	2:w:71:PHE:N	2.70	0.50
2:w:201:LEU:HD12	2:w:226:ALA:HB2	1.94	0.50
2:a:200:TYR:CE1	2:a:228:GLY:HA2	2.47	0.49
2:f:69:GLN:C	2:f:71:PHE:N	2.70	0.49
2:j:128:ILE:HG22	2:j:129:ASP:N	2.26	0.49
2:k:14:ILE:HG21	2:k:44:LEU:HD22	1.92	0.49
2:l:201:LEU:HA	2:l:226:ALA:HA	1.94	0.49
2:q:201:LEU:HA	2:q:226:ALA:HA	1.94	0.49
2:r:200:TYR:CE1	2:r:228:GLY:HA2	2.47	0.49
2:s:77:HIS:HD2	2:s:78:MET:HG3	1.77	0.49
2:t:201:LEU:HA	2:t:226:ALA:HA	1.94	0.49
2:v:69:GLN:C	2:v:71:PHE:H	2.19	0.49
2:a:77:HIS:HD2	2:a:78:MET:HG3	1.77	0.49
1:F:347:GLY:O	1:F:351:THR:HG23	2.12	0.49
2:f:128:ILE:HG22	2:f:129:ASP:N	2.26	0.49
2:g:200:TYR:CE1	2:g:228:GLY:HA2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:69:GLN:C	2:h:71:PHE:H	2.19	0.49
2:h:201:LEU:HA	2:h:226:ALA:HA	1.94	0.49
1:K:347:GLY:O	1:K:351:THR:HG23	2.12	0.49
2:m:128:ILE:HG22	2:m:129:ASP:N	2.26	0.49
1:Q:347:GLY:O	1:Q:351:THR:HG23	2.12	0.49
2:q:77:HIS:HD2	2:q:78:MET:HG3	1.77	0.49
2:q:128:ILE:HG22	2:q:129:ASP:N	2.26	0.49
2:v:201:LEU:HA	2:v:226:ALA:HA	1.94	0.49
1:C:347:GLY:O	1:C:351:THR:HG23	2.12	0.49
2:l:200:TYR:CE1	2:l:228:GLY:HA2	2.47	0.49
1:N:161:TRP:HE1	2:n:73:ARG:HD2	1.77	0.49
2:p:150:VAL:HA	2:p:165:PHE:HB3	1.95	0.49
2:p:200:TYR:CE1	2:p:228:GLY:HA2	2.47	0.49
2:v:150:VAL:HA	2:v:165:PHE:HB3	1.95	0.49
1:X:347:GLY:O	1:X:351:THR:HG23	2.12	0.49
2:y:150:VAL:HA	2:y:165:PHE:HB3	1.95	0.49
2:y:200:TYR:CE1	2:y:228:GLY:HA2	2.47	0.49
1:A:344:LYS:HE2	1:E:242:ASP:HB3	1.93	0.49
2:b:166:LYS:HD2	2:b:178:LEU:HB3	1.95	0.49
2:d:201:LEU:HD12	2:d:226:ALA:HB2	1.94	0.49
2:e:128:ILE:HG22	2:e:129:ASP:N	2.26	0.49
2:h:150:VAL:HA	2:h:165:PHE:HB3	1.95	0.49
2:n:150:VAL:HA	2:n:165:PHE:HB3	1.94	0.49
2:n:201:LEU:HD12	2:n:226:ALA:HB2	1.94	0.49
2:o:166:LYS:HD2	2:o:178:LEU:HB3	1.95	0.49
2:r:77:HIS:HD2	2:r:78:MET:HG3	1.77	0.49
1:T:347:GLY:O	1:T:351:THR:HG23	2.12	0.49
2:x:150:VAL:HA	2:x:165:PHE:HB3	1.95	0.49
2:c:201:LEU:HD12	2:c:226:ALA:HB2	1.94	0.49
2:e:94:GLN:HA	2:e:184:GLN:O	2.13	0.49
2:f:201:LEU:HD12	2:f:226:ALA:HB2	1.94	0.49
2:g:94:GLN:HA	2:g:184:GLN:O	2.13	0.49
2:i:166:LYS:HD2	2:i:178:LEU:HB3	1.95	0.49
1:J:67:ASP:O	1:N:71:VAL:CG1	2.56	0.49
2:j:94:GLN:HA	2:j:184:GLN:O	2.13	0.49
2:k:150:VAL:HA	2:k:165:PHE:HB3	1.95	0.49
2:p:166:LYS:HD2	2:p:178:LEU:HB3	1.95	0.49
1:S:67:ASP:O	1:Y:71:VAL:CG1	2.56	0.49
2:s:166:LYS:HD2	2:s:178:LEU:HB3	1.95	0.49
2:w:94:GLN:HA	2:w:184:GLN:O	2.13	0.49
2:y:166:LYS:HD2	2:y:178:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:O	1:P:71:VAL:CG1	2.56	0.49
2:c:94:GLN:HA	2:c:184:GLN:O	2.13	0.49
2:d:150:VAL:HA	2:d:165:PHE:HB3	1.95	0.49
2:e:201:LEU:HA	2:e:226:ALA:HA	1.94	0.49
1:G:347:GLY:O	1:G:351:THR:HG23	2.12	0.49
2:g:69:GLN:C	2:g:71:PHE:N	2.70	0.49
1:I:347:GLY:O	1:I:351:THR:HG23	2.12	0.49
2:l:94:GLN:HA	2:l:184:GLN:O	2.13	0.49
2:m:94:GLN:HA	2:m:184:GLN:O	2.13	0.49
2:m:201:LEU:HA	2:m:226:ALA:HA	1.94	0.49
2:a:201:LEU:HD12	2:a:226:ALA:HB2	1.94	0.49
2:b:128:ILE:HG22	2:b:129:ASP:N	2.26	0.49
2:c:69:GLN:C	2:c:71:PHE:N	2.70	0.49
2:c:200:TYR:CE1	2:c:228:GLY:HA2	2.47	0.49
2:d:94:GLN:HA	2:d:184:GLN:O	2.13	0.49
2:n:15:LEU:HD11	2:n:30:ARG:HD2	1.95	0.49
2:n:94:GLN:HA	2:n:184:GLN:O	2.13	0.49
2:p:77:HIS:HD2	2:p:78:MET:HG3	1.77	0.49
2:r:201:LEU:HD12	2:r:226:ALA:HB2	1.94	0.49
2:t:69:GLN:C	2:t:71:PHE:N	2.70	0.49
2:t:94:GLN:HA	2:t:184:GLN:O	2.13	0.49
2:t:201:LEU:HD12	2:t:226:ALA:HB2	1.94	0.49
2:v:53:LEU:HD12	2:v:54:PRO:HD2	1.95	0.49
2:y:69:GLN:C	2:y:71:PHE:N	2.70	0.49
2:b:15:LEU:HD11	2:b:30:ARG:HD2	1.95	0.49
1:D:71:VAL:CG1	1:W:67:ASP:O	2.56	0.49
2:d:15:LEU:HD11	2:d:30:ARG:HD2	1.95	0.49
2:h:53:LEU:HD12	2:h:54:PRO:HD2	1.95	0.49
2:j:15:LEU:HD11	2:j:30:ARG:HD2	1.95	0.49
1:L:148:ARG:NH1	1:L:181:GLN:O	2.46	0.49
1:L:347:GLY:O	1:L:351:THR:HG23	2.12	0.49
2:l:69:GLN:C	2:l:71:PHE:N	2.70	0.49
1:O:347:GLY:O	1:O:351:THR:HG23	2.12	0.49
2:o:77:HIS:HD2	2:o:78:MET:HG3	1.77	0.49
2:p:94:GLN:HA	2:p:184:GLN:O	2.13	0.49
2:t:200:TYR:CE1	2:t:228:GLY:HA2	2.47	0.49
1:V:242:ASP:HB3	1:Y:344:LYS:HE2	1.93	0.49
2:w:15:LEU:HD11	2:w:30:ARG:HD2	1.95	0.49
2:w:150:VAL:HA	2:w:165:PHE:HB3	1.95	0.49
2:y:94:GLN:HA	2:y:184:GLN:O	2.13	0.49
2:c:53:LEU:HD12	2:c:54:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:201:LEU:HD12	2:g:226:ALA:HB2	1.94	0.49
1:H:165:LEU:O	1:H:169:GLU:HG2	2.13	0.49
1:H:242:ASP:HB3	1:P:344:LYS:HE2	1.93	0.49
1:J:165:LEU:O	1:J:169:GLU:HG2	2.13	0.49
2:j:150:VAL:HA	2:j:165:PHE:HB3	1.95	0.49
2:j:166:LYS:HD2	2:j:178:LEU:HB3	1.95	0.49
1:M:161:TRP:HE1	2:m:73:ARG:HD2	1.77	0.49
2:p:69:GLN:C	2:p:71:PHE:N	2.70	0.49
2:q:200:TYR:CE1	2:q:228:GLY:HA2	2.47	0.49
2:q:201:LEU:HD12	2:q:226:ALA:HB2	1.94	0.49
2:s:128:ILE:HG22	2:s:129:ASP:N	2.26	0.49
1:V:165:LEU:O	1:V:169:GLU:HG2	2.13	0.49
2:v:77:HIS:HD2	2:v:78:MET:HG3	1.77	0.49
2:v:94:GLN:HA	2:v:184:GLN:O	2.13	0.49
2:v:201:LEU:HD12	2:v:226:ALA:HB2	1.94	0.49
1:W:165:LEU:O	1:W:169:GLU:HG2	2.13	0.49
2:x:200:TYR:CE1	2:x:228:GLY:HA2	2.47	0.49
2:y:77:HIS:HD2	2:y:78:MET:HG3	1.77	0.49
2:a:128:ILE:HG22	2:a:129:ASP:N	2.26	0.49
1:C:148:ARG:NH1	1:C:181:GLN:O	2.46	0.49
2:c:15:LEU:HD11	2:c:30:ARG:HD2	1.95	0.49
2:e:15:LEU:HD11	2:e:30:ARG:HD2	1.95	0.49
2:f:200:TYR:CE1	2:f:228:GLY:HA2	2.47	0.49
2:h:94:GLN:HA	2:h:184:GLN:O	2.13	0.49
2:h:201:LEU:HD12	2:h:226:ALA:HB2	1.94	0.49
2:i:77:HIS:HD2	2:i:78:MET:HG3	1.77	0.49
2:k:200:TYR:CE1	2:k:228:GLY:HA2	2.47	0.49
2:l:201:LEU:HD12	2:l:226:ALA:HB2	1.94	0.49
2:m:201:LEU:HD12	2:m:226:ALA:HB2	1.94	0.49
2:s:15:LEU:HD11	2:s:30:ARG:HD2	1.95	0.49
2:s:94:GLN:HA	2:s:184:GLN:O	2.13	0.49
2:s:200:TYR:CE1	2:s:228:GLY:HA2	2.47	0.49
1:T:148:ARG:NH1	1:T:181:GLN:O	2.46	0.49
1:T:242:ASP:OD1	1:T:242:ASP:N	2.46	0.49
2:t:53:LEU:HD12	2:t:54:PRO:HD2	1.95	0.49
2:w:166:LYS:HD2	2:w:178:LEU:HB3	1.95	0.49
2:w:201:LEU:HA	2:w:226:ALA:HA	1.94	0.49
2:a:94:GLN:HA	2:a:184:GLN:O	2.13	0.48
2:b:200:TYR:CE1	2:b:228:GLY:HA2	2.47	0.48
1:C:242:ASP:OD1	1:C:242:ASP:N	2.46	0.48
2:c:165:PHE:CD2	2:c:167:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:166:LYS:HD2	2:f:178:LEU:HB3	1.95	0.48
2:g:53:LEU:HD12	2:g:54:PRO:HD2	1.95	0.48
2:g:77:HIS:HD2	2:g:78:MET:HG3	1.77	0.48
2:g:128:ILE:HG22	2:g:129:ASP:N	2.26	0.48
2:h:69:GLN:C	2:h:71:PHE:N	2.70	0.48
2:h:77:HIS:HD2	2:h:78:MET:HG3	1.77	0.48
2:j:201:LEU:HA	2:j:226:ALA:HA	1.94	0.48
2:l:166:LYS:HD2	2:l:178:LEU:HB3	1.95	0.48
2:m:166:LYS:HD2	2:m:178:LEU:HB3	1.95	0.48
2:q:166:LYS:HD2	2:q:178:LEU:HB3	1.95	0.48
2:r:94:GLN:HA	2:r:184:GLN:O	2.13	0.48
2:t:15:LEU:HD11	2:t:30:ARG:HD2	1.95	0.48
2:t:165:PHE:CD2	2:t:167:ILE:HD11	2.48	0.48
2:w:53:LEU:HD12	2:w:54:PRO:HD2	1.95	0.48
1:D:71:VAL:HA	1:W:70:ALA:CB	2.44	0.48
2:e:201:LEU:HD12	2:e:226:ALA:HB2	1.94	0.48
2:j:53:LEU:HD12	2:j:54:PRO:HD2	1.95	0.48
2:k:53:LEU:HD12	2:k:54:PRO:HD2	1.95	0.48
2:l:77:HIS:HD2	2:l:78:MET:HG3	1.77	0.48
2:l:128:ILE:HG22	2:l:129:ASP:N	2.26	0.48
2:l:165:PHE:CD2	2:l:167:ILE:HD11	2.48	0.48
2:m:15:LEU:HD11	2:m:30:ARG:HD2	1.95	0.48
2:o:53:LEU:HD12	2:o:54:PRO:HD2	1.95	0.48
2:o:201:LEU:HD12	2:o:226:ALA:HB2	1.94	0.48
2:q:150:VAL:HA	2:q:165:PHE:HB3	1.95	0.48
2:r:128:ILE:HG22	2:r:129:ASP:N	2.26	0.48
1:V:161:TRP:HE1	2:v:73:ARG:HD2	1.79	0.48
2:v:69:GLN:C	2:v:71:PHE:N	2.70	0.48
1:A:70:ALA:CB	1:M:71:VAL:HA	2.44	0.48
2:a:53:LEU:HD12	2:a:54:PRO:HD2	1.95	0.48
2:b:94:GLN:HA	2:b:184:GLN:O	2.13	0.48
2:e:165:PHE:CD2	2:e:167:ILE:HD11	2.48	0.48
1:G:165:LEU:O	1:G:169:GLU:HG2	2.13	0.48
2:g:165:PHE:CD2	2:g:167:ILE:HD11	2.48	0.48
1:H:161:TRP:HE1	2:h:73:ARG:HD2	1.79	0.48
2:i:201:LEU:HD12	2:i:226:ALA:HB2	1.94	0.48
1:J:70:ALA:CB	1:N:71:VAL:HA	2.44	0.48
1:L:70:ALA:CB	1:V:71:VAL:HA	2.44	0.48
1:L:165:LEU:O	1:L:169:GLU:HG2	2.13	0.48
2:l:15:LEU:HD11	2:l:30:ARG:HD2	1.95	0.48
2:m:165:PHE:CD2	2:m:167:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:165:PHE:CD2	2:s:167:ILE:HD11	2.48	0.48
2:w:165:PHE:CD2	2:w:167:ILE:HD11	2.48	0.48
2:x:53:LEU:HD12	2:x:54:PRO:HD2	1.95	0.48
1:B:70:ALA:CB	1:P:71:VAL:HA	2.44	0.48
2:b:165:PHE:CD2	2:b:167:ILE:HD11	2.48	0.48
1:D:148:ARG:NH1	1:D:181:GLN:O	2.46	0.48
2:d:201:LEU:HA	2:d:226:ALA:HA	1.94	0.48
2:e:166:LYS:HD2	2:e:178:LEU:HB3	1.95	0.48
2:f:150:VAL:HA	2:f:165:PHE:HB3	1.95	0.48
1:G:70:ALA:CB	1:H:71:VAL:HA	2.44	0.48
1:G:161:TRP:HE1	2:g:73:ARG:HD2	1.78	0.48
2:g:15:LEU:HD11	2:g:30:ARG:HD2	1.95	0.48
2:i:53:LEU:HD12	2:i:54:PRO:HD2	1.95	0.48
2:j:165:PHE:CD2	2:j:167:ILE:HD11	2.48	0.48
2:l:150:VAL:HA	2:l:165:PHE:HB3	1.95	0.48
2:o:150:VAL:HA	2:o:165:PHE:HB3	1.95	0.48
2:r:53:LEU:HD12	2:r:54:PRO:HD2	1.95	0.48
2:r:165:PHE:CD2	2:r:167:ILE:HD11	2.48	0.48
1:S:70:ALA:CB	1:Y:71:VAL:HA	2.44	0.48
2:a:165:PHE:CD2	2:a:167:ILE:HD11	2.48	0.48
1:B:165:LEU:O	1:B:169:GLU:HG2	2.13	0.48
1:C:70:ALA:CB	1:X:71:VAL:HA	2.44	0.48
1:F:70:ALA:CB	1:O:71:VAL:HA	2.44	0.48
2:g:150:VAL:HA	2:g:165:PHE:HB3	1.94	0.48
2:g:166:LYS:HD2	2:g:178:LEU:HB3	1.95	0.48
2:h:166:LYS:HD2	2:h:178:LEU:HB3	1.95	0.48
1:I:71:VAL:HA	1:Q:70:ALA:CB	2.44	0.48
2:i:150:VAL:HA	2:i:165:PHE:HB3	1.95	0.48
1:K:71:VAL:CG1	1:T:67:ASP:O	2.56	0.48
1:K:71:VAL:HA	1:T:70:ALA:CB	2.44	0.48
2:k:15:LEU:HD11	2:k:30:ARG:HD2	1.95	0.48
2:l:53:LEU:HD12	2:l:54:PRO:HD2	1.95	0.48
2:m:150:VAL:HA	2:m:165:PHE:HB3	1.95	0.48
1:N:148:ARG:NH1	1:N:181:GLN:O	2.46	0.48
2:n:201:LEU:HA	2:n:226:ALA:HA	1.94	0.48
2:q:15:LEU:HD11	2:q:30:ARG:HD2	1.95	0.48
2:q:53:LEU:HD12	2:q:54:PRO:HD2	1.95	0.48
2:t:166:LYS:HD2	2:t:178:LEU:HB3	1.95	0.48
2:v:166:LYS:HD2	2:v:178:LEU:HB3	1.95	0.48
2:x:15:LEU:HD11	2:x:30:ARG:HD2	1.95	0.48
2:x:201:LEU:HA	2:x:226:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:y:165:PHE:CD2	2:y:167:ILE:HD11	2.48	0.48
2:c:150:VAL:HA	2:c:165:PHE:HB3	1.95	0.48
2:c:166:LYS:HD2	2:c:178:LEU:HB3	1.95	0.48
1:D:70:ALA:CB	1:W:71:VAL:HA	2.44	0.48
2:f:15:LEU:HD11	2:f:30:ARG:HD2	1.95	0.48
1:J:71:VAL:HA	1:N:70:ALA:CB	2.44	0.48
2:k:201:LEU:HA	2:k:226:ALA:HA	1.94	0.48
2:p:165:PHE:CD2	2:p:167:ILE:HD11	2.48	0.48
1:Q:161:TRP:HE1	2:q:73:ARG:HD2	1.79	0.48
2:r:150:VAL:HA	2:r:165:PHE:HB3	1.95	0.48
1:T:165:LEU:O	1:T:169:GLU:HG2	2.13	0.48
2:w:200:TYR:CE1	2:w:228:GLY:HA2	2.47	0.48
1:C:71:VAL:CG1	1:X:67:ASP:O	2.56	0.48
1:C:165:LEU:O	1:C:169:GLU:HG2	2.13	0.48
1:D:165:LEU:O	1:D:169:GLU:HG2	2.13	0.48
2:d:165:PHE:CD2	2:d:167:ILE:HD11	2.48	0.48
2:f:53:LEU:HD12	2:f:54:PRO:HD2	1.95	0.48
1:G:71:VAL:HA	1:H:70:ALA:CB	2.44	0.48
2:i:200:TYR:CE1	2:i:228:GLY:HA2	2.47	0.48
1:K:70:ALA:CB	1:T:71:VAL:HA	2.44	0.48
1:L:71:VAL:HA	1:V:70:ALA:CB	2.44	0.48
1:M:148:ARG:NH1	1:M:181:GLN:O	2.46	0.48
2:n:53:LEU:HD12	2:n:54:PRO:HD2	1.95	0.48
2:n:165:PHE:CD2	2:n:167:ILE:HD11	2.48	0.48
2:o:165:PHE:CD2	2:o:167:ILE:HD11	2.48	0.48
1:Q:165:LEU:O	1:Q:169:GLU:HG2	2.13	0.48
2:r:166:LYS:HD2	2:r:178:LEU:HB3	1.95	0.48
1:S:165:LEU:O	1:S:169:GLU:HG2	2.13	0.48
2:t:150:VAL:HA	2:t:165:PHE:HB3	1.95	0.48
1:W:148:ARG:NH1	1:W:181:GLN:O	2.46	0.48
2:x:166:LYS:HD2	2:x:178:LEU:HB3	1.95	0.48
2:y:201:LEU:HA	2:y:226:ALA:HA	1.94	0.48
1:A:71:VAL:HA	1:M:70:ALA:CB	2.44	0.48
2:a:42:LEU:HD23	2:a:222:GLU:OE2	2.14	0.48
2:a:150:VAL:HA	2:a:165:PHE:HB3	1.95	0.48
2:a:166:LYS:HD2	2:a:178:LEU:HB3	1.95	0.48
1:C:67:ASP:O	1:X:71:VAL:CG1	2.56	0.48
1:C:71:VAL:HA	1:X:70:ALA:CB	2.44	0.48
2:d:53:LEU:HD12	2:d:54:PRO:HD2	1.95	0.48
2:e:53:LEU:HD12	2:e:54:PRO:HD2	1.95	0.48
1:F:165:LEU:O	1:F:169:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:161:TRP:HE1	2:i:73:ARG:HD2	1.79	0.48
2:i:165:PHE:CD2	2:i:167:ILE:HD11	2.48	0.48
1:J:148:ARG:NH1	1:J:181:GLN:O	2.46	0.48
2:j:200:TYR:CE1	2:j:228:GLY:HA2	2.47	0.48
2:k:166:LYS:HD2	2:k:178:LEU:HB3	1.95	0.48
1:M:165:LEU:O	1:M:169:GLU:HG2	2.13	0.48
1:N:165:LEU:O	1:N:169:GLU:HG2	2.13	0.48
1:N:168:VAL:HG21	1:N:200:ILE:HD12	1.96	0.48
2:o:200:TYR:CE1	2:o:228:GLY:HA2	2.47	0.48
2:r:42:LEU:HD23	2:r:222:GLU:OE2	2.14	0.48
2:s:150:VAL:HA	2:s:165:PHE:HB3	1.95	0.48
2:x:94:GLN:HA	2:x:184:GLN:O	2.13	0.48
2:b:150:VAL:HA	2:b:165:PHE:HB3	1.95	0.48
1:D:168:VAL:HG21	1:D:200:ILE:HD12	1.96	0.48
1:E:148:ARG:NH1	1:E:181:GLN:O	2.46	0.48
1:E:165:LEU:O	1:E:169:GLU:HG2	2.13	0.48
2:f:42:LEU:HD23	2:f:222:GLU:OE2	2.14	0.48
2:i:22:VAL:HA	2:i:127:GLY:O	2.14	0.48
2:k:22:VAL:HA	2:k:127:GLY:O	2.14	0.48
1:O:161:TRP:HE1	2:o:73:ARG:HD2	1.79	0.48
1:P:148:ARG:NH1	1:P:181:GLN:O	2.46	0.48
2:p:201:LEU:HA	2:p:226:ALA:HA	1.94	0.48
1:X:165:LEU:O	1:X:169:GLU:HG2	2.13	0.48
2:x:22:VAL:HA	2:x:127:GLY:O	2.14	0.48
2:x:165:PHE:CD2	2:x:167:ILE:HD11	2.48	0.48
2:c:77:HIS:HD2	2:c:78:MET:HG3	1.77	0.48
2:d:166:LYS:HD2	2:d:178:LEU:HB3	1.95	0.48
1:E:161:TRP:HE1	2:e:73:ARG:HD2	1.79	0.48
2:e:150:VAL:HA	2:e:165:PHE:HB3	1.95	0.48
1:F:71:VAL:HA	1:O:70:ALA:CB	2.44	0.48
1:F:161:TRP:HE1	2:f:73:ARG:HD2	1.79	0.48
1:F:168:VAL:HG21	1:F:200:ILE:HD12	1.96	0.48
1:H:148:ARG:NH1	1:H:181:GLN:O	2.46	0.48
1:I:70:ALA:CB	1:Q:71:VAL:HA	2.44	0.48
1:I:165:LEU:O	1:I:169:GLU:HG2	2.13	0.48
2:i:42:LEU:HD23	2:i:222:GLU:OE2	2.14	0.48
2:j:22:VAL:HA	2:j:127:GLY:O	2.14	0.48
1:K:67:ASP:O	1:T:71:VAL:CG1	2.56	0.48
1:K:165:LEU:O	1:K:169:GLU:HG2	2.13	0.48
2:k:94:GLN:HA	2:k:184:GLN:O	2.13	0.48
2:k:165:PHE:CD2	2:k:167:ILE:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:53:LEU:HD12	2:m:54:PRO:HD2	1.95	0.48
2:o:22:VAL:HA	2:o:127:GLY:O	2.14	0.48
2:o:42:LEU:HD23	2:o:222:GLU:OE2	2.14	0.48
1:Q:168:VAL:HG21	1:Q:200:ILE:HD12	1.96	0.48
2:q:94:GLN:HA	2:q:184:GLN:O	2.13	0.48
2:s:42:LEU:HD23	2:s:222:GLU:OE2	2.14	0.48
2:s:53:LEU:HD12	2:s:54:PRO:HD2	1.95	0.48
2:v:15:LEU:HD11	2:v:30:ARG:HD2	1.95	0.48
2:w:22:VAL:HA	2:w:127:GLY:O	2.14	0.48
1:A:168:VAL:HG21	1:A:200:ILE:HD12	1.96	0.47
1:E:71:VAL:HA	1:R:70:ALA:CB	2.44	0.47
1:E:168:VAL:HG21	1:E:200:ILE:HD12	1.96	0.47
2:h:15:LEU:HD11	2:h:30:ARG:HD2	1.95	0.47
1:L:161:TRP:HE1	2:l:73:ARG:HD2	1.79	0.47
1:M:168:VAL:HG21	1:M:200:ILE:HD12	1.96	0.47
2:n:22:VAL:HA	2:n:127:GLY:O	2.14	0.47
2:n:166:LYS:HD2	2:n:178:LEU:HB3	1.95	0.47
1:O:165:LEU:O	1:O:169:GLU:HG2	2.13	0.47
2:o:94:GLN:HA	2:o:184:GLN:O	2.13	0.47
2:q:42:LEU:HD23	2:q:222:GLU:OE2	2.14	0.47
2:t:77:HIS:HD2	2:t:78:MET:HG3	1.77	0.47
1:Y:148:ARG:NH1	1:Y:181:GLN:O	2.46	0.47
2:a:15:LEU:HD11	2:a:30:ARG:HD2	1.95	0.47
2:b:42:LEU:HD23	2:b:222:GLU:OE2	2.14	0.47
2:b:53:LEU:HD12	2:b:54:PRO:HD2	1.95	0.47
1:C:161:TRP:HE1	2:c:73:ARG:HD2	1.79	0.47
2:c:22:VAL:HA	2:c:127:GLY:O	2.14	0.47
2:d:42:LEU:HD23	2:d:222:GLU:OE2	2.14	0.47
2:f:94:GLN:HA	2:f:184:GLN:O	2.13	0.47
2:g:22:VAL:HA	2:g:127:GLY:O	2.14	0.47
2:h:165:PHE:CD2	2:h:167:ILE:HD11	2.48	0.47
2:l:22:VAL:HA	2:l:127:GLY:O	2.14	0.47
1:M:242:ASP:HB3	1:R:344:LYS:HE2	1.95	0.47
1:P:161:TRP:HE1	2:p:73:ARG:HD2	1.79	0.47
2:q:22:VAL:HA	2:q:127:GLY:O	2.14	0.47
1:R:168:VAL:HG21	1:R:200:ILE:HD12	1.96	0.47
2:r:15:LEU:HD11	2:r:30:ARG:HD2	1.95	0.47
2:t:22:VAL:HA	2:t:127:GLY:O	2.14	0.47
1:V:148:ARG:NH1	1:V:181:GLN:O	2.46	0.47
1:W:161:TRP:HE1	2:w:73:ARG:HD2	1.79	0.47
1:Y:161:TRP:HE1	2:y:73:ARG:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:22:VAL:HA	2:d:127:GLY:O	2.14	0.47
2:e:77:HIS:HD2	2:e:78:MET:HG3	1.77	0.47
2:i:94:GLN:HA	2:i:184:GLN:O	2.13	0.47
2:m:77:HIS:HD2	2:m:78:MET:HG3	1.77	0.47
2:n:42:LEU:HD23	2:n:222:GLU:OE2	2.14	0.47
2:o:15:LEU:HD11	2:o:30:ARG:HD2	1.95	0.47
1:P:165:LEU:O	1:P:169:GLU:HG2	2.13	0.47
2:p:15:LEU:HD11	2:p:30:ARG:HD2	1.95	0.47
2:t:42:LEU:HD23	2:t:222:GLU:OE2	2.14	0.47
2:v:165:PHE:CD2	2:v:167:ILE:HD11	2.48	0.47
2:c:42:LEU:HD23	2:c:222:GLU:OE2	2.14	0.47
2:i:15:LEU:HD11	2:i:30:ARG:HD2	1.95	0.47
1:J:161:TRP:HE1	2:j:73:ARG:HD2	1.79	0.47
1:T:161:TRP:HE1	2:t:73:ARG:HD2	1.79	0.47
2:y:15:LEU:HD11	2:y:30:ARG:HD2	1.95	0.47
2:a:22:VAL:HA	2:a:127:GLY:O	2.14	0.47
2:f:22:VAL:HA	2:f:127:GLY:O	2.14	0.47
2:g:42:LEU:HD23	2:g:222:GLU:OE2	2.14	0.47
2:i:69:GLN:C	2:i:71:PHE:N	2.70	0.47
1:R:165:LEU:O	1:R:169:GLU:HG2	2.13	0.47
1:S:71:VAL:HA	1:Y:70:ALA:CB	2.44	0.47
2:w:42:LEU:HD23	2:w:222:GLU:OE2	2.14	0.47
1:Y:165:LEU:O	1:Y:169:GLU:HG2	2.13	0.47
2:y:22:VAL:HA	2:y:127:GLY:O	2.14	0.47
2:f:165:PHE:CD2	2:f:167:ILE:HD11	2.48	0.47
1:H:168:VAL:HG21	1:H:200:ILE:HD12	1.96	0.47
2:j:42:LEU:HD23	2:j:222:GLU:OE2	2.14	0.47
2:k:42:LEU:HD23	2:k:222:GLU:OE2	2.14	0.47
2:l:42:LEU:HD23	2:l:222:GLU:OE2	2.14	0.47
2:p:22:VAL:HA	2:p:127:GLY:O	2.14	0.47
2:q:165:PHE:CD2	2:q:167:ILE:HD11	2.48	0.47
2:r:22:VAL:HA	2:r:127:GLY:O	2.14	0.47
2:s:22:VAL:HA	2:s:127:GLY:O	2.14	0.47
2:v:42:LEU:HD23	2:v:222:GLU:OE2	2.14	0.47
1:A:161:TRP:HE1	2:a:73:ARG:HD2	1.79	0.47
1:A:165:LEU:O	1:A:169:GLU:HG2	2.13	0.47
1:B:71:VAL:HA	1:P:70:ALA:CB	2.44	0.47
1:B:161:TRP:HE1	2:b:73:ARG:HD2	1.79	0.47
2:b:22:VAL:HA	2:b:127:GLY:O	2.14	0.47
1:C:73:MET:HB3	1:C:108:PHE:CE2	2.50	0.47
2:d:165:PHE:HD2	2:d:167:ILE:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:MET:HB3	1:G:108:PHE:CE2	2.50	0.47
2:h:42:LEU:HD23	2:h:222:GLU:OE2	2.14	0.47
1:I:67:ASP:O	1:Q:71:VAL:CG1	2.56	0.47
1:I:73:MET:HB3	1:I:108:PHE:CE2	2.50	0.47
1:L:73:MET:HB3	1:L:108:PHE:CE2	2.50	0.47
1:M:73:MET:HB3	1:M:108:PHE:CE2	2.50	0.47
2:m:207:LEU:HG	2:m:220:LEU:HD12	1.97	0.47
1:O:73:MET:HB3	1:O:108:PHE:CE2	2.50	0.47
2:o:69:GLN:C	2:o:71:PHE:N	2.70	0.47
1:S:148:ARG:NH1	1:S:181:GLN:O	2.46	0.47
1:S:161:TRP:HE1	2:s:73:ARG:HD2	1.79	0.47
1:T:73:MET:HB3	1:T:108:PHE:CE2	2.50	0.47
1:V:168:VAL:HG21	1:V:200:ILE:HD12	1.96	0.47
1:W:168:VAL:HG21	1:W:200:ILE:HD12	1.96	0.47
2:x:42:LEU:HD23	2:x:222:GLU:OE2	2.14	0.47
1:A:73:MET:HB3	1:A:108:PHE:CE2	2.50	0.47
1:B:148:ARG:NH1	1:B:181:GLN:O	2.46	0.47
1:E:71:VAL:CG1	1:R:67:ASP:O	2.59	0.47
1:E:73:MET:HB3	1:E:108:PHE:CE2	2.50	0.47
2:e:207:LEU:HG	2:e:220:LEU:HD12	1.97	0.47
1:J:168:VAL:HG21	1:J:200:ILE:HD12	1.96	0.47
1:K:161:TRP:HE1	2:k:73:ARG:HD2	1.79	0.47
2:n:165:PHE:HD2	2:n:167:ILE:HD11	1.80	0.47
1:P:168:VAL:HG21	1:P:200:ILE:HD12	1.96	0.47
1:R:73:MET:HB3	1:R:108:PHE:CE2	2.50	0.47
2:v:22:VAL:HA	2:v:127:GLY:O	2.14	0.47
1:Y:168:VAL:HG21	1:Y:200:ILE:HD12	1.96	0.47
2:y:53:LEU:HD12	2:y:54:PRO:HD2	1.95	0.47
2:e:22:VAL:HA	2:e:127:GLY:O	2.14	0.47
2:h:22:VAL:HA	2:h:127:GLY:O	2.14	0.47
1:I:168:VAL:HG21	1:I:200:ILE:HD12	1.96	0.47
1:O:168:VAL:HG21	1:O:200:ILE:HD12	1.96	0.47
2:p:42:LEU:HD23	2:p:222:GLU:OE2	2.14	0.47
2:p:53:LEU:HD12	2:p:54:PRO:HD2	1.95	0.47
2:p:207:LEU:HG	2:p:220:LEU:HD12	1.97	0.47
1:V:73:MET:HB3	1:V:108:PHE:CE2	2.50	0.47
2:y:207:LEU:HG	2:y:220:LEU:HD12	1.97	0.47
2:e:42:LEU:HD23	2:e:222:GLU:OE2	2.14	0.47
1:F:73:MET:HB3	1:F:108:PHE:CE2	2.50	0.47
1:H:73:MET:HB3	1:H:108:PHE:CE2	2.50	0.47
2:h:165:PHE:HD2	2:h:167:ILE:HD11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:207:LEU:HG	2:h:220:LEU:HD12	1.97	0.47
1:K:168:VAL:HG21	1:K:200:ILE:HD12	1.96	0.47
2:m:42:LEU:HD23	2:m:222:GLU:OE2	2.14	0.47
2:o:207:LEU:HG	2:o:220:LEU:HD12	1.97	0.47
1:Q:73:MET:HB3	1:Q:108:PHE:CE2	2.50	0.47
2:v:165:PHE:HD2	2:v:167:ILE:HD11	1.80	0.47
2:v:207:LEU:HG	2:v:220:LEU:HD12	1.97	0.47
2:a:165:PHE:HD2	2:a:167:ILE:HD11	1.80	0.46
1:C:168:VAL:HG21	1:C:200:ILE:HD12	1.96	0.46
1:F:71:VAL:CG1	1:O:67:ASP:O	2.56	0.46
1:G:168:VAL:HG21	1:G:200:ILE:HD12	1.96	0.46
2:g:165:PHE:HD2	2:g:167:ILE:HD11	1.80	0.46
2:i:207:LEU:HG	2:i:220:LEU:HD12	1.97	0.46
1:L:168:VAL:HG21	1:L:200:ILE:HD12	1.96	0.46
2:m:22:VAL:HA	2:m:127:GLY:O	2.14	0.46
1:T:168:VAL:HG21	1:T:200:ILE:HD12	1.96	0.46
1:X:161:TRP:HE1	2:x:73:ARG:HD2	1.79	0.46
1:X:168:VAL:HG21	1:X:200:ILE:HD12	1.96	0.46
2:y:42:LEU:HD23	2:y:222:GLU:OE2	2.14	0.46
1:B:168:VAL:HG21	1:B:200:ILE:HD12	1.96	0.46
2:l:165:PHE:HD2	2:l:167:ILE:HD11	1.80	0.46
2:r:165:PHE:HD2	2:r:167:ILE:HD11	1.80	0.46
1:Y:73:MET:HB3	1:Y:108:PHE:CE2	2.50	0.46
1:A:71:VAL:CG1	1:M:67:ASP:O	2.56	0.46
1:N:73:MET:HB3	1:N:108:PHE:CE2	2.50	0.46
1:P:73:MET:HB3	1:P:108:PHE:CE2	2.50	0.46
1:R:148:ARG:NH1	1:R:181:GLN:O	2.46	0.46
1:S:168:VAL:HG21	1:S:200:ILE:HD12	1.96	0.46
2:w:165:PHE:HD2	2:w:167:ILE:HD11	1.80	0.46
2:x:165:PHE:HD2	2:x:167:ILE:HD11	1.80	0.46
2:x:207:LEU:HG	2:x:220:LEU:HD12	1.97	0.46
1:A:148:ARG:NH1	1:A:181:GLN:O	2.46	0.46
1:D:73:MET:HB3	1:D:108:PHE:CE2	2.50	0.46
2:j:165:PHE:HD2	2:j:167:ILE:HD11	1.80	0.46
2:k:207:LEU:HG	2:k:220:LEU:HD12	1.97	0.46
2:l:207:LEU:HG	2:l:220:LEU:HD12	1.97	0.46
2:m:150:VAL:HG13	2:m:165:PHE:CD1	2.51	0.46
1:R:161:TRP:HE1	2:r:73:ARG:HD2	1.79	0.46
1:X:148:ARG:NH1	1:X:181:GLN:O	2.46	0.46
2:e:150:VAL:HG13	2:e:165:PHE:CD1	2.51	0.46
2:g:207:LEU:HG	2:g:220:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:150:VAL:HG13	2:h:165:PHE:CD1	2.51	0.46
1:J:73:MET:HB3	1:J:108:PHE:CE2	2.50	0.46
2:k:150:VAL:HG13	2:k:165:PHE:CD1	2.51	0.46
2:k:165:PHE:HD2	2:k:167:ILE:HD11	1.80	0.46
2:r:150:VAL:HG13	2:r:165:PHE:CD1	2.51	0.46
2:v:150:VAL:HG13	2:v:165:PHE:CD1	2.51	0.46
2:w:207:LEU:HG	2:w:220:LEU:HD12	1.97	0.46
2:a:150:VAL:HG13	2:a:165:PHE:CD1	2.51	0.46
2:a:207:LEU:HG	2:a:220:LEU:HD12	1.97	0.46
2:c:150:VAL:HG13	2:c:165:PHE:CD1	2.51	0.46
2:f:150:VAL:HG13	2:f:165:PHE:CD1	2.51	0.46
2:i:150:VAL:HG13	2:i:165:PHE:CD1	2.51	0.46
2:j:207:LEU:HG	2:j:220:LEU:HD12	1.97	0.46
1:K:73:MET:HB3	1:K:108:PHE:CE2	2.50	0.46
1:K:148:ARG:NH1	1:K:181:GLN:O	2.46	0.46
2:o:150:VAL:HG13	2:o:165:PHE:CD1	2.51	0.46
2:q:150:VAL:HG13	2:q:165:PHE:CD1	2.51	0.46
2:r:207:LEU:HG	2:r:220:LEU:HD12	1.97	0.46
1:S:73:MET:HB3	1:S:108:PHE:CE2	2.50	0.46
2:t:150:VAL:HG13	2:t:165:PHE:CD1	2.51	0.46
1:W:73:MET:HB3	1:W:108:PHE:CE2	2.50	0.46
2:w:77:HIS:HD2	2:w:78:MET:HG3	1.77	0.46
1:X:279:SER:O	1:X:279:SER:OG	2.34	0.46
2:x:150:VAL:HG13	2:x:165:PHE:CD1	2.51	0.46
1:B:73:MET:HB3	1:B:108:PHE:CE2	2.50	0.46
2:c:43:THR:O	2:c:44:LEU:HD23	2.16	0.46
2:f:165:PHE:HD2	2:f:167:ILE:HD11	1.80	0.46
2:j:43:THR:O	2:j:44:LEU:HD23	2.16	0.46
1:K:279:SER:O	1:K:279:SER:OG	2.34	0.46
2:q:165:PHE:HD2	2:q:167:ILE:HD11	1.80	0.46
2:w:43:THR:O	2:w:44:LEU:HD23	2.16	0.46
1:F:67:ASP:O	1:O:71:VAL:CG1	2.56	0.46
2:s:43:THR:O	2:s:44:LEU:HD23	2.16	0.46
2:t:43:THR:O	2:t:44:LEU:HD23	2.16	0.46
1:X:73:MET:HB3	1:X:108:PHE:CE2	2.50	0.46
2:c:154:ALA:HB1	2:c:195:LEU:HD11	1.98	0.46
2:g:150:VAL:HG13	2:g:165:PHE:CD1	2.51	0.46
2:j:77:HIS:HD2	2:j:78:MET:HG3	1.77	0.46
2:j:94:GLN:HB3	2:j:185:ASN:HD22	1.81	0.46
1:S:71:VAL:CG1	1:Y:67:ASP:O	2.56	0.46
2:t:154:ALA:HB1	2:t:195:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:w:94:GLN:HB3	2:w:185:ASN:HD22	1.81	0.46
2:b:43:THR:O	2:b:44:LEU:HD23	2.16	0.46
2:b:207:LEU:HG	2:b:220:LEU:HD12	1.97	0.46
1:F:279:SER:O	1:F:279:SER:OG	2.34	0.46
2:g:64:LEU:O	2:g:66:CRO:HA31	2.16	0.46
2:p:43:THR:O	2:p:44:LEU:HD23	2.16	0.46
2:p:94:GLN:HB3	2:p:185:ASN:HD22	1.81	0.46
1:Q:279:SER:O	1:Q:279:SER:OG	2.34	0.46
2:q:94:GLN:HB3	2:q:185:ASN:HD22	1.81	0.46
2:v:94:GLN:HB3	2:v:185:ASN:HD22	1.81	0.46
2:v:154:ALA:HB1	2:v:195:LEU:HD11	1.98	0.46
2:y:43:THR:O	2:y:44:LEU:HD23	2.16	0.46
2:y:94:GLN:HB3	2:y:185:ASN:HD22	1.81	0.46
2:a:43:THR:O	2:a:44:LEU:HD23	2.16	0.45
2:a:94:GLN:HB3	2:a:185:ASN:HD22	1.81	0.45
1:B:71:VAL:CG1	1:P:67:ASP:O	2.56	0.45
2:b:69:GLN:C	2:b:71:PHE:N	2.70	0.45
2:c:94:GLN:HB3	2:c:185:ASN:HD22	1.81	0.45
2:f:94:GLN:HB3	2:f:185:ASN:HD22	1.81	0.45
2:f:207:LEU:HG	2:f:220:LEU:HD12	1.97	0.45
1:G:279:SER:O	1:G:279:SER:OG	2.34	0.45
2:h:94:GLN:HB3	2:h:185:ASN:HD22	1.81	0.45
2:h:154:ALA:HB1	2:h:195:LEU:HD11	1.98	0.45
2:i:43:THR:O	2:i:44:LEU:HD23	2.16	0.45
2:k:69:GLN:C	2:k:71:PHE:N	2.70	0.45
2:l:64:LEU:O	2:l:66:CRO:HA31	2.16	0.45
2:m:165:PHE:HD2	2:m:167:ILE:HD11	1.80	0.45
2:o:43:THR:O	2:o:44:LEU:HD23	2.16	0.45
2:o:165:PHE:HD2	2:o:167:ILE:HD11	1.80	0.45
2:p:64:LEU:O	2:p:66:CRO:HA31	2.16	0.45
2:r:94:GLN:HB3	2:r:185:ASN:HD22	1.81	0.45
2:s:207:LEU:HG	2:s:220:LEU:HD12	1.97	0.45
2:t:94:GLN:HB3	2:t:185:ASN:HD22	1.81	0.45
2:w:154:ALA:HB1	2:w:195:LEU:HD11	1.98	0.45
2:x:69:GLN:C	2:x:71:PHE:N	2.70	0.45
2:y:64:LEU:O	2:y:66:CRO:HA31	2.16	0.45
2:a:154:ALA:HB1	2:a:195:LEU:HD11	1.98	0.45
2:d:43:THR:O	2:d:44:LEU:HD23	2.16	0.45
2:d:64:LEU:O	2:d:66:CRO:HA31	2.16	0.45
2:h:43:THR:O	2:h:44:LEU:HD23	2.16	0.45
2:h:213:GLU:OE2	2:h:217:HIS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:VAL:CG1	1:Q:67:ASP:O	2.56	0.45
2:i:165:PHE:HD2	2:i:167:ILE:HD11	1.80	0.45
2:j:154:ALA:HB1	2:j:195:LEU:HD11	1.98	0.45
2:k:213:GLU:OE2	2:k:217:HIS:HB3	2.17	0.45
1:L:279:SER:O	1:L:279:SER:OG	2.34	0.45
2:l:150:VAL:HG13	2:l:165:PHE:CD1	2.51	0.45
1:M:279:SER:O	1:M:279:SER:OG	2.34	0.45
2:m:94:GLN:HB3	2:m:185:ASN:HD22	1.81	0.45
2:n:43:THR:O	2:n:44:LEU:HD23	2.16	0.45
2:n:64:LEU:O	2:n:66:CRO:HA31	2.16	0.45
2:q:207:LEU:HG	2:q:220:LEU:HD12	1.97	0.45
2:r:43:THR:O	2:r:44:LEU:HD23	2.16	0.45
2:r:154:ALA:HB1	2:r:195:LEU:HD11	1.98	0.45
2:v:213:GLU:OE2	2:v:217:HIS:HB3	2.17	0.45
2:x:213:GLU:OE2	2:x:217:HIS:HB3	2.17	0.45
2:e:165:PHE:HD2	2:e:167:ILE:HD11	1.80	0.45
2:f:43:THR:O	2:f:44:LEU:HD23	2.16	0.45
2:i:213:GLU:OE2	2:i:217:HIS:HB3	2.17	0.45
1:J:279:SER:O	1:J:279:SER:OG	2.34	0.45
2:o:213:GLU:OE2	2:o:217:HIS:HB3	2.17	0.45
2:s:150:VAL:HG13	2:s:165:PHE:CD1	2.51	0.45
2:x:64:LEU:O	2:x:66:CRO:HA31	2.16	0.45
2:d:150:VAL:HG13	2:d:165:PHE:CD1	2.51	0.45
1:E:279:SER:O	1:E:279:SER:OG	2.34	0.45
2:e:43:THR:O	2:e:44:LEU:HD23	2.16	0.45
2:k:64:LEU:O	2:k:66:CRO:HA31	2.16	0.45
2:n:150:VAL:HG13	2:n:165:PHE:CD1	2.51	0.45
2:n:207:LEU:HG	2:n:220:LEU:HD12	1.97	0.45
2:p:165:PHE:HD2	2:p:167:ILE:HD11	1.80	0.45
2:q:43:THR:O	2:q:44:LEU:HD23	2.16	0.45
2:s:165:PHE:HD2	2:s:167:ILE:HD11	1.80	0.45
2:v:43:THR:O	2:v:44:LEU:HD23	2.16	0.45
2:y:150:VAL:HG13	2:y:165:PHE:CD1	2.51	0.45
2:a:64:LEU:O	2:a:66:CRO:HA31	2.16	0.45
2:b:150:VAL:HG13	2:b:165:PHE:CD1	2.51	0.45
2:c:64:LEU:O	2:c:66:CRO:HA31	2.16	0.45
2:e:94:GLN:HB3	2:e:185:ASN:HD22	1.81	0.45
2:i:80:ARG:HA	2:i:194:LEU:HD23	1.99	0.45
2:i:94:GLN:HB3	2:i:185:ASN:HD22	1.81	0.45
2:k:94:GLN:HB3	2:k:185:ASN:HD22	1.81	0.45
1:M:118:TRP:CE2	2:m:43:THR:OG1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:154:ALA:HB1	2:n:195:LEU:HD11	1.98	0.45
2:o:94:GLN:HB3	2:o:185:ASN:HD22	1.81	0.45
2:p:150:VAL:HG13	2:p:165:PHE:CD1	2.51	0.45
2:p:213:GLU:OE2	2:p:217:HIS:HB3	2.17	0.45
2:t:207:LEU:HG	2:t:220:LEU:HD12	1.97	0.45
2:y:165:PHE:HD2	2:y:167:ILE:HD11	1.80	0.45
2:c:207:LEU:HG	2:c:220:LEU:HD12	1.97	0.45
1:E:71:VAL:HA	1:R:70:ALA:HB1	1.99	0.45
2:m:43:THR:O	2:m:44:LEU:HD23	2.16	0.45
2:o:80:ARG:HA	2:o:194:LEU:HD23	1.99	0.45
2:o:154:ALA:HB1	2:o:195:LEU:HD11	1.98	0.45
2:q:154:ALA:HB1	2:q:195:LEU:HD11	1.98	0.45
2:r:64:LEU:O	2:r:66:CRO:HA31	2.16	0.45
2:t:64:LEU:O	2:t:66:CRO:HA31	2.16	0.45
2:x:94:GLN:HB3	2:x:185:ASN:HD22	1.81	0.45
2:y:213:GLU:OE2	2:y:217:HIS:HB3	2.17	0.45
2:c:165:PHE:HD2	2:c:167:ILE:HD11	1.80	0.45
2:d:154:ALA:HB1	2:d:195:LEU:HD11	1.98	0.45
2:d:207:LEU:HG	2:d:220:LEU:HD12	1.97	0.45
2:g:213:GLU:OE2	2:g:217:HIS:HB3	2.17	0.45
2:i:154:ALA:HB1	2:i:195:LEU:HD11	1.98	0.45
2:l:213:GLU:OE2	2:l:217:HIS:HB3	2.17	0.45
2:r:80:ARG:HA	2:r:194:LEU:HD23	1.99	0.45
2:a:80:ARG:HA	2:a:194:LEU:HD23	1.99	0.45
2:b:165:PHE:HD2	2:b:167:ILE:HD11	1.80	0.45
2:d:94:GLN:HB3	2:d:185:ASN:HD22	1.81	0.45
2:f:154:ALA:HB1	2:f:195:LEU:HD11	1.98	0.45
2:l:94:GLN:HB3	2:l:185:ASN:HD22	1.81	0.45
1:P:215:GLU:HG3	1:P:271:GLN:NE2	2.32	0.45
1:R:279:SER:O	1:R:279:SER:OG	2.34	0.45
2:t:165:PHE:HD2	2:t:167:ILE:HD11	1.80	0.45
2:w:80:ARG:HA	2:w:194:LEU:HD23	1.99	0.45
2:w:150:VAL:HG13	2:w:165:PHE:CD1	2.51	0.45
1:Y:215:GLU:HG3	1:Y:271:GLN:NE2	2.32	0.45
1:B:215:GLU:HG3	1:B:271:GLN:NE2	2.32	0.45
1:C:71:VAL:HA	1:X:70:ALA:HB1	1.99	0.45
1:F:355:LYS:HE3	1:F:355:LYS:HB3	1.85	0.45
1:J:71:VAL:HA	1:N:70:ALA:HB1	1.99	0.45
2:j:80:ARG:HA	2:j:194:LEU:HD23	1.99	0.45
2:j:150:VAL:HG13	2:j:165:PHE:CD1	2.51	0.45
1:K:70:ALA:HB1	1:T:71:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:71:VAL:HA	1:T:70:ALA:HB1	1.99	0.45
2:n:94:GLN:HB3	2:n:185:ASN:HD22	1.81	0.45
1:S:215:GLU:HG3	1:S:271:GLN:NE2	2.32	0.45
2:s:154:ALA:HB1	2:s:195:LEU:HD11	1.98	0.45
2:t:213:GLU:OE2	2:t:217:HIS:HB3	2.17	0.45
1:A:279:SER:O	1:A:279:SER:OG	2.34	0.45
2:a:213:GLU:OE2	2:a:217:HIS:HB3	2.17	0.45
1:C:70:ALA:HB1	1:X:71:VAL:HA	1.99	0.45
1:D:70:ALA:HB1	1:W:71:VAL:HA	1.99	0.45
1:E:70:ALA:CB	1:R:71:VAL:HA	2.47	0.45
2:e:154:ALA:HB1	2:e:195:LEU:HD11	1.98	0.45
1:F:70:ALA:HB1	1:O:71:VAL:HA	1.99	0.45
1:G:71:VAL:HA	1:H:70:ALA:HB1	1.99	0.45
1:I:71:VAL:HA	1:Q:70:ALA:HB1	1.99	0.45
2:j:64:LEU:O	2:j:66:CRO:HA31	2.16	0.45
2:k:154:ALA:HB1	2:k:195:LEU:HD11	1.98	0.45
2:l:112:VAL:HG12	2:l:121:ASN:CG	2.42	0.45
2:q:64:LEU:O	2:q:66:CRO:HA31	2.16	0.45
2:r:213:GLU:OE2	2:r:217:HIS:HB3	2.17	0.45
2:s:112:VAL:HG12	2:s:121:ASN:CG	2.42	0.45
1:V:279:SER:O	1:V:279:SER:OG	2.34	0.45
2:w:64:LEU:O	2:w:66:CRO:HA31	2.16	0.45
1:A:70:ALA:HB1	1:M:71:VAL:HA	1.99	0.44
1:A:215:GLU:HG3	1:A:271:GLN:NE2	2.32	0.44
2:b:112:VAL:HG12	2:b:121:ASN:CG	2.42	0.44
2:b:154:ALA:HB1	2:b:195:LEU:HD11	1.98	0.44
2:c:213:GLU:OE2	2:c:217:HIS:HB3	2.17	0.44
1:D:71:VAL:HA	1:W:70:ALA:HB1	1.99	0.44
2:d:213:GLU:OE2	2:d:217:HIS:HB3	2.17	0.44
2:f:64:LEU:O	2:f:66:CRO:HA31	2.16	0.44
2:g:94:GLN:HB3	2:g:185:ASN:HD22	1.81	0.44
2:g:112:VAL:HG12	2:g:121:ASN:CG	2.42	0.44
2:h:80:ARG:HA	2:h:194:LEU:HD23	1.99	0.44
1:J:70:ALA:HB1	1:N:71:VAL:HA	1.99	0.44
1:L:71:VAL:HA	1:V:70:ALA:HB1	1.99	0.44
2:m:154:ALA:HB1	2:m:195:LEU:HD11	1.98	0.44
2:q:213:GLU:OE2	2:q:217:HIS:HB3	2.17	0.44
2:w:112:VAL:HG12	2:w:121:ASN:CG	2.42	0.44
2:w:213:GLU:OE2	2:w:217:HIS:HB3	2.17	0.44
2:x:154:ALA:HB1	2:x:195:LEU:HD11	1.98	0.44
2:y:141:LEU:HD21	2:y:169:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:94:GLN:HB3	2:b:185:ASN:HD22	1.81	0.44
2:c:112:VAL:HG12	2:c:121:ASN:CG	2.42	0.44
1:D:279:SER:O	1:D:279:SER:OG	2.34	0.44
2:e:64:LEU:O	2:e:66:CRO:HA31	2.16	0.44
2:e:82:ASP:OD1	2:e:82:ASP:N	2.49	0.44
1:H:279:SER:O	1:H:279:SER:OG	2.34	0.44
2:j:112:VAL:HG12	2:j:121:ASN:CG	2.42	0.44
2:j:213:GLU:OE2	2:j:217:HIS:HB3	2.17	0.44
2:k:141:LEU:HD21	2:k:169:HIS:HB3	1.99	0.44
1:M:215:GLU:HG3	1:M:271:GLN:NE2	2.32	0.44
2:m:64:LEU:O	2:m:66:CRO:HA31	2.17	0.44
2:m:80:ARG:HA	2:m:194:LEU:HD23	1.99	0.44
2:p:141:LEU:HD21	2:p:169:HIS:HB3	1.99	0.44
1:R:215:GLU:HG3	1:R:271:GLN:NE2	2.32	0.44
2:t:112:VAL:HG12	2:t:121:ASN:CG	2.42	0.44
2:v:80:ARG:HA	2:v:194:LEU:HD23	1.99	0.44
1:W:215:GLU:HG3	1:W:271:GLN:NE2	2.32	0.44
2:x:43:THR:O	2:x:44:LEU:HD23	2.16	0.44
1:B:71:VAL:HA	1:P:70:ALA:HB1	1.99	0.44
2:d:80:ARG:HA	2:d:194:LEU:HD23	1.99	0.44
1:E:215:GLU:HG3	1:E:271:GLN:NE2	2.32	0.44
2:e:80:ARG:HA	2:e:194:LEU:HD23	1.99	0.44
2:f:14:ILE:HG12	2:f:16:VAL:HG23	2.00	0.44
2:f:213:GLU:OE2	2:f:217:HIS:HB3	2.17	0.44
1:I:215:GLU:HG3	1:I:271:GLN:NE2	2.32	0.44
2:k:43:THR:O	2:k:44:LEU:HD23	2.16	0.44
2:l:154:ALA:HB1	2:l:195:LEU:HD11	1.98	0.44
1:O:215:GLU:HG3	1:O:271:GLN:NE2	2.32	0.44
2:q:80:ARG:HA	2:q:194:LEU:HD23	1.99	0.44
2:r:112:VAL:HG12	2:r:121:ASN:CG	2.42	0.44
2:s:213:GLU:OE2	2:s:217:HIS:HB3	2.17	0.44
2:x:141:LEU:HD21	2:x:169:HIS:HB3	1.99	0.44
2:a:95:GLU:O	2:a:183:GLN:HA	2.18	0.44
2:c:95:GLU:O	2:c:183:GLN:HA	2.18	0.44
2:e:112:VAL:HG12	2:e:121:ASN:CG	2.42	0.44
2:h:14:ILE:HG12	2:h:16:VAL:HG23	2.00	0.44
1:J:215:GLU:HG3	1:J:271:GLN:NE2	2.32	0.44
2:l:141:LEU:HD21	2:l:169:HIS:HB3	1.99	0.44
2:m:112:VAL:HG12	2:m:121:ASN:CG	2.42	0.44
1:N:215:GLU:HG3	1:N:271:GLN:NE2	2.32	0.44
1:N:279:SER:O	1:N:279:SER:OG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:213:GLU:OE2	2:n:217:HIS:HB3	2.17	0.44
2:r:95:GLU:O	2:r:183:GLN:HA	2.18	0.44
1:S:71:VAL:HA	1:Y:70:ALA:HB1	1.99	0.44
2:t:95:GLU:O	2:t:183:GLN:HA	2.18	0.44
2:v:14:ILE:HG12	2:v:16:VAL:HG23	2.00	0.44
2:y:95:GLU:O	2:y:183:GLN:HA	2.18	0.44
2:a:112:VAL:HG12	2:a:121:ASN:CG	2.42	0.44
1:C:215:GLU:HG3	1:C:271:GLN:NE2	2.32	0.44
1:D:215:GLU:HG3	1:D:271:GLN:NE2	2.32	0.44
2:d:141:LEU:HD21	2:d:169:HIS:HB3	1.99	0.44
2:e:213:GLU:OE2	2:e:217:HIS:HB3	2.17	0.44
1:F:148:ARG:NH1	1:F:181:GLN:O	2.46	0.44
2:g:95:GLU:O	2:g:183:GLN:HA	2.18	0.44
2:g:141:LEU:HD21	2:g:169:HIS:HB3	1.99	0.44
2:g:154:ALA:HB1	2:g:195:LEU:HD11	1.98	0.44
1:I:148:ARG:NH1	1:I:181:GLN:O	2.46	0.44
1:K:215:GLU:HG3	1:K:271:GLN:NE2	2.32	0.44
2:l:95:GLU:O	2:l:183:GLN:HA	2.18	0.44
2:n:95:GLU:O	2:n:183:GLN:HA	2.18	0.44
2:p:95:GLU:O	2:p:183:GLN:HA	2.18	0.44
1:Q:355:LYS:HE3	1:Q:355:LYS:HB3	1.85	0.44
2:q:14:ILE:HG12	2:q:16:VAL:HG23	2.00	0.44
1:R:355:LYS:HB3	1:R:355:LYS:HE3	1.85	0.44
2:s:94:GLN:HB3	2:s:185:ASN:HD22	1.81	0.44
1:A:355:LYS:HE3	1:A:355:LYS:HB3	1.85	0.44
2:a:14:ILE:HG12	2:a:16:VAL:HG23	2.00	0.44
1:B:70:ALA:HB1	1:P:71:VAL:HA	1.99	0.44
2:b:80:ARG:HA	2:b:194:LEU:HD23	1.99	0.44
2:c:80:ARG:HA	2:c:194:LEU:HD23	1.99	0.44
2:e:141:LEU:HD21	2:e:169:HIS:HB3	1.99	0.44
2:f:80:ARG:HA	2:f:194:LEU:HD23	1.99	0.44
2:f:112:VAL:HG12	2:f:121:ASN:CG	2.42	0.44
2:h:64:LEU:O	2:h:66:CRO:HA31	2.16	0.44
2:i:95:GLU:O	2:i:183:GLN:HA	2.18	0.44
2:j:95:GLU:O	2:j:183:GLN:HA	2.18	0.44
2:m:213:GLU:OE2	2:m:217:HIS:HB3	2.17	0.44
2:n:141:LEU:HD21	2:n:169:HIS:HB3	1.99	0.44
2:o:14:ILE:HG12	2:o:16:VAL:HG23	2.00	0.44
2:o:95:GLU:O	2:o:183:GLN:HA	2.18	0.44
2:p:112:VAL:HG12	2:p:121:ASN:CG	2.42	0.44
2:p:154:ALA:HB1	2:p:195:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:14:ILE:HG12	2:r:16:VAL:HG23	2.00	0.44
1:S:70:ALA:HB1	1:Y:71:VAL:HA	1.99	0.44
1:T:215:GLU:HG3	1:T:271:GLN:NE2	2.32	0.44
2:t:80:ARG:HA	2:t:194:LEU:HD23	1.99	0.44
2:v:64:LEU:O	2:v:66:CRO:HA31	2.16	0.44
2:w:95:GLU:O	2:w:183:GLN:HA	2.18	0.44
1:X:215:GLU:HG3	1:X:271:GLN:NE2	2.32	0.44
2:y:112:VAL:HG12	2:y:121:ASN:CG	2.42	0.44
2:d:95:GLU:O	2:d:183:GLN:HA	2.18	0.44
1:F:71:VAL:HA	1:O:70:ALA:HB1	1.99	0.44
2:g:80:ARG:HA	2:g:194:LEU:HD23	1.99	0.44
2:h:95:GLU:O	2:h:183:GLN:HA	2.18	0.44
2:i:14:ILE:HG12	2:i:16:VAL:HG23	2.00	0.44
2:k:112:VAL:HG12	2:k:121:ASN:CG	2.42	0.44
1:L:215:GLU:HG3	1:L:271:GLN:NE2	2.32	0.44
2:l:80:ARG:HA	2:l:194:LEU:HD23	1.99	0.44
2:m:141:LEU:HD21	2:m:169:HIS:HB3	1.99	0.44
2:n:80:ARG:HA	2:n:194:LEU:HD23	1.99	0.44
2:n:112:VAL:HG12	2:n:121:ASN:CG	2.42	0.44
1:T:355:LYS:HE3	1:T:355:LYS:HB3	1.85	0.44
2:v:112:VAL:HG12	2:v:121:ASN:CG	2.42	0.44
2:x:112:VAL:HG12	2:x:121:ASN:CG	2.42	0.44
2:y:154:ALA:HB1	2:y:195:LEU:HD11	1.98	0.44
2:y:197:ASP:O	2:y:199:HIS:ND1	2.51	0.44
2:b:213:GLU:OE2	2:b:217:HIS:HB3	2.17	0.44
1:C:355:LYS:HE3	1:C:355:LYS:HB3	1.85	0.44
2:d:112:VAL:HG12	2:d:121:ASN:CG	2.42	0.44
1:F:215:GLU:HG3	1:F:271:GLN:NE2	2.32	0.44
1:G:215:GLU:HG3	1:G:271:GLN:NE2	2.32	0.44
2:g:43:THR:O	2:g:44:LEU:HD23	2.16	0.44
1:I:70:ALA:HB1	1:Q:71:VAL:HA	1.99	0.44
2:k:95:GLU:O	2:k:183:GLN:HA	2.18	0.44
2:k:210:ASP:H	2:k:217:HIS:CD2	2.36	0.44
1:O:148:ARG:NH1	1:O:181:GLN:O	2.46	0.44
2:o:64:LEU:O	2:o:66:CRO:HA31	2.16	0.44
2:p:98:ILE:CG1	2:p:106:TYR:HB2	2.40	0.44
2:p:197:ASP:O	2:p:199:HIS:ND1	2.51	0.44
1:Q:148:ARG:NH1	1:Q:181:GLN:O	2.46	0.44
2:q:112:VAL:HG12	2:q:121:ASN:CG	2.42	0.44
2:v:95:GLU:O	2:v:183:GLN:HA	2.18	0.44
2:x:95:GLU:O	2:x:183:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:x:210:ASP:H	2:x:217:HIS:CD2	2.36	0.44
2:b:197:ASP:O	2:b:199:HIS:ND1	2.51	0.44
1:E:67:ASP:O	1:R:71:VAL:CG1	2.59	0.44
2:f:210:ASP:H	2:f:217:HIS:CD2	2.36	0.44
2:h:112:VAL:HG12	2:h:121:ASN:CG	2.42	0.44
2:h:210:ASP:H	2:h:217:HIS:CD2	2.36	0.44
2:i:64:LEU:O	2:i:66:CRO:HA31	2.16	0.44
2:i:197:ASP:O	2:i:199:HIS:ND1	2.51	0.44
1:L:70:ALA:HB1	1:V:71:VAL:HA	1.99	0.44
2:l:43:THR:O	2:l:44:LEU:HD23	2.16	0.44
2:m:210:ASP:H	2:m:217:HIS:CD2	2.36	0.44
2:p:210:ASP:H	2:p:217:HIS:CD2	2.36	0.44
2:q:210:ASP:H	2:q:217:HIS:CD2	2.36	0.44
2:s:197:ASP:O	2:s:199:HIS:ND1	2.51	0.44
2:v:210:ASP:H	2:v:217:HIS:CD2	2.36	0.44
2:c:210:ASP:H	2:c:217:HIS:CD2	2.36	0.43
2:e:197:ASP:O	2:e:199:HIS:ND1	2.51	0.43
2:e:210:ASP:H	2:e:217:HIS:CD2	2.36	0.43
1:G:70:ALA:HB1	1:H:71:VAL:HA	1.99	0.43
2:g:210:ASP:H	2:g:217:HIS:CD2	2.36	0.43
1:H:215:GLU:HG3	1:H:271:GLN:NE2	2.32	0.43
2:m:136:ILE:H	2:m:136:ILE:HD12	1.83	0.43
2:o:197:ASP:O	2:o:199:HIS:ND1	2.51	0.43
2:p:14:ILE:HG12	2:p:16:VAL:HG23	2.00	0.43
1:Q:215:GLU:HG3	1:Q:271:GLN:NE2	2.32	0.43
2:s:64:LEU:O	2:s:66:CRO:HA31	2.16	0.43
2:s:80:ARG:HA	2:s:194:LEU:HD23	1.99	0.43
2:x:197:ASP:O	2:x:199:HIS:ND1	2.51	0.43
2:y:14:ILE:HG12	2:y:16:VAL:HG23	2.00	0.43
2:y:210:ASP:H	2:y:217:HIS:CD2	2.36	0.43
2:b:141:LEU:HD21	2:b:169:HIS:HB3	1.99	0.43
1:D:167:ILE:HA	1:D:170:VAL:HG12	2.00	0.43
2:e:136:ILE:H	2:e:136:ILE:HD12	1.83	0.43
1:F:167:ILE:HA	1:F:170:VAL:HG12	2.00	0.43
1:G:148:ARG:NH1	1:G:181:GLN:O	2.46	0.43
1:H:355:LYS:HE3	1:H:355:LYS:HB3	1.85	0.43
1:K:167:ILE:HA	1:K:170:VAL:HG12	2.00	0.43
2:k:197:ASP:O	2:k:199:HIS:ND1	2.51	0.43
1:L:167:ILE:HA	1:L:170:VAL:HG12	2.00	0.43
2:l:210:ASP:H	2:l:217:HIS:CD2	2.36	0.43
2:o:112:VAL:HG12	2:o:121:ASN:CG	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:69:GLN:C	2:s:71:PHE:N	2.70	0.43
2:t:141:LEU:HD21	2:t:169:HIS:HB3	1.99	0.43
2:t:210:ASP:H	2:t:217:HIS:CD2	2.36	0.43
1:W:279:SER:O	1:W:279:SER:OG	2.34	0.43
2:x:98:ILE:CG1	2:x:106:TYR:HB2	2.40	0.43
2:y:98:ILE:CG1	2:y:106:TYR:HB2	2.40	0.43
1:A:71:VAL:HA	1:M:70:ALA:HB1	1.99	0.43
1:D:67:ASP:O	1:W:71:VAL:CG1	2.56	0.43
1:G:167:ILE:HA	1:G:170:VAL:HG12	2.00	0.43
2:g:14:ILE:HD11	2:g:68:VAL:HG11	2.00	0.43
2:i:112:VAL:HG12	2:i:121:ASN:CG	2.42	0.43
1:K:252:TYR:O	1:K:256:GLN:HG2	2.19	0.43
2:k:14:ILE:HG12	2:k:16:VAL:HG23	2.00	0.43
2:l:14:ILE:HD11	2:l:68:VAL:HG11	2.01	0.43
2:m:197:ASP:O	2:m:199:HIS:ND1	2.51	0.43
1:N:167:ILE:HA	1:N:170:VAL:HG12	2.00	0.43
2:p:80:ARG:HA	2:p:194:LEU:HD23	1.99	0.43
2:p:136:ILE:H	2:p:136:ILE:HD12	1.83	0.43
1:Q:167:ILE:HA	1:Q:170:VAL:HG12	2.00	0.43
1:V:215:GLU:HG3	1:V:271:GLN:NE2	2.32	0.43
1:X:167:ILE:HA	1:X:170:VAL:HG12	2.00	0.43
1:X:252:TYR:O	1:X:256:GLN:HG2	2.19	0.43
2:x:14:ILE:HG12	2:x:16:VAL:HG23	2.00	0.43
2:a:210:ASP:H	2:a:217:HIS:CD2	2.36	0.43
1:B:252:TYR:O	1:B:256:GLN:HG2	2.19	0.43
2:b:64:LEU:O	2:b:66:CRO:HA31	2.16	0.43
2:c:141:LEU:HD21	2:c:169:HIS:HB3	1.99	0.43
2:c:197:ASP:O	2:c:199:HIS:ND1	2.51	0.43
2:i:210:ASP:H	2:i:217:HIS:CD2	2.36	0.43
2:o:210:ASP:H	2:o:217:HIS:CD2	2.36	0.43
2:q:197:ASP:O	2:q:199:HIS:ND1	2.51	0.43
1:R:252:TYR:O	1:R:256:GLN:HG2	2.19	0.43
1:S:252:TYR:O	1:S:256:GLN:HG2	2.19	0.43
2:v:197:ASP:O	2:v:199:HIS:ND1	2.51	0.43
2:y:80:ARG:HA	2:y:194:LEU:HD23	1.99	0.43
2:y:136:ILE:HD12	2:y:136:ILE:H	1.83	0.43
1:A:252:TYR:O	1:A:256:GLN:HG2	2.19	0.43
1:D:243:ASP:OD1	1:D:243:ASP:N	2.52	0.43
1:D:252:TYR:O	1:D:256:GLN:HG2	2.19	0.43
2:f:141:LEU:HD21	2:f:169:HIS:HB3	1.99	0.43
2:f:197:ASP:O	2:f:199:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:197:ASP:O	2:h:199:HIS:ND1	2.51	0.43
1:I:177:ASP:OD1	1:I:177:ASP:N	2.49	0.43
2:j:141:LEU:HD21	2:j:169:HIS:HB3	1.99	0.43
2:j:197:ASP:O	2:j:199:HIS:ND1	2.51	0.43
2:k:98:ILE:CG1	2:k:106:TYR:HB2	2.40	0.43
2:l:197:ASP:O	2:l:199:HIS:ND1	2.51	0.43
2:m:14:ILE:HG12	2:m:16:VAL:HG23	2.00	0.43
2:m:14:ILE:HD11	2:m:68:VAL:HG11	2.01	0.43
1:N:243:ASP:OD1	1:N:243:ASP:N	2.52	0.43
1:N:252:TYR:O	1:N:256:GLN:HG2	2.19	0.43
2:r:210:ASP:H	2:r:217:HIS:CD2	2.36	0.43
1:V:355:LYS:HE3	1:V:355:LYS:HB3	1.85	0.43
2:w:141:LEU:HD21	2:w:169:HIS:HB3	1.99	0.43
2:w:197:ASP:O	2:w:199:HIS:ND1	2.51	0.43
1:X:266:LYS:HB3	1:X:266:LYS:HE3	1.86	0.43
2:a:136:ILE:HD12	2:a:136:ILE:H	1.83	0.43
1:B:167:ILE:HA	1:B:170:VAL:HG12	2.00	0.43
2:d:208:SER:OG	2:d:209:LYS:N	2.52	0.43
2:e:14:ILE:HG12	2:e:16:VAL:HG23	2.00	0.43
2:e:14:ILE:HD11	2:e:68:VAL:HG11	2.01	0.43
2:g:197:ASP:O	2:g:199:HIS:ND1	2.51	0.43
2:i:68:VAL:C	2:i:70:CYS:N	2.77	0.43
2:i:141:LEU:HD21	2:i:169:HIS:HB3	1.99	0.43
1:J:71:VAL:CG1	1:N:67:ASP:O	2.56	0.43
1:K:356:MET:HE3	1:R:363:LEU:HD12	2.01	0.43
2:k:68:VAL:C	2:k:70:CYS:N	2.77	0.43
2:n:197:ASP:O	2:n:199:HIS:ND1	2.51	0.43
2:n:208:SER:OG	2:n:209:LYS:N	2.52	0.43
2:o:68:VAL:C	2:o:70:CYS:N	2.77	0.43
2:q:141:LEU:HD21	2:q:169:HIS:HB3	1.99	0.43
2:s:141:LEU:HD21	2:s:169:HIS:HB3	1.99	0.43
2:t:197:ASP:O	2:t:199:HIS:ND1	2.51	0.43
2:x:68:VAL:C	2:x:70:CYS:N	2.77	0.43
2:x:80:ARG:HA	2:x:194:LEU:HD23	1.99	0.43
2:y:14:ILE:HD11	2:y:68:VAL:HG11	2.01	0.43
2:b:136:ILE:H	2:b:136:ILE:HD12	1.83	0.43
2:d:197:ASP:O	2:d:199:HIS:ND1	2.51	0.43
2:e:78:MET:HG2	2:e:229:ILE:HD13	2.01	0.43
2:f:95:GLU:O	2:f:183:GLN:HA	2.18	0.43
1:H:363:LEU:HD12	1:P:356:MET:HE3	2.01	0.43
2:k:14:ILE:HD11	2:k:68:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:106:TYR:CE2	2:k:125:LEU:HD21	2.54	0.43
2:m:78:MET:HG2	2:m:229:ILE:HD13	2.01	0.43
2:m:95:GLU:O	2:m:183:GLN:HA	2.18	0.43
1:N:363:LEU:HD12	1:W:356:MET:HE3	2.01	0.43
1:O:177:ASP:N	1:O:177:ASP:OD1	2.49	0.43
2:o:141:LEU:HD21	2:o:169:HIS:HB3	1.99	0.43
2:p:14:ILE:HD11	2:p:68:VAL:HG11	2.01	0.43
2:q:95:GLU:O	2:q:183:GLN:HA	2.18	0.43
2:r:136:ILE:H	2:r:136:ILE:HD12	1.83	0.43
1:T:167:ILE:HA	1:T:170:VAL:HG12	2.00	0.43
1:V:363:LEU:HD12	1:Y:356:MET:HE3	2.01	0.43
2:v:141:LEU:HD21	2:v:169:HIS:HB3	1.99	0.43
2:x:106:TYR:CE2	2:x:125:LEU:HD21	2.54	0.43
1:Y:252:TYR:O	1:Y:256:GLN:HG2	2.19	0.43
2:a:208:SER:OG	2:a:209:LYS:N	2.52	0.43
2:b:210:ASP:H	2:b:217:HIS:CD2	2.36	0.43
1:C:167:ILE:HA	1:C:170:VAL:HG12	2.00	0.43
2:c:14:ILE:HG12	2:c:16:VAL:HG23	2.00	0.43
1:D:363:LEU:HD12	1:J:356:MET:HE3	2.01	0.43
2:d:14:ILE:HG12	2:d:16:VAL:HG23	2.00	0.43
2:d:136:ILE:H	2:d:136:ILE:HD12	1.83	0.43
1:E:252:TYR:O	1:E:256:GLN:HG2	2.19	0.43
2:e:95:GLU:O	2:e:183:GLN:HA	2.18	0.43
2:g:106:TYR:CE2	2:g:125:LEU:HD21	2.54	0.43
1:H:252:TYR:O	1:H:256:GLN:HG2	2.19	0.43
2:h:141:LEU:HD21	2:h:169:HIS:HB3	1.99	0.43
2:i:106:TYR:CE2	2:i:125:LEU:HD21	2.54	0.43
2:j:208:SER:OG	2:j:209:LYS:N	2.52	0.43
2:k:80:ARG:HA	2:k:194:LEU:HD23	1.99	0.43
2:l:106:TYR:CE2	2:l:125:LEU:HD21	2.54	0.43
2:n:14:ILE:HG12	2:n:16:VAL:HG23	2.00	0.43
1:P:252:TYR:O	1:P:256:GLN:HG2	2.19	0.43
2:r:141:LEU:HD21	2:r:169:HIS:HB3	1.99	0.43
2:r:208:SER:OG	2:r:209:LYS:N	2.52	0.43
1:S:167:ILE:HA	1:S:170:VAL:HG12	2.00	0.43
2:w:208:SER:OG	2:w:209:LYS:N	2.52	0.43
2:x:14:ILE:HD11	2:x:68:VAL:HG11	2.01	0.43
2:a:141:LEU:HD21	2:a:169:HIS:HB3	1.99	0.43
2:b:106:TYR:CE2	2:b:125:LEU:HD21	2.54	0.43
2:d:78:MET:HG2	2:d:229:ILE:HD13	2.01	0.43
1:E:167:ILE:HA	1:E:170:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:TYR:O	1:G:256:GLN:HG2	2.19	0.43
1:I:167:ILE:HA	1:I:170:VAL:HG12	2.00	0.43
1:I:279:SER:O	1:I:279:SER:OG	2.34	0.43
1:I:356:MET:HE3	1:J:363:LEU:HD12	2.01	0.43
2:i:78:MET:HG2	2:i:229:ILE:HD13	2.01	0.43
1:K:266:LYS:HB3	1:K:266:LYS:HE3	1.86	0.43
1:L:71:VAL:CG1	1:V:67:ASP:O	2.56	0.43
1:M:252:TYR:O	1:M:256:GLN:HG2	2.19	0.43
2:n:136:ILE:HD12	2:n:136:ILE:H	1.83	0.43
2:o:14:ILE:HD11	2:o:68:VAL:HG11	2.01	0.43
2:o:106:TYR:CE2	2:o:125:LEU:HD21	2.54	0.43
2:p:78:MET:HG2	2:p:229:ILE:HD13	2.01	0.43
2:p:106:TYR:CE2	2:p:125:LEU:HD21	2.54	0.43
2:s:136:ILE:H	2:s:136:ILE:HD12	1.83	0.43
2:s:210:ASP:H	2:s:217:HIS:CD2	2.36	0.43
2:t:14:ILE:HG12	2:t:16:VAL:HG23	2.00	0.43
1:V:252:TYR:O	1:V:256:GLN:HG2	2.19	0.43
2:w:14:ILE:HG12	2:w:16:VAL:HG23	2.00	0.43
2:w:78:MET:HG2	2:w:229:ILE:HD13	2.01	0.43
2:y:78:MET:HG2	2:y:229:ILE:HD13	2.01	0.43
2:y:106:TYR:CE2	2:y:125:LEU:HD21	2.54	0.43
1:B:266:LYS:HB3	1:B:266:LYS:HE3	1.86	0.43
2:b:14:ILE:HG12	2:b:16:VAL:HG23	2.00	0.43
2:b:95:GLU:O	2:b:183:GLN:HA	2.18	0.43
2:e:106:TYR:CE2	2:e:125:LEU:HD21	2.54	0.43
1:F:85:VAL:O	1:F:117:LEU:HB2	2.19	0.43
1:F:118:TRP:CE2	2:f:43:THR:OG1	2.72	0.43
1:F:252:TYR:O	1:F:256:GLN:HG2	2.19	0.43
2:f:78:MET:HG2	2:f:229:ILE:HD13	2.01	0.43
1:G:85:VAL:O	1:G:117:LEU:HB2	2.19	0.43
2:g:68:VAL:C	2:g:70:CYS:N	2.77	0.43
2:g:136:ILE:H	2:g:136:ILE:HD12	1.83	0.43
2:i:14:ILE:HD11	2:i:68:VAL:HG11	2.01	0.43
2:i:82:ASP:OD1	2:i:82:ASP:N	2.49	0.43
1:J:85:VAL:O	1:J:117:LEU:HB2	2.19	0.43
2:j:14:ILE:HG12	2:j:16:VAL:HG23	2.00	0.43
2:j:78:MET:HG2	2:j:229:ILE:HD13	2.01	0.43
2:j:106:TYR:CE2	2:j:125:LEU:HD21	2.54	0.43
1:L:85:VAL:O	1:L:117:LEU:HB2	2.19	0.43
1:L:252:TYR:O	1:L:256:GLN:HG2	2.19	0.43
2:l:136:ILE:H	2:l:136:ILE:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:167:ILE:HA	1:M:170:VAL:HG12	2.00	0.43
2:n:78:MET:HG2	2:n:229:ILE:HD13	2.01	0.43
1:O:167:ILE:HA	1:O:170:VAL:HG12	2.00	0.43
1:O:279:SER:O	1:O:279:SER:OG	2.34	0.43
1:O:356:MET:HE3	1:W:363:LEU:HD12	2.01	0.43
2:o:78:MET:HG2	2:o:229:ILE:HD13	2.01	0.43
2:p:82:ASP:OD1	2:p:82:ASP:N	2.49	0.43
1:Q:85:VAL:O	1:Q:117:LEU:HB2	2.19	0.43
2:q:78:MET:HG2	2:q:229:ILE:HD13	2.01	0.43
2:s:106:TYR:CE2	2:s:125:LEU:HD21	2.54	0.43
1:W:85:VAL:O	1:W:117:LEU:HB2	2.19	0.43
2:w:106:TYR:CE2	2:w:125:LEU:HD21	2.54	0.43
1:A:167:ILE:HA	1:A:170:VAL:HG12	2.00	0.42
1:A:363:LEU:HD12	1:X:356:MET:HE3	2.01	0.42
2:b:208:SER:OG	2:b:209:LYS:N	2.52	0.42
2:g:14:ILE:HG12	2:g:16:VAL:HG23	2.00	0.42
2:h:106:TYR:CE2	2:h:125:LEU:HD21	2.54	0.42
1:J:266:LYS:HB3	1:J:266:LYS:HE3	1.86	0.42
2:m:106:TYR:CE2	2:m:125:LEU:HD21	2.54	0.42
2:n:210:ASP:H	2:n:217:HIS:CD2	2.36	0.42
1:P:166:GLU:CD	1:P:166:GLU:H	2.27	0.42
1:Q:252:TYR:O	1:Q:256:GLN:HG2	2.19	0.42
2:s:95:GLU:O	2:s:183:GLN:HA	2.18	0.42
2:s:208:SER:OG	2:s:209:LYS:N	2.52	0.42
1:V:167:ILE:HA	1:V:170:VAL:HG12	2.00	0.42
2:v:106:TYR:CE2	2:v:125:LEU:HD21	2.54	0.42
2:w:210:ASP:H	2:w:217:HIS:CD2	2.36	0.42
1:Y:166:GLU:CD	1:Y:166:GLU:H	2.27	0.42
2:f:68:VAL:C	2:f:70:CYS:N	2.77	0.42
1:H:167:ILE:HA	1:H:170:VAL:HG12	2.00	0.42
2:h:208:SER:OG	2:h:209:LYS:N	2.52	0.42
2:k:208:SER:OG	2:k:209:LYS:N	2.52	0.42
1:M:363:LEU:HD12	1:R:356:MET:HE3	2.01	0.42
2:p:208:SER:OG	2:p:209:LYS:N	2.52	0.42
1:R:167:ILE:HA	1:R:170:VAL:HG12	2.00	0.42
2:s:14:ILE:HG12	2:s:16:VAL:HG23	2.00	0.42
2:v:208:SER:OG	2:v:209:LYS:N	2.52	0.42
2:x:208:SER:OG	2:x:209:LYS:N	2.52	0.42
1:Y:85:VAL:O	1:Y:117:LEU:HB2	2.19	0.42
2:y:82:ASP:OD1	2:y:82:ASP:N	2.49	0.42
1:B:166:GLU:H	1:B:166:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLN:C	1:D:285:SER:HB3	2.45	0.42
1:B:285:SER:HB3	1:D:281:GLN:C	2.45	0.42
1:C:166:GLU:CD	1:C:166:GLU:H	2.27	0.42
1:C:252:TYR:O	1:C:256:GLN:HG2	2.19	0.42
1:C:363:LEU:HD12	1:M:356:MET:HE3	2.01	0.42
2:c:78:MET:HG2	2:c:229:ILE:HD13	2.01	0.42
2:c:106:TYR:CE2	2:c:125:LEU:HD21	2.54	0.42
2:d:106:TYR:CE2	2:d:125:LEU:HD21	2.54	0.42
2:d:210:ASP:H	2:d:217:HIS:CD2	2.36	0.42
2:f:208:SER:OG	2:f:209:LYS:N	2.52	0.42
1:G:71:VAL:CG1	1:H:67:ASP:O	2.56	0.42
1:G:118:TRP:CE2	2:g:43:THR:OG1	2.72	0.42
1:I:252:TYR:O	1:I:256:GLN:HG2	2.19	0.42
2:j:210:ASP:H	2:j:217:HIS:CD2	2.36	0.42
2:l:68:VAL:C	2:l:70:CYS:N	2.77	0.42
1:M:85:VAL:O	1:M:117:LEU:HB2	2.19	0.42
1:N:285:SER:HB3	1:S:281:GLN:C	2.45	0.42
1:O:285:SER:HB3	1:V:281:GLN:C	2.45	0.42
2:o:82:ASP:OD1	2:o:82:ASP:N	2.49	0.42
1:P:85:VAL:O	1:P:117:LEU:HB2	2.19	0.42
1:Q:281:GLN:C	1:R:285:SER:HB3	2.44	0.42
2:r:197:ASP:O	2:r:199:HIS:ND1	2.51	0.42
1:S:85:VAL:O	1:S:117:LEU:HB2	2.19	0.42
1:T:166:GLU:H	1:T:166:GLU:CD	2.27	0.42
2:w:136:ILE:H	2:w:136:ILE:HD12	1.83	0.42
1:Y:167:ILE:HA	1:Y:170:VAL:HG12	2.00	0.42
2:y:208:SER:OG	2:y:209:LYS:N	2.52	0.42
2:a:197:ASP:O	2:a:199:HIS:ND1	2.51	0.42
1:B:85:VAL:O	1:B:117:LEU:HB2	2.19	0.42
2:b:82:ASP:OD1	2:b:82:ASP:N	2.49	0.42
2:c:136:ILE:H	2:c:136:ILE:HD12	1.83	0.42
1:D:356:MET:HE3	1:F:363:LEU:HD12	2.01	0.42
1:E:356:MET:HE3	1:T:363:LEU:HD12	2.01	0.42
2:e:208:SER:OG	2:e:209:LYS:N	2.52	0.42
2:f:106:TYR:CE2	2:f:125:LEU:HD21	2.54	0.42
1:G:67:ASP:O	1:H:71:VAL:CG1	2.56	0.42
1:H:281:GLN:C	1:I:285:SER:HB3	2.45	0.42
2:h:68:VAL:C	2:h:70:CYS:N	2.77	0.42
1:J:167:ILE:HA	1:J:170:VAL:HG12	2.00	0.42
2:j:14:ILE:HD11	2:j:68:VAL:HG11	2.01	0.42
2:l:78:MET:HG2	2:l:229:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:208:SER:OG	2:m:209:LYS:N	2.52	0.42
1:N:85:VAL:O	1:N:117:LEU:HB2	2.19	0.42
1:N:281:GLN:C	1:S:285:SER:HB3	2.45	0.42
2:n:106:TYR:CE2	2:n:125:LEU:HD21	2.54	0.42
1:O:252:TYR:O	1:O:256:GLN:HG2	2.19	0.42
1:P:167:ILE:HA	1:P:170:VAL:HG12	2.00	0.42
1:Q:266:LYS:HE3	1:Q:266:LYS:HB3	1.86	0.42
1:Q:285:SER:HB3	1:R:281:GLN:C	2.45	0.42
2:q:68:VAL:C	2:q:70:CYS:N	2.77	0.42
2:q:106:TYR:CE2	2:q:125:LEU:HD21	2.54	0.42
2:q:208:SER:OG	2:q:209:LYS:N	2.52	0.42
1:S:166:GLU:CD	1:S:166:GLU:H	2.27	0.42
1:T:252:TYR:O	1:T:256:GLN:HG2	2.19	0.42
2:t:106:TYR:CE2	2:t:125:LEU:HD21	2.54	0.42
1:V:166:GLU:CD	1:V:166:GLU:H	2.27	0.42
2:w:14:ILE:HD11	2:w:68:VAL:HG11	2.01	0.42
1:X:166:GLU:H	1:X:166:GLU:CD	2.27	0.42
1:A:281:GLN:C	1:F:285:SER:HB3	2.45	0.42
1:B:363:LEU:HD12	1:G:356:MET:HE3	2.01	0.42
1:D:85:VAL:O	1:D:117:LEU:HB2	2.19	0.42
1:E:85:VAL:O	1:E:117:LEU:HB2	2.19	0.42
1:H:266:LYS:HE3	1:H:266:LYS:HB3	1.86	0.42
2:j:136:ILE:H	2:j:136:ILE:HD12	1.83	0.42
1:K:166:GLU:CD	1:K:166:GLU:H	2.27	0.42
1:K:285:SER:HB3	1:P:281:GLN:C	2.45	0.42
1:L:242:ASP:OD1	1:L:242:ASP:N	2.46	0.42
1:L:285:SER:HB3	1:M:281:GLN:C	2.45	0.42
1:L:356:MET:HE3	1:S:363:LEU:HD12	2.01	0.42
1:N:118:TRP:CE2	2:n:43:THR:OG1	2.72	0.42
1:N:166:GLU:CD	1:N:166:GLU:H	2.27	0.42
1:N:356:MET:HE3	1:Q:363:LEU:HD12	2.01	0.42
2:t:78:MET:HG2	2:t:229:ILE:HD13	2.01	0.42
1:W:167:ILE:HA	1:W:170:VAL:HG12	2.00	0.42
1:X:285:SER:HB3	1:Y:281:GLN:C	2.45	0.42
1:A:285:SER:HB3	1:F:281:GLN:C	2.45	0.42
1:D:166:GLU:H	1:D:166:GLU:CD	2.27	0.42
1:E:281:GLN:C	1:G:285:SER:HB3	2.45	0.42
1:E:285:SER:HB3	1:G:281:GLN:C	2.45	0.42
2:g:78:MET:HG2	2:g:229:ILE:HD13	2.01	0.42
1:H:166:GLU:CD	1:H:166:GLU:H	2.27	0.42
2:h:136:ILE:H	2:h:136:ILE:HD12	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:78:MET:HG2	2:k:229:ILE:HD13	2.01	0.42
2:k:136:ILE:H	2:k:136:ILE:HD12	1.83	0.42
2:l:14:ILE:HG12	2:l:16:VAL:HG23	2.00	0.42
2:t:136:ILE:H	2:t:136:ILE:HD12	1.83	0.42
2:v:68:VAL:C	2:v:70:CYS:N	2.77	0.42
2:v:136:ILE:H	2:v:136:ILE:HD12	1.83	0.42
2:c:14:ILE:HD11	2:c:68:VAL:HG11	2.01	0.42
1:L:281:GLN:C	1:M:285:SER:HB3	2.45	0.42
2:n:14:ILE:HD11	2:n:68:VAL:HG11	2.01	0.42
1:T:356:MET:HE3	1:X:363:LEU:HD12	2.01	0.42
2:v:14:ILE:HD11	2:v:68:VAL:HG11	2.01	0.42
1:W:266:LYS:HB3	1:W:266:LYS:HE3	1.86	0.42
2:x:78:MET:HG2	2:x:229:ILE:HD13	2.01	0.42
2:x:136:ILE:H	2:x:136:ILE:HD12	1.83	0.42
1:A:85:VAL:O	1:A:117:LEU:HB2	2.19	0.42
2:a:14:ILE:HD11	2:a:68:VAL:HG11	2.01	0.42
2:c:68:VAL:C	2:c:70:CYS:N	2.77	0.42
2:c:208:SER:OG	2:c:209:LYS:N	2.52	0.42
2:f:14:ILE:HD11	2:f:68:VAL:HG11	2.01	0.42
1:G:242:ASP:OD1	1:G:242:ASP:N	2.46	0.42
1:I:85:VAL:O	1:I:117:LEU:HB2	2.19	0.42
2:l:98:ILE:CG1	2:l:106:TYR:HB2	2.40	0.42
2:q:14:ILE:HD11	2:q:68:VAL:HG11	2.01	0.42
2:q:136:ILE:HD12	2:q:136:ILE:H	1.83	0.42
1:S:279:SER:O	1:S:279:SER:OG	2.34	0.42
2:s:68:VAL:C	2:s:70:CYS:N	2.77	0.42
2:t:208:SER:OG	2:t:209:LYS:N	2.52	0.42
1:V:85:VAL:O	1:V:117:LEU:HB2	2.19	0.42
1:A:356:MET:HE3	1:E:363:LEU:HD12	2.01	0.42
2:b:68:VAL:C	2:b:70:CYS:N	2.77	0.42
1:C:356:MET:HE3	1:K:363:LEU:HD12	2.01	0.42
2:d:14:ILE:HD11	2:d:68:VAL:HG11	2.01	0.42
2:f:136:ILE:HD12	2:f:136:ILE:H	1.83	0.42
2:g:98:ILE:CG1	2:g:106:TYR:HB2	2.40	0.42
1:H:85:VAL:O	1:H:117:LEU:HB2	2.19	0.42
2:h:14:ILE:HD11	2:h:68:VAL:HG11	2.01	0.42
2:i:136:ILE:HD12	2:i:136:ILE:H	1.83	0.42
1:K:85:VAL:O	1:K:117:LEU:HB2	2.19	0.42
1:L:67:ASP:O	1:V:71:VAL:CG1	2.56	0.42
2:l:208:SER:OG	2:l:209:LYS:N	2.52	0.42
1:M:166:GLU:H	1:M:166:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:355:LYS:HE3	1:M:355:LYS:HB3	1.85	0.42
1:P:243:ASP:OD1	1:P:243:ASP:N	2.52	0.42
1:R:85:VAL:O	1:R:117:LEU:HB2	2.19	0.42
2:r:14:ILE:HD11	2:r:68:VAL:HG11	2.01	0.42
2:t:14:ILE:HD11	2:t:68:VAL:HG11	2.01	0.42
1:Y:177:ASP:OD1	1:Y:177:ASP:N	2.49	0.42
2:a:106:TYR:CE2	2:a:125:LEU:HD21	2.54	0.42
1:B:279:SER:O	1:B:279:SER:OG	2.34	0.42
2:c:4:GLY:HA3	2:c:86:SER:HA	2.02	0.42
1:E:166:GLU:H	1:E:166:GLU:CD	2.27	0.42
2:e:68:VAL:C	2:e:70:CYS:N	2.77	0.42
1:F:266:LYS:HE3	1:F:266:LYS:HB3	1.86	0.42
2:g:208:SER:OG	2:g:209:LYS:N	2.52	0.42
1:H:285:SER:HB3	1:I:281:GLN:C	2.45	0.42
2:h:78:MET:HG2	2:h:229:ILE:HD13	2.01	0.42
1:J:252:TYR:O	1:J:256:GLN:HG2	2.19	0.42
2:j:68:VAL:C	2:j:70:CYS:N	2.77	0.42
1:K:131:HIS:HB2	1:K:134:ILE:HD12	2.02	0.42
1:K:177:ASP:OD1	1:K:177:ASP:N	2.49	0.42
1:L:166:GLU:H	1:L:166:GLU:CD	2.27	0.42
1:O:85:VAL:O	1:O:117:LEU:HB2	2.19	0.42
2:p:68:VAL:C	2:p:70:CYS:N	2.77	0.42
2:t:4:GLY:HA3	2:t:86:SER:HA	2.02	0.42
1:W:252:TYR:O	1:W:256:GLN:HG2	2.19	0.42
2:w:68:VAL:C	2:w:70:CYS:N	2.77	0.42
1:X:131:HIS:HB2	1:X:134:ILE:HD12	2.02	0.42
1:Y:243:ASP:OD1	1:Y:243:ASP:N	2.52	0.42
2:y:68:VAL:C	2:y:70:CYS:N	2.77	0.42
1:B:248:ASN:HB2	1:B:369:ASP:OD1	2.20	0.41
2:b:14:ILE:HD11	2:b:68:VAL:HG11	2.01	0.41
1:C:281:GLN:C	1:J:285:SER:HB3	2.45	0.41
1:D:131:HIS:HB2	1:D:134:ILE:HD12	2.02	0.41
1:F:356:MET:HE3	1:I:363:LEU:HD12	2.01	0.41
1:G:166:GLU:H	1:G:166:GLU:CD	2.27	0.41
2:g:25:HIS:ND1	2:g:54:PRO:HG3	2.35	0.41
1:I:266:LYS:HB3	1:I:266:LYS:HE3	1.86	0.41
2:i:25:HIS:ND1	2:i:54:PRO:HG3	2.35	0.41
2:i:208:SER:OG	2:i:209:LYS:N	2.52	0.41
1:J:248:ASN:HB2	1:J:369:ASP:OD1	2.20	0.41
2:j:4:GLY:HA3	2:j:86:SER:HA	2.02	0.41
1:K:248:ASN:HB2	1:K:369:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:131:HIS:HB2	1:N:134:ILE:HD12	2.02	0.41
1:O:281:GLN:C	1:V:285:SER:HB3	2.45	0.41
1:O:363:LEU:HD12	1:Q:356:MET:HE3	2.01	0.41
2:o:25:HIS:ND1	2:o:54:PRO:HG3	2.35	0.41
2:o:136:ILE:H	2:o:136:ILE:HD12	1.83	0.41
2:o:208:SER:OG	2:o:209:LYS:N	2.52	0.41
1:P:177:ASP:OD1	1:P:177:ASP:N	2.49	0.41
2:r:106:TYR:CE2	2:r:125:LEU:HD21	2.54	0.41
1:S:248:ASN:HB2	1:S:369:ASP:OD1	2.20	0.41
1:T:285:SER:HB3	1:W:281:GLN:C	2.45	0.41
1:V:266:LYS:HE3	1:V:266:LYS:HB3	1.86	0.41
2:v:78:MET:HG2	2:v:229:ILE:HD13	2.01	0.41
2:v:98:ILE:CG1	2:v:106:TYR:HB2	2.40	0.41
1:W:243:ASP:OD1	1:W:243:ASP:N	2.52	0.41
1:W:248:ASN:HB2	1:W:369:ASP:OD1	2.20	0.41
2:w:4:GLY:HA3	2:w:86:SER:HA	2.02	0.41
1:X:85:VAL:O	1:X:117:LEU:HB2	2.19	0.41
1:X:248:ASN:HB2	1:X:369:ASP:OD1	2.20	0.41
1:X:281:GLN:C	1:Y:285:SER:HB3	2.45	0.41
1:Y:131:HIS:HB2	1:Y:134:ILE:HD12	2.02	0.41
2:a:25:HIS:ND1	2:a:54:PRO:HG3	2.35	0.41
2:b:78:MET:HG2	2:b:229:ILE:HD13	2.01	0.41
1:C:248:ASN:HB2	1:C:369:ASP:OD1	2.20	0.41
1:C:285:SER:HB3	1:J:281:GLN:C	2.45	0.41
1:G:131:HIS:HB2	1:G:134:ILE:HD12	2.02	0.41
2:g:4:GLY:HA3	2:g:86:SER:HA	2.02	0.41
2:h:4:GLY:HA3	2:h:86:SER:HA	2.02	0.41
2:h:25:HIS:ND1	2:h:54:PRO:HG3	2.35	0.41
1:K:281:GLN:C	1:P:285:SER:HB3	2.45	0.41
1:L:131:HIS:HB2	1:L:134:ILE:HD12	2.02	0.41
2:l:25:HIS:ND1	2:l:54:PRO:HG3	2.35	0.41
1:P:131:HIS:HB2	1:P:134:ILE:HD12	2.02	0.41
1:P:248:ASN:HB2	1:P:369:ASP:OD1	2.20	0.41
2:r:25:HIS:ND1	2:r:54:PRO:HG3	2.35	0.41
1:T:281:GLN:C	1:W:285:SER:HB3	2.45	0.41
2:t:68:VAL:C	2:t:70:CYS:N	2.77	0.41
2:v:4:GLY:HA3	2:v:86:SER:HA	2.02	0.41
2:v:25:HIS:ND1	2:v:54:PRO:HG3	2.35	0.41
1:X:177:ASP:OD1	1:X:177:ASP:N	2.49	0.41
1:Y:248:ASN:HB2	1:Y:369:ASP:OD1	2.20	0.41
2:j:25:HIS:ND1	2:j:54:PRO:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:25:HIS:ND1	2:n:54:PRO:HG3	2.35	0.41
2:s:78:MET:HG2	2:s:229:ILE:HD13	2.01	0.41
1:T:248:ASN:HB2	1:T:369:ASP:OD1	2.20	0.41
2:w:25:HIS:ND1	2:w:54:PRO:HG3	2.35	0.41
2:x:4:GLY:HA3	2:x:86:SER:HA	2.02	0.41
1:C:85:VAL:O	1:C:117:LEU:HB2	2.19	0.41
2:d:25:HIS:ND1	2:d:54:PRO:HG3	2.35	0.41
2:k:4:GLY:HA3	2:k:86:SER:HA	2.02	0.41
2:n:68:VAL:C	2:n:70:CYS:N	2.77	0.41
2:s:14:ILE:HD11	2:s:68:VAL:HG11	2.01	0.41
1:T:85:VAL:O	1:T:117:LEU:HB2	2.19	0.41
2:w:98:ILE:CG1	2:w:106:TYR:HB2	2.40	0.41
1:A:248:ASN:HB2	1:A:369:ASP:OD1	2.20	0.41
1:E:70:ALA:CB	1:R:74:ALA:HB3	2.51	0.41
1:E:355:LYS:HE3	1:E:355:LYS:HB3	1.85	0.41
1:G:363:LEU:HD12	1:S:356:MET:HE3	2.01	0.41
1:H:356:MET:HE3	1:Y:363:LEU:HD12	2.01	0.41
1:L:248:ASN:HB2	1:L:369:ASP:OD1	2.20	0.41
2:l:4:GLY:HA3	2:l:86:SER:HA	2.02	0.41
1:V:116:ASP:OD1	1:V:117:LEU:N	2.54	0.41
1:V:248:ASN:HB2	1:V:369:ASP:OD1	2.20	0.41
2:x:25:HIS:ND1	2:x:54:PRO:HG3	2.35	0.41
2:a:78:MET:HG2	2:a:229:ILE:HD13	2.01	0.41
1:B:356:MET:HE3	1:L:363:LEU:HD12	2.01	0.41
1:G:248:ASN:HB2	1:G:369:ASP:OD1	2.20	0.41
1:H:248:ASN:HB2	1:H:369:ASP:OD1	2.20	0.41
2:h:98:ILE:CG1	2:h:106:TYR:HB2	2.40	0.41
1:I:166:GLU:CD	1:I:166:GLU:H	2.27	0.41
2:i:199:HIS:HB2	2:i:227:ALA:O	2.21	0.41
2:k:25:HIS:ND1	2:k:54:PRO:HG3	2.35	0.41
1:O:166:GLU:H	1:O:166:GLU:CD	2.27	0.41
2:o:199:HIS:HB2	2:o:227:ALA:O	2.21	0.41
1:R:248:ASN:HB2	1:R:369:ASP:OD1	2.20	0.41
2:r:78:MET:HG2	2:r:229:ILE:HD13	2.01	0.41
2:y:87:ALA:C	2:y:90:GLU:HB3	2.46	0.41
1:A:131:HIS:HB2	1:A:134:ILE:HD12	2.02	0.41
2:b:199:HIS:HB2	2:b:227:ALA:O	2.21	0.41
1:D:116:ASP:OD1	1:D:117:LEU:N	2.54	0.41
1:F:166:GLU:H	1:F:166:GLU:CD	2.27	0.41
1:G:266:LYS:HB3	1:G:266:LYS:HE3	1.86	0.41
2:m:68:VAL:C	2:m:70:CYS:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:ASP:OD1	1:N:117:LEU:N	2.54	0.41
1:O:266:LYS:HB3	1:O:266:LYS:HE3	1.86	0.41
1:P:363:LEU:HD12	1:V:356:MET:HE3	2.01	0.41
2:p:87:ALA:C	2:p:90:GLU:HB3	2.46	0.41
2:p:199:HIS:HB2	2:p:227:ALA:O	2.21	0.41
2:r:98:ILE:CG1	2:r:106:TYR:HB2	2.40	0.41
2:s:25:HIS:ND1	2:s:54:PRO:HG3	2.35	0.41
2:s:199:HIS:HB2	2:s:227:ALA:O	2.21	0.41
2:t:25:HIS:ND1	2:t:54:PRO:HG3	2.35	0.41
2:y:199:HIS:HB2	2:y:227:ALA:O	2.21	0.41
1:A:166:GLU:CD	1:A:166:GLU:H	2.27	0.41
2:b:25:HIS:ND1	2:b:54:PRO:HG3	2.35	0.41
2:c:25:HIS:ND1	2:c:54:PRO:HG3	2.35	0.41
2:d:68:VAL:C	2:d:70:CYS:N	2.77	0.41
2:d:199:HIS:HB2	2:d:227:ALA:O	2.21	0.41
2:e:199:HIS:HB2	2:e:227:ALA:O	2.21	0.41
1:J:166:GLU:H	1:J:166:GLU:CD	2.27	0.41
2:j:98:ILE:CG1	2:j:106:TYR:HB2	2.40	0.41
1:N:248:ASN:HB2	1:N:369:ASP:OD1	2.20	0.41
1:O:248:ASN:HB2	1:O:369:ASP:OD1	2.20	0.41
1:Q:166:GLU:H	1:Q:166:GLU:CD	2.27	0.41
1:R:131:HIS:HB2	1:R:134:ILE:HD12	2.02	0.41
1:T:131:HIS:HB2	1:T:134:ILE:HD12	2.02	0.41
1:T:279:SER:O	1:T:279:SER:OG	2.34	0.41
2:y:25:HIS:ND1	2:y:54:PRO:HG3	2.35	0.41
2:a:4:GLY:HA3	2:a:86:SER:HA	2.02	0.41
2:a:40:GLY:HA2	2:a:71:PHE:O	2.21	0.41
1:C:131:HIS:HB2	1:C:134:ILE:HD12	2.02	0.41
2:c:87:ALA:C	2:c:90:GLU:HB3	2.46	0.41
2:c:199:HIS:HB2	2:c:227:ALA:O	2.21	0.41
1:D:248:ASN:HB2	1:D:369:ASP:OD1	2.20	0.41
1:E:131:HIS:HB2	1:E:134:ILE:HD12	2.02	0.41
2:e:25:HIS:ND1	2:e:54:PRO:HG3	2.35	0.41
2:e:98:ILE:CG1	2:e:106:TYR:HB2	2.40	0.41
1:F:116:ASP:OD1	1:F:117:LEU:N	2.54	0.41
1:F:131:HIS:HB2	1:F:134:ILE:HD12	2.02	0.41
1:F:177:ASP:OD1	1:F:177:ASP:N	2.49	0.41
2:f:4:GLY:HA3	2:f:86:SER:HA	2.02	0.41
2:f:87:ALA:C	2:f:90:GLU:HB3	2.46	0.41
2:h:40:GLY:HA2	2:h:71:PHE:O	2.21	0.41
2:h:199:HIS:HB2	2:h:227:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:ASN:HB2	1:I:369:ASP:OD1	2.20	0.41
2:i:87:ALA:C	2:i:90:GLU:HB3	2.46	0.41
1:J:131:HIS:HB2	1:J:134:ILE:HD12	2.02	0.41
1:M:131:HIS:HB2	1:M:134:ILE:HD12	2.02	0.41
2:m:199:HIS:HB2	2:m:227:ALA:O	2.21	0.41
2:n:199:HIS:HB2	2:n:227:ALA:O	2.21	0.41
2:o:87:ALA:C	2:o:90:GLU:HB3	2.46	0.41
2:p:25:HIS:ND1	2:p:54:PRO:HG3	2.35	0.41
1:Q:131:HIS:HB2	1:Q:134:ILE:HD12	2.02	0.41
1:Q:177:ASP:N	1:Q:177:ASP:OD1	2.49	0.41
2:q:4:GLY:HA3	2:q:86:SER:HA	2.02	0.41
2:q:87:ALA:C	2:q:90:GLU:HB3	2.46	0.41
1:R:166:GLU:H	1:R:166:GLU:CD	2.27	0.41
2:r:4:GLY:HA3	2:r:86:SER:HA	2.02	0.41
2:r:40:GLY:HA2	2:r:71:PHE:O	2.21	0.41
2:s:87:ALA:C	2:s:90:GLU:HB3	2.46	0.41
2:t:87:ALA:C	2:t:90:GLU:HB3	2.46	0.41
2:t:199:HIS:HB2	2:t:227:ALA:O	2.21	0.41
2:v:40:GLY:HA2	2:v:71:PHE:O	2.21	0.41
2:v:199:HIS:HB2	2:v:227:ALA:O	2.21	0.41
1:W:131:HIS:HB2	1:W:134:ILE:HD12	2.02	0.41
1:W:166:GLU:H	1:W:166:GLU:CD	2.27	0.41
2:a:98:ILE:CG1	2:a:106:TYR:HB2	2.40	0.41
2:b:4:GLY:HA3	2:b:86:SER:HA	2.02	0.41
1:C:279:SER:O	1:C:279:SER:OG	2.34	0.41
2:f:25:HIS:ND1	2:f:54:PRO:HG3	2.35	0.41
1:L:266:LYS:HB3	1:L:266:LYS:HE3	1.86	0.41
2:n:4:GLY:HA3	2:n:86:SER:HA	2.02	0.41
1:P:279:SER:O	1:P:279:SER:OG	2.34	0.41
2:p:40:GLY:HA2	2:p:71:PHE:O	2.21	0.41
1:Q:116:ASP:OD1	1:Q:117:LEU:N	2.54	0.41
2:q:25:HIS:ND1	2:q:54:PRO:HG3	2.35	0.41
2:q:199:HIS:HB2	2:q:227:ALA:O	2.21	0.41
2:t:98:ILE:CG1	2:t:106:TYR:HB2	2.40	0.41
2:y:40:GLY:HA2	2:y:71:PHE:O	2.21	0.41
2:a:68:VAL:C	2:a:70:CYS:N	2.77	0.40
1:B:131:HIS:HB2	1:B:134:ILE:HD12	2.02	0.40
1:E:248:ASN:HB2	1:E:369:ASP:OD1	2.20	0.40
2:e:4:GLY:HA3	2:e:86:SER:HA	2.02	0.40
2:f:199:HIS:HB2	2:f:227:ALA:O	2.21	0.40
1:G:355:LYS:HE3	1:G:355:LYS:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:87:ALA:C	2:n:90:GLU:HB3	2.46	0.40
2:r:68:VAL:C	2:r:70:CYS:N	2.77	0.40
1:S:131:HIS:HB2	1:S:134:ILE:HD12	2.02	0.40
2:b:87:ALA:C	2:b:90:GLU:HB3	2.46	0.40
2:c:40:GLY:HA2	2:c:71:PHE:O	2.21	0.40
2:d:87:ALA:C	2:d:90:GLU:HB3	2.46	0.40
2:e:87:ALA:C	2:e:90:GLU:HB3	2.46	0.40
2:m:4:GLY:HA3	2:m:86:SER:HA	2.02	0.40
2:m:25:HIS:ND1	2:m:54:PRO:HG3	2.35	0.40
2:s:4:GLY:HA3	2:s:86:SER:HA	2.02	0.40
1:Y:279:SER:O	1:Y:279:SER:OG	2.34	0.40
2:b:40:GLY:HA2	2:b:71:PHE:O	2.21	0.40
2:d:4:GLY:HA3	2:d:86:SER:HA	2.02	0.40
1:E:70:ALA:HB1	1:R:71:VAL:HA	2.03	0.40
2:g:40:GLY:HA2	2:g:71:PHE:O	2.21	0.40
1:H:131:HIS:HB2	1:H:134:ILE:HD12	2.02	0.40
2:k:40:GLY:HA2	2:k:71:PHE:O	2.21	0.40
2:l:40:GLY:HA2	2:l:71:PHE:O	2.21	0.40
1:M:248:ASN:HB2	1:M:369:ASP:OD1	2.20	0.40
2:m:87:ALA:C	2:m:90:GLU:HB3	2.46	0.40
2:o:4:GLY:HA3	2:o:86:SER:HA	2.02	0.40
2:t:40:GLY:HA2	2:t:71:PHE:O	2.21	0.40
1:V:131:HIS:HB2	1:V:134:ILE:HD12	2.02	0.40
2:x:40:GLY:HA2	2:x:71:PHE:O	2.21	0.40
2:c:81:HIS:O	2:c:196:PRO:HB3	2.22	0.40
2:c:98:ILE:CG1	2:c:106:TYR:HB2	2.40	0.40
1:D:56:GLU:HG2	1:D:72:LEU:HD11	2.04	0.40
1:D:161:TRP:HE1	2:d:73:ARG:CD	2.32	0.40
2:f:81:HIS:O	2:f:196:PRO:HB3	2.22	0.40
2:i:4:GLY:HA3	2:i:86:SER:HA	2.02	0.40
2:m:98:ILE:CG1	2:m:106:TYR:HB2	2.40	0.40
1:N:56:GLU:HG2	1:N:72:LEU:HD11	2.04	0.40
2:q:81:HIS:O	2:q:196:PRO:HB3	2.22	0.40
1:R:243:ASP:OD1	1:R:243:ASP:N	2.52	0.40
1:S:56:GLU:HG2	1:S:72:LEU:HD11	2.04	0.40
2:s:40:GLY:HA2	2:s:71:PHE:O	2.21	0.40
2:t:81:HIS:O	2:t:196:PRO:HB3	2.22	0.40
2:v:87:ALA:C	2:v:90:GLU:HB3	2.46	0.40
1:W:56:GLU:HG2	1:W:72:LEU:HD11	2.04	0.40
2:w:40:GLY:HA2	2:w:71:PHE:O	2.21	0.40
2:a:81:HIS:O	2:a:196:PRO:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:199:HIS:HB2	2:a:227:ALA:O	2.21	0.40
1:B:56:GLU:HG2	1:B:72:LEU:HD11	2.04	0.40
1:C:266:LYS:HE3	1:C:266:LYS:HB3	1.86	0.40
2:d:66:CRO:OH	2:d:148:HIS:HB2	2.22	0.40
2:d:81:HIS:O	2:d:196:PRO:HB3	2.22	0.40
2:e:81:HIS:O	2:e:196:PRO:HB3	2.22	0.40
1:G:116:ASP:OD1	1:G:117:LEU:N	2.54	0.40
1:J:56:GLU:HG2	1:J:72:LEU:HD11	2.04	0.40
2:j:40:GLY:HA2	2:j:71:PHE:O	2.21	0.40
1:K:116:ASP:OD1	1:K:117:LEU:N	2.54	0.40
1:L:116:ASP:OD1	1:L:117:LEU:N	2.54	0.40
2:m:81:HIS:O	2:m:196:PRO:HB3	2.22	0.40
2:n:81:HIS:O	2:n:196:PRO:HB3	2.22	0.40
2:p:66:CRO:OH	2:p:148:HIS:HB2	2.22	0.40
2:r:81:HIS:O	2:r:196:PRO:HB3	2.22	0.40
2:y:66:CRO:OH	2:y:148:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	B	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	C	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	D	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	E	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	F	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	G	319/394 (81%)	306 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	I	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	J	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	K	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	L	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	M	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	N	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	O	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	P	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	Q	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	R	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	S	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	T	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	V	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	W	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	X	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
1	Y	319/394 (81%)	306 (96%)	13 (4%)	0	100	100
2	a	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	b	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	c	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	d	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	e	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	f	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	g	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	h	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	i	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	j	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	k	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	l	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	m	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	n	224/234 (96%)	210 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	o	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	p	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	q	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	r	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	s	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	t	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	v	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	w	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	x	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
2	y	224/234 (96%)	210 (94%)	14 (6%)	0	100	100
All	All	13032/15072 (86%)	12384 (95%)	648 (5%)	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	257/315 (82%)	257 (100%)	0	100	100
1	B	257/315 (82%)	257 (100%)	0	100	100
1	C	257/315 (82%)	257 (100%)	0	100	100
1	D	257/315 (82%)	257 (100%)	0	100	100
1	E	257/315 (82%)	257 (100%)	0	100	100
1	F	257/315 (82%)	257 (100%)	0	100	100
1	G	257/315 (82%)	257 (100%)	0	100	100
1	H	257/315 (82%)	257 (100%)	0	100	100
1	I	257/315 (82%)	257 (100%)	0	100	100
1	J	257/315 (82%)	257 (100%)	0	100	100
1	K	257/315 (82%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	257/315 (82%)	257 (100%)	0	100	100
1	M	257/315 (82%)	257 (100%)	0	100	100
1	N	257/315 (82%)	257 (100%)	0	100	100
1	O	257/315 (82%)	257 (100%)	0	100	100
1	P	257/315 (82%)	257 (100%)	0	100	100
1	Q	257/315 (82%)	257 (100%)	0	100	100
1	R	257/315 (82%)	257 (100%)	0	100	100
1	S	257/315 (82%)	257 (100%)	0	100	100
1	T	257/315 (82%)	257 (100%)	0	100	100
1	V	257/315 (82%)	257 (100%)	0	100	100
1	W	257/315 (82%)	257 (100%)	0	100	100
1	X	257/315 (82%)	257 (100%)	0	100	100
1	Y	257/315 (82%)	257 (100%)	0	100	100
2	a	199/204 (98%)	199 (100%)	0	100	100
2	b	199/204 (98%)	199 (100%)	0	100	100
2	c	199/204 (98%)	199 (100%)	0	100	100
2	d	199/204 (98%)	199 (100%)	0	100	100
2	e	199/204 (98%)	199 (100%)	0	100	100
2	f	199/204 (98%)	199 (100%)	0	100	100
2	g	199/204 (98%)	199 (100%)	0	100	100
2	h	199/204 (98%)	199 (100%)	0	100	100
2	i	199/204 (98%)	199 (100%)	0	100	100
2	j	199/204 (98%)	199 (100%)	0	100	100
2	k	199/204 (98%)	199 (100%)	0	100	100
2	l	199/204 (98%)	199 (100%)	0	100	100
2	m	199/204 (98%)	199 (100%)	0	100	100
2	n	199/204 (98%)	199 (100%)	0	100	100
2	o	199/204 (98%)	199 (100%)	0	100	100
2	p	199/204 (98%)	199 (100%)	0	100	100
2	q	199/204 (98%)	199 (100%)	0	100	100
2	r	199/204 (98%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	s	199/204 (98%)	199 (100%)	0	100	100
2	t	199/204 (98%)	199 (100%)	0	100	100
2	v	199/204 (98%)	199 (100%)	0	100	100
2	w	199/204 (98%)	199 (100%)	0	100	100
2	x	199/204 (98%)	199 (100%)	0	100	100
2	y	199/204 (98%)	199 (100%)	0	100	100
All	All	10944/12456 (88%)	10944 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (312) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	113	ASN
1	A	124	HIS
1	A	164	HIS
1	A	195	ASN
1	A	273	GLN
1	A	303	HIS
1	A	334	HIS
1	A	349	HIS
2	a	77	HIS
2	a	121	ASN
2	a	177	GLN
2	a	185	ASN
2	a	217	HIS
1	B	113	ASN
1	B	124	HIS
1	B	164	HIS
1	B	195	ASN
1	B	273	GLN
1	B	303	HIS
1	B	334	HIS
1	B	349	HIS
2	b	77	HIS
2	b	121	ASN
2	b	177	GLN
2	b	185	ASN
2	b	217	HIS

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Mol	Chain	Res	Type
1	C	113	ASN
1	C	124	HIS
1	C	164	HIS
1	C	195	ASN
1	C	273	GLN
1	C	334	HIS
1	C	349	HIS
2	c	77	HIS
2	c	121	ASN
2	c	177	GLN
2	c	185	ASN
2	c	217	HIS
1	D	113	ASN
1	D	124	HIS
1	D	164	HIS
1	D	195	ASN
1	D	273	GLN
1	D	303	HIS
1	D	334	HIS
1	D	349	HIS
2	d	77	HIS
2	d	121	ASN
2	d	177	GLN
2	d	185	ASN
2	d	217	HIS
1	E	113	ASN
1	E	124	HIS
1	E	164	HIS
1	E	195	ASN
1	E	273	GLN
1	E	303	HIS
1	E	334	HIS
1	E	349	HIS
2	e	77	HIS
2	e	121	ASN
2	e	177	GLN
2	e	185	ASN
2	e	217	HIS
1	F	98	HIS
1	F	113	ASN
1	F	124	HIS
1	F	164	HIS

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Mol	Chain	Res	Type
1	F	195	ASN
1	F	273	GLN
1	F	303	HIS
1	F	334	HIS
1	F	349	HIS
2	f	77	HIS
2	f	121	ASN
2	f	177	GLN
2	f	185	ASN
2	f	217	HIS
1	G	113	ASN
1	G	124	HIS
1	G	164	HIS
1	G	195	ASN
1	G	273	GLN
1	G	303	HIS
1	G	334	HIS
1	G	349	HIS
2	g	77	HIS
2	g	121	ASN
2	g	177	GLN
2	g	185	ASN
2	g	217	HIS
1	H	113	ASN
1	H	124	HIS
1	H	164	HIS
1	H	195	ASN
1	H	273	GLN
1	H	303	HIS
1	H	334	HIS
1	H	349	HIS
2	h	77	HIS
2	h	121	ASN
2	h	177	GLN
2	h	185	ASN
2	h	217	HIS
1	I	113	ASN
1	I	124	HIS
1	I	164	HIS
1	I	195	ASN
1	I	273	GLN
1	I	303	HIS

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Mol	Chain	Res	Type
1	I	334	HIS
1	I	349	HIS
2	i	77	HIS
2	i	121	ASN
2	i	177	GLN
2	i	185	ASN
2	i	217	HIS
1	J	113	ASN
1	J	124	HIS
1	J	164	HIS
1	J	195	ASN
1	J	273	GLN
1	J	303	HIS
1	J	334	HIS
1	J	349	HIS
2	j	77	HIS
2	j	121	ASN
2	j	177	GLN
2	j	185	ASN
2	j	217	HIS
1	K	113	ASN
1	K	124	HIS
1	K	164	HIS
1	K	195	ASN
1	K	273	GLN
1	K	303	HIS
1	K	334	HIS
1	K	349	HIS
2	k	77	HIS
2	k	121	ASN
2	k	177	GLN
2	k	185	ASN
2	k	217	HIS
1	L	113	ASN
1	L	124	HIS
1	L	164	HIS
1	L	195	ASN
1	L	273	GLN
1	L	303	HIS
1	L	334	HIS
1	L	349	HIS
2	l	77	HIS

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Mol	Chain	Res	Type
2	l	121	ASN
2	l	177	GLN
2	l	185	ASN
2	l	217	HIS
1	M	113	ASN
1	M	124	HIS
1	M	164	HIS
1	M	195	ASN
1	M	273	GLN
1	M	303	HIS
1	M	334	HIS
1	M	349	HIS
2	m	77	HIS
2	m	121	ASN
2	m	177	GLN
2	m	185	ASN
2	m	217	HIS
1	N	113	ASN
1	N	124	HIS
1	N	164	HIS
1	N	195	ASN
1	N	273	GLN
1	N	303	HIS
1	N	334	HIS
1	N	349	HIS
2	n	77	HIS
2	n	121	ASN
2	n	177	GLN
2	n	185	ASN
2	n	217	HIS
1	O	113	ASN
1	O	124	HIS
1	O	164	HIS
1	O	195	ASN
1	O	273	GLN
1	O	334	HIS
1	O	349	HIS
2	o	77	HIS
2	o	121	ASN
2	o	177	GLN
2	o	185	ASN
2	o	217	HIS

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Mol	Chain	Res	Type
1	P	113	ASN
1	P	124	HIS
1	P	164	HIS
1	P	195	ASN
1	P	273	GLN
1	P	334	HIS
1	P	349	HIS
2	p	77	HIS
2	p	121	ASN
2	p	177	GLN
2	p	185	ASN
2	p	217	HIS
1	Q	98	HIS
1	Q	113	ASN
1	Q	124	HIS
1	Q	164	HIS
1	Q	195	ASN
1	Q	273	GLN
1	Q	303	HIS
1	Q	334	HIS
1	Q	349	HIS
2	q	77	HIS
2	q	121	ASN
2	q	177	GLN
2	q	185	ASN
2	q	217	HIS
1	R	98	HIS
1	R	113	ASN
1	R	124	HIS
1	R	164	HIS
1	R	195	ASN
1	R	273	GLN
1	R	303	HIS
1	R	334	HIS
1	R	349	HIS
2	r	77	HIS
2	r	121	ASN
2	r	177	GLN
2	r	185	ASN
2	r	217	HIS
1	S	113	ASN
1	S	124	HIS

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Mol	Chain	Res	Type
1	S	164	HIS
1	S	195	ASN
1	S	273	GLN
1	S	303	HIS
1	S	334	HIS
1	S	349	HIS
2	s	77	HIS
2	s	121	ASN
2	s	177	GLN
2	s	185	ASN
2	s	217	HIS
1	T	113	ASN
1	T	124	HIS
1	T	164	HIS
1	T	195	ASN
1	T	273	GLN
1	T	303	HIS
1	T	334	HIS
1	T	349	HIS
2	t	77	HIS
2	t	121	ASN
2	t	177	GLN
2	t	185	ASN
2	t	217	HIS
1	V	113	ASN
1	V	124	HIS
1	V	164	HIS
1	V	195	ASN
1	V	273	GLN
1	V	303	HIS
1	V	334	HIS
1	V	349	HIS
2	v	77	HIS
2	v	121	ASN
2	v	177	GLN
2	v	185	ASN
2	v	217	HIS
1	W	113	ASN
1	W	124	HIS
1	W	164	HIS
1	W	195	ASN
1	W	273	GLN

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Mol	Chain	Res	Type
1	W	303	HIS
1	W	334	HIS
1	W	349	HIS
2	w	77	HIS
2	w	121	ASN
2	w	177	GLN
2	w	185	ASN
2	w	217	HIS
1	X	113	ASN
1	X	124	HIS
1	X	164	HIS
1	X	195	ASN
1	X	273	GLN
1	X	303	HIS
1	X	334	HIS
1	X	349	HIS
2	x	77	HIS
2	x	121	ASN
2	x	177	GLN
2	x	185	ASN
2	x	217	HIS
1	Y	113	ASN
1	Y	124	HIS
1	Y	164	HIS
1	Y	195	ASN
1	Y	273	GLN
1	Y	334	HIS
1	Y	349	HIS
2	y	77	HIS
2	y	121	ASN
2	y	177	GLN
2	y	185	ASN
2	y	217	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CRO	m	66	2	23,23,24	3.19	6 (26%)	30,32,34	3.95	9 (30%)
2	CRO	d	66	2	23,23,24	3.19	6 (26%)	30,32,34	3.98	9 (30%)
2	CRO	h	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	n	66	2	23,23,24	3.19	6 (26%)	30,32,34	3.99	9 (30%)
2	CRO	a	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	c	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	i	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	p	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	v	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	e	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	r	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	o	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	j	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	q	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	t	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	x	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	g	66	2	23,23,24	3.20	6 (26%)	30,32,34	3.97	9 (30%)
2	CRO	w	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	y	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	l	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	b	66	2	23,23,24	3.20	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	k	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)
2	CRO	f	66	2	23,23,24	3.19	6 (26%)	30,32,34	3.98	9 (30%)
2	CRO	s	66	2	23,23,24	3.18	6 (26%)	30,32,34	3.96	9 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CRO	m	66	2	-	0/12/31/32	0/2/2/2
2	CRO	d	66	2	-	0/12/31/32	0/2/2/2
2	CRO	h	66	2	-	0/12/31/32	0/2/2/2
2	CRO	n	66	2	-	0/12/31/32	0/2/2/2
2	CRO	a	66	2	-	0/12/31/32	0/2/2/2
2	CRO	c	66	2	-	0/12/31/32	0/2/2/2
2	CRO	i	66	2	-	0/12/31/32	0/2/2/2
2	CRO	p	66	2	-	0/12/31/32	0/2/2/2
2	CRO	v	66	2	-	0/12/31/32	0/2/2/2
2	CRO	e	66	2	-	0/12/31/32	0/2/2/2
2	CRO	r	66	2	-	0/12/31/32	0/2/2/2
2	CRO	o	66	2	-	0/12/31/32	0/2/2/2
2	CRO	j	66	2	-	0/12/31/32	0/2/2/2
2	CRO	q	66	2	-	0/12/31/32	0/2/2/2
2	CRO	t	66	2	-	0/12/31/32	0/2/2/2
2	CRO	x	66	2	-	0/12/31/32	0/2/2/2
2	CRO	g	66	2	-	0/12/31/32	0/2/2/2
2	CRO	w	66	2	-	0/12/31/32	0/2/2/2
2	CRO	y	66	2	-	0/12/31/32	0/2/2/2
2	CRO	l	66	2	-	0/12/31/32	0/2/2/2
2	CRO	b	66	2	-	0/12/31/32	0/2/2/2
2	CRO	k	66	2	-	0/12/31/32	0/2/2/2
2	CRO	f	66	2	-	0/12/31/32	0/2/2/2
2	CRO	s	66	2	-	0/12/31/32	0/2/2/2

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	66	CRO	CB2-CA2	12.41	1.45	1.35
2	g	66	CRO	CB2-CA2	12.39	1.45	1.35
2	d	66	CRO	CB2-CA2	12.36	1.45	1.35
2	n	66	CRO	CB2-CA2	12.35	1.45	1.35
2	m	66	CRO	CB2-CA2	12.35	1.45	1.35
2	f	66	CRO	CB2-CA2	12.33	1.45	1.35
2	a	66	CRO	CB2-CA2	12.32	1.45	1.35
2	c	66	CRO	CB2-CA2	12.32	1.45	1.35
2	e	66	CRO	CB2-CA2	12.32	1.45	1.35
2	h	66	CRO	CB2-CA2	12.32	1.45	1.35
2	i	66	CRO	CB2-CA2	12.32	1.45	1.35
2	j	66	CRO	CB2-CA2	12.32	1.45	1.35
2	k	66	CRO	CB2-CA2	12.32	1.45	1.35
2	l	66	CRO	CB2-CA2	12.32	1.45	1.35
2	o	66	CRO	CB2-CA2	12.32	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	p	66	CRO	CB2-CA2	12.32	1.45	1.35
2	q	66	CRO	CB2-CA2	12.32	1.45	1.35
2	r	66	CRO	CB2-CA2	12.32	1.45	1.35
2	s	66	CRO	CB2-CA2	12.32	1.45	1.35
2	t	66	CRO	CB2-CA2	12.32	1.45	1.35
2	v	66	CRO	CB2-CA2	12.32	1.45	1.35
2	w	66	CRO	CB2-CA2	12.32	1.45	1.35
2	x	66	CRO	CB2-CA2	12.32	1.45	1.35
2	y	66	CRO	CB2-CA2	12.32	1.45	1.35
2	g	66	CRO	C2-N3	-5.39	1.27	1.39
2	b	66	CRO	C2-N3	-5.39	1.27	1.39
2	f	66	CRO	C2-N3	-5.38	1.27	1.39
2	a	66	CRO	C2-N3	-5.38	1.27	1.39
2	c	66	CRO	C2-N3	-5.38	1.27	1.39
2	e	66	CRO	C2-N3	-5.38	1.27	1.39
2	h	66	CRO	C2-N3	-5.38	1.27	1.39
2	i	66	CRO	C2-N3	-5.38	1.27	1.39
2	j	66	CRO	C2-N3	-5.38	1.27	1.39
2	k	66	CRO	C2-N3	-5.38	1.27	1.39
2	l	66	CRO	C2-N3	-5.38	1.27	1.39
2	o	66	CRO	C2-N3	-5.38	1.27	1.39
2	p	66	CRO	C2-N3	-5.38	1.27	1.39
2	q	66	CRO	C2-N3	-5.38	1.27	1.39
2	r	66	CRO	C2-N3	-5.38	1.27	1.39
2	s	66	CRO	C2-N3	-5.38	1.27	1.39
2	t	66	CRO	C2-N3	-5.38	1.27	1.39
2	v	66	CRO	C2-N3	-5.38	1.27	1.39
2	w	66	CRO	C2-N3	-5.38	1.27	1.39
2	x	66	CRO	C2-N3	-5.38	1.27	1.39
2	y	66	CRO	C2-N3	-5.38	1.27	1.39
2	n	66	CRO	C2-N3	-5.38	1.27	1.39
2	m	66	CRO	C2-N3	-5.37	1.27	1.39
2	d	66	CRO	C2-N3	-5.36	1.27	1.39
2	n	66	CRO	CA2-C2	-4.20	1.44	1.48
2	b	66	CRO	CA2-C2	-4.17	1.44	1.48
2	g	66	CRO	CA2-C2	-4.17	1.44	1.48
2	m	66	CRO	CA2-C2	-4.16	1.44	1.48
2	a	66	CRO	CA2-C2	-4.14	1.44	1.48
2	c	66	CRO	CA2-C2	-4.14	1.44	1.48
2	e	66	CRO	CA2-C2	-4.14	1.44	1.48
2	h	66	CRO	CA2-C2	-4.14	1.44	1.48
2	i	66	CRO	CA2-C2	-4.14	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	66	CRO	CA2-C2	-4.14	1.44	1.48
2	k	66	CRO	CA2-C2	-4.14	1.44	1.48
2	l	66	CRO	CA2-C2	-4.14	1.44	1.48
2	o	66	CRO	CA2-C2	-4.14	1.44	1.48
2	p	66	CRO	CA2-C2	-4.14	1.44	1.48
2	q	66	CRO	CA2-C2	-4.14	1.44	1.48
2	r	66	CRO	CA2-C2	-4.14	1.44	1.48
2	s	66	CRO	CA2-C2	-4.14	1.44	1.48
2	t	66	CRO	CA2-C2	-4.14	1.44	1.48
2	v	66	CRO	CA2-C2	-4.14	1.44	1.48
2	w	66	CRO	CA2-C2	-4.14	1.44	1.48
2	x	66	CRO	CA2-C2	-4.14	1.44	1.48
2	y	66	CRO	CA2-C2	-4.14	1.44	1.48
2	d	66	CRO	CA2-C2	-4.13	1.44	1.48
2	f	66	CRO	CA2-C2	-4.12	1.44	1.48
2	g	66	CRO	CA2-N2	-3.25	1.31	1.38
2	d	66	CRO	CA2-N2	-3.24	1.31	1.38
2	m	66	CRO	CA2-N2	-3.24	1.31	1.38
2	b	66	CRO	CA2-N2	-3.24	1.31	1.38
2	f	66	CRO	CA2-N2	-3.24	1.31	1.38
2	a	66	CRO	CA2-N2	-3.23	1.31	1.38
2	c	66	CRO	CA2-N2	-3.23	1.31	1.38
2	e	66	CRO	CA2-N2	-3.23	1.31	1.38
2	h	66	CRO	CA2-N2	-3.23	1.31	1.38
2	i	66	CRO	CA2-N2	-3.23	1.31	1.38
2	j	66	CRO	CA2-N2	-3.23	1.31	1.38
2	k	66	CRO	CA2-N2	-3.23	1.31	1.38
2	l	66	CRO	CA2-N2	-3.23	1.31	1.38
2	o	66	CRO	CA2-N2	-3.23	1.31	1.38
2	p	66	CRO	CA2-N2	-3.23	1.31	1.38
2	q	66	CRO	CA2-N2	-3.23	1.31	1.38
2	r	66	CRO	CA2-N2	-3.23	1.31	1.38
2	s	66	CRO	CA2-N2	-3.23	1.31	1.38
2	t	66	CRO	CA2-N2	-3.23	1.31	1.38
2	v	66	CRO	CA2-N2	-3.23	1.31	1.38
2	w	66	CRO	CA2-N2	-3.23	1.31	1.38
2	x	66	CRO	CA2-N2	-3.23	1.31	1.38
2	y	66	CRO	CA2-N2	-3.23	1.31	1.38
2	n	66	CRO	CA2-N2	-3.19	1.31	1.38
2	n	66	CRO	CA1-C1	-2.31	1.48	1.51
2	m	66	CRO	CA1-C1	-2.29	1.48	1.51
2	f	66	CRO	CA1-C1	-2.28	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	66	CRO	CA1-C1	-2.27	1.48	1.51
2	c	66	CRO	CA1-C1	-2.27	1.48	1.51
2	e	66	CRO	CA1-C1	-2.27	1.48	1.51
2	h	66	CRO	CA1-C1	-2.27	1.48	1.51
2	i	66	CRO	CA1-C1	-2.27	1.48	1.51
2	j	66	CRO	CA1-C1	-2.27	1.48	1.51
2	k	66	CRO	CA1-C1	-2.27	1.48	1.51
2	l	66	CRO	CA1-C1	-2.27	1.48	1.51
2	o	66	CRO	CA1-C1	-2.27	1.48	1.51
2	p	66	CRO	CA1-C1	-2.27	1.48	1.51
2	q	66	CRO	CA1-C1	-2.27	1.48	1.51
2	r	66	CRO	CA1-C1	-2.27	1.48	1.51
2	s	66	CRO	CA1-C1	-2.27	1.48	1.51
2	t	66	CRO	CA1-C1	-2.27	1.48	1.51
2	v	66	CRO	CA1-C1	-2.27	1.48	1.51
2	w	66	CRO	CA1-C1	-2.27	1.48	1.51
2	x	66	CRO	CA1-C1	-2.27	1.48	1.51
2	y	66	CRO	CA1-C1	-2.27	1.48	1.51
2	g	66	CRO	CA1-C1	-2.27	1.48	1.51
2	d	66	CRO	CA1-C1	-2.25	1.48	1.51
2	b	66	CRO	CA1-C1	-2.25	1.48	1.51
2	n	66	CRO	CA3-N3	-2.13	1.43	1.47
2	d	66	CRO	CA3-N3	-2.13	1.43	1.47
2	m	66	CRO	CA3-N3	-2.11	1.43	1.47
2	f	66	CRO	CA3-N3	-2.11	1.43	1.47
2	a	66	CRO	CA3-N3	-2.09	1.43	1.47
2	c	66	CRO	CA3-N3	-2.09	1.43	1.47
2	e	66	CRO	CA3-N3	-2.09	1.43	1.47
2	h	66	CRO	CA3-N3	-2.09	1.43	1.47
2	i	66	CRO	CA3-N3	-2.09	1.43	1.47
2	j	66	CRO	CA3-N3	-2.09	1.43	1.47
2	k	66	CRO	CA3-N3	-2.09	1.43	1.47
2	l	66	CRO	CA3-N3	-2.09	1.43	1.47
2	o	66	CRO	CA3-N3	-2.09	1.43	1.47
2	p	66	CRO	CA3-N3	-2.09	1.43	1.47
2	q	66	CRO	CA3-N3	-2.09	1.43	1.47
2	r	66	CRO	CA3-N3	-2.09	1.43	1.47
2	s	66	CRO	CA3-N3	-2.09	1.43	1.47
2	t	66	CRO	CA3-N3	-2.09	1.43	1.47
2	v	66	CRO	CA3-N3	-2.09	1.43	1.47
2	w	66	CRO	CA3-N3	-2.09	1.43	1.47
2	x	66	CRO	CA3-N3	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	y	66	CRO	CA3-N3	-2.09	1.43	1.47
2	g	66	CRO	CA3-N3	-2.09	1.43	1.47
2	b	66	CRO	CA3-N3	-2.07	1.43	1.47

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	66	CRO	O2-C2-CA2	-14.34	122.91	130.96
2	d	66	CRO	O2-C2-CA2	-14.29	122.94	130.96
2	f	66	CRO	O2-C2-CA2	-14.29	122.94	130.96
2	g	66	CRO	O2-C2-CA2	-14.28	122.94	130.96
2	a	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	c	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	e	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	h	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	i	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	j	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	k	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	l	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	o	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	p	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	q	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	r	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	s	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	t	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	v	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	w	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	x	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	y	66	CRO	O2-C2-CA2	-14.27	122.95	130.96
2	m	66	CRO	O2-C2-CA2	-14.25	122.96	130.96
2	b	66	CRO	O2-C2-CA2	-14.24	122.97	130.96
2	n	66	CRO	CA2-C2-N3	13.04	109.53	103.37
2	f	66	CRO	CA2-C2-N3	13.00	109.52	103.37
2	g	66	CRO	CA2-C2-N3	12.99	109.51	103.37
2	b	66	CRO	CA2-C2-N3	12.97	109.50	103.37
2	d	66	CRO	CA2-C2-N3	12.96	109.50	103.37
2	a	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	c	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	e	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	h	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	i	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	j	66	CRO	CA2-C2-N3	12.93	109.48	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	l	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	o	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	p	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	q	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	r	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	s	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	t	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	v	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	w	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	x	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	y	66	CRO	CA2-C2-N3	12.93	109.48	103.37
2	m	66	CRO	CA2-C2-N3	12.87	109.46	103.37
2	f	66	CRO	C2-N3-C1	-5.86	105.00	107.97
2	d	66	CRO	C2-N3-C1	-5.86	105.00	107.97
2	g	66	CRO	C2-N3-C1	-5.82	105.02	107.97
2	n	66	CRO	C2-N3-C1	-5.80	105.03	107.97
2	b	66	CRO	C2-N3-C1	-5.78	105.04	107.97
2	a	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	c	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	e	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	h	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	i	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	j	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	k	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	l	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	o	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	p	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	q	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	r	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	s	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	t	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	v	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	w	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	x	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	y	66	CRO	C2-N3-C1	-5.75	105.06	107.97
2	m	66	CRO	C2-N3-C1	-5.71	105.07	107.97
2	f	66	CRO	N3-C1-N2	3.69	114.01	111.45
2	d	66	CRO	N3-C1-N2	3.69	114.01	111.45
2	n	66	CRO	N3-C1-N2	3.64	113.97	111.45
2	b	66	CRO	N3-C1-N2	3.64	113.97	111.45
2	g	66	CRO	N3-C1-N2	3.63	113.97	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	c	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	e	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	h	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	i	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	j	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	k	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	l	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	o	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	p	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	q	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	r	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	s	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	t	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	v	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	w	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	x	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	y	66	CRO	N3-C1-N2	3.63	113.97	111.45
2	m	66	CRO	N3-C1-N2	3.61	113.95	111.45
2	d	66	CRO	C2-CA2-N2	-3.14	106.74	108.93
2	n	66	CRO	C2-CA2-N2	-3.12	106.75	108.93
2	a	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	c	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	e	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	h	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	i	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	j	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	k	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	l	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	o	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	p	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	q	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	r	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	s	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	t	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	v	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	w	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	x	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	y	66	CRO	C2-CA2-N2	-3.11	106.76	108.93
2	f	66	CRO	C2-CA2-N2	-3.10	106.76	108.93
2	g	66	CRO	C2-CA2-N2	-3.10	106.76	108.93
2	b	66	CRO	C2-CA2-N2	-3.10	106.76	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	66	CRO	C2-CA2-N2	-3.02	106.82	108.93
2	n	66	CRO	CB2-CA2-C2	2.93	125.78	122.28
2	d	66	CRO	CB2-CA2-C2	2.91	125.75	122.28
2	a	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	c	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	e	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	h	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	i	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	j	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	k	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	l	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	m	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	o	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	p	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	q	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	r	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	s	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	t	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	v	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	w	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	x	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	y	66	CRO	CB2-CA2-C2	2.90	125.74	122.28
2	b	66	CRO	CB2-CA2-C2	2.90	125.73	122.28
2	f	66	CRO	CB2-CA2-C2	2.90	125.73	122.28
2	g	66	CRO	CB2-CA2-C2	2.88	125.71	122.28
2	b	66	CRO	O3-C3-CA3	-2.72	118.19	126.39
2	f	66	CRO	O3-C3-CA3	-2.71	118.19	126.39
2	d	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	a	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	c	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	e	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	h	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	i	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	j	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	k	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	l	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	o	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	p	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	q	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	r	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	s	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	t	66	CRO	O3-C3-CA3	-2.71	118.20	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	w	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	x	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	y	66	CRO	O3-C3-CA3	-2.71	118.20	126.39
2	m	66	CRO	O3-C3-CA3	-2.71	118.21	126.39
2	g	66	CRO	O3-C3-CA3	-2.71	118.21	126.39
2	n	66	CRO	O3-C3-CA3	-2.69	118.26	126.39
2	b	66	CRO	OG1-CB1-CA1	2.41	114.20	109.04
2	n	66	CRO	OG1-CB1-CA1	2.40	114.19	109.04
2	a	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	c	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	e	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	h	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	i	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	j	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	k	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	l	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	o	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	p	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	q	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	r	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	s	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	t	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	v	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	w	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	x	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	y	66	CRO	OG1-CB1-CA1	2.39	114.16	109.04
2	g	66	CRO	OG1-CB1-CA1	2.38	114.15	109.04
2	m	66	CRO	OG1-CB1-CA1	2.38	114.14	109.04
2	d	66	CRO	OG1-CB1-CA1	2.38	114.13	109.04
2	f	66	CRO	OG1-CB1-CA1	2.36	114.10	109.04
2	g	66	CRO	CA3-N3-C2	2.34	129.17	123.80
2	f	66	CRO	CA3-N3-C2	2.34	129.17	123.80
2	n	66	CRO	CA3-N3-C2	2.33	129.14	123.80
2	a	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	c	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	e	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	h	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	i	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	j	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	k	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	l	66	CRO	CA3-N3-C2	2.32	129.13	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	o	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	p	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	q	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	r	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	s	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	t	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	v	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	w	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	x	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	y	66	CRO	CA3-N3-C2	2.32	129.13	123.80
2	b	66	CRO	CA3-N3-C2	2.32	129.12	123.80
2	d	66	CRO	CA3-N3-C2	2.32	129.12	123.80
2	m	66	CRO	CA3-N3-C2	2.31	129.09	123.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	m	66	CRO	1	0
2	d	66	CRO	2	0
2	h	66	CRO	1	0
2	n	66	CRO	1	0
2	a	66	CRO	1	0
2	c	66	CRO	1	0
2	i	66	CRO	1	0
2	p	66	CRO	2	0
2	v	66	CRO	1	0
2	e	66	CRO	1	0
2	r	66	CRO	1	0
2	o	66	CRO	1	0
2	j	66	CRO	1	0
2	q	66	CRO	1	0
2	t	66	CRO	1	0
2	x	66	CRO	1	0
2	g	66	CRO	1	0
2	w	66	CRO	1	0
2	y	66	CRO	2	0
2	l	66	CRO	1	0
2	b	66	CRO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	k	66	CRO	1	0
2	f	66	CRO	1	0
2	s	66	CRO	1	0

## 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.



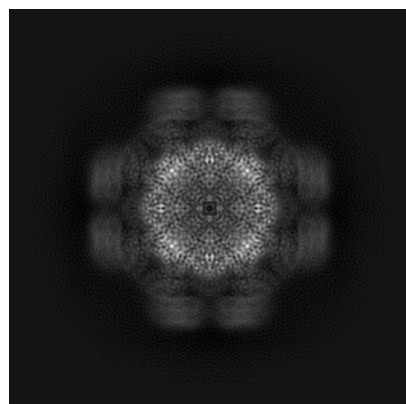
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61130. These allow visual inspection of the internal detail of the map and identification of artifacts.

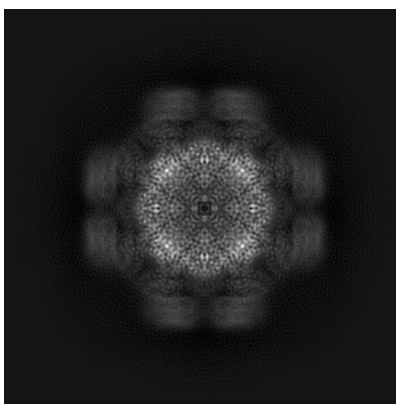
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

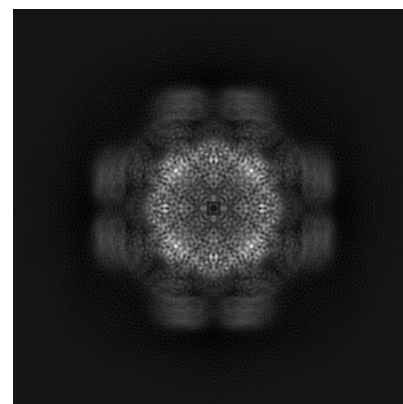
#### 6.1.1 Primary map



X

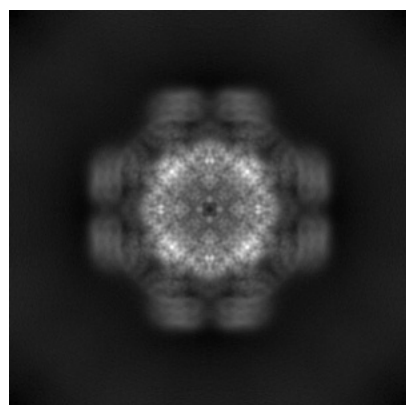


Y

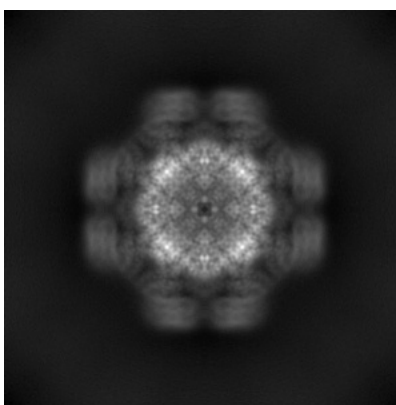


Z

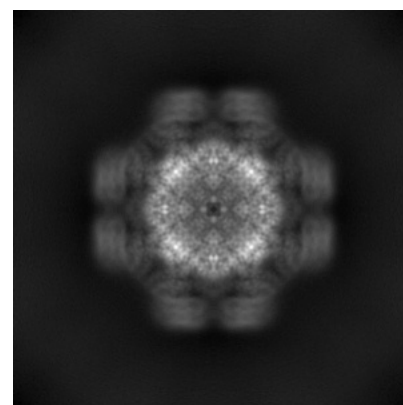
#### 6.1.2 Raw map



X



Y



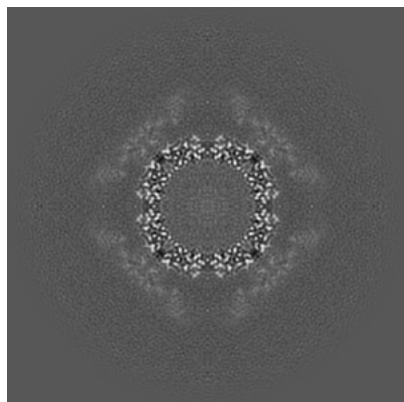
Z

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

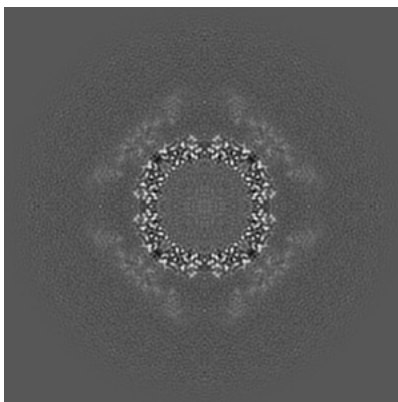


## 6.2 Central slices [i](#)

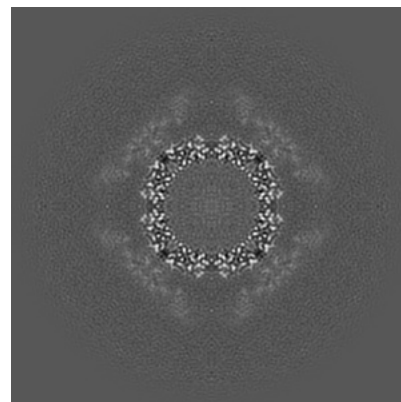
### 6.2.1 Primary map



X Index: 160

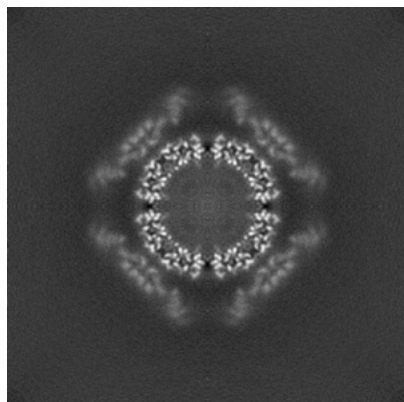


Y Index: 160

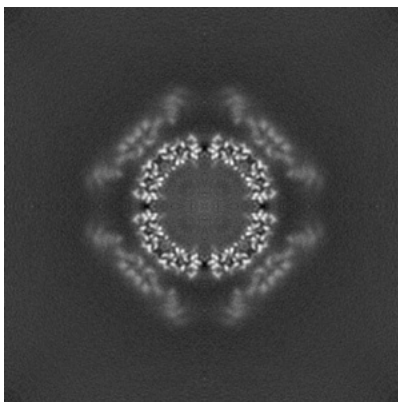


Z Index: 160

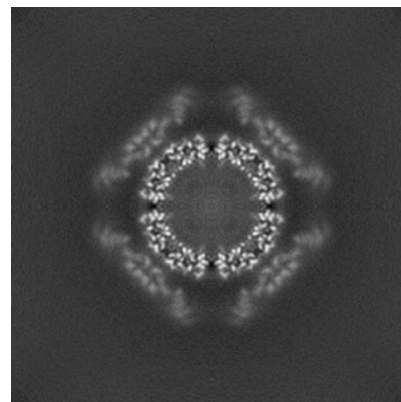
### 6.2.2 Raw map



X Index: 160



Y Index: 160

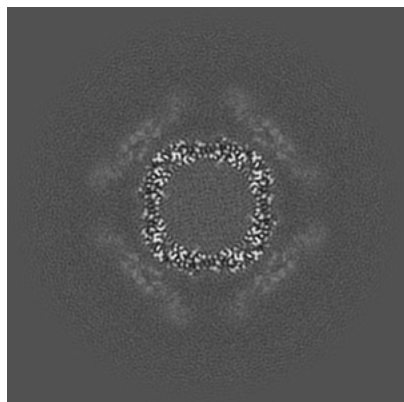


Z Index: 160

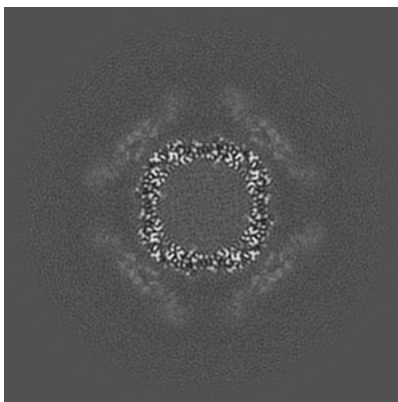
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

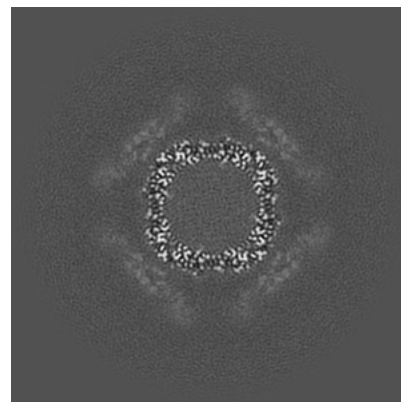
### 6.3.1 Primary map



X Index: 158

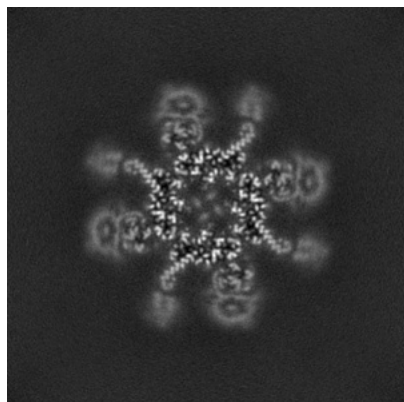


Y Index: 158

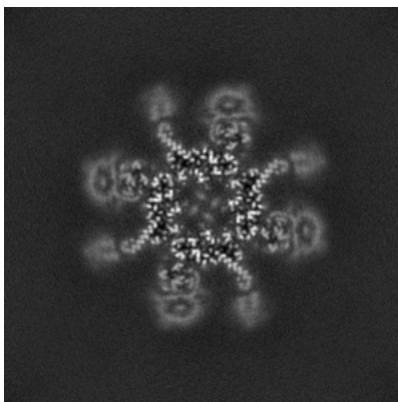


Z Index: 158

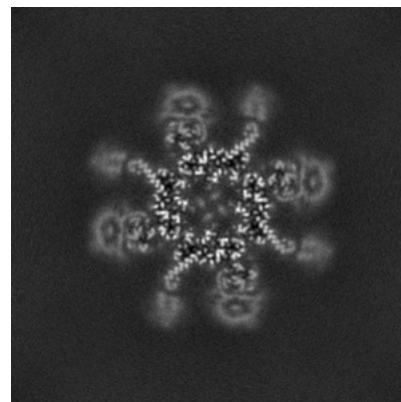
### 6.3.2 Raw map



X Index: 127



Y Index: 193

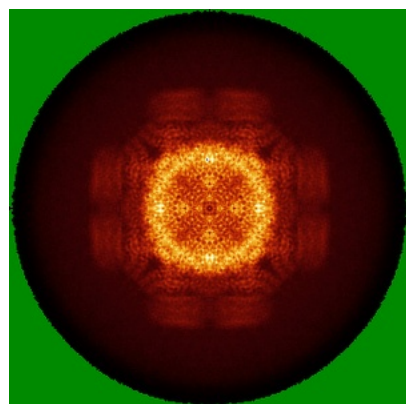


Z Index: 127

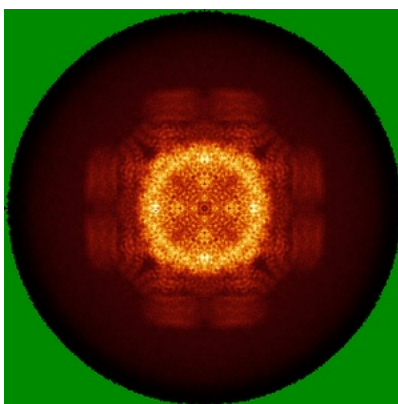
The images above show the largest variance slices of the map in three orthogonal directions.

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

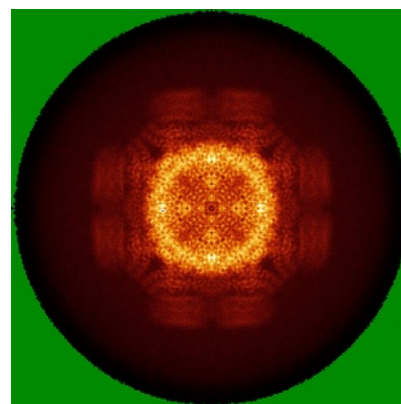
### 6.4.1 Primary map



X

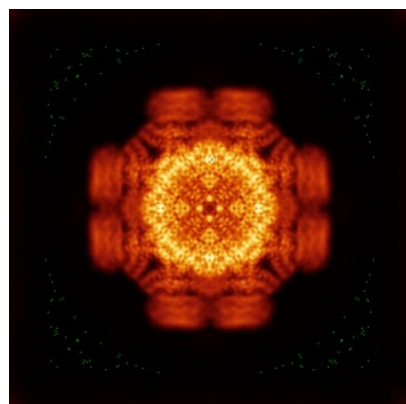


Y

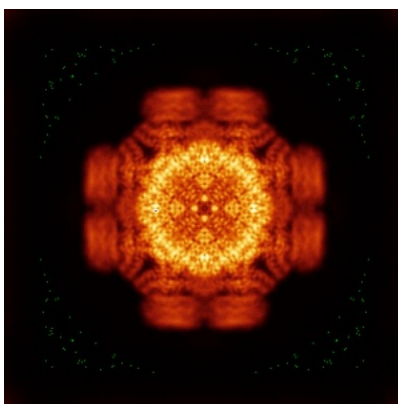


Z

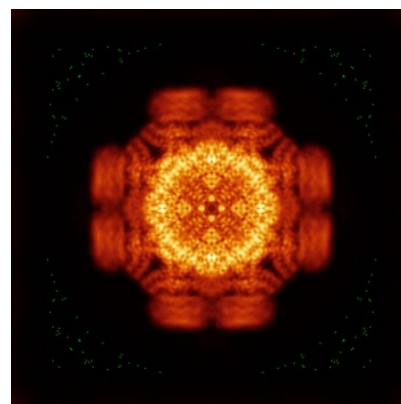
### 6.4.2 Raw map



X



Y

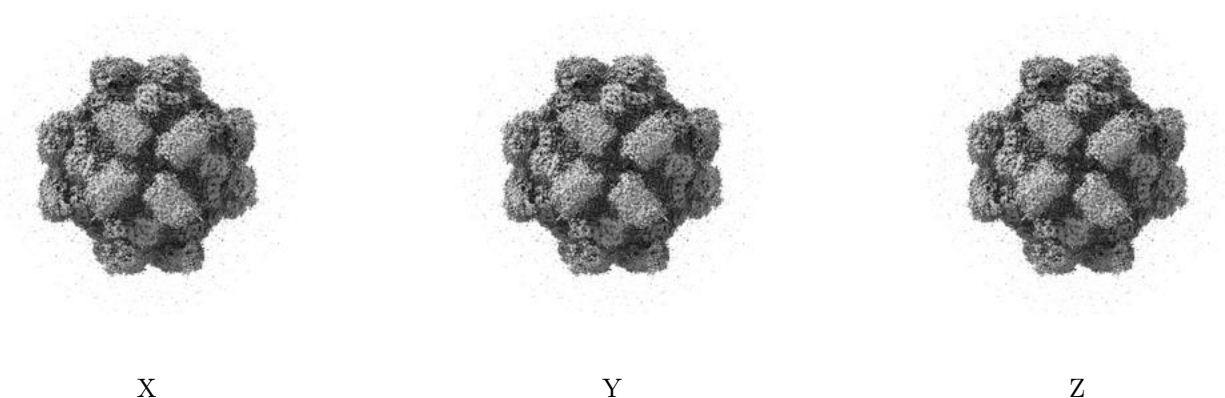


Z

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.

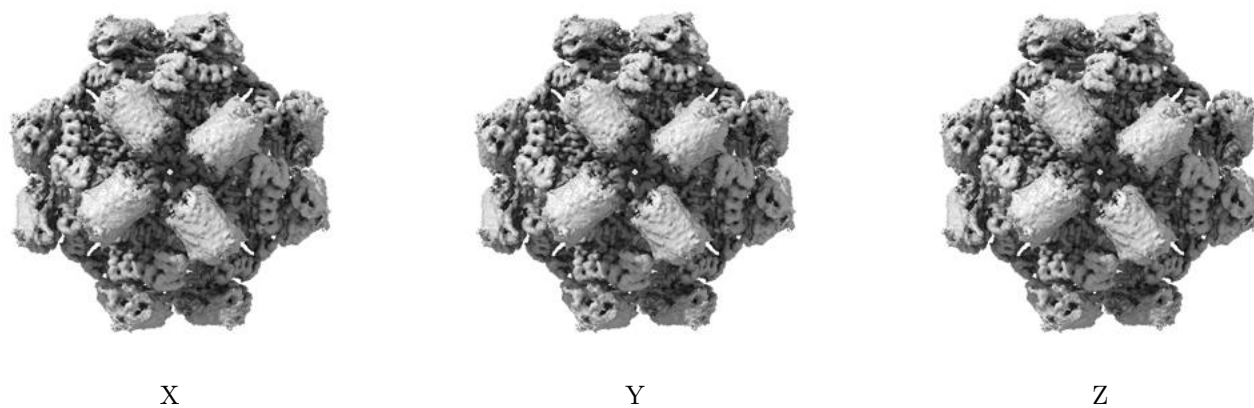
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

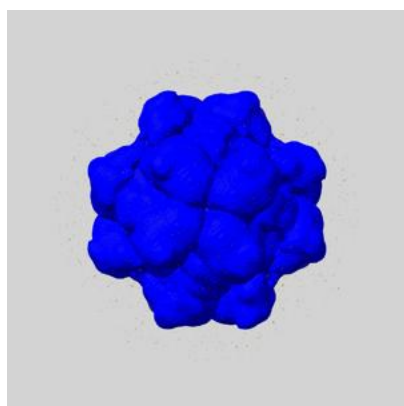
## 6.6 Mask visualisation [i](#)

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

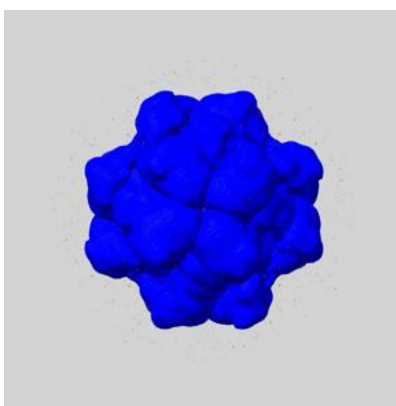
A mask typically either:

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

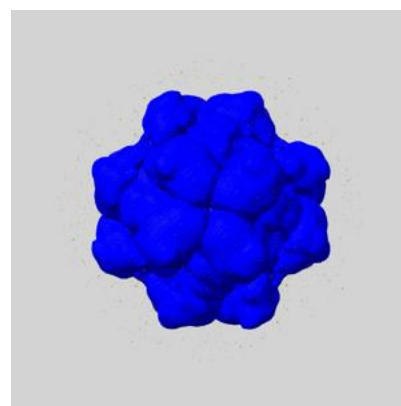
### 6.6.1 emd\_61130\_msk\_1.map [i](#)



X



Y

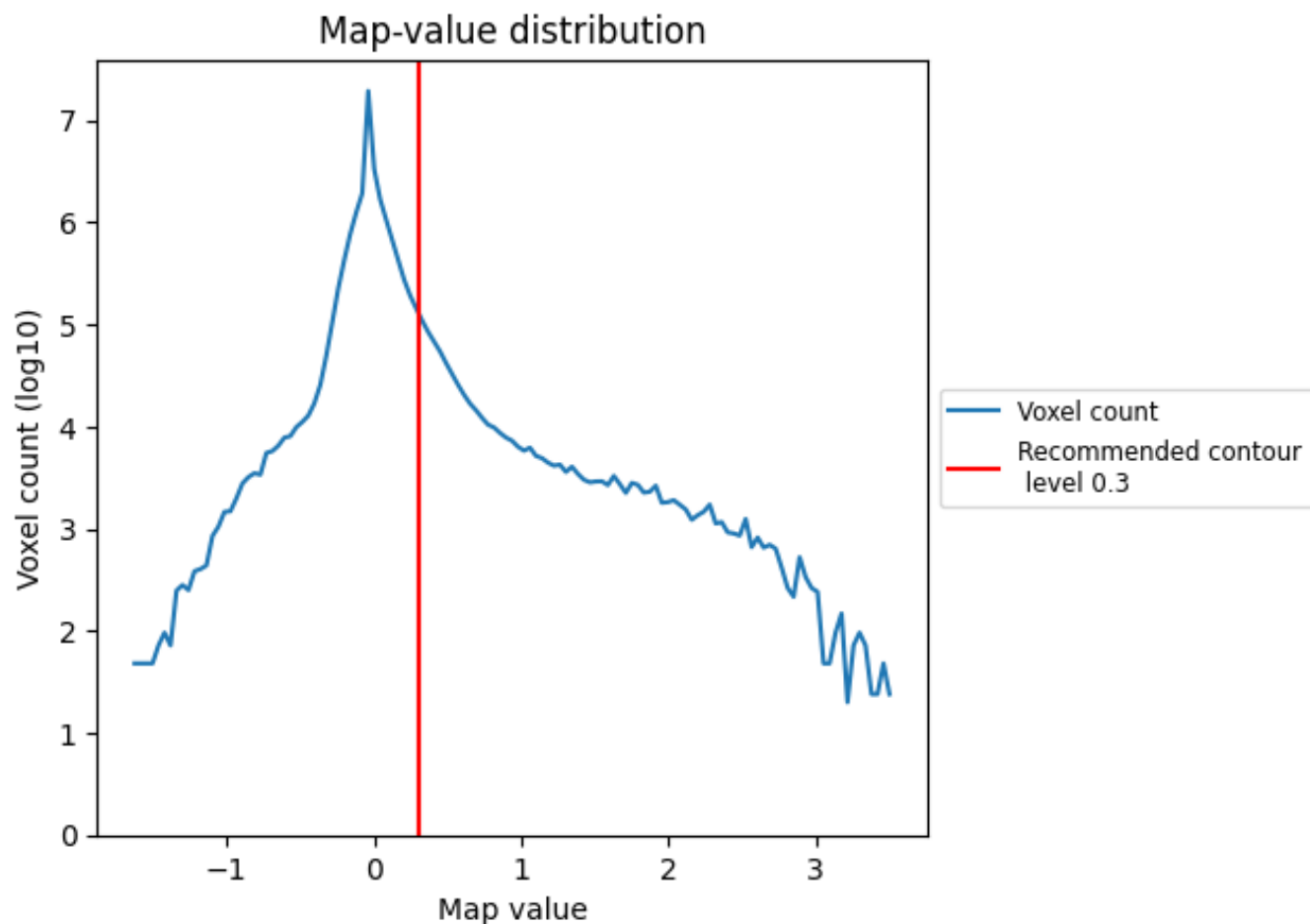


Z

## 7 Map analysis [i](#)

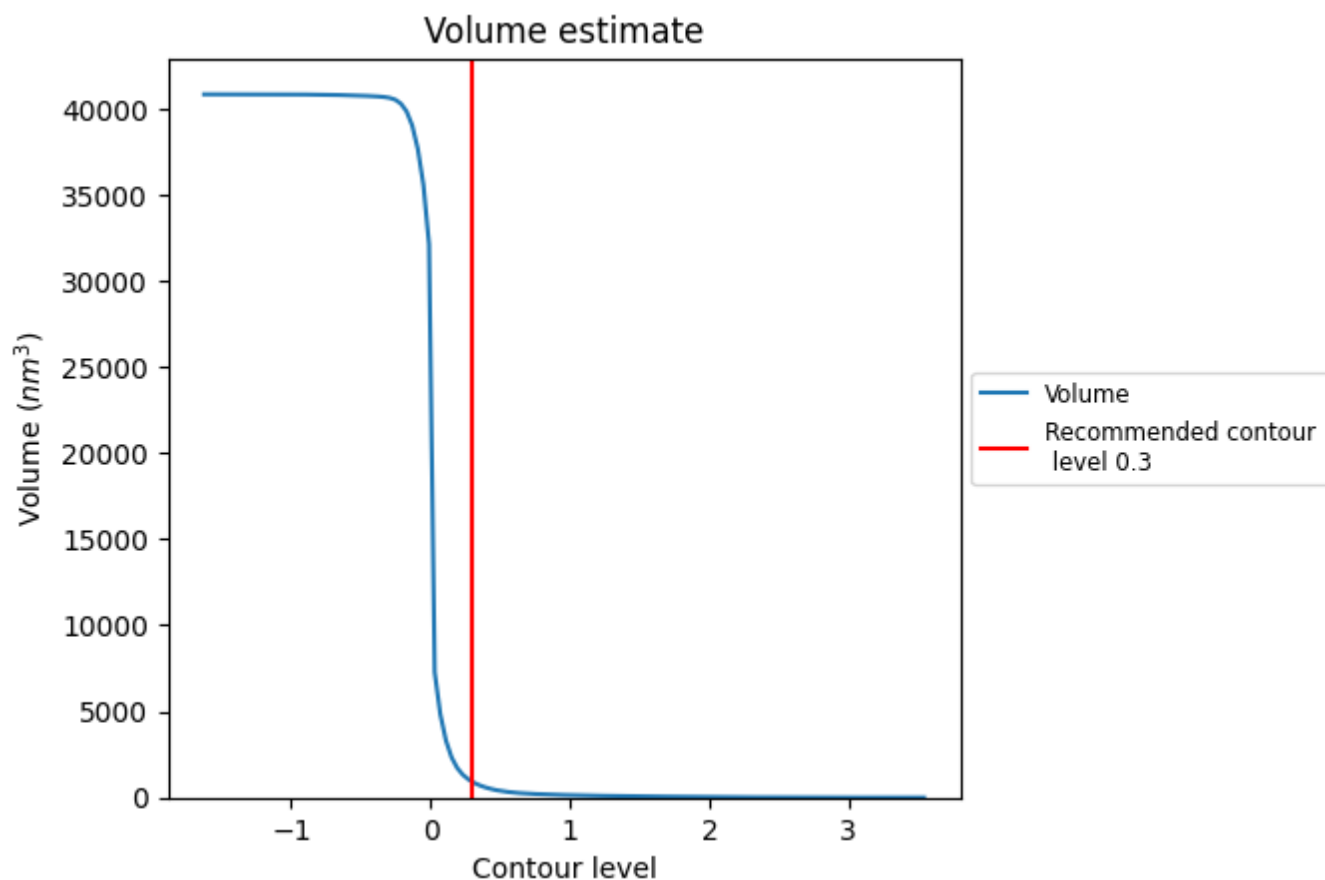
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

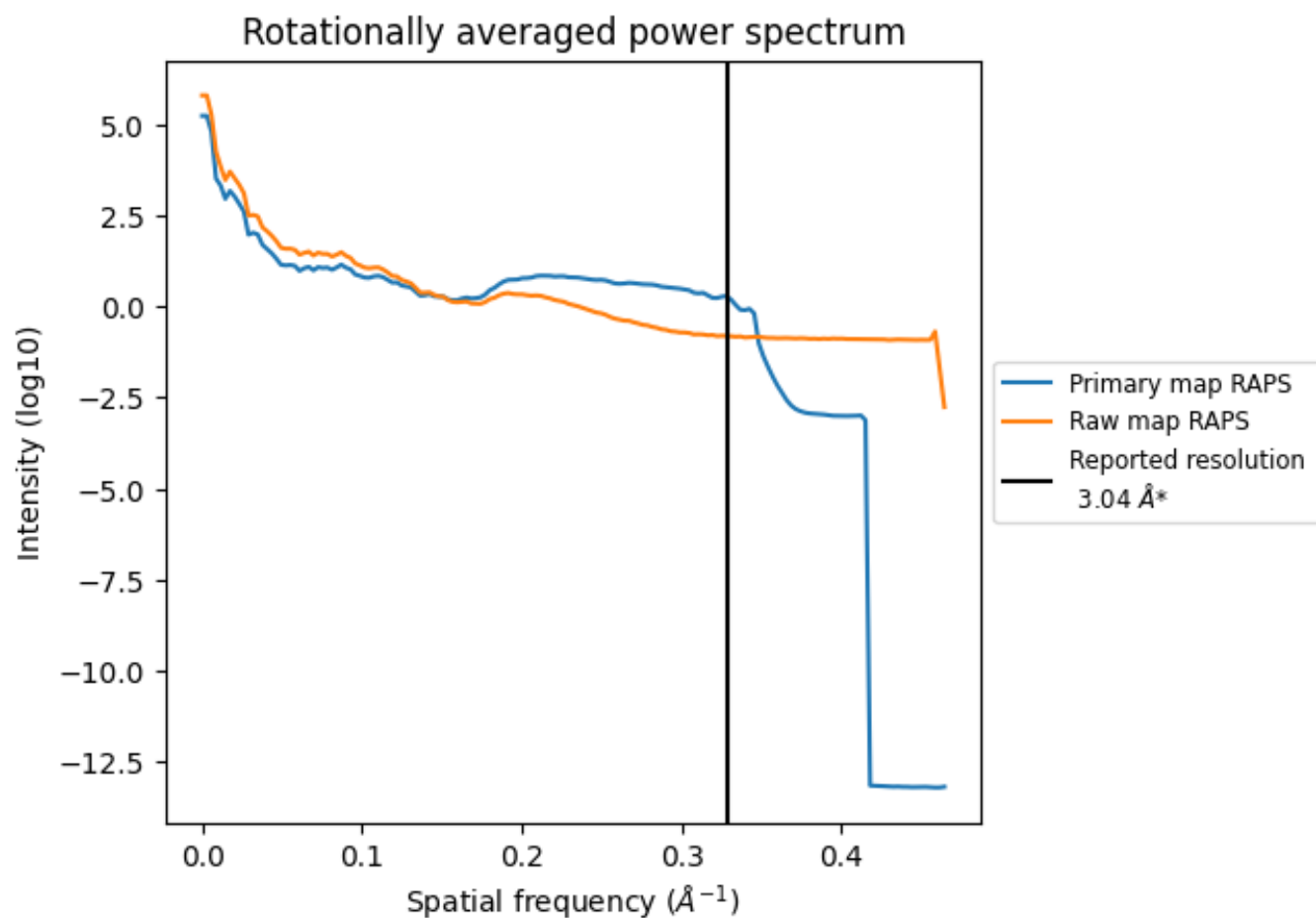
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 920  $\text{nm}^3$ ; this corresponds to an approximate mass of 831 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 ⓘ



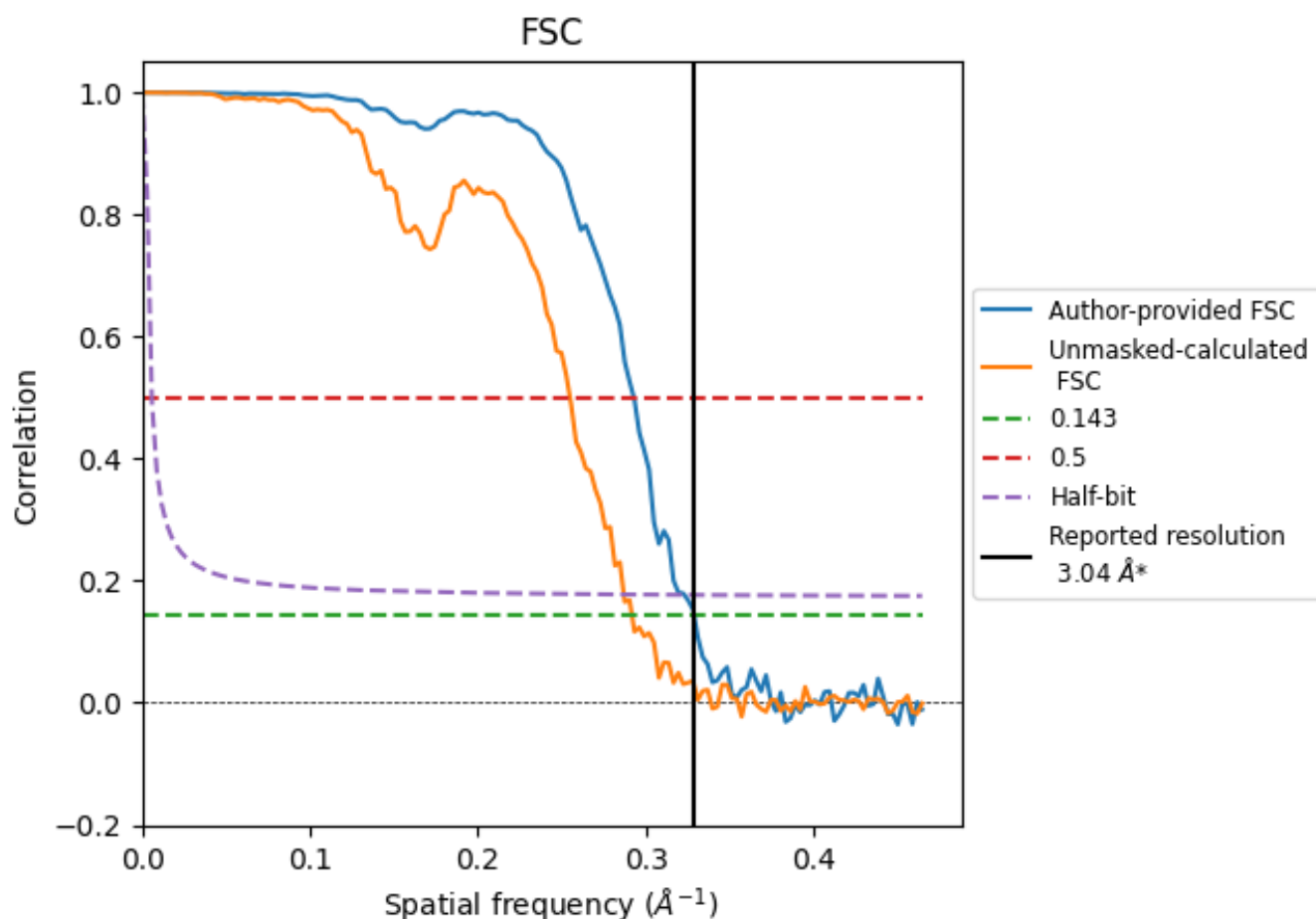
\*Reported resolution corresponds to spatial frequency of 0.329  $\text{\AA}^{-1}$



## 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  $0.329 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

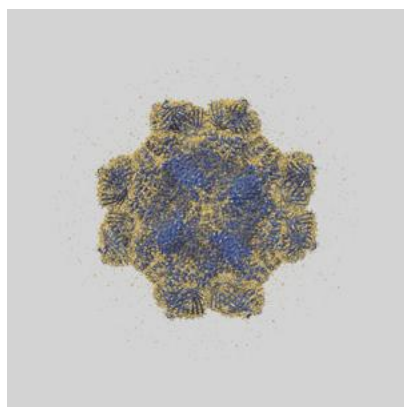
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.41	3.10
Unmasked-calculated*	3.43	3.92	3.48

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 3.04 by more than 10 %

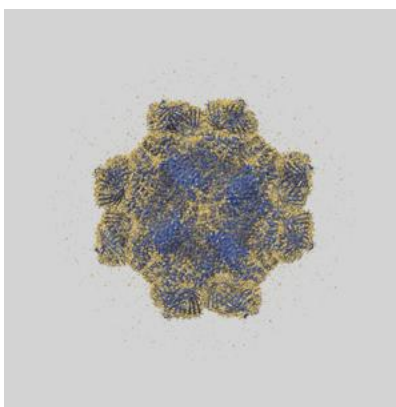
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61130 and PDB model 9J48. Per-residue inclusion information can be found in [section 3](#) on [page 34](#).

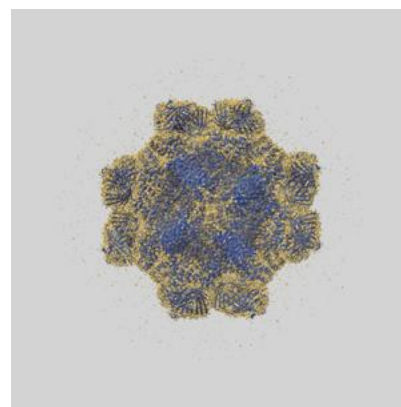
### 9.1 Map-model overlay [i](#)



X



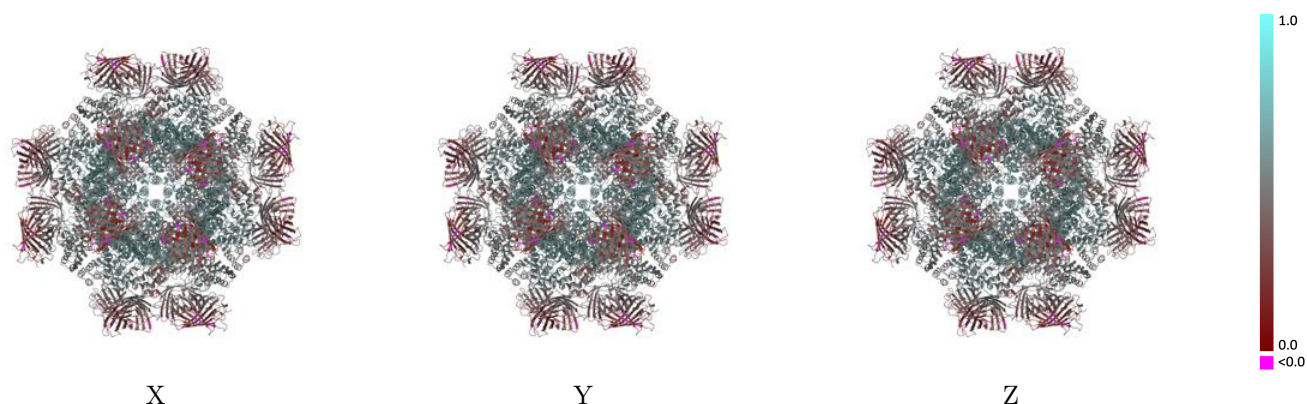
Y



Z

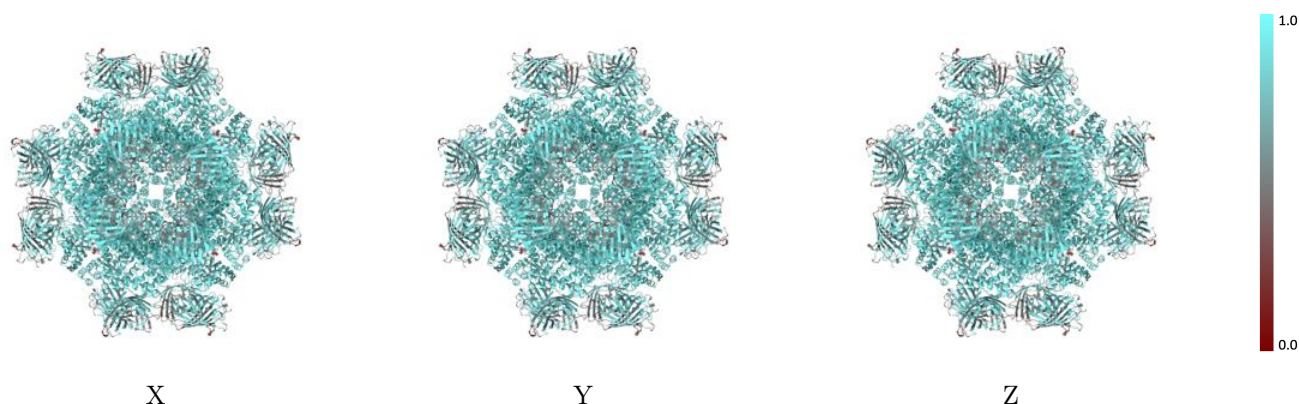
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



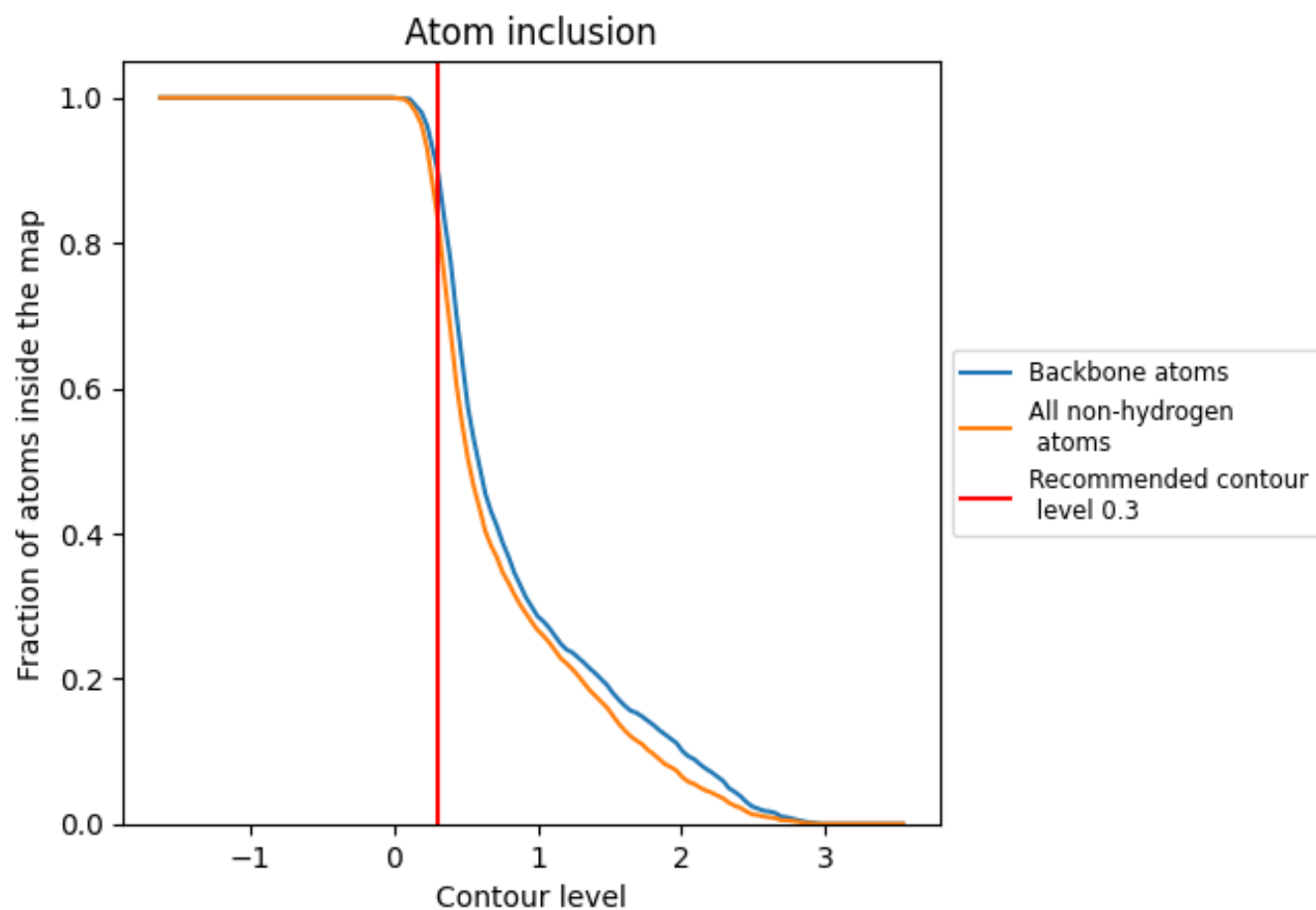
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8400	 0.4750
A	 0.9570	 0.5730
B	 0.9570	 0.5710
C	 0.9570	 0.5720
D	 0.9570	 0.5730
E	 0.9570	 0.5740
F	 0.9570	 0.5710
G	 0.9570	 0.5750
H	 0.9570	 0.5730
I	 0.9570	 0.5730
J	 0.9570	 0.5740
K	 0.9570	 0.5730
L	 0.9570	 0.5740
M	 0.9570	 0.5740
N	 0.9570	 0.5710
O	 0.9570	 0.5730
P	 0.9570	 0.5720
Q	 0.9570	 0.5740
R	 0.9570	 0.5740
S	 0.9570	 0.5730
T	 0.9570	 0.5720
V	 0.9570	 0.5720
W	 0.9570	 0.5710
X	 0.9570	 0.5730
Y	 0.9570	 0.5720
a	 0.6810	 0.3440
b	 0.6850	 0.3420
c	 0.6810	 0.3430
d	 0.6890	 0.3450
e	 0.6810	 0.3410
f	 0.6830	 0.3400
g	 0.6850	 0.3440
h	 0.6810	 0.3430
i	 0.6810	 0.3390
j	 0.6810	 0.3410



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Chain	Atom inclusion	Q-score
k	 0.6810	 0.3410
l	 0.6810	 0.3400
m	 0.6890	 0.3430
n	 0.6830	 0.3430
o	 0.6810	 0.3390
p	 0.6810	 0.3400
q	 0.6810	 0.3400
r	 0.6810	 0.3410
s	 0.6810	 0.3420
t	 0.6810	 0.3420
v	 0.6810	 0.3420
w	 0.6810	 0.3400
x	 0.6810	 0.3420
y	 0.6810	 0.3420