



Full wwPDB EM Validation Report ⓘ

Jul 14, 2025 – 10:47 AM JST

PDB ID : 9IUE / pdb_00009iue
EMDB ID : EMD-60898
Title : cryo-EM structure of FtsE/X and ZipA complex in filament
Authors : Zhu, K.F.; Li, J.W.; Luo, M.
Deposited on : 2024-07-20
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
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) : 2.44

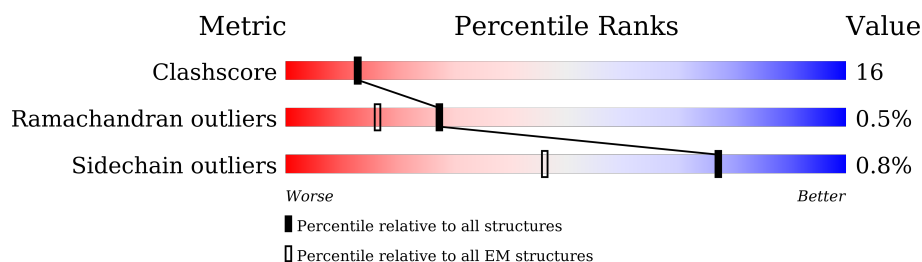
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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




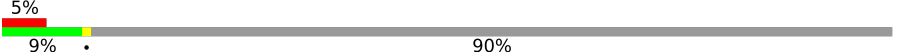



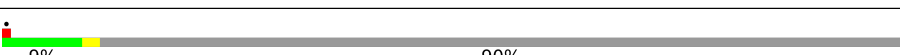
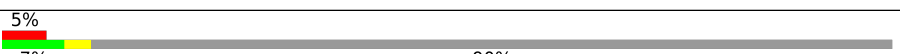
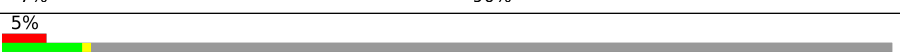
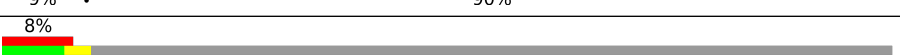
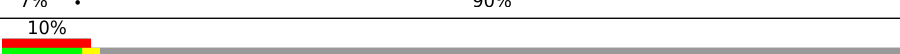


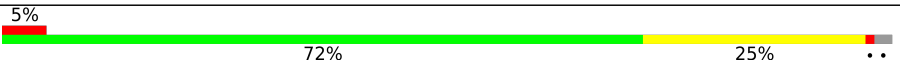


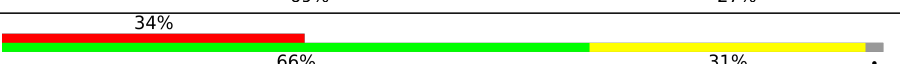









Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	1	328	6% . 90%
1	2	328	9% . 90%
1	E	328	5% 7% . 90%
1	F	328	5% 9% . 90%
1	K	328	8% 7% . 90%
1	L	328	10% 9% . 90%
1	Q	328	7% . 90%
1	R	328	9% . 90%



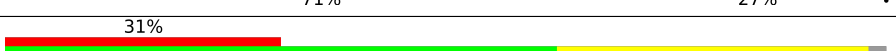
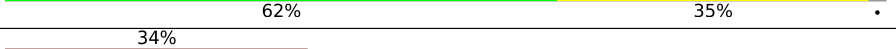


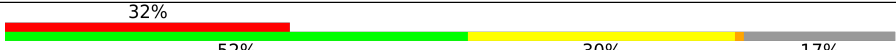




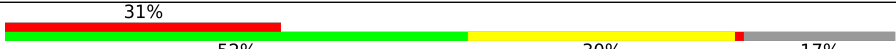
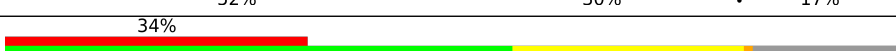





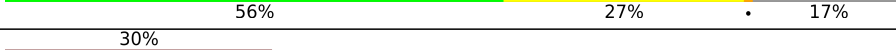
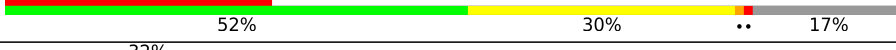

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Mol	Chain	Length	Quality of chain
1	W	328	
1	X	328	
1	c	328	
1	d	328	
1	i	328	
1	j	328	
1	o	328	
1	p	328	
1	u	328	
1	v	328	
2	5	226	
2	6	226	
2	G	226	
2	H	226	
2	M	226	
2	N	226	
2	S	226	
2	T	226	
2	Y	226	
2	Z	226	
2	e	226	
2	f	226	
2	k	226	
2	l	226	
2	q	226	

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Mol	Chain	Length	Quality of chain
2	r	226	
2	w	226	
2	x	226	
3	A	352	
3	B	352	
3	C	352	
3	D	352	
3	I	352	
3	J	352	
3	O	352	
3	P	352	
3	U	352	
3	V	352	
3	a	352	
3	b	352	
3	g	352	
3	h	352	
3	m	352	
3	n	352	
3	s	352	
3	t	352	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 75492 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 Cell division protein ZipA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	2	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	E	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	F	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	K	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	L	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	Q	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	R	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	W	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	X	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	c	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	d	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	i	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	j	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	o	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	p	33	Total	C	N	O	S	0	0
			263	175	46	41	1		
1	u	33	Total	C	N	O	S	0	0
			263	175	46	41	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	v	33	Total	C	N	O	S	0	0
			263	175	46	41	1		

- Molecule 2 is a protein called Cell division ATP-binding protein FtsE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	6	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	G	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	H	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	M	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	N	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	S	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	T	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	Y	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	Z	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	e	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	f	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	k	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	l	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	q	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	r	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		
2	w	222	Total	C	N	O	S	0	0
			1713	1080	319	306	8		
2	x	221	Total	C	N	O	S	0	0
			1709	1078	318	305	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	-3	SER	-	expression tag	UNP W1F1D8
5	0	VAL	THR	conflict	UNP W1F1D8
6	-3	SER	-	expression tag	UNP W1F1D8
6	0	VAL	THR	conflict	UNP W1F1D8
G	-3	SER	-	expression tag	UNP W1F1D8
G	0	VAL	THR	conflict	UNP W1F1D8
H	-3	SER	-	expression tag	UNP W1F1D8
H	0	VAL	THR	conflict	UNP W1F1D8
M	-3	SER	-	expression tag	UNP W1F1D8
M	0	VAL	THR	conflict	UNP W1F1D8
N	-3	SER	-	expression tag	UNP W1F1D8
N	0	VAL	THR	conflict	UNP W1F1D8
S	-3	SER	-	expression tag	UNP W1F1D8
S	0	VAL	THR	conflict	UNP W1F1D8
T	-3	SER	-	expression tag	UNP W1F1D8
T	0	VAL	THR	conflict	UNP W1F1D8
Y	-3	SER	-	expression tag	UNP W1F1D8
Y	0	VAL	THR	conflict	UNP W1F1D8
Z	-3	SER	-	expression tag	UNP W1F1D8
Z	0	VAL	THR	conflict	UNP W1F1D8
e	-3	SER	-	expression tag	UNP W1F1D8
e	0	VAL	THR	conflict	UNP W1F1D8
f	-3	SER	-	expression tag	UNP W1F1D8
f	0	VAL	THR	conflict	UNP W1F1D8
k	-3	SER	-	expression tag	UNP W1F1D8
k	0	VAL	THR	conflict	UNP W1F1D8
l	-3	SER	-	expression tag	UNP W1F1D8
l	0	VAL	THR	conflict	UNP W1F1D8
q	-3	SER	-	expression tag	UNP W1F1D8
q	0	VAL	THR	conflict	UNP W1F1D8
r	-3	SER	-	expression tag	UNP W1F1D8
r	0	VAL	THR	conflict	UNP W1F1D8
w	-3	SER	-	expression tag	UNP W1F1D8
w	0	VAL	THR	conflict	UNP W1F1D8
x	-3	SER	-	expression tag	UNP W1F1D8
x	0	VAL	THR	conflict	UNP W1F1D8

- Molecule 3 is a protein called Cell division protein FtsX.

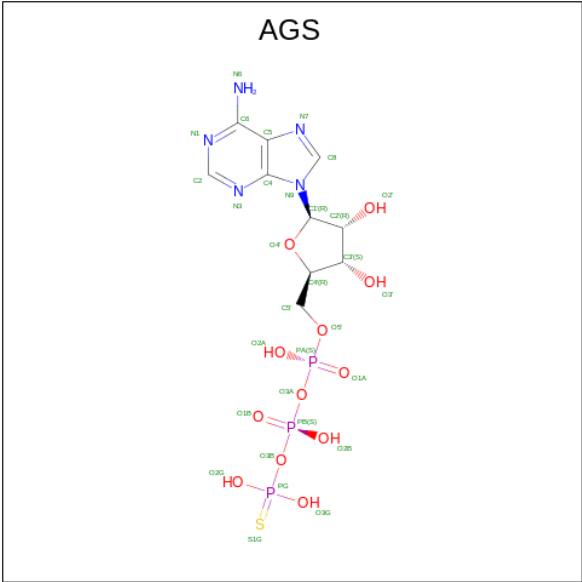
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	C	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	D	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	I	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	J	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	O	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	P	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	U	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	V	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	a	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	b	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	g	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	h	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	m	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	n	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		
3	s	292	Total	C	N	O	S	0	0
			2204	1425	371	400	8		
3	t	293	Total	C	N	O	S	0	0
			2174	1412	360	393	9		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	H	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	M	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	N	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	S	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	T	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	Y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	Z	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	e	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	f	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	k	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	l	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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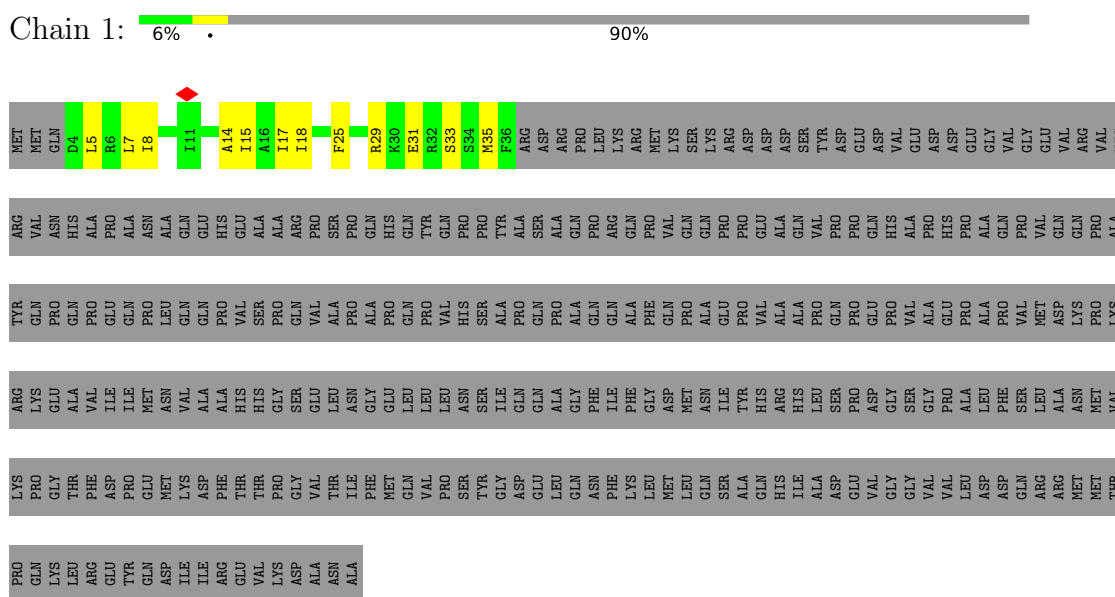
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Mol	Chain	Residues	Atoms						AltConf
4	q	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	r	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	w	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
4	x	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

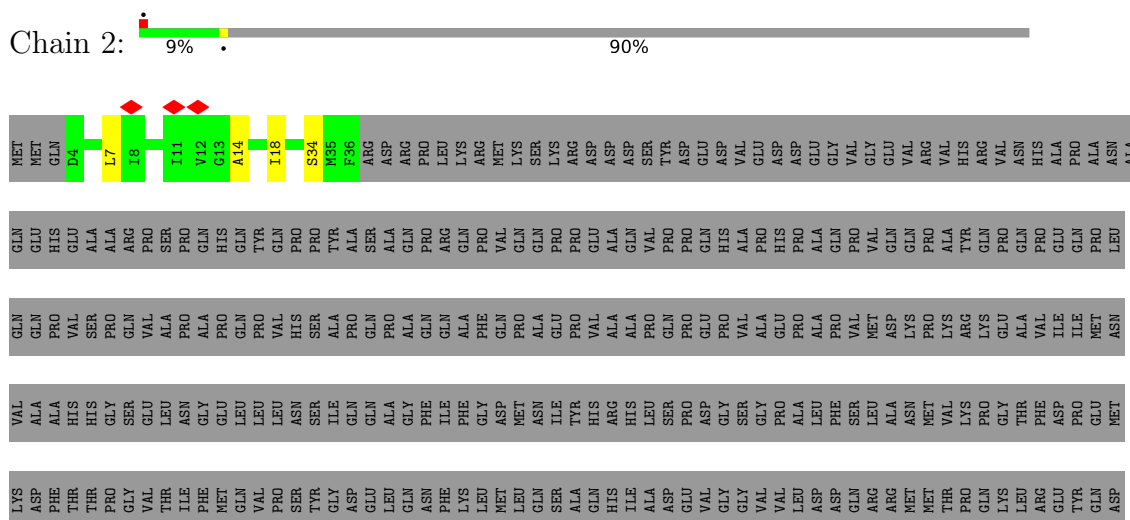
3 Residue-property plots [i](#)

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

• Molecule 1: Cell division protein ZipA



• Molecule 1: Cell division protein ZipA





LEU ARG
GLU TYR
GLN ASP
TLE TLE
ARG
GLU VAL
LYS
ASP
ASN
ALA

● Molecule 1: Cell division protein ZipA



GLU	VAL	LYS	ASP	ALA	ASN	ALA	THR	THR	HIS	HIS	VAL	SER	GLN	PRO	ALA	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
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● Molecule 1: Cell division protein ZipA



ARG	ARG	MET	MET	THR	PRO	GLN	LYS	LEU	LEU	ARG	GLU	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	ARG	GLU	THR	THR	PRO	GLY	GLY	VAL	THR	THR	GLN	ASP	ILE	ILE	
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● Molecule 1: Cell division protein ZipA



MET	MET	GLN	D4	L7	I8	I9	I10	I11	V12	G13	A14	I15	A16	I17	I18	A19	L20	L21	S33	S34	M35	F36	ARG	ASP	ARG	PRO	GLU	LEU	LYS	ARG	MET	LYS	LYS	SER	LYS	ARG	ASP	ASP	ASP	THR	ASP	GLU	ASP	VAL	GLU	ASP	GLY	GLY	VAL	VAL	GLY	GLY	VAL	VAL	GLY	VAL	ARG	HIS	ARG	VAL	VAL
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LYS	GLY	GLU	PRO	ASN
LEU	THR	ALA	GLN	HIS
ARG	PHE	VAL	PRO	ALA
GLU	ASP	ILE	GLU	PRO
TYR	PRO	ILE	GLN	ALA
GLN	GLI	MET	PRO	ASN
ASP	MET	ASN	LEU	ALA
ILE	LYS	VAL	GLN	GLN
ILE	ASP	ALA	GLN	GLU
ARG	PHE	ALA	PRO	HIS
GLU	THR	HIS	VAL	GLU
VAL	THR	HIS	SER	ALA
LYS	PRO	GLY	PRO	ALA
ARG	GLY	SER	GLN	ARG
ALA	VAL	GLU	VAL	PRO
ASN	THR	LEU	ALA	SER
ALA	ILE	ASN	PRO	PRO
	PHE	GLY	ALA	GLN
	MET	GLU	PRO	HIS
	GLN	LEU	GLN	GLN
	VAL	LEU	PRO	TYR
	PRO	LEU	VAL	GLN
	SER	ASN	HIS	PRO
	TYR	SER	SER	PRO
	GLY	ILE	ALA	TYR
	ASP	GLN	PRO	ALA
	GLU	GLN	GLN	SER
	LEU	ALA	PRO	ALA
	GLN	GLY	ALA	GLN
	ASN	PHE	GLN	PRO
	PHE	ILE	GLN	ARG
	LYS	PHE	ALA	GLN
	LEU	GLY	PHE	PRO
	MET	MET	GLN	VAL
	LEU	ASN	PRO	GLN
	SER	ILE	ALA	GLN
	GLN	ASN	ALA	GLN
	SER	GLY	PRO	PRO
	ALA	TYR	VAL	PRO
	GLN	HIS	GLU	ALA
	ILE	HIS	ALA	GLN
	ALA	LEU	PRO	VAL
	ASP	SER	GLN	PRO
	GLU	PRO	GLN	PRO
	VAL	ASP	GLU	GLN
	GLY	GLY	PRO	HIS
	GLY	SER	VAL	ALA
	VAL	GLY	ALA	PRO
	VAL	PRO	GLU	HIS
	LEU	ALA	PRO	PRO
	ASP	LEU	ALA	ALA
	ASP	PHE	PRO	GLN
	GLN	SER	VAL	PRO
	ARG	LEU	MET	VAL
	ARG	ALA	ASP	GLN
	MET	ASN	LYS	GLN
	MET	MET	PRO	ALA
	THR	VAL	LYS	ALA
	PRO	VAL	TYR	GLN

- Molecule 1: Cell division protein ZipA

[illegible]

- Molecule 1: Cell division protein ZipA

[illegible]

[illegible]

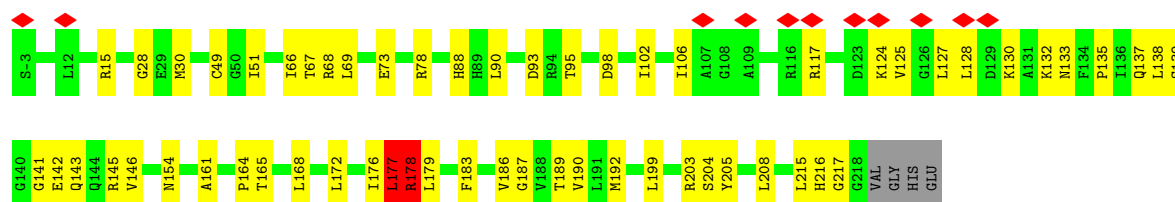
- Molecule 1: Cell division protein ZipA



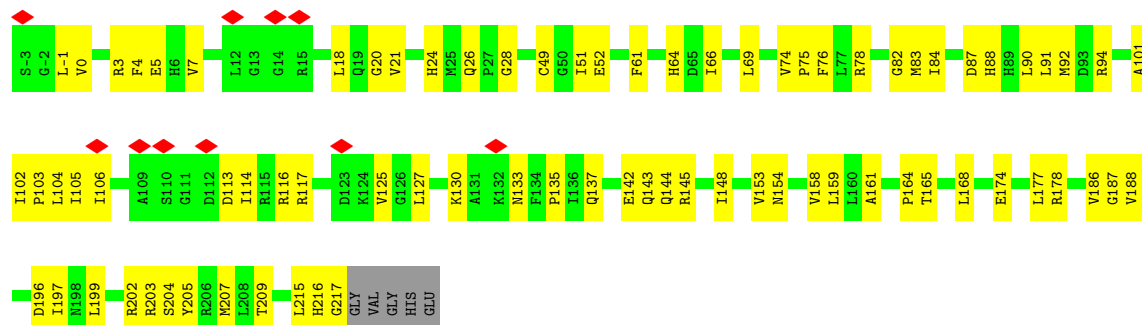
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GLU	ASP	ILE	ILE	GLN	GLU	ALA	D4
TYR	PRO	ASP	ILE	MET	PRO	ASN	I8
GLN	GLU	GLU	MET	ASN	LEU	ALA	I9
ASP	MET	ILE	VAL	ASN	GLN	GLN	I10
ILE	ILE	ASP	ALA	VAL	GLN	GLU	I11
ARG	PHE	ASP	ALA	PRO	PRO	HIS	I12
GLU	THR	THR	HIS	VAL	GLU	GLU	V12
VAL	THR	THR	HIS	SER	ALA	ALA	G13
LYS	PRO	GLY	GLY	PRO	PRO	ALA	A14
ASP	GLY	SER	SER	GLN	ARG	ARG	I15
ALA	ALA	ALA	GLU	VAL	VAL	SER	A16
ASN	THR	THR	LEU	ALA	ALA	SER	I17
ALA	ILE	ILE	ASN	PRO	PRO	PRO	I18
	PHE	PHE	GLY	ALA	ALA	GLN	I19
	MET	GLU	GLU	PRO	GLN	HIS	G19
	GLU	VAL	LEU	PRO	GLN	PRO	L20
	VAL	VAL	LEU	VAL	VAL	GLN	L21
	SER	ASN	ASN	HIS	PRO	PRO	
	TYR	GLY	ILE	SER	TYR	TYR	R32
	GLY	GLU	ILE	GLN	ALA	ALA	S33
	GLU	GLU	GLN	GLN	SER	SER	S34
	LEU	ALA	ALA	PRO	ALA	GLN	K35
	GLN	GLY	PHE	ALA	PRO	PRO	F36
	ASN	ASN	PHE	GLN	GLN	ARG	ASP
	PHE	TYR	ILE	ALA	ALA	GLN	ARG
	LEU	LEU	GLY	PHE	GLN	PRO	PRO
	MET	MET	ASP	GLN	VAL	VAL	PRO
	LEU	LEU	MET	PRO	GLN	GLN	LEU
	GLN	GLN	ASN	ALA	ALA	GLN	LYS
	ALA	ALA	ILE	ILE	ALA	VAL	ARG
	ASP	ASP	LEU	LEU	PRO	GLN	LYS
	VAL	VAL	PRO	PRO	GLN	PRO	ASP
	GLU	GLU	ASP	GLU	PRO	ASP	ASP
	GLY	GLY	GLY	ASP	GLU	HIS	SER
	GLY	SER	SER	VAL	PRO	TYR	TYR
	VAL	VAL	GLY	ALA	ALA	PRO	ASP
	LEU	LEU	PRO	PRO	HIS	HIS	GLU
	ASP	ASP	ALA	ALA	ALA	VAL	ASP
	ASP	PHE	LEU	PRO	ALA	VAL	VAL
	GLN	SER	PHE	PRO	GLN	GLU	GLU
	THR	THR	LEU	VAL	VAL	ASP	ASP
	PRO	PRO	LEU	MET	MET	GLY	GLY
	GLN	GLN	PRO	VAL	VAL	VAL	VAL
				ARG	ARG	ARG	ARG
							HIS
							ARG

- Molecule 1: Cell division protein ZipA

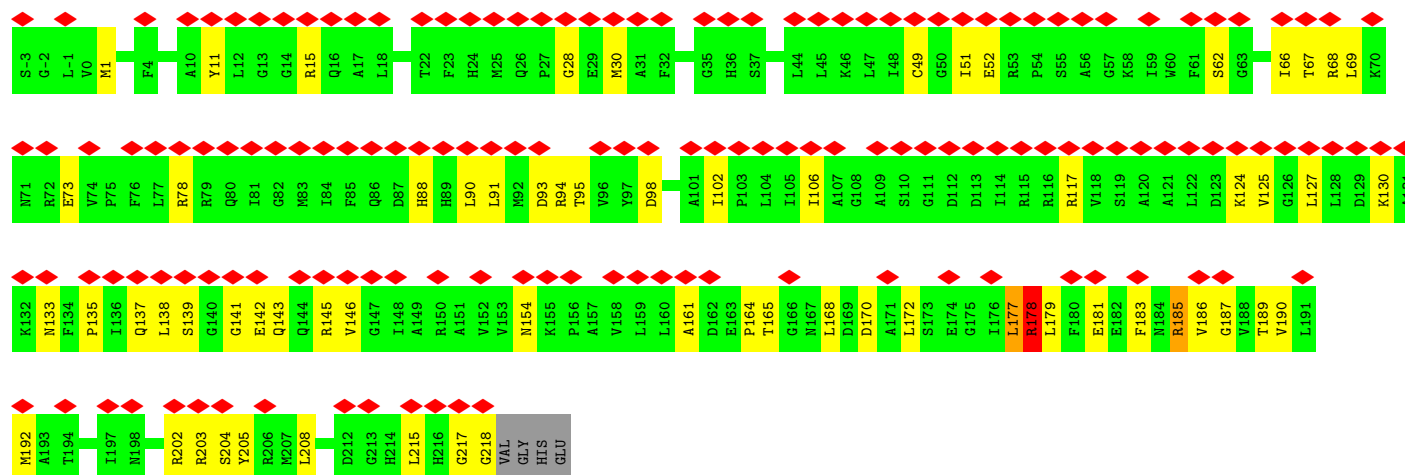
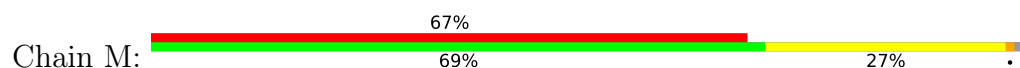
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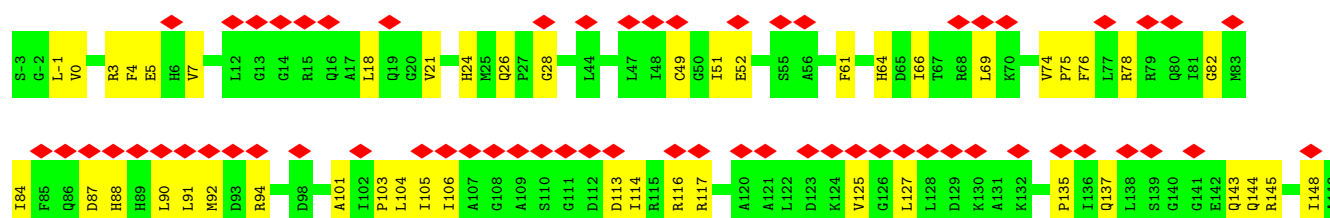
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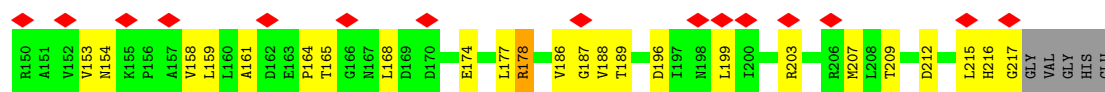


• Molecule 2: Cell division ATP-binding protein FtsE



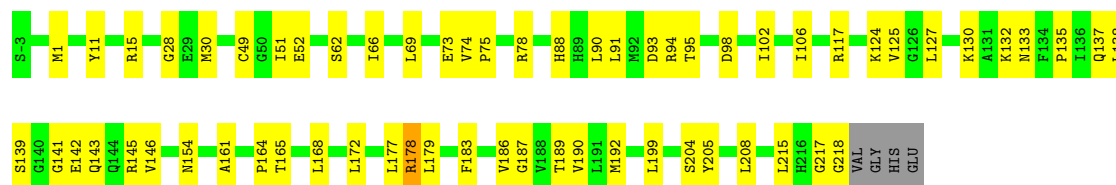
• Molecule 2: Cell division ATP-binding protein FtsE





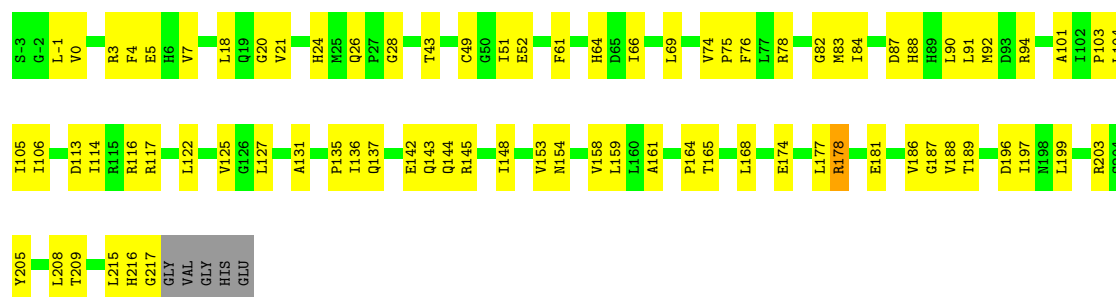
• Molecule 2: Cell division ATP-binding protein FtsE

Chain S: 71% 27%



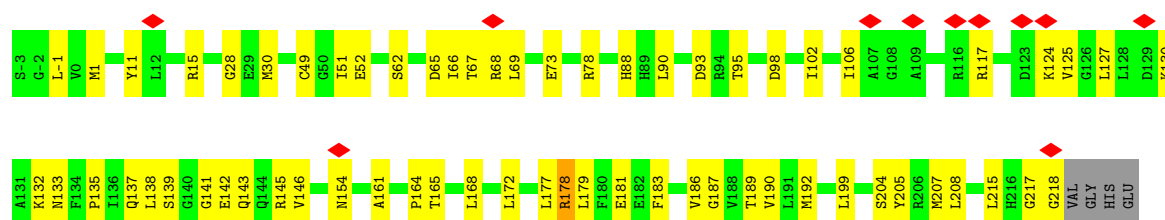
• Molecule 2: Cell division ATP-binding protein FtsE

Chain T: 62% 35%



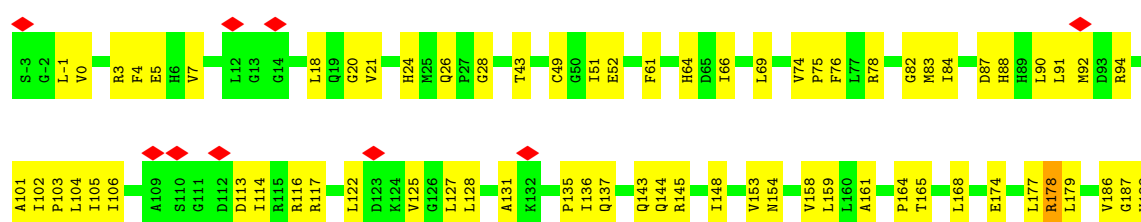
• Molecule 2: Cell division ATP-binding protein FtsE

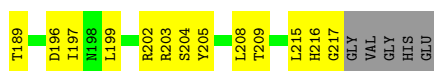
Chain Y: 5% 70% 28%



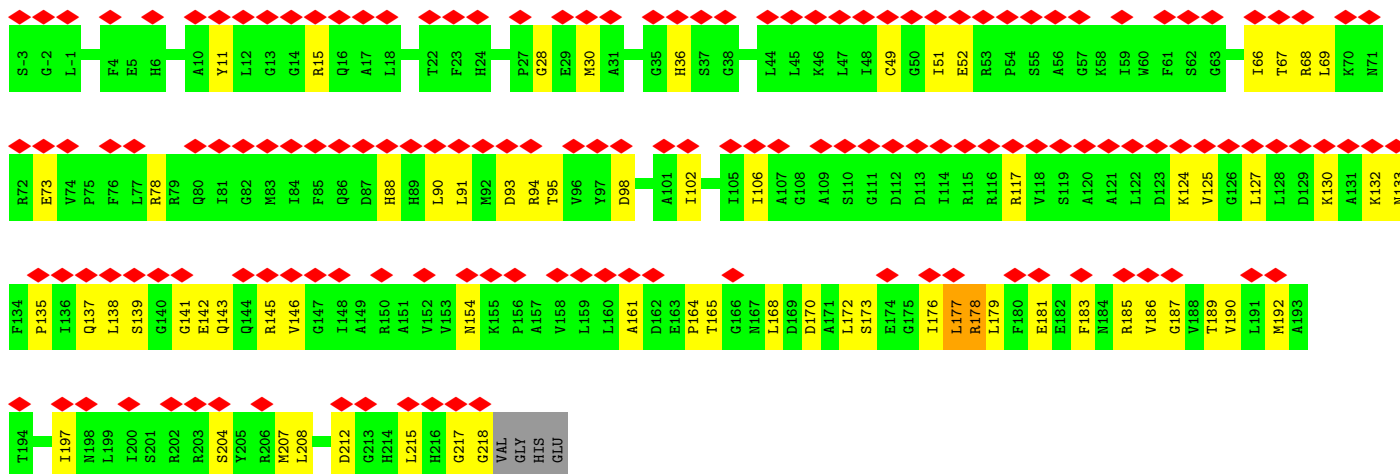
• Molecule 2: Cell division ATP-binding protein FtsE

Chain Z: 61% 36%

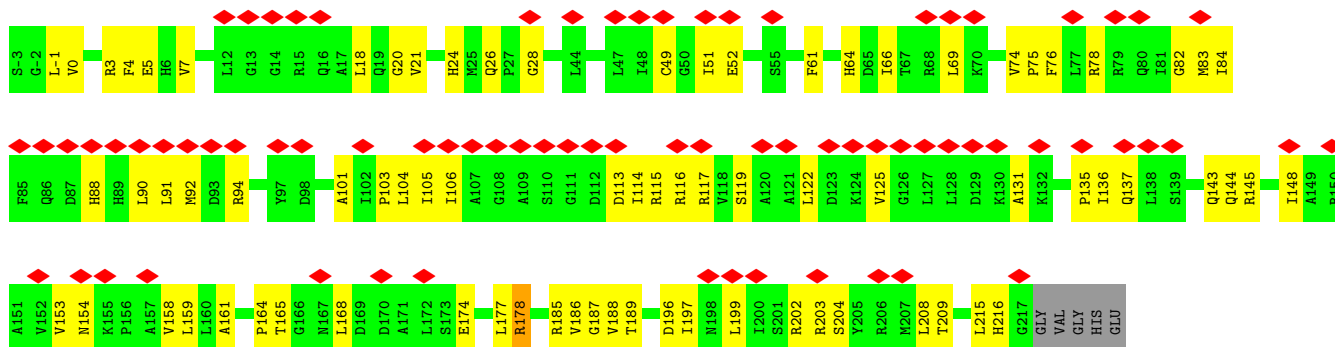




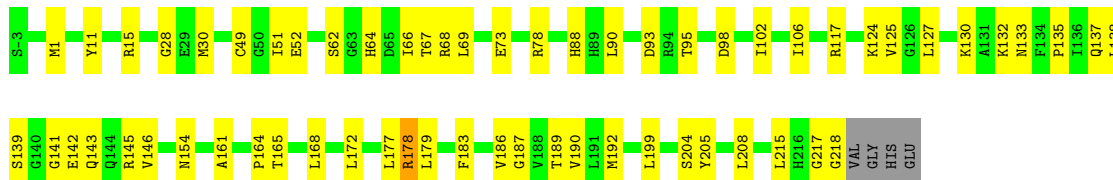
• Molecule 2: Cell division ATP-binding protein FtsE



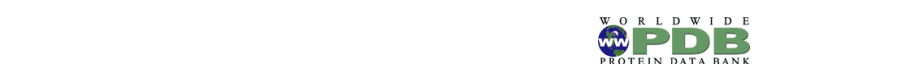
• Molecule 2: Cell division ATP-binding protein FtsE

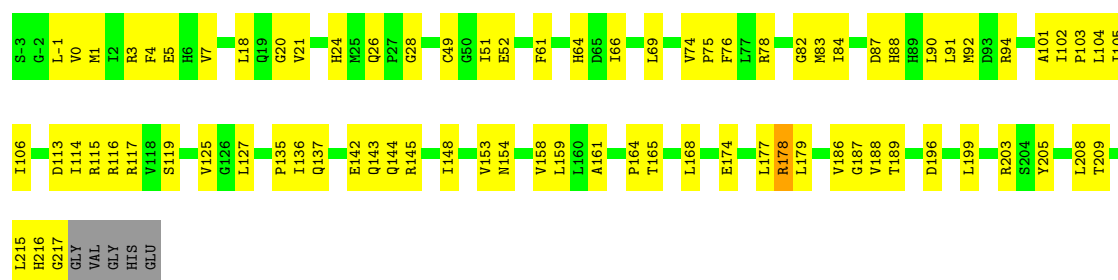


• Molecule 2: Cell division ATP-binding protein FtsE



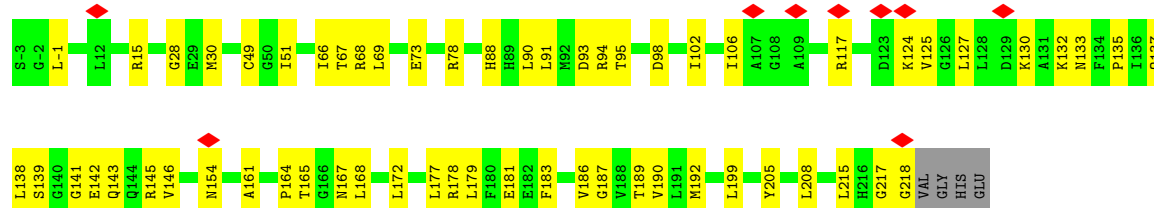
• Molecule 2: Cell division ATP-binding protein FtsE





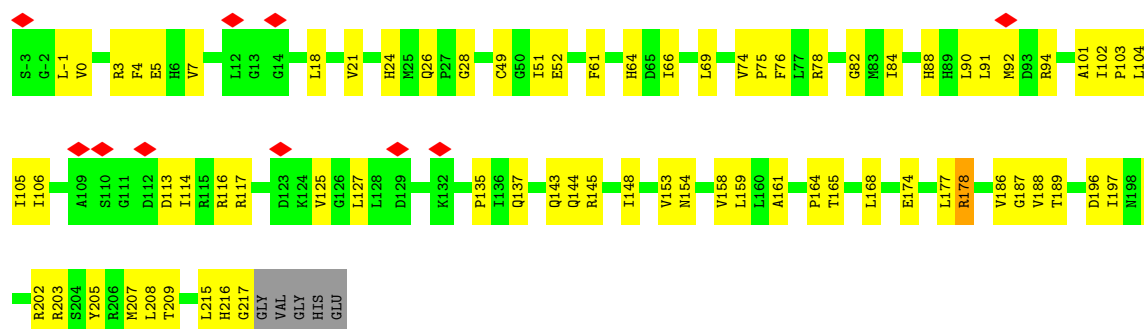
• Molecule 2: Cell division ATP-binding protein FtsE

Chain q: 72% 27%



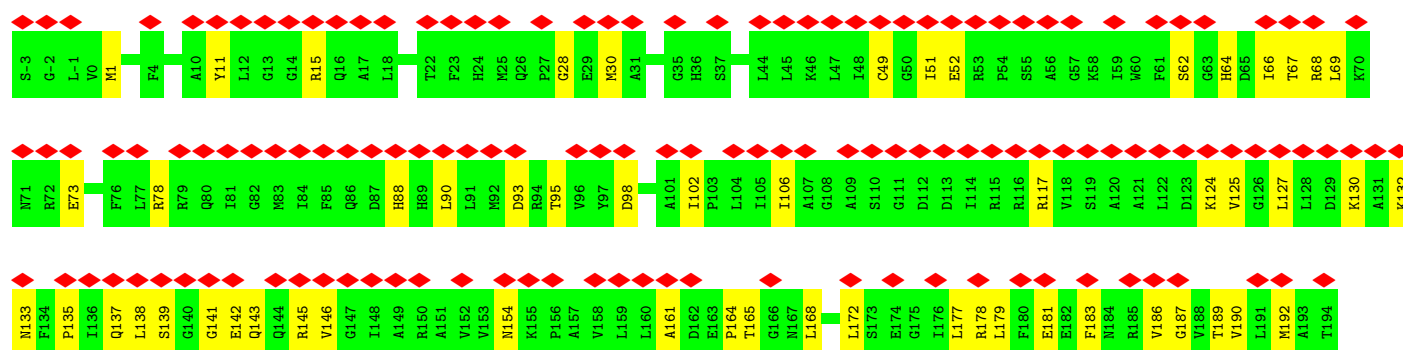
• Molecule 2: Cell division ATP-binding protein FtsE

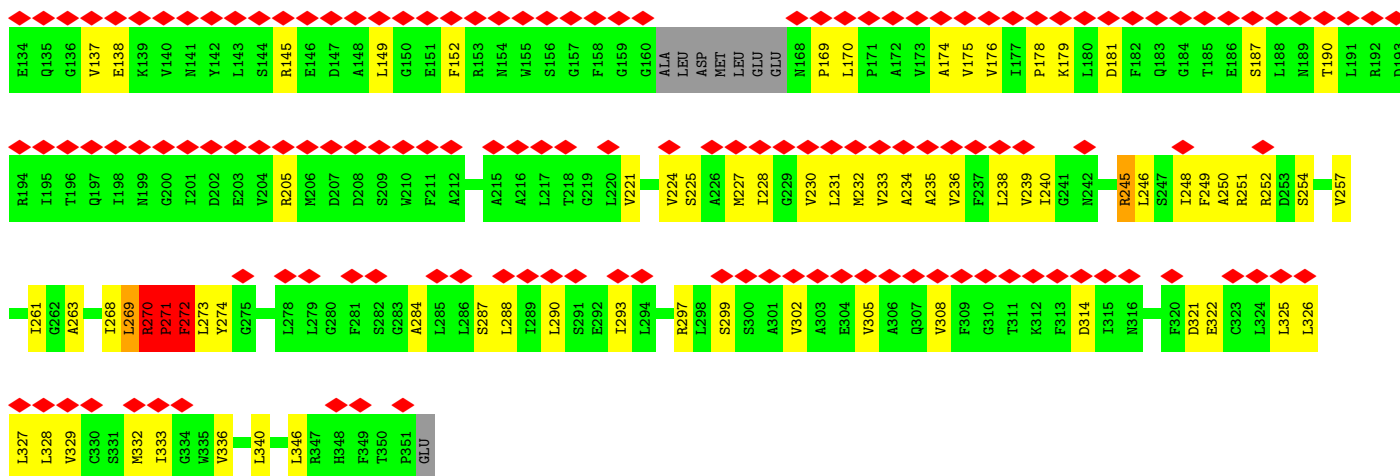
Chain r: 65% 32%



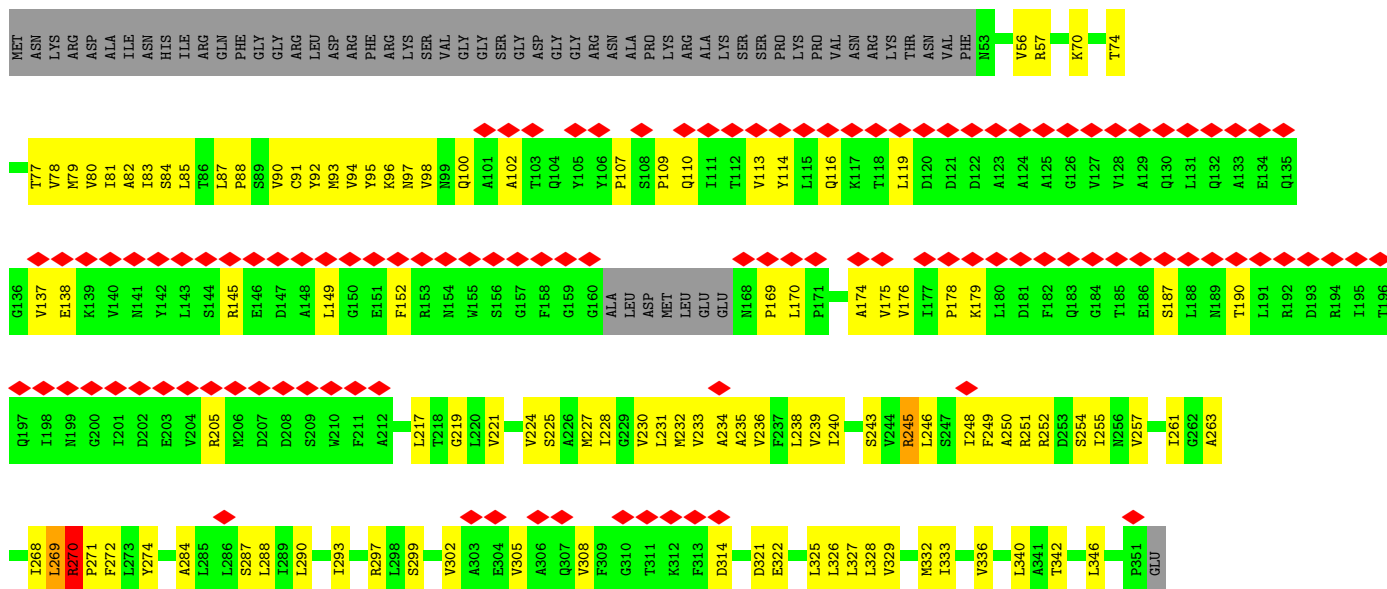
• Molecule 2: Cell division ATP-binding protein FtsE

Chain w: 66% 27%

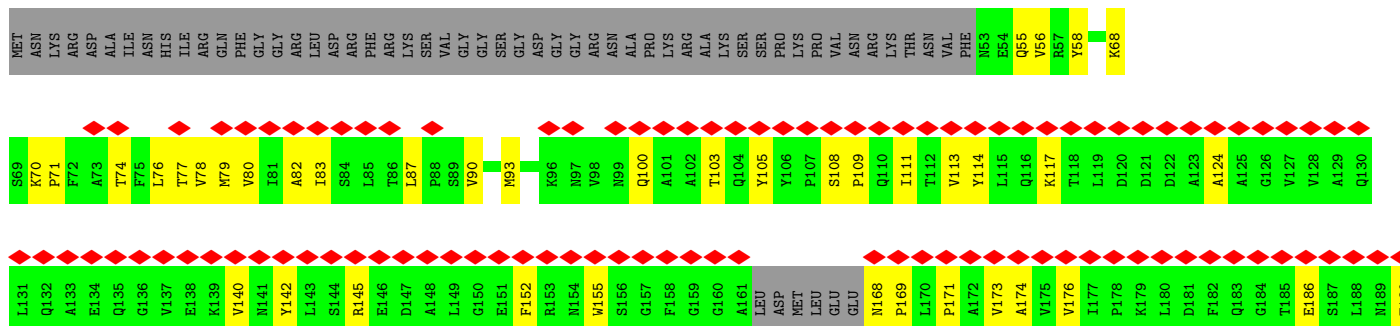


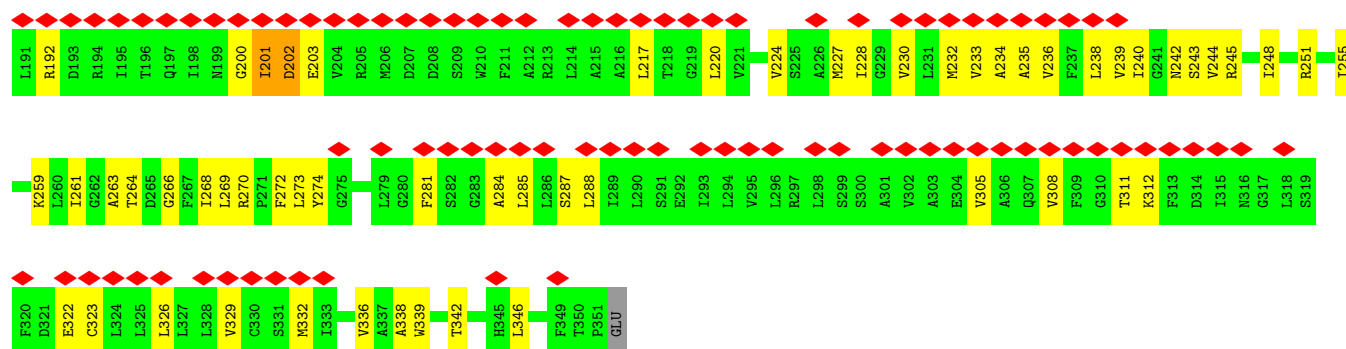


• Molecule 3: Cell division protein FtsX

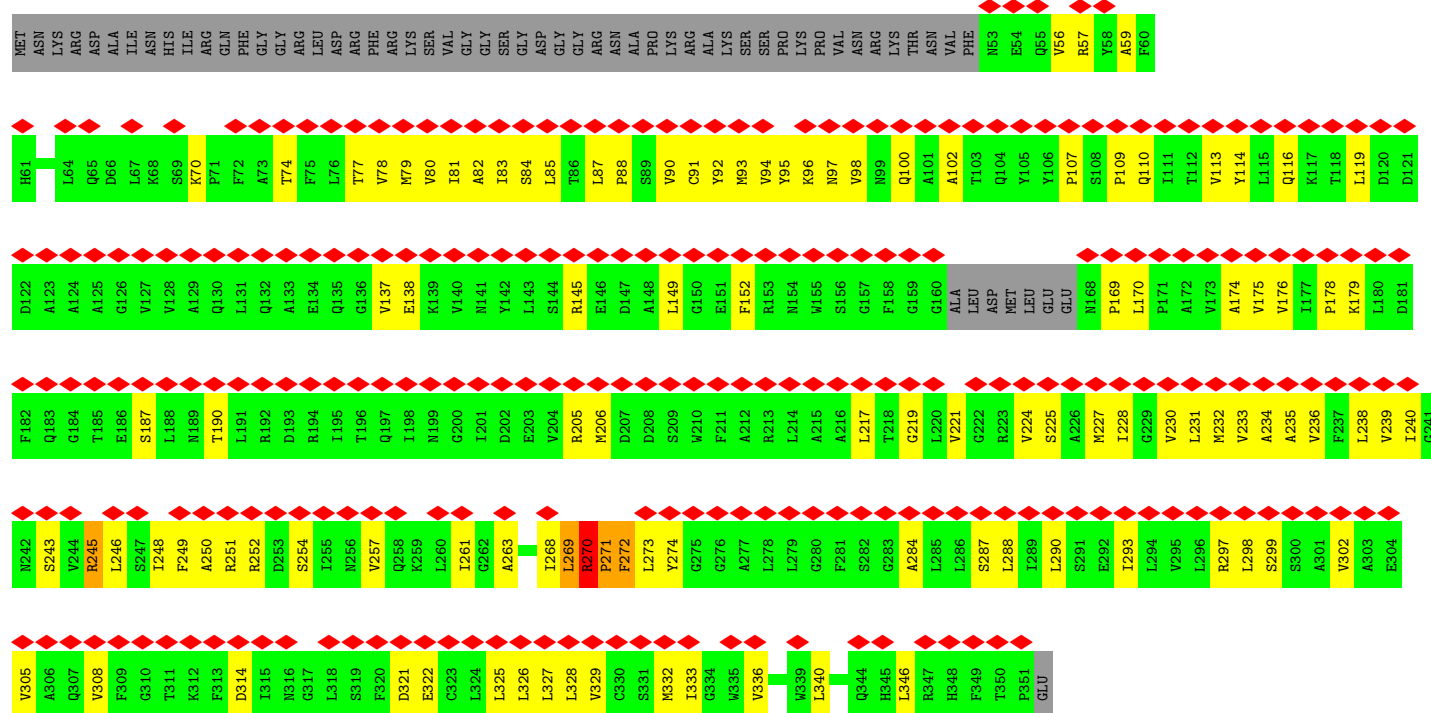
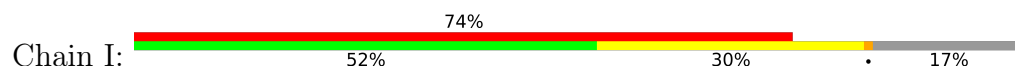


• Molecule 3: Cell division protein FtsX

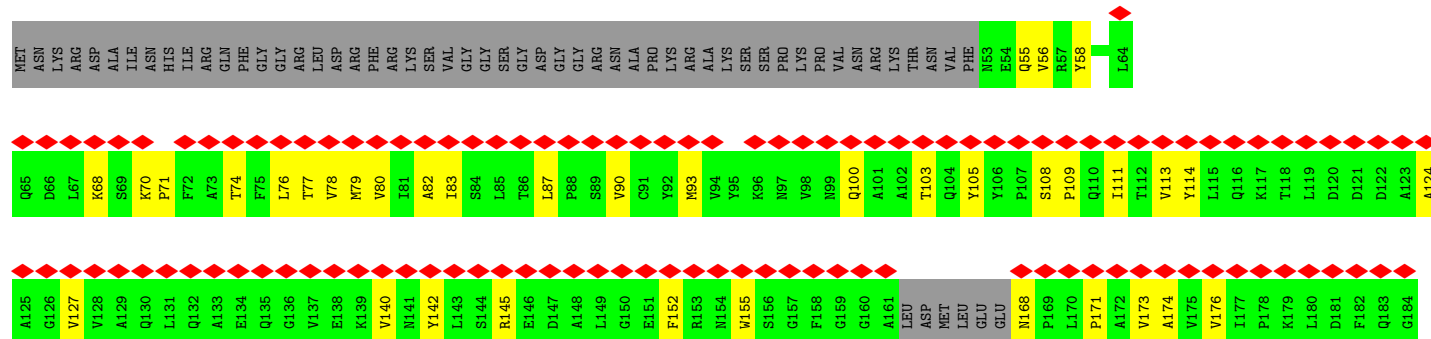


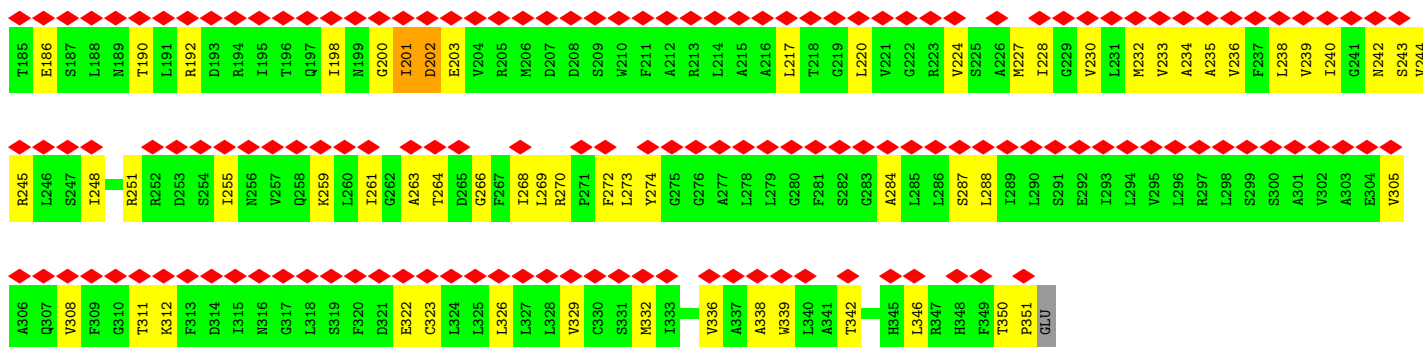


• Molecule 3: Cell division protein FtsX

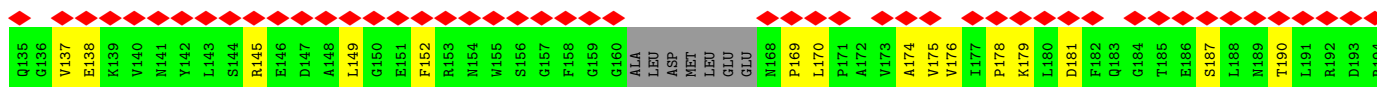
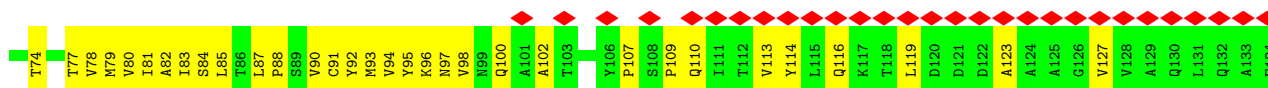
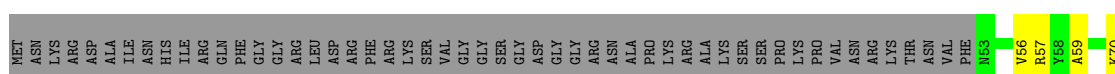


• Molecule 3: Cell division protein FtsX

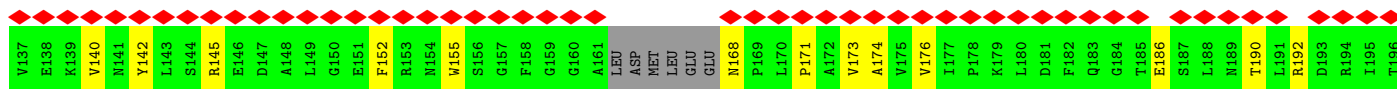
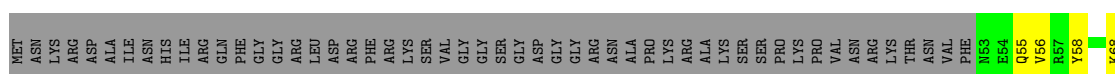




• Molecule 3: Cell division protein FtsX

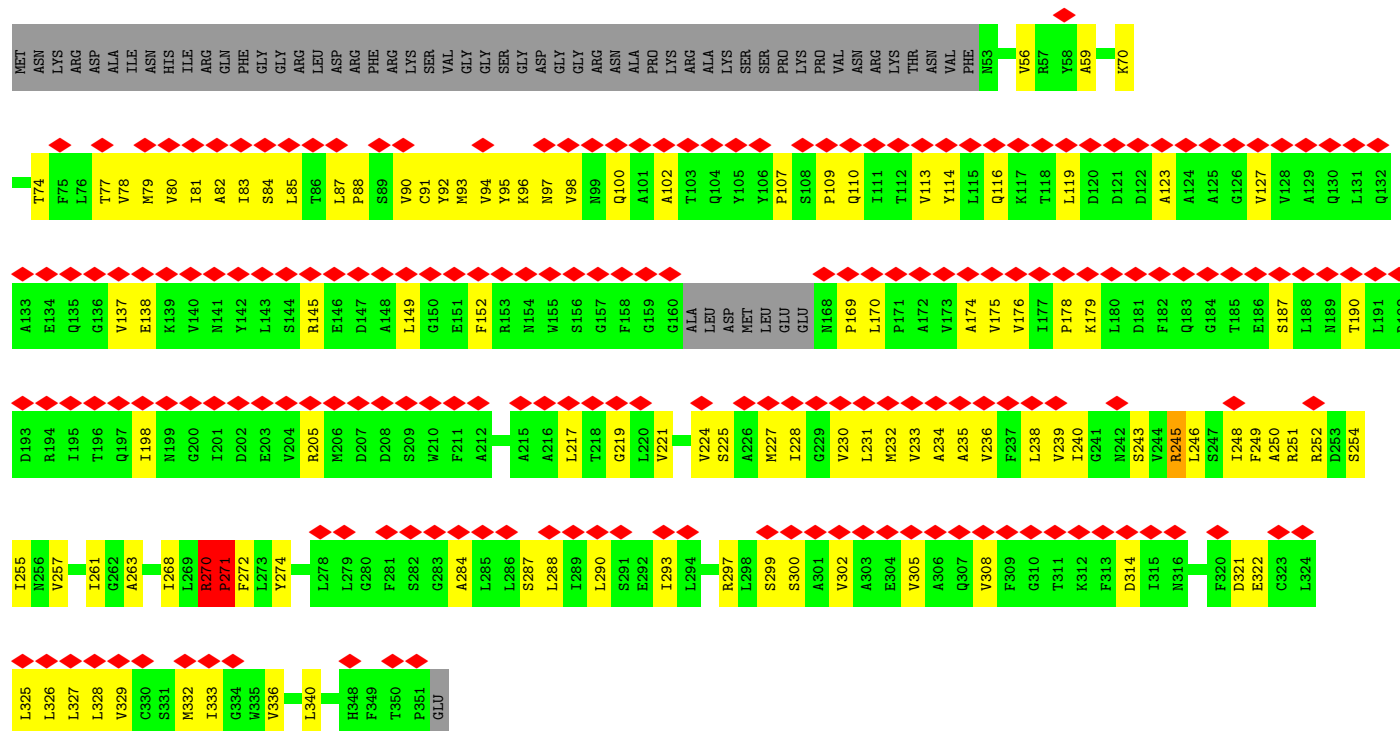


• Molecule 3: Cell division protein FtsX

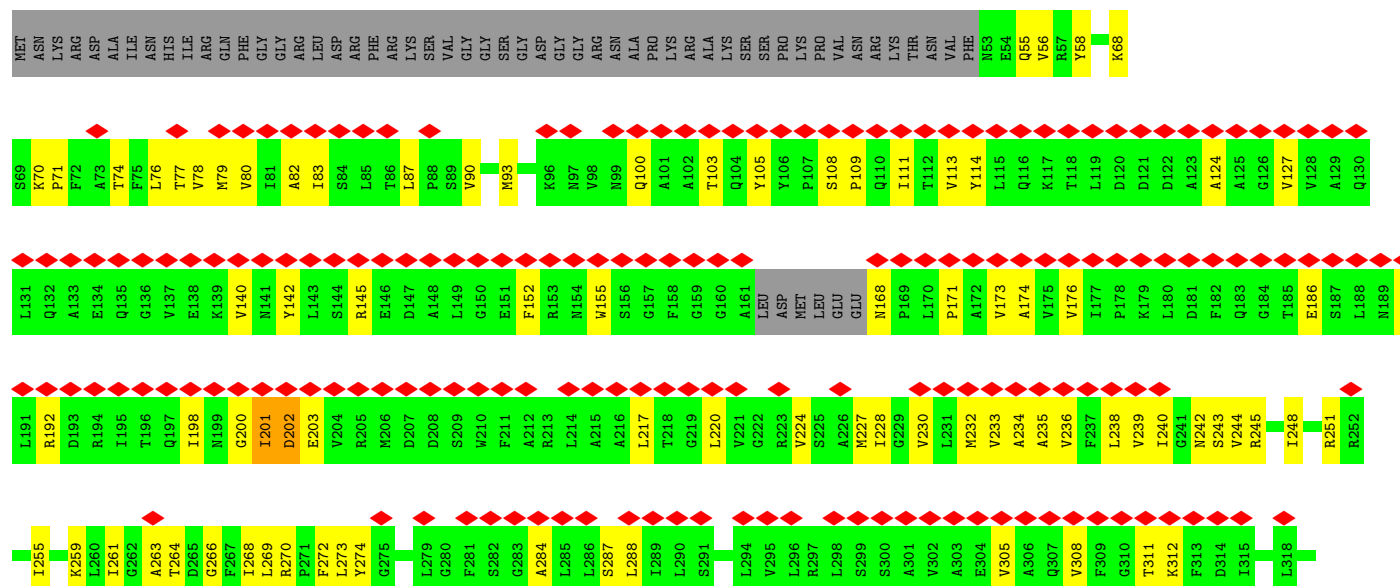


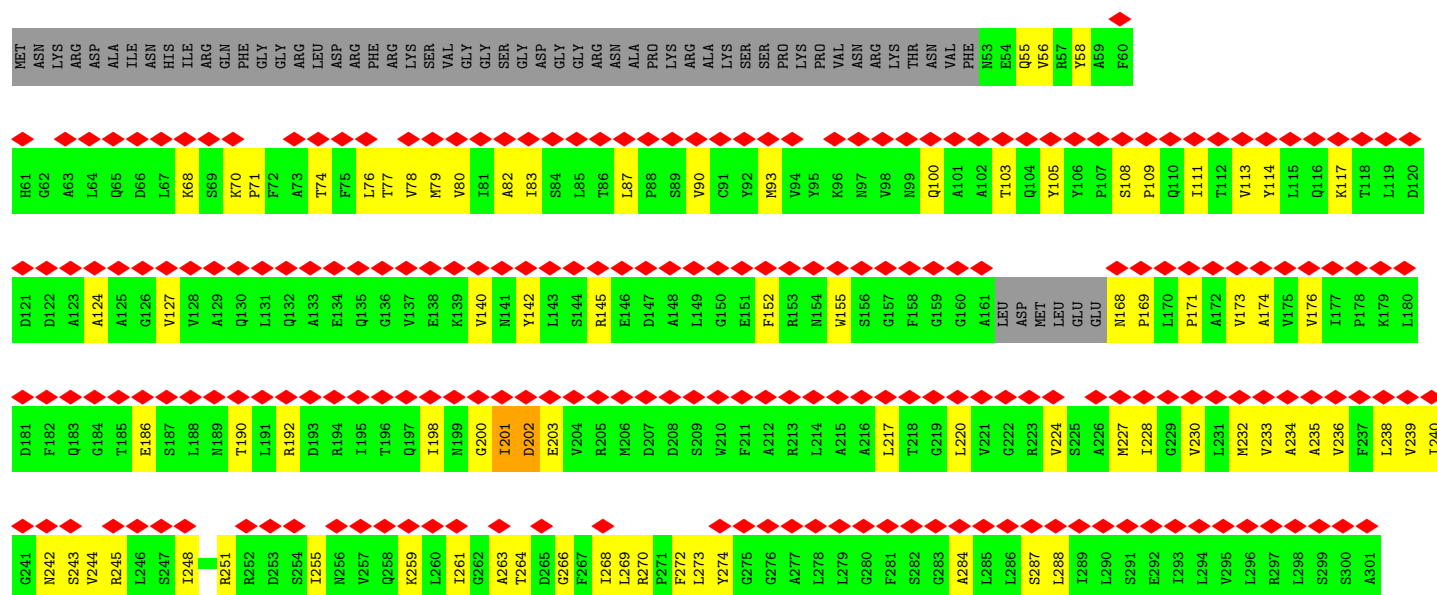
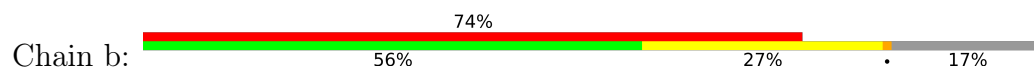
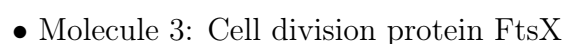
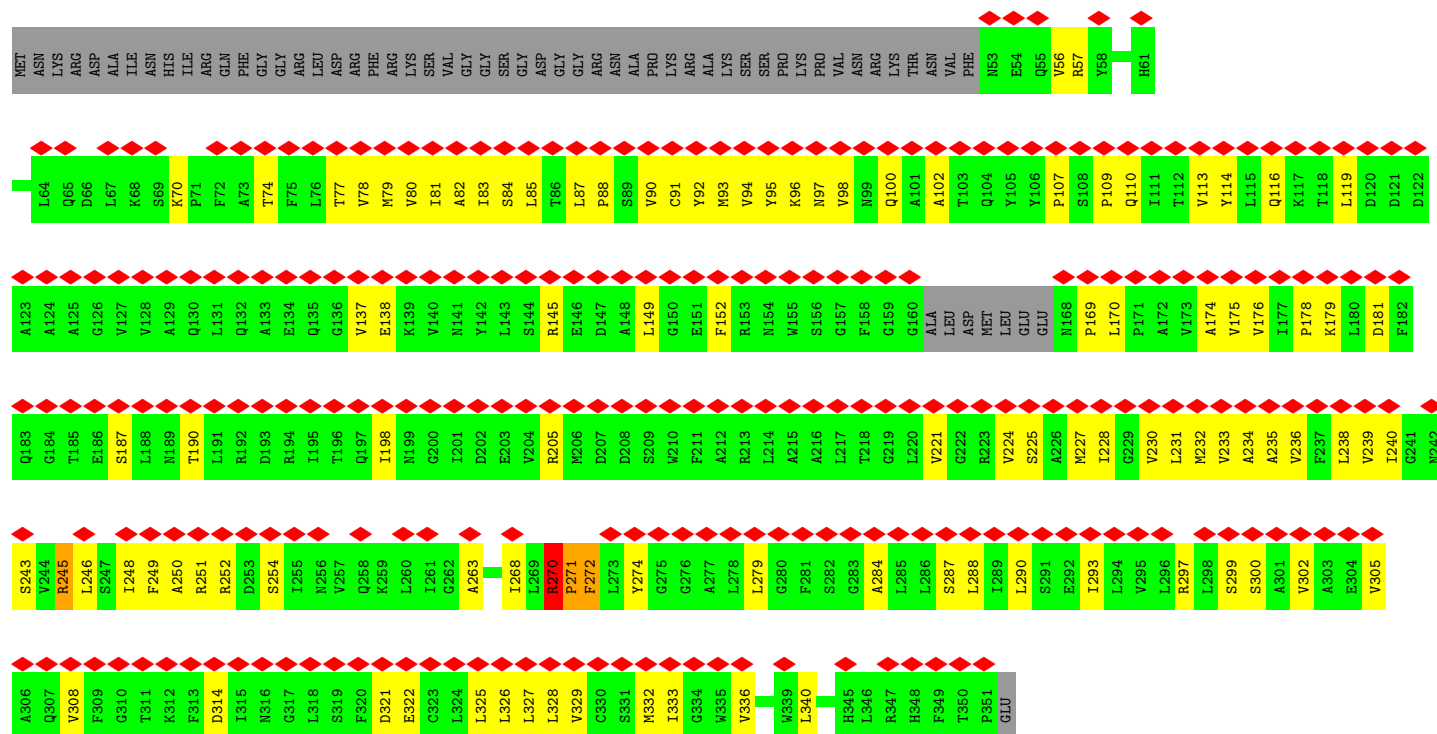
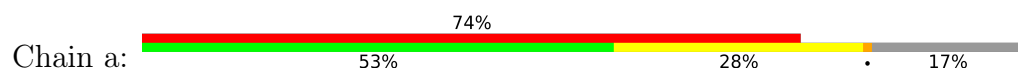
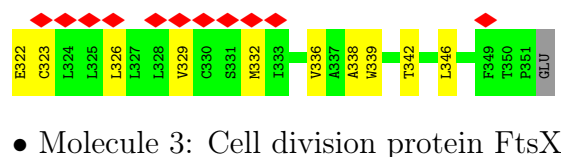


• Molecule 3: Cell division protein FtsX



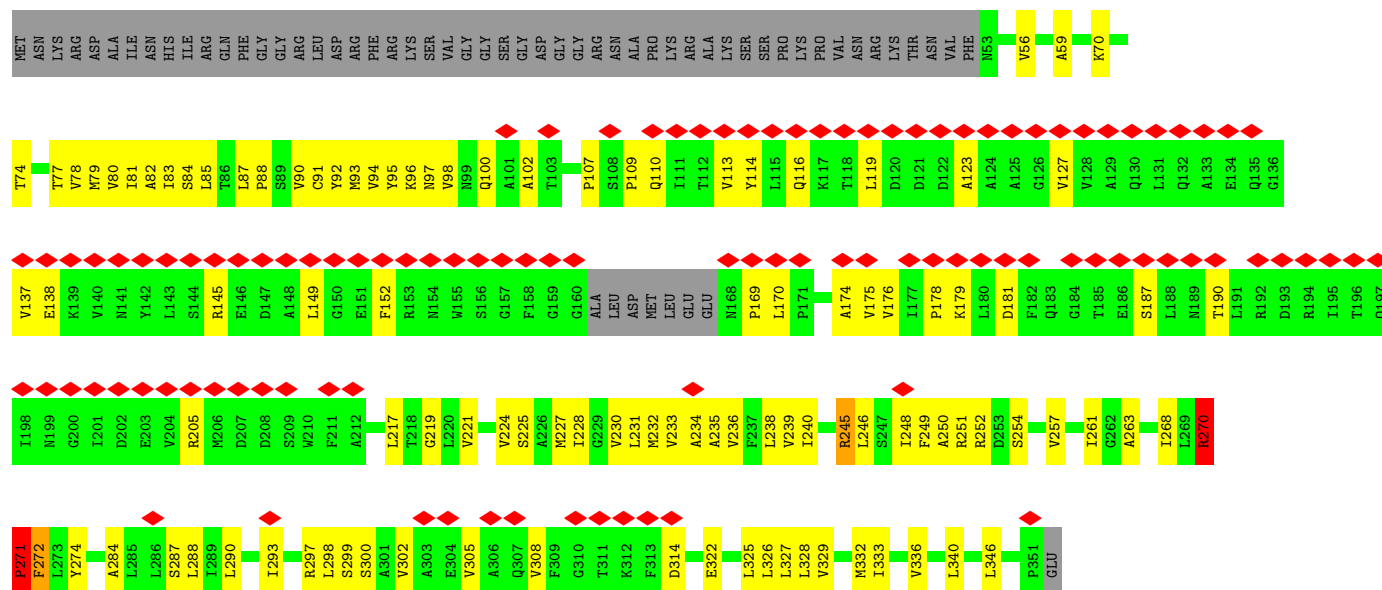
• Molecule 3: Cell division protein FtsX



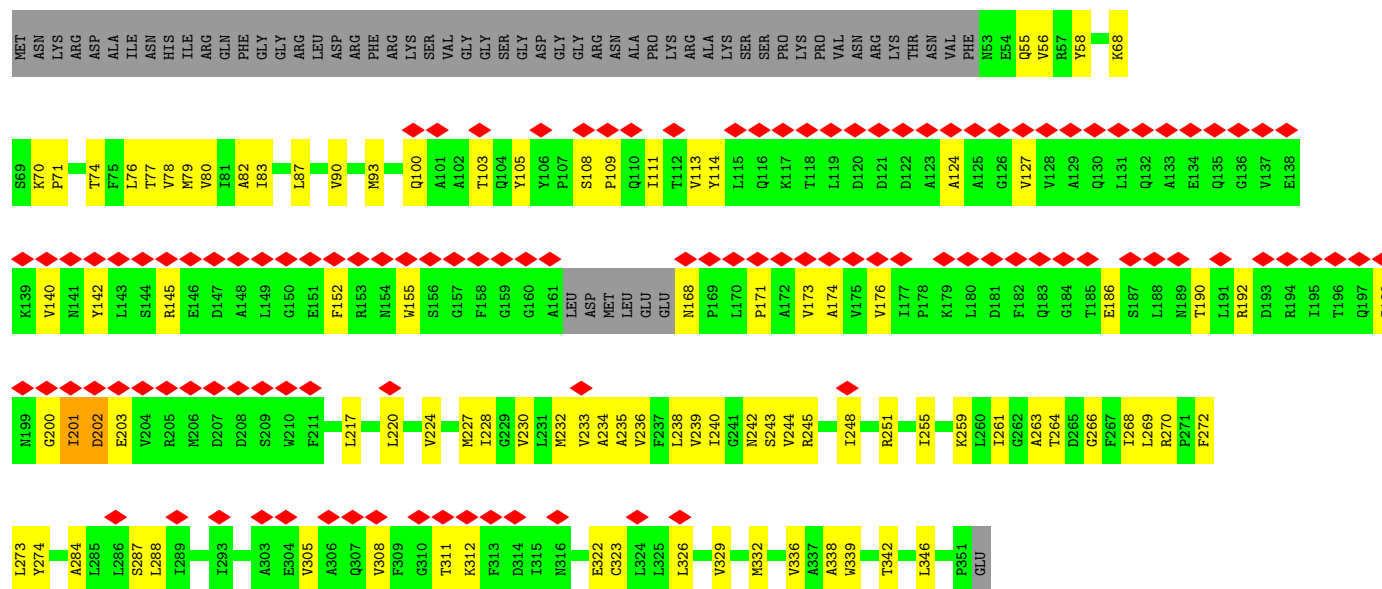




• Molecule 3: Cell division protein FtsX

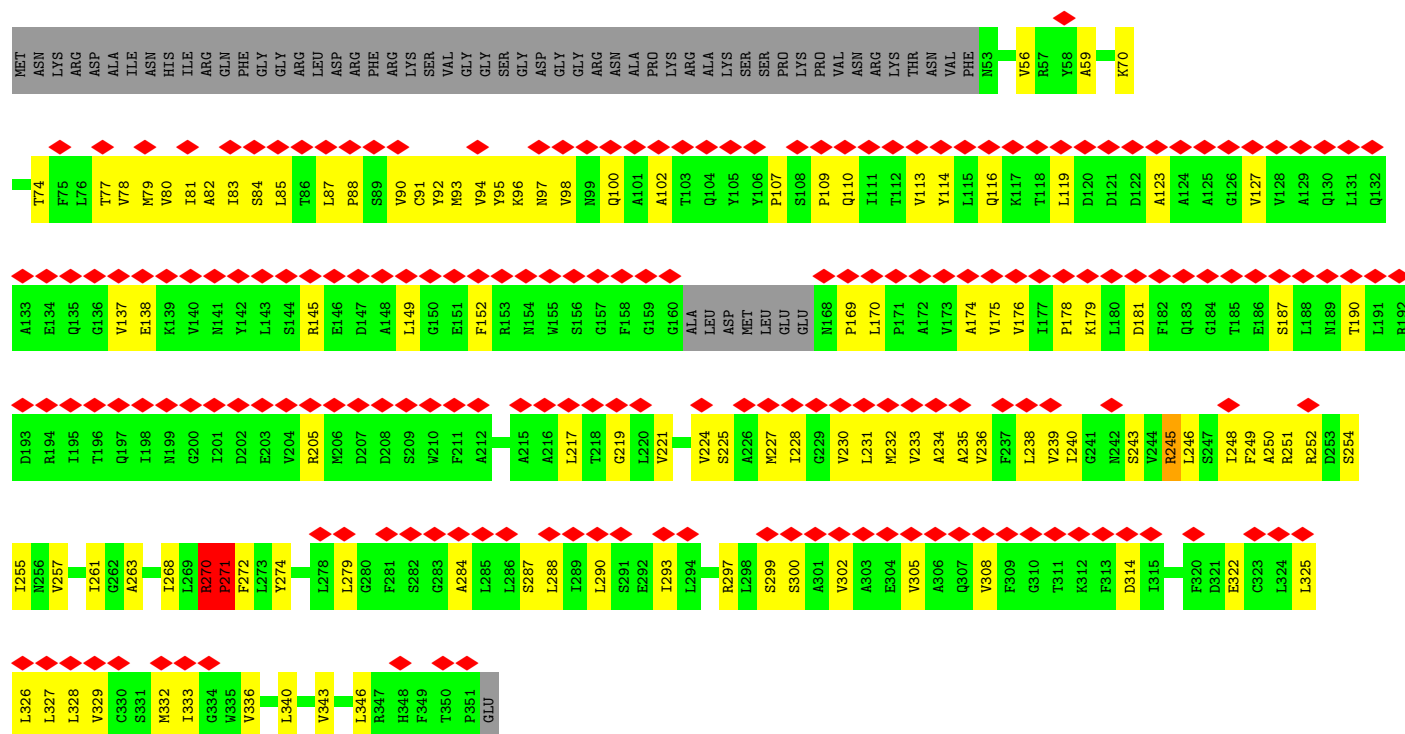


• Molecule 3: Cell division protein FtsX

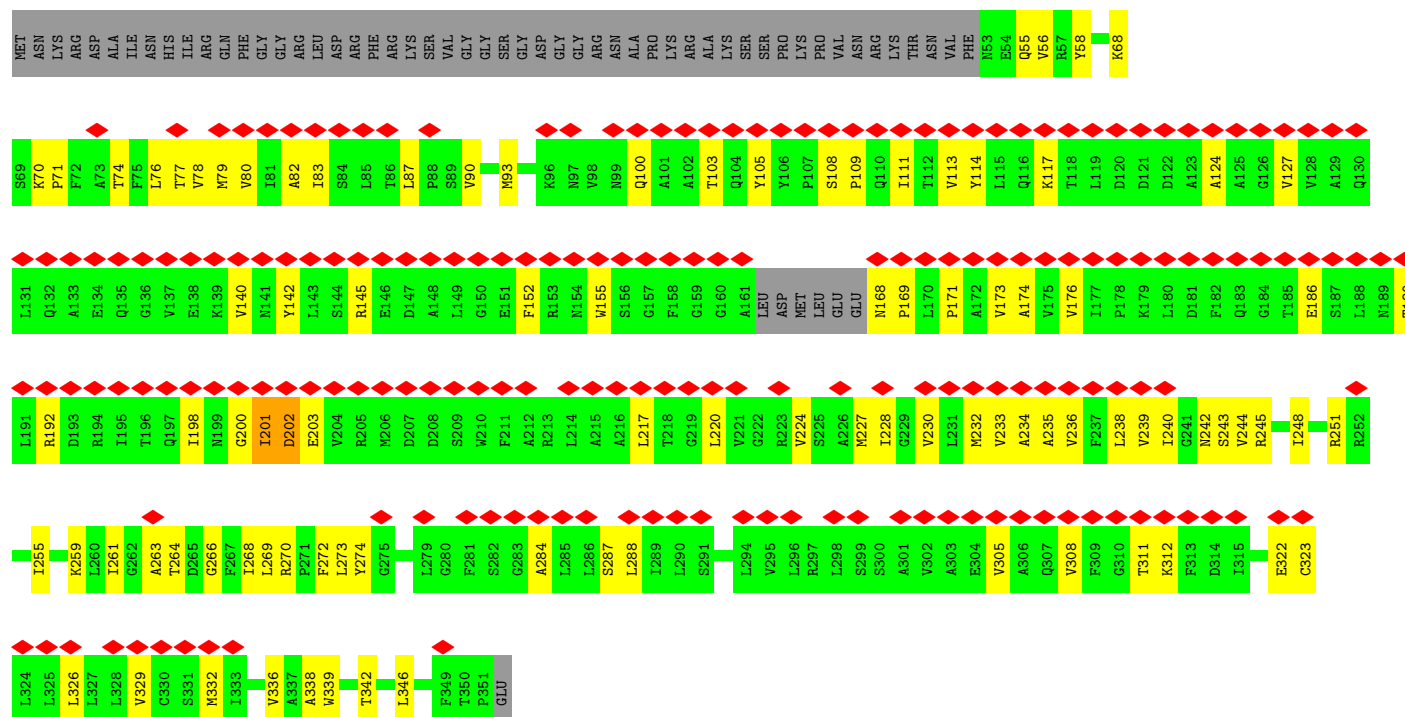


• Molecule 3: Cell division protein FtsX



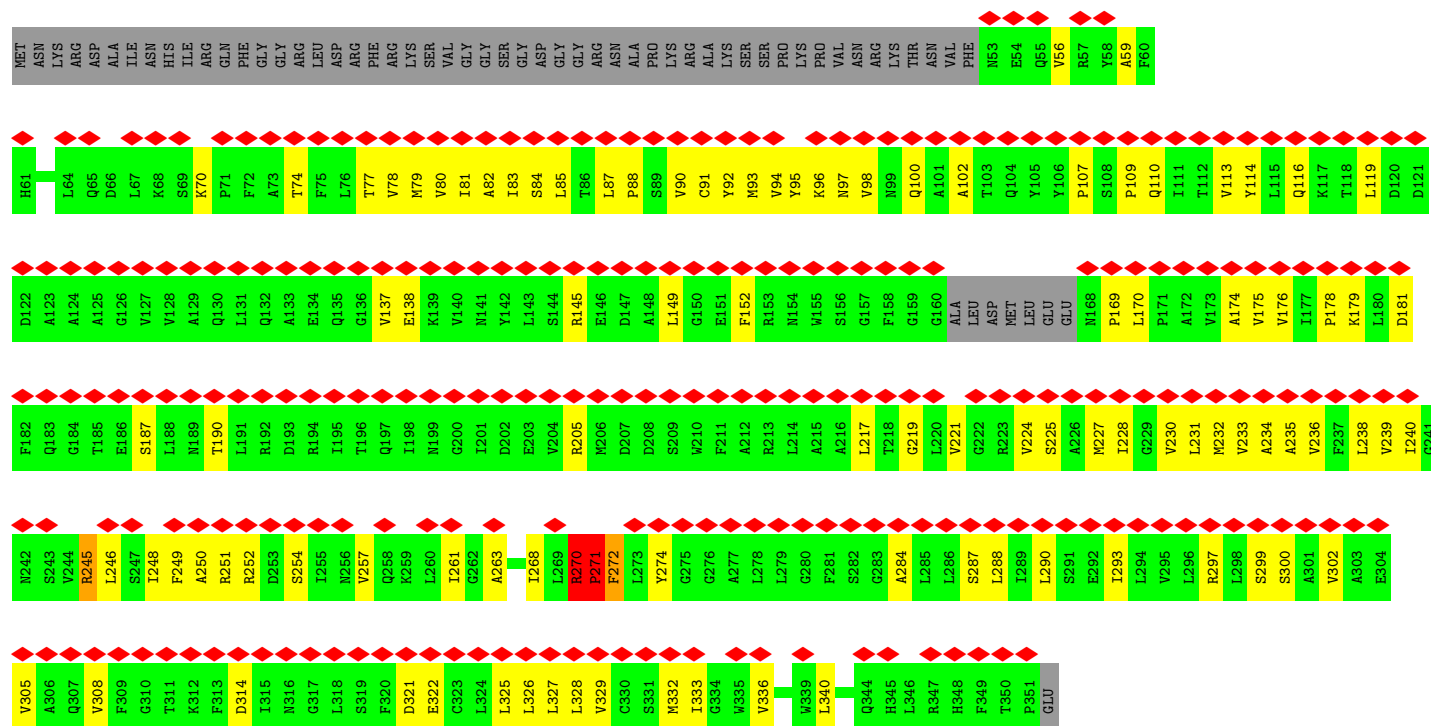


- Molecule 3: Cell division protein FtsX

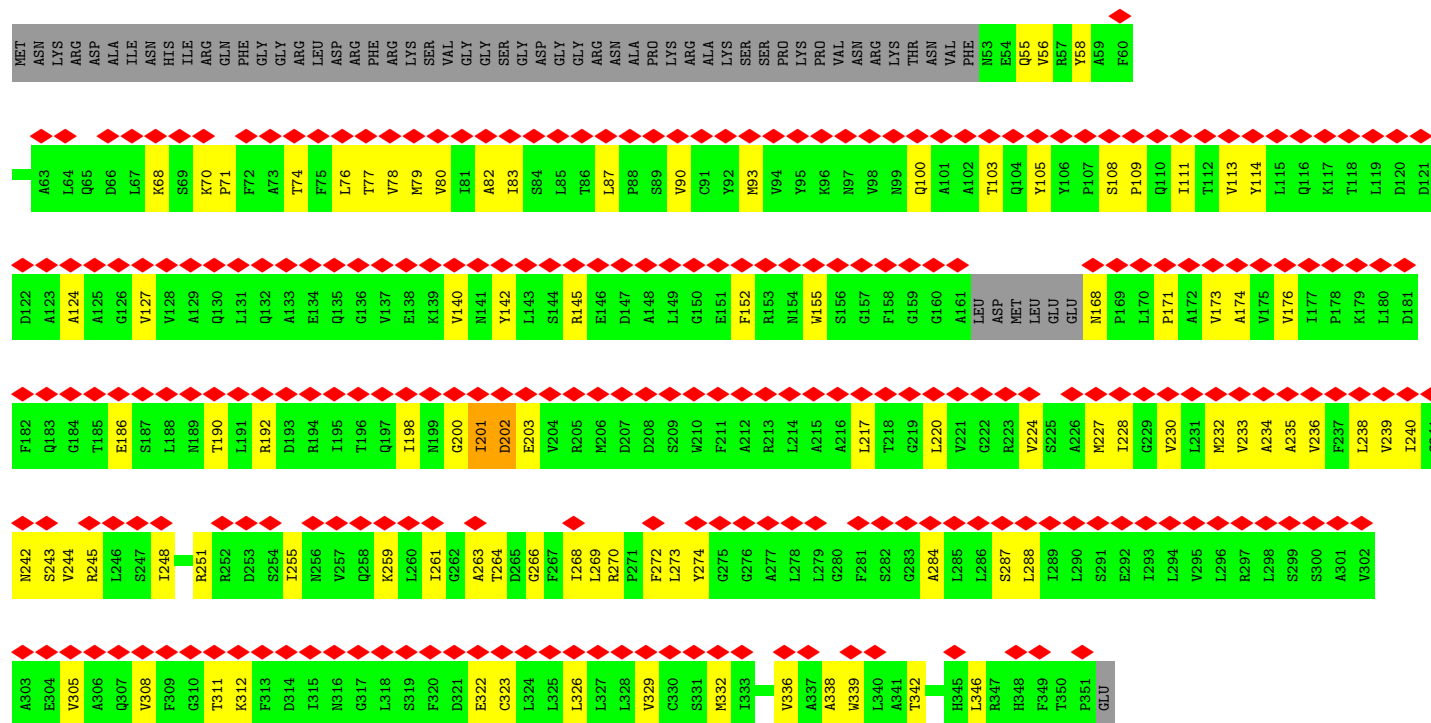


- Molecule 3: Cell division protein FtsX





• Molecule 3: Cell division protein FtsX



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Property	Value	Source
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.764	Depositor
Minimum map value	-0.847	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.10	0/267	0.29	0/359
1	2	0.12	0/267	0.32	0/359
1	E	0.11	0/267	0.29	0/359
1	F	0.12	0/267	0.32	0/359
1	K	0.11	0/267	0.29	0/359
1	L	0.13	0/267	0.33	0/359
1	Q	0.11	0/267	0.29	0/359
1	R	0.13	0/267	0.32	0/359
1	W	0.11	0/267	0.30	0/359
1	X	0.13	0/267	0.33	0/359
1	c	0.11	0/267	0.30	0/359
1	d	0.12	0/267	0.32	0/359
1	i	0.11	0/267	0.30	0/359
1	j	0.12	0/267	0.32	0/359
1	o	0.11	0/267	0.30	0/359
1	p	0.12	0/267	0.32	0/359
1	u	0.11	0/267	0.30	0/359
1	v	0.13	0/267	0.32	0/359
2	5	0.23	0/1742	0.44	0/2346
2	6	0.21	0/1738	0.44	0/2341
2	G	0.26	0/1742	0.50	1/2346 (0.0%)
2	H	0.21	0/1738	0.42	0/2341
2	M	0.29	0/1742	0.50	0/2346
2	N	0.22	0/1738	0.40	0/2341
2	S	0.23	0/1742	0.44	0/2346
2	T	0.21	0/1738	0.43	1/2341 (0.0%)
2	Y	0.23	0/1742	0.45	0/2346
2	Z	0.23	0/1738	0.44	0/2341
2	e	0.30	0/1742	0.49	0/2346
2	f	0.25	0/1738	0.42	0/2341
2	k	0.23	0/1742	0.44	0/2346
2	l	0.21	0/1738	0.43	0/2341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	q	0.23	0/1742	0.45	0/2346
2	r	0.21	0/1738	0.43	0/2341
2	w	0.23	0/1742	0.44	0/2346
2	x	0.22	0/1738	0.40	0/2341
3	A	0.18	0/2214	0.44	0/3021
3	B	0.25	0/2244	0.66	4/3056 (0.1%)
3	C	0.20	0/2244	0.50	0/3056
3	D	0.18	0/2214	0.43	0/3021
3	I	0.21	0/2244	0.53	1/3056 (0.0%)
3	J	0.18	0/2214	0.43	0/3021
3	O	0.18	0/2244	0.54	2/3056 (0.1%)
3	P	0.18	0/2214	0.44	0/3021
3	U	0.18	0/2244	0.54	3/3056 (0.1%)
3	V	0.18	0/2214	0.43	0/3021
3	a	0.20	0/2244	0.54	1/3056 (0.0%)
3	b	0.18	0/2214	0.44	0/3021
3	g	0.20	0/2244	0.55	1/3056 (0.0%)
3	h	0.18	0/2214	0.44	0/3021
3	m	0.18	0/2244	0.54	3/3056 (0.1%)
3	n	0.18	0/2214	0.44	0/3021
3	s	0.20	0/2244	0.54	2/3056 (0.1%)
3	t	0.18	0/2214	0.44	0/3021
All	All	0.21	0/76248	0.47	19/103338 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	5	0	1
2	6	0	1
2	G	0	1
2	H	0	1
2	M	0	2
2	N	0	1
2	S	0	1
2	T	0	1
2	Y	0	1
2	Z	0	1
2	e	0	1
2	f	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	k	0	1
2	l	0	1
2	q	0	1
2	r	0	1
2	w	0	1
2	x	0	1
3	B	0	1
3	C	0	1
3	I	0	1
3	O	0	1
3	U	0	1
3	a	0	1
3	g	0	1
3	m	0	1
3	s	0	1
All	All	0	29

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	272	PHE	CA-C-N	-14.65	100.76	120.54
3	B	272	PHE	C-N-CA	-14.65	100.76	120.54
3	B	271	PRO	N-CA-C	-7.54	96.93	112.47
3	U	271	PRO	CB-CA-C	6.52	122.32	111.56
3	g	270	ARG	CB-CA-C	6.50	122.98	110.17
3	m	271	PRO	CB-CA-C	6.49	122.27	111.56
3	O	271	PRO	CA-N-CD	-6.44	102.99	112.00
3	m	271	PRO	CA-N-CD	-6.20	103.32	112.00
3	I	270	ARG	CB-CA-C	6.20	122.37	110.17
3	U	271	PRO	CA-N-CD	-6.06	103.51	112.00
3	s	270	ARG	CB-CA-C	5.97	121.93	110.17
3	a	270	ARG	CB-CA-C	5.89	121.78	110.17
3	U	270	ARG	CB-CA-C	5.79	121.58	110.17
3	m	270	ARG	CB-CA-C	5.64	121.28	110.17
3	O	270	ARG	CB-CA-C	5.58	121.17	110.17
2	G	177	LEU	N-CA-C	-5.10	106.16	112.38
3	B	272	PHE	N-CA-CB	5.09	119.10	110.49
3	s	271	PRO	CA-N-CD	-5.04	104.95	112.00
2	T	181	GLU	N-CA-C	-5.01	105.73	111.14

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	5	178	ARG	Sidechain
2	6	178	ARG	Sidechain
3	B	270	ARG	Sidechain
3	C	270	ARG	Sidechain
2	G	178	ARG	Sidechain
2	H	178	ARG	Sidechain
3	I	270	ARG	Sidechain
2	M	178	ARG	Sidechain
2	M	185	ARG	Sidechain
2	N	178	ARG	Sidechain
3	O	270	ARG	Sidechain
2	S	178	ARG	Sidechain
2	T	178	ARG	Sidechain
3	U	270	ARG	Sidechain
2	Y	178	ARG	Sidechain
2	Z	178	ARG	Sidechain
3	a	270	ARG	Sidechain
2	e	178	ARG	Sidechain
2	f	178	ARG	Sidechain
2	f	202	ARG	Sidechain
3	g	270	ARG	Sidechain
2	k	178	ARG	Sidechain
2	l	178	ARG	Sidechain
3	m	270	ARG	Sidechain
2	q	178	ARG	Sidechain
2	r	178	ARG	Sidechain
3	s	270	ARG	Sidechain
2	w	178	ARG	Sidechain
2	x	178	ARG	Sidechain

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	1	263	0	287	11	0
1	2	263	0	287	3	0
1	E	263	0	287	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	263	0	287	3	0
1	K	263	0	287	10	0
1	L	263	0	287	3	0
1	Q	263	0	287	9	0
1	R	263	0	287	2	0
1	W	263	0	287	10	0
1	X	263	0	287	3	0
1	c	263	0	287	10	0
1	d	263	0	287	2	0
1	i	263	0	287	9	0
1	j	263	0	287	4	0
1	o	263	0	287	8	0
1	p	263	0	287	2	0
1	u	263	0	287	9	0
1	v	263	0	287	4	0
2	5	1713	0	1756	58	0
2	6	1709	0	1753	52	0
2	G	1713	0	1756	52	0
2	H	1709	0	1753	61	0
2	M	1713	0	1756	62	0
2	N	1709	0	1753	51	0
2	S	1713	0	1756	52	0
2	T	1709	0	1753	57	0
2	Y	1713	0	1756	60	0
2	Z	1709	0	1753	61	0
2	e	1713	0	1756	57	0
2	f	1709	0	1753	55	0
2	k	1713	0	1756	55	0
2	l	1709	0	1753	58	0
2	q	1713	0	1756	52	0
2	r	1709	0	1753	55	0
2	w	1713	0	1756	54	0
2	x	1709	0	1753	59	0
3	A	2174	0	2173	78	0
3	B	2204	0	2224	107	0
3	C	2204	0	2224	95	0
3	D	2174	0	2173	77	0
3	I	2204	0	2224	102	0
3	J	2174	0	2173	77	0
3	O	2204	0	2224	98	0
3	P	2174	0	2173	72	0
3	U	2204	0	2224	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	V	2174	0	2173	76	0
3	a	2204	0	2224	99	0
3	b	2174	0	2173	75	0
3	g	2204	0	2224	100	0
3	h	2174	0	2173	79	0
3	m	2204	0	2224	101	0
3	n	2174	0	2173	79	0
3	s	2204	0	2224	97	0
3	t	2174	0	2173	77	0
4	5	31	0	12	0	0
4	6	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
4	M	31	0	12	0	0
4	N	31	0	12	0	0
4	S	31	0	12	0	0
4	T	31	0	12	1	0
4	Y	31	0	12	0	0
4	Z	31	0	12	1	0
4	e	31	0	12	0	0
4	f	31	0	12	0	0
4	k	31	0	12	0	0
4	l	31	0	12	0	0
4	q	31	0	12	0	0
4	r	31	0	12	0	0
4	w	31	0	12	0	0
4	x	31	0	12	0	0
All	All	75492	0	76536	2476	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 16.

All (2476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:204:SER:O	2:Y:218:GLY:HA3	1.28	1.31
2:M:218:GLY:HA3	2:w:204:SER:O	1.37	1.25
2:Y:204:SER:O	2:q:218:GLY:HA3	1.31	1.24
2:5:218:GLY:HA3	2:k:204:SER:O	1.35	1.23
2:S:204:SER:O	2:k:218:GLY:HA3	1.39	1.22
2:5:204:SER:O	2:S:218:GLY:HA3	1.37	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:246:LEU:HG	3:B:272:PHE:HZ	1.31	0.92
3:m:270:ARG:C	3:m:272:PHE:H	1.77	0.92
3:U:270:ARG:C	3:U:272:PHE:H	1.77	0.91
2:G:205:TYR:CE1	2:Y:217:GLY:HA3	2.06	0.91
3:O:270:ARG:C	3:O:272:PHE:H	1.78	0.91
2:5:51:ILE:HA	2:5:78:ARG:NH2	1.89	0.88
3:a:270:ARG:HB3	3:a:271:PRO:HD2	1.53	0.88
2:G:51:ILE:HA	2:G:78:ARG:NH2	1.88	0.88
3:g:270:ARG:HB3	3:g:271:PRO:HD2	1.55	0.88
2:k:51:ILE:HA	2:k:78:ARG:NH2	1.88	0.88
2:M:51:ILE:HA	2:M:78:ARG:NH2	1.88	0.87
2:e:51:ILE:HA	2:e:78:ARG:NH2	1.88	0.87
2:q:51:ILE:HA	2:q:78:ARG:NH2	1.89	0.87
2:w:51:ILE:HA	2:w:78:ARG:NH2	1.89	0.87
2:S:51:ILE:HA	2:S:78:ARG:NH2	1.88	0.86
3:O:270:ARG:HB3	3:O:271:PRO:HD2	1.57	0.86
2:Y:51:ILE:HA	2:Y:78:ARG:NH2	1.89	0.85
3:s:270:ARG:HB3	3:s:271:PRO:HD2	1.59	0.85
3:I:270:ARG:HB3	3:I:271:PRO:HD2	1.57	0.85
3:A:76:LEU:HA	3:A:79:MET:HE3	1.59	0.84
3:D:76:LEU:HA	3:D:79:MET:HE3	1.59	0.84
3:U:270:ARG:HB3	3:U:271:PRO:HD2	1.59	0.84
3:B:246:LEU:HG	3:B:272:PHE:CZ	2.11	0.84
3:J:76:LEU:HA	3:J:79:MET:HE3	1.59	0.84
3:n:76:LEU:HA	3:n:79:MET:HE3	1.59	0.84
3:m:270:ARG:HB3	3:m:271:PRO:HD2	1.60	0.83
3:h:76:LEU:HA	3:h:79:MET:HE3	1.59	0.83
3:t:76:LEU:HA	3:t:79:MET:HE3	1.59	0.83
3:V:76:LEU:HA	3:V:79:MET:HE3	1.59	0.82
2:e:204:SER:O	2:w:218:GLY:HA3	1.78	0.82
3:P:76:LEU:HA	3:P:79:MET:HE3	1.59	0.82
3:b:76:LEU:HA	3:b:79:MET:HE3	1.59	0.82
3:m:138:GLU:H	3:m:179:LYS:HZ1	1.26	0.81
3:g:138:GLU:H	3:g:179:LYS:HZ1	1.29	0.81
2:G:205:TYR:HE1	2:Y:217:GLY:HA3	1.42	0.80
3:U:138:GLU:H	3:U:179:LYS:HZ1	1.28	0.80
2:l:28:GLY:H	2:l:189:THR:HG22	1.47	0.80
2:x:28:GLY:H	2:x:189:THR:HG22	1.47	0.80
2:6:28:GLY:H	2:6:189:THR:HG22	1.47	0.79
2:N:28:GLY:H	2:N:189:THR:HG22	1.47	0.79
2:r:28:GLY:H	2:r:189:THR:HG22	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:GLY:H	2:H:189:THR:HG22	1.48	0.79
3:O:138:GLU:H	3:O:179:LYS:HZ1	1.29	0.79
2:f:28:GLY:H	2:f:189:THR:HG22	1.47	0.78
3:B:138:GLU:H	3:B:179:LYS:HZ1	1.29	0.78
2:Z:28:GLY:H	2:Z:189:THR:HG22	1.47	0.78
2:T:28:GLY:H	2:T:189:THR:HG22	1.48	0.78
2:k:51:ILE:HG12	2:k:78:ARG:NH2	2.00	0.76
2:e:51:ILE:HG12	2:e:78:ARG:NH2	2.01	0.76
2:l:127:LEU:HD11	2:l:142:GLU:HB3	1.68	0.76
2:G:51:ILE:HG12	2:G:78:ARG:NH2	2.01	0.76
2:M:51:ILE:HG12	2:M:78:ARG:NH2	2.01	0.76
2:S:51:ILE:HG12	2:S:78:ARG:NH2	2.01	0.76
2:5:51:ILE:HG12	2:5:78:ARG:NH2	2.01	0.76
3:U:270:ARG:C	3:U:272:PHE:N	2.42	0.76
2:q:51:ILE:HG12	2:q:78:ARG:NH2	2.01	0.76
2:w:51:ILE:HG12	2:w:78:ARG:NH2	2.01	0.76
2:M:30:MET:HG3	2:M:190:VAL:HB	1.69	0.75
2:5:30:MET:HG3	2:5:190:VAL:HB	1.69	0.75
2:G:30:MET:HG3	2:G:190:VAL:HB	1.69	0.75
2:Y:51:ILE:HG12	2:Y:78:ARG:NH2	2.01	0.75
2:k:30:MET:HG3	2:k:190:VAL:HB	1.69	0.75
3:m:270:ARG:C	3:m:272:PHE:N	2.43	0.75
2:Y:30:MET:HG3	2:Y:190:VAL:HB	1.69	0.75
2:q:30:MET:HG3	2:q:190:VAL:HB	1.69	0.74
2:w:30:MET:HG3	2:w:190:VAL:HB	1.69	0.74
2:e:30:MET:HG3	2:e:190:VAL:HB	1.69	0.74
2:S:30:MET:HG3	2:S:190:VAL:HB	1.69	0.74
3:B:240:ILE:HD11	3:B:340:LEU:HD11	1.70	0.74
3:C:138:GLU:H	3:C:179:LYS:HZ1	1.33	0.74
3:C:240:ILE:HD11	3:C:340:LEU:HD11	1.70	0.74
3:O:240:ILE:HD11	3:O:340:LEU:HD11	1.70	0.74
3:U:240:ILE:HD11	3:U:340:LEU:HD11	1.70	0.74
3:a:138:GLU:H	3:a:179:LYS:HZ1	1.32	0.74
2:M:204:SER:O	2:e:218:GLY:HA3	1.87	0.73
3:I:138:GLU:H	3:I:179:LYS:HZ1	1.33	0.73
3:P:288:LEU:HD21	3:P:323:CYS:HA	1.70	0.73
3:a:240:ILE:HD11	3:a:340:LEU:HD11	1.70	0.73
3:A:288:LEU:HD21	3:A:323:CYS:HA	1.70	0.73
3:I:240:ILE:HD11	3:I:340:LEU:HD11	1.70	0.73
3:D:288:LEU:HD21	3:D:323:CYS:HA	1.70	0.73
3:b:288:LEU:HD21	3:b:323:CYS:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:288:LEU:HD21	3:J:323:CYS:HA	1.70	0.73
2:Y:51:ILE:HA	2:Y:78:ARG:HH21	1.53	0.73
2:S:51:ILE:HA	2:S:78:ARG:HH21	1.53	0.73
2:w:51:ILE:HA	2:w:78:ARG:HH21	1.53	0.73
2:6:127:LEU:HD11	2:6:142:GLU:HB3	1.70	0.73
2:T:127:LEU:HD11	2:T:142:GLU:HB3	1.70	0.73
3:V:288:LEU:HD21	3:V:323:CYS:HA	1.70	0.73
2:e:51:ILE:HA	2:e:78:ARG:HH21	1.53	0.73
2:k:51:ILE:HA	2:k:78:ARG:HH21	1.53	0.73
3:n:288:LEU:HD21	3:n:323:CYS:HA	1.70	0.72
3:O:270:ARG:O	3:O:272:PHE:N	2.20	0.72
3:t:288:LEU:HD21	3:t:323:CYS:HA	1.70	0.72
2:G:51:ILE:HA	2:G:78:ARG:HH21	1.53	0.72
3:h:288:LEU:HD21	3:h:323:CYS:HA	1.70	0.72
2:q:28:GLY:H	2:q:189:THR:HG22	1.55	0.72
2:k:28:GLY:H	2:k:189:THR:HG22	1.55	0.72
2:M:28:GLY:H	2:M:189:THR:HG22	1.55	0.72
3:s:138:GLU:H	3:s:179:LYS:HZ1	1.34	0.71
2:G:28:GLY:H	2:G:189:THR:HG22	1.55	0.71
2:5:28:GLY:H	2:5:189:THR:HG22	1.55	0.71
3:g:240:ILE:HD11	3:g:340:LEU:HD11	1.70	0.71
3:m:240:ILE:HD11	3:m:340:LEU:HD11	1.70	0.71
2:q:51:ILE:HA	2:q:78:ARG:HH21	1.53	0.71
3:s:240:ILE:HD11	3:s:340:LEU:HD11	1.70	0.71
2:w:28:GLY:H	2:w:189:THR:HG22	1.54	0.71
2:5:51:ILE:HA	2:5:78:ARG:HH21	1.53	0.71
3:P:82:ALA:HA	3:P:287:SER:HB2	1.73	0.71
2:Y:28:GLY:H	2:Y:189:THR:HG22	1.55	0.71
3:b:82:ALA:HA	3:b:287:SER:HB2	1.73	0.71
2:r:104:LEU:HD21	2:r:117:ARG:HE	1.56	0.71
3:m:270:ARG:O	3:m:272:PHE:N	2.24	0.71
2:N:104:LEU:HD21	2:N:117:ARG:HE	1.56	0.70
3:V:82:ALA:HA	3:V:287:SER:HB2	1.73	0.70
3:U:270:ARG:O	3:U:272:PHE:N	2.24	0.70
2:Z:104:LEU:HD21	2:Z:117:ARG:HE	1.56	0.70
2:f:104:LEU:HD21	2:f:117:ARG:HE	1.56	0.70
2:e:28:GLY:H	2:e:189:THR:HG22	1.55	0.70
2:x:104:LEU:HD21	2:x:117:ARG:HE	1.56	0.70
2:6:104:LEU:HD21	2:6:117:ARG:HE	1.56	0.70
2:M:51:ILE:HA	2:M:78:ARG:HH21	1.53	0.70
2:S:28:GLY:H	2:S:189:THR:HG22	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:82:ALA:HA	3:A:287:SER:HB2	1.73	0.69
2:l:104:LEU:HD21	2:l:117:ARG:HE	1.56	0.69
3:t:82:ALA:HA	3:t:287:SER:HB2	1.73	0.69
2:H:104:LEU:HD21	2:H:117:ARG:HE	1.56	0.69
3:J:82:ALA:HA	3:J:287:SER:HB2	1.73	0.69
3:g:305:VAL:HG21	3:h:220:LEU:HB3	1.75	0.69
3:D:82:ALA:HA	3:D:287:SER:HB2	1.73	0.69
3:O:87:LEU:HD22	3:P:87:LEU:HD23	1.75	0.69
2:T:104:LEU:HD21	2:T:117:ARG:HE	1.56	0.69
3:a:87:LEU:HD22	3:b:87:LEU:HD23	1.75	0.69
3:h:82:ALA:HA	3:h:287:SER:HB2	1.73	0.69
3:n:82:ALA:HA	3:n:287:SER:HB2	1.73	0.69
3:s:87:LEU:HD22	3:t:87:LEU:HD23	1.75	0.69
3:s:305:VAL:HG21	3:t:220:LEU:HB3	1.75	0.69
3:m:87:LEU:HD22	3:n:87:LEU:HD23	1.75	0.69
3:U:87:LEU:HD22	3:V:87:LEU:HD23	1.75	0.69
3:m:305:VAL:HG21	3:n:220:LEU:HB3	1.75	0.69
2:H:174:GLU:OE2	2:H:203:ARG:NH2	2.26	0.69
3:g:87:LEU:HD22	3:h:87:LEU:HD23	1.75	0.69
2:6:174:GLU:OE2	2:6:203:ARG:NH2	2.26	0.69
3:D:228:ILE:O	3:D:232:MET:HG2	1.94	0.68
2:N:174:GLU:OE2	2:N:203:ARG:NH2	2.26	0.68
2:l:174:GLU:OE2	2:l:203:ARG:NH2	2.26	0.68
2:x:174:GLU:OE2	2:x:203:ARG:NH2	2.26	0.68
2:H:202:ARG:HG2	2:r:197:ILE:HD13	1.75	0.68
2:Z:174:GLU:OE2	2:Z:203:ARG:NH2	2.26	0.68
2:r:174:GLU:OE2	2:r:203:ARG:NH2	2.26	0.68
2:T:174:GLU:OE2	2:T:203:ARG:NH2	2.26	0.68
3:U:305:VAL:HG21	3:V:220:LEU:HB3	1.75	0.68
3:O:305:VAL:HG21	3:P:220:LEU:HB3	1.75	0.68
2:f:174:GLU:OE2	2:f:203:ARG:NH2	2.26	0.68
3:A:228:ILE:O	3:A:232:MET:HG2	1.94	0.68
2:G:205:TYR:HE1	2:Y:217:GLY:CA	2.07	0.68
3:I:305:VAL:HG21	3:J:220:LEU:HB3	1.75	0.68
3:P:228:ILE:O	3:P:232:MET:HG2	1.94	0.68
3:a:305:VAL:HG21	3:b:220:LEU:HB3	1.75	0.68
3:B:305:VAL:HG21	3:D:220:LEU:HB3	1.74	0.67
3:A:87:LEU:HD23	3:C:87:LEU:HD22	1.75	0.67
3:A:220:LEU:HB3	3:C:305:VAL:HG21	1.75	0.67
3:B:87:LEU:HD22	3:D:87:LEU:HD23	1.75	0.67
3:b:228:ILE:O	3:b:232:MET:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:268:ILE:HD11	3:b:346:LEU:HD11	1.76	0.67
3:I:87:LEU:HD22	3:J:87:LEU:HD23	1.75	0.67
3:h:228:ILE:O	3:h:232:MET:HG2	1.94	0.67
3:n:268:ILE:HD11	3:n:346:LEU:HD11	1.76	0.67
3:J:228:ILE:O	3:J:232:MET:HG2	1.94	0.67
3:h:268:ILE:HD11	3:h:346:LEU:HD11	1.76	0.67
3:V:228:ILE:O	3:V:232:MET:HG2	1.94	0.67
3:t:228:ILE:O	3:t:232:MET:HG2	1.94	0.67
3:P:268:ILE:HD11	3:P:346:LEU:HD11	1.76	0.67
3:n:228:ILE:O	3:n:232:MET:HG2	1.94	0.67
3:V:268:ILE:HD11	3:V:346:LEU:HD11	1.76	0.66
3:t:268:ILE:HD11	3:t:346:LEU:HD11	1.76	0.66
2:Y:205:TYR:CE1	2:q:217:GLY:HA3	2.31	0.66
3:J:268:ILE:HD11	3:J:346:LEU:HD11	1.76	0.66
3:A:268:ILE:HD11	3:A:346:LEU:HD11	1.76	0.66
3:B:271:PRO:HG2	3:B:272:PHE:CD2	2.31	0.66
3:D:268:ILE:HD11	3:D:346:LEU:HD11	1.76	0.66
3:A:236:VAL:O	3:A:240:ILE:HG12	1.96	0.65
3:D:236:VAL:O	3:D:240:ILE:HG12	1.96	0.65
3:b:74:THR:O	3:b:78:VAL:HG23	1.97	0.65
3:g:270:ARG:O	3:g:272:PHE:N	2.29	0.65
3:t:74:THR:O	3:t:78:VAL:HG23	1.97	0.65
3:D:74:THR:O	3:D:78:VAL:HG23	1.97	0.65
2:H:49:CYS:HB2	2:H:51:ILE:HG13	1.79	0.65
2:M:161:ALA:HB1	2:M:164:PRO:HG3	1.79	0.65
2:q:161:ALA:HB1	2:q:164:PRO:HG3	1.79	0.65
2:5:218:GLY:CA	2:k:204:SER:O	2.30	0.65
3:J:74:THR:O	3:J:78:VAL:HG23	1.97	0.65
3:J:236:VAL:O	3:J:240:ILE:HG12	1.96	0.65
2:N:49:CYS:HB2	2:N:51:ILE:HG13	1.79	0.65
3:P:74:THR:O	3:P:78:VAL:HG23	1.97	0.65
3:h:74:THR:O	3:h:78:VAL:HG23	1.97	0.65
3:h:236:VAL:O	3:h:240:ILE:HG12	1.96	0.65
3:m:236:VAL:HG22	3:m:333:ILE:HG21	1.79	0.65
2:5:161:ALA:HB1	2:5:164:PRO:HG3	1.79	0.65
2:k:161:ALA:HB1	2:k:164:PRO:HG3	1.79	0.65
3:n:236:VAL:O	3:n:240:ILE:HG12	1.96	0.65
3:C:236:VAL:HG22	3:C:333:ILE:HG21	1.79	0.65
3:V:74:THR:O	3:V:78:VAL:HG23	1.97	0.65
2:Z:49:CYS:HB2	2:Z:51:ILE:HG13	1.79	0.65
3:g:270:ARG:O	3:g:271:PRO:C	2.40	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:t:236:VAL:O	3:t:240:ILE:HG12	1.96	0.65
3:A:74:THR:O	3:A:78:VAL:HG23	1.97	0.65
2:w:161:ALA:HB1	2:w:164:PRO:HG3	1.79	0.65
2:6:49:CYS:HB2	2:6:51:ILE:HG13	1.79	0.65
2:G:161:ALA:HB1	2:G:164:PRO:HG3	1.79	0.65
3:g:236:VAL:HG22	3:g:333:ILE:HG21	1.79	0.65
3:s:236:VAL:HG22	3:s:333:ILE:HG21	1.79	0.65
2:G:51:ILE:CA	2:G:78:ARG:HH21	2.10	0.64
3:I:236:VAL:HG22	3:I:333:ILE:HG21	1.79	0.64
2:f:49:CYS:HB2	2:f:51:ILE:HG13	1.79	0.64
3:B:236:VAL:HG22	3:B:333:ILE:HG21	1.79	0.64
3:J:244:VAL:O	3:J:248:ILE:HG13	1.98	0.64
3:P:236:VAL:O	3:P:240:ILE:HG12	1.96	0.64
2:T:49:CYS:HB2	2:T:51:ILE:HG13	1.79	0.64
2:5:51:ILE:CA	2:5:78:ARG:HH21	2.10	0.64
3:A:244:VAL:O	3:A:248:ILE:HG13	1.98	0.64
2:M:218:GLY:CA	2:w:204:SER:O	2.31	0.64
3:b:236:VAL:O	3:b:240:ILE:HG12	1.96	0.64
3:b:244:VAL:O	3:b:248:ILE:HG13	1.97	0.64
2:e:161:ALA:HB1	2:e:164:PRO:HG3	1.79	0.64
3:a:236:VAL:HG22	3:a:333:ILE:HG21	1.79	0.64
2:k:51:ILE:CA	2:k:78:ARG:HH21	2.10	0.64
3:D:244:VAL:O	3:D:248:ILE:HG13	1.98	0.64
1:E:25:PHE:HD2	1:E:29:ARG:HH21	1.45	0.64
2:M:51:ILE:CA	2:M:78:ARG:HH21	2.10	0.64
2:S:161:ALA:HB1	2:S:164:PRO:HG3	1.79	0.64
3:n:74:THR:O	3:n:78:VAL:HG23	1.97	0.64
3:t:244:VAL:O	3:t:248:ILE:HG13	1.98	0.64
3:I:270:ARG:HB3	3:I:271:PRO:CD	2.28	0.64
3:I:299:SER:HA	3:I:302:VAL:HG22	1.80	0.64
3:U:299:SER:HA	3:U:302:VAL:HG22	1.80	0.64
3:V:236:VAL:O	3:V:240:ILE:HG12	1.96	0.64
2:Y:51:ILE:CA	2:Y:78:ARG:HH21	2.10	0.64
1:c:35:MET:HE2	2:f:64:HIS:HB3	1.80	0.64
3:g:87:LEU:HA	3:g:90:VAL:HG22	1.80	0.64
2:l:49:CYS:HB2	2:l:51:ILE:HG13	1.79	0.64
1:1:35:MET:HE2	2:6:64:HIS:HB3	1.80	0.64
3:C:299:SER:HA	3:C:302:VAL:HG22	1.80	0.64
2:S:51:ILE:CA	2:S:78:ARG:HH21	2.10	0.64
3:U:236:VAL:HG22	3:U:333:ILE:HG21	1.79	0.64
1:W:35:MET:HE2	2:Z:64:HIS:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:161:ALA:HB1	2:Y:164:PRO:HG3	1.79	0.64
3:a:299:SER:HA	3:a:302:VAL:HG22	1.80	0.64
3:h:244:VAL:O	3:h:248:ILE:HG13	1.98	0.64
1:K:35:MET:HE2	2:N:64:HIS:HB3	1.81	0.63
3:O:236:VAL:HG22	3:O:333:ILE:HG21	1.79	0.63
3:s:87:LEU:HA	3:s:90:VAL:HG22	1.80	0.63
3:B:299:SER:HA	3:B:302:VAL:HG22	1.81	0.63
3:V:244:VAL:O	3:V:248:ILE:HG13	1.98	0.63
2:r:49:CYS:HB2	2:r:51:ILE:HG13	1.79	0.63
2:w:51:ILE:CA	2:w:78:ARG:HH21	2.11	0.63
3:P:244:VAL:O	3:P:248:ILE:HG13	1.97	0.63
1:Q:35:MET:HE2	2:T:64:HIS:HB3	1.80	0.63
3:g:299:SER:HA	3:g:302:VAL:HG22	1.80	0.63
2:x:49:CYS:HB2	2:x:51:ILE:HG13	1.79	0.63
3:m:87:LEU:HA	3:m:90:VAL:HG22	1.80	0.63
1:o:35:MET:HE2	2:r:64:HIS:HB3	1.80	0.63
3:O:299:SER:HA	3:O:302:VAL:HG22	1.80	0.63
2:e:51:ILE:CA	2:e:78:ARG:HH21	2.10	0.63
1:i:35:MET:HE2	2:l:64:HIS:HB3	1.80	0.63
3:n:244:VAL:O	3:n:248:ILE:HG13	1.98	0.63
3:B:85:LEU:HA	3:B:88:PRO:HG2	1.81	0.63
3:B:271:PRO:HD2	3:B:272:PHE:N	2.12	0.63
3:m:299:SER:HA	3:m:302:VAL:HG22	1.80	0.63
3:s:85:LEU:HA	3:s:88:PRO:HG2	1.81	0.63
3:C:328:LEU:O	3:C:332:MET:HG2	1.98	0.63
1:E:35:MET:HE2	2:H:64:HIS:HB3	1.81	0.63
3:I:85:LEU:HA	3:I:88:PRO:HG2	1.81	0.63
3:I:328:LEU:O	3:I:332:MET:HG2	1.98	0.63
3:U:328:LEU:O	3:U:332:MET:HG2	1.98	0.63
3:g:85:LEU:HA	3:g:88:PRO:HG2	1.81	0.63
3:s:91:CYS:SG	3:s:228:ILE:HD13	2.39	0.63
3:s:328:LEU:O	3:s:332:MET:HG2	1.98	0.63
2:q:51:ILE:CA	2:q:78:ARG:HH21	2.11	0.63
3:s:299:SER:HA	3:s:302:VAL:HG22	1.80	0.63
3:U:91:CYS:SG	3:U:228:ILE:HD13	2.39	0.63
3:m:85:LEU:HA	3:m:88:PRO:HG2	1.81	0.63
1:u:35:MET:HE2	2:x:64:HIS:HB3	1.80	0.63
3:B:91:CYS:SG	3:B:228:ILE:HD13	2.39	0.62
3:C:85:LEU:HA	3:C:88:PRO:HG2	1.81	0.62
3:g:91:CYS:SG	3:g:228:ILE:HD13	2.39	0.62
1:i:25:PHE:HD2	1:i:29:ARG:HH21	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:328:LEU:O	3:m:332:MET:HG2	1.98	0.62
3:C:90:VAL:HA	3:C:93:MET:HG2	1.81	0.62
3:I:90:VAL:HA	3:I:93:MET:HG2	1.81	0.62
3:B:328:LEU:O	3:B:332:MET:HG2	1.98	0.62
2:H:197:ILE:HD13	2:Z:202:ARG:HG2	1.81	0.62
3:O:91:CYS:SG	3:O:228:ILE:HD13	2.39	0.62
1:c:25:PHE:HD2	1:c:29:ARG:HH21	1.45	0.62
3:g:328:LEU:O	3:g:332:MET:HG2	1.98	0.62
1:1:25:PHE:HD2	1:1:29:ARG:HH21	1.45	0.62
3:C:87:LEU:HA	3:C:90:VAL:HG22	1.80	0.62
3:I:87:LEU:HA	3:I:90:VAL:HG22	1.80	0.62
2:M:51:ILE:CA	2:M:78:ARG:NH2	2.62	0.62
3:a:328:LEU:O	3:a:332:MET:HG2	1.98	0.62
1:o:25:PHE:HD2	1:o:29:ARG:HH21	1.45	0.62
1:u:25:PHE:HD2	1:u:29:ARG:HH21	1.45	0.62
3:O:90:VAL:HA	3:O:93:MET:HG2	1.81	0.62
1:W:25:PHE:HD2	1:W:29:ARG:HH21	1.45	0.62
3:m:91:CYS:SG	3:m:228:ILE:HD13	2.39	0.62
3:B:87:LEU:HA	3:B:90:VAL:HG22	1.80	0.62
3:B:90:VAL:HA	3:B:93:MET:HG2	1.81	0.62
3:U:87:LEU:HA	3:U:90:VAL:HG22	1.80	0.62
2:l:104:LEU:HD11	2:l:117:ARG:HB2	1.82	0.62
2:x:104:LEU:HD11	2:x:117:ARG:HB2	1.82	0.62
3:O:87:LEU:HA	3:O:90:VAL:HG22	1.80	0.62
3:U:90:VAL:HA	3:U:93:MET:HG2	1.81	0.62
2:q:51:ILE:CA	2:q:78:ARG:NH2	2.63	0.62
2:5:51:ILE:CA	2:5:78:ARG:NH2	2.62	0.62
3:I:91:CYS:SG	3:I:228:ILE:HD13	2.39	0.62
3:J:235:ALA:O	3:J:239:VAL:HG23	2.00	0.62
1:K:25:PHE:HD2	1:K:29:ARG:HH21	1.45	0.62
3:O:328:LEU:O	3:O:332:MET:HG2	1.98	0.62
3:V:235:ALA:O	3:V:239:VAL:HG23	2.00	0.62
3:a:90:VAL:HA	3:a:93:MET:HG2	1.81	0.62
3:a:91:CYS:SG	3:a:228:ILE:HD13	2.39	0.62
3:O:85:LEU:HA	3:O:88:PRO:HG2	1.81	0.62
2:T:104:LEU:HD11	2:T:117:ARG:HB2	1.82	0.62
3:a:87:LEU:HA	3:a:90:VAL:HG22	1.80	0.62
3:A:235:ALA:O	3:A:239:VAL:HG23	2.00	0.62
3:C:91:CYS:SG	3:C:228:ILE:HD13	2.39	0.62
1:Q:25:PHE:HD2	1:Q:29:ARG:HH21	1.45	0.62
3:U:85:LEU:HA	3:U:88:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:96:LYS:NZ	3:U:322:GLU:OE1	2.33	0.62
2:Z:104:LEU:HD11	2:Z:117:ARG:HB2	1.82	0.62
3:C:96:LYS:NZ	3:C:322:GLU:OE1	2.33	0.61
3:a:85:LEU:HA	3:a:88:PRO:HG2	1.81	0.61
2:f:104:LEU:HD11	2:f:117:ARG:HB2	1.82	0.61
3:n:235:ALA:O	3:n:239:VAL:HG23	2.00	0.61
2:r:104:LEU:HD11	2:r:117:ARG:HB2	1.82	0.61
2:e:51:ILE:CA	2:e:78:ARG:NH2	2.62	0.61
3:m:96:LYS:NZ	3:m:322:GLU:OE1	2.33	0.61
3:I:96:LYS:NZ	3:I:322:GLU:OE1	2.33	0.61
3:P:235:ALA:O	3:P:239:VAL:HG23	2.00	0.61
3:B:96:LYS:NZ	3:B:322:GLU:OE1	2.33	0.61
3:O:96:LYS:NZ	3:O:322:GLU:OE1	2.33	0.61
3:O:109:PRO:HG2	3:O:178:PRO:HD2	1.82	0.61
3:U:109:PRO:HG2	3:U:178:PRO:HD2	1.82	0.61
3:h:338:ALA:O	3:h:342:THR:HG22	2.01	0.61
3:t:235:ALA:O	3:t:239:VAL:HG23	2.00	0.61
3:D:235:ALA:O	3:D:239:VAL:HG23	2.00	0.61
2:M:51:ILE:HG12	2:M:78:ARG:CZ	2.31	0.61
2:T:88:HIS:HB2	2:T:90:LEU:HD13	1.82	0.61
3:a:109:PRO:HG2	3:a:178:PRO:HD2	1.82	0.61
3:b:235:ALA:O	3:b:239:VAL:HG23	2.00	0.61
3:g:109:PRO:HG2	3:g:178:PRO:HD2	1.82	0.61
3:s:109:PRO:HG2	3:s:178:PRO:HD2	1.82	0.61
3:J:338:ALA:O	3:J:342:THR:HG22	2.01	0.61
3:V:105:TYR:HE1	3:V:109:PRO:HD3	1.65	0.61
3:m:109:PRO:HG2	3:m:178:PRO:HD2	1.82	0.61
3:n:332:MET:HA	3:n:332:MET:HE3	1.83	0.61
3:n:338:ALA:O	3:n:342:THR:HG22	2.01	0.61
3:t:338:ALA:O	3:t:342:THR:HG22	2.01	0.61
2:5:51:ILE:HG12	2:5:78:ARG:CZ	2.31	0.61
2:G:51:ILE:HG12	2:G:78:ARG:CZ	2.31	0.61
2:H:88:HIS:HB2	2:H:90:LEU:HD13	1.82	0.61
2:N:104:LEU:HD11	2:N:117:ARG:HB2	1.82	0.61
3:V:332:MET:HA	3:V:332:MET:HE3	1.83	0.61
2:f:88:HIS:HB2	2:f:90:LEU:HD13	1.82	0.61
3:h:332:MET:HA	3:h:332:MET:HE3	1.83	0.61
3:t:105:TYR:HE1	3:t:109:PRO:HD3	1.65	0.61
3:t:332:MET:HA	3:t:332:MET:HE3	1.83	0.61
2:6:88:HIS:HB2	2:6:90:LEU:HD13	1.82	0.61
3:A:338:ALA:O	3:A:342:THR:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:271:PRO:CD	3:B:272:PHE:N	2.58	0.61
2:H:104:LEU:HD11	2:H:117:ARG:HB2	1.82	0.61
3:V:338:ALA:O	3:V:342:THR:HG22	2.01	0.61
3:g:96:LYS:NZ	3:g:322:GLU:OE1	2.33	0.61
3:h:235:ALA:O	3:h:239:VAL:HG23	2.00	0.61
3:O:245:ARG:HH12	3:O:249:PHE:HA	1.66	0.61
3:P:332:MET:HA	3:P:332:MET:HE3	1.83	0.61
2:Z:88:HIS:HB2	2:Z:90:LEU:HD13	1.82	0.61
3:a:245:ARG:HH12	3:a:249:PHE:HA	1.66	0.61
2:q:124:LYS:HE2	2:q:183:PHE:HE1	1.65	0.61
3:C:245:ARG:HH12	3:C:249:PHE:HA	1.66	0.61
2:G:51:ILE:CA	2:G:78:ARG:NH2	2.62	0.61
2:e:51:ILE:HG12	2:e:78:ARG:CZ	2.31	0.61
2:5:217:GLY:HA3	2:k:205:TYR:CE1	2.36	0.60
3:B:245:ARG:HH12	3:B:249:PHE:HA	1.66	0.60
2:H:207:MET:HB3	2:Z:204:SER:HB3	1.82	0.60
3:I:245:ARG:HH12	3:I:249:PHE:HA	1.66	0.60
2:T:113:ASP:OD1	2:T:116:ARG:NH1	2.34	0.60
3:a:96:LYS:NZ	3:a:322:GLU:OE1	2.33	0.60
3:g:90:VAL:HA	3:g:93:MET:HG2	1.81	0.60
3:h:105:TYR:HE1	3:h:109:PRO:HD3	1.65	0.60
2:r:88:HIS:HB2	2:r:90:LEU:HD13	1.82	0.60
2:x:113:ASP:OD1	2:x:116:ARG:NH1	2.34	0.60
2:5:124:LYS:HE2	2:5:183:PHE:HE1	1.65	0.60
2:6:104:LEU:HD11	2:6:117:ARG:HB2	1.82	0.60
3:D:105:TYR:HE1	3:D:109:PRO:HD3	1.65	0.60
3:U:245:ARG:HH12	3:U:249:PHE:HA	1.66	0.60
3:b:332:MET:HA	3:b:332:MET:HE3	1.83	0.60
2:e:124:LYS:HE2	2:e:183:PHE:HE1	1.65	0.60
2:f:113:ASP:OD1	2:f:116:ARG:NH1	2.34	0.60
3:s:90:VAL:HA	3:s:93:MET:HG2	1.81	0.60
2:G:124:LYS:HE2	2:G:183:PHE:HE1	1.65	0.60
3:J:105:TYR:HE1	3:J:109:PRO:HD3	1.65	0.60
2:N:88:HIS:HB2	2:N:90:LEU:HD13	1.82	0.60
3:P:338:ALA:O	3:P:342:THR:HG22	2.01	0.60
3:m:90:VAL:HA	3:m:93:MET:HG2	1.81	0.60
3:n:105:TYR:HE1	3:n:109:PRO:HD3	1.65	0.60
2:x:88:HIS:HB2	2:x:90:LEU:HD13	1.82	0.60
2:S:51:ILE:HG12	2:S:78:ARG:CZ	2.31	0.60
2:Z:113:ASP:OD1	2:Z:116:ARG:NH1	2.34	0.60
2:l:88:HIS:HB2	2:l:90:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:245:ARG:HH12	3:s:249:PHE:HA	1.66	0.60
2:S:49:CYS:HB2	2:S:51:ILE:HG13	1.84	0.60
2:e:49:CYS:HB2	2:e:51:ILE:HG13	1.84	0.60
3:g:245:ARG:HH12	3:g:249:PHE:HA	1.66	0.60
2:k:124:LYS:HE2	2:k:183:PHE:HE1	1.65	0.60
3:s:96:LYS:NZ	3:s:322:GLU:OE1	2.33	0.60
2:l:113:ASP:OD1	2:l:116:ARG:NH1	2.34	0.60
2:q:49:CYS:HB2	2:q:51:ILE:HG13	1.84	0.60
2:w:124:LYS:HE2	2:w:183:PHE:HE1	1.65	0.60
3:A:105:TYR:HE1	3:A:109:PRO:HD3	1.65	0.60
3:A:224:VAL:O	3:A:228:ILE:HG22	2.02	0.60
3:D:338:ALA:O	3:D:342:THR:HG22	2.01	0.60
2:G:49:CYS:HB2	2:G:51:ILE:HG13	1.84	0.60
2:H:113:ASP:OD1	2:H:116:ARG:NH1	2.34	0.60
3:P:105:TYR:HE1	3:P:109:PRO:HD3	1.65	0.60
2:Y:124:LYS:HE2	2:Y:183:PHE:HE1	1.65	0.60
2:Y:51:ILE:HG12	2:Y:78:ARG:CZ	2.31	0.60
2:k:51:ILE:HG12	2:k:78:ARG:CZ	2.31	0.60
2:5:49:CYS:HB2	2:5:51:ILE:HG13	1.84	0.60
3:J:224:VAL:O	3:J:228:ILE:HG22	2.02	0.60
2:M:49:CYS:HB2	2:M:51:ILE:HG13	1.84	0.60
2:M:124:LYS:HE2	2:M:183:PHE:HE1	1.65	0.60
2:M:217:GLY:HA3	2:w:205:TYR:CE1	2.36	0.60
2:N:212:ASP:HB2	2:f:185:ARG:NH2	2.16	0.60
2:S:124:LYS:HE2	2:S:183:PHE:HE1	1.65	0.60
3:b:338:ALA:O	3:b:342:THR:HG22	2.01	0.60
3:B:109:PRO:HG2	3:B:178:PRO:HD2	1.82	0.60
2:Y:49:CYS:HB2	2:Y:51:ILE:HG13	1.84	0.60
3:m:245:ARG:HH12	3:m:249:PHE:HA	1.66	0.60
3:n:224:VAL:O	3:n:228:ILE:HG22	2.02	0.60
2:w:49:CYS:HB2	2:w:51:ILE:HG13	1.84	0.60
3:B:272:PHE:O	3:B:273:LEU:C	2.38	0.59
3:J:332:MET:HE3	3:J:332:MET:HA	1.83	0.59
2:k:49:CYS:HB2	2:k:51:ILE:HG13	1.84	0.59
3:B:113:VAL:HB	3:B:174:ALA:HB3	1.85	0.59
3:D:224:VAL:O	3:D:228:ILE:HG22	2.02	0.59
3:b:105:TYR:HE1	3:b:109:PRO:HD3	1.65	0.59
3:h:224:VAL:O	3:h:228:ILE:HG22	2.02	0.59
2:w:51:ILE:CA	2:w:78:ARG:NH2	2.63	0.59
3:I:113:VAL:HB	3:I:174:ALA:HB3	1.85	0.59
2:q:51:ILE:HG12	2:q:78:ARG:CZ	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:113:ASP:OD1	2:6:116:ARG:NH1	2.34	0.59
3:C:109:PRO:HG2	3:C:178:PRO:HD2	1.82	0.59
2:S:51:ILE:CA	2:S:78:ARG:NH2	2.62	0.59
2:w:51:ILE:HG12	2:w:78:ARG:CZ	2.31	0.59
2:G:15:ARG:NH1	2:H:137:GLN:O	2.36	0.59
3:I:109:PRO:HG2	3:I:178:PRO:HD2	1.82	0.59
2:q:15:ARG:NH1	2:r:137:GLN:O	2.36	0.59
3:C:113:VAL:HB	3:C:174:ALA:HB3	1.84	0.59
3:D:332:MET:HA	3:D:332:MET:HE3	1.83	0.59
2:Y:15:ARG:NH1	2:Z:137:GLN:O	2.36	0.59
2:k:15:ARG:NH1	2:l:137:GLN:O	2.36	0.59
2:w:15:ARG:NH1	2:x:137:GLN:O	2.36	0.59
3:A:332:MET:HA	3:A:332:MET:HE3	1.83	0.59
2:N:113:ASP:OD1	2:N:116:ARG:NH1	2.34	0.59
3:b:224:VAL:O	3:b:228:ILE:HG22	2.02	0.59
3:t:224:VAL:O	3:t:228:ILE:HG22	2.02	0.59
3:P:224:VAL:O	3:P:228:ILE:HG22	2.02	0.59
2:r:113:ASP:OD1	2:r:116:ARG:NH1	2.34	0.59
3:g:113:VAL:HB	3:g:174:ALA:HB3	1.84	0.59
2:S:15:ARG:NH1	2:T:137:GLN:O	2.36	0.58
2:e:170:ASP:OD1	2:x:202:ARG:NH2	2.36	0.58
2:k:51:ILE:CA	2:k:78:ARG:NH2	2.62	0.58
2:5:15:ARG:NH1	2:6:137:GLN:O	2.36	0.58
2:5:205:TYR:CE1	2:S:217:GLY:HA3	2.37	0.58
2:M:204:SER:HB3	2:e:207:MET:HB3	1.85	0.58
3:O:113:VAL:HB	3:O:174:ALA:HB3	1.85	0.58
2:M:15:ARG:NH1	2:N:137:GLN:O	2.36	0.58
3:s:113:VAL:HB	3:s:174:ALA:HB3	1.85	0.58
3:m:113:VAL:HB	3:m:174:ALA:HB3	1.85	0.58
2:e:15:ARG:NH1	2:f:137:GLN:O	2.36	0.58
3:D:245:ARG:NH1	3:D:245:ARG:O	2.37	0.58
3:U:113:VAL:HB	3:U:174:ALA:HB3	1.85	0.58
2:Y:204:SER:O	2:q:218:GLY:CA	2.27	0.58
2:M:30:MET:HE1	2:M:181:GLU:HG2	1.86	0.58
3:V:224:VAL:O	3:V:228:ILE:HG22	2.02	0.58
3:a:113:VAL:HB	3:a:174:ALA:HB3	1.85	0.58
3:B:270:ARG:HA	3:B:273:LEU:H	1.69	0.57
2:G:205:TYR:CE1	2:Y:217:GLY:CA	2.81	0.57
3:a:74:THR:O	3:a:78:VAL:HG22	2.05	0.57
3:t:152:PHE:HA	3:t:155:TRP:HD1	1.69	0.57
3:B:236:VAL:HG22	3:B:333:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:161:ALA:HB1	2:N:164:PRO:HG3	1.87	0.57
3:P:261:ILE:HD12	2:T:103:PRO:HG3	1.87	0.57
2:6:161:ALA:HB1	2:6:164:PRO:HG3	1.87	0.57
3:B:74:THR:O	3:B:78:VAL:HG22	2.05	0.57
2:S:205:TYR:CE1	2:k:217:GLY:HA3	2.39	0.57
3:b:201:ILE:O	3:b:203:GLU:N	2.37	0.57
3:g:74:THR:O	3:g:78:VAL:HG22	2.05	0.57
3:s:74:THR:O	3:s:78:VAL:HG22	2.05	0.57
3:A:245:ARG:NH1	3:A:245:ARG:O	2.37	0.57
3:C:236:VAL:HG22	3:C:333:ILE:HD13	1.87	0.57
3:I:83:ILE:HD12	3:J:235:ALA:HB1	1.87	0.57
3:P:201:ILE:O	3:P:203:GLU:N	2.37	0.57
3:b:261:ILE:HD12	2:f:103:PRO:HG3	1.87	0.57
2:q:164:PRO:HG2	2:q:192:MET:HE3	1.87	0.57
3:t:261:ILE:HD12	2:x:103:PRO:HG3	1.87	0.57
3:B:83:ILE:HD12	3:D:235:ALA:HB1	1.87	0.57
2:H:161:ALA:HB1	2:H:164:PRO:HG3	1.87	0.57
3:I:270:ARG:O	3:I:271:PRO:C	2.48	0.57
3:O:74:THR:O	3:O:78:VAL:HG22	2.05	0.57
3:h:152:PHE:HA	3:h:155:TRP:HD1	1.69	0.57
3:m:83:ILE:HD12	3:n:235:ALA:HB1	1.87	0.57
3:n:261:ILE:HD12	2:r:103:PRO:HG3	1.87	0.57
3:I:236:VAL:HG22	3:I:333:ILE:HD13	1.87	0.57
3:O:83:ILE:HD12	3:P:235:ALA:HB1	1.87	0.57
2:T:161:ALA:HB1	2:T:164:PRO:HG3	1.87	0.57
2:f:161:ALA:HB1	2:f:164:PRO:HG3	1.87	0.57
3:t:55:GLN:OE1	3:t:270:ARG:NH2	2.38	0.57
3:C:74:THR:O	3:C:78:VAL:HG22	2.05	0.57
3:V:152:PHE:HA	3:V:155:TRP:HD1	1.69	0.57
3:V:201:ILE:O	3:V:203:GLU:N	2.37	0.57
2:Y:51:ILE:CA	2:Y:78:ARG:NH2	2.62	0.57
2:Z:161:ALA:HB1	2:Z:164:PRO:HG3	1.86	0.57
3:b:152:PHE:HA	3:b:155:TRP:HD1	1.69	0.57
3:h:55:GLN:OE1	3:h:270:ARG:NH2	2.38	0.57
3:m:74:THR:O	3:m:78:VAL:HG22	2.05	0.57
3:s:83:ILE:HD12	3:t:235:ALA:HB1	1.87	0.57
3:U:83:ILE:HD12	3:V:235:ALA:HB1	1.87	0.57
3:V:261:ILE:HD12	2:Z:103:PRO:HG3	1.87	0.57
3:a:83:ILE:HD12	3:b:235:ALA:HB1	1.87	0.57
3:h:261:ILE:HD12	2:l:103:PRO:HG3	1.87	0.57
3:A:235:ALA:HB1	3:C:83:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:VAL:HA	3:C:227:MET:HE2	1.87	0.57
3:J:55:GLN:OE1	3:J:270:ARG:NH2	2.38	0.57
3:P:55:GLN:OE1	3:P:270:ARG:NH2	2.38	0.57
3:U:74:THR:O	3:U:78:VAL:HG22	2.05	0.57
3:V:55:GLN:OE1	3:V:270:ARG:NH2	2.38	0.57
3:n:201:ILE:O	3:n:203:GLU:N	2.37	0.57
3:D:152:PHE:HA	3:D:155:TRP:HD1	1.69	0.56
3:I:224:VAL:HA	3:I:227:MET:HE2	1.87	0.56
3:P:245:ARG:NH1	3:P:245:ARG:O	2.37	0.56
3:b:55:GLN:OE1	3:b:270:ARG:NH2	2.38	0.56
3:g:83:ILE:HD12	3:h:235:ALA:HB1	1.87	0.56
2:k:164:PRO:HG2	2:k:192:MET:HE3	1.87	0.56
3:n:245:ARG:NH1	3:n:245:ARG:O	2.37	0.56
3:J:152:PHE:HA	3:J:155:TRP:HD1	1.69	0.56
3:U:236:VAL:HG22	3:U:333:ILE:HD13	1.87	0.56
3:b:245:ARG:NH1	3:b:245:ARG:O	2.37	0.56
3:h:201:ILE:O	3:h:203:GLU:N	2.37	0.56
2:5:164:PRO:HG2	2:5:192:MET:HE3	1.87	0.56
3:A:55:GLN:OE1	3:A:270:ARG:NH2	2.38	0.56
3:B:224:VAL:HA	3:B:227:MET:HE2	1.87	0.56
3:I:74:THR:O	3:I:78:VAL:HG22	2.04	0.56
3:J:245:ARG:NH1	3:J:245:ARG:O	2.37	0.56
2:M:164:PRO:HG2	2:M:192:MET:HE3	1.87	0.56
3:O:137:VAL:HG21	3:O:176:VAL:HG13	1.87	0.56
3:P:152:PHE:HA	3:P:155:TRP:HD1	1.69	0.56
3:V:245:ARG:NH1	3:V:245:ARG:O	2.37	0.56
3:a:137:VAL:HG21	3:a:176:VAL:HG13	1.87	0.56
3:n:55:GLN:OE1	3:n:270:ARG:NH2	2.38	0.56
3:n:152:PHE:HA	3:n:155:TRP:HD1	1.69	0.56
2:x:87:ASP:OD1	2:x:87:ASP:N	2.36	0.56
3:O:236:VAL:HG22	3:O:333:ILE:HD13	1.87	0.56
3:a:87:LEU:H	3:a:87:LEU:HD12	1.71	0.56
3:a:236:VAL:HG22	3:a:333:ILE:HD13	1.87	0.56
3:t:201:ILE:O	3:t:203:GLU:N	2.37	0.56
3:P:145:ARG:HE	3:P:171:PRO:HA	1.71	0.56
3:U:231:LEU:HD22	3:V:87:LEU:HD21	1.88	0.56
3:g:236:VAL:HG22	3:g:333:ILE:HD13	1.87	0.56
3:A:152:PHE:HA	3:A:155:TRP:HD1	1.69	0.56
3:D:55:GLN:OE1	3:D:270:ARG:NH2	2.38	0.56
3:O:87:LEU:HD12	3:O:87:LEU:H	1.71	0.56
2:T:66:ILE:HG22	2:T:69:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:66:ILE:HG22	2:f:69:LEU:HD13	1.88	0.56
2:l:161:ALA:HB1	2:l:164:PRO:HG3	1.87	0.56
3:m:236:VAL:HG22	3:m:333:ILE:HD13	1.87	0.56
2:r:161:ALA:HB1	2:r:164:PRO:HG3	1.87	0.56
2:6:66:ILE:HG22	2:6:69:LEU:HD13	1.88	0.56
2:H:66:ILE:HG22	2:H:69:LEU:HD13	1.88	0.56
2:N:212:ASP:HB2	2:f:185:ARG:HH22	1.71	0.56
3:O:231:LEU:HD22	3:P:87:LEU:HD21	1.88	0.56
2:w:164:PRO:HG2	2:w:192:MET:HE3	1.87	0.56
2:6:103:PRO:HG3	3:A:261:ILE:HD12	1.87	0.56
3:C:137:VAL:HG21	3:C:176:VAL:HG13	1.87	0.56
3:D:261:ILE:HD12	2:H:103:PRO:HG3	1.87	0.56
3:J:261:ILE:HD12	2:N:103:PRO:HG3	1.87	0.56
3:U:137:VAL:HG21	3:U:176:VAL:HG13	1.87	0.56
3:V:145:ARG:HE	3:V:171:PRO:HA	1.71	0.56
3:h:90:VAL:HA	3:h:93:MET:HG2	1.88	0.56
3:s:236:VAL:HG22	3:s:333:ILE:HD13	1.87	0.56
3:B:87:LEU:H	3:B:87:LEU:HD12	1.71	0.56
3:I:137:VAL:HG21	3:I:176:VAL:HG13	1.87	0.56
3:P:90:VAL:HA	3:P:93:MET:HG2	1.88	0.56
3:V:90:VAL:HA	3:V:93:MET:HG2	1.88	0.56
2:Y:205:TYR:HE1	2:q:217:GLY:HA3	1.71	0.56
3:a:231:LEU:HD22	3:b:87:LEU:HD21	1.88	0.56
3:b:145:ARG:HE	3:b:171:PRO:HA	1.71	0.56
2:e:164:PRO:HG2	2:e:192:MET:HE3	1.87	0.56
3:t:90:VAL:HA	3:t:93:MET:HG2	1.88	0.56
2:x:161:ALA:HB1	2:x:164:PRO:HG3	1.87	0.56
2:G:164:PRO:HG2	2:G:192:MET:HE3	1.87	0.56
3:I:87:LEU:H	3:I:87:LEU:HD12	1.71	0.56
2:N:66:ILE:HG22	2:N:69:LEU:HD13	1.88	0.55
2:Z:66:ILE:HG22	2:Z:69:LEU:HD13	1.88	0.55
3:n:90:VAL:HA	3:n:93:MET:HG2	1.88	0.55
2:r:66:ILE:HG22	2:r:69:LEU:HD13	1.88	0.55
2:x:66:ILE:HG22	2:x:69:LEU:HD13	1.88	0.55
3:B:137:VAL:HG21	3:B:176:VAL:HG13	1.87	0.55
3:b:90:VAL:HA	3:b:93:MET:HG2	1.88	0.55
3:m:224:VAL:HA	3:m:227:MET:HE2	1.87	0.55
3:A:87:LEU:HD21	3:C:231:LEU:HD22	1.88	0.55
3:B:231:LEU:HD22	3:D:87:LEU:HD21	1.88	0.55
3:I:231:LEU:HD22	3:J:87:LEU:HD21	1.88	0.55
3:U:87:LEU:H	3:U:87:LEU:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:66:ILE:HG22	2:l:69:LEU:HD13	1.88	0.55
3:s:137:VAL:HG21	3:s:176:VAL:HG13	1.87	0.55
3:s:268:ILE:C	3:s:270:ARG:H	2.15	0.55
3:B:270:ARG:HB3	3:B:273:LEU:HB2	1.87	0.55
3:C:87:LEU:H	3:C:87:LEU:HD12	1.71	0.55
3:a:224:VAL:HA	3:a:227:MET:HE2	1.87	0.55
3:h:145:ARG:HE	3:h:171:PRO:HA	1.71	0.55
3:t:145:ARG:HE	3:t:171:PRO:HA	1.71	0.55
2:x:165:THR:HA	2:x:168:LEU:HB2	1.88	0.55
1:2:34:SER:OG	2:5:73:GLU:OE2	2.24	0.55
1:F:34:SER:OG	2:G:73:GLU:OE2	2.24	0.55
1:L:34:SER:OG	2:M:73:GLU:OE2	2.24	0.55
2:M:205:TYR:HE1	2:e:217:GLY:HA3	1.72	0.55
2:e:28:GLY:N	2:e:189:THR:HG22	2.22	0.55
2:l:87:ASP:OD1	2:l:87:ASP:N	2.36	0.55
2:N:125:VAL:HB	2:N:145:ARG:HG2	1.89	0.55
2:f:165:THR:HA	2:f:168:LEU:HB2	1.88	0.55
2:l:165:THR:HA	2:l:168:LEU:HB2	1.88	0.55
2:6:125:VAL:HB	2:6:145:ARG:HG2	1.89	0.55
3:D:90:VAL:HA	3:D:93:MET:HG2	1.88	0.55
3:J:201:ILE:O	3:J:203:GLU:N	2.37	0.55
2:S:28:GLY:N	2:S:189:THR:HG22	2.22	0.55
2:S:164:PRO:HG2	2:S:192:MET:HE3	1.87	0.55
2:Y:164:PRO:HG2	2:Y:192:MET:HE3	1.87	0.55
2:e:185:ARG:NH2	2:w:211:SER:OG	2.40	0.55
3:g:137:VAL:HG21	3:g:176:VAL:HG13	1.87	0.55
3:g:231:LEU:HD22	3:h:87:LEU:HD21	1.88	0.55
3:h:245:ARG:NH1	3:h:245:ARG:O	2.37	0.55
3:A:201:ILE:O	3:A:203:GLU:N	2.37	0.55
2:H:125:VAL:HB	2:H:145:ARG:HG2	1.89	0.55
2:T:165:THR:HA	2:T:168:LEU:HB2	1.88	0.55
3:a:268:ILE:C	3:a:270:ARG:H	2.14	0.55
3:a:270:ARG:O	3:a:272:PHE:N	2.40	0.55
3:m:231:LEU:HD22	3:n:87:LEU:HD21	1.88	0.55
2:r:125:VAL:HB	2:r:145:ARG:HG2	1.89	0.55
3:s:231:LEU:HD22	3:t:87:LEU:HD21	1.88	0.55
3:D:145:ARG:HE	3:D:171:PRO:HA	1.71	0.55
3:U:224:VAL:HA	3:U:227:MET:HE2	1.87	0.55
3:U:332:MET:O	3:U:336:VAL:HG12	2.07	0.55
2:Y:186:VAL:HG23	2:Y:187:GLY:H	1.72	0.55
2:Z:165:THR:HA	2:Z:168:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:332:MET:O	3:g:336:VAL:HG12	2.07	0.55
3:D:201:ILE:O	3:D:203:GLU:N	2.37	0.55
3:O:224:VAL:HA	3:O:227:MET:HE2	1.87	0.55
3:g:87:LEU:HD12	3:g:87:LEU:H	1.71	0.55
3:g:224:VAL:HA	3:g:227:MET:HE2	1.87	0.55
2:l:125:VAL:HB	2:l:145:ARG:HG2	1.89	0.55
3:m:137:VAL:HG21	3:m:176:VAL:HG13	1.87	0.55
3:n:145:ARG:HE	3:n:171:PRO:HA	1.71	0.55
2:r:165:THR:HA	2:r:168:LEU:HB2	1.88	0.55
3:t:245:ARG:NH1	3:t:245:ARG:O	2.37	0.55
2:w:186:VAL:HG23	2:w:187:GLY:H	1.72	0.55
3:I:245:ARG:NH1	3:I:248:ILE:O	2.41	0.54
2:5:28:GLY:N	2:5:189:THR:HG22	2.22	0.54
3:C:245:ARG:NH1	3:C:248:ILE:O	2.41	0.54
3:I:332:MET:O	3:I:336:VAL:HG12	2.07	0.54
2:T:209:THR:O	2:T:216:HIS:N	2.40	0.54
2:Z:125:VAL:HB	2:Z:145:ARG:HG2	1.89	0.54
2:f:125:VAL:HB	2:f:145:ARG:HG2	1.89	0.54
3:g:245:ARG:NH1	3:g:248:ILE:O	2.40	0.54
1:j:34:SER:OG	2:k:73:GLU:OE2	2.24	0.54
1:v:34:SER:OG	2:w:73:GLU:OE2	2.24	0.54
2:6:165:THR:HA	2:6:168:LEU:HB2	1.88	0.54
3:C:332:MET:O	3:C:336:VAL:HG12	2.07	0.54
2:N:165:THR:HA	2:N:168:LEU:HB2	1.88	0.54
3:O:332:MET:O	3:O:336:VAL:HG12	2.07	0.54
2:S:186:VAL:HG23	2:S:187:GLY:H	1.72	0.54
2:T:125:VAL:HB	2:T:145:ARG:HG2	1.89	0.54
3:U:245:ARG:NH1	3:U:248:ILE:O	2.40	0.54
2:Z:209:THR:O	2:Z:216:HIS:N	2.40	0.54
3:m:245:ARG:NH1	3:m:248:ILE:O	2.40	0.54
3:m:332:MET:O	3:m:336:VAL:HG12	2.07	0.54
2:r:144:GLN:O	2:r:148:ILE:HD12	2.08	0.54
3:s:224:VAL:HA	3:s:227:MET:HE2	1.87	0.54
3:s:332:MET:O	3:s:336:VAL:HG12	2.07	0.54
3:C:116:GLN:HB3	3:C:119:LEU:HD22	1.90	0.54
2:G:28:GLY:N	2:G:189:THR:HG22	2.22	0.54
2:N:0:VAL:HG21	2:N:3:ARG:HD3	1.89	0.54
2:f:209:THR:O	2:f:216:HIS:N	2.40	0.54
3:s:87:LEU:H	3:s:87:LEU:HD12	1.71	0.54
2:x:125:VAL:HB	2:x:145:ARG:HG2	1.89	0.54
3:C:270:ARG:O	3:C:271:PRO:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:THR:HA	2:H:168:LEU:HB2	1.88	0.54
3:I:116:GLN:HB3	3:I:119:LEU:HD22	1.90	0.54
3:P:100:GLN:O	3:P:103:THR:OG1	2.24	0.54
2:f:144:GLN:O	2:f:148:ILE:HD12	2.08	0.54
3:g:97:ASN:OD1	3:g:98:VAL:N	2.41	0.54
2:k:186:VAL:HG23	2:k:187:GLY:H	1.72	0.54
2:l:144:GLN:O	2:l:148:ILE:HD12	2.08	0.54
3:m:97:ASN:OD1	3:m:98:VAL:N	2.41	0.54
3:A:90:VAL:HA	3:A:93:MET:HG2	1.88	0.54
2:H:144:GLN:O	2:H:148:ILE:HD12	2.08	0.54
3:I:97:ASN:OD1	3:I:98:VAL:N	2.41	0.54
3:J:90:VAL:HA	3:J:93:MET:HG2	1.88	0.54
1:Q:31:GLU:HA	2:T:76:PHE:HZ	1.73	0.54
3:V:234:ALA:O	3:V:238:LEU:HD22	2.08	0.54
1:W:31:GLU:HA	2:Z:76:PHE:HZ	1.73	0.54
3:a:270:ARG:O	3:a:271:PRO:C	2.50	0.54
2:f:0:VAL:HG21	2:f:3:ARG:HD3	1.89	0.54
1:p:34:SER:OG	2:q:73:GLU:OE2	2.24	0.54
2:r:82:GLY:HA3	2:r:159:LEU:HD23	1.89	0.54
3:s:245:ARG:NH1	3:s:248:ILE:O	2.40	0.54
2:x:82:GLY:HA3	2:x:159:LEU:HD23	1.89	0.54
2:6:144:GLN:O	2:6:148:ILE:HD12	2.08	0.54
3:P:234:ALA:O	3:P:238:LEU:HD22	2.08	0.54
2:T:0:VAL:HG21	2:T:3:ARG:HD3	1.89	0.54
2:T:82:GLY:HA3	2:T:159:LEU:HD23	1.89	0.54
2:Y:28:GLY:N	2:Y:189:THR:HG22	2.22	0.54
2:Z:0:VAL:HG21	2:Z:3:ARG:HD3	1.89	0.54
2:l:209:THR:O	2:l:216:HIS:N	2.40	0.54
3:m:82:ALA:HA	3:m:287:SER:HB2	1.89	0.54
3:s:97:ASN:OD1	3:s:98:VAL:N	2.41	0.54
2:6:0:VAL:HG21	2:6:3:ARG:HD3	1.89	0.54
3:C:97:ASN:OD1	3:C:98:VAL:N	2.41	0.54
2:T:144:GLN:O	2:T:148:ILE:HD12	2.08	0.54
3:b:251:ARG:H	3:b:251:ARG:HD3	1.73	0.54
2:x:144:GLN:O	2:x:148:ILE:HD12	2.08	0.54
2:x:209:THR:O	2:x:216:HIS:N	2.40	0.54
3:A:251:ARG:H	3:A:251:ARG:HD3	1.73	0.54
3:B:245:ARG:NH1	3:B:248:ILE:O	2.40	0.54
3:B:332:MET:O	3:B:336:VAL:HG12	2.07	0.54
2:H:82:GLY:HA3	2:H:159:LEU:HD23	1.89	0.54
2:M:186:VAL:HG23	2:M:187:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:144:GLN:O	2:N:148:ILE:HD12	2.08	0.54
3:O:245:ARG:NH1	3:O:248:ILE:O	2.40	0.54
2:T:87:ASP:OD1	2:T:87:ASP:N	2.36	0.54
3:a:97:ASN:OD1	3:a:98:VAL:N	2.41	0.54
1:c:31:GLU:HA	2:f:76:PHE:HZ	1.73	0.54
2:e:186:VAL:HG23	2:e:187:GLY:H	1.72	0.54
3:s:270:ARG:O	3:s:271:PRO:C	2.50	0.54
2:6:82:GLY:HA3	2:6:159:LEU:HD23	1.89	0.54
3:A:145:ARG:HE	3:A:171:PRO:HA	1.71	0.54
3:B:116:GLN:HB3	3:B:119:LEU:HD22	1.90	0.54
3:D:251:ARG:H	3:D:251:ARG:HD3	1.73	0.54
2:G:186:VAL:HG23	2:G:187:GLY:H	1.72	0.54
3:P:251:ARG:HD3	3:P:251:ARG:H	1.73	0.54
2:Z:82:GLY:HA3	2:Z:159:LEU:HD23	1.89	0.54
3:a:235:ALA:O	3:a:239:VAL:HG23	2.08	0.54
3:a:245:ARG:NH1	3:a:248:ILE:O	2.41	0.54
3:a:332:MET:O	3:a:336:VAL:HG12	2.07	0.54
2:q:186:VAL:HG23	2:q:187:GLY:H	1.72	0.54
2:r:209:THR:O	2:r:216:HIS:N	2.40	0.54
2:w:28:GLY:N	2:w:189:THR:HG22	2.22	0.54
2:5:186:VAL:HG23	2:5:187:GLY:H	1.72	0.53
3:J:251:ARG:HD3	3:J:251:ARG:H	1.73	0.53
3:b:234:ALA:O	3:b:238:LEU:HD22	2.08	0.53
3:J:234:ALA:O	3:J:238:LEU:HD22	2.08	0.53
2:f:82:GLY:HA3	2:f:159:LEU:HD23	1.89	0.53
3:m:116:GLN:HB3	3:m:119:LEU:HD22	1.90	0.53
3:A:234:ALA:O	3:A:238:LEU:HD22	2.08	0.53
3:B:97:ASN:OD1	3:B:98:VAL:N	2.41	0.53
1:E:31:GLU:HA	2:H:76:PHE:HZ	1.73	0.53
2:H:205:TYR:HE1	2:r:217:GLY:C	2.17	0.53
2:N:82:GLY:HA3	2:N:159:LEU:HD23	1.89	0.53
3:O:235:ALA:O	3:O:239:VAL:HG23	2.08	0.53
3:U:235:ALA:O	3:U:239:VAL:HG23	2.08	0.53
3:g:116:GLN:HB3	3:g:119:LEU:HD22	1.90	0.53
3:h:251:ARG:HD3	3:h:251:ARG:H	1.73	0.53
2:l:0:VAL:HG21	2:l:3:ARG:HD3	1.89	0.53
3:n:100:GLN:O	3:n:103:THR:OG1	2.24	0.53
3:n:251:ARG:HD3	3:n:251:ARG:H	1.73	0.53
2:r:0:VAL:HG21	2:r:3:ARG:HD3	1.89	0.53
3:t:234:ALA:O	3:t:238:LEU:HD22	2.08	0.53
2:6:209:THR:O	2:6:216:HIS:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:GLU:O	3:D:190:THR:HG22	2.09	0.53
2:H:209:THR:O	2:H:216:HIS:N	2.40	0.53
3:I:92:TYR:CD1	3:I:228:ILE:HD11	2.44	0.53
2:N:209:THR:O	2:N:216:HIS:N	2.40	0.53
3:O:270:ARG:C	3:O:272:PHE:N	2.47	0.53
3:V:251:ARG:H	3:V:251:ARG:HD3	1.73	0.53
3:t:186:GLU:O	3:t:190:THR:HG22	2.09	0.53
3:D:100:GLN:O	3:D:103:THR:OG1	2.24	0.53
3:O:97:ASN:OD1	3:O:98:VAL:N	2.41	0.53
3:U:97:ASN:OD1	3:U:98:VAL:N	2.41	0.53
2:l:51:ILE:HA	2:l:78:ARG:NH2	2.24	0.53
3:t:251:ARG:H	3:t:251:ARG:HD3	1.73	0.53
2:x:0:VAL:HG21	2:x:3:ARG:HD3	1.89	0.53
1:l:31:GLU:HA	2:6:76:PHE:HZ	1.73	0.53
3:A:186:GLU:O	3:A:190:THR:HG22	2.09	0.53
3:C:235:ALA:O	3:C:239:VAL:HG23	2.08	0.53
3:J:145:ARG:HE	3:J:171:PRO:HA	1.71	0.53
3:J:350:THR:O	3:J:351:PRO:C	2.50	0.53
3:O:230:VAL:O	3:O:233:VAL:HG12	2.09	0.53
3:a:230:VAL:O	3:a:233:VAL:HG12	2.09	0.53
3:h:186:GLU:O	3:h:190:THR:HG22	2.09	0.53
2:l:82:GLY:HA3	2:l:159:LEU:HD23	1.89	0.53
3:B:235:ALA:O	3:B:239:VAL:HG23	2.08	0.53
3:C:92:TYR:CD1	3:C:228:ILE:HD11	2.44	0.53
2:H:0:VAL:HG21	2:H:3:ARG:HD3	1.89	0.53
2:H:51:ILE:HA	2:H:78:ARG:NH2	2.24	0.53
3:I:230:VAL:O	3:I:233:VAL:HG12	2.09	0.53
3:I:235:ALA:O	3:I:239:VAL:HG23	2.08	0.53
3:J:186:GLU:O	3:J:190:THR:HG22	2.09	0.53
2:N:196:ASP:OD1	2:N:199:LEU:N	2.42	0.53
3:U:230:VAL:O	3:U:233:VAL:HG12	2.09	0.53
2:Z:144:GLN:O	2:Z:148:ILE:HD12	2.08	0.53
3:b:100:GLN:O	3:b:103:THR:OG1	2.24	0.53
1:d:34:SER:OG	2:e:73:GLU:OE2	2.24	0.53
3:s:116:GLN:HB3	3:s:119:LEU:HD22	1.90	0.53
2:x:51:ILE:HA	2:x:78:ARG:NH2	2.24	0.53
2:e:30:MET:HE1	2:e:181:GLU:HG2	1.89	0.53
2:k:28:GLY:N	2:k:189:THR:HG22	2.22	0.53
3:m:235:ALA:O	3:m:239:VAL:HG23	2.08	0.53
1:u:31:GLU:HA	2:x:76:PHE:HZ	1.73	0.53
2:6:51:ILE:HA	2:6:78:ARG:NH2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:TYR:HD2	2:H:105:ILE:HG21	1.74	0.53
3:D:234:ALA:O	3:D:238:LEU:HD22	2.08	0.53
1:R:34:SER:OG	2:S:73:GLU:OE2	2.24	0.53
3:U:116:GLN:HB3	3:U:119:LEU:HD22	1.90	0.53
3:a:116:GLN:HB3	3:a:119:LEU:HD22	1.90	0.53
3:h:234:ALA:O	3:h:238:LEU:HD22	2.08	0.53
2:r:51:ILE:HA	2:r:78:ARG:NH2	2.24	0.53
3:s:230:VAL:O	3:s:233:VAL:HG12	2.09	0.53
2:6:196:ASP:OD1	2:6:199:LEU:N	2.42	0.52
3:C:230:VAL:O	3:C:233:VAL:HG12	2.09	0.52
3:O:116:GLN:HB3	3:O:119:LEU:HD22	1.90	0.52
3:P:186:GLU:O	3:P:190:THR:HG22	2.09	0.52
2:Y:208:LEU:HD23	2:Y:215:LEU:HD11	1.91	0.52
2:6:105:ILE:HG21	3:A:58:TYR:HD2	1.75	0.52
3:B:96:LYS:O	3:B:100:GLN:HG2	2.09	0.52
3:J:263:ALA:HA	2:N:106:ILE:HG23	1.91	0.52
1:K:31:GLU:HA	2:N:76:PHE:HZ	1.73	0.52
2:Z:51:ILE:HA	2:Z:78:ARG:NH2	2.24	0.52
3:g:92:TYR:CD1	3:g:228:ILE:HD11	2.44	0.52
3:g:230:VAL:O	3:g:233:VAL:HG12	2.09	0.52
1:i:31:GLU:HA	2:l:76:PHE:HZ	1.73	0.52
3:m:87:LEU:H	3:m:87:LEU:HD12	1.74	0.52
3:n:234:ALA:O	3:n:238:LEU:HD22	2.08	0.52
3:s:92:TYR:CD1	3:s:228:ILE:HD11	2.44	0.52
3:s:235:ALA:O	3:s:239:VAL:HG23	2.08	0.52
2:N:51:ILE:HA	2:N:78:ARG:NH2	2.24	0.52
1:X:34:SER:OG	2:Y:73:GLU:OE2	2.24	0.52
2:Z:196:ASP:OD1	2:Z:199:LEU:N	2.42	0.52
3:b:186:GLU:O	3:b:190:THR:HG22	2.09	0.52
2:f:51:ILE:HA	2:f:78:ARG:NH2	2.24	0.52
3:B:92:TYR:CD1	3:B:228:ILE:HD11	2.44	0.52
3:b:113:VAL:HB	3:b:174:ALA:HB3	1.91	0.52
2:x:135:PRO:O	2:x:143:GLN:NE2	2.38	0.52
2:M:178:ARG:HH12	2:M:203:ARG:HH12	1.56	0.52
2:Y:127:LEU:HD11	2:Y:142:GLU:OE2	2.10	0.52
3:a:92:TYR:CD1	3:a:228:ILE:HD11	2.44	0.52
3:n:58:TYR:CD2	2:r:105:ILE:HG21	2.45	0.52
3:n:113:VAL:HB	3:n:174:ALA:HB3	1.91	0.52
3:n:186:GLU:O	3:n:190:THR:HG22	2.09	0.52
2:q:28:GLY:N	2:q:189:THR:HG22	2.22	0.52
3:B:230:VAL:O	3:B:233:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:58:TYR:HD2	2:N:105:ILE:HG21	1.75	0.52
2:S:127:LEU:HD11	2:S:142:GLU:OE2	2.10	0.52
3:h:58:TYR:CD2	2:l:105:ILE:HG21	2.45	0.52
3:h:113:VAL:HB	3:h:174:ALA:HB3	1.91	0.52
2:6:105:ILE:HG21	3:A:58:TYR:CD2	2.45	0.52
2:6:106:ILE:HG23	3:A:263:ALA:HA	1.91	0.52
3:V:186:GLU:O	3:V:190:THR:HG22	2.09	0.52
3:V:263:ALA:HA	2:Z:106:ILE:HG23	1.91	0.52
2:e:127:LEU:HD11	2:e:142:GLU:OE2	2.10	0.52
3:A:100:GLN:O	3:A:103:THR:OG1	2.24	0.52
3:I:96:LYS:O	3:I:100:GLN:HG2	2.09	0.52
3:J:58:TYR:CD2	2:N:105:ILE:HG21	2.45	0.52
2:T:51:ILE:HA	2:T:78:ARG:NH2	2.24	0.52
3:U:92:TYR:CD1	3:U:228:ILE:HD11	2.44	0.52
2:Z:87:ASP:OD1	2:Z:87:ASP:N	2.36	0.52
3:m:92:TYR:CD1	3:m:228:ILE:HD11	2.44	0.52
3:C:88:PRO:HA	3:C:228:ILE:HD12	1.92	0.52
3:D:58:TYR:CD2	2:H:105:ILE:HG21	2.45	0.52
3:I:88:PRO:HA	3:I:228:ILE:HD12	1.92	0.52
3:O:92:TYR:CD1	3:O:228:ILE:HD11	2.44	0.52
3:U:96:LYS:O	3:U:100:GLN:HG2	2.09	0.52
3:V:58:TYR:CD2	2:Z:105:ILE:HG21	2.45	0.52
3:V:113:VAL:HB	3:V:174:ALA:HB3	1.91	0.52
3:V:239:VAL:O	3:V:243:SER:OG	2.21	0.52
3:b:58:TYR:HD2	2:f:105:ILE:HG21	1.75	0.52
2:q:208:LEU:HD23	2:q:215:LEU:HD11	1.91	0.52
3:t:113:VAL:HB	3:t:174:ALA:HB3	1.91	0.52
2:6:87:ASP:OD1	2:6:87:ASP:N	2.36	0.52
3:C:269:LEU:HG	3:C:342:THR:OG1	2.09	0.52
3:D:263:ALA:HA	2:H:106:ILE:HG23	1.91	0.52
2:N:135:PRO:O	2:N:143:GLN:NE2	2.38	0.52
3:P:58:TYR:CD2	2:T:105:ILE:HG21	2.45	0.52
2:S:208:LEU:HD23	2:S:215:LEU:HD11	1.91	0.52
3:g:235:ALA:O	3:g:239:VAL:HG23	2.08	0.52
3:m:230:VAL:O	3:m:233:VAL:HG12	2.09	0.52
3:t:58:TYR:CD2	2:x:105:ILE:HG21	2.45	0.52
3:B:88:PRO:HA	3:B:228:ILE:HD12	1.92	0.51
2:H:196:ASP:OD1	2:H:199:LEU:N	2.42	0.51
3:P:113:VAL:HB	3:P:174:ALA:HB3	1.91	0.51
3:P:263:ALA:HA	2:T:106:ILE:HG23	1.91	0.51
3:h:58:TYR:HD2	2:l:105:ILE:HG21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:263:ALA:HA	2:l:106:ILE:HG23	1.91	0.51
2:k:208:LEU:HD23	2:k:215:LEU:HD11	1.91	0.51
2:l:135:PRO:O	2:l:143:GLN:NE2	2.38	0.51
3:n:58:TYR:HD2	2:r:105:ILE:HG21	1.75	0.51
3:s:270:ARG:O	3:s:272:PHE:N	2.43	0.51
3:b:58:TYR:CD2	2:f:105:ILE:HG21	2.45	0.51
1:o:31:GLU:HA	2:r:76:PHE:HZ	1.73	0.51
2:G:217:GLY:HA3	2:q:205:TYR:CE1	2.46	0.51
3:J:113:VAL:HB	3:J:174:ALA:HB3	1.91	0.51
3:P:58:TYR:HD2	2:T:105:ILE:HG21	1.75	0.51
2:T:196:ASP:OD1	2:T:199:LEU:N	2.42	0.51
3:U:88:PRO:HA	3:U:228:ILE:HD12	1.92	0.51
3:m:96:LYS:O	3:m:100:GLN:HG2	2.09	0.51
3:t:263:ALA:HA	2:x:106:ILE:HG23	1.91	0.51
2:w:208:LEU:HD23	2:w:215:LEU:HD11	1.91	0.51
2:G:127:LEU:HD11	2:G:142:GLU:OE2	2.10	0.51
3:O:96:LYS:O	3:O:100:GLN:HG2	2.09	0.51
3:P:248:ILE:HB	3:P:272:PHE:HB3	1.92	0.51
3:V:248:ILE:HB	3:V:272:PHE:HB3	1.92	0.51
2:Y:66:ILE:HG22	2:Y:69:LEU:HD13	1.93	0.51
3:a:88:PRO:HA	3:a:228:ILE:HD12	1.92	0.51
3:n:263:ALA:HA	2:r:106:ILE:HG23	1.91	0.51
3:t:58:TYR:HD2	2:x:105:ILE:HG21	1.74	0.51
3:A:113:VAL:HB	3:A:174:ALA:HB3	1.91	0.51
3:B:271:PRO:HD2	3:B:272:PHE:HB2	1.92	0.51
2:M:217:GLY:HA3	2:w:205:TYR:HE1	1.76	0.51
2:S:66:ILE:HG22	2:S:69:LEU:HD13	1.93	0.51
2:e:66:ILE:HG22	2:e:69:LEU:HD13	1.93	0.51
3:g:88:PRO:HA	3:g:228:ILE:HD12	1.92	0.51
3:m:88:PRO:HA	3:m:228:ILE:HD12	1.92	0.51
3:C:96:LYS:O	3:C:100:GLN:HG2	2.09	0.51
2:M:208:LEU:HD23	2:M:215:LEU:HD11	1.91	0.51
3:a:96:LYS:O	3:a:100:GLN:HG2	2.09	0.51
2:e:208:LEU:HD23	2:e:215:LEU:HD11	1.91	0.51
2:f:135:PRO:O	2:f:143:GLN:NE2	2.38	0.51
2:5:127:LEU:HD11	2:5:142:GLU:OE2	2.10	0.51
3:D:248:ILE:HB	3:D:272:PHE:HB3	1.92	0.51
3:V:58:TYR:HD2	2:Z:105:ILE:HG21	1.74	0.51
3:O:88:PRO:HA	3:O:228:ILE:HD12	1.92	0.51
1:Q:15:ILE:O	1:Q:18:ILE:HG22	2.11	0.51
1:W:15:ILE:O	1:W:18:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:248:ILE:HB	3:b:272:PHE:HB3	1.92	0.51
3:s:88:PRO:HA	3:s:228:ILE:HD12	1.92	0.51
3:D:113:VAL:HB	3:D:174:ALA:HB3	1.91	0.51
2:H:24:HIS:HD2	2:H:26:GLN:HE22	1.58	0.51
3:J:100:GLN:O	3:J:103:THR:OG1	2.24	0.51
2:M:127:LEU:HD11	2:M:142:GLU:OE2	2.10	0.51
2:T:135:PRO:O	2:T:143:GLN:NE2	2.38	0.51
1:c:15:ILE:O	1:c:18:ILE:HG22	2.11	0.51
1:o:15:ILE:O	1:o:18:ILE:HG22	2.11	0.51
2:q:127:LEU:HD11	2:q:142:GLU:OE2	2.10	0.51
2:r:196:ASP:OD1	2:r:199:LEU:N	2.42	0.51
2:w:127:LEU:HD11	2:w:142:GLU:OE2	2.10	0.51
3:U:221:VAL:O	3:U:224:VAL:HG12	2.11	0.51
3:b:263:ALA:HA	2:f:106:ILE:HG23	1.91	0.51
3:g:187:SER:O	3:g:190:THR:OG1	2.28	0.51
3:s:96:LYS:O	3:s:100:GLN:HG2	2.09	0.51
2:G:208:LEU:HD23	2:G:215:LEU:HD11	1.91	0.50
3:g:96:LYS:O	3:g:100:GLN:HG2	2.09	0.50
2:k:127:LEU:HD11	2:k:142:GLU:OE2	2.10	0.50
2:l:24:HIS:HD2	2:l:26:GLN:HE22	1.58	0.50
3:s:187:SER:O	3:s:190:THR:OG1	2.28	0.50
3:t:100:GLN:O	3:t:103:THR:OG1	2.24	0.50
2:x:196:ASP:OD1	2:x:199:LEU:N	2.42	0.50
2:5:66:ILE:HG22	2:5:69:LEU:HD13	1.93	0.50
2:5:208:LEU:HD23	2:5:215:LEU:HD11	1.91	0.50
2:G:66:ILE:HG22	2:G:69:LEU:HD13	1.93	0.50
3:O:221:VAL:O	3:O:224:VAL:HG12	2.11	0.50
2:r:24:HIS:HD2	2:r:26:GLN:HE22	1.58	0.50
3:t:322:GLU:O	3:t:326:LEU:HG	2.12	0.50
2:x:24:HIS:HD2	2:x:26:GLN:HE22	1.58	0.50
2:6:135:PRO:O	2:6:143:GLN:NE2	2.38	0.50
3:B:314:ASP:N	3:B:314:ASP:OD1	2.45	0.50
3:D:332:MET:O	3:D:336:VAL:HG12	2.12	0.50
2:M:66:ILE:HG22	2:M:69:LEU:HD13	1.93	0.50
3:O:314:ASP:OD1	3:O:314:ASP:N	2.45	0.50
3:a:221:VAL:O	3:a:224:VAL:HG12	2.11	0.50
2:f:24:HIS:HD2	2:f:26:GLN:HE22	1.58	0.50
2:f:196:ASP:OD1	2:f:199:LEU:N	2.42	0.50
3:A:248:ILE:HB	3:A:272:PHE:HB3	1.92	0.50
1:K:15:ILE:O	1:K:18:ILE:HG22	2.11	0.50
1:L:14:ALA:O	1:L:18:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:14:ALA:O	1:v:18:ILE:HG12	2.12	0.50
3:C:314:ASP:N	3:C:314:ASP:OD1	2.45	0.50
1:E:15:ILE:O	1:E:18:ILE:HG22	2.11	0.50
2:M:28:GLY:N	2:M:189:THR:HG22	2.22	0.50
2:Z:24:HIS:HD2	2:Z:26:GLN:HE22	1.58	0.50
3:m:314:ASP:N	3:m:314:ASP:OD1	2.45	0.50
3:t:248:ILE:HB	3:t:272:PHE:HB3	1.92	0.50
1:2:14:ALA:O	1:2:18:ILE:HG12	2.12	0.50
3:I:314:ASP:OD1	3:I:314:ASP:N	2.45	0.50
3:J:248:ILE:HB	3:J:272:PHE:HB3	1.92	0.50
2:T:24:HIS:HD2	2:T:26:GLN:HE22	1.58	0.50
3:a:314:ASP:OD1	3:a:314:ASP:N	2.45	0.50
3:m:246:LEU:HB3	3:m:250:ALA:HB3	1.94	0.50
3:s:246:LEU:HB3	3:s:250:ALA:HB3	1.94	0.50
2:H:28:GLY:N	2:H:189:THR:HG22	2.23	0.50
3:b:322:GLU:O	3:b:326:LEU:HG	2.12	0.50
3:h:77:THR:HA	3:h:80:VAL:HG12	1.93	0.50
2:l:196:ASP:OD1	2:l:199:LEU:N	2.42	0.50
3:s:82:ALA:HA	3:s:287:SER:HB2	1.93	0.50
3:I:149:LEU:HD23	3:I:170:LEU:HD23	1.94	0.50
3:g:246:LEU:HB3	3:g:250:ALA:HB3	1.93	0.50
3:h:248:ILE:HB	3:h:272:PHE:HB3	1.92	0.50
1:i:15:ILE:O	1:i:18:ILE:HG22	2.11	0.50
1:j:14:ALA:O	1:j:18:ILE:HG12	2.12	0.50
2:q:66:ILE:HG22	2:q:69:LEU:HD13	1.93	0.50
1:1:15:ILE:O	1:1:18:ILE:HG22	2.11	0.50
3:A:77:THR:HA	3:A:80:VAL:HG12	1.93	0.50
3:B:114:TYR:OH	3:B:205:ARG:NH2	2.45	0.50
3:C:149:LEU:HD23	3:C:170:LEU:HD23	1.94	0.50
3:C:152:PHE:HB2	3:C:170:LEU:HD21	1.94	0.50
3:C:221:VAL:O	3:C:224:VAL:HG12	2.11	0.50
1:F:14:ALA:O	1:F:18:ILE:HG12	2.12	0.50
3:I:70:LYS:O	3:I:74:THR:OG1	2.27	0.50
3:J:322:GLU:O	3:J:326:LEU:HG	2.11	0.50
2:Z:4:PHE:HD2	2:Z:7:VAL:HG11	1.77	0.50
3:g:82:ALA:HA	3:g:287:SER:HB2	1.93	0.50
3:t:77:THR:HA	3:t:80:VAL:HG12	1.93	0.50
2:w:66:ILE:HG22	2:w:69:LEU:HD13	1.93	0.50
2:x:4:PHE:HD2	2:x:7:VAL:HG11	1.77	0.50
3:A:332:MET:O	3:A:336:VAL:HG12	2.12	0.49
3:I:152:PHE:HB2	3:I:170:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:221:VAL:O	3:I:224:VAL:HG12	2.11	0.49
3:J:77:THR:HA	3:J:80:VAL:HG12	1.93	0.49
3:O:82:ALA:HA	3:O:287:SER:HB2	1.94	0.49
3:U:82:ALA:HA	3:U:287:SER:HB2	1.93	0.49
3:g:314:ASP:OD1	3:g:314:ASP:N	2.45	0.49
2:l:4:PHE:HD2	2:l:7:VAL:HG11	1.77	0.49
3:n:248:ILE:HB	3:n:272:PHE:HB3	1.92	0.49
1:p:14:ALA:O	1:p:18:ILE:HG12	2.12	0.49
3:B:152:PHE:HB2	3:B:170:LEU:HD21	1.94	0.49
3:D:77:THR:HA	3:D:80:VAL:HG12	1.93	0.49
2:H:202:ARG:HG2	2:r:197:ILE:CD1	2.41	0.49
3:O:152:PHE:HB2	3:O:170:LEU:HD21	1.94	0.49
3:U:152:PHE:HB2	3:U:170:LEU:HD21	1.94	0.49
2:Z:135:PRO:O	2:Z:143:GLN:NE2	2.38	0.49
2:k:66:ILE:HG22	2:k:69:LEU:HD13	1.93	0.49
3:m:152:PHE:HB2	3:m:170:LEU:HD21	1.94	0.49
3:n:105:TYR:CE1	3:n:109:PRO:HD3	2.47	0.49
2:r:135:PRO:O	2:r:143:GLN:NE2	2.38	0.49
1:u:15:ILE:O	1:u:18:ILE:HG22	2.11	0.49
2:6:24:HIS:HD2	2:6:26:GLN:HE22	1.58	0.49
3:B:221:VAL:O	3:B:224:VAL:HG12	2.11	0.49
2:H:87:ASP:OD1	2:H:87:ASP:N	2.36	0.49
3:I:82:ALA:HA	3:I:287:SER:HB2	1.93	0.49
2:N:24:HIS:HD2	2:N:26:GLN:HE22	1.58	0.49
3:O:284:ALA:HB3	3:O:327:LEU:HD23	1.94	0.49
2:T:28:GLY:N	2:T:189:THR:HG22	2.23	0.49
3:U:149:LEU:HD23	3:U:170:LEU:HD23	1.94	0.49
3:U:233:VAL:O	3:U:236:VAL:HB	2.13	0.49
3:V:273:LEU:HD21	3:V:339:TRP:HB2	1.94	0.49
3:a:82:ALA:HA	3:a:287:SER:HB2	1.93	0.49
3:a:152:PHE:HB2	3:a:170:LEU:HD21	1.94	0.49
1:d:14:ALA:O	1:d:18:ILE:HG12	2.12	0.49
3:g:152:PHE:HB2	3:g:170:LEU:HD21	1.94	0.49
3:h:105:TYR:CE1	3:h:109:PRO:HD3	2.47	0.49
3:h:332:MET:O	3:h:336:VAL:HG12	2.12	0.49
3:m:221:VAL:O	3:m:224:VAL:HG12	2.11	0.49
3:n:77:THR:HA	3:n:80:VAL:HG12	1.93	0.49
3:s:152:PHE:HB2	3:s:170:LEU:HD21	1.94	0.49
2:T:4:PHE:HD2	2:T:7:VAL:HG11	1.77	0.49
3:b:332:MET:O	3:b:336:VAL:HG12	2.12	0.49
3:n:332:MET:O	3:n:336:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:s:284:ALA:HB3	3:s:327:LEU:HD23	1.94	0.49
3:t:105:TYR:CE1	3:t:109:PRO:HD3	2.47	0.49
2:5:205:TYR:HE1	2:S:217:GLY:HA3	1.78	0.49
3:B:284:ALA:HB3	3:B:327:LEU:HD23	1.94	0.49
3:C:70:LYS:O	3:C:74:THR:OG1	2.27	0.49
3:I:233:VAL:O	3:I:236:VAL:HB	2.13	0.49
3:O:116:GLN:HB3	3:O:119:LEU:HB3	1.94	0.49
3:U:284:ALA:HB3	3:U:327:LEU:HD23	1.94	0.49
1:X:14:ALA:O	1:X:18:ILE:HG12	2.12	0.49
3:a:116:GLN:HB3	3:a:119:LEU:HB3	1.94	0.49
3:B:116:GLN:HB3	3:B:119:LEU:HB3	1.94	0.49
3:B:246:LEU:HB3	3:B:250:ALA:HB3	1.94	0.49
3:C:246:LEU:HB3	3:C:250:ALA:HB3	1.94	0.49
2:M:202:ARG:HG2	2:e:197:ILE:HG22	1.94	0.49
2:M:205:TYR:CE1	2:e:217:GLY:HA3	2.47	0.49
1:R:14:ALA:O	1:R:18:ILE:HG12	2.12	0.49
3:V:77:THR:HA	3:V:80:VAL:HG12	1.93	0.49
3:a:284:ALA:HB3	3:a:327:LEU:HD23	1.94	0.49
2:f:28:GLY:N	2:f:189:THR:HG22	2.23	0.49
3:g:114:TYR:OH	3:g:205:ARG:NH2	2.45	0.49
3:g:284:ALA:HB3	3:g:327:LEU:HD23	1.94	0.49
2:r:4:PHE:HD2	2:r:7:VAL:HG11	1.77	0.49
3:s:116:GLN:HB3	3:s:119:LEU:HB3	1.94	0.49
3:s:314:ASP:N	3:s:314:ASP:OD1	2.45	0.49
3:t:332:MET:O	3:t:336:VAL:HG12	2.12	0.49
3:B:82:ALA:HA	3:B:287:SER:HB2	1.93	0.49
3:C:82:ALA:HA	3:C:287:SER:HB2	1.93	0.49
3:C:233:VAL:O	3:C:236:VAL:HB	2.12	0.49
3:C:284:ALA:HB3	3:C:327:LEU:HD23	1.94	0.49
2:H:217:GLY:C	2:Z:205:TYR:HE1	2.20	0.49
3:J:273:LEU:HD21	3:J:339:TRP:HB2	1.94	0.49
3:O:233:VAL:O	3:O:236:VAL:HB	2.12	0.49
3:P:332:MET:O	3:P:336:VAL:HG12	2.12	0.49
3:U:114:TYR:OH	3:U:205:ARG:NH2	2.45	0.49
3:g:221:VAL:O	3:g:224:VAL:HG12	2.11	0.49
3:m:114:TYR:OH	3:m:205:ARG:NH2	2.45	0.49
3:B:149:LEU:HD23	3:B:170:LEU:HD23	1.94	0.49
3:C:79:MET:O	3:C:83:ILE:HG23	2.13	0.49
3:C:114:TYR:OH	3:C:205:ARG:NH2	2.45	0.49
3:D:273:LEU:HD21	3:D:339:TRP:HB2	1.94	0.49
3:I:246:LEU:HB3	3:I:250:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:273:LEU:HD21	3:P:339:TRP:HB2	1.94	0.49
2:S:133:ASN:HB3	2:S:137:GLN:NE2	2.28	0.49
3:U:116:GLN:HB3	3:U:119:LEU:HB3	1.94	0.49
3:b:77:THR:HA	3:b:80:VAL:HG12	1.93	0.49
3:m:284:ALA:HB3	3:m:327:LEU:HD23	1.94	0.49
3:s:233:VAL:O	3:s:236:VAL:HB	2.13	0.49
3:t:273:LEU:HD21	3:t:339:TRP:HB2	1.94	0.49
3:J:332:MET:O	3:J:336:VAL:HG12	2.12	0.49
2:N:207:MET:HB3	2:f:204:SER:HB3	1.95	0.49
3:V:332:MET:O	3:V:336:VAL:HG12	2.12	0.49
2:Z:74:VAL:HG23	2:Z:75:PRO:HD3	1.95	0.49
3:a:246:LEU:HB3	3:a:250:ALA:HB3	1.93	0.49
3:g:116:GLN:HB3	3:g:119:LEU:HB3	1.94	0.49
3:h:273:LEU:HD21	3:h:339:TRP:HB2	1.94	0.49
3:s:114:TYR:OH	3:s:205:ARG:NH2	2.45	0.49
3:s:221:VAL:O	3:s:224:VAL:HG12	2.11	0.49
2:5:217:GLY:HA3	2:k:205:TYR:HE1	1.77	0.49
3:B:91:CYS:HA	3:B:94:VAL:HG22	1.95	0.49
2:H:18:LEU:HD22	2:H:21:VAL:HG21	1.95	0.49
3:I:91:CYS:HA	3:I:94:VAL:HG22	1.95	0.49
3:P:105:TYR:CE1	3:P:109:PRO:HD3	2.47	0.49
3:U:314:ASP:N	3:U:314:ASP:OD1	2.45	0.49
2:Y:133:ASN:HB3	2:Y:137:GLN:NE2	2.28	0.49
2:Z:18:LEU:HD22	2:Z:21:VAL:HG21	1.95	0.49
2:e:133:ASN:HB3	2:e:137:GLN:NE2	2.28	0.49
3:g:268:ILE:C	3:g:270:ARG:H	2.20	0.49
3:g:270:ARG:HB3	3:g:271:PRO:CD	2.33	0.49
2:l:18:LEU:HD22	2:l:21:VAL:HG21	1.95	0.49
3:m:116:GLN:HB3	3:m:119:LEU:HB3	1.94	0.49
3:m:149:LEU:HD23	3:m:170:LEU:HD23	1.94	0.49
2:r:18:LEU:HD22	2:r:21:VAL:HG21	1.95	0.49
2:6:18:LEU:HD22	2:6:21:VAL:HG21	1.95	0.48
3:C:91:CYS:HA	3:C:94:VAL:HG22	1.95	0.48
3:I:79:MET:O	3:I:83:ILE:HG23	2.13	0.48
3:I:269:LEU:O	3:I:273:LEU:HG	2.12	0.48
2:f:4:PHE:HD2	2:f:7:VAL:HG11	1.77	0.48
2:f:74:VAL:HG23	2:f:75:PRO:HD3	1.95	0.48
3:g:233:VAL:O	3:g:236:VAL:HB	2.12	0.48
3:B:79:MET:O	3:B:83:ILE:HG23	2.13	0.48
3:I:114:TYR:OH	3:I:205:ARG:NH2	2.45	0.48
3:I:224:VAL:O	3:I:228:ILE:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:270:ARG:O	3:I:272:PHE:N	2.46	0.48
3:J:74:THR:O	3:J:77:THR:OG1	2.29	0.48
2:N:18:LEU:HD22	2:N:21:VAL:HG21	1.95	0.48
3:O:114:TYR:OH	3:O:205:ARG:NH2	2.45	0.48
3:O:149:LEU:HD23	3:O:170:LEU:HD23	1.94	0.48
3:U:224:VAL:O	3:U:228:ILE:HG23	2.13	0.48
3:a:187:SER:O	3:a:190:THR:OG1	2.28	0.48
3:g:149:LEU:HD23	3:g:170:LEU:HD23	1.94	0.48
2:x:18:LEU:HD22	2:x:21:VAL:HG21	1.95	0.48
3:I:284:ALA:HB3	3:I:327:LEU:HD23	1.94	0.48
2:T:18:LEU:HD22	2:T:21:VAL:HG21	1.95	0.48
3:B:233:VAL:O	3:B:236:VAL:HB	2.13	0.48
3:C:224:VAL:O	3:C:228:ILE:HG23	2.13	0.48
3:O:246:LEU:HB3	3:O:250:ALA:HB3	1.93	0.48
3:P:77:THR:HA	3:P:80:VAL:HG12	1.94	0.48
2:T:74:VAL:HG23	2:T:75:PRO:HD3	1.95	0.48
3:U:91:CYS:HA	3:U:94:VAL:HG22	1.95	0.48
2:f:18:LEU:HD22	2:f:21:VAL:HG21	1.95	0.48
3:m:79:MET:O	3:m:83:ILE:HG23	2.13	0.48
3:n:311:THR:OG1	3:n:312:LYS:N	2.46	0.48
3:s:79:MET:O	3:s:83:ILE:HG23	2.13	0.48
3:A:266:GLY:HA2	3:A:269:LEU:HD12	1.96	0.48
3:A:273:LEU:HD21	3:A:339:TRP:HB2	1.94	0.48
3:C:116:GLN:HB3	3:C:119:LEU:HB3	1.94	0.48
2:G:133:ASN:HB3	2:G:137:GLN:NE2	2.28	0.48
2:G:176:ILE:C	2:G:178:ARG:N	2.69	0.48
2:N:92:MET:HA	2:N:92:MET:HE3	1.96	0.48
3:O:187:SER:O	3:O:190:THR:OG1	2.28	0.48
3:U:187:SER:O	3:U:190:THR:OG1	2.28	0.48
3:a:91:CYS:HA	3:a:94:VAL:HG22	1.95	0.48
3:a:149:LEU:HD23	3:a:170:LEU:HD23	1.94	0.48
3:b:273:LEU:HD21	3:b:339:TRP:HB2	1.94	0.48
3:g:224:VAL:O	3:g:228:ILE:HG23	2.13	0.48
3:n:117:LYS:NZ	3:n:169:PRO:O	2.44	0.48
3:n:273:LEU:HD21	3:n:339:TRP:HB2	1.94	0.48
3:s:224:VAL:O	3:s:228:ILE:HG23	2.13	0.48
3:D:266:GLY:HA2	3:D:269:LEU:HD12	1.96	0.48
3:I:116:GLN:HB3	3:I:119:LEU:HB3	1.94	0.48
3:J:266:GLY:HA2	3:J:269:LEU:HD12	1.96	0.48
3:U:246:LEU:HB3	3:U:250:ALA:HB3	1.94	0.48
3:a:233:VAL:O	3:a:236:VAL:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:88:HIS:NE2	2:e:143:GLN:OE1	2.47	0.48
2:l:74:VAL:HG23	2:l:75:PRO:HD3	1.95	0.48
3:m:224:VAL:O	3:m:228:ILE:HG23	2.13	0.48
2:r:74:VAL:HG23	2:r:75:PRO:HD3	1.95	0.48
2:6:28:GLY:N	2:6:189:THR:HG22	2.23	0.48
3:B:70:LYS:O	3:B:74:THR:OG1	2.27	0.48
3:I:302:VAL:HG12	3:J:220:LEU:HD12	1.96	0.48
2:N:4:PHE:HD2	2:N:7:VAL:HG11	1.77	0.48
3:U:234:ALA:HB2	3:V:83:ILE:HG21	1.95	0.48
3:h:200:GLY:C	3:h:202:ASP:H	2.22	0.48
3:n:200:GLY:C	3:n:202:ASP:H	2.22	0.48
2:q:133:ASN:HB3	2:q:137:GLN:NE2	2.28	0.48
2:q:181:GLU:OE2	2:q:205:TYR:OH	2.23	0.48
3:s:91:CYS:HA	3:s:94:VAL:HG22	1.95	0.48
2:5:133:ASN:HB3	2:5:137:GLN:NE2	2.28	0.48
2:6:92:MET:HA	2:6:92:MET:HE3	1.96	0.48
2:M:133:ASN:HB3	2:M:137:GLN:NE2	2.28	0.48
3:O:91:CYS:HA	3:O:94:VAL:HG22	1.95	0.48
3:P:200:GLY:C	3:P:202:ASP:H	2.22	0.48
2:S:88:HIS:NE2	2:S:143:GLN:OE1	2.47	0.48
2:S:204:SER:O	2:k:218:GLY:CA	2.33	0.48
3:V:200:GLY:C	3:V:202:ASP:H	2.22	0.48
3:b:200:GLY:C	3:b:202:ASP:H	2.22	0.48
3:g:234:ALA:HB2	3:h:83:ILE:HG21	1.95	0.48
3:h:311:THR:OG1	3:h:312:LYS:N	2.46	0.48
3:m:233:VAL:O	3:m:236:VAL:HB	2.12	0.48
3:s:149:LEU:HD23	3:s:170:LEU:HD23	1.94	0.48
3:s:234:ALA:HB2	3:t:83:ILE:HG21	1.95	0.48
3:t:200:GLY:C	3:t:202:ASP:H	2.22	0.48
3:D:200:GLY:C	3:D:202:ASP:H	2.22	0.48
3:O:224:VAL:O	3:O:228:ILE:HG23	2.13	0.48
2:T:92:MET:HA	2:T:92:MET:HE3	1.96	0.48
3:a:79:MET:O	3:a:83:ILE:HG23	2.13	0.48
3:a:114:TYR:OH	3:a:205:ARG:NH2	2.45	0.48
3:b:105:TYR:CE1	3:b:109:PRO:HD3	2.47	0.48
2:f:92:MET:HA	2:f:92:MET:HE3	1.96	0.48
3:s:70:LYS:O	3:s:74:THR:OG1	2.27	0.48
2:x:74:VAL:HG23	2:x:75:PRO:HD3	1.95	0.48
2:6:4:PHE:HD2	2:6:7:VAL:HG11	1.77	0.48
3:A:83:ILE:HG21	3:C:234:ALA:HB2	1.95	0.48
3:A:200:GLY:C	3:A:202:ASP:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:220:LEU:HD12	3:C:302:VAL:HG12	1.96	0.48
2:G:177:LEU:HD21	2:G:203:ARG:HE	1.79	0.48
3:a:70:LYS:HD2	3:a:70:LYS:HA	1.71	0.48
3:g:91:CYS:HA	3:g:94:VAL:HG22	1.95	0.48
3:m:88:PRO:HD3	3:m:231:LEU:CD2	2.44	0.48
3:m:302:VAL:HG12	3:n:220:LEU:HD12	1.96	0.48
3:t:239:VAL:O	3:t:243:SER:OG	2.21	0.48
3:A:105:TYR:CE1	3:A:109:PRO:HD3	2.47	0.47
3:B:88:PRO:HD3	3:B:231:LEU:CD2	2.44	0.47
3:B:224:VAL:O	3:B:228:ILE:HG23	2.13	0.47
3:C:88:PRO:HD3	3:C:231:LEU:CD2	2.44	0.47
3:D:240:ILE:O	3:D:244:VAL:HG22	2.14	0.47
2:H:92:MET:HA	2:H:92:MET:HE3	1.96	0.47
3:I:234:ALA:HB2	3:J:83:ILE:HG21	1.95	0.47
3:J:200:GLY:C	3:J:202:ASP:H	2.22	0.47
2:N:127:LEU:HD23	2:N:127:LEU:HA	1.74	0.47
3:O:88:PRO:HD3	3:O:231:LEU:CD2	2.44	0.47
3:a:88:PRO:HD3	3:a:231:LEU:CD2	2.44	0.47
3:b:266:GLY:HA2	3:b:269:LEU:HD12	1.96	0.47
3:g:79:MET:O	3:g:83:ILE:HG23	2.13	0.47
3:n:266:GLY:HA2	3:n:269:LEU:HD12	1.96	0.47
2:q:88:HIS:NE2	2:q:143:GLN:OE1	2.47	0.47
2:w:88:HIS:NE2	2:w:143:GLN:OE1	2.47	0.47
2:w:133:ASN:HB3	2:w:137:GLN:NE2	2.28	0.47
3:A:240:ILE:O	3:A:244:VAL:HG22	2.15	0.47
2:M:88:HIS:NE2	2:M:143:GLN:OE1	2.47	0.47
3:P:311:THR:OG1	3:P:312:LYS:N	2.46	0.47
3:U:79:MET:O	3:U:83:ILE:HG23	2.13	0.47
2:k:90:LEU:HD21	2:k:146:VAL:HG12	1.97	0.47
3:m:234:ALA:HB2	3:n:83:ILE:HG21	1.95	0.47
3:t:311:THR:OG1	3:t:312:LYS:N	2.46	0.47
2:w:90:LEU:HD21	2:w:146:VAL:HG12	1.97	0.47
3:A:284:ALA:O	3:A:288:LEU:HB2	2.15	0.47
3:D:111:ILE:HD12	3:D:176:VAL:HB	1.96	0.47
2:G:88:HIS:NE2	2:G:143:GLN:OE1	2.47	0.47
2:H:4:PHE:HD2	2:H:7:VAL:HG11	1.77	0.47
3:J:111:ILE:HD12	3:J:176:VAL:HB	1.97	0.47
3:J:284:ALA:O	3:J:288:LEU:HB2	2.15	0.47
3:O:79:MET:O	3:O:83:ILE:HG23	2.13	0.47
3:U:149:LEU:HA	3:U:170:LEU:HD23	1.97	0.47
3:U:268:ILE:C	3:U:270:ARG:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:88:HIS:NE2	2:Y:143:GLN:OE1	2.47	0.47
3:a:224:VAL:O	3:a:228:ILE:HG23	2.13	0.47
2:f:3:ARG:NH1	2:f:5:GLU:OE2	2.47	0.47
3:h:111:ILE:HD12	3:h:176:VAL:HB	1.97	0.47
2:k:133:ASN:HB3	2:k:137:GLN:NE2	2.28	0.47
2:r:3:ARG:NH1	2:r:5:GLU:OE2	2.47	0.47
3:t:111:ILE:HD12	3:t:176:VAL:HB	1.97	0.47
2:5:88:HIS:NE2	2:5:143:GLN:OE1	2.47	0.47
3:A:111:ILE:HD12	3:A:176:VAL:HB	1.97	0.47
3:B:234:ALA:HB2	3:D:83:ILE:HG21	1.95	0.47
2:H:135:PRO:O	2:H:143:GLN:NE2	2.38	0.47
2:N:74:VAL:HG23	2:N:75:PRO:HD3	1.95	0.47
3:U:88:PRO:HD3	3:U:231:LEU:CD2	2.44	0.47
3:h:228:ILE:HG12	3:h:232:MET:SD	2.55	0.47
2:k:88:HIS:NE2	2:k:143:GLN:OE1	2.47	0.47
3:n:284:ALA:O	3:n:288:LEU:HB2	2.15	0.47
3:t:228:ILE:HG12	3:t:232:MET:SD	2.55	0.47
2:x:3:ARG:NH1	2:x:5:GLU:OE2	2.47	0.47
2:6:74:VAL:HG23	2:6:75:PRO:HD3	1.95	0.47
3:D:322:GLU:O	3:D:326:LEU:HG	2.15	0.47
3:J:240:ILE:O	3:J:244:VAL:HG22	2.15	0.47
3:O:149:LEU:HA	3:O:170:LEU:HD23	1.97	0.47
3:O:234:ALA:HB2	3:P:83:ILE:HG21	1.95	0.47
3:P:266:GLY:HA2	3:P:269:LEU:HD12	1.96	0.47
3:P:284:ALA:O	3:P:288:LEU:HB2	2.15	0.47
3:V:111:ILE:HD12	3:V:176:VAL:HB	1.97	0.47
3:V:228:ILE:HG12	3:V:232:MET:SD	2.55	0.47
2:Z:92:MET:HE3	2:Z:92:MET:HA	1.96	0.47
3:g:88:PRO:HD3	3:g:231:LEU:CD2	2.44	0.47
3:B:57:ARG:HE	3:B:57:ARG:HB2	1.57	0.47
3:B:302:VAL:HG12	3:D:220:LEU:HD12	1.96	0.47
2:G:90:LEU:HD21	2:G:146:VAL:HG12	1.97	0.47
2:H:74:VAL:HG23	2:H:75:PRO:HD3	1.95	0.47
3:I:88:PRO:HD3	3:I:231:LEU:CD2	2.44	0.47
2:T:3:ARG:NH1	2:T:5:GLU:OE2	2.47	0.47
3:V:311:THR:OG1	3:V:312:LYS:N	2.46	0.47
3:a:149:LEU:HA	3:a:170:LEU:HD23	1.97	0.47
3:a:302:VAL:HG12	3:b:220:LEU:HD12	1.96	0.47
3:b:284:ALA:O	3:b:288:LEU:HB2	2.15	0.47
2:e:170:ASP:CG	2:x:202:ARG:NH2	2.73	0.47
3:g:149:LEU:HA	3:g:170:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:284:ALA:O	3:h:288:LEU:HB2	2.15	0.47
2:q:177:LEU:HD22	2:q:199:LEU:HG	1.96	0.47
3:s:149:LEU:HA	3:s:170:LEU:HD23	1.97	0.47
2:H:202:ARG:C	2:r:207:MET:HE1	2.40	0.47
2:N:28:GLY:N	2:N:189:THR:HG22	2.23	0.47
2:N:186:VAL:HG23	2:N:187:GLY:H	1.80	0.47
3:P:111:ILE:HD12	3:P:176:VAL:HB	1.96	0.47
3:V:284:ALA:O	3:V:288:LEU:HB2	2.15	0.47
3:b:111:ILE:HD12	3:b:176:VAL:HB	1.96	0.47
3:b:228:ILE:HG12	3:b:232:MET:SD	2.55	0.47
3:b:240:ILE:O	3:b:244:VAL:HG22	2.15	0.47
3:g:70:LYS:O	3:g:74:THR:OG1	2.27	0.47
3:g:302:VAL:HG12	3:h:220:LEU:HD12	1.96	0.47
2:k:177:LEU:HD22	2:k:199:LEU:HG	1.96	0.47
2:l:92:MET:HA	2:l:92:MET:HE3	1.96	0.47
2:l:186:VAL:HG23	2:l:187:GLY:H	1.80	0.47
3:n:111:ILE:HD12	3:n:176:VAL:HB	1.97	0.47
3:n:228:ILE:HG12	3:n:232:MET:SD	2.55	0.47
3:n:240:ILE:O	3:n:244:VAL:HG22	2.15	0.47
2:r:92:MET:HA	2:r:92:MET:HE3	1.96	0.47
3:t:240:ILE:O	3:t:244:VAL:HG22	2.15	0.47
2:w:177:LEU:HD22	2:w:199:LEU:HG	1.97	0.47
2:x:186:VAL:HG23	2:x:187:GLY:H	1.80	0.47
3:B:56:VAL:HG13	3:B:274:TYR:HE2	1.80	0.47
2:H:3:ARG:NH1	2:H:5:GLU:OE2	2.47	0.47
2:S:177:LEU:HD22	2:S:199:LEU:HG	1.96	0.47
3:m:91:CYS:HA	3:m:94:VAL:HG22	1.95	0.47
3:m:149:LEU:HA	3:m:170:LEU:HD23	1.97	0.47
2:q:90:LEU:HD21	2:q:146:VAL:HG12	1.97	0.47
3:t:284:ALA:O	3:t:288:LEU:HB2	2.15	0.47
2:x:92:MET:HA	2:x:92:MET:HE3	1.96	0.47
3:A:228:ILE:HG12	3:A:232:MET:SD	2.55	0.47
3:D:192:ARG:HD3	3:D:192:ARG:HA	1.76	0.47
3:D:228:ILE:HG12	3:D:232:MET:SD	2.55	0.47
3:D:284:ALA:O	3:D:288:LEU:HB2	2.15	0.47
3:J:105:TYR:CE1	3:J:109:PRO:HD3	2.47	0.47
2:N:3:ARG:NH1	2:N:5:GLU:OE2	2.47	0.47
2:S:161:ALA:HB3	2:S:192:MET:HA	1.97	0.47
2:Y:181:GLU:OE2	2:Y:205:TYR:OH	2.23	0.47
3:a:234:ALA:HB2	3:b:83:ILE:HG21	1.95	0.47
2:l:3:ARG:NH1	2:l:5:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:115:ARG:O	2:l:119:SER:OG	2.31	0.47
3:s:56:VAL:HG13	3:s:274:TYR:HE2	1.80	0.47
3:t:266:GLY:HA2	3:t:269:LEU:HD12	1.96	0.47
2:w:11:TYR:OH	2:w:52:GLU:OE2	2.28	0.47
3:C:56:VAL:HG13	3:C:274:TYR:HE2	1.80	0.47
3:C:57:ARG:HE	3:C:57:ARG:HB2	1.57	0.47
2:G:161:ALA:HB3	2:G:192:MET:HA	1.97	0.47
3:O:56:VAL:HG13	3:O:274:TYR:HE2	1.80	0.47
3:V:322:GLU:O	3:V:326:LEU:HG	2.15	0.47
2:Y:90:LEU:HD21	2:Y:146:VAL:HG12	1.97	0.47
2:Z:3:ARG:NH1	2:Z:5:GLU:OE2	2.47	0.47
3:a:70:LYS:O	3:a:74:THR:OG1	2.27	0.47
3:b:114:TYR:HE1	3:b:173:VAL:HG13	1.80	0.47
2:e:161:ALA:HB3	2:e:192:MET:HA	1.97	0.47
3:h:240:ILE:O	3:h:244:VAL:HG22	2.14	0.47
3:h:266:GLY:HA2	3:h:269:LEU:HD12	1.96	0.47
3:m:268:ILE:C	3:m:270:ARG:H	2.23	0.47
3:s:88:PRO:HD3	3:s:231:LEU:CD2	2.44	0.47
2:5:161:ALA:HB3	2:5:192:MET:HA	1.97	0.46
2:6:3:ARG:NH1	2:6:5:GLU:OE2	2.47	0.46
3:C:329:VAL:HG12	3:C:333:ILE:HD11	1.97	0.46
3:D:140:VAL:HG22	3:D:176:VAL:HG22	1.97	0.46
2:G:130:LYS:HD2	2:G:138:LEU:HD22	1.97	0.46
3:I:329:VAL:HG12	3:I:333:ILE:HD11	1.97	0.46
3:J:114:TYR:HE1	3:J:173:VAL:HG13	1.80	0.46
2:M:51:ILE:HA	2:M:78:ARG:HH22	1.77	0.46
2:M:90:LEU:HD21	2:M:146:VAL:HG12	1.97	0.46
3:O:302:VAL:HG12	3:P:220:LEU:HD12	1.96	0.46
3:V:240:ILE:O	3:V:244:VAL:HG22	2.15	0.46
2:Y:177:LEU:HD22	2:Y:199:LEU:HG	1.96	0.46
3:m:297:ARG:O	3:m:300:SER:OG	2.31	0.46
2:6:186:VAL:HG23	2:6:187:GLY:H	1.80	0.46
2:M:161:ALA:HB3	2:M:192:MET:HA	1.97	0.46
3:O:70:LYS:O	3:O:74:THR:OG1	2.27	0.46
3:P:228:ILE:HG12	3:P:232:MET:SD	2.55	0.46
2:S:90:LEU:HD21	2:S:146:VAL:HG12	1.97	0.46
2:S:130:LYS:HD2	2:S:138:LEU:HD22	1.97	0.46
3:U:297:ARG:O	3:U:300:SER:OG	2.31	0.46
3:V:266:GLY:HA2	3:V:269:LEU:HD12	1.96	0.46
3:a:56:VAL:HG13	3:a:274:TYR:HE2	1.80	0.46
3:g:56:VAL:HG13	3:g:274:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:114:TYR:HE1	3:n:173:VAL:HG13	1.80	0.46
2:r:186:VAL:HG23	2:r:187:GLY:H	1.80	0.46
3:A:114:TYR:HE1	3:A:173:VAL:HG13	1.80	0.46
3:A:140:VAL:HG22	3:A:176:VAL:HG22	1.97	0.46
3:A:227:MET:HE3	3:C:297:ARG:NH2	2.30	0.46
3:B:93:MET:HA	3:B:96:LYS:HE3	1.98	0.46
3:I:56:VAL:HG13	3:I:274:TYR:HE2	1.80	0.46
3:I:57:ARG:HE	3:I:57:ARG:HB2	1.57	0.46
2:M:130:LYS:HD2	2:M:138:LEU:HD22	1.97	0.46
3:P:114:TYR:HE1	3:P:173:VAL:HG13	1.80	0.46
3:P:240:ILE:O	3:P:244:VAL:HG22	2.15	0.46
3:V:100:GLN:O	3:V:103:THR:OG1	2.24	0.46
1:W:33:SER:O	1:W:33:SER:OG	2.33	0.46
2:Z:104:LEU:HD13	2:Z:114:ILE:HA	1.98	0.46
3:a:297:ARG:NH2	3:b:227:MET:HE3	2.31	0.46
2:e:130:LYS:HD2	2:e:138:LEU:HD22	1.97	0.46
2:e:173:SER:O	2:e:177:LEU:HB3	2.14	0.46
3:h:114:TYR:HE1	3:h:173:VAL:HG13	1.80	0.46
2:k:161:ALA:HB3	2:k:192:MET:HA	1.97	0.46
3:t:114:TYR:HE1	3:t:173:VAL:HG13	1.80	0.46
2:5:130:LYS:HD2	2:5:138:LEU:HD22	1.97	0.46
3:B:149:LEU:HA	3:B:170:LEU:HD23	1.97	0.46
3:B:297:ARG:NH2	3:D:227:MET:HE3	2.31	0.46
3:C:93:MET:HA	3:C:96:LYS:HE3	1.98	0.46
3:I:149:LEU:HA	3:I:170:LEU:HD23	1.97	0.46
3:O:325:LEU:O	3:O:329:VAL:HG23	2.16	0.46
2:Y:161:ALA:HB3	2:Y:192:MET:HA	1.97	0.46
2:Z:186:VAL:HG23	2:Z:187:GLY:H	1.80	0.46
3:a:325:LEU:O	3:a:329:VAL:HG23	2.16	0.46
3:s:84:SER:HB2	3:s:235:ALA:HB2	1.97	0.46
3:s:302:VAL:HG12	3:t:220:LEU:HD12	1.96	0.46
3:t:74:THR:O	3:t:77:THR:OG1	2.29	0.46
3:A:117:LYS:NZ	3:A:169:PRO:O	2.44	0.46
3:B:84:SER:HB2	3:B:235:ALA:HB2	1.97	0.46
3:J:140:VAL:HG22	3:J:176:VAL:HG22	1.97	0.46
3:O:57:ARG:HE	3:O:57:ARG:HB2	1.57	0.46
3:O:77:THR:HA	3:O:80:VAL:HG12	1.98	0.46
3:P:140:VAL:HG22	3:P:176:VAL:HG22	1.97	0.46
3:P:322:GLU:O	3:P:326:LEU:HG	2.16	0.46
3:U:325:LEU:O	3:U:329:VAL:HG23	2.16	0.46
3:V:326:LEU:HA	3:V:329:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:130:LYS:HD3	2:Y:133:ASN:ND2	2.31	0.46
2:Y:130:LYS:HD2	2:Y:138:LEU:HD22	1.97	0.46
3:a:270:ARG:HB3	3:a:271:PRO:CD	2.33	0.46
2:e:130:LYS:HD3	2:e:133:ASN:ND2	2.31	0.46
2:k:141:GLY:HA3	2:k:172:LEU:HD23	1.98	0.46
3:s:297:ARG:NH2	3:t:227:MET:HE3	2.30	0.46
2:5:90:LEU:HD21	2:5:146:VAL:HG12	1.97	0.46
3:B:325:LEU:O	3:B:329:VAL:HG23	2.16	0.46
3:B:329:VAL:HG12	3:B:333:ILE:HD11	1.97	0.46
3:C:84:SER:HB2	3:C:235:ALA:HB2	1.97	0.46
3:C:149:LEU:HA	3:C:170:LEU:HD23	1.97	0.46
3:I:93:MET:HA	3:I:96:LYS:HE3	1.98	0.46
3:J:228:ILE:HG12	3:J:232:MET:SD	2.55	0.46
3:V:140:VAL:HG22	3:V:176:VAL:HG22	1.97	0.46
3:a:84:SER:HB2	3:a:235:ALA:HB2	1.97	0.46
2:f:104:LEU:HD13	2:f:114:ILE:HA	1.98	0.46
3:g:84:SER:HB2	3:g:235:ALA:HB2	1.97	0.46
3:h:239:VAL:O	3:h:243:SER:OG	2.21	0.46
2:l:104:LEU:HD13	2:l:114:ILE:HA	1.98	0.46
3:A:192:ARG:HD3	3:A:192:ARG:HA	1.76	0.46
3:B:85:LEU:HG	3:B:326:LEU:HD11	1.98	0.46
3:D:230:VAL:HA	3:D:233:VAL:HG22	1.98	0.46
3:I:84:SER:HB2	3:I:235:ALA:HB2	1.97	0.46
3:I:297:ARG:NH2	3:J:227:MET:HE3	2.31	0.46
3:O:268:ILE:C	3:O:270:ARG:H	2.24	0.46
3:P:255:ILE:HG23	3:P:268:ILE:HD12	1.98	0.46
2:T:104:LEU:HD13	2:T:114:ILE:HA	1.98	0.46
3:U:56:VAL:HG13	3:U:274:TYR:HE2	1.80	0.46
3:U:77:THR:HA	3:U:80:VAL:HG12	1.98	0.46
3:b:140:VAL:HG22	3:b:176:VAL:HG22	1.97	0.46
3:b:255:ILE:HG23	3:b:268:ILE:HD12	1.98	0.46
3:b:326:LEU:HA	3:b:329:VAL:HG12	1.98	0.46
2:e:90:LEU:HD21	2:e:146:VAL:HG12	1.97	0.46
3:m:56:VAL:HG13	3:m:274:TYR:HE2	1.80	0.46
3:n:322:GLU:O	3:n:326:LEU:HG	2.15	0.46
2:q:141:GLY:HA3	2:q:172:LEU:HD23	1.98	0.46
2:w:161:ALA:HB3	2:w:192:MET:HA	1.97	0.46
2:x:104:LEU:HD13	2:x:114:ILE:HA	1.98	0.46
3:B:234:ALA:HB2	3:D:83:ILE:HD12	1.98	0.46
3:C:85:LEU:HG	3:C:326:LEU:HD11	1.98	0.46
2:G:130:LYS:HD3	2:G:133:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:205:TYR:CE1	2:Y:217:GLY:C	2.93	0.46
3:I:85:LEU:HG	3:I:326:LEU:HD11	1.98	0.46
2:N:104:LEU:HD13	2:N:114:ILE:HA	1.98	0.46
3:O:297:ARG:NH2	3:P:227:MET:HE3	2.31	0.46
2:S:130:LYS:HD3	2:S:133:ASN:ND2	2.31	0.46
2:S:205:TYR:HE1	2:k:217:GLY:HA3	1.79	0.46
2:k:130:LYS:HD3	2:k:133:ASN:ND2	2.31	0.46
3:m:84:SER:HB2	3:m:235:ALA:HB2	1.97	0.46
2:q:161:ALA:HB3	2:q:192:MET:HA	1.98	0.46
3:s:91:CYS:HA	3:s:94:VAL:CG2	2.46	0.46
3:s:325:LEU:O	3:s:329:VAL:HG23	2.16	0.46
2:w:130:LYS:HD3	2:w:133:ASN:ND2	2.31	0.46
2:w:130:LYS:HD2	2:w:138:LEU:HD22	1.97	0.46
2:6:127:LEU:HD23	2:6:127:LEU:HA	1.74	0.46
3:A:230:VAL:HA	3:A:233:VAL:HG22	1.98	0.46
2:G:125:VAL:HB	2:G:145:ARG:HG2	1.98	0.46
2:H:186:VAL:HG23	2:H:187:GLY:H	1.80	0.46
3:I:234:ALA:HB2	3:J:83:ILE:HD12	1.98	0.46
2:T:186:VAL:HG23	2:T:187:GLY:H	1.80	0.46
3:U:249:PHE:HB2	3:U:252:ARG:HB3	1.98	0.46
3:U:302:VAL:HG12	3:V:220:LEU:HD12	1.96	0.46
3:V:255:ILE:HG23	3:V:268:ILE:HD12	1.98	0.46
2:Y:125:VAL:HB	2:Y:145:ARG:HG2	1.98	0.46
2:w:141:GLY:HA3	2:w:172:LEU:HD23	1.98	0.46
2:5:177:LEU:HD22	2:5:199:LEU:HG	1.96	0.46
2:5:204:SER:O	2:S:218:GLY:CA	2.32	0.46
3:A:232:MET:HG2	3:A:232:MET:H	1.60	0.46
3:A:322:GLU:O	3:A:326:LEU:HG	2.16	0.46
3:B:187:SER:O	3:B:190:THR:OG1	2.28	0.46
3:D:117:LYS:NZ	3:D:169:PRO:O	2.44	0.46
2:H:104:LEU:HD13	2:H:114:ILE:HA	1.98	0.46
3:J:230:VAL:HA	3:J:233:VAL:HG22	1.98	0.46
2:M:204:SER:HB3	2:e:207:MET:HE3	1.97	0.46
3:O:84:SER:HB2	3:O:235:ALA:HB2	1.97	0.46
3:P:326:LEU:HA	3:P:329:VAL:HG12	1.98	0.46
2:T:127:LEU:HA	2:T:127:LEU:HD23	1.74	0.46
3:U:95:TYR:CE1	3:U:221:VAL:HG23	2.51	0.46
3:g:91:CYS:HA	3:g:94:VAL:CG2	2.46	0.46
3:g:297:ARG:NH2	3:h:227:MET:HE3	2.30	0.46
2:r:104:LEU:HD13	2:r:114:ILE:HA	1.98	0.46
2:5:141:GLY:HA3	2:5:172:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:104:LEU:HD13	2:6:114:ILE:HA	1.98	0.45
3:I:187:SER:O	3:I:190:THR:OG1	2.28	0.45
3:O:329:VAL:HG12	3:O:333:ILE:HD11	1.98	0.45
3:P:230:VAL:HA	3:P:233:VAL:HG22	1.98	0.45
2:S:125:VAL:HB	2:S:145:ARG:HG2	1.98	0.45
3:U:70:LYS:HA	3:U:70:LYS:HD2	1.71	0.45
3:U:84:SER:HB2	3:U:235:ALA:HB2	1.97	0.45
3:a:77:THR:HA	3:a:80:VAL:HG12	1.98	0.45
2:e:141:GLY:HA3	2:e:172:LEU:HD23	1.98	0.45
3:h:322:GLU:O	3:h:326:LEU:HG	2.16	0.45
3:m:85:LEU:HG	3:m:326:LEU:HD11	1.98	0.45
3:m:325:LEU:O	3:m:329:VAL:HG23	2.16	0.45
3:A:83:ILE:HD12	3:C:234:ALA:HB2	1.98	0.45
3:B:91:CYS:HA	3:B:94:VAL:CG2	2.46	0.45
3:C:91:CYS:HA	3:C:94:VAL:CG2	2.46	0.45
3:C:187:SER:O	3:C:190:THR:OG1	2.28	0.45
3:D:326:LEU:HA	3:D:329:VAL:HG12	1.98	0.45
2:M:130:LYS:HD3	2:M:133:ASN:ND2	2.31	0.45
2:M:141:GLY:HA3	2:M:172:LEU:HD23	1.98	0.45
3:V:114:TYR:HE1	3:V:173:VAL:HG13	1.81	0.45
2:Y:141:GLY:HA3	2:Y:172:LEU:HD23	1.98	0.45
2:f:186:VAL:HG23	2:f:187:GLY:H	1.80	0.45
3:g:83:ILE:HG13	3:g:84:SER:N	2.32	0.45
3:g:325:LEU:O	3:g:329:VAL:HG23	2.16	0.45
2:l:83:MET:HE3	2:l:83:MET:HB2	1.89	0.45
3:m:70:LYS:O	3:m:74:THR:OG1	2.27	0.45
2:q:130:LYS:HD2	2:q:138:LEU:HD22	1.97	0.45
2:5:135:PRO:O	2:5:143:GLN:NE2	2.50	0.45
3:B:77:THR:HA	3:B:80:VAL:HG12	1.98	0.45
3:D:114:TYR:HE1	3:D:173:VAL:HG13	1.80	0.45
3:J:311:THR:OG1	3:J:312:LYS:N	2.46	0.45
2:N:92:MET:HE1	2:N:135:PRO:HB2	1.99	0.45
3:U:93:MET:HA	3:U:96:LYS:HE3	1.98	0.45
3:U:329:VAL:HG12	3:U:333:ILE:HD11	1.97	0.45
3:V:227:MET:O	3:V:230:VAL:HG12	2.16	0.45
3:b:311:THR:OG1	3:b:312:LYS:N	2.46	0.45
3:g:85:LEU:HG	3:g:326:LEU:HD11	1.98	0.45
3:h:140:VAL:HG22	3:h:176:VAL:HG22	1.97	0.45
2:k:130:LYS:HD2	2:k:138:LEU:HD22	1.97	0.45
3:m:83:ILE:HG13	3:m:84:SER:N	2.32	0.45
3:n:227:MET:O	3:n:230:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:130:LYS:HD3	2:q:133:ASN:ND2	2.31	0.45
2:r:92:MET:HE1	2:r:135:PRO:HB2	1.99	0.45
2:5:130:LYS:HD3	2:5:133:ASN:ND2	2.31	0.45
2:6:92:MET:HE1	2:6:135:PRO:HB2	1.99	0.45
3:B:263:ALA:HA	2:G:106:ILE:HG23	1.98	0.45
2:G:177:LEU:HD22	2:G:199:LEU:HG	1.98	0.45
3:P:259:LYS:HD3	3:P:268:ILE:HD13	1.99	0.45
2:T:92:MET:HE1	2:T:135:PRO:HB2	1.99	0.45
3:U:91:CYS:HA	3:U:94:VAL:CG2	2.46	0.45
2:Z:92:MET:HE1	2:Z:135:PRO:HB2	1.99	0.45
3:b:259:LYS:HD3	3:b:268:ILE:HD13	1.99	0.45
3:g:270:ARG:C	3:g:272:PHE:N	2.75	0.45
3:m:93:MET:HA	3:m:96:LYS:HE3	1.98	0.45
3:n:140:VAL:HG22	3:n:176:VAL:HG22	1.97	0.45
2:r:28:GLY:N	2:r:189:THR:HG22	2.23	0.45
3:s:83:ILE:HG13	3:s:84:SER:N	2.32	0.45
3:t:140:VAL:HG22	3:t:176:VAL:HG22	1.97	0.45
2:5:11:TYR:OH	2:5:52:GLU:OE2	2.28	0.45
2:5:125:VAL:HB	2:5:145:ARG:HG2	1.98	0.45
3:C:288:LEU:HD12	3:C:326:LEU:HD23	1.99	0.45
3:I:91:CYS:HA	3:I:94:VAL:CG2	2.46	0.45
3:I:288:LEU:HD12	3:I:326:LEU:HD23	1.99	0.45
3:I:325:LEU:O	3:I:329:VAL:HG23	2.16	0.45
3:J:326:LEU:HA	3:J:329:VAL:HG12	1.98	0.45
2:M:135:PRO:O	2:M:143:GLN:NE2	2.50	0.45
3:O:95:TYR:CE1	3:O:221:VAL:HG23	2.51	0.45
3:O:297:ARG:O	3:O:300:SER:OG	2.31	0.45
3:V:230:VAL:HA	3:V:233:VAL:HG22	1.98	0.45
3:a:93:MET:HA	3:a:96:LYS:HE3	1.98	0.45
3:a:329:VAL:HG12	3:a:333:ILE:HD11	1.98	0.45
3:h:227:MET:O	3:h:230:VAL:HG12	2.16	0.45
3:m:329:VAL:HG12	3:m:333:ILE:HD11	1.97	0.45
3:s:85:LEU:HG	3:s:326:LEU:HD11	1.98	0.45
3:t:227:MET:O	3:t:230:VAL:HG12	2.16	0.45
3:t:326:LEU:HA	3:t:329:VAL:HG12	1.98	0.45
2:x:92:MET:HE1	2:x:135:PRO:HB2	1.99	0.45
3:A:239:VAL:O	3:A:243:SER:OG	2.21	0.45
3:A:326:LEU:HA	3:A:329:VAL:HG12	1.98	0.45
3:C:325:LEU:O	3:C:329:VAL:HG23	2.16	0.45
2:G:93:ASP:OD1	2:G:93:ASP:C	2.60	0.45
2:G:141:GLY:HA3	2:G:172:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:MET:HE1	2:H:135:PRO:HB2	1.99	0.45
3:U:70:LYS:O	3:U:74:THR:OG1	2.27	0.45
3:U:297:ARG:NH2	3:V:227:MET:HE3	2.31	0.45
3:a:83:ILE:HG13	3:a:84:SER:N	2.32	0.45
3:b:230:VAL:HA	3:b:233:VAL:HG22	1.98	0.45
2:e:125:VAL:HB	2:e:145:ARG:HG2	1.98	0.45
3:h:326:LEU:HA	3:h:329:VAL:HG12	1.98	0.45
2:k:93:ASP:OD1	2:k:93:ASP:C	2.60	0.45
2:l:92:MET:HE1	2:l:135:PRO:HB2	1.99	0.45
3:n:79:MET:O	3:n:83:ILE:HG13	2.17	0.45
1:o:33:SER:O	1:o:33:SER:OG	2.33	0.45
2:q:93:ASP:OD1	2:q:93:ASP:C	2.60	0.45
2:5:132:LYS:HA	2:5:132:LYS:HD3	1.84	0.45
3:B:271:PRO:HD2	3:B:272:PHE:CB	2.46	0.45
2:H:204:SER:HB3	2:r:207:MET:HB3	1.99	0.45
3:I:77:THR:HA	3:I:80:VAL:HG12	1.98	0.45
3:J:259:LYS:HD3	3:J:268:ILE:HD13	1.99	0.45
2:M:125:VAL:HB	2:M:145:ARG:HG2	1.98	0.45
3:O:249:PHE:HB2	3:O:252:ARG:HB3	1.98	0.45
3:P:227:MET:O	3:P:230:VAL:HG12	2.16	0.45
2:S:141:GLY:HA3	2:S:172:LEU:HD23	1.98	0.45
2:Z:127:LEU:HD23	2:Z:127:LEU:HA	1.74	0.45
3:a:57:ARG:HE	3:a:57:ARG:HB2	1.57	0.45
2:f:92:MET:HE1	2:f:135:PRO:HB2	1.99	0.45
3:g:77:THR:HA	3:g:80:VAL:HG12	1.98	0.45
3:g:95:TYR:CE1	3:g:221:VAL:HG23	2.51	0.45
3:h:79:MET:O	3:h:83:ILE:HG13	2.17	0.45
3:h:255:ILE:HG23	3:h:268:ILE:HD12	1.98	0.45
2:l:84:ILE:HG12	2:l:148:ILE:HG13	1.98	0.45
3:t:255:ILE:HG23	3:t:268:ILE:HD12	1.98	0.45
2:w:93:ASP:OD1	2:w:93:ASP:C	2.60	0.45
3:A:255:ILE:HG23	3:A:268:ILE:HD12	1.98	0.45
3:A:259:LYS:HD3	3:A:268:ILE:HD13	1.99	0.45
3:D:74:THR:O	3:D:77:THR:OG1	2.29	0.45
3:D:79:MET:O	3:D:83:ILE:HG13	2.17	0.45
3:D:255:ILE:HG23	3:D:268:ILE:HD12	1.98	0.45
2:H:24:HIS:CD2	2:H:26:GLN:HE22	2.35	0.45
3:I:263:ALA:HA	2:M:106:ILE:HG23	1.98	0.45
3:J:227:MET:O	3:J:230:VAL:HG12	2.16	0.45
3:O:85:LEU:HG	3:O:326:LEU:HD11	1.98	0.45
3:U:110:GLN:HE22	3:U:175:VAL:HG13	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:259:LYS:HD3	3:V:268:ILE:HD13	1.99	0.45
2:Y:93:ASP:C	2:Y:93:ASP:OD1	2.60	0.45
3:a:85:LEU:HG	3:a:326:LEU:HD11	1.97	0.45
3:a:263:ALA:HA	2:e:106:ILE:HG23	1.98	0.45
3:g:93:MET:HA	3:g:96:LYS:HE3	1.98	0.45
3:g:110:GLN:HE22	3:g:175:VAL:HG13	1.82	0.45
3:g:249:PHE:HB2	3:g:252:ARG:HB3	1.98	0.45
3:g:297:ARG:O	3:g:300:SER:OG	2.31	0.45
3:h:259:LYS:HD3	3:h:268:ILE:HD13	1.99	0.45
3:m:77:THR:HA	3:m:80:VAL:HG12	1.98	0.45
3:n:255:ILE:HG23	3:n:268:ILE:HD12	1.98	0.45
3:s:95:TYR:CE1	3:s:221:VAL:HG23	2.51	0.45
2:x:84:ILE:HG12	2:x:148:ILE:HG13	1.99	0.45
2:5:106:ILE:HG23	3:C:263:ALA:HA	1.98	0.45
3:A:79:MET:O	3:A:83:ILE:HG13	2.17	0.45
3:B:95:TYR:CE1	3:B:221:VAL:HG23	2.51	0.45
2:H:127:LEU:HD21	2:H:142:GLU:HG2	1.99	0.45
3:I:249:PHE:HB2	3:I:252:ARG:HB3	1.98	0.45
3:J:192:ARG:HD3	3:J:192:ARG:HA	1.76	0.45
3:J:255:ILE:HG23	3:J:268:ILE:HD12	1.98	0.45
3:O:91:CYS:HA	3:O:94:VAL:CG2	2.46	0.45
3:O:93:MET:HA	3:O:96:LYS:HE3	1.98	0.45
3:U:85:LEU:HG	3:U:326:LEU:HD11	1.98	0.45
3:V:82:ALA:CA	3:V:287:SER:HB2	2.44	0.45
3:a:91:CYS:HA	3:a:94:VAL:CG2	2.46	0.45
3:b:227:MET:O	3:b:230:VAL:HG12	2.16	0.45
3:m:95:TYR:CE1	3:m:221:VAL:HG23	2.51	0.45
3:m:249:PHE:HB2	3:m:252:ARG:HB3	1.98	0.45
3:n:259:LYS:HD3	3:n:268:ILE:HD13	1.99	0.45
3:s:110:GLN:HE22	3:s:175:VAL:HG13	1.82	0.45
3:t:79:MET:O	3:t:83:ILE:HG13	2.17	0.45
2:5:51:ILE:HA	2:5:78:ARG:HH22	1.77	0.45
3:A:227:MET:O	3:A:230:VAL:HG12	2.16	0.45
3:B:288:LEU:HD12	3:B:326:LEU:HD23	1.99	0.45
3:C:77:THR:HA	3:C:80:VAL:HG12	1.98	0.45
3:D:259:LYS:HD3	3:D:268:ILE:HD13	1.99	0.45
3:I:95:TYR:CE1	3:I:221:VAL:HG23	2.51	0.45
3:J:79:MET:O	3:J:83:ILE:HG13	2.17	0.45
2:M:185:ARG:HH12	2:e:212:ASP:HB2	1.81	0.45
2:S:93:ASP:C	2:S:93:ASP:OD1	2.60	0.45
3:b:79:MET:O	3:b:83:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:115:ARG:O	2:f:119:SER:OG	2.31	0.45
3:g:234:ALA:HB2	3:h:83:ILE:HD12	1.98	0.45
3:m:59:ALA:HA	3:m:271:PRO:HG3	1.98	0.45
3:m:91:CYS:HA	3:m:94:VAL:CG2	2.46	0.45
3:m:297:ARG:NH2	3:n:227:MET:HE3	2.31	0.45
3:n:326:LEU:HA	3:n:329:VAL:HG12	1.98	0.45
2:r:84:ILE:HG12	2:r:148:ILE:HG13	1.98	0.45
3:s:249:PHE:HB2	3:s:252:ARG:HB3	1.98	0.45
3:t:259:LYS:HD3	3:t:268:ILE:HD13	1.99	0.45
2:5:93:ASP:OD1	2:5:93:ASP:C	2.60	0.44
3:B:110:GLN:HE22	3:B:175:VAL:HG13	1.82	0.44
3:B:328:LEU:HD23	3:B:328:LEU:HA	1.87	0.44
3:C:110:GLN:HE22	3:C:175:VAL:HG13	1.82	0.44
2:N:84:ILE:HG12	2:N:148:ILE:HG13	1.98	0.44
3:O:83:ILE:HG13	3:O:84:SER:N	2.32	0.44
3:P:242:ASN:OD1	3:P:243:SER:N	2.51	0.44
2:T:43:THR:OG1	4:T:301:AGS:O1A	2.31	0.44
3:b:242:ASN:OD1	3:b:243:SER:N	2.51	0.44
3:g:329:VAL:HG12	3:g:333:ILE:HD11	1.98	0.44
3:m:110:GLN:HE22	3:m:175:VAL:HG13	1.82	0.44
3:s:77:THR:HA	3:s:80:VAL:HG12	1.98	0.44
3:s:329:VAL:HG12	3:s:333:ILE:HD11	1.98	0.44
3:t:242:ASN:OD1	3:t:243:SER:N	2.51	0.44
3:B:249:PHE:HB2	3:B:252:ARG:HB3	1.98	0.44
3:I:83:ILE:HG13	3:I:84:SER:N	2.32	0.44
3:O:110:GLN:HE22	3:O:175:VAL:HG13	1.82	0.44
3:O:234:ALA:HB2	3:P:83:ILE:HD12	1.98	0.44
3:O:263:ALA:HA	2:S:106:ILE:HG23	1.98	0.44
3:a:95:TYR:CE1	3:a:221:VAL:HG23	2.51	0.44
3:b:74:THR:O	3:b:77:THR:OG1	2.29	0.44
2:f:84:ILE:HG12	2:f:148:ILE:HG13	1.98	0.44
3:m:263:ALA:HA	2:q:106:ILE:HG23	1.98	0.44
3:n:232:MET:HG2	3:n:232:MET:H	1.60	0.44
3:s:93:MET:HA	3:s:96:LYS:HE3	1.98	0.44
3:A:311:THR:OG1	3:A:312:LYS:N	2.46	0.44
3:D:105:TYR:CE1	3:D:109:PRO:HD3	2.47	0.44
3:D:242:ASN:OD1	3:D:243:SER:N	2.51	0.44
3:O:288:LEU:HD12	3:O:326:LEU:HD23	1.99	0.44
3:U:234:ALA:HB2	3:V:83:ILE:HD12	1.98	0.44
3:U:288:LEU:HD12	3:U:326:LEU:HD23	1.99	0.44
3:V:79:MET:O	3:V:83:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:288:LEU:HD12	3:a:326:LEU:HD23	1.99	0.44
2:e:93:ASP:C	2:e:93:ASP:OD1	2.60	0.44
3:g:263:ALA:HA	2:k:106:ILE:HG23	1.98	0.44
3:h:230:VAL:HA	3:h:233:VAL:HG22	1.98	0.44
3:h:242:ASN:OD1	3:h:243:SER:N	2.50	0.44
2:k:51:ILE:HA	2:k:78:ARG:HH22	1.76	0.44
2:k:51:ILE:N	2:k:78:ARG:HH21	2.16	0.44
3:m:234:ALA:HB2	3:n:83:ILE:HD12	1.98	0.44
2:q:125:VAL:HB	2:q:145:ARG:HG2	1.98	0.44
3:s:234:ALA:HB2	3:t:83:ILE:HD12	1.98	0.44
3:s:263:ALA:HA	2:w:106:ILE:HG23	1.98	0.44
1:v:7:LEU:HD23	1:v:7:LEU:HA	1.87	0.44
3:B:81:ILE:HD12	3:B:84:SER:OG	2.18	0.44
3:C:83:ILE:HG13	3:C:84:SER:N	2.32	0.44
3:D:227:MET:O	3:D:230:VAL:HG12	2.16	0.44
1:E:33:SER:O	1:E:33:SER:OG	2.33	0.44
3:I:110:GLN:HE22	3:I:175:VAL:HG13	1.82	0.44
2:T:84:ILE:HG12	2:T:148:ILE:HG13	1.98	0.44
3:a:110:GLN:HE22	3:a:175:VAL:HG13	1.82	0.44
3:a:234:ALA:HB2	3:b:83:ILE:HD12	1.98	0.44
3:a:249:PHE:HB2	3:a:252:ARG:HB3	1.98	0.44
3:a:297:ARG:O	3:a:300:SER:OG	2.31	0.44
3:n:230:VAL:HA	3:n:233:VAL:HG22	1.98	0.44
3:s:81:ILE:HD12	3:s:84:SER:OG	2.18	0.44
2:w:125:VAL:HB	2:w:145:ARG:HG2	1.98	0.44
2:x:83:MET:HE3	2:x:83:MET:HB2	1.89	0.44
2:6:24:HIS:CD2	2:6:26:GLN:HE22	2.35	0.44
2:6:84:ILE:HG12	2:6:148:ILE:HG13	1.98	0.44
3:C:249:PHE:HB2	3:C:252:ARG:HB3	1.98	0.44
3:U:321:ASP:OD1	3:U:322:GLU:N	2.47	0.44
2:Y:68:ARG:HA	2:Y:68:ARG:HD3	1.78	0.44
3:a:81:ILE:HD12	3:a:84:SER:OG	2.18	0.44
2:q:132:LYS:HA	2:q:132:LYS:HD3	1.84	0.44
3:t:230:VAL:HA	3:t:233:VAL:HG22	1.98	0.44
3:B:70:LYS:HA	3:B:70:LYS:HD2	1.71	0.44
3:I:245:ARG:HB3	3:I:272:PHE:CZ	2.52	0.44
2:M:93:ASP:OD1	2:M:93:ASP:C	2.60	0.44
3:P:79:MET:O	3:P:83:ILE:HG13	2.17	0.44
2:T:91:LEU:HD13	2:T:94:ARG:NH1	2.33	0.44
3:U:81:ILE:HD12	3:U:84:SER:OG	2.18	0.44
3:U:83:ILE:HG13	3:U:84:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:28:GLY:N	2:Z:189:THR:HG22	2.23	0.44
2:k:132:LYS:HA	2:k:132:LYS:HD3	1.85	0.44
2:r:24:HIS:CD2	2:r:26:GLN:HE22	2.35	0.44
3:B:83:ILE:HG13	3:B:84:SER:N	2.32	0.44
3:C:95:TYR:CE1	3:C:221:VAL:HG23	2.52	0.44
2:H:84:ILE:HG12	2:H:148:ILE:HG13	1.98	0.44
3:O:81:ILE:HD12	3:O:84:SER:OG	2.18	0.44
3:V:105:TYR:CE1	3:V:109:PRO:HD3	2.47	0.44
2:Z:24:HIS:CD2	2:Z:26:GLN:HE22	2.35	0.44
2:f:91:LEU:HD13	2:f:94:ARG:NH1	2.33	0.44
3:g:81:ILE:HD12	3:g:84:SER:OG	2.18	0.44
2:k:125:VAL:HB	2:k:145:ARG:HG2	1.98	0.44
2:k:135:PRO:O	2:k:143:GLN:NE2	2.50	0.44
3:n:74:THR:O	3:n:77:THR:OG1	2.29	0.44
2:H:91:LEU:HD13	2:H:94:ARG:NH1	2.33	0.44
1:K:8:ILE:H	1:K:8:ILE:HG12	1.64	0.44
3:O:102:ALA:O	3:O:107:PRO:HG2	2.18	0.44
3:V:192:ARG:HD3	3:V:192:ARG:HA	1.76	0.44
3:V:242:ASN:OD1	3:V:243:SER:N	2.51	0.44
2:Y:117:ARG:NH2	2:Y:154:ASN:OD1	2.51	0.44
2:e:51:ILE:HA	2:e:78:ARG:HH22	1.77	0.44
2:e:117:ARG:NH2	2:e:154:ASN:OD1	2.51	0.44
3:n:239:VAL:O	3:n:243:SER:OG	2.21	0.44
3:s:181:ASP:OD1	3:s:181:ASP:N	2.48	0.44
2:x:127:LEU:HD23	2:x:127:LEU:HA	1.74	0.44
3:B:321:ASP:OD1	3:B:322:GLU:N	2.47	0.44
3:P:70:LYS:O	3:P:74:THR:HG23	2.18	0.44
3:V:70:LYS:O	3:V:74:THR:HG23	2.18	0.44
2:Z:84:ILE:HG12	2:Z:148:ILE:HG13	1.99	0.44
3:a:102:ALA:O	3:a:107:PRO:HG2	2.18	0.44
3:b:70:LYS:O	3:b:74:THR:HG23	2.18	0.44
2:f:24:HIS:CD2	2:f:26:GLN:HE22	2.35	0.44
3:A:242:ASN:OD1	3:A:243:SER:N	2.51	0.43
3:D:273:LEU:HD23	3:D:273:LEU:HA	1.84	0.43
3:U:59:ALA:HA	3:U:271:PRO:HG3	2.00	0.43
3:U:102:ALA:O	3:U:107:PRO:HG2	2.18	0.43
2:Y:51:ILE:N	2:Y:78:ARG:HH21	2.16	0.43
2:Y:135:PRO:O	2:Y:143:GLN:NE2	2.50	0.43
2:Z:83:MET:HE3	2:Z:83:MET:HB2	1.89	0.43
2:e:51:ILE:N	2:e:78:ARG:HH21	2.16	0.43
3:m:288:LEU:HD12	3:m:326:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:135:PRO:O	2:q:143:GLN:NE2	2.50	0.43
3:s:297:ARG:O	3:s:300:SER:OG	2.31	0.43
2:6:205:TYR:HE1	2:l:217:GLY:C	2.26	0.43
3:B:245:ARG:HB3	3:B:272:PHE:CE2	2.52	0.43
3:D:70:LYS:O	3:D:74:THR:HG23	2.18	0.43
2:G:204:SER:HB3	2:Y:207:MET:HB3	2.00	0.43
3:I:268:ILE:C	3:I:270:ARG:N	2.76	0.43
2:N:24:HIS:CD2	2:N:26:GLN:HE22	2.35	0.43
1:Q:8:ILE:H	1:Q:8:ILE:HG12	1.64	0.43
2:S:51:ILE:N	2:S:78:ARG:HH21	2.16	0.43
2:S:117:ARG:NH2	2:S:154:ASN:OD1	2.51	0.43
2:Z:91:LEU:HD13	2:Z:94:ARG:NH1	2.33	0.43
3:g:288:LEU:HD12	3:g:326:LEU:HD23	1.99	0.43
3:n:70:LYS:O	3:n:74:THR:HG23	2.18	0.43
2:w:51:ILE:N	2:w:78:ARG:HH21	2.17	0.43
2:w:68:ARG:HA	2:w:68:ARG:HD3	1.78	0.43
2:w:132:LYS:HA	2:w:132:LYS:HD3	1.85	0.43
2:x:216:HIS:HB3	2:x:217:GLY:H	1.64	0.43
3:C:81:ILE:HD12	3:C:84:SER:OG	2.18	0.43
1:K:17:ILE:C	1:K:17:ILE:HD12	2.44	0.43
2:M:11:TYR:OH	2:M:52:GLU:OE2	2.29	0.43
2:N:216:HIS:HB3	2:N:217:GLY:H	1.64	0.43
3:P:192:ARG:HA	3:P:192:ARG:HD3	1.76	0.43
2:T:24:HIS:CD2	2:T:26:GLN:HE22	2.35	0.43
3:U:263:ALA:HA	2:Y:106:ILE:HG23	1.98	0.43
3:V:74:THR:O	3:V:77:THR:OG1	2.29	0.43
3:I:81:ILE:HD12	3:I:84:SER:OG	2.18	0.43
3:J:242:ASN:OD1	3:J:243:SER:N	2.51	0.43
3:O:270:ARG:CB	3:O:271:PRO:HD2	2.40	0.43
3:V:68:LYS:O	3:V:71:PRO:HD3	2.19	0.43
3:b:264:THR:HG22	3:b:266:GLY:H	1.84	0.43
3:g:102:ALA:O	3:g:107:PRO:HG2	2.18	0.43
3:h:68:LYS:O	3:h:71:PRO:HD3	2.19	0.43
3:h:70:LYS:O	3:h:74:THR:HG23	2.18	0.43
1:i:17:ILE:C	1:i:17:ILE:HD12	2.44	0.43
2:k:117:ARG:NH2	2:k:154:ASN:OD1	2.51	0.43
3:m:81:ILE:HD12	3:m:84:SER:OG	2.18	0.43
3:n:242:ASN:OD1	3:n:243:SER:N	2.50	0.43
3:n:273:LEU:HD23	3:n:273:LEU:HA	1.84	0.43
2:w:135:PRO:O	2:w:143:GLN:NE2	2.50	0.43
1:l:17:ILE:C	1:l:17:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:ALA:CA	3:D:287:SER:HB2	2.44	0.43
1:E:17:ILE:C	1:E:17:ILE:HD12	2.44	0.43
2:G:165:THR:HA	2:G:168:LEU:HB2	2.00	0.43
3:P:68:LYS:O	3:P:71:PRO:HD3	2.19	0.43
3:U:305:VAL:O	3:U:308:VAL:HG22	2.19	0.43
2:Y:11:TYR:OH	2:Y:52:GLU:OE2	2.28	0.43
3:a:305:VAL:O	3:a:308:VAL:HG22	2.19	0.43
2:l:24:HIS:CD2	2:l:26:GLN:HE22	2.35	0.43
3:t:68:LYS:O	3:t:71:PRO:HD3	2.19	0.43
2:w:117:ARG:NH2	2:w:154:ASN:OD1	2.51	0.43
2:5:51:ILE:N	2:5:78:ARG:HH21	2.16	0.43
2:5:165:THR:HA	2:5:168:LEU:HB2	2.00	0.43
2:6:91:LEU:HD13	2:6:94:ARG:NH1	2.33	0.43
2:6:217:GLY:C	2:T:205:TYR:HE1	2.27	0.43
3:B:225:SER:HA	3:B:228:ILE:HG12	2.01	0.43
3:B:290:LEU:HA	3:B:293:ILE:HG12	2.00	0.43
3:C:305:VAL:O	3:C:308:VAL:HG22	2.19	0.43
3:D:264:THR:HG22	3:D:266:GLY:H	1.84	0.43
3:J:264:THR:HG22	3:J:266:GLY:H	1.84	0.43
2:M:51:ILE:N	2:M:78:ARG:HH21	2.16	0.43
3:P:82:ALA:CA	3:P:287:SER:HB2	2.44	0.43
2:T:83:MET:HE3	2:T:83:MET:HB2	1.90	0.43
2:Z:197:ILE:HD13	2:r:202:ARG:HG2	1.99	0.43
3:b:117:LYS:NZ	3:b:169:PRO:O	2.44	0.43
3:m:225:SER:HA	3:m:228:ILE:HG12	2.01	0.43
3:n:68:LYS:O	3:n:71:PRO:HD3	2.19	0.43
2:q:51:ILE:HA	2:q:78:ARG:HH22	1.77	0.43
2:q:51:ILE:N	2:q:78:ARG:HH21	2.16	0.43
2:r:91:LEU:HD13	2:r:94:ARG:NH1	2.33	0.43
3:s:102:ALA:O	3:s:107:PRO:HG2	2.18	0.43
3:t:70:LYS:O	3:t:74:THR:HG23	2.18	0.43
2:x:91:LEU:HD13	2:x:94:ARG:NH1	2.33	0.43
1:F:7:LEU:HD23	1:F:7:LEU:HA	1.87	0.43
2:G:132:LYS:HA	2:G:132:LYS:HD3	1.84	0.43
2:H:127:LEU:HD23	2:H:127:LEU:HA	1.74	0.43
3:I:305:VAL:O	3:I:308:VAL:HG22	2.19	0.43
3:J:232:MET:HG2	3:J:232:MET:H	1.60	0.43
2:M:165:THR:HA	2:M:168:LEU:HB2	2.00	0.43
3:P:264:THR:HG22	3:P:266:GLY:H	1.84	0.43
2:Y:-1:LEU:HD12	2:Y:-1:LEU:HA	1.89	0.43
2:Y:165:THR:HA	2:Y:168:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:68:LYS:O	3:b:71:PRO:HD3	2.19	0.43
3:b:305:VAL:O	3:b:308:VAL:HG22	2.19	0.43
2:e:165:THR:HA	2:e:168:LEU:HB2	2.00	0.43
2:k:165:THR:HA	2:k:168:LEU:HB2	2.00	0.43
3:n:192:ARG:HD3	3:n:192:ARG:HA	1.76	0.43
1:o:17:ILE:C	1:o:17:ILE:HD12	2.44	0.43
2:q:165:THR:HA	2:q:168:LEU:HB2	2.00	0.43
3:t:192:ARG:HD3	3:t:192:ARG:HA	1.76	0.43
2:w:165:THR:HA	2:w:168:LEU:HB2	2.00	0.43
3:A:82:ALA:CA	3:A:287:SER:HB2	2.44	0.43
3:A:264:THR:HG22	3:A:266:GLY:H	1.84	0.43
3:B:102:ALA:O	3:B:107:PRO:HG2	2.18	0.43
3:B:305:VAL:O	3:B:308:VAL:HG22	2.19	0.43
3:D:305:VAL:O	3:D:308:VAL:HG22	2.19	0.43
3:D:311:THR:OG1	3:D:312:LYS:N	2.46	0.43
2:G:216:HIS:CG	2:G:217:GLY:H	2.37	0.43
3:I:321:ASP:OD1	3:I:322:GLU:N	2.47	0.43
3:P:305:VAL:O	3:P:308:VAL:HG22	2.19	0.43
2:S:165:THR:HA	2:S:168:LEU:HB2	2.00	0.43
3:U:90:VAL:O	3:U:94:VAL:HG22	2.19	0.43
3:U:290:LEU:HA	3:U:293:ILE:HG12	2.00	0.43
2:Z:43:THR:OG1	4:Z:301:AGS:O1A	2.31	0.43
2:e:132:LYS:HD3	2:e:132:LYS:HA	1.84	0.43
3:h:305:VAL:O	3:h:308:VAL:HG22	2.19	0.43
3:m:102:ALA:O	3:m:107:PRO:HG2	2.18	0.43
2:q:117:ARG:NH2	2:q:154:ASN:OD1	2.51	0.43
3:s:288:LEU:HD12	3:s:326:LEU:HD23	1.99	0.43
1:u:17:ILE:C	1:u:17:ILE:HD12	2.44	0.43
3:C:225:SER:HA	3:C:228:ILE:HG12	2.01	0.43
2:H:83:MET:HE3	2:H:83:MET:HB2	1.90	0.43
3:V:259:LYS:HA	3:V:259:LYS:HD2	1.86	0.43
3:a:225:SER:HA	3:a:228:ILE:HG12	2.01	0.43
2:f:83:MET:HE3	2:f:83:MET:HB2	1.90	0.43
2:f:136:ILE:HD12	2:f:136:ILE:HA	1.93	0.43
3:g:181:ASP:OD1	3:g:181:ASP:N	2.48	0.43
2:l:28:GLY:N	2:l:189:THR:HG22	2.23	0.43
3:t:305:VAL:O	3:t:308:VAL:HG22	2.19	0.43
2:5:117:ARG:NH2	2:5:154:ASN:OD1	2.51	0.43
3:A:305:VAL:O	3:A:308:VAL:HG22	2.19	0.43
3:C:221:VAL:HA	3:C:224:VAL:HG12	2.01	0.43
3:D:217:LEU:O	3:D:220:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:117:ARG:NH2	2:G:154:ASN:OD1	2.51	0.43
3:I:90:VAL:O	3:I:94:VAL:HG22	2.19	0.43
3:J:239:VAL:O	3:J:243:SER:OG	2.21	0.43
3:O:145:ARG:NH2	3:O:169:PRO:O	2.52	0.43
3:O:290:LEU:HA	3:O:293:ILE:HG12	2.00	0.43
3:O:305:VAL:O	3:O:308:VAL:HG22	2.19	0.43
2:S:132:LYS:HA	2:S:132:LYS:HD3	1.85	0.43
3:U:145:ARG:NH2	3:U:169:PRO:O	2.52	0.43
1:X:7:LEU:HD23	1:X:7:LEU:HA	1.87	0.43
3:a:221:VAL:HA	3:a:224:VAL:HG12	2.01	0.43
3:m:290:LEU:HA	3:m:293:ILE:HG12	2.00	0.43
3:n:305:VAL:O	3:n:308:VAL:HG22	2.19	0.43
2:6:101:ALA:O	2:6:105:ILE:HG13	2.19	0.42
3:A:70:LYS:O	3:A:74:THR:HG23	2.18	0.42
3:B:221:VAL:HA	3:B:224:VAL:HG12	2.01	0.42
3:C:90:VAL:O	3:C:94:VAL:HG22	2.19	0.42
3:D:68:LYS:O	3:D:71:PRO:HD3	2.19	0.42
3:I:102:ALA:O	3:I:107:PRO:HG2	2.18	0.42
2:M:117:ARG:NH2	2:M:154:ASN:OD1	2.51	0.42
2:N:87:ASP:OD1	2:N:87:ASP:N	2.36	0.42
3:O:90:VAL:O	3:O:94:VAL:HG22	2.19	0.42
2:S:11:TYR:OH	2:S:52:GLU:OE2	2.28	0.42
3:a:145:ARG:NH2	3:a:169:PRO:O	2.52	0.42
3:h:82:ALA:CA	3:h:287:SER:HB2	2.44	0.42
3:m:80:VAL:HG22	3:m:238:LEU:HD11	2.01	0.42
3:m:187:SER:O	3:m:190:THR:OG1	2.28	0.42
3:m:221:VAL:HA	3:m:224:VAL:HG12	2.01	0.42
3:m:305:VAL:O	3:m:308:VAL:HG22	2.19	0.42
2:r:101:ALA:O	2:r:105:ILE:HG13	2.19	0.42
3:s:92:TYR:HD1	3:s:228:ILE:HD11	1.84	0.42
3:t:82:ALA:CA	3:t:287:SER:HB2	2.44	0.42
2:x:61:PHE:HE1	2:x:158:VAL:HG11	1.84	0.42
1:1:33:SER:O	1:1:33:SER:OG	2.33	0.42
2:H:61:PHE:HE1	2:H:158:VAL:HG11	1.84	0.42
3:I:225:SER:HA	3:I:228:ILE:HG12	2.01	0.42
3:J:68:LYS:O	3:J:71:PRO:HD3	2.19	0.42
3:J:70:LYS:O	3:J:74:THR:HG23	2.18	0.42
3:O:59:ALA:HB1	3:O:271:PRO:HD3	2.00	0.42
3:U:92:TYR:HD1	3:U:228:ILE:HD11	1.84	0.42
3:V:305:VAL:O	3:V:308:VAL:HG22	2.19	0.42
2:Z:216:HIS:HB3	2:Z:217:GLY:H	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:101:ALA:O	2:f:105:ILE:HG13	2.19	0.42
3:g:145:ARG:NH2	3:g:169:PRO:O	2.52	0.42
3:h:192:ARG:HA	3:h:192:ARG:HD3	1.76	0.42
2:l:61:PHE:HE1	2:l:158:VAL:HG11	1.84	0.42
2:l:91:LEU:HD13	2:l:94:ARG:NH1	2.33	0.42
3:m:70:LYS:HD2	3:m:70:LYS:HA	1.71	0.42
3:m:145:ARG:NH2	3:m:169:PRO:O	2.52	0.42
3:s:290:LEU:HA	3:s:293:ILE:HG12	2.00	0.42
3:t:217:LEU:O	3:t:220:LEU:HD23	2.19	0.42
1:u:14:ALA:HA	1:u:17:ILE:HG13	2.01	0.42
2:x:24:HIS:CD2	2:x:26:GLN:HE22	2.35	0.42
2:x:115:ARG:O	2:x:119:SER:OG	2.31	0.42
3:A:217:LEU:O	3:A:220:LEU:HD23	2.19	0.42
3:C:102:ALA:O	3:C:107:PRO:HG2	2.18	0.42
3:I:221:VAL:HA	3:I:224:VAL:HG12	2.01	0.42
3:J:305:VAL:O	3:J:308:VAL:HG22	2.19	0.42
2:M:177:LEU:HD23	2:M:177:LEU:HA	1.86	0.42
2:N:91:LEU:HD13	2:N:94:ARG:NH1	2.33	0.42
3:O:92:TYR:HD1	3:O:228:ILE:HD11	1.85	0.42
3:O:225:SER:HA	3:O:228:ILE:HG12	2.01	0.42
3:O:279:LEU:HD12	3:O:279:LEU:HA	1.93	0.42
2:T:177:LEU:HD22	2:T:199:LEU:HG	2.01	0.42
2:Z:52:GLU:OE2	2:Z:52:GLU:HA	2.20	0.42
3:a:80:VAL:HG22	3:a:238:LEU:HD11	2.01	0.42
1:c:7:LEU:HD23	1:c:7:LEU:HA	1.93	0.42
2:f:61:PHE:HE1	2:f:158:VAL:HG11	1.84	0.42
2:f:177:LEU:HD22	2:f:199:LEU:HG	2.01	0.42
3:g:92:TYR:HD1	3:g:228:ILE:HD11	1.85	0.42
3:h:217:LEU:O	3:h:220:LEU:HD23	2.19	0.42
3:s:145:ARG:NH2	3:s:169:PRO:O	2.52	0.42
3:s:221:VAL:HA	3:s:224:VAL:HG12	2.01	0.42
2:x:101:ALA:O	2:x:105:ILE:HG13	2.19	0.42
2:5:125:VAL:HG12	2:5:179:LEU:HD21	2.02	0.42
3:A:74:THR:O	3:A:77:THR:OG1	2.29	0.42
2:G:51:ILE:N	2:G:78:ARG:HH21	2.16	0.42
2:H:101:ALA:O	2:H:105:ILE:HG13	2.19	0.42
3:I:78:VAL:O	3:I:81:ILE:HG22	2.20	0.42
3:I:290:LEU:HA	3:I:293:ILE:HG12	2.00	0.42
2:N:101:ALA:O	2:N:105:ILE:HG13	2.19	0.42
1:Q:17:ILE:HD12	1:Q:17:ILE:C	2.44	0.42
2:T:101:ALA:O	2:T:105:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:221:VAL:HA	3:U:224:VAL:HG12	2.01	0.42
2:Z:7:VAL:O	2:Z:20:GLY:N	2.53	0.42
2:Z:177:LEU:HD22	2:Z:199:LEU:HG	2.01	0.42
3:b:192:ARG:HA	3:b:192:ARG:HD3	1.76	0.42
1:c:17:ILE:C	1:c:17:ILE:HD12	2.44	0.42
3:g:90:VAL:O	3:g:94:VAL:HG22	2.19	0.42
3:g:221:VAL:HA	3:g:224:VAL:HG12	2.01	0.42
3:g:290:LEU:HA	3:g:293:ILE:HG12	2.00	0.42
2:k:139:SER:OG	2:k:142:GLU:HG3	2.19	0.42
2:l:101:ALA:O	2:l:105:ILE:HG13	2.19	0.42
3:m:90:VAL:O	3:m:94:VAL:HG22	2.19	0.42
2:q:102:ILE:O	2:q:106:ILE:HG12	2.20	0.42
2:w:1:MET:O	2:w:62:SER:N	2.52	0.42
2:x:52:GLU:HA	2:x:52:GLU:OE2	2.20	0.42
2:5:102:ILE:O	2:5:106:ILE:HG12	2.20	0.42
2:6:61:PHE:HE1	2:6:158:VAL:HG11	1.84	0.42
3:C:78:VAL:O	3:C:81:ILE:HG22	2.20	0.42
3:I:145:ARG:NH2	3:I:169:PRO:O	2.52	0.42
3:J:217:LEU:O	3:J:220:LEU:HD23	2.19	0.42
2:M:102:ILE:O	2:M:106:ILE:HG12	2.20	0.42
3:O:80:VAL:HG22	3:O:238:LEU:HD11	2.01	0.42
3:O:221:VAL:HA	3:O:224:VAL:HG12	2.01	0.42
2:T:52:GLU:HA	2:T:52:GLU:OE2	2.20	0.42
2:T:61:PHE:HE1	2:T:158:VAL:HG11	1.84	0.42
3:a:279:LEU:HD12	3:a:279:LEU:HA	1.93	0.42
1:j:7:LEU:HD23	1:j:7:LEU:HA	1.87	0.42
3:m:78:VAL:O	3:m:81:ILE:HG22	2.20	0.42
2:q:-1:LEU:HD12	2:q:-1:LEU:HA	1.89	0.42
3:s:90:VAL:O	3:s:94:VAL:HG22	2.19	0.42
3:A:68:LYS:O	3:A:71:PRO:HD3	2.19	0.42
3:C:290:LEU:HA	3:C:293:ILE:HG12	2.00	0.42
3:D:239:VAL:O	3:D:243:SER:OG	2.21	0.42
2:G:135:PRO:O	2:G:143:GLN:NE2	2.50	0.42
3:J:82:ALA:CA	3:J:287:SER:HB2	2.44	0.42
1:L:7:LEU:HD23	1:L:7:LEU:HA	1.87	0.42
2:M:178:ARG:O	2:M:179:LEU:C	2.63	0.42
2:S:135:PRO:O	2:S:143:GLN:NE2	2.50	0.42
3:U:78:VAL:O	3:U:81:ILE:HG22	2.20	0.42
3:V:217:LEU:O	3:V:220:LEU:HD23	2.19	0.42
3:a:90:VAL:O	3:a:94:VAL:HG22	2.19	0.42
3:b:82:ALA:CA	3:b:287:SER:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:k:102:ILE:O	2:k:106:ILE:HG12	2.20	0.42
2:l:52:GLU:HA	2:l:52:GLU:OE2	2.20	0.42
3:n:82:ALA:CA	3:n:287:SER:HB2	2.44	0.42
2:q:139:SER:OG	2:q:142:GLU:HG3	2.20	0.42
3:s:225:SER:HA	3:s:228:ILE:HG12	2.01	0.42
2:w:139:SER:OG	2:w:142:GLU:HG3	2.20	0.42
3:D:56:VAL:HG13	3:D:274:TYR:HE2	1.85	0.42
2:M:205:TYR:HE1	2:e:217:GLY:CA	2.32	0.42
2:N:61:PHE:HE1	2:N:158:VAL:HG11	1.84	0.42
3:O:78:VAL:O	3:O:81:ILE:HG22	2.20	0.42
3:P:217:LEU:O	3:P:220:LEU:HD23	2.19	0.42
2:T:136:ILE:HD12	2:T:136:ILE:HA	1.93	0.42
2:T:197:ILE:HD12	2:T:197:ILE:HA	1.87	0.42
3:a:78:VAL:O	3:a:81:ILE:HG22	2.20	0.42
1:i:14:ALA:HA	1:i:17:ILE:HG13	2.01	0.42
3:n:264:THR:HG22	3:n:266:GLY:H	1.84	0.42
2:r:61:PHE:HE1	2:r:158:VAL:HG11	1.84	0.42
2:w:181:GLU:OE2	2:w:205:TYR:OH	2.23	0.42
2:x:136:ILE:HD12	2:x:136:ILE:HA	1.93	0.42
2:6:83:MET:HE3	2:6:83:MET:HB2	1.90	0.42
3:B:90:VAL:O	3:B:94:VAL:HG22	2.19	0.42
3:B:92:TYR:CE1	3:B:228:ILE:HD11	2.55	0.42
3:C:92:TYR:CE1	3:C:228:ILE:HD11	2.55	0.42
3:D:124:ALA:HB1	3:D:142:TYR:CZ	2.55	0.42
1:E:14:ALA:HA	1:E:17:ILE:HG13	2.01	0.42
2:M:68:ARG:HA	2:M:68:ARG:HD3	1.78	0.42
2:T:7:VAL:O	2:T:20:GLY:N	2.53	0.42
3:V:264:THR:HG22	3:V:266:GLY:H	1.84	0.42
2:Y:205:TYR:CE1	2:q:217:GLY:CA	3.02	0.42
3:a:290:LEU:HA	3:a:293:ILE:HG12	2.00	0.42
2:e:95:THR:HG23	2:e:98:ASP:H	1.85	0.42
3:g:78:VAL:O	3:g:81:ILE:HG22	2.20	0.42
3:g:225:SER:HA	3:g:228:ILE:HG12	2.01	0.42
1:i:7:LEU:HD23	1:i:7:LEU:HA	1.93	0.42
3:s:78:VAL:O	3:s:81:ILE:HG22	2.20	0.42
3:s:305:VAL:O	3:s:308:VAL:HG22	2.19	0.42
3:t:105:TYR:HE1	3:t:108:SER:HA	1.85	0.42
2:w:102:ILE:O	2:w:106:ILE:HG12	2.20	0.42
1:1:8:ILE:H	1:1:8:ILE:HG12	1.64	0.42
1:1:14:ALA:HA	1:1:17:ILE:HG13	2.01	0.42
2:5:128:LEU:HD12	2:5:128:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:78:VAL:O	3:B:81:ILE:HG22	2.20	0.42
3:C:80:VAL:O	3:C:83:ILE:HG12	2.20	0.42
3:C:145:ARG:NH2	3:C:169:PRO:O	2.52	0.42
3:C:321:ASP:OD1	3:C:322:GLU:N	2.47	0.42
2:G:102:ILE:O	2:G:106:ILE:HG12	2.20	0.42
3:I:92:TYR:CE1	3:I:228:ILE:HD11	2.55	0.42
2:N:153:VAL:O	2:N:154:ASN:HB2	2.20	0.42
3:O:92:TYR:CE1	3:O:228:ILE:HD11	2.55	0.42
3:U:80:VAL:HG22	3:U:238:LEU:HD11	2.01	0.42
3:a:92:TYR:CE1	3:a:228:ILE:HD11	2.55	0.42
3:a:92:TYR:HD1	3:a:228:ILE:HD11	1.85	0.42
2:f:52:GLU:HA	2:f:52:GLU:OE2	2.20	0.42
3:g:80:VAL:HG22	3:g:238:LEU:HD11	2.01	0.42
2:l:7:VAL:O	2:l:20:GLY:N	2.53	0.42
3:m:251:ARG:HG2	3:m:254:SER:OG	2.20	0.42
2:G:51:ILE:HA	2:G:78:ARG:HH22	1.77	0.42
3:I:80:VAL:O	3:I:83:ILE:HG12	2.20	0.42
2:N:52:GLU:HA	2:N:52:GLU:OE2	2.20	0.42
1:Q:5:LEU:HD12	1:Q:5:LEU:H	1.85	0.42
2:S:51:ILE:HA	2:S:78:ARG:HH22	1.77	0.42
2:S:95:THR:HG23	2:S:98:ASP:H	1.85	0.42
3:U:80:VAL:O	3:U:83:ILE:HG12	2.20	0.42
3:U:92:TYR:CE1	3:U:228:ILE:HD11	2.55	0.42
3:b:56:VAL:HG13	3:b:274:TYR:HE2	1.85	0.42
3:b:124:ALA:HB1	3:b:142:TYR:CZ	2.55	0.42
3:b:217:LEU:O	3:b:220:LEU:HD23	2.19	0.42
2:e:102:ILE:O	2:e:106:ILE:HG12	2.20	0.42
3:g:110:GLN:HA	3:g:110:GLN:OE1	2.20	0.42
3:g:305:VAL:O	3:g:308:VAL:HG22	2.19	0.42
3:h:56:VAL:HG13	3:h:274:TYR:HE2	1.85	0.42
3:h:100:GLN:O	3:h:103:THR:OG1	2.24	0.42
3:m:92:TYR:CE1	3:m:228:ILE:HD11	2.55	0.42
3:m:92:TYR:HD1	3:m:228:ILE:HD11	1.84	0.42
3:n:56:VAL:HG13	3:n:274:TYR:HE2	1.85	0.42
3:n:217:LEU:O	3:n:220:LEU:HD23	2.19	0.42
1:o:14:ALA:HA	1:o:17:ILE:HG13	2.01	0.42
3:s:110:GLN:HA	3:s:110:GLN:OE1	2.20	0.42
3:t:108:SER:HA	3:t:109:PRO:HD3	1.93	0.42
3:t:264:THR:HG22	3:t:266:GLY:H	1.84	0.42
2:6:52:GLU:HA	2:6:52:GLU:OE2	2.20	0.41
3:C:110:GLN:OE1	3:C:110:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:128:LEU:HD12	2:G:128:LEU:HA	1.85	0.41
3:I:110:GLN:OE1	3:I:110:GLN:HA	2.20	0.41
2:M:178:ARG:HH11	2:e:36:HIS:HB3	1.85	0.41
2:M:217:GLY:CA	2:w:205:TYR:HE1	2.32	0.41
2:S:125:VAL:HG12	2:S:179:LEU:HD21	2.02	0.41
2:Y:205:TYR:HE1	2:q:217:GLY:CA	2.31	0.41
2:Z:61:PHE:HE1	2:Z:158:VAL:HG11	1.84	0.41
3:a:181:ASP:OD1	3:a:181:ASP:N	2.48	0.41
3:a:251:ARG:HG2	3:a:254:SER:OG	2.20	0.41
1:c:14:ALA:HA	1:c:17:ILE:HG13	2.01	0.41
2:f:153:VAL:O	2:f:154:ASN:HB2	2.20	0.41
3:g:92:TYR:CE1	3:g:228:ILE:HD11	2.55	0.41
3:h:74:THR:O	3:h:77:THR:OG1	2.29	0.41
3:s:78:VAL:HA	3:s:81:ILE:HG22	2.02	0.41
3:t:56:VAL:HG13	3:t:274:TYR:HE2	1.85	0.41
2:x:7:VAL:O	2:x:20:GLY:N	2.53	0.41
2:6:153:VAL:O	2:6:154:ASN:HB2	2.20	0.41
3:C:328:LEU:HD23	3:C:328:LEU:HA	1.87	0.41
2:H:7:VAL:O	2:H:20:GLY:N	2.53	0.41
2:H:52:GLU:HA	2:H:52:GLU:OE2	2.20	0.41
3:I:92:TYR:HD1	3:I:228:ILE:HD11	1.84	0.41
3:I:251:ARG:HG2	3:I:254:SER:OG	2.20	0.41
2:M:139:SER:OG	2:M:142:GLU:HG3	2.20	0.41
3:O:80:VAL:O	3:O:83:ILE:HG12	2.20	0.41
3:P:56:VAL:HG13	3:P:274:TYR:HE2	1.85	0.41
1:W:17:ILE:C	1:W:17:ILE:HD12	2.44	0.41
2:Z:101:ALA:O	2:Z:105:ILE:HG13	2.19	0.41
3:a:305:VAL:HG11	3:b:220:LEU:HD22	2.03	0.41
1:c:5:LEU:HD12	1:c:5:LEU:H	1.85	0.41
3:g:251:ARG:HG2	3:g:254:SER:OG	2.20	0.41
3:h:105:TYR:HE1	3:h:108:SER:HA	1.85	0.41
2:k:1:MET:O	2:k:62:SER:N	2.52	0.41
2:l:127:LEU:HA	2:l:127:LEU:HD23	1.74	0.41
3:m:279:LEU:HD12	3:m:279:LEU:HA	1.94	0.41
2:r:52:GLU:OE2	2:r:52:GLU:HA	2.20	0.41
3:s:92:TYR:CE1	3:s:228:ILE:HD11	2.55	0.41
2:x:153:VAL:O	2:x:154:ASN:HB2	2.20	0.41
2:5:139:SER:OG	2:5:142:GLU:HG3	2.20	0.41
3:A:56:VAL:HG13	3:A:274:TYR:HE2	1.85	0.41
3:A:124:ALA:HB1	3:A:142:TYR:CZ	2.55	0.41
3:B:92:TYR:HD1	3:B:228:ILE:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:VAL:HG22	3:C:238:LEU:HD11	2.01	0.41
3:J:105:TYR:HE1	3:J:108:SER:HA	1.85	0.41
2:M:67:THR:O	2:M:68:ARG:HD3	2.21	0.41
3:O:251:ARG:HG2	3:O:254:SER:OG	2.20	0.41
1:Q:14:ALA:HA	1:Q:17:ILE:HG13	2.01	0.41
3:U:198:ILE:HD13	3:U:198:ILE:HA	1.93	0.41
2:Z:-1:LEU:H	2:Z:-1:LEU:HD23	1.86	0.41
3:a:82:ALA:O	3:a:287:SER:OG	2.31	0.41
3:h:264:THR:HG22	3:h:266:GLY:H	1.84	0.41
2:r:153:VAL:O	2:r:154:ASN:HB2	2.20	0.41
3:s:80:VAL:HG22	3:s:238:LEU:HD11	2.01	0.41
3:t:124:ALA:HB1	3:t:142:TYR:CZ	2.55	0.41
2:5:67:THR:O	2:5:68:ARG:HD3	2.21	0.41
3:B:80:VAL:O	3:B:83:ILE:HG12	2.20	0.41
3:B:145:ARG:NH2	3:B:169:PRO:O	2.52	0.41
3:B:305:VAL:HG11	3:D:220:LEU:HD22	2.03	0.41
3:I:78:VAL:HA	3:I:81:ILE:HG22	2.02	0.41
1:K:33:SER:O	1:K:33:SER:OG	2.33	0.41
2:M:217:GLY:C	2:w:205:TYR:CE1	2.98	0.41
2:S:102:ILE:O	2:S:106:ILE:HG12	2.20	0.41
2:T:153:VAL:O	2:T:154:ASN:HB2	2.20	0.41
2:T:217:GLY:C	2:l:205:TYR:HE1	2.28	0.41
3:U:225:SER:HA	3:U:228:ILE:HG12	2.01	0.41
2:Y:90:LEU:HD23	2:Y:90:LEU:HA	1.79	0.41
2:Y:95:THR:HG23	2:Y:98:ASP:H	1.85	0.41
3:a:321:ASP:OD1	3:a:322:GLU:N	2.47	0.41
3:b:264:THR:HG21	1:c:31:GLU:HG2	2.02	0.41
1:c:33:SER:O	1:c:33:SER:OG	2.33	0.41
3:g:78:VAL:HA	3:g:81:ILE:HG22	2.02	0.41
3:h:108:SER:HA	3:h:109:PRO:HD3	1.93	0.41
2:k:67:THR:O	2:k:68:ARG:HD3	2.21	0.41
2:k:68:ARG:HD3	2:k:68:ARG:HA	1.78	0.41
2:q:67:THR:O	2:q:68:ARG:HD3	2.21	0.41
3:s:59:ALA:HA	3:s:271:PRO:HG3	2.02	0.41
2:x:28:GLY:N	2:x:189:THR:HG22	2.23	0.41
2:5:68:ARG:HD3	2:5:68:ARG:HA	1.78	0.41
3:B:80:VAL:HG22	3:B:238:LEU:HD11	2.01	0.41
3:B:269:LEU:O	3:B:271:PRO:HD3	2.21	0.41
3:C:251:ARG:HG2	3:C:254:SER:OG	2.20	0.41
2:G:67:THR:O	2:G:68:ARG:HD3	2.21	0.41
2:G:95:THR:HG23	2:G:98:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:177:LEU:HD22	2:H:199:LEU:HG	2.01	0.41
1:K:14:ALA:HA	1:K:17:ILE:HG13	2.01	0.41
2:M:217:GLY:CA	2:w:205:TYR:CE1	3.03	0.41
3:O:305:VAL:HG11	3:P:220:LEU:HD22	2.03	0.41
3:P:124:ALA:HB1	3:P:142:TYR:CZ	2.55	0.41
3:P:264:THR:HG21	1:Q:31:GLU:HG2	2.02	0.41
1:W:5:LEU:HD12	1:W:5:LEU:H	1.85	0.41
1:W:14:ALA:HA	1:W:17:ILE:HG13	2.01	0.41
2:Y:139:SER:OG	2:Y:142:GLU:HG3	2.20	0.41
3:a:110:GLN:OE1	3:a:110:GLN:HA	2.20	0.41
2:e:11:TYR:OH	2:e:52:GLU:OE2	2.28	0.41
2:e:178:ARG:HA	2:e:181:GLU:HG3	2.02	0.41
3:g:70:LYS:HD2	3:g:70:LYS:HA	1.71	0.41
2:l:179:LEU:HD12	2:l:179:LEU:HA	1.96	0.41
3:m:80:VAL:O	3:m:83:ILE:HG12	2.20	0.41
3:m:110:GLN:OE1	3:m:110:GLN:HA	2.20	0.41
3:m:257:VAL:O	3:m:261:ILE:HG12	2.21	0.41
3:s:80:VAL:O	3:s:83:ILE:HG12	2.20	0.41
3:t:127:VAL:HG11	3:t:198:ILE:HD13	2.03	0.41
1:u:5:LEU:HD12	1:u:5:LEU:H	1.85	0.41
2:x:-1:LEU:HD23	2:x:-1:LEU:H	1.85	0.41
3:A:220:LEU:HD22	3:C:305:VAL:HG11	2.03	0.41
3:B:251:ARG:HG2	3:B:254:SER:OG	2.20	0.41
3:B:257:VAL:O	3:B:261:ILE:HG12	2.21	0.41
3:B:271:PRO:HG2	3:B:272:PHE:HD2	1.80	0.41
3:D:264:THR:HG21	1:E:31:GLU:HG2	2.02	0.41
2:G:139:SER:OG	2:G:142:GLU:HG3	2.19	0.41
3:I:80:VAL:HG22	3:I:238:LEU:HD11	2.01	0.41
3:U:246:LEU:HD23	3:U:246:LEU:HA	1.94	0.41
2:Y:132:LYS:HA	2:Y:132:LYS:HD3	1.85	0.41
2:f:7:VAL:O	2:f:20:GLY:N	2.53	0.41
3:g:80:VAL:O	3:g:83:ILE:HG12	2.20	0.41
3:h:124:ALA:HB1	3:h:142:TYR:CZ	2.55	0.41
3:h:127:VAL:HG11	3:h:198:ILE:HD13	2.03	0.41
3:h:259:LYS:HA	3:h:259:LYS:HD2	1.86	0.41
2:l:102:ILE:O	2:l:106:ILE:HG12	2.21	0.41
3:n:124:ALA:HB1	3:n:142:TYR:CZ	2.55	0.41
3:n:127:VAL:HG11	3:n:198:ILE:HD13	2.03	0.41
2:r:177:LEU:HD22	2:r:199:LEU:HG	2.01	0.41
3:s:251:ARG:HG2	3:s:254:SER:OG	2.20	0.41
2:x:177:LEU:HD22	2:x:199:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:31:GLU:HG2	3:A:264:THR:HG21	2.02	0.41
3:A:105:TYR:HE1	3:A:108:SER:HA	1.85	0.41
3:B:269:LEU:HD12	3:B:269:LEU:HA	1.86	0.41
3:C:268:ILE:HB	3:C:346:LEU:HD11	2.03	0.41
3:I:268:ILE:HB	3:I:346:LEU:HD11	2.03	0.41
2:T:208:LEU:HD23	2:T:215:LEU:HD11	2.03	0.41
3:U:82:ALA:O	3:U:287:SER:OG	2.31	0.41
3:V:56:VAL:HG13	3:V:274:TYR:HE2	1.85	0.41
3:V:105:TYR:HE1	3:V:108:SER:HA	1.85	0.41
3:V:127:VAL:HG11	3:V:198:ILE:HD13	2.03	0.41
2:Z:153:VAL:O	2:Z:154:ASN:HB2	2.20	0.41
3:a:80:VAL:O	3:a:83:ILE:HG12	2.20	0.41
1:i:5:LEU:HD12	1:i:5:LEU:H	1.85	0.41
2:k:125:VAL:HG12	2:k:179:LEU:HD21	2.01	0.41
2:l:-1:LEU:HD23	2:l:-1:LEU:H	1.86	0.41
2:l:177:LEU:HD22	2:l:199:LEU:HG	2.01	0.41
3:n:105:TYR:HE1	3:n:108:SER:HA	1.85	0.41
3:s:245:ARG:NH1	3:s:245:ARG:HB2	2.36	0.41
3:t:232:MET:HG2	3:t:232:MET:H	1.60	0.41
2:x:102:ILE:O	2:x:106:ILE:HG12	2.21	0.41
3:A:273:LEU:HD23	3:A:273:LEU:HA	1.84	0.41
3:B:110:GLN:OE1	3:B:110:GLN:HA	2.20	0.41
3:C:255:ILE:HD11	3:C:272:PHE:HE2	1.86	0.41
3:C:257:VAL:O	3:C:261:ILE:HG12	2.21	0.41
1:E:5:LEU:HD12	1:E:5:LEU:H	1.85	0.41
2:H:153:VAL:O	2:H:154:ASN:HB2	2.20	0.41
2:H:215:LEU:HG	2:H:216:HIS:N	2.36	0.41
3:I:246:LEU:HD23	3:I:246:LEU:HA	1.94	0.41
3:P:127:VAL:HG11	3:P:198:ILE:HD13	2.03	0.41
2:S:139:SER:OG	2:S:142:GLU:HG3	2.20	0.41
2:T:-1:LEU:HD23	2:T:-1:LEU:H	1.86	0.41
3:U:245:ARG:NH1	3:U:245:ARG:HB2	2.36	0.41
3:V:124:ALA:HB1	3:V:142:TYR:CZ	2.55	0.41
3:V:264:THR:HG21	1:W:31:GLU:HG2	2.02	0.41
2:Y:102:ILE:O	2:Y:106:ILE:HG12	2.20	0.41
2:Z:122:LEU:HD13	2:Z:131:ALA:HB2	2.03	0.41
2:f:-1:LEU:H	2:f:-1:LEU:HD23	1.86	0.41
2:f:122:LEU:HD13	2:f:131:ALA:HB2	2.03	0.41
3:g:245:ARG:HH12	3:g:249:PHE:CA	2.33	0.41
3:g:245:ARG:NH1	3:g:245:ARG:HB2	2.36	0.41
2:l:136:ILE:HD12	2:l:136:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:125:VAL:HG12	2:q:179:LEU:HD21	2.02	0.41
3:s:245:ARG:HH12	3:s:249:PHE:CA	2.33	0.41
3:s:257:VAL:O	3:s:261:ILE:HG12	2.21	0.41
2:w:67:THR:O	2:w:68:ARG:HD3	2.21	0.41
2:x:208:LEU:HD23	2:x:215:LEU:HD11	2.03	0.41
2:5:95:THR:HG23	2:5:98:ASP:H	1.85	0.41
2:5:217:GLY:CA	2:k:205:TYR:CE1	3.04	0.41
3:A:145:ARG:NH2	3:A:168:ASN:O	2.54	0.41
3:A:259:LYS:HA	3:A:259:LYS:HD2	1.86	0.41
3:B:245:ARG:HH12	3:B:249:PHE:CA	2.33	0.41
3:B:268:ILE:HB	3:B:346:LEU:HD11	2.03	0.41
3:C:78:VAL:HA	3:C:81:ILE:HG22	2.02	0.41
3:D:259:LYS:HD2	3:D:259:LYS:HA	1.86	0.41
3:I:59:ALA:HA	3:I:271:PRO:HD3	2.02	0.41
3:I:305:VAL:HG11	3:J:220:LEU:HD22	2.03	0.41
3:J:56:VAL:HG13	3:J:274:TYR:HE2	1.85	0.41
3:J:124:ALA:HB1	3:J:142:TYR:CZ	2.55	0.41
3:J:145:ARG:NH2	3:J:168:ASN:O	2.54	0.41
3:J:264:THR:HG21	1:K:31:GLU:HG2	2.02	0.41
1:K:5:LEU:HD12	1:K:5:LEU:H	1.85	0.41
3:O:245:ARG:NH1	3:O:245:ARG:HB2	2.36	0.41
3:O:255:ILE:HD11	3:O:272:PHE:CE2	2.56	0.41
3:P:145:ARG:NH2	3:P:168:ASN:O	2.54	0.41
2:T:122:LEU:HD13	2:T:131:ALA:HB2	2.03	0.41
3:U:110:GLN:HA	3:U:110:GLN:OE1	2.20	0.41
2:Y:1:MET:O	2:Y:62:SER:N	2.52	0.41
2:Y:67:THR:O	2:Y:68:ARG:HD3	2.21	0.41
2:Y:125:VAL:HG12	2:Y:179:LEU:HD21	2.02	0.41
2:Z:102:ILE:O	2:Z:106:ILE:HG12	2.21	0.41
3:a:198:ILE:HD13	3:a:198:ILE:HA	1.93	0.41
3:a:268:ILE:C	3:a:270:ARG:N	2.79	0.41
3:b:105:TYR:HE1	3:b:108:SER:HA	1.85	0.41
3:b:145:ARG:NH2	3:b:168:ASN:O	2.54	0.41
3:b:259:LYS:HD2	3:b:259:LYS:HA	1.86	0.41
2:e:139:SER:OG	2:e:142:GLU:HG3	2.19	0.41
2:f:197:ILE:HD12	2:f:197:ILE:HA	1.87	0.41
2:f:208:LEU:HD23	2:f:215:LEU:HD11	2.03	0.41
3:g:59:ALA:HB1	3:g:271:PRO:HD3	2.03	0.41
2:l:153:VAL:O	2:l:154:ASN:HB2	2.20	0.41
2:l:208:LEU:HD23	2:l:215:LEU:HD11	2.03	0.41
3:m:78:VAL:HA	3:m:81:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:108:SER:HA	3:n:109:PRO:HD3	1.93	0.41
3:s:70:LYS:HD2	3:s:70:LYS:HA	1.71	0.41
3:s:270:ARG:C	3:s:272:PHE:N	2.79	0.41
3:t:145:ARG:NH2	3:t:168:ASN:O	2.54	0.41
3:t:264:THR:HG21	1:u:31:GLU:HG2	2.02	0.41
2:w:125:VAL:HG12	2:w:179:LEU:HD21	2.02	0.41
2:6:177:LEU:HD22	2:6:199:LEU:HG	2.01	0.41
3:J:127:VAL:HG11	3:J:198:ILE:HD13	2.03	0.41
2:N:215:LEU:HG	2:N:216:HIS:N	2.36	0.41
3:U:255:ILE:HD11	3:U:272:PHE:CE2	2.56	0.41
1:W:8:ILE:H	1:W:8:ILE:HG12	1.64	0.41
2:Z:208:LEU:HD23	2:Z:215:LEU:HD11	2.03	0.41
3:a:245:ARG:NH1	3:a:245:ARG:HB2	2.36	0.41
2:e:67:THR:O	2:e:68:ARG:HD3	2.21	0.41
2:e:135:PRO:O	2:e:143:GLN:NE2	2.50	0.41
3:g:257:VAL:O	3:g:261:ILE:HG12	2.21	0.41
3:h:145:ARG:NH2	3:h:168:ASN:O	2.54	0.41
3:h:264:THR:HG21	1:i:31:GLU:HG2	2.02	0.41
3:m:123:ALA:O	3:m:127:VAL:HG23	2.21	0.41
3:m:181:ASP:OD1	3:m:181:ASP:N	2.48	0.41
2:r:-1:LEU:HD23	2:r:-1:LEU:H	1.85	0.41
2:r:208:LEU:HD23	2:r:215:LEU:HD11	2.03	0.41
2:r:215:LEU:HG	2:r:216:HIS:N	2.36	0.41
2:5:90:LEU:HD23	2:5:90:LEU:HA	1.79	0.40
2:5:181:GLU:OE2	2:5:205:TYR:OH	2.23	0.40
3:A:127:VAL:HG11	3:A:198:ILE:HD13	2.03	0.40
3:B:170:LEU:HD12	3:B:170:LEU:HA	1.92	0.40
3:C:92:TYR:HD1	3:C:228:ILE:HD11	1.85	0.40
3:C:217:LEU:C	3:C:219:GLY:H	2.29	0.40
3:C:245:ARG:NH1	3:C:245:ARG:HB2	2.36	0.40
3:D:105:TYR:HE1	3:D:108:SER:HA	1.85	0.40
3:I:217:LEU:C	3:I:219:GLY:H	2.30	0.40
3:I:245:ARG:NH1	3:I:245:ARG:HB2	2.36	0.40
2:M:1:MET:O	2:M:62:SER:N	2.52	0.40
3:O:110:GLN:OE1	3:O:110:GLN:HA	2.20	0.40
2:T:216:HIS:HB3	2:T:217:GLY:H	1.64	0.40
3:b:127:VAL:HG11	3:b:198:ILE:HD13	2.03	0.40
3:g:91:CYS:SG	3:g:224:VAL:HG13	2.61	0.40
3:g:217:LEU:C	3:g:219:GLY:H	2.29	0.40
3:m:217:LEU:C	3:m:219:GLY:H	2.29	0.40
3:m:245:ARG:NH1	3:m:245:ARG:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:95:THR:HG23	2:q:98:ASP:H	1.85	0.40
2:r:102:ILE:O	2:r:106:ILE:HG12	2.21	0.40
2:x:215:LEU:HG	2:x:216:HIS:N	2.36	0.40
2:6:215:LEU:HG	2:6:216:HIS:N	2.36	0.40
3:B:78:VAL:HA	3:B:81:ILE:HG22	2.02	0.40
3:C:245:ARG:HH12	3:C:249:PHE:CA	2.33	0.40
2:H:-1:LEU:H	2:H:-1:LEU:HD23	1.86	0.40
3:I:257:VAL:O	3:I:261:ILE:HG12	2.21	0.40
2:M:91:LEU:HD13	2:M:94:ARG:HH12	1.86	0.40
2:N:177:LEU:HD22	2:N:199:LEU:HG	2.01	0.40
3:U:251:ARG:HG2	3:U:254:SER:OG	2.20	0.40
3:U:257:VAL:O	3:U:261:ILE:HG12	2.21	0.40
3:V:145:ARG:NH2	3:V:168:ASN:O	2.54	0.40
3:a:270:ARG:C	3:a:272:PHE:N	2.78	0.40
3:h:248:ILE:HG13	3:h:248:ILE:H	1.76	0.40
3:m:91:CYS:SG	3:m:224:VAL:HG13	2.61	0.40
3:n:264:THR:HG21	1:o:31:GLU:HG2	2.02	0.40
2:r:127:LEU:HD23	2:r:127:LEU:HA	1.74	0.40
3:t:273:LEU:HD23	3:t:273:LEU:HA	1.84	0.40
1:u:8:ILE:H	1:u:8:ILE:HG12	1.64	0.40
2:x:74:VAL:N	2:x:75:PRO:HD2	2.36	0.40
1:1:5:LEU:H	1:1:5:LEU:HD12	1.85	0.40
2:6:-1:LEU:H	2:6:-1:LEU:HD23	1.85	0.40
3:B:181:ASP:OD1	3:B:181:ASP:N	2.48	0.40
3:C:88:PRO:HD3	3:C:231:LEU:HD21	2.03	0.40
3:D:145:ARG:NH2	3:D:168:ASN:O	2.54	0.40
3:D:281:PHE:O	3:D:285:LEU:HD23	2.22	0.40
3:I:245:ARG:HH12	3:I:249:PHE:CA	2.33	0.40
2:M:95:THR:HG23	2:M:98:ASP:H	1.85	0.40
3:O:198:ILE:HD13	3:O:198:ILE:HA	1.93	0.40
3:P:105:TYR:HE1	3:P:108:SER:HA	1.85	0.40
3:U:123:ALA:O	3:U:127:VAL:HG23	2.21	0.40
3:U:217:LEU:C	3:U:219:GLY:H	2.30	0.40
2:Z:128:LEU:HD12	2:Z:128:LEU:HA	1.92	0.40
2:e:91:LEU:HD13	2:e:94:ARG:HH12	1.86	0.40
2:f:74:VAL:N	2:f:75:PRO:HD2	2.36	0.40
3:g:123:ALA:O	3:g:127:VAL:HG23	2.21	0.40
3:h:232:MET:HG2	3:h:232:MET:H	1.60	0.40
2:k:11:TYR:OH	2:k:52:GLU:OE2	2.28	0.40
2:l:1:MET:HE2	2:l:1:MET:HB2	2.01	0.40
3:m:255:ILE:HD11	3:m:272:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:340:LEU:HA	3:m:343:VAL:HG22	2.03	0.40
3:I:88:PRO:HD3	3:I:231:LEU:HD21	2.04	0.40
2:S:91:LEU:HD13	2:S:94:ARG:HH12	1.86	0.40
3:U:78:VAL:HA	3:U:81:ILE:HG22	2.02	0.40
3:U:81:ILE:HD12	3:U:81:ILE:HA	1.87	0.40
3:U:91:CYS:SG	3:U:224:VAL:HG13	2.61	0.40
3:U:305:VAL:HG11	3:V:220:LEU:HD22	2.03	0.40
3:V:273:LEU:HD23	3:V:273:LEU:HA	1.84	0.40
2:Z:179:LEU:HD12	2:Z:179:LEU:HA	1.96	0.40
2:Z:217:GLY:C	2:r:205:TYR:HE1	2.30	0.40
3:a:81:ILE:HD12	3:a:81:ILE:HA	1.87	0.40
3:g:268:ILE:HB	3:g:346:LEU:HD11	2.03	0.40
3:g:298:LEU:HD22	3:h:224:VAL:HG22	2.04	0.40
2:k:95:THR:HG23	2:k:98:ASP:H	1.85	0.40
2:l:215:LEU:HG	2:l:216:HIS:N	2.36	0.40
3:m:305:VAL:HG11	3:n:220:LEU:HD22	2.03	0.40
3:n:145:ARG:NH2	3:n:168:ASN:O	2.54	0.40
2:q:91:LEU:HD13	2:q:94:ARG:HH12	1.86	0.40
2:q:167:ASN:OD1	2:q:167:ASN:N	2.55	0.40
3:s:91:CYS:SG	3:s:224:VAL:HG13	2.61	0.40
3:t:248:ILE:HG13	3:t:248:ILE:H	1.76	0.40
2:w:95:THR:HG23	2:w:98:ASP:H	1.85	0.40
2:x:130:LYS:HD3	2:x:133:ASN:OD1	2.22	0.40
1:1:7:LEU:HD23	1:1:7:LEU:HA	1.93	0.40
1:2:7:LEU:HD23	1:2:7:LEU:HA	1.87	0.40
2:5:1:MET:O	2:5:62:SER:N	2.52	0.40
2:5:91:LEU:HD13	2:5:94:ARG:HH12	1.86	0.40
2:5:217:GLY:CA	2:k:205:TYR:HE1	2.34	0.40
2:6:7:VAL:O	2:6:20:GLY:N	2.53	0.40
3:B:88:PRO:HD3	3:B:231:LEU:HD21	2.04	0.40
2:H:51:ILE:HA	2:H:78:ARG:HH21	1.86	0.40
2:H:102:ILE:O	2:H:106:ILE:HG12	2.21	0.40
2:H:130:LYS:HD3	2:H:133:ASN:OD1	2.22	0.40
3:I:91:CYS:SG	3:I:224:VAL:HG13	2.61	0.40
3:I:298:LEU:HD22	3:J:224:VAL:HG22	2.04	0.40
2:N:-1:LEU:HD23	2:N:-1:LEU:H	1.85	0.40
3:O:123:ALA:O	3:O:127:VAL:HG23	2.22	0.40
3:O:181:ASP:OD1	3:O:181:ASP:N	2.48	0.40
3:O:257:VAL:O	3:O:261:ILE:HG12	2.21	0.40
2:S:1:MET:O	2:S:62:SER:N	2.52	0.40
2:S:74:VAL:N	2:S:75:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:65:ASP:OD1	2:Y:67:THR:OG1	2.37	0.40
2:Z:136:ILE:HD12	2:Z:136:ILE:HA	1.93	0.40
3:h:273:LEU:HD23	3:h:273:LEU:HA	1.84	0.40
1:j:35:MET:O	2:k:64:HIS:NE2	2.55	0.40
3:m:268:ILE:HB	3:m:346:LEU:HD11	2.03	0.40
3:n:248:ILE:HG13	3:n:248:ILE:H	1.76	0.40
3:s:217:LEU:C	3:s:219:GLY:H	2.30	0.40
3:s:321:ASP:OD1	3:s:322:GLU:N	2.47	0.40
1:v:35:MET:O	2:w:64:HIS:NE2	2.55	0.40
2:x:179:LEU:HD12	2:x:179:LEU:HA	1.96	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	1	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	2	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	E	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	F	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	K	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	L	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	Q	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	R	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	W	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	X	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	c	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	d	31/328 (10%)	29 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	j	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	o	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	p	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
1	u	31/328 (10%)	30 (97%)	1 (3%)	0	100	100
1	v	31/328 (10%)	29 (94%)	2 (6%)	0	100	100
2	5	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	6	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	G	220/226 (97%)	205 (93%)	15 (7%)	0	100	100
2	H	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	M	220/226 (97%)	208 (94%)	12 (6%)	0	100	100
2	N	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	S	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	T	219/226 (97%)	208 (95%)	11 (5%)	0	100	100
2	Y	220/226 (97%)	208 (94%)	12 (6%)	0	100	100
2	Z	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	e	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	f	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	k	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	l	219/226 (97%)	208 (95%)	11 (5%)	0	100	100
2	q	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	r	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
2	w	220/226 (97%)	207 (94%)	13 (6%)	0	100	100
2	x	219/226 (97%)	209 (95%)	10 (5%)	0	100	100
3	A	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	B	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	13	42
3	C	288/352 (82%)	265 (92%)	21 (7%)	2 (1%)	19	50
3	D	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	I	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	34
3	J	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	O	288/352 (82%)	264 (92%)	21 (7%)	3 (1%)	13	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	U	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	13	42
3	V	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	a	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	34
3	b	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	g	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	34
3	h	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	m	288/352 (82%)	263 (91%)	22 (8%)	3 (1%)	13	42
3	n	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
3	s	288/352 (82%)	263 (91%)	21 (7%)	4 (1%)	9	34
3	t	289/352 (82%)	275 (95%)	12 (4%)	2 (1%)	19	50
All	All	9702/16308 (60%)	9118 (94%)	536 (6%)	48 (0%)	27	56

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	201	ILE
3	B	272	PHE
3	D	201	ILE
3	I	270	ARG
3	I	271	PRO
3	J	201	ILE
3	O	270	ARG
3	O	271	PRO
3	P	201	ILE
3	U	271	PRO
3	V	201	ILE
3	a	271	PRO
3	b	201	ILE
3	g	270	ARG
3	g	271	PRO
3	h	201	ILE
3	m	271	PRO
3	n	201	ILE
3	s	271	PRO
3	t	201	ILE
3	I	272	PHE
3	a	270	ARG

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Mol	Chain	Res	Type
3	s	270	ARG
3	A	202	ASP
3	C	270	ARG
3	D	202	ASP
3	J	202	ASP
3	P	202	ASP
3	V	202	ASP
3	a	272	PHE
3	b	202	ASP
3	g	272	PHE
3	h	202	ASP
3	n	202	ASP
3	s	272	PHE
3	t	202	ASP
3	B	245	ARG
3	B	271	PRO
3	C	245	ARG
3	I	245	ARG
3	O	245	ARG
3	U	245	ARG
3	U	270	ARG
3	a	245	ARG
3	g	245	ARG
3	m	245	ARG
3	s	245	ARG
3	m	270	ARG

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	1	28/279 (10%)	28 (100%)	0	100	100
1	2	28/279 (10%)	28 (100%)	0	100	100
1	E	28/279 (10%)	28 (100%)	0	100	100
1	F	28/279 (10%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	28/279 (10%)	28 (100%)	0	100	100
1	L	28/279 (10%)	28 (100%)	0	100	100
1	Q	28/279 (10%)	28 (100%)	0	100	100
1	R	28/279 (10%)	28 (100%)	0	100	100
1	W	28/279 (10%)	28 (100%)	0	100	100
1	X	28/279 (10%)	28 (100%)	0	100	100
1	c	28/279 (10%)	28 (100%)	0	100	100
1	d	28/279 (10%)	28 (100%)	0	100	100
1	i	28/279 (10%)	28 (100%)	0	100	100
1	j	28/279 (10%)	28 (100%)	0	100	100
1	o	28/279 (10%)	28 (100%)	0	100	100
1	p	28/279 (10%)	27 (96%)	1 (4%)	30	57
1	u	28/279 (10%)	28 (100%)	0	100	100
1	v	28/279 (10%)	28 (100%)	0	100	100
2	5	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	6	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	G	181/184 (98%)	178 (98%)	3 (2%)	56	74
2	H	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	M	181/184 (98%)	178 (98%)	3 (2%)	56	74
2	N	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	S	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	T	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	Y	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	Z	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	e	181/184 (98%)	178 (98%)	3 (2%)	56	74
2	f	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	k	181/184 (98%)	180 (99%)	1 (1%)	84	90
2	l	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	q	181/184 (98%)	181 (100%)	0	100	100
2	r	181/184 (98%)	179 (99%)	2 (1%)	70	82
2	w	181/184 (98%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	x	181/184 (98%)	179 (99%)	2 (1%)	70	82
3	A	222/289 (77%)	222 (100%)	0	100	100
3	B	231/289 (80%)	228 (99%)	3 (1%)	65	79
3	C	231/289 (80%)	228 (99%)	3 (1%)	65	79
3	D	222/289 (77%)	222 (100%)	0	100	100
3	I	231/289 (80%)	226 (98%)	5 (2%)	47	69
3	J	222/289 (77%)	222 (100%)	0	100	100
3	O	231/289 (80%)	227 (98%)	4 (2%)	56	74
3	P	222/289 (77%)	222 (100%)	0	100	100
3	U	231/289 (80%)	228 (99%)	3 (1%)	65	79
3	V	222/289 (77%)	222 (100%)	0	100	100
3	a	231/289 (80%)	228 (99%)	3 (1%)	65	79
3	b	222/289 (77%)	222 (100%)	0	100	100
3	g	231/289 (80%)	228 (99%)	3 (1%)	65	79
3	h	222/289 (77%)	222 (100%)	0	100	100
3	m	231/289 (80%)	227 (98%)	4 (2%)	56	74
3	n	222/289 (77%)	222 (100%)	0	100	100
3	s	231/289 (80%)	229 (99%)	2 (1%)	75	85
3	t	222/289 (77%)	222 (100%)	0	100	100
All	All	7839/13536 (58%)	7779 (99%)	60 (1%)	77	87

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5	178	ARG
2	6	188	VAL
3	B	232	MET
3	B	269	LEU
3	B	270	ARG
3	C	232	MET
3	C	243	SER
3	C	269	LEU
2	G	177	LEU
2	G	178	ARG
2	G	179	LEU

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Mol	Chain	Res	Type
2	H	188	VAL
3	I	206	MET
3	I	232	MET
3	I	243	SER
3	I	269	LEU
3	I	270	ARG
2	M	170	ASP
2	M	177	LEU
2	M	178	ARG
2	N	178	ARG
2	N	188	VAL
3	O	232	MET
3	O	243	SER
3	O	270	ARG
3	O	271	PRO
2	S	178	ARG
2	T	178	ARG
2	T	188	VAL
3	U	232	MET
3	U	243	SER
3	U	271	PRO
2	Y	178	ARG
2	Z	178	ARG
2	Z	188	VAL
3	a	232	MET
3	a	243	SER
3	a	270	ARG
2	e	176	ILE
2	e	177	LEU
2	e	179	LEU
2	f	178	ARG
2	f	188	VAL
3	g	232	MET
3	g	270	ARG
3	g	271	PRO
2	k	178	ARG
2	l	178	ARG
2	l	188	VAL
3	m	232	MET
3	m	243	SER
3	m	270	ARG
3	m	271	PRO

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Mol	Chain	Res	Type
1	p	21	LEU
2	r	178	ARG
2	r	188	VAL
3	s	232	MET
3	s	270	ARG
2	x	178	ARG
2	x	188	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	5	71	ASN
2	5	214	HIS
2	6	26	GLN
2	6	214	HIS
3	B	132	GLN
3	B	242	ASN
3	C	132	GLN
3	C	242	ASN
2	G	71	ASN
2	G	214	HIS
2	H	26	GLN
2	H	214	HIS
3	I	132	GLN
3	I	242	ASN
2	M	71	ASN
2	M	214	HIS
2	N	26	GLN
2	N	214	HIS
3	O	132	GLN
3	O	242	ASN
2	S	71	ASN
2	S	214	HIS
2	T	26	GLN
2	T	214	HIS
3	U	132	GLN
3	U	242	ASN
2	Y	71	ASN
2	Y	214	HIS
2	Z	26	GLN
2	Z	214	HIS
3	a	132	GLN

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Mol	Chain	Res	Type
3	a	242	ASN
2	e	71	ASN
2	f	26	GLN
2	f	214	HIS
2	f	216	HIS
3	g	132	GLN
3	g	242	ASN
2	k	71	ASN
2	k	214	HIS
2	l	26	GLN
2	l	184	ASN
2	l	214	HIS
3	m	132	GLN
3	m	242	ASN
2	q	71	ASN
2	q	214	HIS
2	r	26	GLN
2	r	214	HIS
2	r	216	HIS
3	s	132	GLN
3	s	242	ASN
2	w	71	ASN
2	x	26	GLN
2	x	214	HIS
2	x	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands 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
4	AGS	r	301	-	26,33,33	0.73	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	q	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	6	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	M	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	S	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	k	301	-	26,33,33	0.73	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	Z	301	-	26,33,33	0.75	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	e	301	-	26,33,33	0.73	1 (3%)	26,52,52	1.03	2 (7%)
4	AGS	N	301	-	26,33,33	0.75	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	l	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	T	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	f	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	H	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)
4	AGS	w	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	Y	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	G	301	-	26,33,33	0.75	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	5	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.02	2 (7%)
4	AGS	x	301	-	26,33,33	0.74	1 (3%)	26,52,52	1.06	2 (7%)

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
4	AGS	r	301	-	-	4/17/38/38	0/3/3/3
4	AGS	q	301	-	-	6/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	6	301	-	-	4/17/38/38	0/3/3/3
4	AGS	M	301	-	-	6/17/38/38	0/3/3/3
4	AGS	S	301	-	-	6/17/38/38	0/3/3/3
4	AGS	k	301	-	-	6/17/38/38	0/3/3/3
4	AGS	Z	301	-	-	4/17/38/38	0/3/3/3
4	AGS	e	301	-	-	6/17/38/38	0/3/3/3
4	AGS	N	301	-	-	4/17/38/38	0/3/3/3
4	AGS	l	301	-	-	4/17/38/38	0/3/3/3
4	AGS	T	301	-	-	4/17/38/38	0/3/3/3
4	AGS	f	301	-	-	4/17/38/38	0/3/3/3
4	AGS	H	301	-	-	4/17/38/38	0/3/3/3
4	AGS	w	301	-	-	6/17/38/38	0/3/3/3
4	AGS	Y	301	-	-	6/17/38/38	0/3/3/3
4	AGS	G	301	-	-	6/17/38/38	0/3/3/3
4	AGS	5	301	-	-	6/17/38/38	0/3/3/3
4	AGS	x	301	-	-	4/17/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	301	AGS	PG-S1G	2.11	1.95	1.90
4	G	301	AGS	PG-S1G	2.09	1.95	1.90
4	Z	301	AGS	PG-S1G	2.08	1.95	1.90
4	q	301	AGS	PG-S1G	2.08	1.95	1.90
4	6	301	AGS	PG-S1G	2.07	1.95	1.90
4	x	301	AGS	PG-S1G	2.07	1.95	1.90
4	f	301	AGS	PG-S1G	2.07	1.95	1.90
4	M	301	AGS	PG-S1G	2.06	1.95	1.90
4	l	301	AGS	PG-S1G	2.06	1.95	1.90
4	T	301	AGS	PG-S1G	2.06	1.95	1.90
4	r	301	AGS	PG-S1G	2.06	1.95	1.90
4	e	301	AGS	PG-S1G	2.05	1.95	1.90
4	5	301	AGS	PG-S1G	2.05	1.95	1.90
4	Y	301	AGS	PG-S1G	2.04	1.95	1.90
4	H	301	AGS	PG-S1G	2.04	1.95	1.90
4	w	301	AGS	PG-S1G	2.04	1.95	1.90
4	S	301	AGS	PG-S1G	2.03	1.95	1.90
4	k	301	AGS	PG-S1G	2.02	1.95	1.90

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	l	301	AGS	PA-O3A-PB	-3.81	119.75	132.83
4	f	301	AGS	PA-O3A-PB	-3.81	119.75	132.83
4	r	301	AGS	PA-O3A-PB	-3.81	119.76	132.83
4	H	301	AGS	PA-O3A-PB	-3.80	119.77	132.83
4	N	301	AGS	PA-O3A-PB	-3.80	119.78	132.83
4	6	301	AGS	PA-O3A-PB	-3.80	119.80	132.83
4	Z	301	AGS	PA-O3A-PB	-3.80	119.80	132.83
4	T	301	AGS	PA-O3A-PB	-3.80	119.80	132.83
4	x	301	AGS	PA-O3A-PB	-3.79	119.84	132.83
4	G	301	AGS	PA-O3A-PB	-3.73	120.04	132.83
4	M	301	AGS	PA-O3A-PB	-3.72	120.07	132.83
4	e	301	AGS	PA-O3A-PB	-3.72	120.07	132.83
4	q	301	AGS	PA-O3A-PB	-3.72	120.07	132.83
4	5	301	AGS	PA-O3A-PB	-3.72	120.08	132.83
4	k	301	AGS	PA-O3A-PB	-3.71	120.08	132.83
4	Y	301	AGS	PA-O3A-PB	-3.71	120.08	132.83
4	w	301	AGS	PA-O3A-PB	-3.71	120.09	132.83
4	S	301	AGS	PA-O3A-PB	-3.71	120.10	132.83
4	f	301	AGS	C5-C6-N6	2.31	123.86	120.35
4	T	301	AGS	C5-C6-N6	2.30	123.84	120.35
4	r	301	AGS	C5-C6-N6	2.29	123.84	120.35
4	l	301	AGS	C5-C6-N6	2.29	123.84	120.35
4	Z	301	AGS	C5-C6-N6	2.29	123.83	120.35
4	x	301	AGS	C5-C6-N6	2.29	123.83	120.35
4	6	301	AGS	C5-C6-N6	2.28	123.82	120.35
4	N	301	AGS	C5-C6-N6	2.28	123.82	120.35
4	e	301	AGS	C5-C6-N6	2.28	123.81	120.35
4	w	301	AGS	C5-C6-N6	2.26	123.79	120.35
4	S	301	AGS	C5-C6-N6	2.26	123.79	120.35
4	5	301	AGS	C5-C6-N6	2.26	123.79	120.35
4	Y	301	AGS	C5-C6-N6	2.26	123.79	120.35
4	k	301	AGS	C5-C6-N6	2.26	123.78	120.35
4	H	301	AGS	C5-C6-N6	2.25	123.77	120.35
4	G	301	AGS	C5-C6-N6	2.25	123.77	120.35
4	M	301	AGS	C5-C6-N6	2.24	123.76	120.35
4	q	301	AGS	C5-C6-N6	2.24	123.75	120.35

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	301	AGS	PB-O3B-PG-O2G
4	5	301	AGS	PB-O3B-PG-O3G
4	5	301	AGS	C5'-O5'-PA-O1A
4	5	301	AGS	O4'-C4'-C5'-O5'
4	6	301	AGS	PB-O3B-PG-O2G
4	6	301	AGS	PB-O3B-PG-O3G
4	6	301	AGS	C5'-O5'-PA-O1A
4	G	301	AGS	PB-O3B-PG-O2G
4	G	301	AGS	PB-O3B-PG-O3G
4	G	301	AGS	C5'-O5'-PA-O1A
4	G	301	AGS	O4'-C4'-C5'-O5'
4	H	301	AGS	PB-O3B-PG-O2G
4	H	301	AGS	PB-O3B-PG-O3G
4	H	301	AGS	C5'-O5'-PA-O1A
4	M	301	AGS	PB-O3B-PG-O2G
4	M	301	AGS	PB-O3B-PG-O3G
4	M	301	AGS	C5'-O5'-PA-O1A
4	M	301	AGS	O4'-C4'-C5'-O5'
4	N	301	AGS	PB-O3B-PG-O2G
4	N	301	AGS	PB-O3B-PG-O3G
4	N	301	AGS	C5'-O5'-PA-O1A
4	S	301	AGS	PB-O3B-PG-O2G
4	S	301	AGS	PB-O3B-PG-O3G
4	S	301	AGS	C5'-O5'-PA-O1A
4	S	301	AGS	O4'-C4'-C5'-O5'
4	T	301	AGS	PB-O3B-PG-O2G
4	T	301	AGS	PB-O3B-PG-O3G
4	T	301	AGS	C5'-O5'-PA-O1A
4	Y	301	AGS	PB-O3B-PG-O2G
4	Y	301	AGS	PB-O3B-PG-O3G
4	Y	301	AGS	C5'-O5'-PA-O1A
4	Y	301	AGS	O4'-C4'-C5'-O5'
4	Z	301	AGS	PB-O3B-PG-O2G
4	Z	301	AGS	PB-O3B-PG-O3G
4	Z	301	AGS	C5'-O5'-PA-O1A
4	e	301	AGS	PB-O3B-PG-O2G
4	e	301	AGS	PB-O3B-PG-O3G
4	e	301	AGS	C5'-O5'-PA-O1A
4	e	301	AGS	O4'-C4'-C5'-O5'
4	f	301	AGS	PB-O3B-PG-O2G
4	f	301	AGS	PB-O3B-PG-O3G
4	f	301	AGS	C5'-O5'-PA-O1A
4	k	301	AGS	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
4	k	301	AGS	PB-O3B-PG-O3G
4	k	301	AGS	C5'-O5'-PA-O1A
4	k	301	AGS	O4'-C4'-C5'-O5'
4	l	301	AGS	PB-O3B-PG-O2G
4	l	301	AGS	PB-O3B-PG-O3G
4	l	301	AGS	C5'-O5'-PA-O1A
4	q	301	AGS	PB-O3B-PG-O2G
4	q	301	AGS	PB-O3B-PG-O3G
4	q	301	AGS	C5'-O5'-PA-O1A
4	q	301	AGS	O4'-C4'-C5'-O5'
4	r	301	AGS	PB-O3B-PG-O2G
4	r	301	AGS	PB-O3B-PG-O3G
4	r	301	AGS	C5'-O5'-PA-O1A
4	w	301	AGS	PB-O3B-PG-O2G
4	w	301	AGS	PB-O3B-PG-O3G
4	w	301	AGS	C5'-O5'-PA-O1A
4	w	301	AGS	O4'-C4'-C5'-O5'
4	x	301	AGS	PB-O3B-PG-O2G
4	x	301	AGS	PB-O3B-PG-O3G
4	x	301	AGS	C5'-O5'-PA-O1A
4	5	301	AGS	C3'-C4'-C5'-O5'
4	G	301	AGS	C3'-C4'-C5'-O5'
4	M	301	AGS	C3'-C4'-C5'-O5'
4	S	301	AGS	C3'-C4'-C5'-O5'
4	Y	301	AGS	C3'-C4'-C5'-O5'
4	e	301	AGS	C3'-C4'-C5'-O5'
4	k	301	AGS	C3'-C4'-C5'-O5'
4	q	301	AGS	C3'-C4'-C5'-O5'
4	w	301	AGS	C3'-C4'-C5'-O5'
4	5	301	AGS	C5'-O5'-PA-O3A
4	6	301	AGS	C5'-O5'-PA-O3A
4	G	301	AGS	C5'-O5'-PA-O3A
4	H	301	AGS	C5'-O5'-PA-O3A
4	M	301	AGS	C5'-O5'-PA-O3A
4	N	301	AGS	C5'-O5'-PA-O3A
4	S	301	AGS	C5'-O5'-PA-O3A
4	T	301	AGS	C5'-O5'-PA-O3A
4	Y	301	AGS	C5'-O5'-PA-O3A
4	Z	301	AGS	C5'-O5'-PA-O3A
4	e	301	AGS	C5'-O5'-PA-O3A
4	f	301	AGS	C5'-O5'-PA-O3A
4	k	301	AGS	C5'-O5'-PA-O3A

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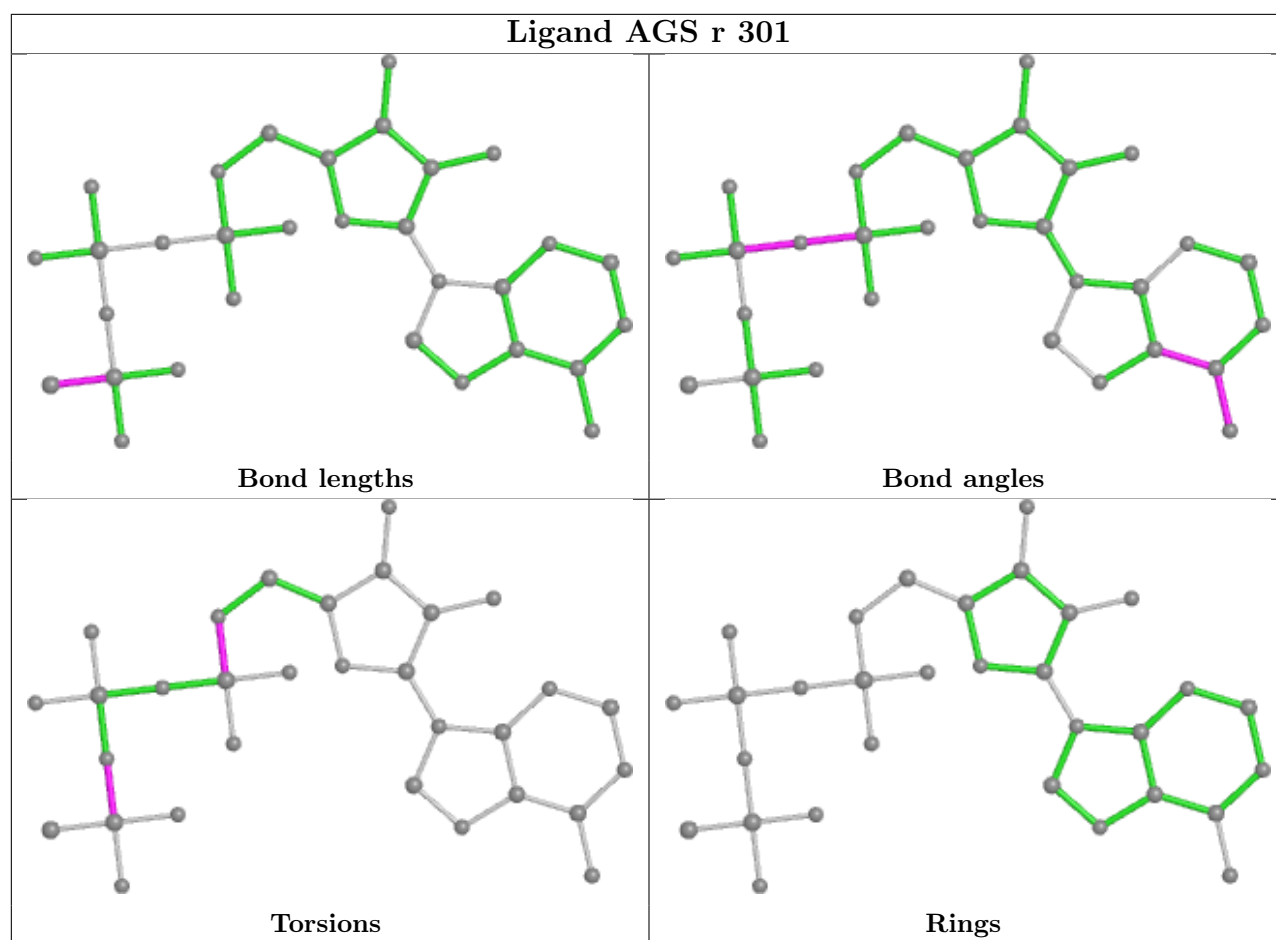
Mol	Chain	Res	Type	Atoms
4	l	301	AGS	C5'-O5'-PA-O3A
4	q	301	AGS	C5'-O5'-PA-O3A
4	r	301	AGS	C5'-O5'-PA-O3A
4	w	301	AGS	C5'-O5'-PA-O3A
4	x	301	AGS	C5'-O5'-PA-O3A

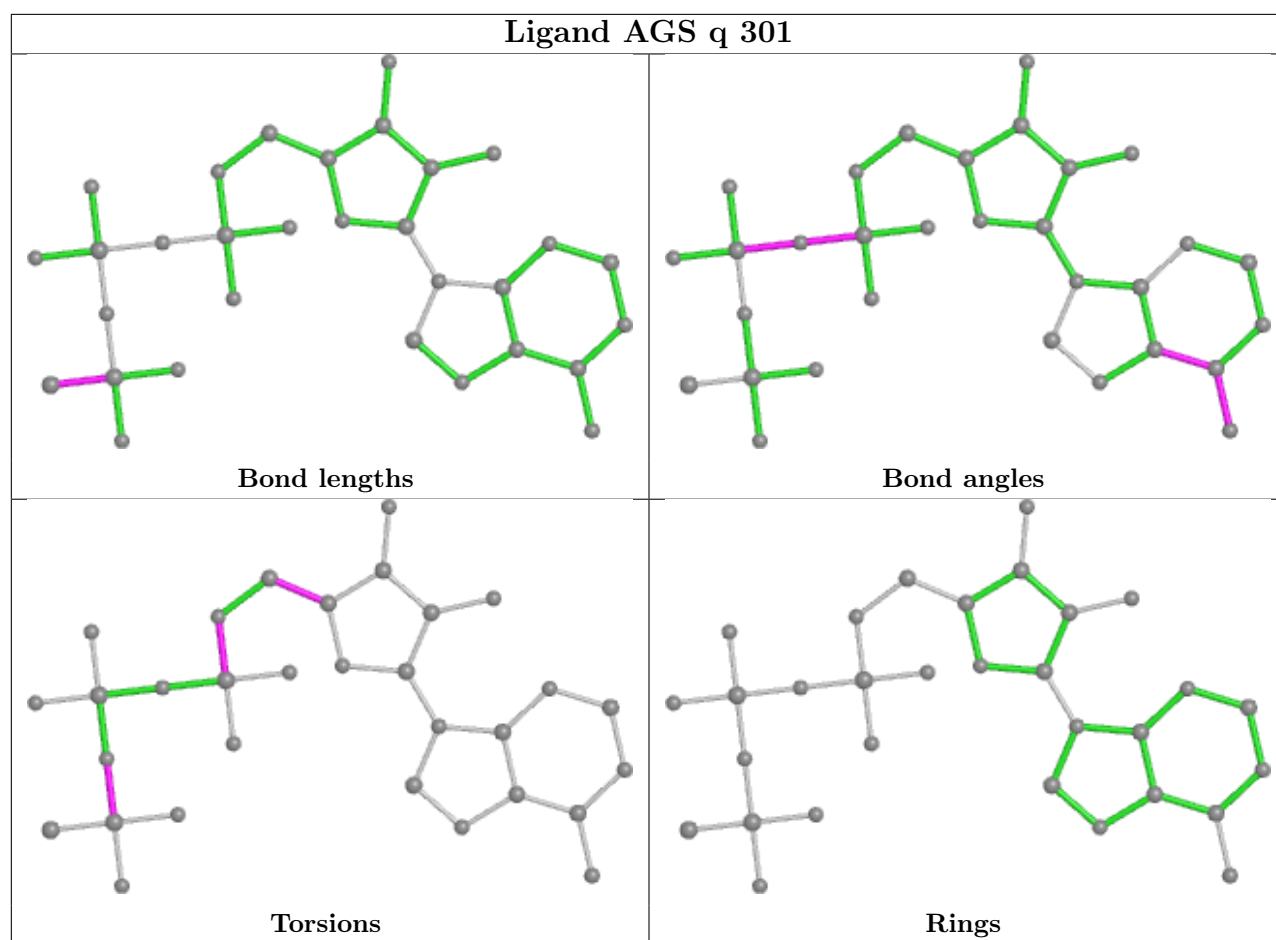
There are no ring outliers.

2 monomers are involved in 2 short contacts:

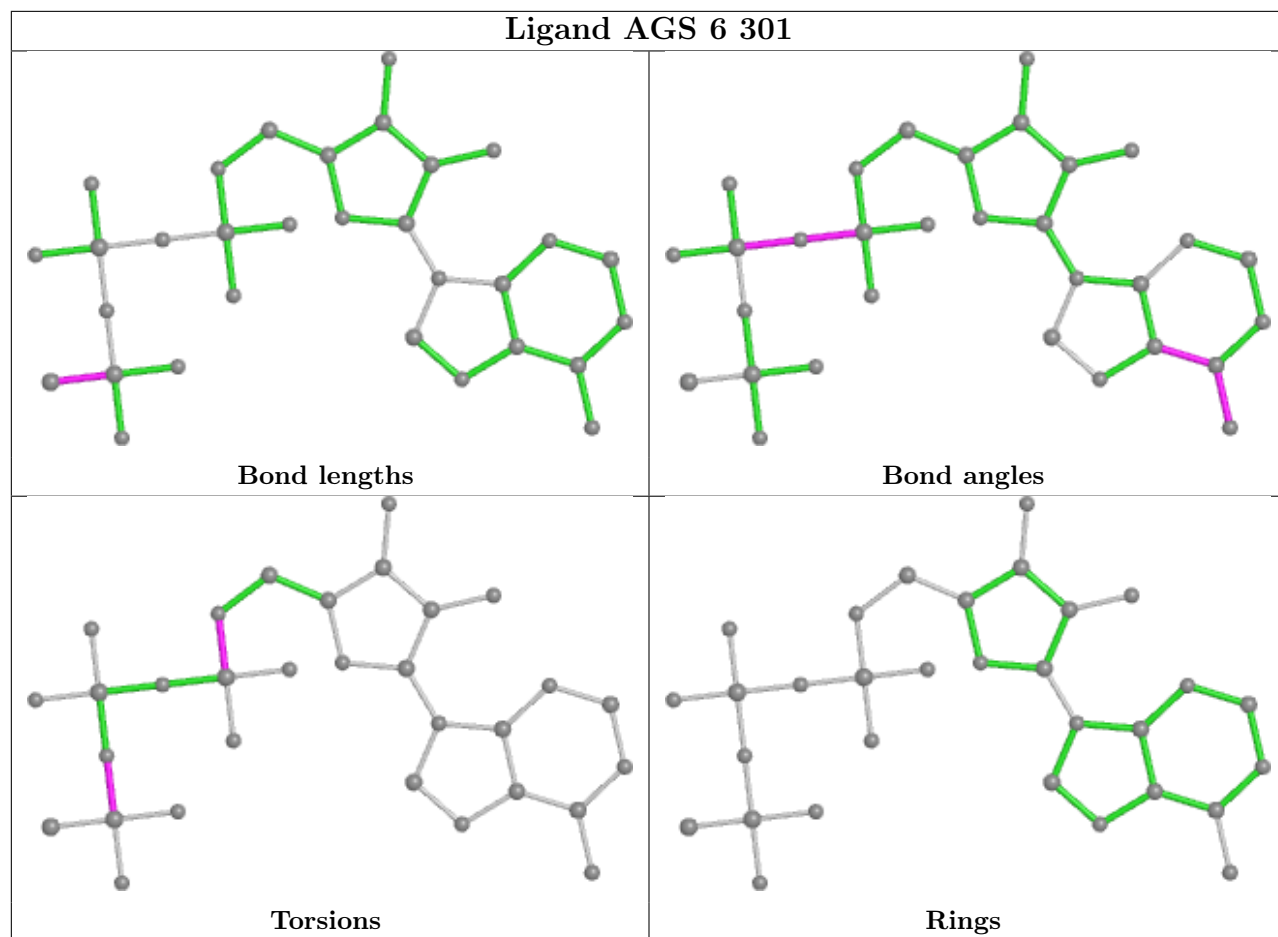
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Z	301	AGS	1	0
4	T	301	AGS	1	0

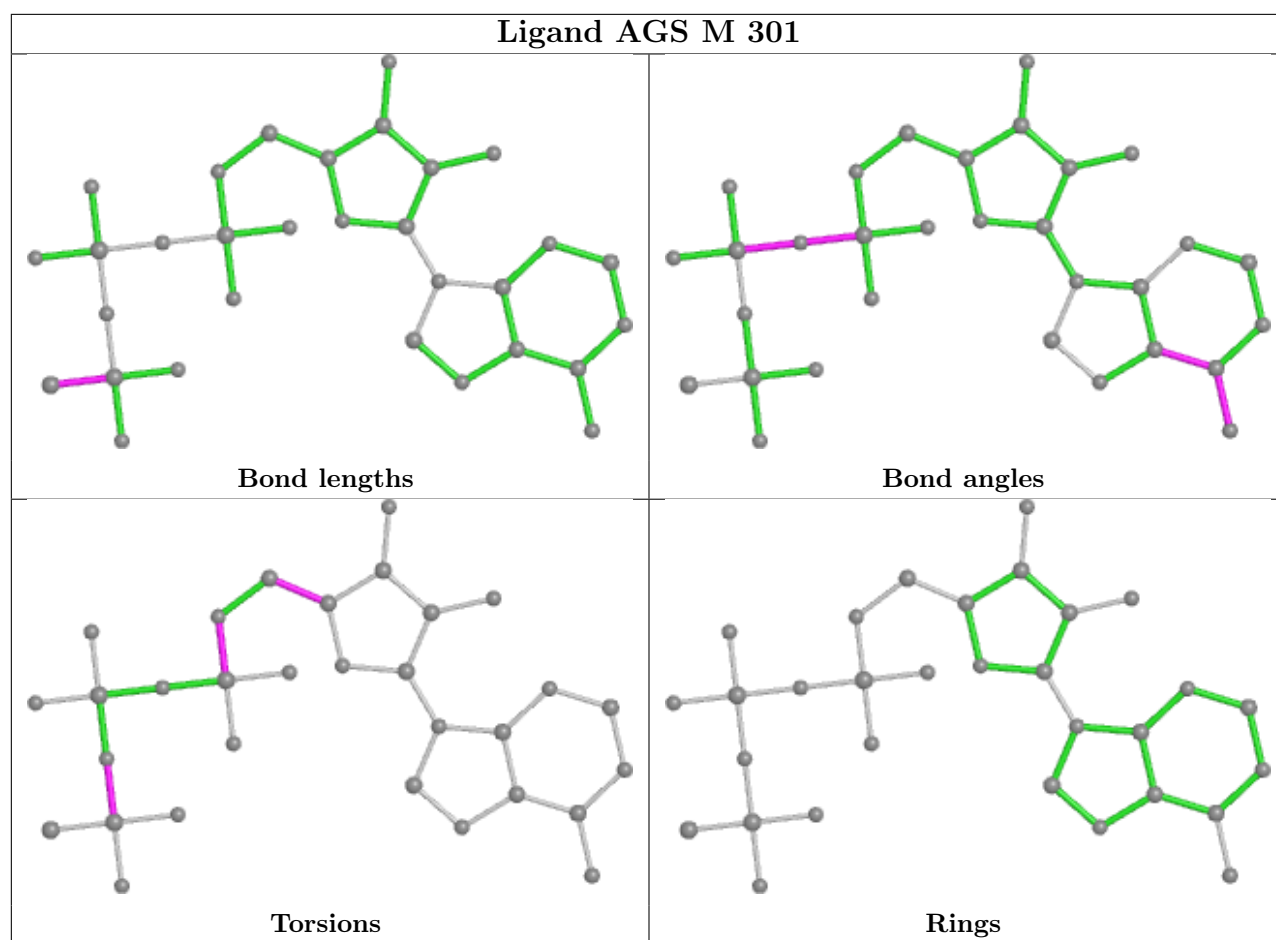
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



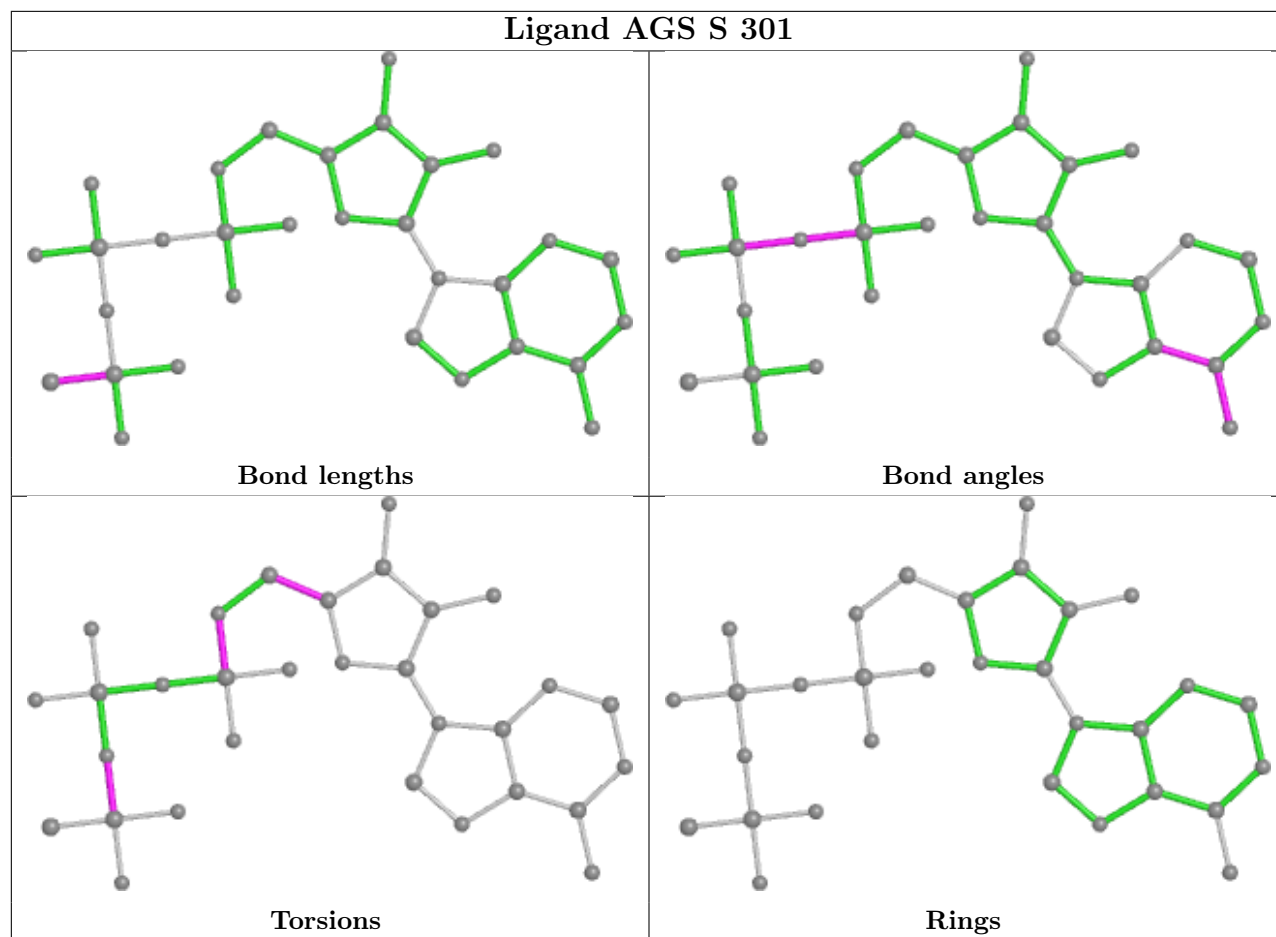


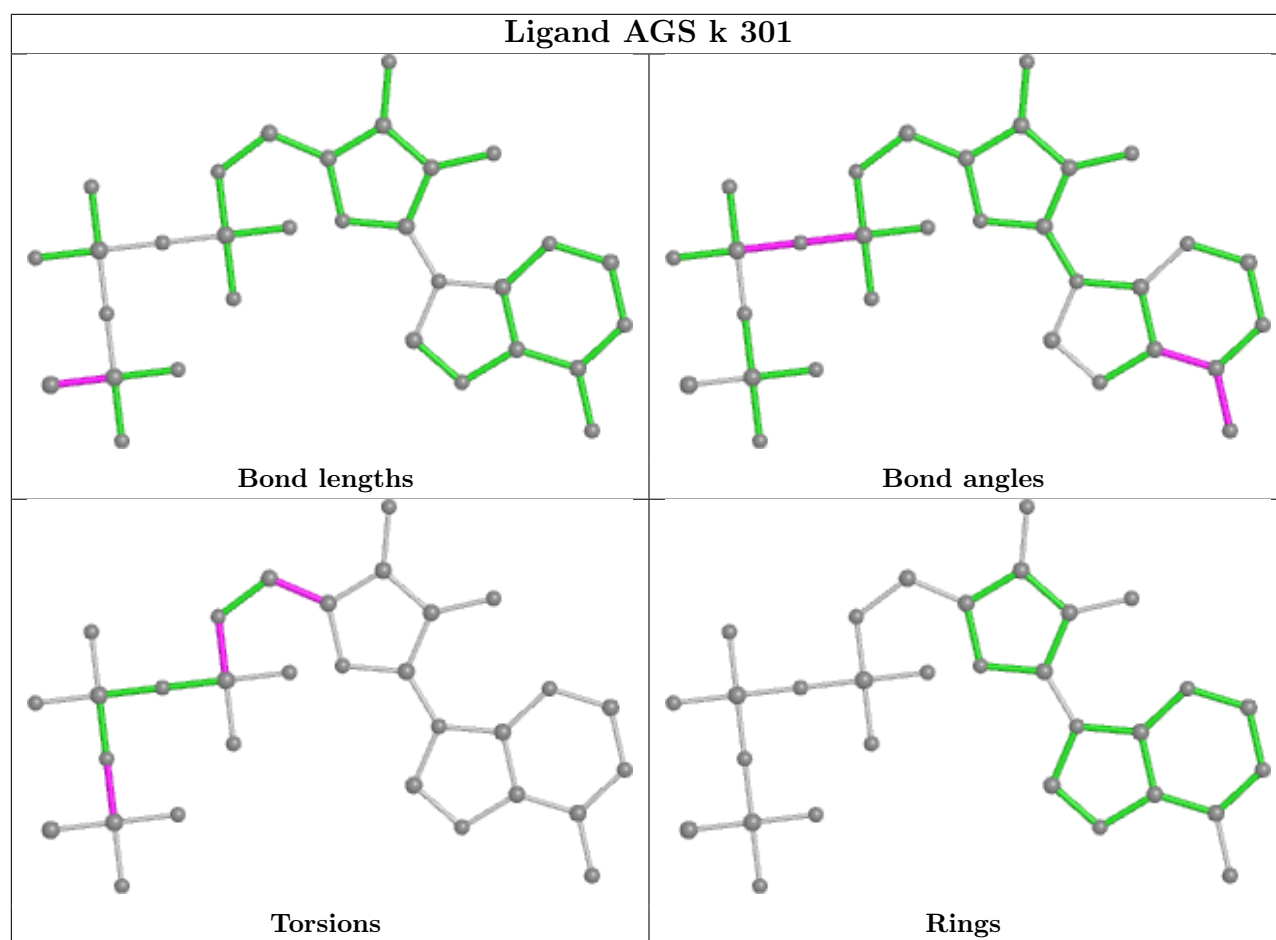
Ligand AGS 6 301



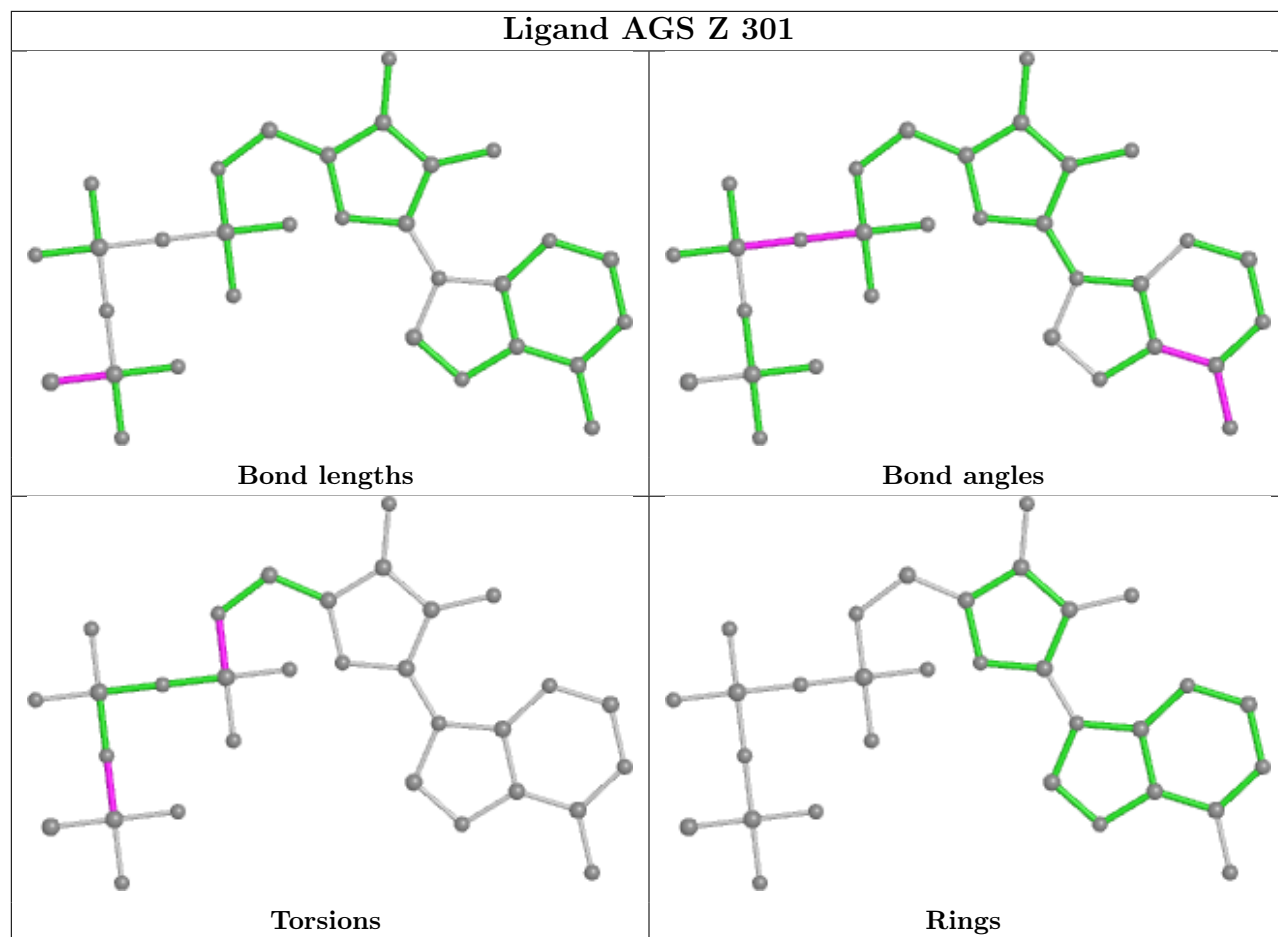


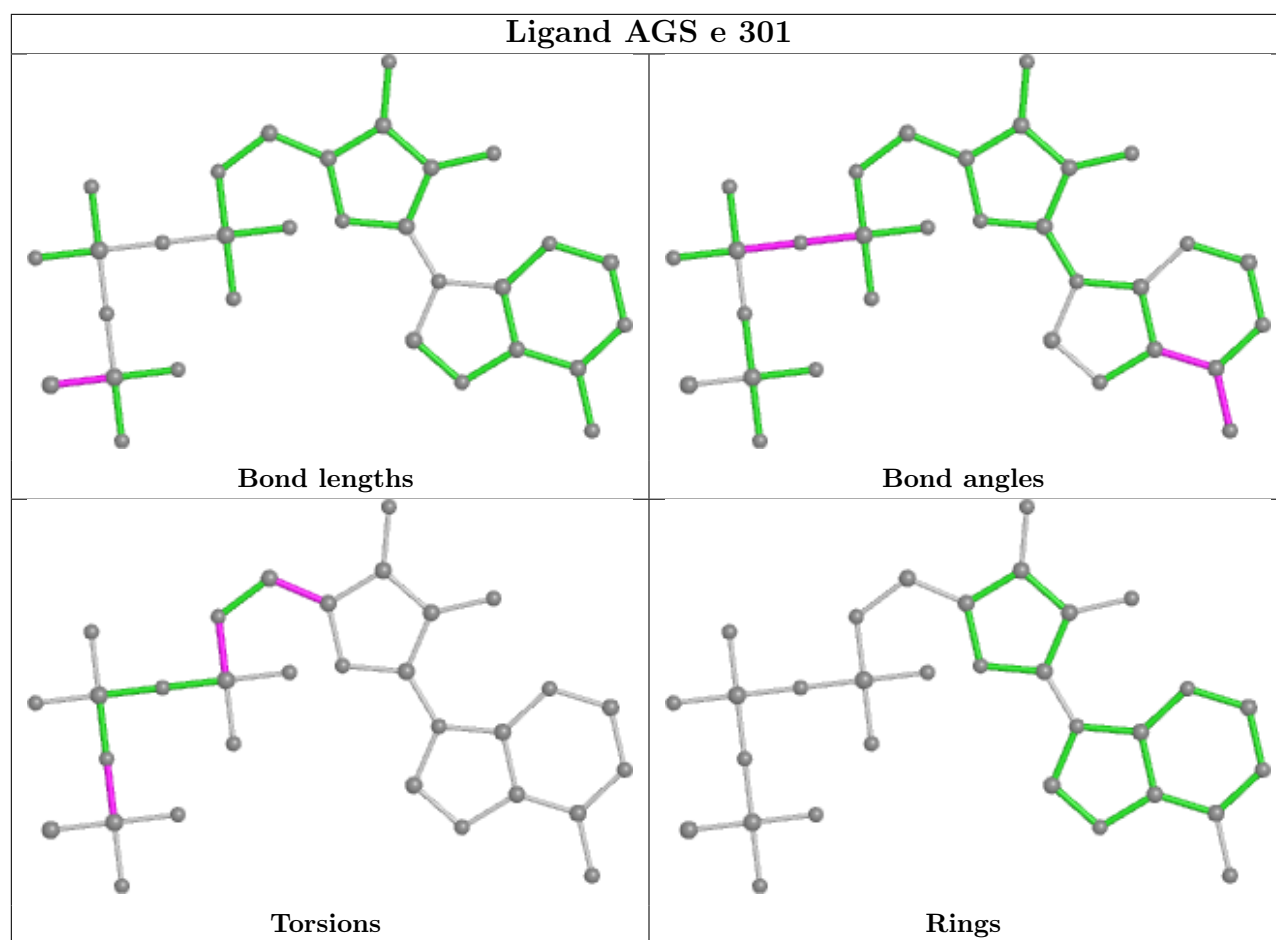
Ligand AGS S 301

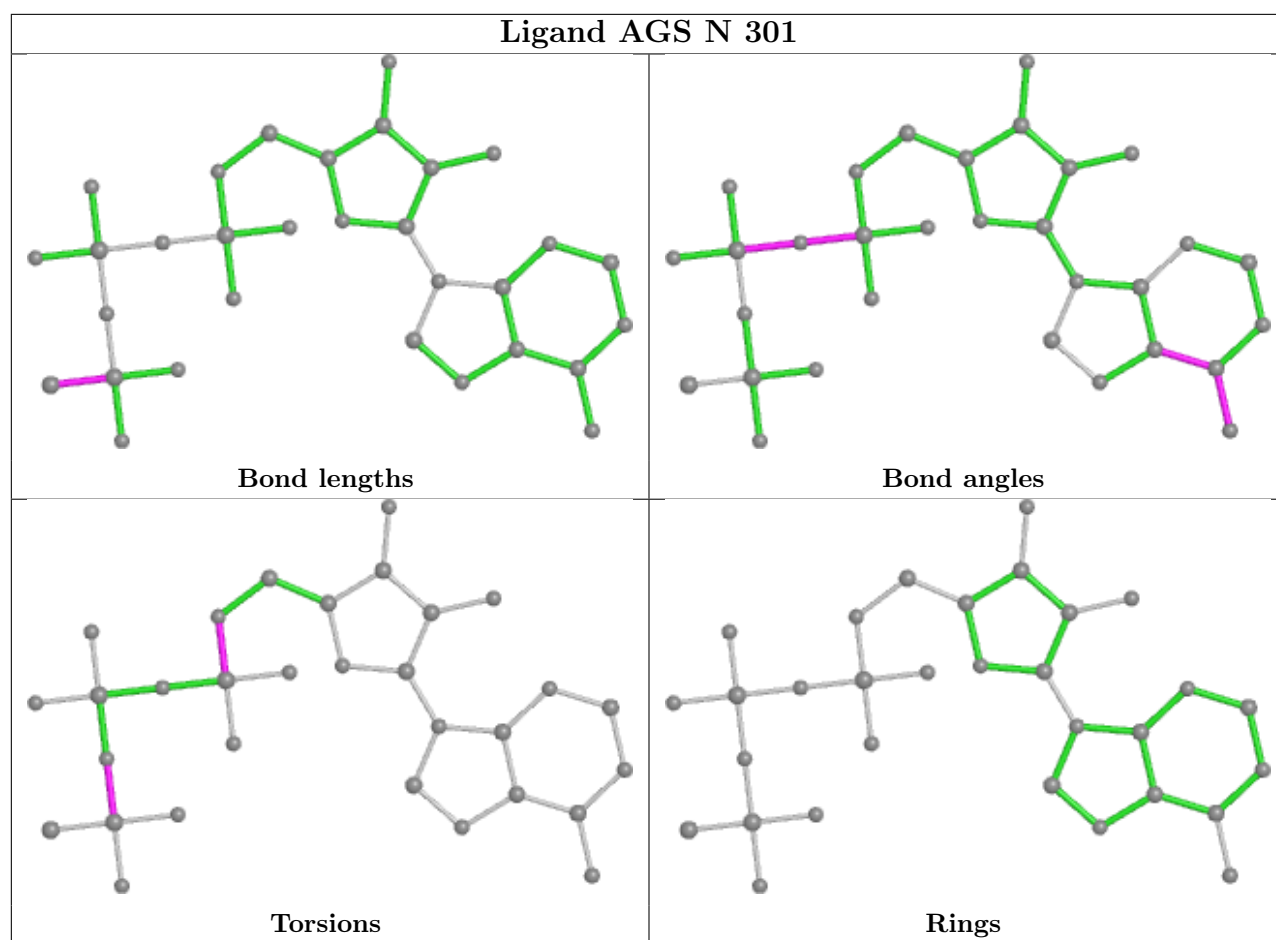


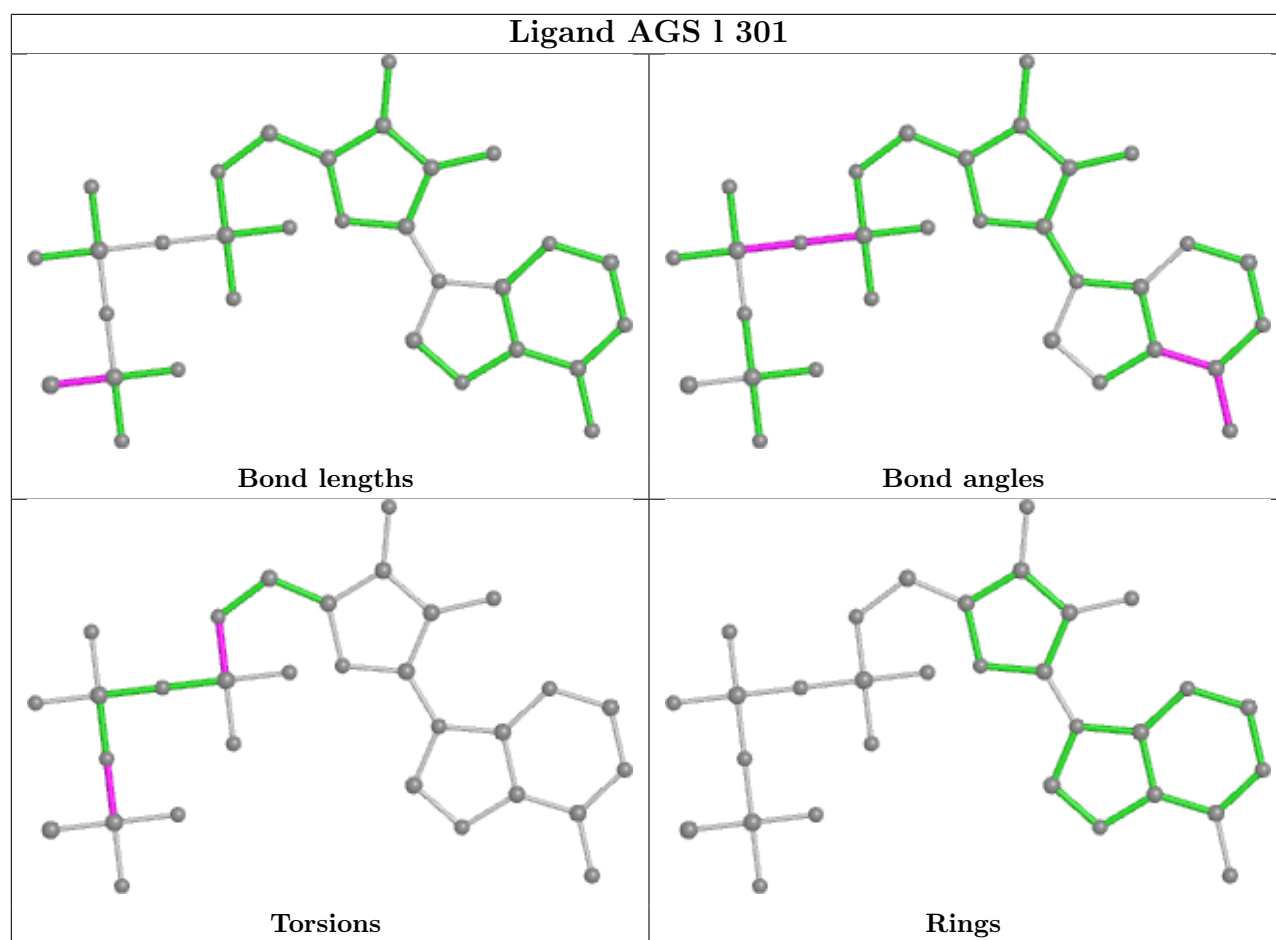


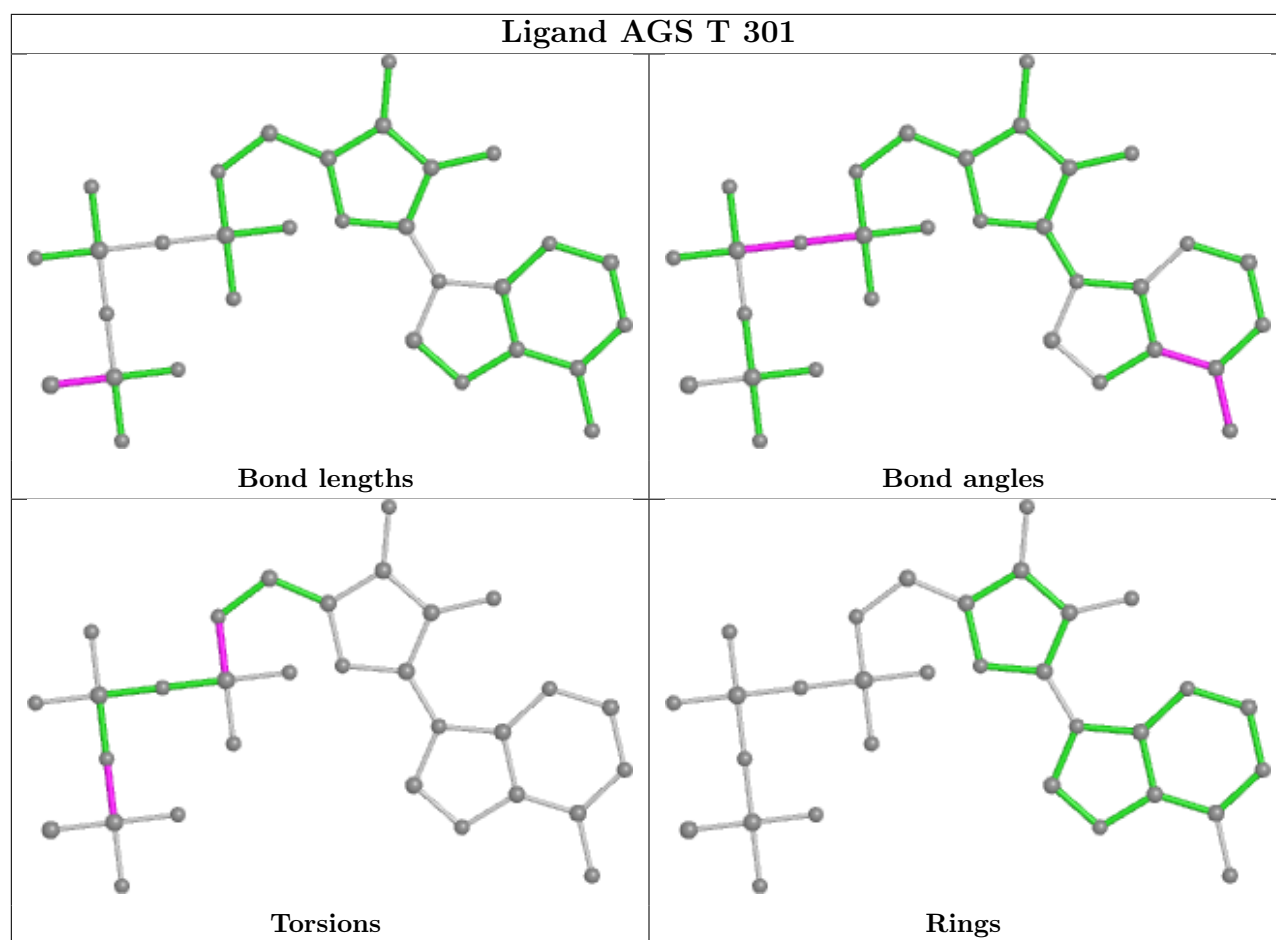
Ligand AGS Z 301



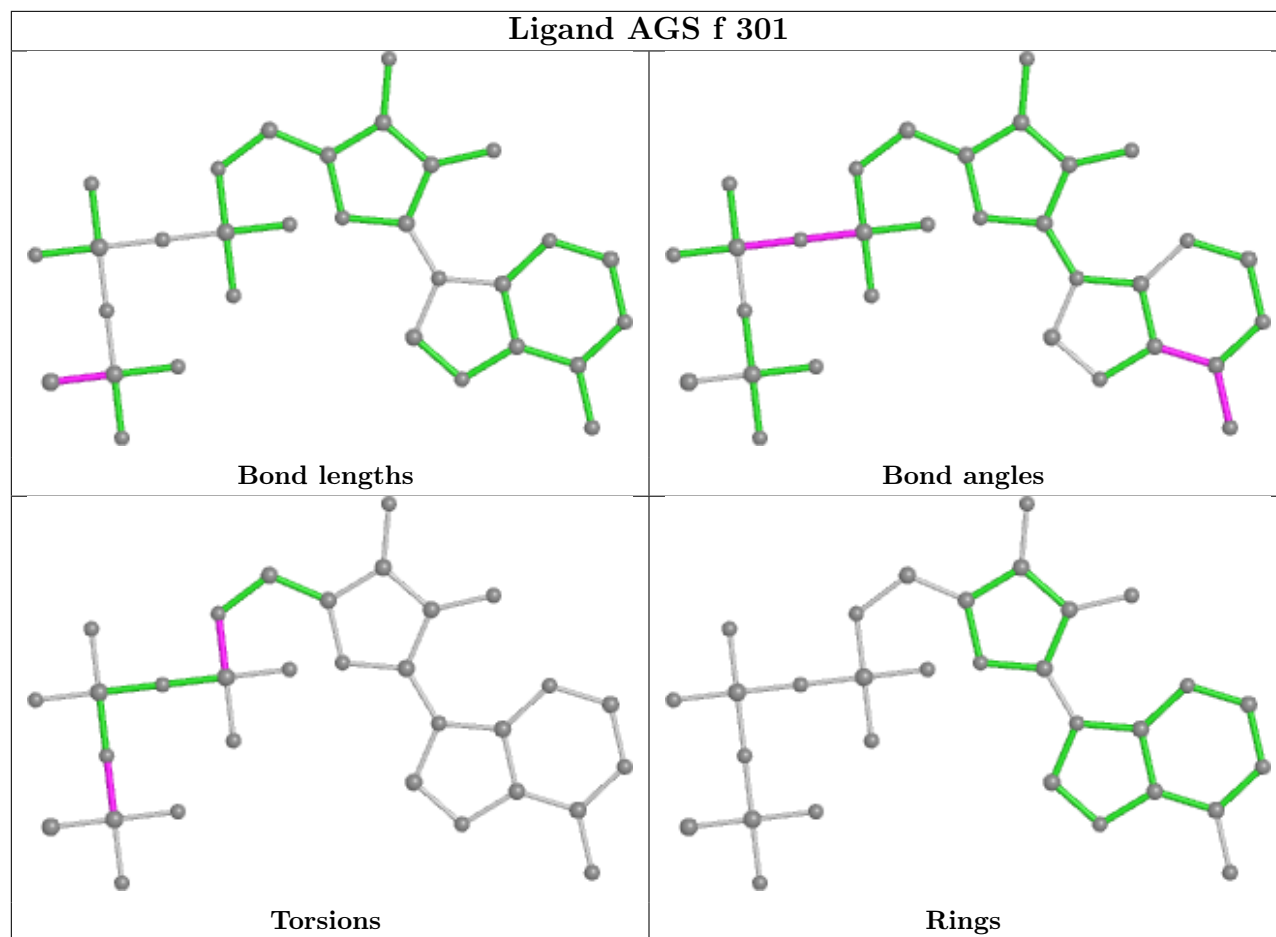


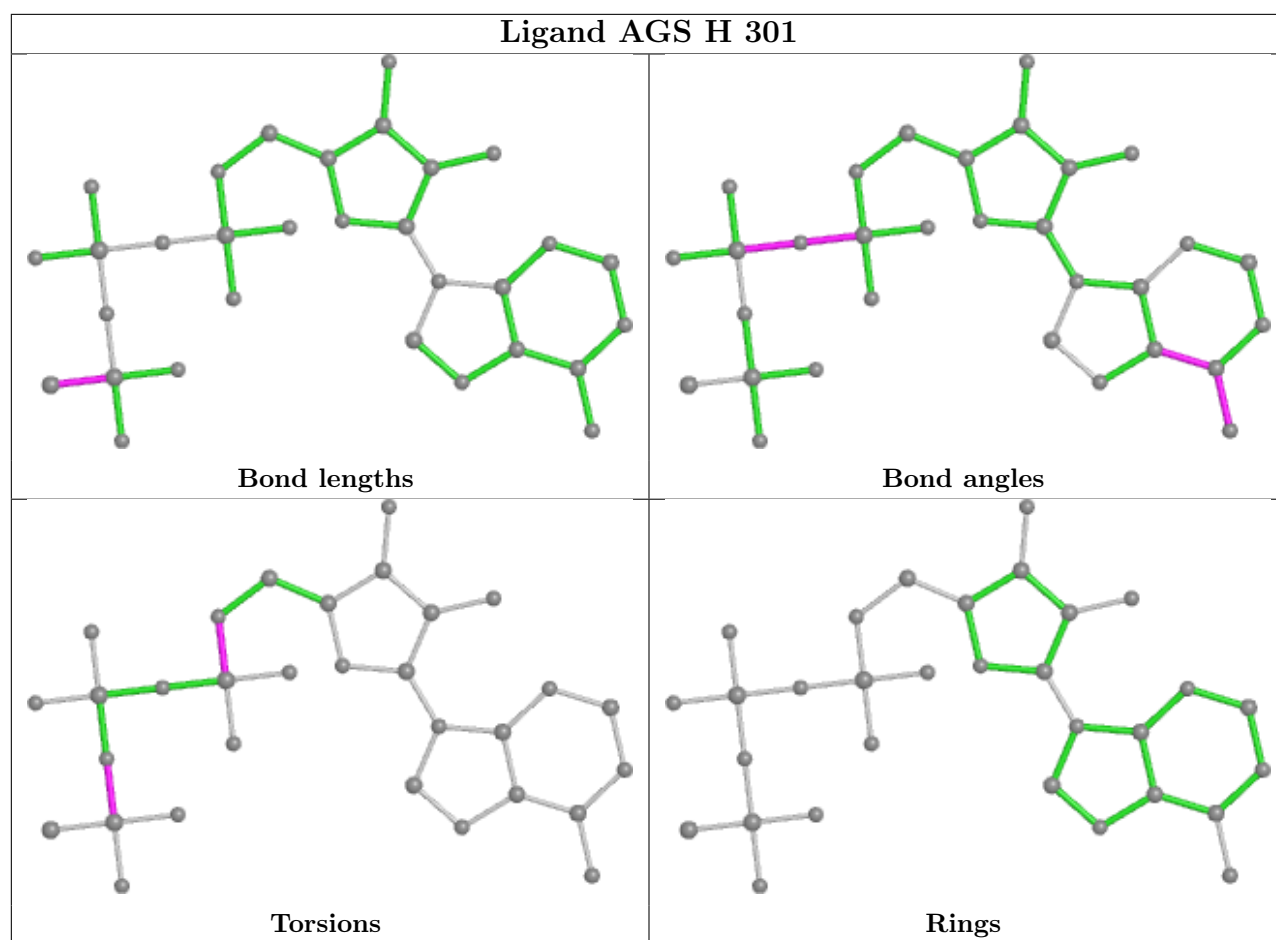


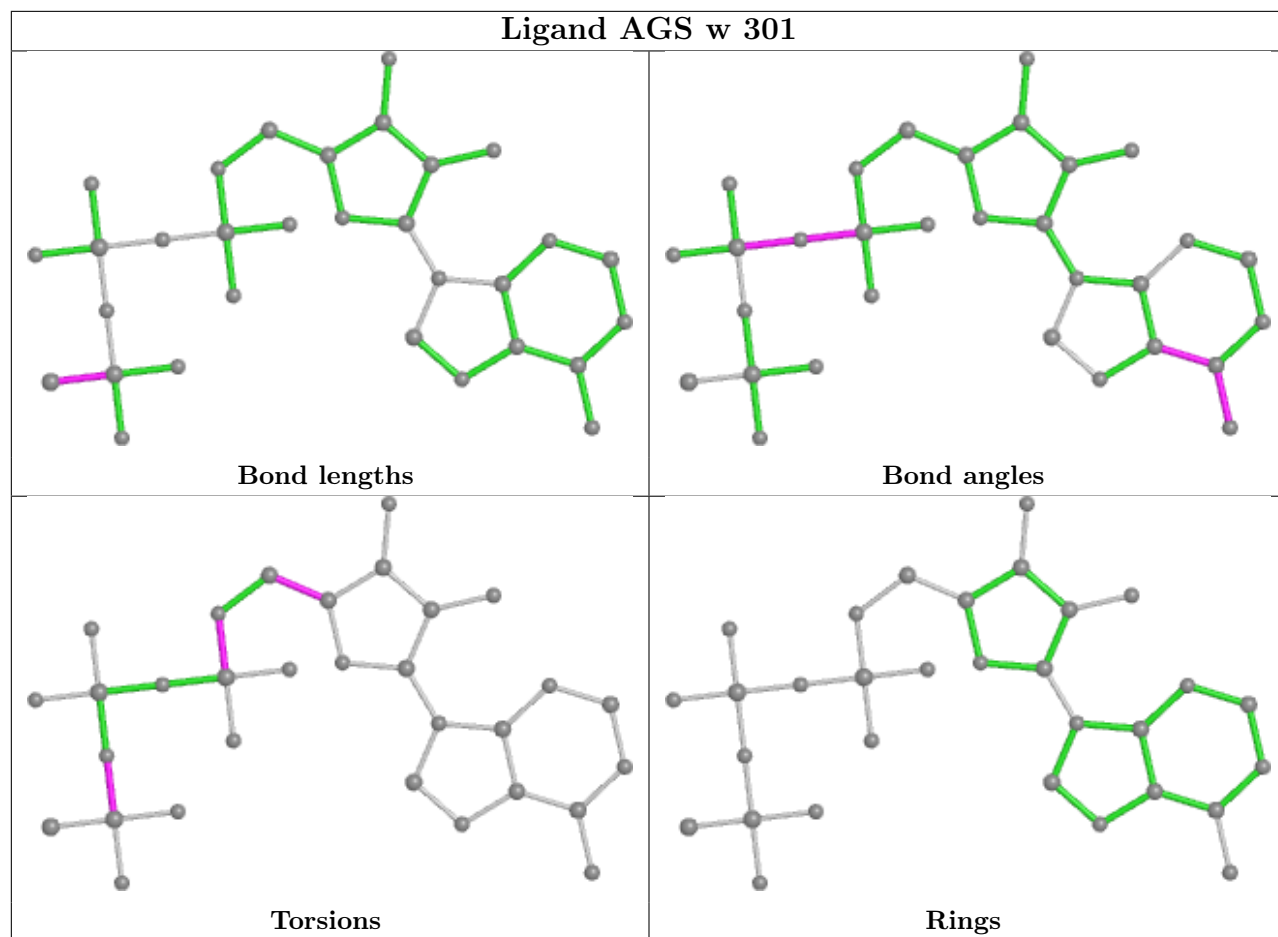


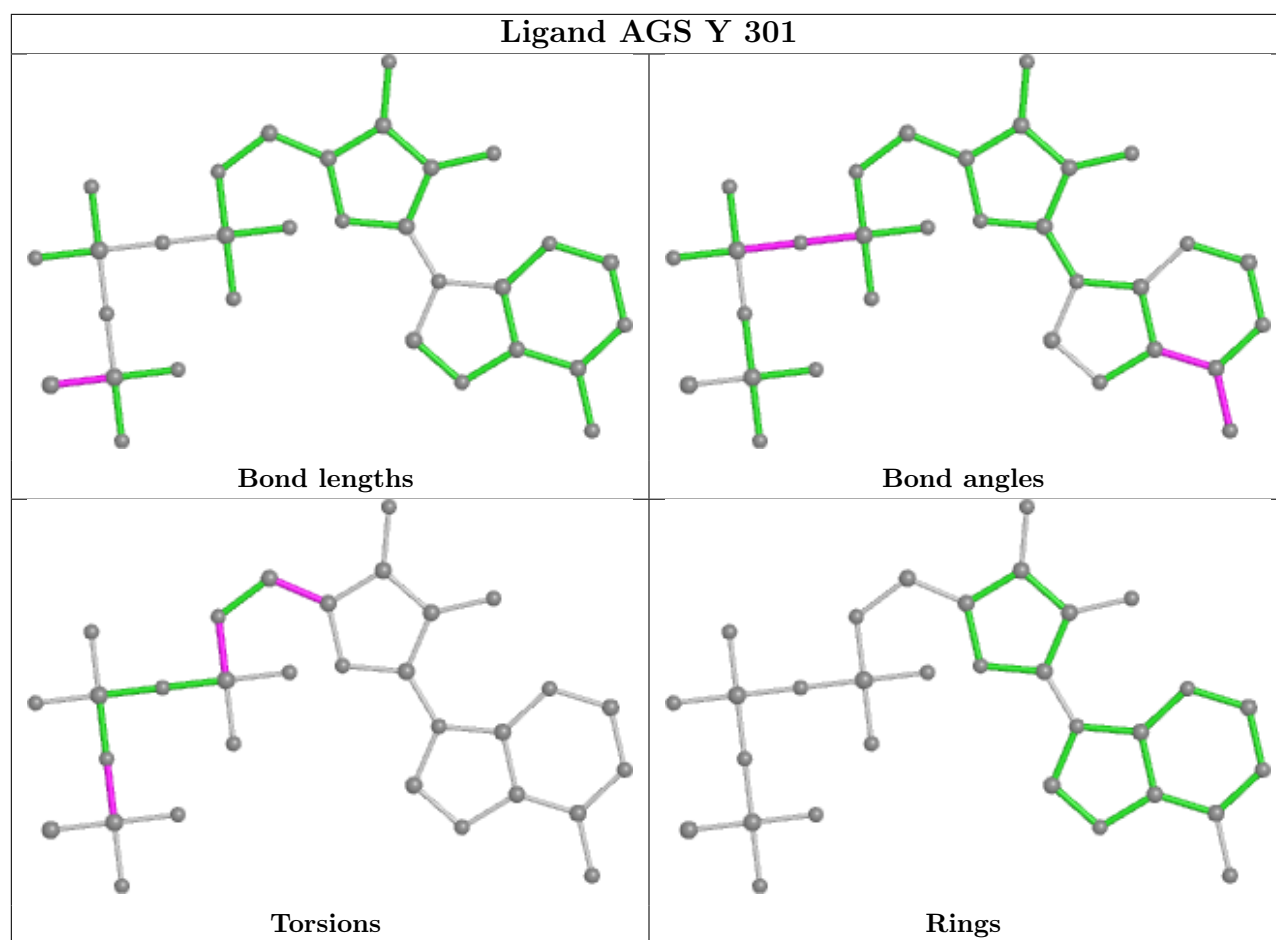


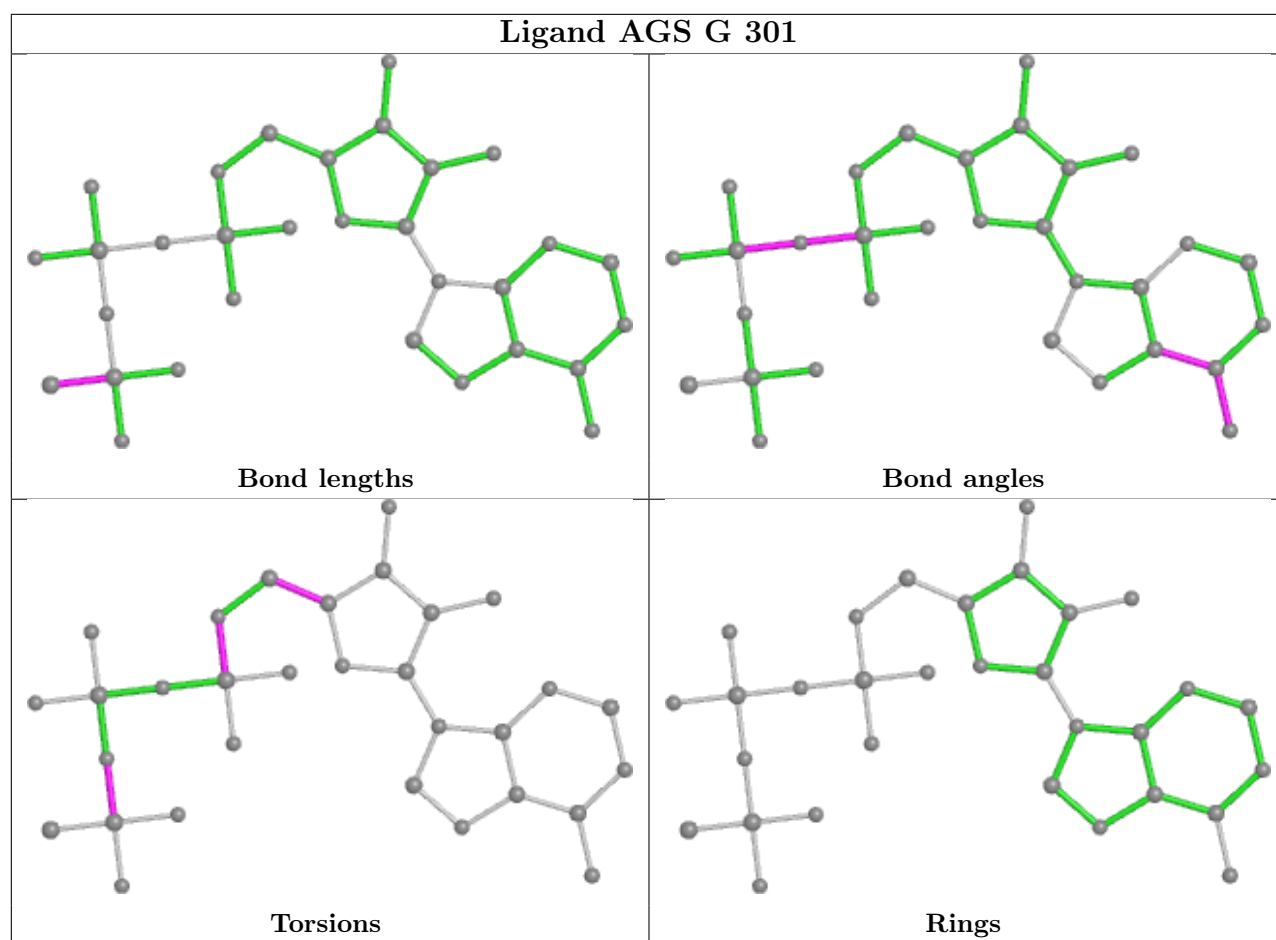
Ligand AGS f 301

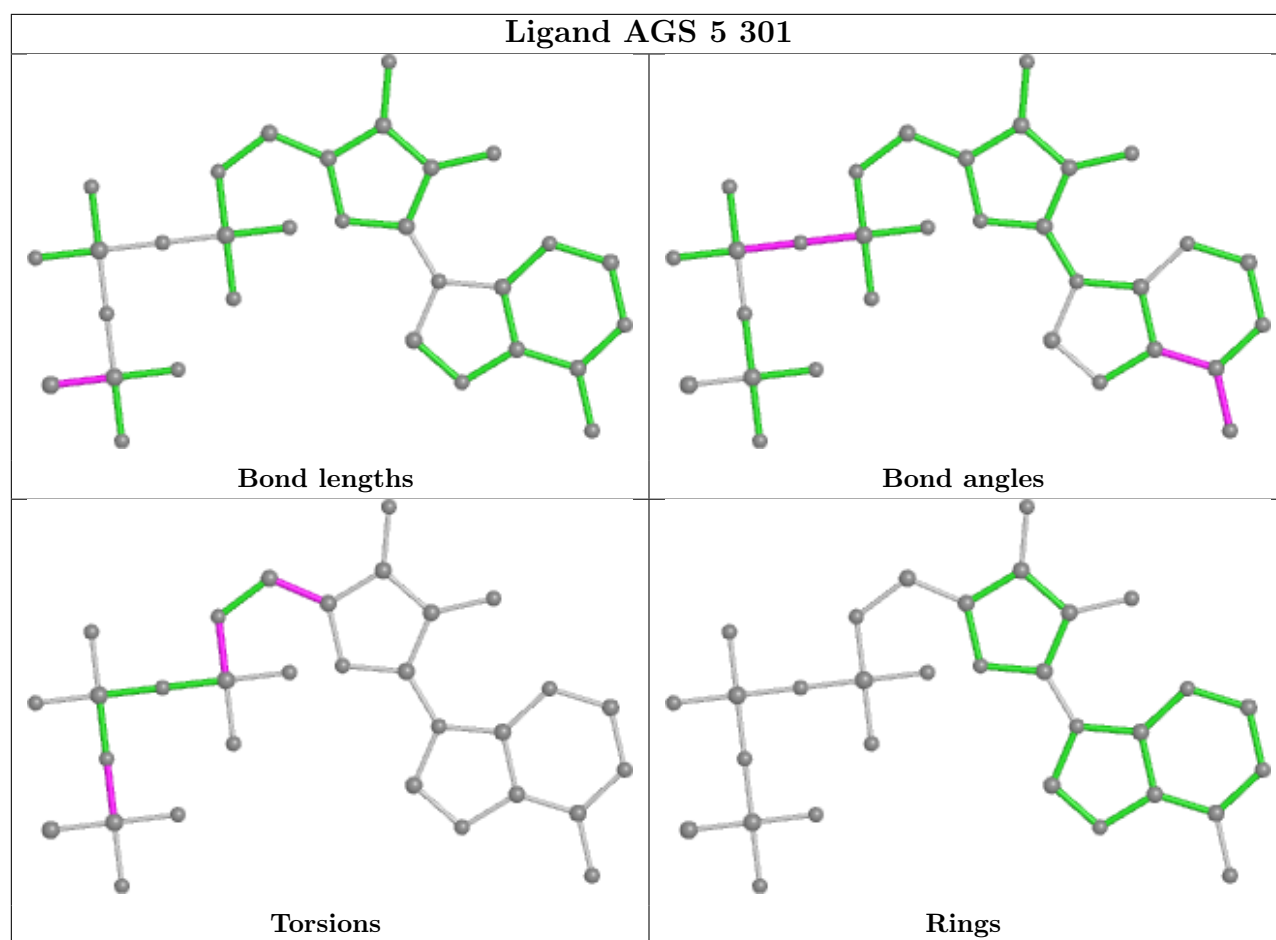


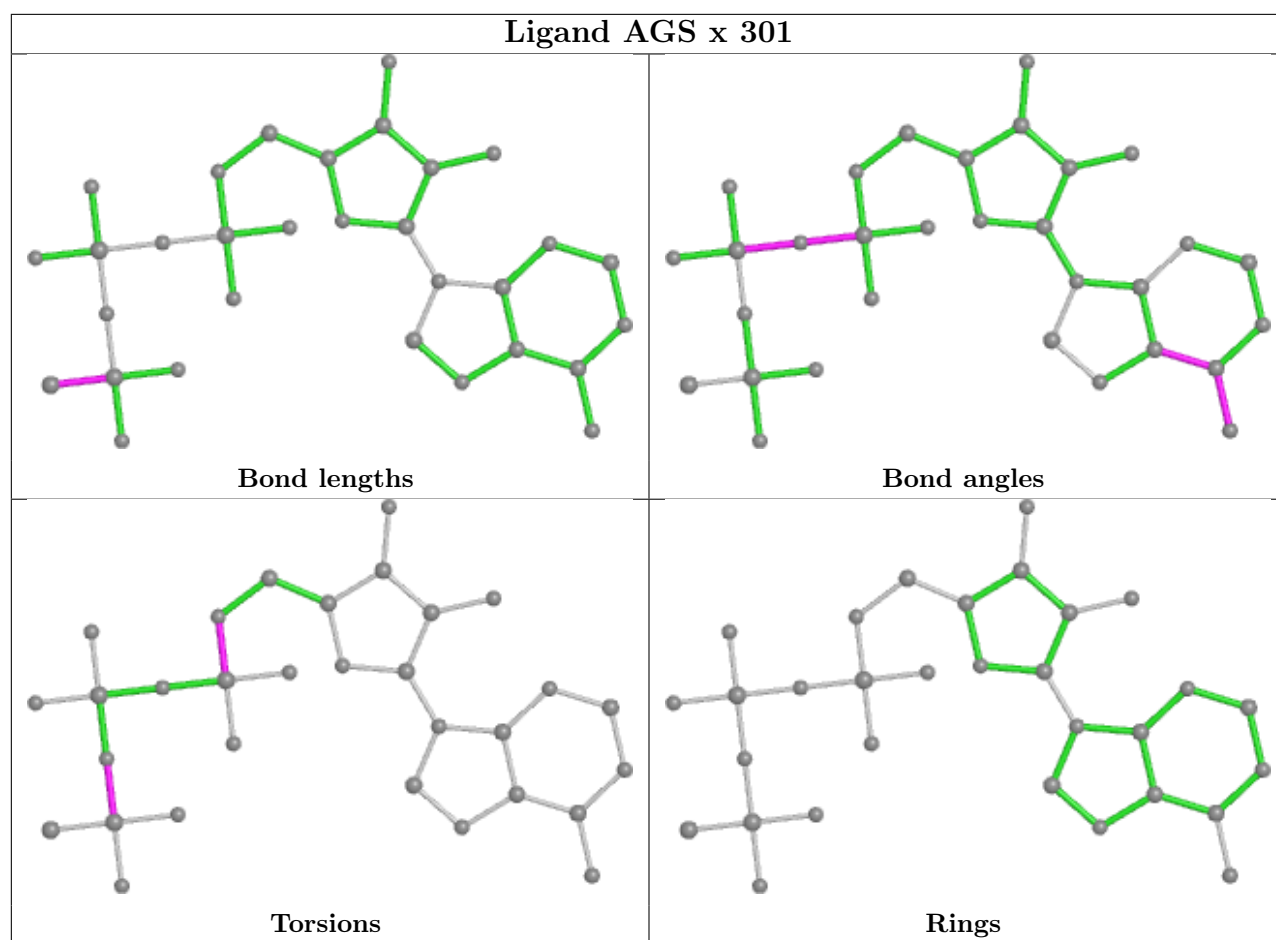












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

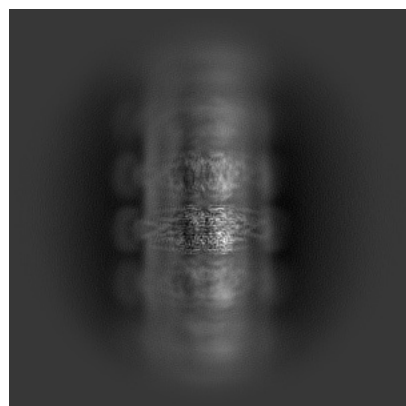
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60898. These allow visual inspection of the internal detail of the map and identification of artifacts.

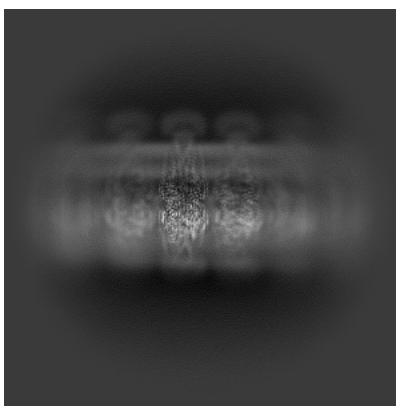
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

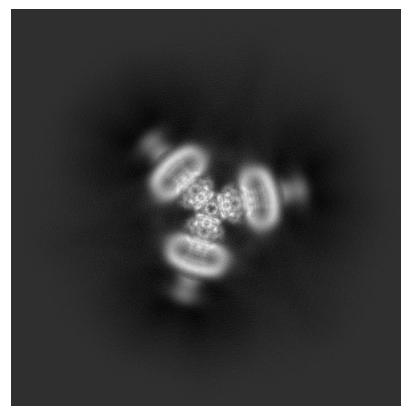
6.1.1 Primary map



X

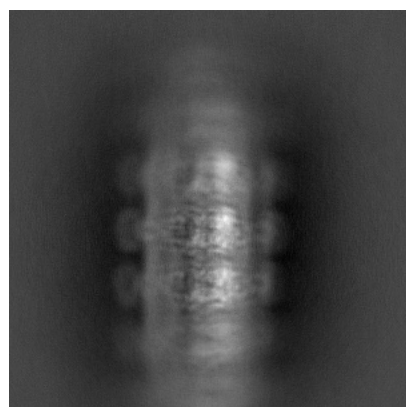


Y

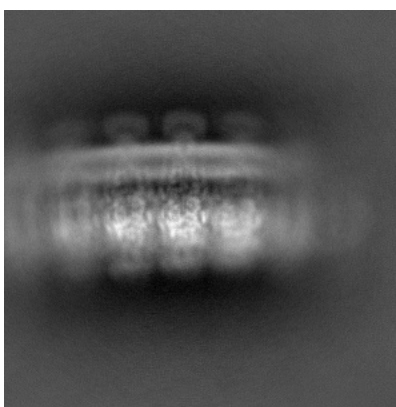


Z

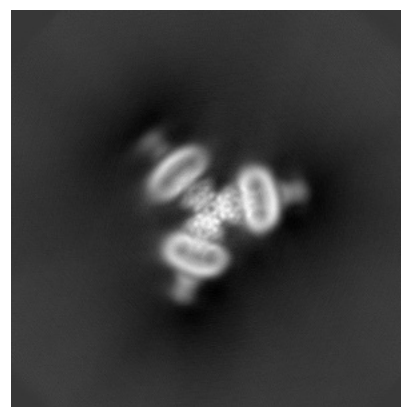
6.1.2 Raw map



X



Y

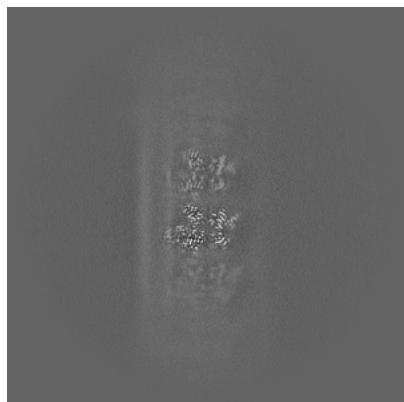


Z

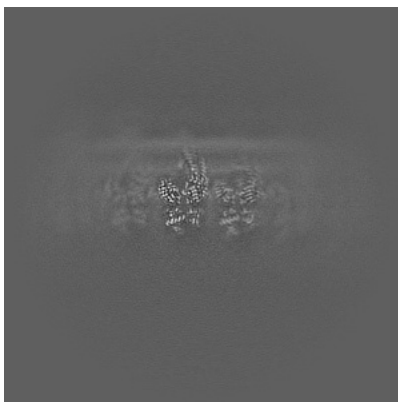
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

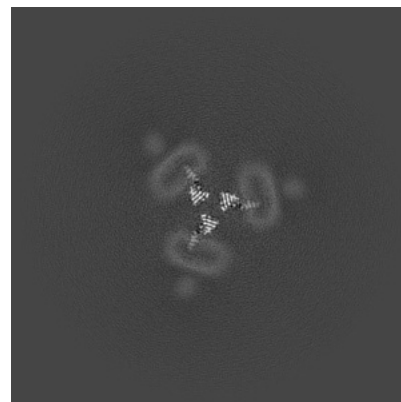
6.2.1 Primary map



X Index: 256

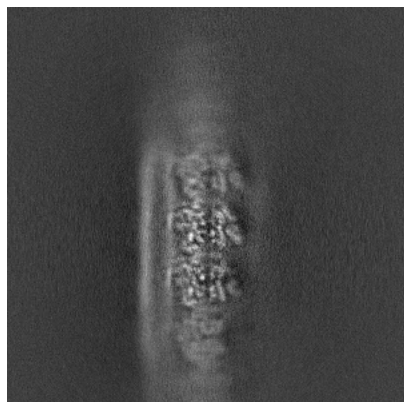


Y Index: 256

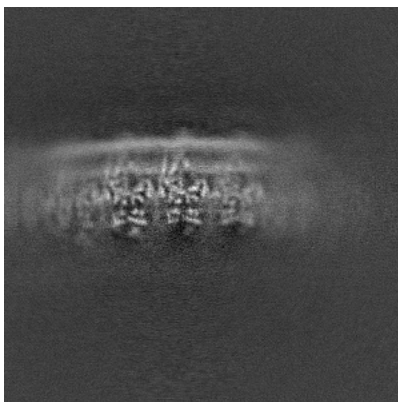


Z Index: 256

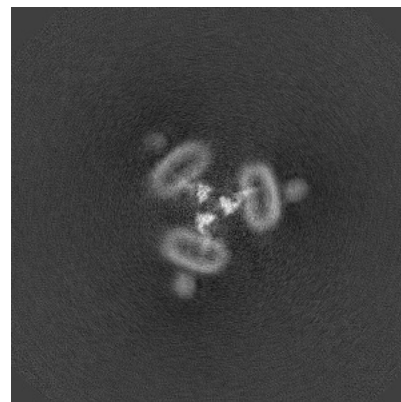
6.2.2 Raw map



X Index: 256



Y Index: 256

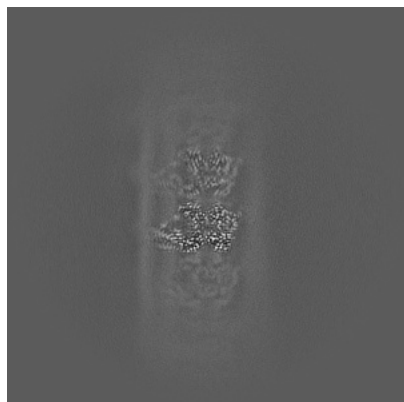


Z Index: 256

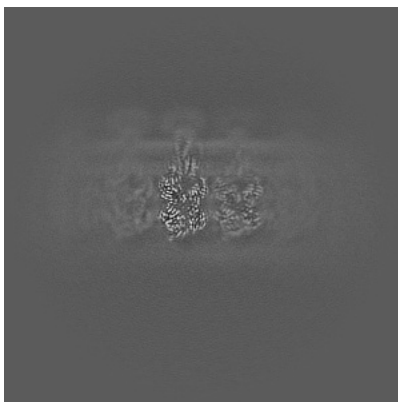
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

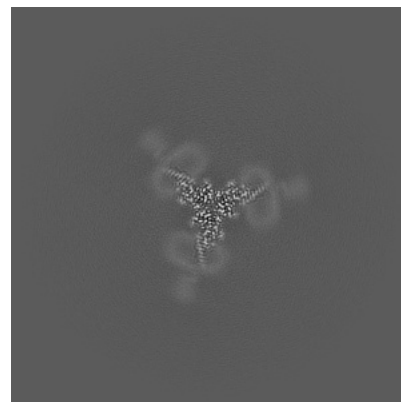
6.3.1 Primary map



X Index: 248

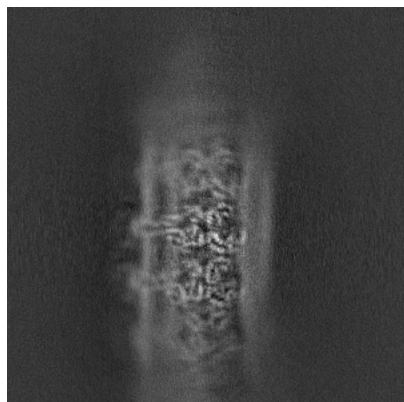


Y Index: 266

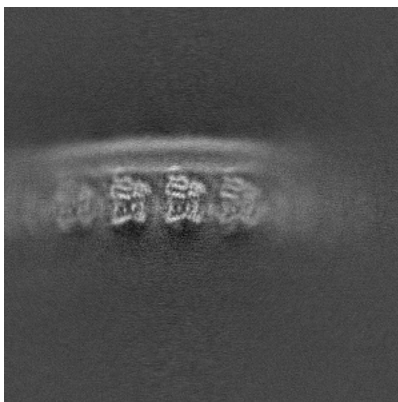


Z Index: 215

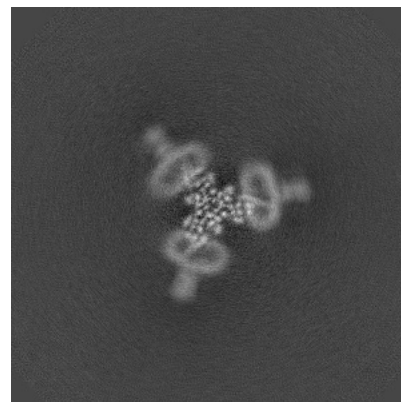
6.3.2 Raw map



X Index: 239



Y Index: 248

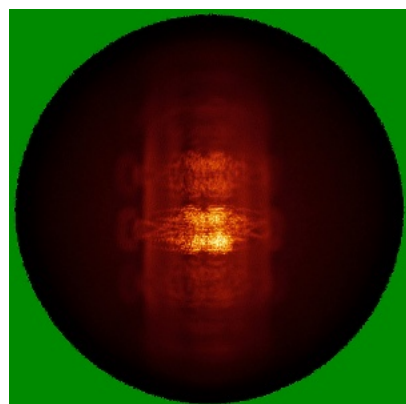


Z Index: 216

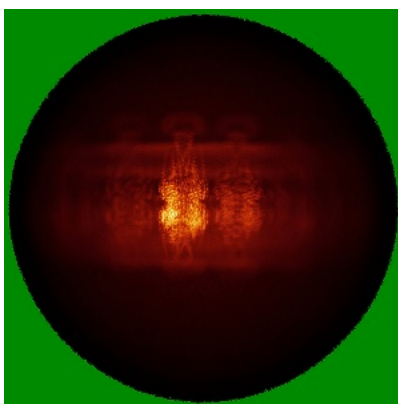
The images above show the largest variance slices of the map in three orthogonal directions.

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

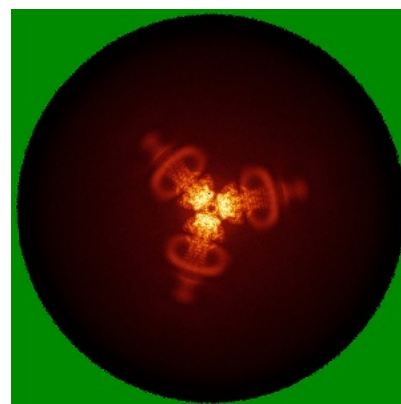
6.4.1 Primary map



X

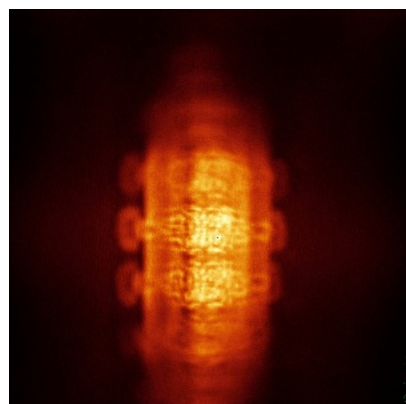


Y

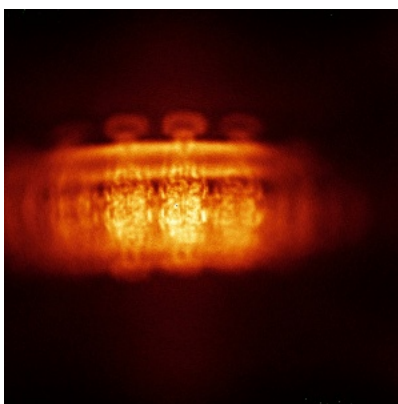


Z

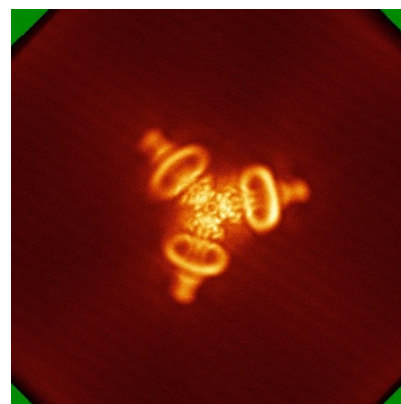
6.4.2 Raw map



X



Y

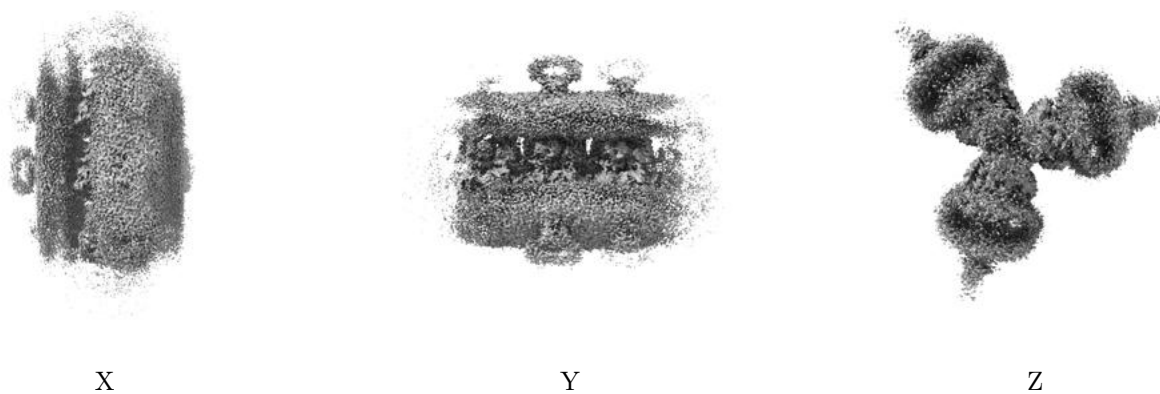


Z

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.

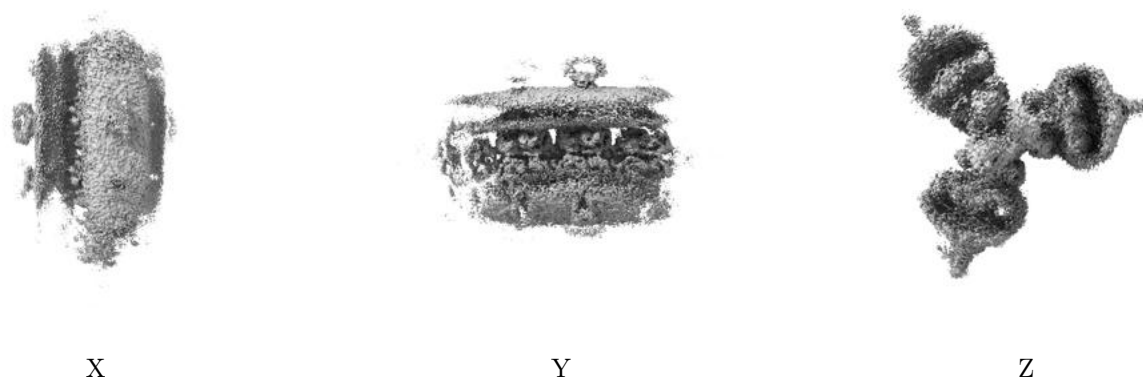
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

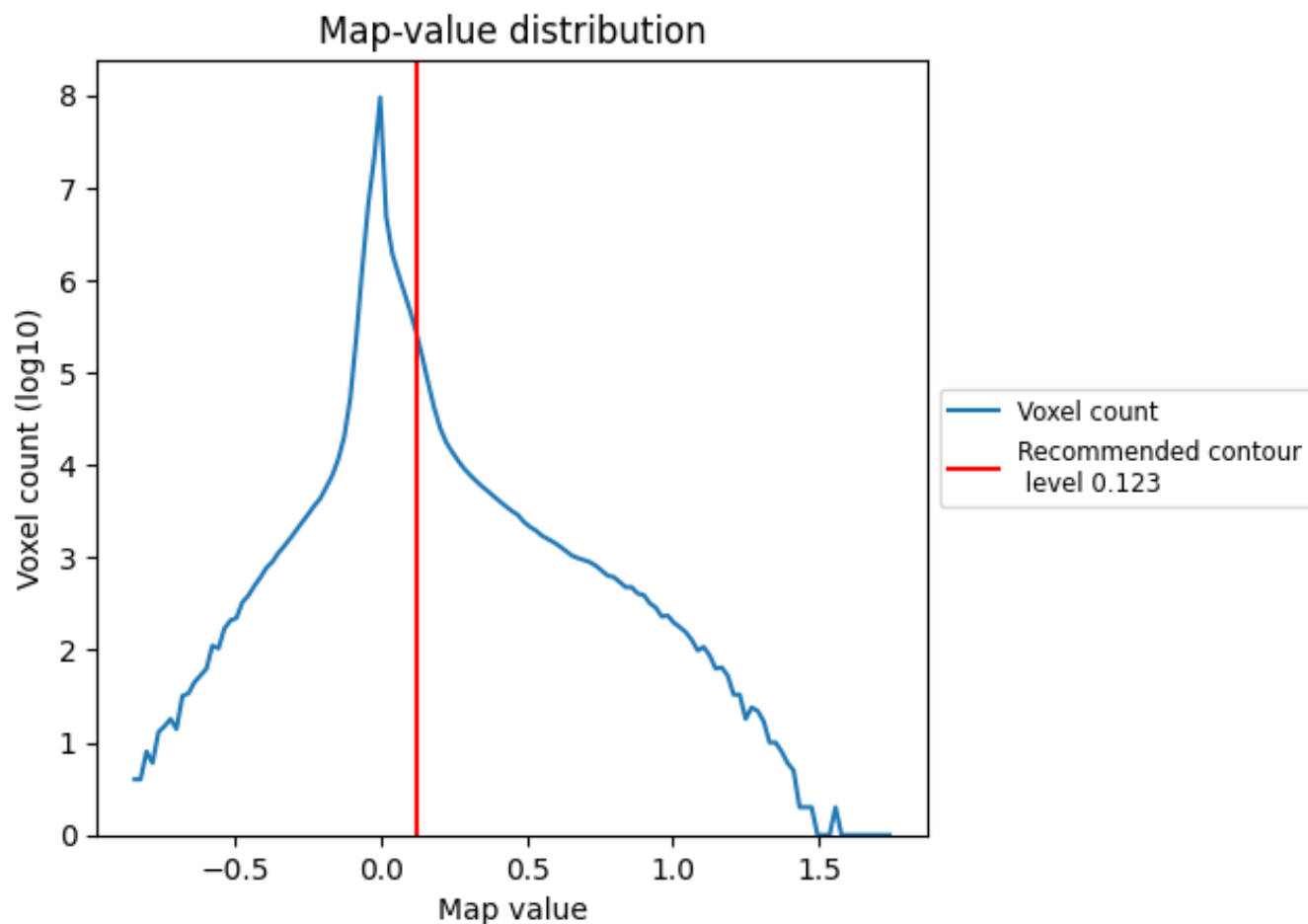
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

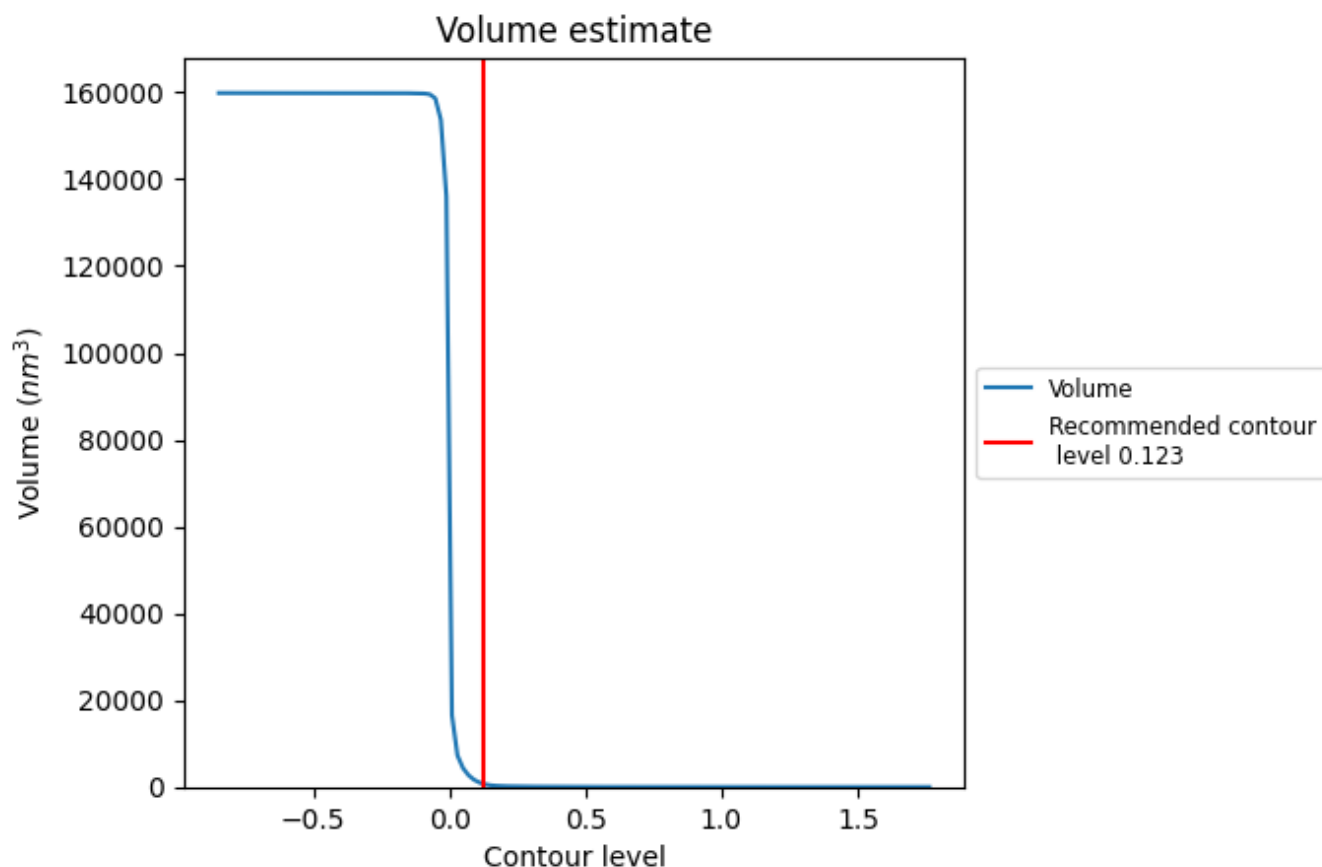
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

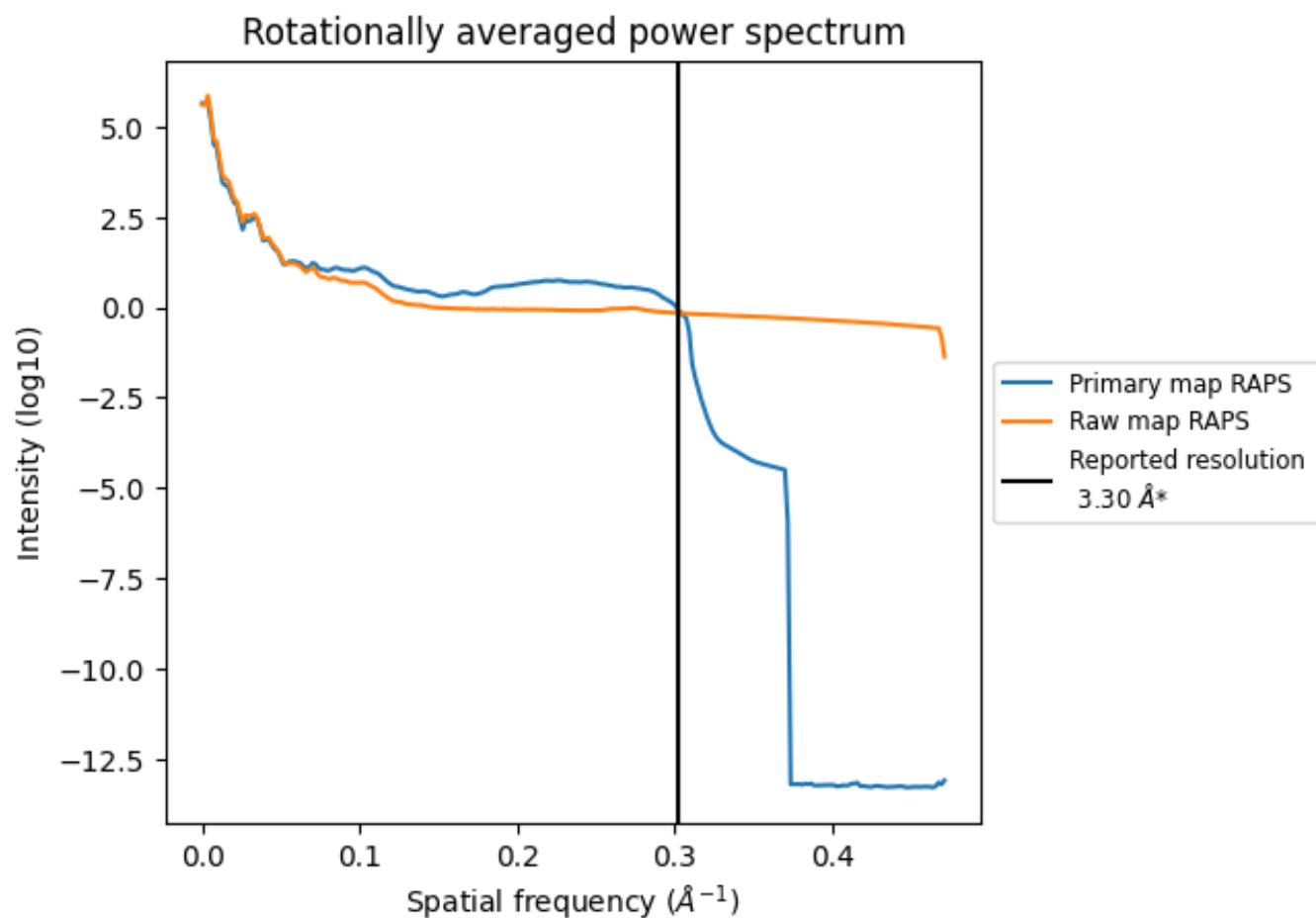
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 777 nm³; this corresponds to an approximate mass of 701 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

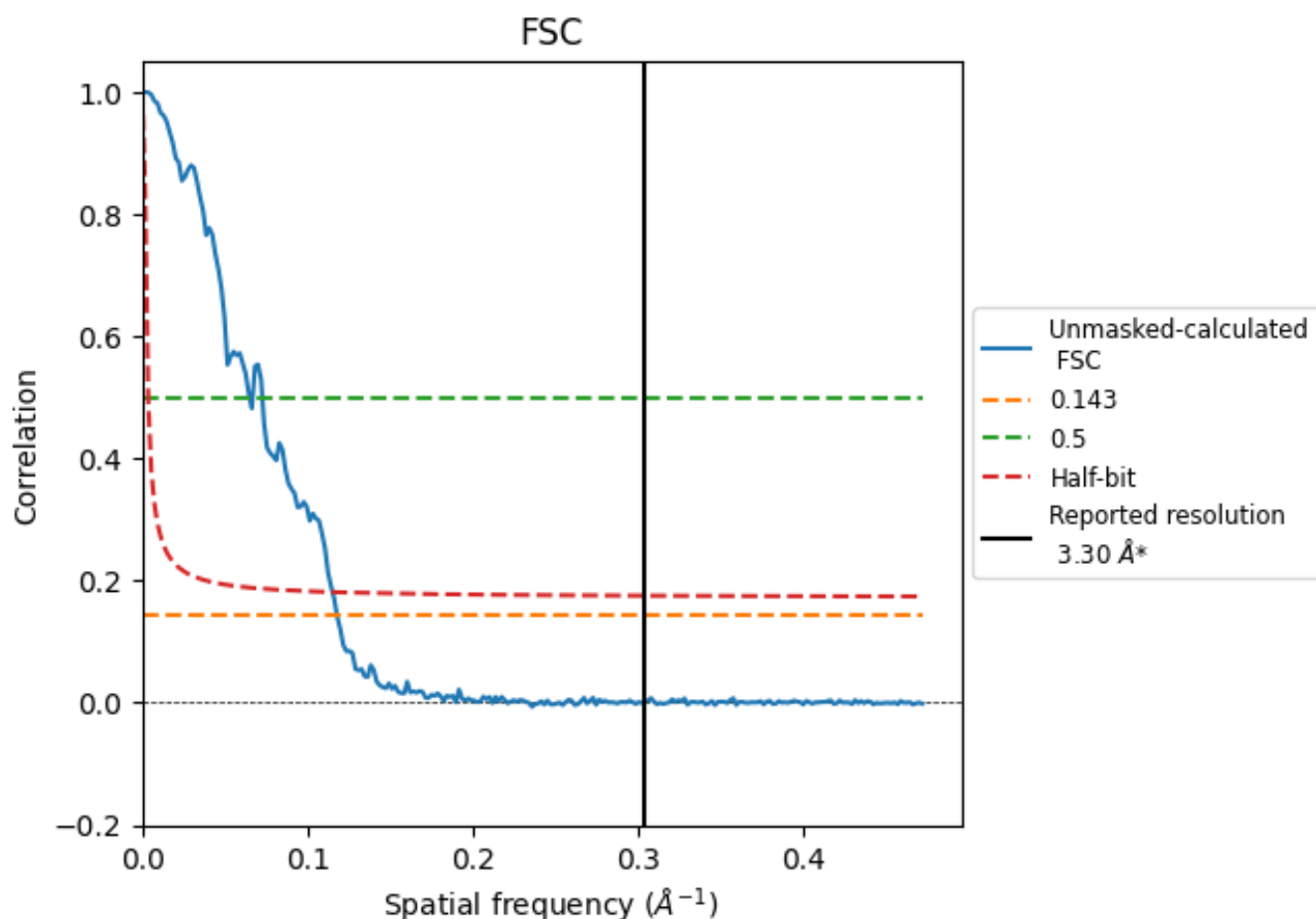


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

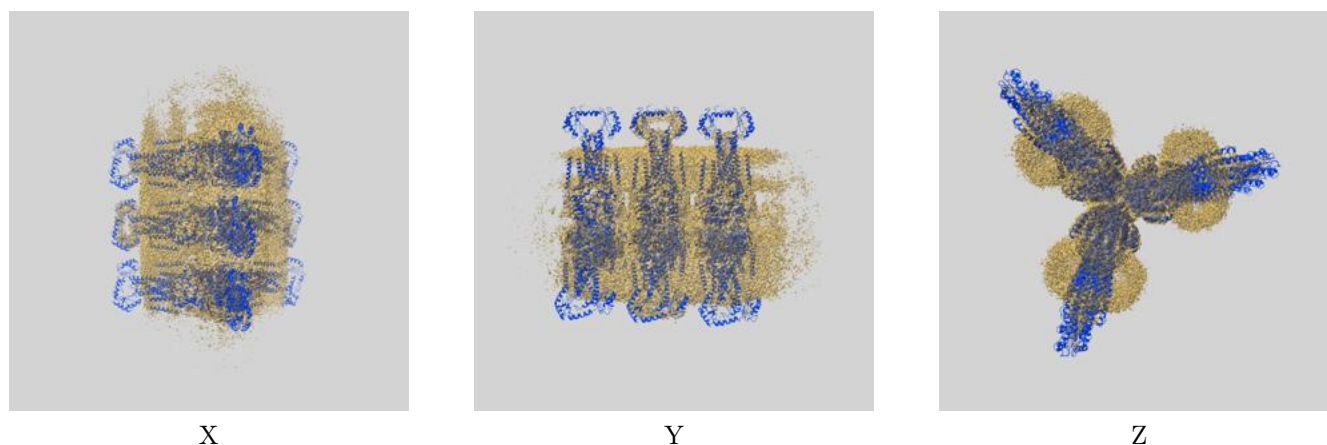
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.49	15.41	8.69

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

9 Map-model fit [i](#)

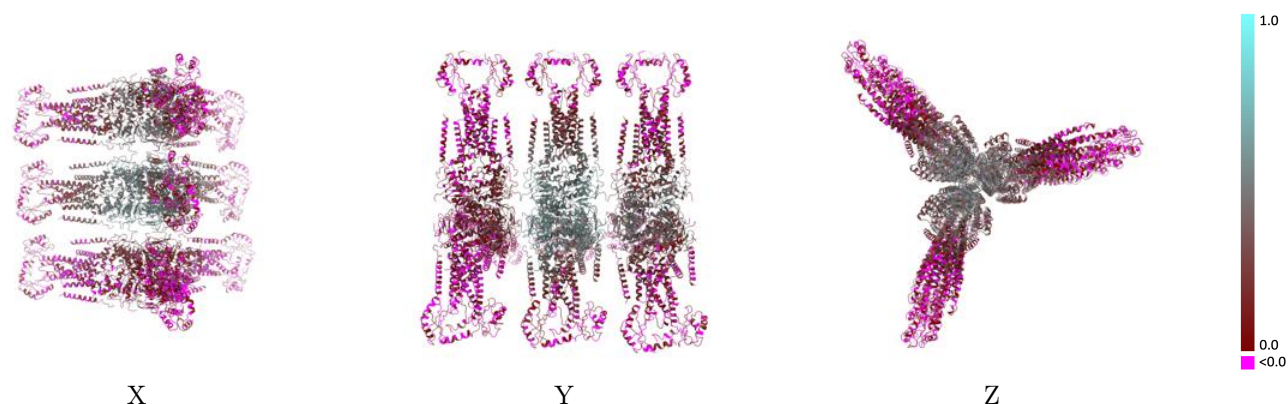
This section contains information regarding the fit between EMDB map EMD-60898 and PDB model 9IUE. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



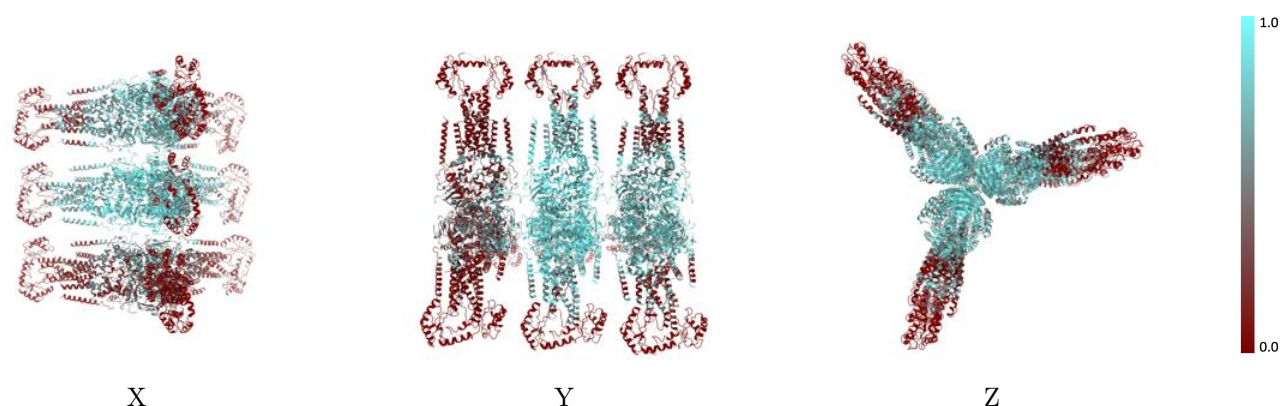
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



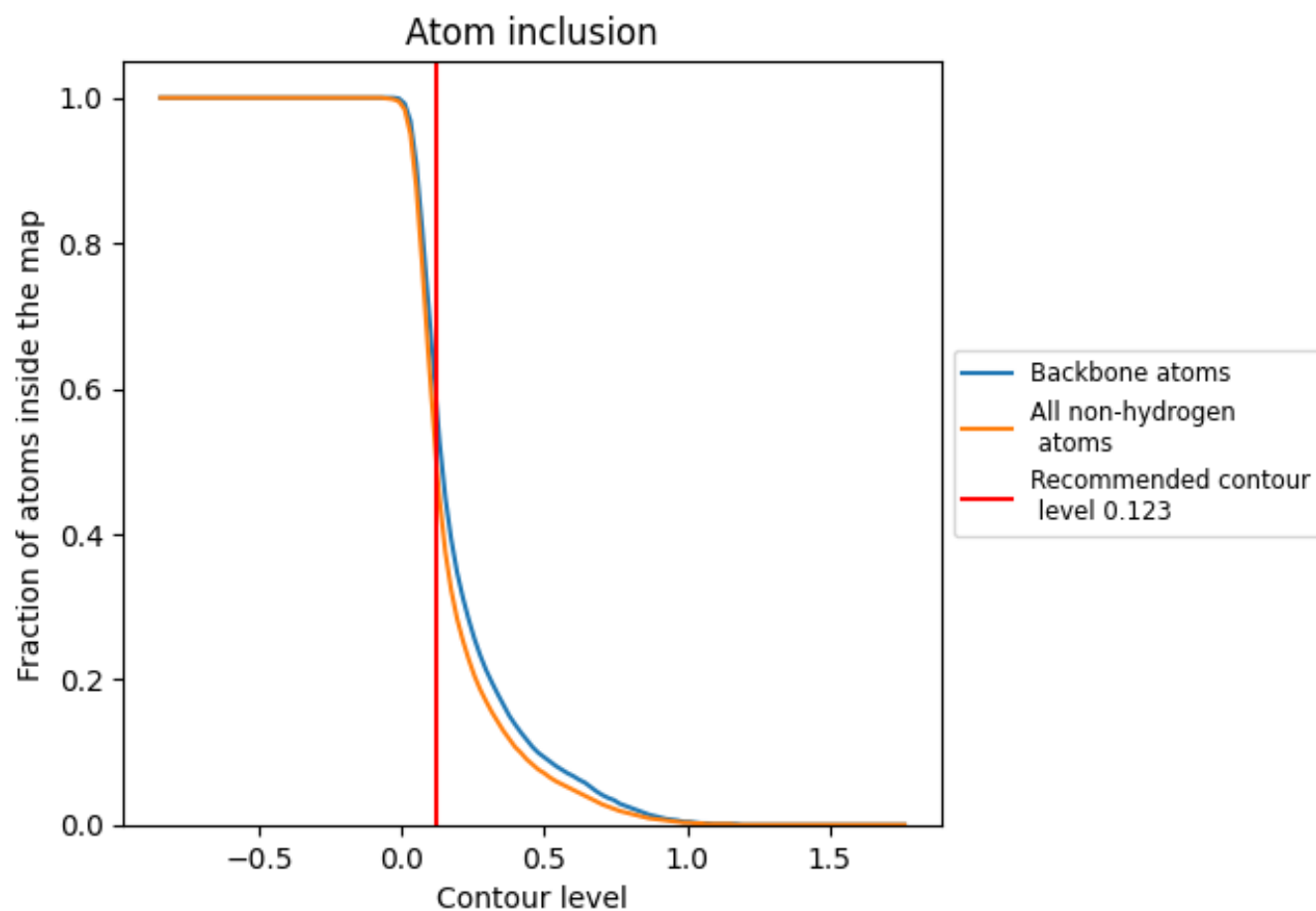
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.123).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% 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 (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2200
1	 0.7770	 0.3660
2	 0.7930	 0.3450
5	 0.9450	 0.5500
6	 0.9360	 0.5370
A	 0.5160	 0.2080
B	 0.2940	 0.0820
C	 0.5440	 0.2250
D	 0.2910	 0.0910
E	 0.4060	 0.1280
F	 0.4530	 0.1310
G	 0.7720	 0.3700
H	 0.7850	 0.3790
I	 0.1120	 0.0350
J	 0.1240	 0.0470
K	 0.2540	 0.0700
L	 0.1090	 0.0390
M	 0.3230	 0.1160
N	 0.5030	 0.1950
O	 0.5430	 0.2260
P	 0.5140	 0.2090
Q	 0.7770	 0.3630
R	 0.7970	 0.3480
S	 0.9440	 0.5470
T	 0.9340	 0.5330
U	 0.2930	 0.0820
V	 0.2930	 0.0890
W	 0.4100	 0.1220
X	 0.4490	 0.1330
Y	 0.7850	 0.3810
Z	 0.7860	 0.3810
a	 0.1120	 0.0310
b	 0.1280	 0.0510
c	 0.2660	 0.0710
d	 0.1090	 0.0220



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Chain	Atom inclusion	Q-score
e	 0.3230	 0.1170
f	 0.4990	 0.1920
g	 0.5480	 0.2250
h	 0.5190	 0.2100
i	 0.7850	 0.3630
j	 0.7810	 0.3430
k	 0.9430	 0.5470
l	 0.9330	 0.5330
m	 0.2970	 0.0820
n	 0.2940	 0.0920
o	 0.4180	 0.1270
p	 0.4410	 0.1340
q	 0.7840	 0.3810
r	 0.7920	 0.3840
s	 0.1130	 0.0340
t	 0.1330	 0.0520
u	 0.2500	 0.0760
v	 0.0980	 0.0330
w	 0.3260	 0.1160
x	 0.5080	 0.1980