



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:46 AM UTC

PDB ID : 5VU2 / pdb_00005vu2
EMDB ID : EMD-8734
Title : Electron cryo-microscopy of "immature" Chikungunya VLP
Authors : Rossmann, M.G.; Yap, M.L.
Deposited on : 2017-05-18
Resolution : 6.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

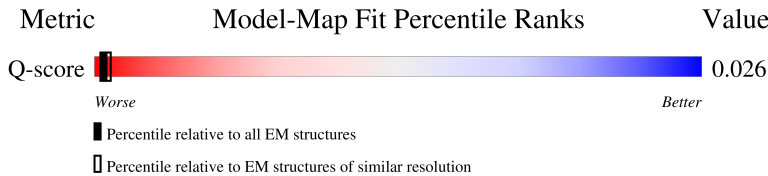
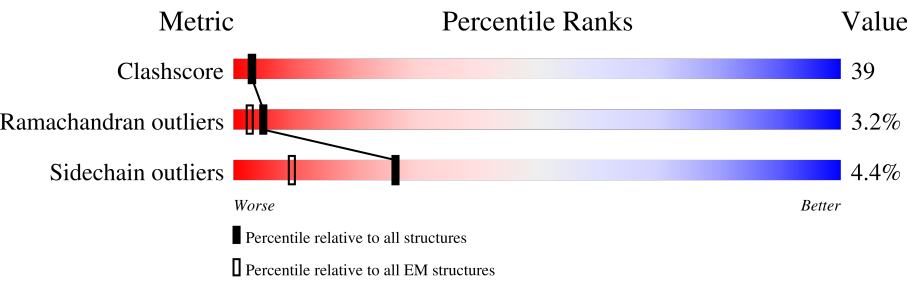
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	503 (6.30 - 7.30)

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

Mol	Chain	Length	Quality of chain
1	A	866	21% 37% 61%
1	B	866	21% 36% 61%
1	C	866	20% 36% 61%
1	D	866	21% 35% 61%

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Mol	Chain	Length	Quality of chain
1	M	866	
1	N	866	
1	O	866	
1	P	866	
2	U	60	
2	V	60	
2	W	60	
2	X	60	
3	I	149	
3	J	149	
3	K	149	
3	L	149	
4	E	46	
4	F	46	
4	G	46	
4	H	46	
5	Q	81	
5	R	81	
5	S	81	
5	T	81	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32676 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 E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	A	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	B	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	N	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	C	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	O	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		
1	D	341	Total	C	N	O	S	0	0
			2691	1677	487	507	20		
1	P	382	Total	C	N	O	S	1	0
			2911	1839	487	561	24		

- Molecule 2 is a protein called E3 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	V	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	W	60	Total	C	N	O	S	0	0
			477	296	81	91	9		
2	X	60	Total	C	N	O	S	0	0
			477	296	81	91	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	64	GLU	-	expression tag	UNP C7S7A1
V	64	GLU	-	expression tag	UNP C7S7A1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	64	GLU	-	expression tag	UNP C7S7A1
X	64	GLU	-	expression tag	UNP C7S7A1

- Molecule 3 is a protein called capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	J	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	K	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		
3	L	149	Total	C	N	O	S	0	0
			1141	723	201	211	6		

- Molecule 4 is a protein called E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	F	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	G	46	Total	C	N	O	S	0	0
			336	218	57	59	2		
4	H	46	Total	C	N	O	S	0	0
			336	218	57	59	2		

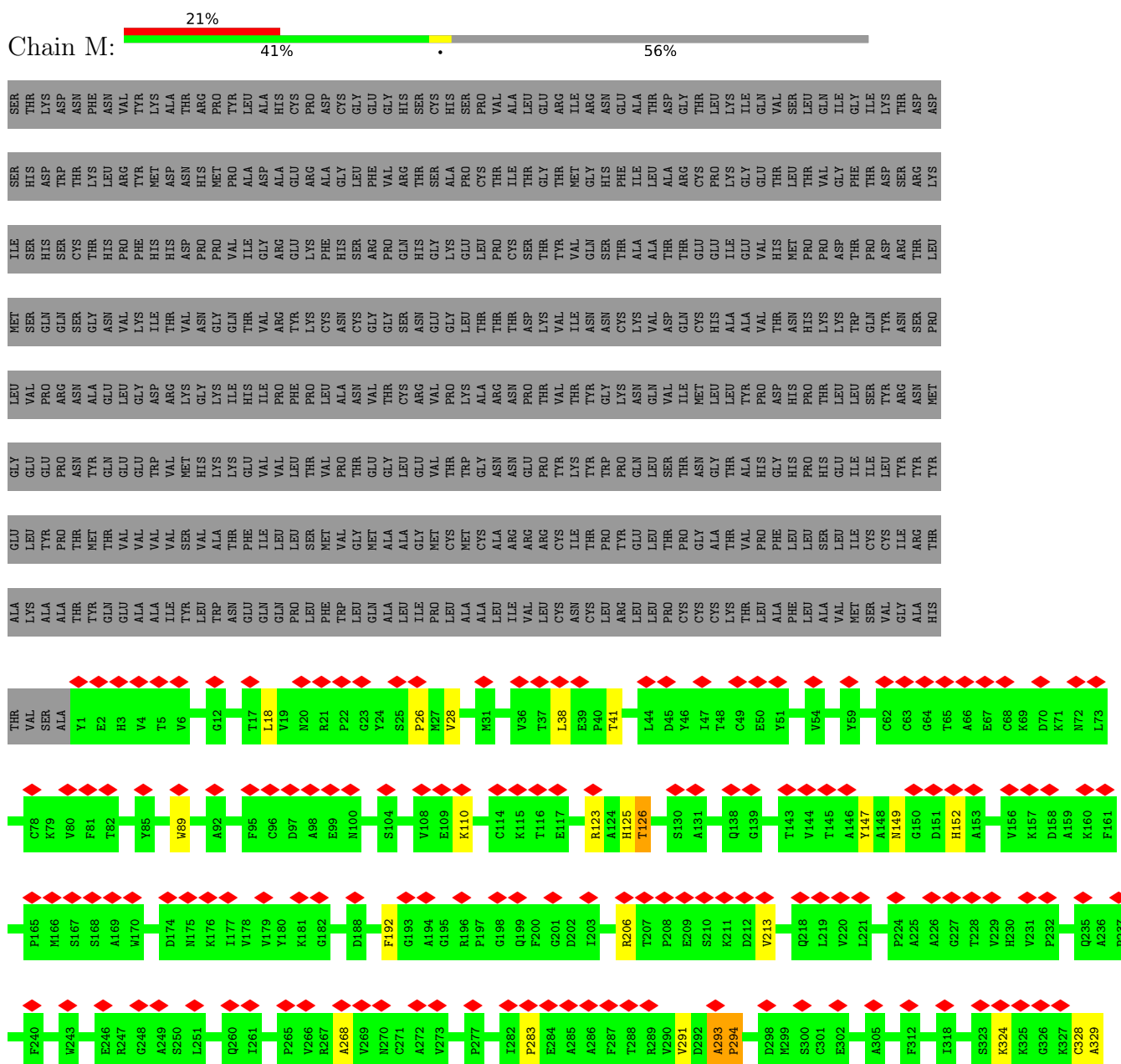
- Molecule 5 is a protein called E2 envelope glycoprotein.

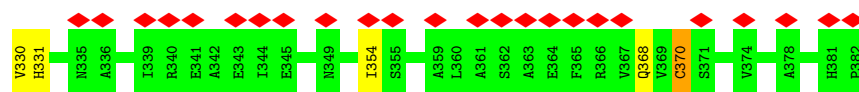
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	R	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	S	81	Total	C	N	O	S	0	0
			613	396	101	108	8		
5	T	81	Total	C	N	O	S	0	0
			613	396	101	108	8		

3 Residue-property plots

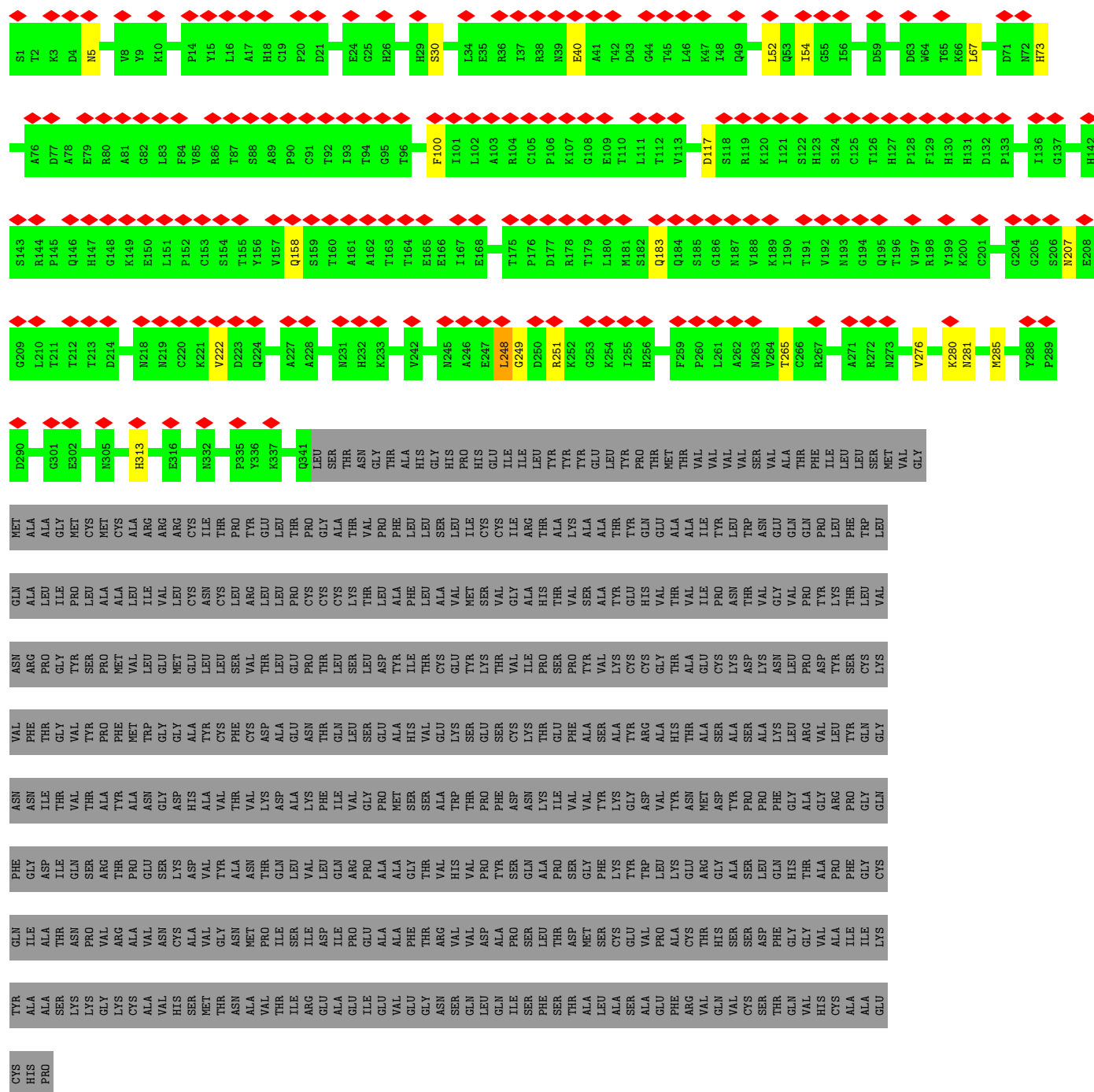
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: E1 envelope glycoprotein



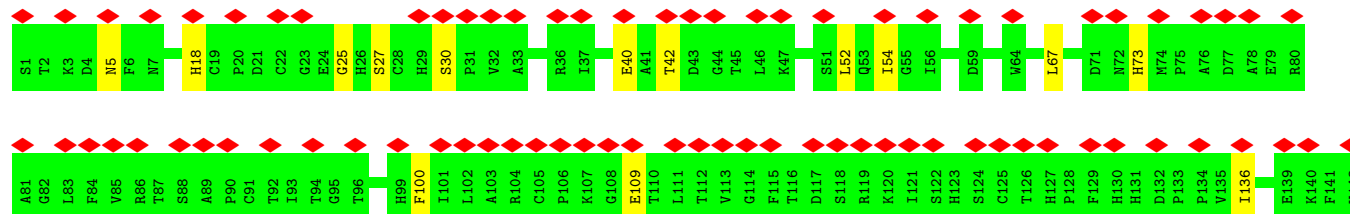


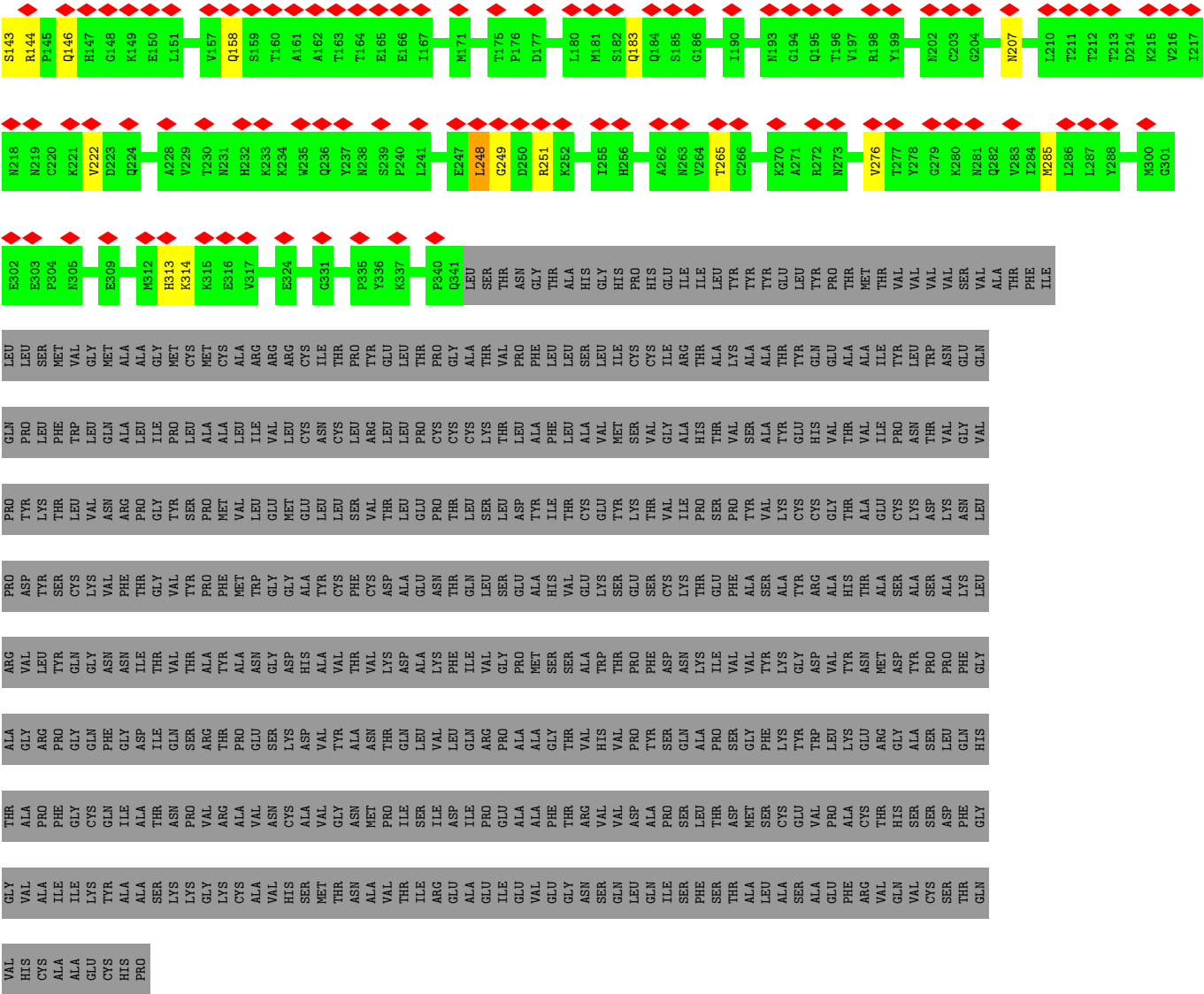
• Molecule 1: E1 envelope glycoprotein

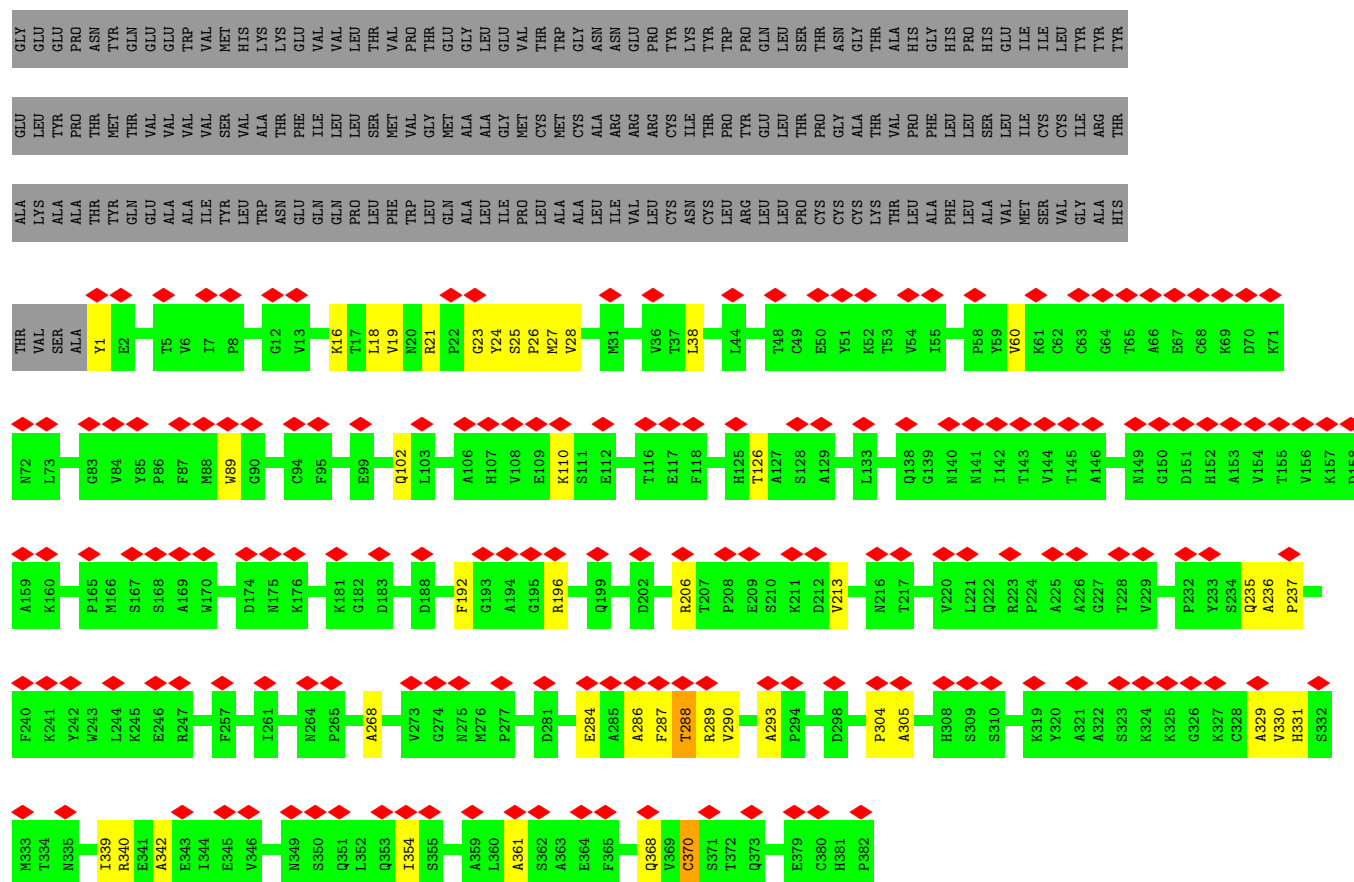


• Molecule 1: E1 envelope glycoprotein

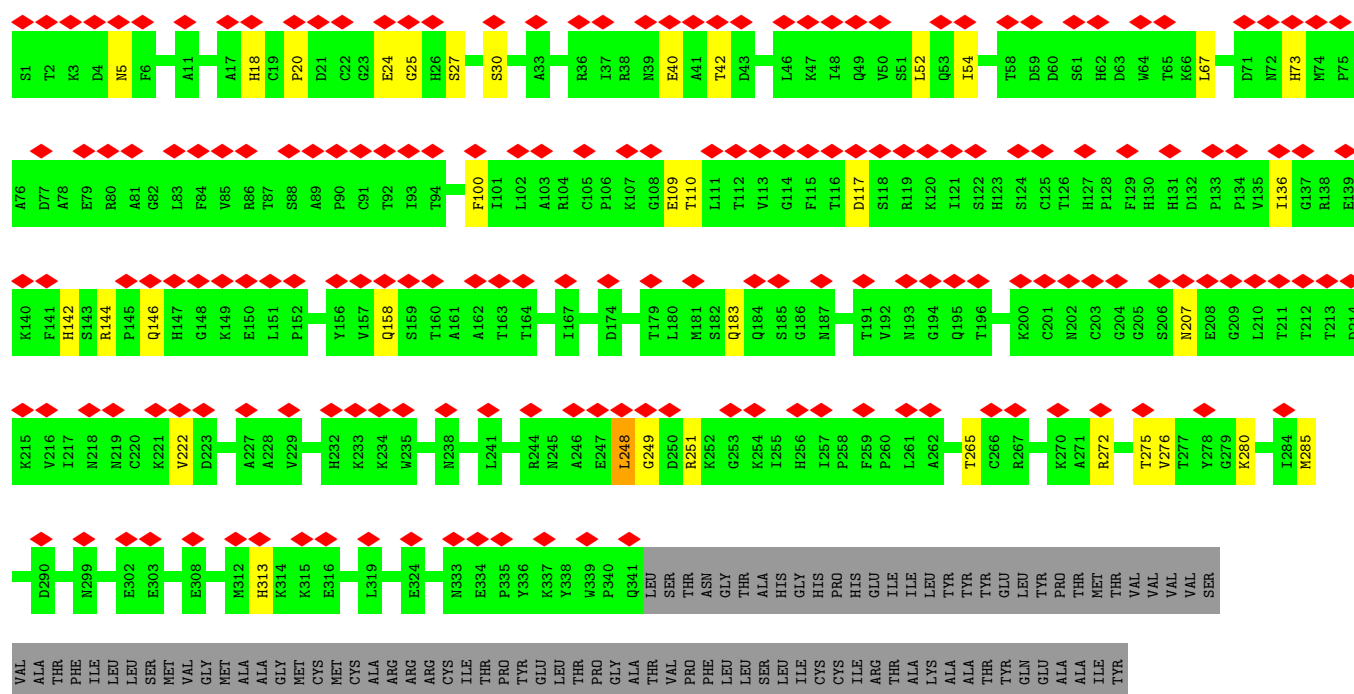








• Molecule 1: E1 envelope glycoprotein

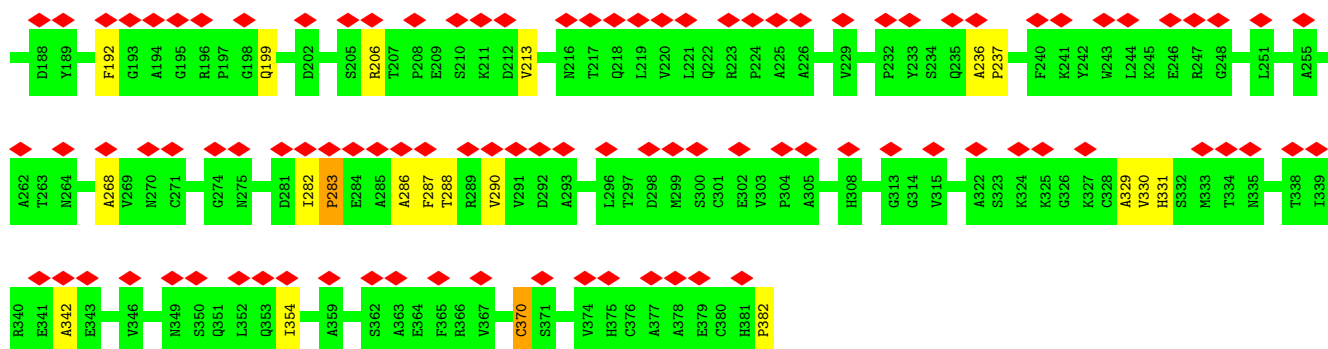


VAL	SER	ALA	TYR	ALA	LYS	ASN	LEU
SER	SER	SER	PRO	SER	ASP	THR	TRP
CYS	ASP	LEU	PRO	ALA	LYS	ASN	ASN
THR	PHE	GLN	PHE	LYS	ASN	GLY	GLU
GLN	GLY	HIS	GLY	LEU	LEU	VAL	GLN
VAL	GLY	THR	ALA	ARG	PRO	PRO	GLN
HIS	VAL	ALA	GLY	VAL	ASP	TYR	PRO
CYS	ALA	PRO	ARG	LEU	LYS	LEU	LEU
ALA	ILE	PHE	PRO	TYR	SER	THR	THR
ALA	ILE	GLY	GLY	GLN	CYS	LEU	PHE
GLU	LYS	CYS	GLN	GLY	LYS	VAL	LEU
CYS	TYR	GLN	PHE	ASN	VAL	ASN	GLN
HIS	ALA	ILE	GLY	ASN	PHE	ARG	ALA
PRO	ALA	THR	ASP	ILE	THR	GLY	LEU
	SER	THR	ILE	THR	VAL	TYR	PRO
	SER	THR	ILE	THR	GLY	GLY	LEU
	LYS	ASN	GLN	VAL	VAL	TYR	SER
	LYS	PRO	SER	THR	PRO	PRO	ALA
	GLY	VAL	ARG	ALA	ALA	PRO	ALA
	LYS	ARG	THR	TYR	PHE	MET	ALA
	CYS	VAL	PRO	ASN	TRP	VAL	LEU
	ALA	VAL	GLU	ASN	GLY	LEU	LEU
	VAL	ASN	SER	ASP	GLY	MET	VAL
	HIS	CYS	LYS	ASP	ALA	GLY	VAL
	SER	ALA	ASP	HIS	ALA	MET	CYS
	MET	VAL	VAL	ALA	TYR	LEU	ASN
	THR	THR	TYR	VAL	CYS	LEU	CYS
	ASN	ASN	ALA	THR	PHE	SER	ARG
	ALA	MET	ASN	VAL	CYS	VAL	LEU
	VAL	PRO	THR	LYS	ASP	THR	LEU
	THR	ILE	GLN	ASP	ALA	LEU	LEU
	ILE	SER	LEU	ALA	GLY	PRO	PRO
	ARG	ILE	VAL	LYS	ASN	GLU	CYS
	GLU	ASP	LEU	PHE	THR	THR	CYS
	ALA	ILE	GLN	ILE	GLN	LEU	CYS
	GLU	PRO	ARG	VAL	LEU	SER	LYS
	ILE	GLU	PRO	GLY	SER	ASP	THR
	GLU	ALA	ALA	PRO	GLY	LEU	ALA
	VAL	ALA	ALA	MET	ALA	TYR	VAL
	GLY	PHE	GLY	SER	HIS	ILE	PHE
	ASN	ARG	VAL	ALA	VAL	THR	LEU
	SER	VAL	HIS	TRP	LYS	CYS	ALA
	GLN	VAL	VAL	THR	GLY	VAL	VAL
	LEU	ASP	PRO	THR	SER	GLY	VAL
	LEU	VAL	PRO	GLU	LYS	THR	THR
	GLN	VAL	VAL	GLU	THR	GLY	THR
	GLN	ALA	TYR	PHE	VAL	VAL	SER
	ILE	PRO	GLN	ASN	CYS	ILE	ALA
	SER	SER	SER	ASN	LYS	PRO	HIS
	PHE	LEU	ALA	LYS	THR	ILE	ALA
	THR	THR	THR	ILE	THR	GLY	THR
	ALA	ASP	ASP	VAL	PHE	SER	SER
	LEU	MET	GLY	VAL	ALA	TYR	VAL
	SER	SER	SER	THR	GLY	VAL	TYR
	ALA	CYS	LYS	LYS	ALA	LYS	TYR
	SER	GLY	TYR	GLY	TYR	CYS	GLY
	ALA	VAL	THR	ASP	ARG	CYS	HIS
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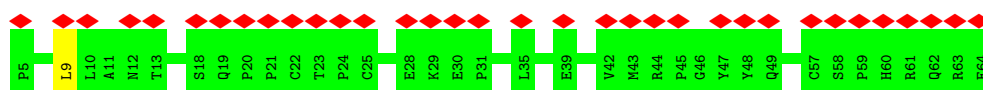
- Molecule 1: E1 envelope glycoprotein



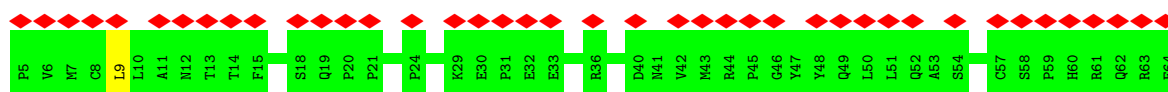
W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108	E109	K110	S111	E112	S113	C114	K115	T116	E117	T126	K132	Y137	Q138	G139	T143	V144	T145	D151	H152	A153	V154	T155	V156	K157	D158	A159	K160	P165	M166	W89	G90	G91	C94	F95	C96	D97	Q102	L103	S104	E105	A106	H107	V108
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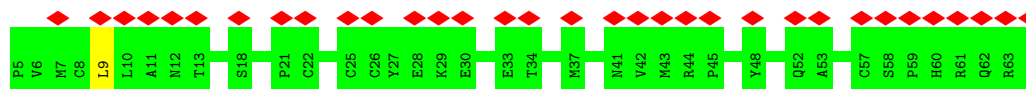
- Molecule 2: E3 envelope glycoprotein



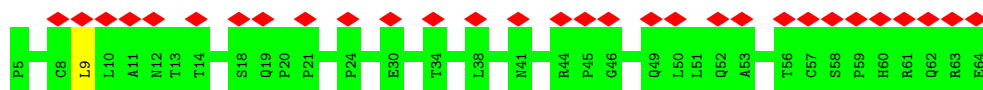
- Molecule 2: E3 envelope glycoprotein



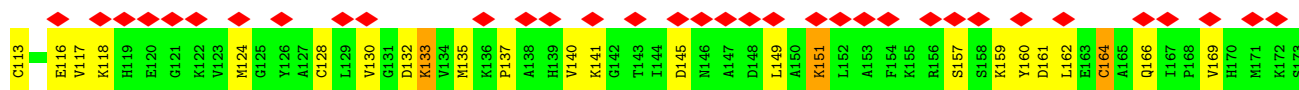
- Molecule 2: E3 envelope glycoprotein



- Molecule 2: E3 envelope glycoprotein

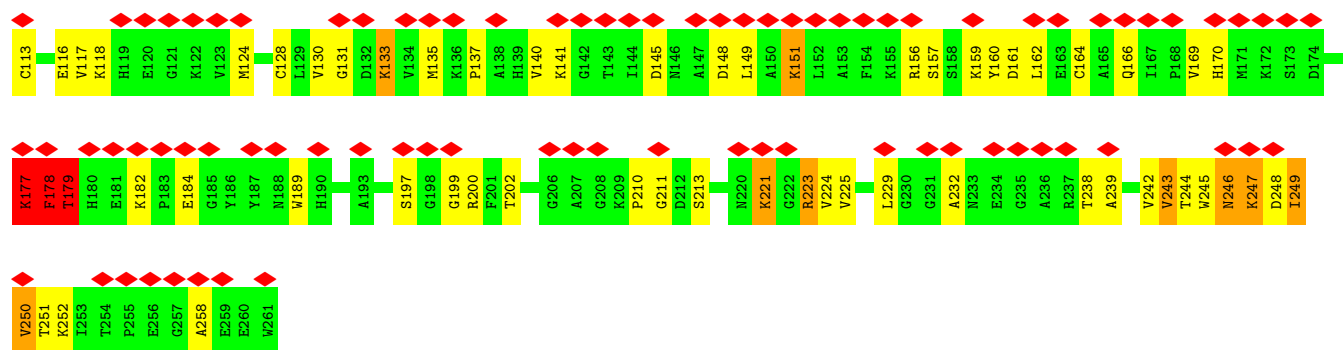


- Molecule 3: capsid protein

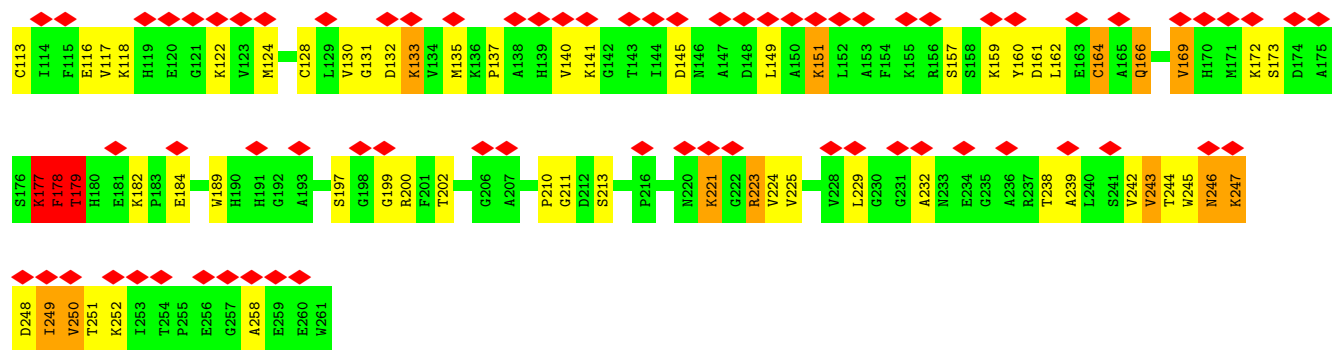




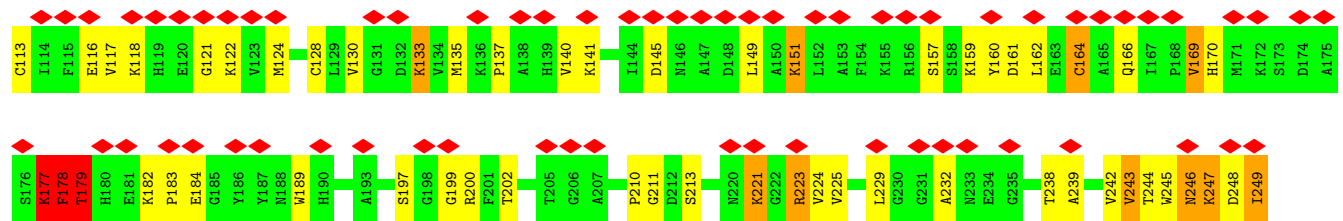
• Molecule 3: capsid protein

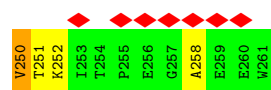


• Molecule 3: capsid protein

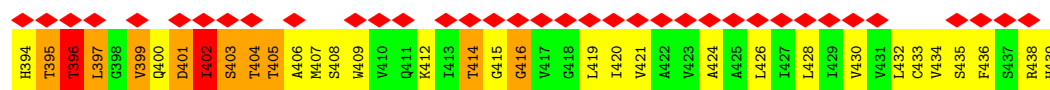
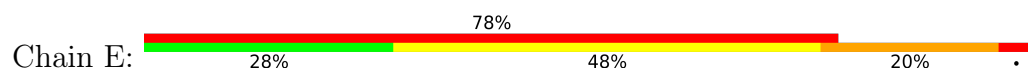


• Molecule 3: capsid protein

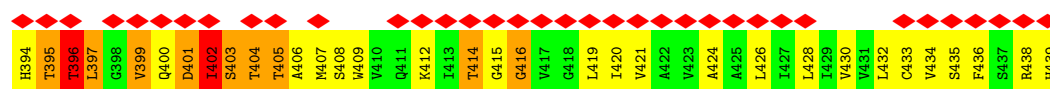
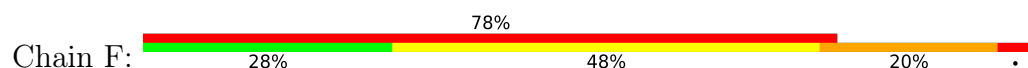




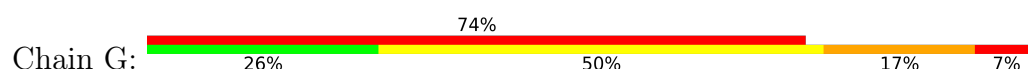
• Molecule 4: E1 envelope glycoprotein



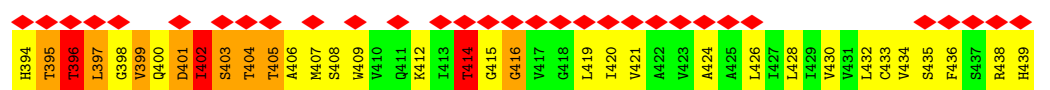
• Molecule 4: E1 envelope glycoprotein



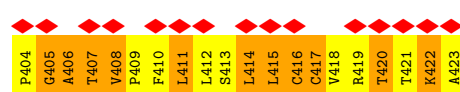
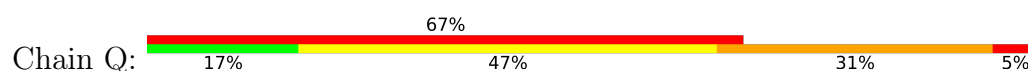
• Molecule 4: E1 envelope glycoprotein



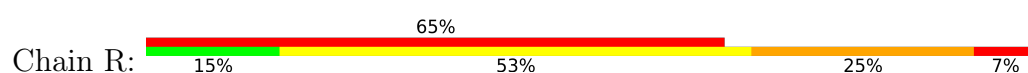
• Molecule 4: E1 envelope glycoprotein

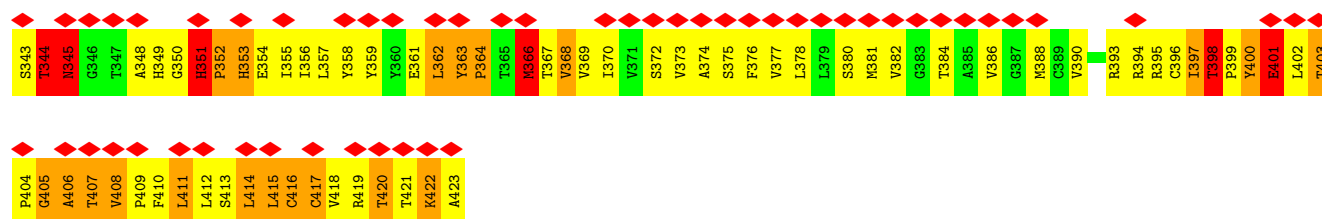


• Molecule 5: E2 envelope glycoprotein

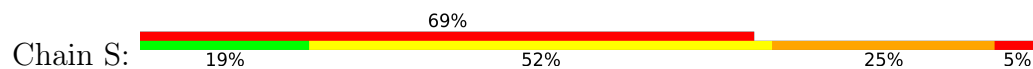


• Molecule 5: E2 envelope glycoprotein

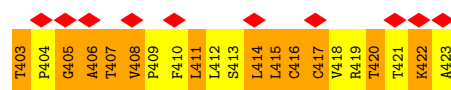
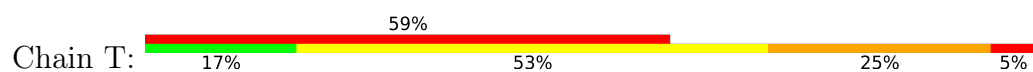




• Molecule 5: E2 envelope glycoprotein



• Molecule 5: E2 envelope glycoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72944	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.000	Depositor
Minimum map value	-5.000	Depositor
Average map value	0.029	Depositor
Map value standard deviation	0.438	Depositor
Recommended contour level	1	Depositor
Map size (Å)	998.39996, 998.39996, 998.39996	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/2763	1.12	4/3760 (0.1%)
1	B	0.69	0/2763	1.12	4/3760 (0.1%)
1	C	0.69	0/2763	1.12	3/3760 (0.1%)
1	D	0.69	0/2763	1.12	4/3760 (0.1%)
1	M	0.64	0/2984	1.06	2/4069 (0.0%)
1	N	0.64	0/2984	1.06	2/4069 (0.0%)
1	O	0.64	0/2984	1.04	0/4069
1	P	0.64	0/2984	1.04	2/4069 (0.0%)
2	U	0.72	0/489	1.27	0/665
2	V	0.72	0/489	1.27	0/665
2	W	0.73	0/489	1.27	0/665
2	X	0.72	0/489	1.27	0/665
3	I	0.83	4/1169 (0.3%)	2.15	12/1577 (0.8%)
3	J	0.83	4/1169 (0.3%)	2.15	12/1577 (0.8%)
3	K	0.83	4/1169 (0.3%)	2.15	12/1577 (0.8%)
3	L	0.83	4/1169 (0.3%)	2.15	12/1577 (0.8%)
4	E	1.16	7/340 (2.1%)	1.58	13/464 (2.8%)
4	F	1.16	7/340 (2.1%)	1.58	13/464 (2.8%)
4	G	1.16	7/340 (2.1%)	1.58	13/464 (2.8%)
4	H	1.16	7/340 (2.1%)	1.58	13/464 (2.8%)
5	Q	0.46	1/627 (0.2%)	0.74	0/858
5	R	0.44	1/627 (0.2%)	0.72	0/858
5	S	0.44	1/627 (0.2%)	0.73	0/858
5	T	0.44	1/627 (0.2%)	0.71	0/858
All	All	0.71	48/33488 (0.1%)	1.30	121/45572 (0.3%)

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
3	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2
3	K	0	2
3	L	0	2
4	E	0	1
4	F	0	1
4	G	0	1
4	H	0	1
All	All	0	12

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	178	PHE	C-N	9.49	1.47	1.33
3	K	178	PHE	C-N	9.46	1.47	1.33
3	I	178	PHE	C-N	9.38	1.46	1.33
3	L	178	PHE	C-N	9.38	1.46	1.33
4	F	396	THR	N-CA	7.11	1.55	1.46
4	H	396	THR	N-CA	7.09	1.55	1.46
4	E	396	THR	N-CA	7.08	1.55	1.46
4	G	396	THR	N-CA	7.05	1.55	1.46
3	J	113	CYS	CB-SG	-6.96	1.58	1.81
3	K	113	CYS	CB-SG	-6.96	1.58	1.81
3	L	113	CYS	CB-SG	-6.93	1.58	1.81
3	I	113	CYS	CB-SG	-6.90	1.58	1.81
4	H	402	ILE	N-CA	6.64	1.54	1.46
4	F	402	ILE	N-CA	6.63	1.54	1.46
4	G	402	ILE	N-CA	6.62	1.54	1.46
4	E	402	ILE	N-CA	6.60	1.54	1.46
3	J	177	LYS	C-N	-6.36	1.24	1.33
3	I	177	LYS	C-N	-6.30	1.24	1.33
4	E	403	SER	CA-C	6.28	1.61	1.52
4	G	403	SER	CA-C	6.27	1.61	1.52
3	L	177	LYS	C-N	-6.27	1.25	1.33
4	H	403	SER	CA-C	6.24	1.61	1.52
3	K	177	LYS	C-N	-6.21	1.25	1.33
4	F	403	SER	CA-C	6.20	1.61	1.52
4	G	402	ILE	CA-C	6.03	1.60	1.52
4	H	402	ILE	CA-C	6.01	1.60	1.52
4	E	402	ILE	CA-C	6.01	1.60	1.52
4	F	402	ILE	CA-C	6.00	1.60	1.52
4	E	400	GLN	CA-C	5.97	1.60	1.52
4	F	400	GLN	CA-C	5.96	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	400	GLN	CA-C	5.96	1.60	1.52
3	J	128	CYS	CB-SG	-5.93	1.61	1.81
3	I	128	CYS	CB-SG	-5.92	1.61	1.81
4	G	400	GLN	CA-C	5.91	1.60	1.52
3	L	128	CYS	CB-SG	-5.90	1.61	1.81
3	K	128	CYS	CB-SG	-5.90	1.61	1.81
5	R	345	ASN	N-CA	5.76	1.52	1.46
5	S	345	ASN	N-CA	5.75	1.52	1.46
5	Q	345	ASN	N-CA	5.75	1.52	1.46
5	T	345	ASN	N-CA	5.73	1.52	1.46
4	H	400	GLN	CA-CB	5.38	1.62	1.53
4	G	400	GLN	CA-CB	5.38	1.62	1.53
4	F	400	GLN	CA-CB	5.36	1.62	1.53
4	E	400	GLN	CA-CB	5.35	1.62	1.53
4	H	401	ASP	CA-C	5.32	1.59	1.52
4	E	401	ASP	CA-C	5.31	1.59	1.52
4	G	401	ASP	CA-C	5.29	1.59	1.52
4	F	401	ASP	CA-C	5.27	1.59	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	177	LYS	O-C-N	-46.10	61.27	122.59
3	K	177	LYS	O-C-N	-46.08	61.31	122.59
3	L	177	LYS	O-C-N	-46.05	61.35	122.59
3	J	177	LYS	O-C-N	-46.04	61.35	122.59
3	J	178	PHE	O-C-N	-31.62	80.54	122.59
3	L	178	PHE	O-C-N	-31.57	80.60	122.59
3	K	178	PHE	O-C-N	-31.57	80.60	122.59
3	I	178	PHE	O-C-N	-31.53	80.66	122.59
3	K	177	LYS	CA-C-N	28.30	175.60	121.54
3	K	177	LYS	C-N-CA	28.30	175.60	121.54
3	L	177	LYS	CA-C-N	28.30	175.59	121.54
3	L	177	LYS	C-N-CA	28.30	175.59	121.54
3	I	177	LYS	CA-C-N	28.28	175.56	121.54
3	I	177	LYS	C-N-CA	28.28	175.56	121.54
3	J	177	LYS	CA-C-N	28.27	175.53	121.54
3	J	177	LYS	C-N-CA	28.27	175.53	121.54
3	J	178	PHE	CA-C-N	14.30	148.85	121.54
3	J	178	PHE	C-N-CA	14.30	148.85	121.54
3	I	178	PHE	CA-C-N	14.26	148.78	121.54
3	I	178	PHE	C-N-CA	14.26	148.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	178	PHE	CA-C-N	14.24	148.74	121.54
3	K	178	PHE	C-N-CA	14.24	148.74	121.54
3	L	178	PHE	CA-C-N	14.23	148.72	121.54
3	L	178	PHE	C-N-CA	14.23	148.72	121.54
3	I	128	CYS	CA-CB-SG	11.61	141.11	114.40
3	J	128	CYS	CA-CB-SG	11.61	141.10	114.40
3	K	128	CYS	CA-CB-SG	11.60	141.07	114.40
3	L	128	CYS	CA-CB-SG	11.56	141.00	114.40
4	G	402	ILE	N-CA-C	10.37	130.92	109.34
4	E	402	ILE	N-CA-C	10.37	130.91	109.34
4	H	402	ILE	N-CA-C	10.36	130.90	109.34
4	F	402	ILE	N-CA-C	10.35	130.88	109.34
4	E	395	THR	N-CA-C	8.57	122.28	107.28
4	F	395	THR	N-CA-C	8.57	122.27	107.28
4	H	395	THR	N-CA-C	8.56	122.25	107.28
4	G	395	THR	N-CA-C	8.55	122.24	107.28
4	H	403	SER	N-CA-C	8.05	127.95	110.80
4	F	403	SER	N-CA-C	8.05	127.94	110.80
4	G	403	SER	N-CA-C	8.04	127.93	110.80
4	E	403	SER	N-CA-C	8.03	127.90	110.80
4	E	414	THR	N-CA-C	6.88	120.67	109.59
4	H	414	THR	N-CA-C	6.88	120.66	109.59
4	F	414	THR	N-CA-C	6.86	120.63	109.59
4	G	414	THR	N-CA-C	6.86	120.64	109.59
4	F	396	THR	CA-C-N	-6.59	108.94	121.54
4	F	396	THR	C-N-CA	-6.59	108.94	121.54
4	H	396	THR	CA-C-N	-6.57	108.99	121.54
4	H	396	THR	C-N-CA	-6.57	108.99	121.54
4	G	396	THR	CA-C-N	-6.56	109.01	121.54
4	G	396	THR	C-N-CA	-6.56	109.01	121.54
4	E	396	THR	CA-C-N	-6.54	109.04	121.54
4	E	396	THR	C-N-CA	-6.54	109.04	121.54
4	F	396	THR	N-CA-CB	6.47	121.43	110.49
4	E	396	THR	N-CA-CB	6.47	121.42	110.49
4	H	396	THR	N-CA-CB	6.46	121.41	110.49
4	G	396	THR	N-CA-CB	6.44	121.38	110.49
4	G	395	THR	CA-C-N	6.44	133.83	121.54
4	G	395	THR	C-N-CA	6.44	133.83	121.54
4	E	395	THR	CA-C-N	6.42	133.81	121.54
4	E	395	THR	C-N-CA	6.42	133.81	121.54
4	H	395	THR	CA-C-N	6.42	133.80	121.54
4	H	395	THR	C-N-CA	6.42	133.80	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	395	THR	CA-C-N	6.42	133.80	121.54
4	F	395	THR	C-N-CA	6.42	133.80	121.54
3	K	113	CYS	CA-CB-SG	6.38	129.08	114.40
3	I	113	CYS	CA-CB-SG	6.38	129.07	114.40
3	J	113	CYS	CA-CB-SG	6.33	128.95	114.40
3	L	113	CYS	CA-CB-SG	6.32	128.94	114.40
1	C	30	SER	N-CA-C	6.27	117.70	109.93
1	B	30	SER	N-CA-C	6.26	117.69	109.93
1	A	30	SER	N-CA-C	6.25	117.69	109.93
1	D	30	SER	N-CA-C	6.22	117.64	109.93
1	C	100	PHE	N-CA-C	5.83	118.97	109.59
4	G	400	GLN	CB-CG-CD	5.81	122.47	112.60
4	E	400	GLN	CB-CG-CD	5.80	122.47	112.60
4	H	400	GLN	CB-CG-CD	5.80	122.46	112.60
4	F	400	GLN	CB-CG-CD	5.80	122.45	112.60
1	A	100	PHE	N-CA-C	5.78	118.89	109.59
1	B	100	PHE	N-CA-C	5.78	118.89	109.59
1	D	100	PHE	N-CA-C	5.77	118.88	109.59
3	K	249	ILE	N-CA-C	5.74	118.18	109.12
3	J	249	ILE	N-CA-C	5.72	118.16	109.12
3	I	249	ILE	N-CA-C	5.70	118.13	109.12
3	L	249	ILE	N-CA-C	5.64	118.03	109.12
1	N	283	PRO	CA-C-N	5.60	128.05	120.38
1	N	283	PRO	C-N-CA	5.60	128.05	120.38
1	P	283	PRO	CA-C-N	5.58	128.03	120.38
1	P	283	PRO	C-N-CA	5.58	128.03	120.38
1	M	283	PRO	CA-C-N	5.55	127.98	120.38
1	M	283	PRO	C-N-CA	5.55	127.98	120.38
4	H	416	GLY	CA-C-N	-5.42	112.21	121.97
4	H	416	GLY	C-N-CA	-5.42	112.21	121.97
4	F	416	GLY	CA-C-N	-5.42	112.22	121.97
4	F	416	GLY	C-N-CA	-5.42	112.22	121.97
4	G	416	GLY	CA-C-N	-5.41	112.23	121.97
4	G	416	GLY	C-N-CA	-5.41	112.23	121.97
4	E	416	GLY	CA-C-N	-5.40	112.24	121.97
4	E	416	GLY	C-N-CA	-5.40	112.24	121.97
3	K	116	GLU	N-CA-C	5.39	118.03	109.24
3	J	116	GLU	N-CA-C	5.38	118.02	109.24
3	L	116	GLU	N-CA-C	5.37	118.00	109.24
3	I	116	GLU	N-CA-C	5.35	117.96	109.24
3	J	243	VAL	N-CA-C	-5.27	100.16	107.80
4	F	416	GLY	N-CA-C	5.27	125.67	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	243	VAL	N-CA-C	-5.27	100.16	107.80
3	K	243	VAL	N-CA-C	-5.26	100.17	107.80
4	H	416	GLY	N-CA-C	5.25	125.63	113.18
4	G	416	GLY	N-CA-C	5.25	125.62	113.18
4	E	416	GLY	N-CA-C	5.24	125.61	113.18
1	A	5	ASN	CA-CB-CG	5.24	117.84	112.60
1	D	5	ASN	CA-CB-CG	5.22	117.82	112.60
1	C	5	ASN	CA-CB-CG	5.22	117.82	112.60
1	B	5	ASN	CA-CB-CG	5.22	117.82	112.60
3	K	242	VAL	N-CA-C	5.19	116.38	108.80
3	I	242	VAL	N-CA-C	5.19	116.37	108.80
3	I	243	VAL	N-CA-C	-5.19	100.28	107.80
3	J	242	VAL	N-CA-C	5.14	116.31	108.80
3	L	242	VAL	N-CA-C	5.11	116.26	108.80
1	A	117	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	117	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	117	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	414	THR	Peptide
4	F	414	THR	Peptide
4	G	414	THR	Peptide
4	H	414	THR	Peptide
3	I	177	LYS	Mainchain
3	I	178	PHE	Mainchain
3	J	177	LYS	Mainchain
3	J	178	PHE	Mainchain
3	K	177	LYS	Mainchain
3	K	178	PHE	Mainchain
3	L	177	LYS	Mainchain
3	L	178	PHE	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2691	0	2608	17	0
1	B	2691	0	2603	59	0
1	C	2691	0	2605	49	0
1	D	2691	0	2603	87	0
1	M	2911	0	2819	105	0
1	N	2911	0	2819	71	0
1	O	2911	0	2819	139	0
1	P	2911	0	2819	71	0
2	U	477	0	457	0	0
2	V	477	0	457	0	0
2	W	477	0	457	0	0
2	X	477	0	457	0	0
3	I	1141	0	1125	173	0
3	J	1141	0	1119	148	0
3	K	1141	0	1124	227	0
3	L	1141	0	1123	173	0
4	E	336	0	361	107	0
4	F	336	0	361	122	0
4	G	336	0	361	137	0
4	H	336	0	361	109	0
5	Q	613	0	630	352	0
5	R	613	0	631	380	0
5	S	613	0	629	406	0
5	T	613	0	631	361	0
All	All	32676	0	31979	2498	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 39.

All (2498) 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)
3:J:160:TYR:CE2	5:R:398:THR:HG23	1.18	1.67
3:K:160:TYR:CZ	5:S:398:THR:HG23	1.24	1.65
3:I:160:TYR:CZ	5:Q:398:THR:HG23	1.27	1.64
4:H:402:ILE:HB	4:H:407:MET:SD	1.34	1.64
3:K:132:ASP:H	5:S:402:LEU:CD1	1.12	1.63
5:Q:349:HIS:CE1	5:Q:358:TYR:CE2	1.79	1.62
4:E:402:ILE:HB	4:E:407:MET:SD	1.34	1.61
1:C:18:HIS:CE1	1:D:146:GLN:NE2	1.68	1.60
3:I:251:THR:CG2	4:E:439:HIS:HB3	1.17	1.59
4:G:399:VAL:HG21	5:S:362:LEU:CD2	1.23	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:CE1	1:D:109:GLU:HG3	1.24	1.59
4:F:402:ILE:HB	4:F:407:MET:SD	1.34	1.58
4:G:402:ILE:HB	4:G:407:MET:SD	1.34	1.56
3:K:160:TYR:CD2	5:S:397:ILE:HG22	1.38	1.55
4:F:421:VAL:HG13	5:R:388:MET:SD	1.48	1.54
1:M:291:VAL:HG22	1:O:304:PRO:CB	1.10	1.53
4:E:421:VAL:HG13	5:Q:388:MET:SD	1.48	1.53
3:L:178:PHE:CZ	5:T:403:THR:HG21	1.44	1.52
4:G:421:VAL:HG13	5:S:388:MET:SD	1.48	1.52
3:J:157:SER:CB	5:R:397:ILE:HD12	1.36	1.52
5:Q:356:ILE:HA	5:Q:359:TYR:CE2	1.45	1.51
1:O:237:PRO:CD	1:D:272:ARG:NH2	1.74	1.50
5:R:349:HIS:CE1	5:R:357:LEU:HB2	1.47	1.50
5:R:351:HIS:HB3	5:R:352:PRO:CD	1.33	1.50
4:H:421:VAL:HG13	5:T:388:MET:SD	1.48	1.50
1:B:142:HIS:NE2	1:D:109:GLU:HG3	1.19	1.49
5:Q:349:HIS:CE1	5:Q:358:TYR:HE2	1.14	1.49
3:K:157:SER:CB	5:S:397:ILE:HD12	1.42	1.48
4:G:399:VAL:CG2	5:S:362:LEU:HD21	1.37	1.48
3:K:160:TYR:CE1	5:S:398:THR:HG23	1.46	1.48
4:G:399:VAL:CG1	5:S:362:LEU:CD1	1.91	1.47
5:S:356:ILE:HA	5:S:359:TYR:CE2	1.48	1.47
3:K:160:TYR:CZ	5:S:398:THR:CG2	1.98	1.47
5:S:406:ALA:CB	5:S:409:PRO:HD2	1.45	1.46
3:I:251:THR:CG2	4:E:439:HIS:CB	1.93	1.46
5:R:356:ILE:HA	5:R:359:TYR:CE2	1.51	1.46
5:R:406:ALA:CB	5:R:409:PRO:HD2	1.45	1.45
3:L:133:LYS:H	5:T:402:LEU:CD1	1.23	1.44
3:I:251:THR:HG23	4:E:439:HIS:CB	1.48	1.44
5:Q:413:SER:HB2	5:Q:417:CYS:SG	1.57	1.44
5:T:406:ALA:CB	5:T:409:PRO:HD2	1.45	1.44
5:T:356:ILE:HA	5:T:359:TYR:CE2	1.51	1.44
3:J:160:TYR:CZ	5:R:398:THR:HG23	1.50	1.44
5:T:413:SER:HB2	5:T:417:CYS:SG	1.57	1.44
5:T:418:VAL:CG1	5:T:419:ARG:HA	1.47	1.44
5:Q:406:ALA:CB	5:Q:409:PRO:HD2	1.45	1.43
3:L:164:CYS:SG	5:T:400:TYR:CZ	2.11	1.43
5:S:418:VAL:CG1	5:S:419:ARG:HA	1.47	1.43
1:B:142:HIS:CE1	1:D:109:GLU:CG	2.00	1.42
3:L:133:LYS:HD2	5:T:402:LEU:CD2	1.49	1.42
5:S:413:SER:HB2	5:S:417:CYS:SG	1.57	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:418:VAL:CG1	5:Q:419:ARG:HA	1.47	1.42
5:R:406:ALA:HB2	5:R:409:PRO:CD	1.49	1.42
5:R:413:SER:HB2	5:R:417:CYS:SG	1.57	1.42
4:G:399:VAL:HG11	5:S:362:LEU:CD1	1.49	1.42
5:Q:406:ALA:HB2	5:Q:409:PRO:CD	1.49	1.42
1:M:149:ASN:HD21	1:N:191:PRO:CG	1.32	1.41
3:J:157:SER:OG	5:R:397:ILE:CG2	1.67	1.41
5:T:406:ALA:HB2	5:T:409:PRO:CD	1.49	1.41
3:L:159:LYS:HZ2	4:H:432:LEU:CD2	1.33	1.41
3:J:160:TYR:CE2	5:R:398:THR:CG2	2.02	1.41
5:R:418:VAL:CG1	5:R:419:ARG:HA	1.47	1.41
3:K:160:TYR:CE2	5:S:398:THR:N	1.85	1.41
3:L:133:LYS:N	5:T:402:LEU:CD1	1.74	1.41
4:H:403:SER:CA	4:H:407:MET:HG2	1.51	1.40
5:S:406:ALA:HB2	5:S:409:PRO:CD	1.49	1.39
5:Q:349:HIS:NE2	5:Q:358:TYR:CE2	1.73	1.39
5:Q:364:PRO:O	5:Q:365:THR:CG2	1.71	1.39
3:J:159:LYS:CD	4:F:432:LEU:HB3	1.50	1.39
5:S:349:HIS:CE1	5:S:354:GLU:C	1.85	1.39
4:E:403:SER:CA	4:E:407:MET:HG2	1.52	1.38
4:G:403:SER:CA	4:G:407:MET:HG2	1.52	1.38
4:F:399:VAL:HG21	5:R:362:LEU:CD2	1.53	1.38
4:F:403:SER:CA	4:F:407:MET:HG2	1.52	1.38
1:D:280:LYS:CE	5:T:343:SER:O	1.69	1.38
3:L:178:PHE:CZ	5:T:403:THR:CG2	2.05	1.37
1:M:291:VAL:CG2	1:O:304:PRO:HB2	1.51	1.37
3:K:132:ASP:N	5:S:402:LEU:CD1	1.82	1.37
3:K:157:SER:CB	5:S:397:ILE:CD1	2.02	1.36
5:S:416:CYS:HA	5:S:417:CYS:C	1.42	1.36
5:T:418:VAL:HG13	5:T:419:ARG:CA	1.56	1.36
1:O:26:PRO:HG2	1:O:370:CYS:O	1.23	1.35
5:Q:349:HIS:NE2	5:Q:358:TYR:HE2	0.86	1.35
5:Q:418:VAL:HG13	5:Q:419:ARG:CA	1.56	1.35
3:L:159:LYS:HZ3	4:H:432:LEU:CD1	1.37	1.35
5:R:416:CYS:HA	5:R:417:CYS:C	1.42	1.35
5:R:418:VAL:HG13	5:R:419:ARG:CA	1.56	1.34
5:T:416:CYS:HA	5:T:417:CYS:C	1.42	1.34
3:K:248:ASP:OD2	5:S:405:GLY:CA	1.74	1.34
4:G:399:VAL:CG2	5:S:362:LEU:HD11	1.55	1.34
1:B:25:GLY:HA3	1:C:144:ARG:O	1.19	1.34
5:S:418:VAL:HG13	5:S:419:ARG:CA	1.56	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:133:LYS:CD	5:T:402:LEU:CD2	2.03	1.33
3:L:159:LYS:NZ	4:H:432:LEU:HD22	1.39	1.33
3:L:178:PHE:HZ	5:T:403:THR:CG2	1.41	1.33
1:M:149:ASN:ND2	1:N:191:PRO:HG2	1.38	1.32
3:I:160:TYR:OH	5:Q:398:THR:HG23	1.28	1.31
1:C:109:GLU:HB3	1:D:142:HIS:CE1	1.66	1.31
5:S:363:TYR:CG	5:S:364:PRO:HD2	1.65	1.31
3:K:164:CYS:SG	5:S:400:TYR:CE2	2.24	1.30
5:R:363:TYR:CG	5:R:364:PRO:HD2	1.63	1.30
3:L:133:LYS:CD	5:T:401:GLU:O	1.79	1.29
3:J:162:LEU:HG	5:R:400:TYR:OH	1.18	1.29
3:J:178:PHE:HZ	5:R:403:THR:CG2	1.45	1.29
3:K:159:LYS:HZ3	4:G:432:LEU:CD1	1.46	1.29
1:M:26:PRO:HG2	1:M:370:CYS:O	1.28	1.29
5:Q:422:LYS:HA	5:Q:423:ALA:C	1.55	1.28
3:K:160:TYR:CD2	5:S:397:ILE:CG2	2.16	1.27
3:L:164:CYS:SG	5:T:400:TYR:CE2	2.27	1.27
5:Q:416:CYS:HA	5:Q:417:CYS:C	1.42	1.27
3:J:160:TYR:CZ	5:R:398:THR:CG2	2.14	1.27
1:M:149:ASN:ND2	1:N:191:PRO:CG	1.95	1.27
1:M:291:VAL:CG2	1:O:304:PRO:CB	2.07	1.27
5:R:349:HIS:CE1	5:R:354:GLU:O	1.82	1.26
3:I:157:SER:OG	5:Q:397:ILE:HG23	1.12	1.26
5:Q:356:ILE:O	5:Q:359:TYR:CD2	1.87	1.26
1:O:237:PRO:HD3	1:D:272:ARG:NH2	0.93	1.26
3:K:164:CYS:SG	5:S:400:TYR:CD2	2.28	1.26
3:I:157:SER:OG	5:Q:397:ILE:CG2	1.82	1.25
3:K:160:TYR:HE2	5:S:398:THR:N	1.23	1.25
3:L:159:LYS:NZ	4:H:432:LEU:HD13	1.49	1.25
5:Q:356:ILE:O	5:Q:359:TYR:HD2	0.95	1.25
3:J:178:PHE:CZ	5:R:403:THR:HG21	1.72	1.25
3:L:159:LYS:NZ	4:H:432:LEU:CD2	1.93	1.25
4:F:399:VAL:CG1	5:R:366:MET:HE2	1.64	1.25
5:S:365:THR:O	5:S:366:MET:HG2	1.31	1.25
1:O:18:LEU:HB2	1:O:331:HIS:CG	1.70	1.25
5:S:422:LYS:HA	5:S:423:ALA:C	1.55	1.25
1:C:18:HIS:HE1	1:D:146:GLN:NE2	0.75	1.25
3:J:162:LEU:CG	5:R:400:TYR:OH	1.85	1.25
5:R:406:ALA:HA	5:R:407:THR:C	1.55	1.24
5:S:406:ALA:HA	5:S:407:THR:C	1.55	1.24
1:N:237:PRO:HG2	1:C:314:LYS:NZ	1.53	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:356:ILE:O	5:R:359:TYR:HD2	1.17	1.24
3:J:157:SER:HB2	5:R:397:ILE:CD1	1.66	1.24
3:L:162:LEU:HB3	5:T:400:TYR:OH	1.32	1.24
3:L:164:CYS:SG	5:T:400:TYR:CE1	2.31	1.23
1:B:94:THR:HG22	1:D:24:GLU:OE1	1.35	1.23
3:I:160:TYR:CZ	5:Q:398:THR:CG2	2.21	1.23
3:I:132:ASP:N	5:Q:402:LEU:HD13	1.43	1.23
1:P:23:GLY:C	1:P:290:VAL:HG23	1.62	1.22
4:G:421:VAL:CG1	5:S:388:MET:SD	2.27	1.22
5:T:406:ALA:HA	5:T:407:THR:C	1.55	1.22
3:L:159:LYS:NZ	4:H:432:LEU:CD1	2.00	1.22
5:T:356:ILE:O	5:T:359:TYR:HD2	1.17	1.22
4:H:421:VAL:CG1	5:T:388:MET:SD	2.27	1.22
5:R:422:LYS:HA	5:R:423:ALA:C	1.55	1.21
5:S:349:HIS:CE1	5:S:354:GLU:O	1.87	1.21
4:F:421:VAL:CG1	5:R:388:MET:SD	2.27	1.21
1:P:26:PRO:HG2	1:P:370:CYS:O	1.39	1.21
3:K:159:LYS:NZ	5:S:394:ARG:O	1.71	1.21
3:I:160:TYR:CE2	5:Q:398:THR:HG23	1.76	1.21
4:E:421:VAL:CG1	5:Q:388:MET:SD	2.27	1.21
3:K:160:TYR:CE2	5:S:398:THR:CA	2.24	1.20
4:G:403:SER:N	4:G:407:MET:CG	2.04	1.20
4:F:403:SER:N	4:F:407:MET:CG	2.04	1.20
4:G:399:VAL:CG2	5:S:362:LEU:CD1	2.18	1.20
4:E:403:SER:N	4:E:407:MET:CG	2.04	1.20
4:F:399:VAL:CG2	5:R:362:LEU:HD11	1.71	1.20
5:T:408:VAL:HB	5:T:409:PRO:CD	1.72	1.20
1:P:382:PRO:HG3	5:T:345:ASN:OD1	1.42	1.20
3:J:133:LYS:HD3	5:R:401:GLU:O	1.03	1.20
5:S:408:VAL:HB	5:S:409:PRO:CD	1.72	1.20
3:J:159:LYS:CD	4:F:436:PHE:HE2	1.45	1.19
3:L:133:LYS:CD	5:T:402:LEU:HD21	1.69	1.19
3:K:159:LYS:CE	4:G:432:LEU:HD13	1.71	1.19
5:Q:406:ALA:HA	5:Q:407:THR:C	1.55	1.19
4:H:403:SER:N	4:H:407:MET:CG	2.04	1.19
5:T:422:LYS:HA	5:T:423:ALA:C	1.55	1.19
3:K:159:LYS:CD	4:G:432:LEU:HD13	1.73	1.19
4:F:402:ILE:CB	4:F:407:MET:SD	2.30	1.19
1:C:109:GLU:CB	1:D:142:HIS:CE1	2.26	1.18
4:E:403:SER:CA	4:E:407:MET:CG	2.21	1.18
4:F:403:SER:CA	4:F:407:MET:CG	2.21	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:399:VAL:CG2	5:R:362:LEU:HD21	1.74	1.18
1:A:280:LYS:HD2	5:Q:343:SER:CB	1.72	1.18
1:O:28:VAL:HG21	1:O:330:VAL:O	1.40	1.18
4:G:403:SER:CA	4:G:407:MET:CG	2.21	1.18
4:H:403:SER:CA	4:H:407:MET:CG	2.21	1.18
4:G:399:VAL:HG21	5:S:362:LEU:CG	1.71	1.18
5:Q:408:VAL:HB	5:Q:409:PRO:CD	1.72	1.18
3:K:162:LEU:HD23	5:S:400:TYR:CE1	1.40	1.17
5:R:408:VAL:CG1	5:R:409:PRO:HD3	1.74	1.17
5:R:408:VAL:HB	5:R:409:PRO:CD	1.72	1.17
4:G:399:VAL:CG1	5:S:362:LEU:HD11	1.59	1.17
1:M:291:VAL:HG22	1:O:304:PRO:CG	1.75	1.17
3:K:248:ASP:HB2	5:S:404:PRO:O	1.41	1.17
5:Q:408:VAL:HB	5:Q:409:PRO:HD2	1.25	1.17
1:P:18:LEU:HB2	1:P:331:HIS:CG	1.77	1.17
3:L:162:LEU:CB	5:T:400:TYR:OH	1.93	1.17
5:Q:408:VAL:CG1	5:Q:409:PRO:HD3	1.74	1.17
3:L:133:LYS:HD3	5:T:401:GLU:O	1.01	1.16
5:S:408:VAL:CG1	5:S:409:PRO:HD3	1.74	1.16
4:H:402:ILE:CB	4:H:407:MET:SD	2.30	1.16
5:Q:359:TYR:O	5:Q:363:TYR:CD2	1.99	1.16
5:T:348:ALA:O	5:T:354:GLU:OE1	1.60	1.16
3:I:132:ASP:OD1	5:Q:402:LEU:CD2	1.93	1.16
3:K:159:LYS:NZ	5:S:394:ARG:C	2.03	1.16
4:E:402:ILE:CB	4:E:407:MET:SD	2.30	1.16
4:G:402:ILE:CB	4:G:407:MET:SD	2.30	1.16
5:T:408:VAL:CG1	5:T:409:PRO:HD3	1.74	1.16
4:G:399:VAL:CB	5:S:362:LEU:HD11	1.76	1.15
5:S:356:ILE:O	5:S:359:TYR:HD2	1.29	1.15
1:D:280:LYS:HE2	5:T:343:SER:C	1.58	1.15
1:B:25:GLY:CA	1:C:144:ARG:O	1.93	1.15
3:I:132:ASP:OD1	5:Q:402:LEU:HD22	0.98	1.15
4:F:403:SER:H	4:F:407:MET:CG	1.59	1.15
4:G:399:VAL:CG2	5:S:362:LEU:CD2	2.06	1.15
1:B:272:ARG:NH2	1:P:237:PRO:CD	2.09	1.15
4:E:403:SER:H	4:E:407:MET:CG	1.59	1.14
3:I:133:LYS:HB2	5:Q:402:LEU:HG	1.27	1.14
4:G:403:SER:H	4:G:407:MET:CG	1.59	1.14
4:G:403:SER:CB	4:G:407:MET:HG2	1.77	1.14
4:H:403:SER:CB	4:H:407:MET:HG2	1.77	1.14
3:J:159:LYS:HD3	4:F:432:LEU:CB	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:403:SER:CB	4:E:407:MET:HG2	1.78	1.13
5:S:352:PRO:HA	5:S:355:ILE:CD1	1.78	1.13
3:K:132:ASP:N	5:S:402:LEU:HD11	1.52	1.13
1:C:109:GLU:HG3	1:D:142:HIS:NE2	1.62	1.13
1:O:23:GLY:C	1:O:290:VAL:HG23	1.73	1.13
3:K:159:LYS:NZ	4:G:432:LEU:CD1	2.12	1.13
3:K:162:LEU:CD2	5:S:400:TYR:CE1	2.31	1.13
4:F:399:VAL:HG22	5:R:362:LEU:HD11	1.22	1.13
4:F:403:SER:CB	4:F:407:MET:HG2	1.78	1.13
3:K:132:ASP:N	5:S:402:LEU:HD13	1.47	1.12
3:K:250:VAL:HG21	5:S:401:GLU:HB2	1.31	1.12
5:R:351:HIS:HB3	5:R:352:PRO:HD3	1.30	1.12
5:T:408:VAL:HB	5:T:409:PRO:HD2	1.25	1.12
3:J:159:LYS:CD	4:F:436:PHE:CE2	2.16	1.12
5:Q:416:CYS:HA	5:Q:417:CYS:O	1.49	1.12
4:H:403:SER:H	4:H:407:MET:HG3	1.12	1.12
3:J:133:LYS:CD	5:R:401:GLU:O	1.95	1.12
3:K:131:GLY:HA3	5:S:402:LEU:CD1	1.78	1.11
1:P:18:LEU:HB2	1:P:331:HIS:CD2	1.84	1.11
3:L:133:LYS:N	5:T:402:LEU:HD11	0.85	1.11
5:R:408:VAL:HB	5:R:409:PRO:HD2	1.25	1.11
5:T:416:CYS:HA	5:T:417:CYS:O	1.49	1.11
1:M:152:HIS:HA	1:N:194:ALA:CB	1.79	1.11
5:R:416:CYS:HA	5:R:417:CYS:O	1.49	1.11
5:Q:352:PRO:HA	5:Q:355:ILE:CD1	1.80	1.11
5:R:351:HIS:CB	5:R:352:PRO:HD2	1.80	1.11
4:H:403:SER:H	4:H:407:MET:CG	1.59	1.11
5:R:407:THR:H	5:R:421:THR:CG2	1.64	1.10
3:K:157:SER:OG	5:S:397:ILE:CD1	1.80	1.10
5:S:416:CYS:HA	5:S:417:CYS:O	1.49	1.10
1:B:272:ARG:NH2	1:P:237:PRO:HD2	1.66	1.09
5:Q:407:THR:H	5:Q:421:THR:CG2	1.64	1.09
3:J:250:VAL:HG12	5:R:398:THR:HG22	1.30	1.09
3:K:159:LYS:HD3	4:G:432:LEU:HD13	1.28	1.09
4:F:399:VAL:HG11	5:R:362:LEU:HD13	1.21	1.09
3:I:159:LYS:HD2	4:E:436:PHE:HZ	1.12	1.09
3:J:157:SER:CB	5:R:397:ILE:CG2	2.29	1.09
3:J:157:SER:CA	5:R:397:ILE:HD12	1.82	1.09
3:K:159:LYS:HZ1	5:S:394:ARG:CB	1.66	1.09
4:F:403:SER:C	4:F:407:MET:HG2	1.78	1.09
5:R:349:HIS:HE1	5:R:357:LEU:CB	1.65	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:407:THR:H	5:T:421:THR:CG2	1.64	1.09
3:K:159:LYS:HB3	4:G:436:PHE:HZ	1.13	1.08
3:K:160:TYR:HD2	5:S:397:ILE:CG2	1.58	1.08
1:P:382:PRO:CG	5:T:345:ASN:OD1	2.02	1.08
5:R:349:HIS:NE2	5:R:354:GLU:O	1.83	1.08
5:S:407:THR:H	5:S:421:THR:CG2	1.64	1.08
3:K:132:ASP:H	5:S:402:LEU:HD11	0.93	1.08
3:L:159:LYS:HZ2	4:H:432:LEU:CG	1.65	1.08
4:G:399:VAL:CG1	5:S:362:LEU:HD13	1.70	1.08
1:A:280:LYS:HD2	5:Q:343:SER:HB3	1.35	1.08
1:O:237:PRO:HD3	1:D:272:ARG:CZ	1.82	1.08
3:I:160:TYR:OH	5:Q:398:THR:CG2	1.99	1.08
5:R:351:HIS:CB	5:R:352:PRO:CD	2.25	1.08
1:O:361:ALA:HB1	5:S:345:ASN:CG	1.78	1.08
4:F:399:VAL:CG1	5:R:362:LEU:HD13	1.82	1.08
3:K:159:LYS:CB	4:G:436:PHE:HZ	1.65	1.07
5:T:351:HIS:HB3	5:T:352:PRO:HD2	1.13	1.07
1:B:272:ARG:CZ	1:P:237:PRO:HD3	1.85	1.07
3:J:160:TYR:CD2	5:R:398:THR:HG23	1.88	1.07
4:E:403:SER:H	4:E:407:MET:HG3	1.12	1.07
4:E:403:SER:C	4:E:407:MET:HG2	1.78	1.07
5:Q:349:HIS:CE1	5:Q:354:GLU:C	2.32	1.07
4:F:403:SER:H	4:F:407:MET:HG3	1.12	1.07
5:R:352:PRO:CA	5:R:355:ILE:HD12	1.84	1.07
4:G:403:SER:C	4:G:407:MET:HG2	1.78	1.07
5:S:408:VAL:CB	5:S:409:PRO:CD	2.30	1.07
5:T:407:THR:N	5:T:421:THR:HG21	1.70	1.07
1:M:41:THR:HA	1:N:43:SER:OG	1.46	1.07
5:S:352:PRO:CA	5:S:355:ILE:HD12	1.81	1.07
5:S:401:GLU:O	5:S:402:LEU:HG	1.55	1.07
4:H:403:SER:C	4:H:407:MET:HG2	1.78	1.07
5:Q:401:GLU:O	5:Q:402:LEU:HG	1.55	1.07
3:I:159:LYS:CD	4:E:436:PHE:HZ	1.68	1.07
5:Q:408:VAL:CB	5:Q:409:PRO:CD	2.30	1.07
4:G:403:SER:H	4:G:407:MET:HG3	1.12	1.07
5:Q:356:ILE:CA	5:Q:359:TYR:HE2	1.66	1.06
5:Q:407:THR:N	5:Q:421:THR:HG21	1.70	1.06
5:S:408:VAL:HB	5:S:409:PRO:HD2	1.25	1.06
3:J:159:LYS:HD2	4:F:436:PHE:CE2	1.73	1.06
4:G:399:VAL:HG21	5:S:362:LEU:CD1	1.81	1.06
1:M:152:HIS:CB	1:N:194:ALA:HB2	1.86	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:130:VAL:O	5:Q:402:LEU:HD12	1.56	1.06
3:J:157:SER:CB	5:R:397:ILE:CD1	2.29	1.06
4:F:399:VAL:HG11	5:R:366:MET:HE2	1.37	1.06
5:R:408:VAL:CB	5:R:409:PRO:CD	2.30	1.06
3:K:159:LYS:HZ2	5:S:394:ARG:C	1.60	1.06
1:M:291:VAL:CG2	1:O:304:PRO:CG	2.33	1.05
1:M:291:VAL:CG2	1:O:304:PRO:HG2	1.86	1.05
1:P:382:PRO:HG3	5:T:345:ASN:CG	1.79	1.05
5:Q:356:ILE:CA	5:Q:359:TYR:CE2	2.37	1.05
5:Q:406:ALA:CA	5:Q:407:THR:C	2.30	1.05
4:F:399:VAL:CG2	5:R:362:LEU:CD1	2.32	1.05
5:R:407:THR:N	5:R:421:THR:HG21	1.69	1.05
3:K:157:SER:HB2	5:S:397:ILE:HD13	1.33	1.05
5:R:416:CYS:CA	5:R:417:CYS:C	2.30	1.05
5:R:356:ILE:O	5:R:359:TYR:CD2	2.09	1.05
5:S:356:ILE:HA	5:S:359:TYR:CD2	1.91	1.05
5:S:407:THR:N	5:S:421:THR:HG21	1.70	1.05
3:I:229:LEU:HD12	3:I:252:LYS:HE3	1.37	1.05
3:K:159:LYS:HZ3	4:G:432:LEU:CD2	1.70	1.05
3:K:159:LYS:HB3	4:G:436:PHE:CZ	1.91	1.05
5:Q:364:PRO:C	5:Q:365:THR:HG23	1.82	1.05
3:K:160:TYR:CE2	5:S:398:THR:HG23	1.92	1.04
5:R:351:HIS:HB3	5:R:352:PRO:HD2	1.05	1.04
1:D:280:LYS:NZ	5:T:343:SER:O	1.90	1.04
1:P:26:PRO:O	1:P:329:ALA:HB2	1.58	1.04
3:K:229:LEU:HD12	3:K:252:LYS:HE3	1.37	1.04
5:R:356:ILE:CA	5:R:359:TYR:CE2	2.41	1.04
4:H:403:SER:OG	4:H:407:MET:HG2	1.57	1.04
5:T:356:ILE:O	5:T:359:TYR:CD2	2.09	1.04
3:K:132:ASP:H	5:S:402:LEU:HD13	1.03	1.04
3:K:159:LYS:HZ1	5:S:394:ARG:HB3	1.17	1.04
5:Q:359:TYR:O	5:Q:363:TYR:CG	2.09	1.04
5:R:401:GLU:O	5:R:402:LEU:HG	1.55	1.04
5:T:401:GLU:O	5:T:402:LEU:HG	1.55	1.04
5:T:402:LEU:O	5:T:403:THR:HG23	1.58	1.04
3:K:157:SER:CA	5:S:397:ILE:HD12	1.88	1.04
3:L:229:LEU:HD12	3:L:252:LYS:HE3	1.37	1.04
5:Q:402:LEU:O	5:Q:403:THR:HG23	1.58	1.04
5:S:416:CYS:CA	5:S:417:CYS:C	2.30	1.04
3:J:178:PHE:HZ	5:R:403:THR:HG21	0.87	1.03
5:Q:352:PRO:CA	5:Q:355:ILE:HD12	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:408:VAL:CB	5:T:409:PRO:CD	2.30	1.03
1:O:236:ALA:HA	1:D:272:ARG:HH22	1.16	1.03
1:O:361:ALA:CB	5:S:345:ASN:CG	2.30	1.03
3:J:229:LEU:HD12	3:J:252:LYS:HE3	1.37	1.03
4:F:399:VAL:HG21	5:R:362:LEU:HD21	1.28	1.03
5:S:406:ALA:CA	5:S:407:THR:C	2.30	1.03
5:T:406:ALA:CA	5:T:407:THR:C	2.30	1.03
1:B:146:GLN:HE21	1:D:20:PRO:HA	1.19	1.03
3:J:159:LYS:HD3	4:F:432:LEU:HB3	1.11	1.03
3:K:157:SER:OG	5:S:397:ILE:HD12	1.07	1.03
3:K:160:TYR:CE2	5:S:398:THR:CB	2.40	1.03
5:R:402:LEU:O	5:R:403:THR:HG23	1.58	1.03
4:G:399:VAL:HG13	5:S:362:LEU:CD1	1.88	1.03
5:T:348:ALA:C	5:T:354:GLU:OE1	2.01	1.03
5:T:356:ILE:CA	5:T:359:TYR:CE2	2.41	1.03
3:L:133:LYS:H	5:T:402:LEU:HD12	1.22	1.03
5:Q:413:SER:HB2	5:Q:417:CYS:CB	1.88	1.03
4:G:396:THR:OG1	4:G:397:LEU:HD22	1.58	1.03
3:L:159:LYS:CE	4:H:432:LEU:HD13	1.88	1.03
5:S:413:SER:HB2	5:S:417:CYS:CB	1.88	1.03
5:T:413:SER:HB2	5:T:417:CYS:CB	1.88	1.03
1:M:291:VAL:CG2	1:O:304:PRO:C	2.32	1.02
3:J:159:LYS:HD2	4:F:432:LEU:HB3	1.41	1.02
4:G:399:VAL:HG23	5:S:362:LEU:HD21	1.39	1.02
5:S:402:LEU:O	5:S:403:THR:HG23	1.58	1.02
4:H:396:THR:OG1	4:H:397:LEU:HD22	1.58	1.02
1:M:293:ALA:O	1:M:324:LYS:HE2	1.59	1.02
1:A:281:ASN:OD1	5:Q:343:SER:HB2	1.59	1.02
4:E:396:THR:OG1	4:E:397:LEU:HD22	1.58	1.02
5:R:413:SER:HB2	5:R:417:CYS:CB	1.88	1.02
3:K:130:VAL:O	5:S:402:LEU:HD12	1.60	1.02
5:R:406:ALA:CA	5:R:407:THR:C	2.30	1.02
1:O:361:ALA:HB1	5:S:345:ASN:OD1	1.59	1.02
5:R:349:HIS:CE1	5:R:357:LEU:CB	2.40	1.02
4:H:399:VAL:CG1	5:T:366:MET:HE2	1.88	1.02
4:E:403:SER:OG	4:E:407:MET:HG2	1.57	1.02
4:F:399:VAL:CG1	5:R:362:LEU:CD1	2.37	1.02
4:F:403:SER:OG	4:F:407:MET:HG2	1.57	1.02
4:G:403:SER:OG	4:G:407:MET:HG2	1.57	1.02
5:T:416:CYS:CA	5:T:417:CYS:C	2.30	1.02
1:M:152:HIS:CD2	1:N:194:ALA:HB2	1.95	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:178:PHE:CZ	5:R:403:THR:CG2	2.35	1.01
5:Q:406:ALA:C	5:Q:410:PHE:CD2	2.38	1.01
5:Q:416:CYS:CA	5:Q:417:CYS:C	2.30	1.01
4:F:396:THR:OG1	4:F:397:LEU:HD22	1.58	1.01
5:T:406:ALA:C	5:T:410:PHE:CD2	2.39	1.01
1:P:28:VAL:HG21	1:P:330:VAL:O	1.61	1.01
5:Q:411:LEU:N	5:Q:413:SER:HB3	1.76	1.01
5:S:356:ILE:CA	5:S:359:TYR:CE2	2.43	1.01
5:S:406:ALA:C	5:S:410:PHE:CD2	2.39	1.01
3:K:159:LYS:NZ	5:S:394:ARG:HB3	1.75	1.01
5:Q:356:ILE:C	5:Q:359:TYR:HD2	1.69	1.01
5:T:411:LEU:N	5:T:413:SER:HB3	1.76	1.01
1:P:18:LEU:HD13	1:P:331:HIS:HB2	1.40	1.00
3:I:251:THR:HG23	4:E:439:HIS:HB2	1.43	1.00
5:R:411:LEU:N	5:R:413:SER:HB3	1.76	1.00
5:S:365:THR:O	5:S:366:MET:CG	2.07	1.00
3:L:159:LYS:NZ	4:H:432:LEU:CG	2.24	1.00
1:B:144:ARG:HE	1:D:25:GLY:HA3	0.85	1.00
5:R:363:TYR:CD1	5:R:364:PRO:HD2	1.96	1.00
5:R:406:ALA:C	5:R:410:PHE:CD2	2.39	1.00
3:I:251:THR:HG21	4:E:439:HIS:CB	1.73	1.00
4:F:399:VAL:CG2	5:R:362:LEU:CD2	2.35	1.00
5:T:351:HIS:HB3	5:T:352:PRO:CD	1.90	1.00
3:J:157:SER:CB	5:R:397:ILE:HG23	1.91	1.00
5:T:422:LYS:CA	5:T:423:ALA:C	2.35	1.00
3:I:132:ASP:H	5:Q:402:LEU:HD13	0.84	1.00
3:I:234:GLU:HA	3:K:169:VAL:O	1.61	1.00
3:L:157:SER:HA	5:T:397:ILE:HD12	1.42	1.00
5:Q:364:PRO:O	5:Q:365:THR:HG23	0.82	1.00
5:R:352:PRO:HA	5:R:355:ILE:HD12	1.03	1.00
5:S:411:LEU:N	5:S:413:SER:HB3	1.76	1.00
3:J:157:SER:HB2	5:R:397:ILE:HD12	1.02	1.00
3:K:248:ASP:OD2	5:S:405:GLY:HA3	0.83	1.00
4:F:432:LEU:O	4:F:436:PHE:CD2	2.15	1.00
3:I:159:LYS:HD2	4:E:436:PHE:CZ	1.97	0.99
3:I:234:GLU:O	3:K:173:SER:HB3	1.62	0.99
3:J:130:VAL:HG13	5:R:401:GLU:OE1	1.60	0.99
1:B:144:ARG:HE	1:D:25:GLY:CA	1.75	0.99
4:G:432:LEU:O	4:G:436:PHE:CD2	2.15	0.99
3:J:229:LEU:CD1	3:J:252:LYS:HE3	1.92	0.99
4:H:432:LEU:O	4:H:436:PHE:CD2	2.15	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:432:LEU:O	4:E:436:PHE:CD2	2.15	0.99
1:O:18:LEU:HB2	1:O:331:HIS:CD2	1.97	0.99
5:R:356:ILE:HA	5:R:359:TYR:CD2	1.97	0.99
1:M:152:HIS:CG	1:N:194:ALA:HB2	1.97	0.99
5:Q:422:LYS:CA	5:Q:423:ALA:C	2.35	0.99
5:R:349:HIS:CA	5:R:354:GLU:HB2	1.60	0.99
1:M:152:HIS:HA	1:N:194:ALA:HB2	1.44	0.99
5:Q:413:SER:CB	5:Q:417:CYS:SG	2.51	0.99
5:T:413:SER:CB	5:T:417:CYS:SG	2.51	0.99
3:K:133:LYS:H	5:S:402:LEU:HD11	1.20	0.99
5:T:356:ILE:HA	5:T:359:TYR:CD2	1.97	0.99
1:C:109:GLU:CB	1:D:142:HIS:NE2	2.26	0.98
3:L:159:LYS:HD3	4:H:432:LEU:HB3	1.44	0.98
3:L:229:LEU:CD1	3:L:252:LYS:HE3	1.92	0.98
5:Q:406:ALA:HB2	5:Q:408:VAL:HB	1.45	0.98
5:R:363:TYR:CD1	5:R:364:PRO:CD	2.47	0.98
3:J:157:SER:OG	5:R:397:ILE:HG21	0.81	0.98
5:T:406:ALA:HA	5:T:408:VAL:N	1.78	0.98
3:K:160:TYR:CZ	5:S:398:THR:CB	2.47	0.98
5:S:422:LYS:CA	5:S:423:ALA:C	2.35	0.98
5:Q:407:THR:HG22	5:Q:421:THR:OG1	1.64	0.98
5:S:406:ALA:HA	5:S:408:VAL:N	1.78	0.98
5:T:406:ALA:HB2	5:T:408:VAL:HB	1.45	0.98
1:O:236:ALA:HA	1:D:272:ARG:NH2	1.79	0.98
5:R:356:ILE:CA	5:R:359:TYR:HE2	1.77	0.98
5:R:413:SER:CB	5:R:417:CYS:SG	2.51	0.98
4:G:399:VAL:HG22	5:S:362:LEU:HD11	1.43	0.98
5:T:356:ILE:CA	5:T:359:TYR:HE2	1.76	0.98
1:M:41:THR:HB	1:N:125:HIS:HE1	1.28	0.98
5:T:407:THR:HG22	5:T:421:THR:OG1	1.64	0.98
1:B:144:ARG:NE	1:D:25:GLY:HA3	1.62	0.98
3:J:151:LYS:HE2	3:J:151:LYS:HA	1.46	0.98
3:I:229:LEU:CD1	3:I:252:LYS:HE3	1.92	0.97
5:R:406:ALA:HA	5:R:408:VAL:N	1.78	0.97
5:S:407:THR:HG22	5:S:421:THR:OG1	1.64	0.97
1:B:142:HIS:NE2	1:D:109:GLU:CG	2.14	0.97
3:K:131:GLY:CA	5:S:402:LEU:CD1	2.40	0.97
3:K:159:LYS:CE	5:S:394:ARG:HB3	1.95	0.97
5:S:406:ALA:HB2	5:S:408:VAL:HB	1.45	0.97
5:S:413:SER:CB	5:S:417:CYS:SG	2.51	0.97
5:T:408:VAL:HG12	5:T:409:PRO:HD3	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:229:LEU:CD1	3:K:252:LYS:HE3	1.92	0.97
5:R:407:THR:HG22	5:R:421:THR:OG1	1.64	0.97
5:R:408:VAL:HG12	5:R:409:PRO:HD3	1.45	0.97
3:K:250:VAL:O	4:G:439:HIS:CE1	2.17	0.97
3:K:151:LYS:HE2	3:K:151:LYS:HA	1.47	0.97
5:T:349:HIS:CE1	5:T:355:ILE:HA	1.98	0.97
1:O:26:PRO:CG	1:O:370:CYS:O	2.12	0.97
1:O:237:PRO:HD3	1:D:272:ARG:HH22	1.30	0.97
3:I:159:LYS:NZ	5:Q:394:ARG:O	1.97	0.97
3:K:160:TYR:CD2	5:S:398:THR:N	2.31	0.97
5:S:408:VAL:HG12	5:S:409:PRO:HD3	1.45	0.97
1:C:109:GLU:CG	1:D:142:HIS:NE2	2.27	0.96
1:O:26:PRO:O	1:O:329:ALA:HB2	1.65	0.96
3:L:178:PHE:CZ	5:T:403:THR:HG22	1.95	0.96
5:Q:408:VAL:HG12	5:Q:409:PRO:HD3	1.45	0.96
5:R:406:ALA:HB2	5:R:408:VAL:HB	1.45	0.96
1:M:291:VAL:HG22	1:O:304:PRO:CA	1.94	0.96
3:J:178:PHE:HA	3:J:224:VAL:O	1.65	0.96
5:Q:406:ALA:HA	5:Q:408:VAL:N	1.78	0.96
1:M:152:HIS:CA	1:N:194:ALA:HB2	1.95	0.96
3:L:178:PHE:HA	3:L:224:VAL:O	1.65	0.96
1:B:24:GLU:O	1:C:144:ARG:HB3	1.63	0.96
3:I:178:PHE:HA	3:I:224:VAL:O	1.65	0.96
5:R:422:LYS:CA	5:R:423:ALA:C	2.35	0.96
1:M:125:HIS:CE1	1:N:41:THR:HB	2.00	0.96
3:I:132:ASP:H	5:Q:402:LEU:CD1	1.78	0.96
3:K:178:PHE:HA	3:K:224:VAL:O	1.65	0.96
3:L:157:SER:CB	5:T:397:ILE:HD12	1.96	0.96
3:L:162:LEU:HG	5:T:400:TYR:HH	1.30	0.96
5:T:363:TYR:CG	5:T:364:PRO:HD2	2.01	0.96
1:M:149:ASN:ND2	1:N:191:PRO:HG3	1.79	0.96
3:I:162:LEU:HD23	5:Q:400:TYR:CE1	2.00	0.95
3:K:131:GLY:CA	5:S:402:LEU:HD13	1.94	0.95
3:K:160:TYR:CE1	5:S:398:THR:CG2	2.34	0.95
3:I:151:LYS:HA	3:I:151:LYS:HE2	1.46	0.95
3:L:133:LYS:CD	5:T:402:LEU:HD23	1.95	0.95
3:K:131:GLY:C	5:S:402:LEU:HD13	1.90	0.95
1:O:18:LEU:HD13	1:O:331:HIS:HB2	1.48	0.95
1:M:147:TYR:HE2	1:N:192:PHE:HB3	1.31	0.95
3:L:159:LYS:HZ2	4:H:432:LEU:HD22	0.87	0.95
4:F:403:SER:C	4:F:407:MET:CG	2.39	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:408:VAL:CG1	5:Q:409:PRO:CD	2.44	0.95
1:B:272:ARG:NH2	1:P:237:PRO:HD3	1.79	0.95
1:N:237:PRO:HG2	1:C:314:LYS:HZ1	1.12	0.95
4:G:403:SER:N	4:G:407:MET:SD	2.40	0.95
5:T:408:VAL:CG1	5:T:409:PRO:CD	2.44	0.95
4:F:403:SER:N	4:F:407:MET:SD	2.40	0.95
4:E:403:SER:C	4:E:407:MET:CG	2.39	0.94
5:T:406:ALA:HB1	5:T:407:THR:O	1.67	0.94
3:J:162:LEU:HG	5:R:400:TYR:HH	1.23	0.94
3:L:133:LYS:HD3	5:T:402:LEU:CD2	1.94	0.94
3:L:164:CYS:SG	5:T:400:TYR:CD2	2.58	0.94
5:S:356:ILE:O	5:S:359:TYR:CD2	2.20	0.94
3:L:133:LYS:CD	5:T:402:LEU:CG	2.45	0.94
3:K:157:SER:CB	5:S:397:ILE:HD13	1.93	0.94
3:K:162:LEU:CD2	5:S:400:TYR:HE1	1.75	0.94
4:F:399:VAL:HG12	5:R:366:MET:HE2	1.48	0.94
4:G:403:SER:C	4:G:407:MET:CG	2.39	0.94
5:R:406:ALA:C	5:R:410:PHE:CE2	2.46	0.94
1:B:146:GLN:NE2	1:D:20:PRO:HA	1.83	0.94
5:Q:410:PHE:C	5:Q:413:SER:HB3	1.93	0.94
5:S:406:ALA:HB1	5:S:407:THR:O	1.67	0.94
5:T:406:ALA:C	5:T:410:PHE:CE2	2.46	0.94
1:N:237:PRO:CG	1:C:314:LYS:NZ	2.31	0.94
5:Q:406:ALA:C	5:Q:410:PHE:CE2	2.46	0.94
5:R:418:VAL:CG1	5:R:419:ARG:CA	2.30	0.94
5:S:406:ALA:C	5:S:410:PHE:CE2	2.46	0.94
5:S:407:THR:N	5:S:421:THR:CG2	2.30	0.94
5:T:402:LEU:C	5:T:403:THR:HG23	1.91	0.94
1:M:291:VAL:HG21	1:O:304:PRO:HG2	1.48	0.93
3:I:160:TYR:CE2	5:Q:398:THR:CA	2.51	0.93
3:L:164:CYS:SG	5:T:400:TYR:CD1	2.61	0.93
4:H:403:SER:N	4:H:407:MET:SD	2.40	0.93
3:I:133:LYS:HD3	5:Q:401:GLU:O	1.67	0.93
3:L:151:LYS:HE2	3:L:151:LYS:HA	1.47	0.93
5:R:408:VAL:CG1	5:R:409:PRO:CD	2.44	0.93
3:L:157:SER:CA	5:T:397:ILE:HD12	1.98	0.93
4:E:403:SER:N	4:E:407:MET:SD	2.40	0.93
5:Q:363:TYR:N	5:Q:364:PRO:HD2	1.81	0.93
5:Q:407:THR:N	5:Q:410:PHE:CD2	2.36	0.93
5:Q:407:THR:CA	5:Q:421:THR:HG21	1.98	0.93
5:R:407:THR:HG23	5:R:421:THR:HB	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:399:VAL:HG21	5:S:362:LEU:HD22	1.50	0.93
5:S:408:VAL:CG1	5:S:409:PRO:CD	2.44	0.93
5:T:407:THR:N	5:T:410:PHE:CD2	2.36	0.93
3:I:178:PHE:CZ	5:Q:403:THR:HG21	2.02	0.93
5:Q:410:PHE:O	5:Q:411:LEU:HG	1.69	0.93
5:S:410:PHE:C	5:S:413:SER:HB3	1.92	0.93
3:J:157:SER:CB	5:R:397:ILE:HG21	1.91	0.93
3:K:159:LYS:CG	4:G:436:PHE:HZ	1.80	0.93
5:R:352:PRO:HA	5:R:355:ILE:CD1	1.95	0.93
5:R:407:THR:N	5:R:410:PHE:CD2	2.36	0.93
5:R:407:THR:CA	5:R:421:THR:HG21	1.98	0.93
5:R:410:PHE:O	5:R:411:LEU:HG	1.69	0.93
5:S:363:TYR:CG	5:S:364:PRO:CD	2.51	0.93
5:T:410:PHE:O	5:T:411:LEU:HG	1.69	0.93
3:I:160:TYR:CE2	5:Q:398:THR:HA	2.03	0.93
5:Q:407:THR:HG23	5:Q:421:THR:HB	1.49	0.93
5:R:402:LEU:C	5:R:403:THR:HG23	1.91	0.93
5:T:407:THR:CA	5:T:421:THR:HG21	1.98	0.93
1:P:382:PRO:HG3	5:T:345:ASN:CB	1.98	0.93
5:Q:402:LEU:C	5:Q:403:THR:HG23	1.91	0.93
5:S:402:LEU:C	5:S:403:THR:HG23	1.91	0.93
3:I:251:THR:HG23	4:E:439:HIS:CG	2.03	0.93
5:S:407:THR:N	5:S:410:PHE:CD2	2.36	0.93
5:S:408:VAL:HG12	5:S:409:PRO:CD	1.99	0.93
4:H:403:SER:C	4:H:407:MET:CG	2.39	0.93
1:B:272:ARG:HH12	1:P:236:ALA:HA	1.34	0.93
5:Q:406:ALA:HB1	5:Q:407:THR:O	1.67	0.92
5:R:410:PHE:C	5:R:413:SER:HB3	1.92	0.92
4:G:403:SER:N	4:G:407:MET:HG3	1.76	0.92
5:S:407:THR:HG23	5:S:421:THR:HB	1.49	0.92
5:S:410:PHE:O	5:S:411:LEU:HG	1.69	0.92
4:H:396:THR:O	4:H:397:LEU:HD13	1.69	0.92
5:T:407:THR:HG23	5:T:421:THR:HB	1.49	0.92
5:R:408:VAL:HG12	5:R:409:PRO:CD	1.99	0.92
4:G:396:THR:O	4:G:397:LEU:HD13	1.69	0.92
5:R:407:THR:N	5:R:421:THR:CG2	2.30	0.92
3:L:133:LYS:HD2	5:T:402:LEU:CG	1.98	0.92
5:Q:352:PRO:HA	5:Q:355:ILE:HD12	0.94	0.92
1:M:26:PRO:CG	1:M:370:CYS:O	2.16	0.92
1:M:125:HIS:HE1	1:N:41:THR:HB	1.35	0.92
1:N:237:PRO:CG	1:C:314:LYS:HZ1	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:361:ALA:CB	5:S:345:ASN:CB	2.48	0.92
3:K:160:TYR:CE2	5:S:397:ILE:HG22	2.04	0.92
5:R:406:ALA:HB1	5:R:407:THR:O	1.67	0.92
5:T:410:PHE:C	5:T:413:SER:HB3	1.92	0.92
5:Q:406:ALA:HB1	5:Q:410:PHE:CD2	2.05	0.92
3:J:157:SER:HB2	5:R:397:ILE:HG23	1.52	0.92
3:K:159:LYS:NZ	4:G:432:LEU:CD2	2.33	0.92
5:Q:408:VAL:HG12	5:Q:409:PRO:CD	1.99	0.92
1:D:280:LYS:CD	5:T:343:SER:O	2.16	0.92
5:S:406:ALA:HB1	5:S:410:PHE:CD2	2.05	0.92
5:S:407:THR:CA	5:S:421:THR:HG21	1.98	0.92
5:T:406:ALA:HB1	5:T:410:PHE:CD2	2.05	0.92
1:M:152:HIS:CD2	1:N:194:ALA:CB	2.50	0.92
3:L:162:LEU:CG	5:T:400:TYR:OH	2.18	0.92
3:K:159:LYS:HZ3	4:G:432:LEU:CG	1.82	0.91
5:Q:359:TYR:C	5:Q:363:TYR:CD2	2.38	0.91
5:T:363:TYR:CD1	5:T:364:PRO:HD2	2.05	0.91
3:K:131:GLY:HA3	5:S:402:LEU:HD13	1.43	0.91
5:R:406:ALA:HB1	5:R:410:PHE:CD2	2.05	0.91
3:L:133:LYS:HD2	5:T:402:LEU:HD21	0.91	0.91
5:R:363:TYR:CG	5:R:364:PRO:CD	2.52	0.91
4:E:396:THR:O	4:E:397:LEU:HD13	1.69	0.91
3:I:160:TYR:HE2	5:Q:398:THR:N	1.67	0.91
3:I:251:THR:HG21	4:E:439:HIS:HB3	0.92	0.91
3:K:131:GLY:HA3	5:S:402:LEU:HD12	1.49	0.91
5:Q:380:SER:O	5:Q:384:THR:HG23	1.71	0.91
1:M:291:VAL:HG23	1:O:304:PRO:C	1.93	0.91
4:F:399:VAL:HG21	5:R:362:LEU:HD22	1.51	0.91
5:T:408:VAL:HG12	5:T:409:PRO:CD	2.00	0.91
3:I:160:TYR:HE2	5:Q:398:THR:CA	1.84	0.91
3:J:160:TYR:CE2	5:R:398:THR:CB	2.54	0.91
5:R:352:PRO:O	5:R:355:ILE:HB	1.71	0.91
4:G:403:SER:OG	4:G:407:MET:N	2.04	0.91
5:S:380:SER:O	5:S:384:THR:HG23	1.71	0.91
4:E:403:SER:OG	4:E:407:MET:N	2.04	0.91
1:P:23:GLY:O	1:P:290:VAL:HG23	1.70	0.90
1:D:280:LYS:HE2	5:T:343:SER:O	1.41	0.90
3:K:131:GLY:C	5:S:402:LEU:CD1	2.45	0.90
5:T:419:ARG:O	5:T:420:THR:HG23	1.71	0.90
3:I:133:LYS:HB2	5:Q:402:LEU:CG	1.79	0.90
3:I:132:ASP:CG	5:Q:402:LEU:HD22	1.96	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:133:LYS:HD2	5:S:402:LEU:HD21	1.53	0.90
4:F:396:THR:O	4:F:397:LEU:HD13	1.69	0.90
3:J:160:TYR:CZ	5:R:398:THR:HG21	2.06	0.90
3:K:122:LYS:HZ1	3:L:169:VAL:HG21	1.37	0.90
5:R:380:SER:O	5:R:384:THR:HG23	1.71	0.90
1:B:146:GLN:HE22	1:D:18:HIS:CE1	1.89	0.90
3:L:178:PHE:CE2	5:T:403:THR:CG2	2.54	0.90
1:P:27:MET:CE	1:P:286:ALA:O	2.19	0.90
5:R:345:ASN:O	5:R:345:ASN:ND2	2.05	0.90
3:K:159:LYS:HD3	4:G:432:LEU:CD1	2.02	0.89
4:H:403:SER:OG	4:H:407:MET:N	2.04	0.89
1:P:26:PRO:CG	1:P:370:CYS:O	2.19	0.89
3:K:133:LYS:N	5:S:402:LEU:HD11	1.87	0.89
4:F:403:SER:OG	4:F:407:MET:N	2.04	0.89
5:T:345:ASN:ND2	5:T:345:ASN:O	2.05	0.89
5:S:345:ASN:O	5:S:345:ASN:ND2	2.05	0.89
3:I:251:THR:CB	4:E:439:HIS:HB3	2.03	0.89
3:K:157:SER:HB2	5:S:397:ILE:CD1	1.88	0.89
3:K:159:LYS:HG2	4:G:436:PHE:CZ	2.06	0.89
3:K:178:PHE:CA	3:K:224:VAL:O	2.21	0.89
5:R:356:ILE:C	5:R:359:TYR:HD2	1.79	0.89
5:S:419:ARG:O	5:S:420:THR:HG23	1.71	0.89
1:M:152:HIS:HA	1:N:194:ALA:HB1	1.52	0.89
1:B:142:HIS:CD2	1:D:109:GLU:HG3	2.08	0.89
3:J:178:PHE:CA	3:J:224:VAL:O	2.21	0.89
5:S:356:ILE:CA	5:S:359:TYR:HE2	1.80	0.89
5:T:356:ILE:C	5:T:359:TYR:HD2	1.79	0.89
1:A:280:LYS:CD	5:Q:343:SER:CB	2.51	0.89
3:K:157:SER:CA	5:S:397:ILE:CD1	2.47	0.89
3:K:159:LYS:HZ3	4:G:432:LEU:HD11	1.34	0.89
5:S:351:HIS:CB	5:S:352:PRO:CD	2.50	0.89
1:M:293:ALA:O	1:M:324:LYS:CE	2.21	0.89
3:I:178:PHE:HZ	5:Q:403:THR:HG21	1.35	0.89
3:K:122:LYS:HG3	3:L:170:HIS:HB3	1.54	0.89
5:R:419:ARG:O	5:R:420:THR:HG23	1.71	0.89
5:T:380:SER:O	5:T:384:THR:HG23	1.71	0.89
5:Q:345:ASN:ND2	5:Q:345:ASN:O	2.06	0.89
5:Q:419:ARG:O	5:Q:420:THR:HG23	1.71	0.89
1:C:109:GLU:CG	1:D:142:HIS:CE1	2.55	0.88
3:L:178:PHE:CA	3:L:224:VAL:O	2.21	0.88
3:I:160:TYR:CD2	5:Q:397:ILE:HG22	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLN:HE22	1:D:18:HIS:HE1	1.13	0.88
1:C:18:HIS:HE1	1:D:146:GLN:HE21	1.18	0.88
4:F:399:VAL:HG21	5:R:362:LEU:CD1	2.00	0.88
5:S:349:HIS:HE1	5:S:354:GLU:O	1.49	0.88
5:T:407:THR:N	5:T:421:THR:CG2	2.30	0.88
3:K:159:LYS:NZ	4:G:432:LEU:HD11	1.83	0.88
3:L:133:LYS:CG	5:T:401:GLU:O	2.21	0.88
5:Q:407:THR:N	5:Q:421:THR:CG2	2.30	0.88
5:S:356:ILE:C	5:S:359:TYR:HD2	1.81	0.88
4:H:403:SER:N	4:H:407:MET:HG3	1.76	0.88
5:Q:411:LEU:HA	5:Q:412:LEU:C	1.98	0.88
5:T:418:VAL:CG1	5:T:419:ARG:CA	2.30	0.88
5:R:349:HIS:CD2	5:R:354:GLU:O	2.27	0.88
5:R:406:ALA:O	5:R:410:PHE:HE2	1.57	0.88
5:T:351:HIS:CB	5:T:352:PRO:HD2	2.03	0.88
3:I:178:PHE:CA	3:I:224:VAL:O	2.21	0.88
3:K:159:LYS:CG	4:G:436:PHE:CZ	2.57	0.88
5:Q:406:ALA:O	5:Q:410:PHE:HE2	1.57	0.88
5:S:407:THR:HA	5:S:421:THR:HG21	1.56	0.88
4:E:403:SER:N	4:E:407:MET:HG3	1.76	0.87
5:S:418:VAL:CG1	5:S:419:ARG:CA	2.30	0.87
3:L:133:LYS:CD	5:T:402:LEU:HG	2.03	0.87
3:L:178:PHE:CE2	5:T:403:THR:HG22	2.09	0.87
5:S:363:TYR:CB	5:S:364:PRO:HD2	2.03	0.87
1:M:147:TYR:CE2	1:N:192:PHE:HB3	2.09	0.87
5:T:352:PRO:HA	5:T:355:ILE:HD12	1.54	0.87
5:T:351:HIS:O	5:T:355:ILE:CD1	2.22	0.87
1:M:293:ALA:HB1	1:M:294:PRO:CD	2.04	0.87
5:T:406:ALA:O	5:T:410:PHE:HE2	1.57	0.87
5:T:407:THR:HA	5:T:421:THR:HG21	1.56	0.87
1:O:237:PRO:CD	1:D:272:ARG:HH22	1.78	0.87
3:L:159:LYS:CD	4:H:432:LEU:HB3	2.05	0.87
4:G:399:VAL:HG11	5:S:362:LEU:HD13	0.88	0.87
1:M:125:HIS:HE1	1:N:41:THR:CB	1.87	0.87
1:B:25:GLY:HA3	1:C:144:ARG:C	2.00	0.87
3:I:234:GLU:HB2	3:K:172:LYS:HB2	1.57	0.86
4:F:421:VAL:HG13	5:R:388:MET:CG	2.05	0.86
5:S:411:LEU:HA	5:S:412:LEU:C	1.98	0.86
1:M:18:LEU:HB2	1:M:331:HIS:ND1	1.90	0.86
5:R:407:THR:HA	5:R:421:THR:HG21	1.56	0.86
5:T:411:LEU:HA	5:T:412:LEU:C	1.98	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:130:VAL:CG1	5:T:401:GLU:OE1	2.23	0.86
4:H:421:VAL:HG13	5:T:388:MET:CG	2.05	0.86
3:K:157:SER:HA	5:S:397:ILE:CD1	2.06	0.86
3:K:248:ASP:CB	5:S:404:PRO:O	2.23	0.86
5:S:406:ALA:O	5:S:410:PHE:HE2	1.57	0.86
1:O:16:LYS:NZ	1:O:340:ARG:HA	1.91	0.86
1:O:237:PRO:CD	1:D:272:ARG:HH21	1.56	0.85
3:I:160:TYR:CE2	5:Q:398:THR:CG2	2.50	0.85
5:Q:418:VAL:CG1	5:Q:419:ARG:CA	2.30	0.85
1:C:109:GLU:HB2	1:D:142:HIS:CD2	2.12	0.85
5:Q:349:HIS:HB3	5:Q:354:GLU:H	1.41	0.85
5:R:411:LEU:HA	5:R:412:LEU:C	1.98	0.85
4:E:421:VAL:HG13	5:Q:388:MET:CG	2.05	0.85
4:E:421:VAL:CG1	5:Q:388:MET:CG	2.54	0.85
4:G:421:VAL:HG13	5:S:388:MET:CG	2.05	0.85
1:M:18:LEU:HD21	1:M:368:GLN:NE2	1.91	0.85
5:Q:407:THR:HA	5:Q:421:THR:HG21	1.56	0.85
3:K:122:LYS:NZ	3:L:169:VAL:HG21	1.91	0.85
1:O:28:VAL:HB	1:O:342:ALA:O	1.77	0.85
3:K:250:VAL:CG2	5:S:401:GLU:HB2	2.07	0.85
3:L:159:LYS:HZ3	4:H:432:LEU:HD13	1.04	0.85
3:I:133:LYS:CG	5:Q:401:GLU:O	2.25	0.85
3:K:160:TYR:CE2	5:S:398:THR:CG2	2.53	0.85
5:S:406:ALA:O	5:S:410:PHE:CE2	2.30	0.85
5:T:406:ALA:O	5:T:410:PHE:CE2	2.30	0.85
5:R:410:PHE:C	5:R:413:SER:CB	2.50	0.85
5:R:351:HIS:O	5:R:355:ILE:HG13	1.77	0.85
5:T:410:PHE:C	5:T:413:SER:CB	2.50	0.85
1:M:41:THR:HB	1:N:125:HIS:CE1	2.12	0.84
1:O:361:ALA:CB	5:S:345:ASN:HB2	2.07	0.84
1:P:26:PRO:O	1:P:329:ALA:CB	2.24	0.84
3:I:250:VAL:O	4:E:439:HIS:CE1	2.30	0.84
4:F:421:VAL:CG1	5:R:388:MET:CG	2.54	0.84
4:G:421:VAL:CG1	5:S:388:MET:CG	2.54	0.84
4:H:421:VAL:CG1	5:T:388:MET:CG	2.54	0.84
1:M:125:HIS:HE1	1:N:41:THR:CG2	1.91	0.84
5:Q:349:HIS:CE1	5:Q:358:TYR:CD2	2.64	0.84
5:Q:410:PHE:C	5:Q:413:SER:CB	2.50	0.84
3:K:159:LYS:HE2	5:S:394:ARG:HB3	1.57	0.84
3:L:162:LEU:HG	5:T:400:TYR:OH	1.78	0.84
1:D:280:LYS:CE	5:T:343:SER:C	2.29	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:406:ALA:O	5:R:410:PHE:CE2	2.30	0.84
5:T:421:THR:O	5:T:422:LYS:HG3	1.78	0.84
5:Q:359:TYR:O	5:Q:363:TYR:CB	2.25	0.84
5:Q:406:ALA:O	5:Q:410:PHE:CE2	2.30	0.84
1:P:382:PRO:CD	5:T:345:ASN:OD1	2.26	0.84
3:L:130:VAL:HG13	5:T:401:GLU:OE1	1.77	0.84
3:L:252:LYS:N	4:H:439:HIS:HB3	1.92	0.84
5:Q:421:THR:O	5:Q:422:LYS:HG3	1.78	0.84
5:R:351:HIS:O	5:R:355:ILE:CD1	2.26	0.84
5:S:410:PHE:C	5:S:413:SER:CB	2.50	0.84
1:B:272:ARG:HH22	1:P:237:PRO:HD2	1.40	0.83
3:J:251:THR:HA	4:F:439:HIS:CD2	1.89	0.83
3:K:159:LYS:HZ1	5:S:394:ARG:C	1.77	0.83
3:J:159:LYS:C	4:F:436:PHE:HE1	1.87	0.83
5:Q:408:VAL:CB	5:Q:409:PRO:HD3	2.04	0.83
5:R:393:ARG:O	5:R:397:ILE:HG12	1.78	0.83
4:G:432:LEU:O	4:G:436:PHE:HD2	1.61	0.83
3:I:132:ASP:N	5:Q:402:LEU:CD1	2.37	0.83
5:S:393:ARG:O	5:S:397:ILE:HG12	1.78	0.83
3:I:159:LYS:CD	4:E:436:PHE:CZ	2.57	0.83
4:G:399:VAL:CB	5:S:362:LEU:CD1	2.46	0.83
4:G:415:GLY:O	4:G:419:LEU:HD12	1.79	0.83
5:T:411:LEU:CA	5:T:412:LEU:C	2.51	0.83
1:O:27:MET:HE1	1:O:286:ALA:O	1.78	0.83
1:O:235:GLN:O	1:D:272:ARG:NH1	2.10	0.83
1:O:237:PRO:HD3	1:D:272:ARG:HH21	1.04	0.83
4:F:415:GLY:O	4:F:419:LEU:HD12	1.79	0.83
5:R:408:VAL:CB	5:R:409:PRO:HD3	2.04	0.83
5:R:421:THR:O	5:R:422:LYS:HG3	1.78	0.83
5:S:421:THR:O	5:S:422:LYS:HG3	1.78	0.83
4:H:415:GLY:O	4:H:419:LEU:HD12	1.79	0.83
5:T:393:ARG:O	5:T:397:ILE:HG12	1.78	0.83
5:Q:356:ILE:HA	5:Q:359:TYR:CD2	2.12	0.83
5:Q:411:LEU:CA	5:Q:412:LEU:C	2.51	0.83
5:Q:356:ILE:C	5:Q:359:TYR:CD2	2.49	0.83
1:M:125:HIS:NE2	1:N:41:THR:O	2.12	0.83
3:K:160:TYR:HH	5:S:398:THR:HG1	0.90	0.83
5:R:367:THR:O	5:R:370:ILE:N	2.10	0.83
5:S:411:LEU:CA	5:S:412:LEU:C	2.51	0.82
3:I:160:TYR:CE2	5:Q:397:ILE:HG22	2.14	0.82
5:R:407:THR:O	5:R:410:PHE:CD2	2.32	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:356:ILE:CA	5:T:359:TYR:CD2	2.62	0.82
5:Q:393:ARG:O	5:Q:397:ILE:HG12	1.78	0.82
5:T:349:HIS:CE1	5:T:354:GLU:C	2.56	0.82
3:J:159:LYS:C	4:F:436:PHE:CE1	2.54	0.82
5:S:407:THR:O	5:S:410:PHE:CD2	2.32	0.82
5:T:407:THR:O	5:T:410:PHE:CD2	2.32	0.82
1:B:25:GLY:C	1:C:144:ARG:O	2.22	0.82
5:Q:349:HIS:HE1	5:Q:358:TYR:CE2	1.55	0.82
1:O:27:MET:CE	1:O:286:ALA:O	2.28	0.82
5:Q:374:ALA:O	5:Q:378:LEU:HG	1.79	0.82
5:R:411:LEU:CA	5:R:412:LEU:C	2.51	0.82
5:Q:407:THR:O	5:Q:410:PHE:CD2	2.32	0.82
5:R:363:TYR:CD1	5:R:364:PRO:HD3	2.14	0.82
5:S:397:ILE:HG22	5:S:398:THR:N	1.95	0.82
3:L:159:LYS:HZ1	4:H:432:LEU:HD22	1.41	0.82
4:G:403:SER:O	4:G:407:MET:HG2	1.80	0.82
5:S:352:PRO:O	5:S:355:ILE:HB	1.79	0.82
3:K:248:ASP:O	5:S:403:THR:OG1	1.98	0.81
4:F:403:SER:N	4:F:407:MET:HG3	1.76	0.81
1:O:24:TYR:CD2	1:O:288:THR:O	2.33	0.81
1:P:23:GLY:C	1:P:290:VAL:CG2	2.51	0.81
5:R:407:THR:N	5:R:410:PHE:HD2	1.78	0.81
3:I:162:LEU:HD23	5:Q:400:TYR:HE1	1.42	0.81
1:O:16:LYS:NZ	1:O:340:ARG:O	2.12	0.81
3:I:133:LYS:CD	5:Q:401:GLU:O	2.28	0.81
3:L:159:LYS:HZ3	4:H:432:LEU:HD11	1.42	0.81
4:E:415:GLY:O	4:E:419:LEU:HD12	1.79	0.81
5:Q:415:LEU:O	5:Q:416:CYS:HB2	1.80	0.81
1:P:27:MET:HE1	1:P:286:ALA:O	1.80	0.81
3:K:159:LYS:NZ	4:G:432:LEU:HD13	1.85	0.81
5:S:374:ALA:O	5:S:378:LEU:HG	1.79	0.81
1:B:21:ASP:OD2	1:C:143:SER:CB	2.27	0.81
1:B:142:HIS:CE1	1:D:109:GLU:CD	2.57	0.81
1:P:382:PRO:HG3	5:T:345:ASN:HB2	1.61	0.81
4:E:403:SER:O	4:E:407:MET:HG2	1.80	0.81
5:S:415:LEU:O	5:S:416:CYS:HB2	1.80	0.81
4:H:403:SER:O	4:H:407:MET:HG2	1.80	0.81
1:M:41:THR:CA	1:N:43:SER:OG	2.25	0.81
1:B:142:HIS:ND1	1:D:109:GLU:HB3	1.95	0.81
3:I:246:ASN:OD1	4:E:439:HIS:HA	1.81	0.81
5:R:397:ILE:HG22	5:R:398:THR:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:HIS:CE1	1:D:109:GLU:CB	2.64	0.81
3:I:160:TYR:HE2	5:Q:398:THR:H	1.26	0.81
4:G:402:ILE:HG21	4:G:407:MET:HE1	1.63	0.81
1:B:142:HIS:ND1	1:D:109:GLU:CB	2.44	0.81
5:R:356:ILE:CA	5:R:359:TYR:CD2	2.62	0.81
5:S:356:ILE:CA	5:S:359:TYR:CD2	2.61	0.81
5:S:406:ALA:C	5:S:410:PHE:HD2	1.87	0.81
5:S:407:THR:N	5:S:410:PHE:HD2	1.78	0.81
5:T:374:ALA:O	5:T:378:LEU:HG	1.79	0.81
5:T:397:ILE:HG22	5:T:398:THR:N	1.95	0.81
3:I:249:ILE:HG22	4:E:439:HIS:CE1	2.16	0.80
3:K:164:CYS:SG	5:S:400:TYR:CZ	2.74	0.80
4:E:432:LEU:O	4:E:436:PHE:HD2	1.61	0.80
5:Q:397:ILE:HG22	5:Q:398:THR:N	1.95	0.80
4:H:432:LEU:O	4:H:436:PHE:HD2	1.61	0.80
1:M:149:ASN:HD21	1:N:191:PRO:HG2	0.63	0.80
5:S:351:HIS:HB3	5:S:352:PRO:HD3	1.62	0.80
3:I:221:LYS:HB2	3:I:221:LYS:NZ	1.96	0.80
1:B:280:LYS:HD2	5:R:343:SER:HB3	1.62	0.80
4:F:399:VAL:HG21	5:R:362:LEU:CG	2.11	0.80
5:R:374:ALA:O	5:R:378:LEU:HG	1.79	0.80
4:G:399:VAL:CG2	5:S:362:LEU:CG	2.43	0.80
4:H:402:ILE:HG21	4:H:407:MET:HE1	1.63	0.80
5:T:406:ALA:CB	5:T:407:THR:O	2.30	0.80
1:P:18:LEU:HD13	1:P:331:HIS:CB	2.11	0.80
5:Q:421:THR:O	5:Q:422:LYS:CG	2.30	0.80
4:F:432:LEU:O	4:F:436:PHE:HD2	1.61	0.80
5:T:421:THR:O	5:T:422:LYS:CG	2.30	0.80
3:J:162:LEU:CB	5:R:400:TYR:OH	2.30	0.80
5:R:415:LEU:O	5:R:416:CYS:HB2	1.80	0.80
5:S:406:ALA:CB	5:S:407:THR:O	2.30	0.80
1:A:281:ASN:OD1	5:Q:343:SER:CB	2.30	0.80
5:Q:419:ARG:O	5:Q:420:THR:CG2	2.30	0.80
5:S:421:THR:O	5:S:422:LYS:CG	2.30	0.80
5:T:349:HIS:CE1	5:T:355:ILE:CA	2.64	0.80
5:T:415:LEU:O	5:T:416:CYS:HB2	1.80	0.80
3:I:159:LYS:HZ3	5:Q:394:ARG:HB3	1.45	0.80
5:Q:349:HIS:HA	5:Q:354:GLU:CG	1.98	0.80
5:Q:406:ALA:CB	5:Q:407:THR:O	2.30	0.80
4:F:403:SER:O	4:F:407:MET:HG2	1.80	0.80
5:S:363:TYR:CD1	5:S:364:PRO:CD	2.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:221:LYS:NZ	3:K:221:LYS:HB2	1.96	0.80
5:Q:406:ALA:C	5:Q:410:PHE:HD2	1.86	0.80
5:Q:417:CYS:O	5:Q:420:THR:CG2	2.30	0.80
5:S:401:GLU:O	5:S:402:LEU:CG	2.30	0.80
4:E:416:GLY:O	4:E:420:ILE:HD12	1.82	0.79
5:R:421:THR:O	5:R:422:LYS:CG	2.30	0.79
5:T:402:LEU:O	5:T:403:THR:CG2	2.30	0.79
5:Q:407:THR:N	5:Q:410:PHE:HD2	1.78	0.79
5:R:406:ALA:CB	5:R:407:THR:O	2.30	0.79
1:O:26:PRO:O	1:O:329:ALA:CB	2.29	0.79
3:I:157:SER:OG	5:Q:397:ILE:HD12	1.81	0.79
3:L:164:CYS:SG	5:T:400:TYR:CG	2.76	0.79
5:R:419:ARG:O	5:R:420:THR:CG2	2.30	0.79
4:G:399:VAL:HG13	5:S:362:LEU:HD11	1.47	0.79
1:C:109:GLU:HG3	1:D:142:HIS:CE1	2.17	0.79
5:S:417:CYS:O	5:S:420:THR:CG2	2.30	0.79
1:A:280:LYS:CD	5:Q:343:SER:HB3	2.10	0.79
5:Q:402:LEU:O	5:Q:403:THR:CG2	2.30	0.79
5:T:419:ARG:O	5:T:420:THR:CG2	2.30	0.79
1:N:237:PRO:HG2	1:C:314:LYS:CE	2.12	0.79
3:I:133:LYS:HG2	5:Q:401:GLU:O	1.83	0.79
3:K:133:LYS:CD	5:S:402:LEU:HD21	2.12	0.79
3:K:248:ASP:CG	5:S:405:GLY:HA3	2.00	0.79
3:L:221:LYS:HB2	3:L:221:LYS:NZ	1.96	0.79
5:Q:407:THR:CG2	5:Q:421:THR:HB	2.11	0.79
5:S:413:SER:CB	5:S:417:CYS:CB	2.61	0.79
5:T:363:TYR:CD1	5:T:364:PRO:CD	2.65	0.79
1:O:236:ALA:CA	1:D:272:ARG:HH22	1.95	0.79
4:F:399:VAL:HG13	5:R:362:LEU:CD1	2.13	0.79
4:G:403:SER:OG	4:G:407:MET:CG	2.31	0.79
5:S:351:HIS:CB	5:S:352:PRO:HD3	2.13	0.79
5:T:407:THR:CG2	5:T:421:THR:HB	2.11	0.79
5:R:407:THR:CG2	5:R:421:THR:HB	2.11	0.79
4:G:416:GLY:O	4:G:420:ILE:HD12	1.82	0.79
5:T:413:SER:CB	5:T:417:CYS:CB	2.61	0.79
5:Q:401:GLU:O	5:Q:402:LEU:CG	2.30	0.79
5:Q:410:PHE:HD1	5:Q:417:CYS:HA	1.48	0.79
4:F:416:GLY:O	4:F:420:ILE:HD12	1.82	0.79
5:R:402:LEU:O	5:R:403:THR:CG2	2.30	0.79
5:S:407:THR:CG2	5:S:421:THR:HB	2.11	0.79
1:P:382:PRO:HD3	5:T:345:ASN:OD1	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:402:LEU:O	5:S:403:THR:CG2	2.30	0.79
5:T:408:VAL:CB	5:T:409:PRO:HD3	2.04	0.79
3:I:178:PHE:CZ	5:Q:403:THR:CG2	2.66	0.78
4:F:403:SER:OG	4:F:407:MET:CG	2.31	0.78
5:R:363:TYR:CB	5:R:364:PRO:HD2	2.12	0.78
5:T:401:GLU:O	5:T:402:LEU:CG	2.30	0.78
5:T:410:PHE:HD1	5:T:417:CYS:HA	1.48	0.78
3:I:178:PHE:HZ	5:Q:403:THR:CG2	1.96	0.78
5:R:401:GLU:O	5:R:402:LEU:CG	2.30	0.78
5:R:417:CYS:O	5:R:420:THR:CG2	2.30	0.78
4:H:416:GLY:O	4:H:420:ILE:HD12	1.82	0.78
5:T:417:CYS:O	5:T:420:THR:CG2	2.30	0.78
3:J:221:LYS:HB2	3:J:221:LYS:NZ	1.96	0.78
3:L:133:LYS:HD3	5:T:402:LEU:HD23	1.59	0.78
4:E:402:ILE:HG21	4:E:407:MET:HE1	1.63	0.78
5:R:413:SER:CB	5:R:417:CYS:CB	2.61	0.78
1:O:236:ALA:HA	1:D:272:ARG:HH12	1.48	0.78
3:I:157:SER:HB3	5:Q:400:TYR:CE2	2.18	0.78
4:F:402:ILE:HG21	4:F:407:MET:HE1	1.63	0.78
5:S:419:ARG:O	5:S:420:THR:CG2	2.30	0.78
3:L:130:VAL:O	5:T:402:LEU:HD12	1.82	0.78
4:E:403:SER:OG	4:E:407:MET:CG	2.31	0.78
5:Q:413:SER:CB	5:Q:417:CYS:CB	2.61	0.78
5:R:410:PHE:O	5:R:411:LEU:CG	2.32	0.78
4:H:403:SER:OG	4:H:407:MET:CG	2.31	0.78
5:R:406:ALA:C	5:R:410:PHE:HD2	1.87	0.78
1:A:280:LYS:CD	5:Q:343:SER:OG	2.32	0.77
4:F:399:VAL:CG1	5:R:366:MET:CE	2.57	0.77
4:H:399:VAL:CB	5:T:366:MET:HE2	2.14	0.77
3:L:133:LYS:HD3	5:T:402:LEU:HG	1.64	0.77
5:T:410:PHE:O	5:T:411:LEU:CG	2.32	0.77
3:J:157:SER:HA	5:R:397:ILE:HD12	1.64	0.77
5:Q:407:THR:O	5:Q:410:PHE:HD2	1.68	0.77
1:O:1:TYR:HB3	1:O:287:PHE:CE2	2.20	0.77
3:K:250:VAL:HG12	5:S:398:THR:HG22	1.67	0.77
3:K:122:LYS:NZ	3:L:169:VAL:CG2	2.48	0.77
3:K:160:TYR:CE2	5:S:398:THR:OG1	2.36	0.77
5:Q:416:CYS:CA	5:Q:417:CYS:O	2.30	0.77
5:T:407:THR:O	5:T:410:PHE:HD2	1.68	0.77
5:S:408:VAL:CB	5:S:409:PRO:HD3	2.04	0.77
3:L:252:LYS:H	4:H:439:HIS:CB	1.96	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:410:PHE:O	5:Q:411:LEU:CG	2.32	0.76
5:R:408:VAL:HG12	5:R:409:PRO:N	2.00	0.76
5:S:410:PHE:HD1	5:S:417:CYS:HA	1.48	0.76
1:B:142:HIS:CG	1:D:109:GLU:HB2	2.21	0.76
1:M:291:VAL:O	1:M:324:LYS:NZ	2.18	0.76
5:S:410:PHE:O	5:S:411:LEU:CG	2.32	0.76
5:T:349:HIS:HE1	5:T:354:GLU:C	1.93	0.76
5:T:351:HIS:O	5:T:355:ILE:HG13	1.85	0.76
5:R:405:GLY:O	5:R:406:ALA:HB3	1.86	0.76
5:R:416:CYS:CA	5:R:417:CYS:O	2.30	0.76
5:S:363:TYR:CD1	5:S:364:PRO:HD2	2.20	0.76
5:S:410:PHE:CD1	5:S:417:CYS:HA	2.21	0.76
5:T:410:PHE:CD1	5:T:417:CYS:HA	2.21	0.76
3:K:131:GLY:CA	5:S:402:LEU:HD12	2.12	0.76
5:T:408:VAL:HG12	5:T:409:PRO:N	2.00	0.76
1:B:142:HIS:CG	1:D:109:GLU:CB	2.69	0.76
1:P:18:LEU:HD22	1:P:331:HIS:HB3	1.67	0.76
3:K:159:LYS:CB	4:G:436:PHE:CZ	2.55	0.76
3:L:133:LYS:HD3	5:T:402:LEU:CG	2.11	0.76
3:L:133:LYS:HB2	5:T:402:LEU:HG	1.68	0.76
4:H:399:VAL:HB	5:T:366:MET:HE2	1.67	0.76
3:I:251:THR:OG1	4:E:439:HIS:ND1	2.18	0.76
4:E:416:GLY:O	4:E:420:ILE:CD1	2.34	0.76
1:O:236:ALA:HA	1:D:272:ARG:NH1	2.00	0.76
3:K:160:TYR:CD2	5:S:398:THR:CA	2.68	0.76
5:Q:405:GLY:O	5:Q:406:ALA:HB3	1.86	0.76
5:R:410:PHE:HD1	5:R:417:CYS:HA	1.48	0.76
5:S:408:VAL:HG12	5:S:409:PRO:N	2.00	0.76
1:B:27:SER:H	1:C:146:GLN:HE21	1.34	0.75
5:Q:363:TYR:H	5:Q:364:PRO:HD2	1.48	0.75
5:T:406:ALA:C	5:T:410:PHE:HD2	1.87	0.75
3:I:159:LYS:HZ2	4:E:432:LEU:HD22	1.50	0.75
5:T:405:GLY:O	5:T:406:ALA:HB3	1.86	0.75
3:J:159:LYS:HD2	4:F:436:PHE:HE2	1.16	0.75
5:T:407:THR:N	5:T:410:PHE:HD2	1.78	0.75
1:O:237:PRO:HD2	1:D:272:ARG:NH2	1.92	0.75
5:T:349:HIS:CE1	5:T:355:ILE:N	2.55	0.75
5:T:416:CYS:CA	5:T:417:CYS:O	2.30	0.75
1:O:361:ALA:HB3	5:S:345:ASN:CG	2.10	0.75
3:I:249:ILE:HG22	4:E:439:HIS:HE1	1.50	0.75
3:K:122:LYS:CG	3:L:170:HIS:HB3	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:351:HIS:HB2	5:Q:352:PRO:HD3	1.68	0.75
4:F:416:GLY:O	4:F:420:ILE:CD1	2.34	0.75
4:H:416:GLY:O	4:H:420:ILE:CD1	2.34	0.75
3:I:157:SER:CB	5:Q:397:ILE:HG23	2.16	0.75
4:H:399:VAL:HG11	5:T:366:MET:HE2	1.67	0.75
1:O:235:GLN:C	1:D:272:ARG:NH1	2.45	0.75
5:Q:410:PHE:CD1	5:Q:417:CYS:HA	2.21	0.75
5:R:407:THR:O	5:R:410:PHE:HD2	1.68	0.75
5:R:410:PHE:CD1	5:R:417:CYS:HA	2.21	0.75
5:S:405:GLY:O	5:S:406:ALA:HB3	1.86	0.75
5:S:416:CYS:CA	5:S:417:CYS:O	2.30	0.75
3:K:130:VAL:CG1	5:S:401:GLU:OE1	2.35	0.74
4:E:402:ILE:CG2	4:E:407:MET:HE1	2.18	0.74
5:S:418:VAL:HG22	5:S:421:THR:H	1.52	0.74
3:I:234:GLU:CB	3:K:172:LYS:HB2	2.17	0.74
3:K:250:VAL:HG21	5:S:401:GLU:CB	2.15	0.74
1:M:293:ALA:O	1:M:324:LYS:NZ	2.20	0.74
3:I:160:TYR:CE2	5:Q:398:THR:N	2.54	0.74
5:Q:418:VAL:HG22	5:Q:421:THR:H	1.52	0.74
5:T:356:ILE:HA	5:T:359:TYR:HE2	0.96	0.74
1:B:288:TYR:OH	1:P:199:GLN:NE2	2.21	0.74
1:O:236:ALA:HA	1:D:272:ARG:CZ	2.18	0.74
5:Q:349:HIS:NE2	5:Q:358:TYR:CZ	2.53	0.74
4:G:416:GLY:O	4:G:420:ILE:CD1	2.34	0.74
5:R:356:ILE:C	5:R:359:TYR:CD2	2.62	0.74
1:P:18:LEU:HB2	1:P:331:HIS:CE1	2.22	0.74
4:F:403:SER:O	4:F:407:MET:CB	2.36	0.74
5:R:349:HIS:NE2	5:R:357:LEU:HB2	2.00	0.74
3:L:178:PHE:C	3:L:224:VAL:O	2.31	0.73
5:Q:349:HIS:CE1	5:Q:358:TYR:CZ	2.71	0.73
4:H:399:VAL:CG1	5:T:366:MET:CE	2.66	0.73
5:R:421:THR:O	5:R:422:LYS:CB	2.36	0.73
4:G:403:SER:O	4:G:407:MET:CB	2.36	0.73
5:T:421:THR:O	5:T:422:LYS:CB	2.36	0.73
1:O:236:ALA:CA	1:D:272:ARG:HH12	2.00	0.73
3:J:178:PHE:C	3:J:224:VAL:O	2.32	0.73
3:K:178:PHE:C	3:K:224:VAL:O	2.32	0.73
5:R:418:VAL:HG22	5:R:420:THR:H	1.53	0.73
5:R:418:VAL:HG22	5:R:421:THR:H	1.52	0.73
5:T:418:VAL:HG22	5:T:421:THR:H	1.52	0.73
1:M:18:LEU:HB2	1:M:331:HIS:CG	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:349:HIS:HB3	5:Q:354:GLU:N	2.02	0.73
5:Q:352:PRO:O	5:Q:355:ILE:N	2.20	0.73
5:S:418:VAL:HG22	5:S:420:THR:H	1.53	0.73
4:H:403:SER:O	4:H:407:MET:CB	2.36	0.73
3:L:179:THR:HG22	3:L:223:ARG:HB3	1.71	0.73
5:S:351:HIS:HB2	5:S:352:PRO:CD	2.17	0.73
5:S:352:PRO:O	5:S:355:ILE:N	2.22	0.73
3:I:179:THR:HG22	3:I:223:ARG:HB3	1.71	0.73
3:K:159:LYS:HZ1	5:S:394:ARG:CA	2.00	0.73
5:R:410:PHE:O	5:R:411:LEU:CB	2.36	0.73
3:K:179:THR:HG22	3:K:223:ARG:HB3	1.71	0.73
5:Q:408:VAL:HG12	5:Q:409:PRO:N	2.00	0.73
5:T:349:HIS:HE1	5:T:354:GLU:O	1.71	0.73
1:C:18:HIS:CE1	1:D:146:GLN:HE21	1.96	0.73
3:L:159:LYS:C	4:H:436:PHE:HE1	1.96	0.73
4:E:403:SER:O	4:E:407:MET:CB	2.36	0.73
5:Q:408:VAL:HB	5:Q:409:PRO:HD3	1.65	0.73
5:S:407:THR:O	5:S:410:PHE:HD2	1.68	0.73
5:T:410:PHE:O	5:T:411:LEU:CB	2.36	0.73
3:K:130:VAL:O	5:S:402:LEU:CD1	2.37	0.72
3:K:164:CYS:SG	5:S:400:TYR:CG	2.82	0.72
5:R:351:HIS:O	5:R:355:ILE:CG1	2.36	0.72
5:S:421:THR:O	5:S:422:LYS:CB	2.36	0.72
1:C:27:SER:HB2	1:D:146:GLN:NE2	2.04	0.72
3:K:160:TYR:CD2	5:S:397:ILE:HG21	2.24	0.72
4:E:403:SER:O	4:E:407:MET:CG	2.37	0.72
1:P:18:LEU:CB	1:P:331:HIS:CG	2.66	0.72
3:I:178:PHE:C	3:I:224:VAL:O	2.32	0.72
3:K:160:TYR:CD1	5:S:398:THR:HG23	2.20	0.72
5:Q:418:VAL:HG22	5:Q:420:THR:H	1.53	0.72
5:T:410:PHE:CD2	5:T:421:THR:HG21	2.24	0.72
1:M:147:TYR:CD2	1:N:192:PHE:O	2.43	0.72
1:B:94:THR:CG2	1:D:24:GLU:OE1	2.27	0.72
1:O:18:LEU:HB2	1:O:331:HIS:ND1	2.03	0.72
5:Q:364:PRO:O	5:Q:365:THR:CB	2.37	0.72
5:R:406:ALA:CB	5:R:410:PHE:CD2	2.73	0.72
5:Q:406:ALA:CB	5:Q:410:PHE:CD2	2.73	0.72
5:Q:421:THR:O	5:Q:422:LYS:CB	2.36	0.72
5:T:372:SER:O	5:T:376:PHE:CD2	2.43	0.72
5:T:408:VAL:HB	5:T:409:PRO:HD3	1.65	0.72
3:K:160:TYR:CZ	5:S:398:THR:OG1	2.31	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:248:ASP:OD2	5:T:405:GLY:HA3	1.89	0.72
5:S:410:PHE:O	5:S:411:LEU:CB	2.36	0.72
1:C:109:GLU:HB3	1:D:142:HIS:ND1	2.03	0.72
1:D:280:LYS:HD2	5:T:343:SER:O	1.88	0.72
4:E:404:THR:O	4:E:405:THR:C	2.33	0.72
5:T:418:VAL:HG22	5:T:420:THR:H	1.53	0.72
1:M:126:THR:HG21	1:N:175:ASN:ND2	2.05	0.72
1:O:18:LEU:CB	1:O:331:HIS:CG	2.63	0.72
1:O:361:ALA:HB2	5:S:345:ASN:HB2	1.71	0.72
4:F:404:THR:O	4:F:405:THR:C	2.33	0.72
5:S:406:ALA:CB	5:S:410:PHE:CD2	2.73	0.72
4:H:404:THR:O	4:H:405:THR:C	2.33	0.72
1:O:18:LEU:HD13	1:O:331:HIS:CB	2.18	0.71
3:J:179:THR:HG22	3:J:223:ARG:HB3	1.71	0.71
5:Q:372:SER:O	5:Q:376:PHE:CD2	2.43	0.71
5:Q:410:PHE:O	5:Q:411:LEU:CB	2.36	0.71
5:R:414:LEU:O	5:R:415:LEU:C	2.33	0.71
5:T:406:ALA:CB	5:T:410:PHE:CD2	2.73	0.71
5:Q:349:HIS:HA	5:Q:354:GLU:HG3	1.69	0.71
5:S:414:LEU:O	5:S:415:LEU:C	2.33	0.71
5:Q:410:PHE:CD2	5:Q:421:THR:HG21	2.25	0.71
5:S:372:SER:O	5:S:376:PHE:CD2	2.43	0.71
5:Q:414:LEU:O	5:Q:415:LEU:C	2.33	0.71
3:L:250:VAL:HG12	5:T:398:THR:HG22	1.71	0.71
5:S:410:PHE:CD2	5:S:421:THR:HG21	2.24	0.71
1:B:272:ARG:NH1	1:P:236:ALA:HA	2.05	0.71
5:R:410:PHE:CD2	5:R:421:THR:HG21	2.24	0.71
4:G:403:SER:O	4:G:407:MET:CG	2.37	0.71
5:S:352:PRO:HA	5:S:355:ILE:HD12	0.87	0.71
4:H:403:SER:O	4:H:407:MET:CG	2.37	0.71
1:B:146:GLN:HE21	1:D:20:PRO:CA	2.00	0.71
5:Q:359:TYR:O	5:Q:363:TYR:HB2	1.89	0.71
5:S:407:THR:CG2	5:S:421:THR:CB	2.69	0.71
1:M:291:VAL:CG2	1:O:304:PRO:CA	2.62	0.71
4:E:397:LEU:HD22	4:E:397:LEU:N	2.06	0.71
4:F:399:VAL:HG12	5:R:366:MET:CE	2.19	0.71
1:A:280:LYS:HD2	5:Q:343:SER:CA	2.21	0.71
1:O:24:TYR:CD2	1:O:287:PHE:O	2.44	0.71
3:L:162:LEU:HD23	5:T:400:TYR:HE1	1.56	0.71
4:G:397:LEU:HD22	4:G:397:LEU:N	2.06	0.71
5:T:411:LEU:N	5:T:413:SER:CB	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:414:LEU:O	5:T:415:LEU:C	2.33	0.71
1:O:18:LEU:HD22	1:O:331:HIS:HB3	1.72	0.71
5:Q:406:ALA:CB	5:Q:408:VAL:HB	2.21	0.71
5:R:411:LEU:N	5:R:413:SER:CB	2.54	0.71
5:S:356:ILE:C	5:S:359:TYR:CD2	2.66	0.70
5:R:367:THR:O	5:R:369:VAL:N	2.24	0.70
5:R:372:SER:O	5:R:376:PHE:CD2	2.43	0.70
5:R:407:THR:CG2	5:R:421:THR:CB	2.69	0.70
5:T:407:THR:CG2	5:T:421:THR:CB	2.69	0.70
3:J:148:ASP:OD1	3:L:121:GLY:HA3	1.90	0.70
3:J:159:LYS:HD3	4:F:436:PHE:HE2	1.53	0.70
4:F:397:LEU:HD22	4:F:397:LEU:N	2.06	0.70
5:R:356:ILE:HA	5:R:359:TYR:HE2	0.96	0.70
5:T:351:HIS:O	5:T:355:ILE:CG1	2.39	0.70
1:M:291:VAL:HG22	1:O:304:PRO:HB2	0.71	0.70
1:P:18:LEU:HD22	1:P:331:HIS:ND1	2.06	0.70
3:J:221:LYS:HB2	3:J:221:LYS:HZ2	1.55	0.70
5:R:406:ALA:CB	5:R:408:VAL:HB	2.21	0.70
1:P:18:LEU:CB	1:P:331:HIS:CE1	2.75	0.70
3:J:157:SER:HB2	5:R:397:ILE:HD13	1.72	0.70
3:K:160:TYR:CD2	5:S:398:THR:HA	2.26	0.70
5:Q:407:THR:CG2	5:Q:421:THR:CB	2.69	0.70
3:J:130:VAL:CG1	5:R:401:GLU:OE1	2.38	0.70
5:Q:402:LEU:C	5:Q:403:THR:CG2	2.64	0.70
5:S:363:TYR:CD1	5:S:364:PRO:HD3	2.25	0.70
1:O:24:TYR:HD2	1:O:288:THR:C	1.99	0.70
5:Q:397:ILE:O	5:Q:398:THR:C	2.34	0.70
1:P:382:PRO:CG	5:T:345:ASN:HB2	2.21	0.70
3:L:157:SER:HA	5:T:397:ILE:CD1	2.21	0.70
5:Q:356:ILE:CA	5:Q:359:TYR:CD2	2.70	0.70
4:F:403:SER:O	4:F:407:MET:CG	2.37	0.70
5:S:356:ILE:HA	5:S:359:TYR:HE2	0.92	0.70
4:H:397:LEU:HD22	4:H:397:LEU:N	2.06	0.70
5:Q:410:PHE:CA	5:Q:413:SER:HB3	2.22	0.70
4:G:404:THR:O	4:G:405:THR:C	2.33	0.70
1:B:143:SER:HB3	1:D:110:THR:HG21	1.72	0.70
3:K:245:TRP:HZ2	5:S:401:GLU:OE1	1.73	0.70
5:S:410:PHE:CA	5:S:413:SER:HB3	2.22	0.70
1:O:24:TYR:CB	1:O:288:THR:O	2.40	0.69
3:K:160:TYR:OH	5:S:398:THR:OG1	1.87	0.69
5:Q:363:TYR:N	5:Q:364:PRO:CD	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:418:VAL:HA	5:T:419:ARG:C	2.17	0.69
1:O:28:VAL:HG11	1:O:342:ALA:HA	1.72	0.69
5:R:397:ILE:O	5:R:398:THR:C	2.34	0.69
5:S:349:HIS:HA	5:S:354:GLU:CG	2.07	0.69
5:S:397:ILE:O	5:S:398:THR:C	2.34	0.69
5:T:397:ILE:O	5:T:398:THR:C	2.34	0.69
1:B:144:ARG:NE	1:D:25:GLY:CA	2.41	0.69
1:O:23:GLY:O	1:O:290:VAL:N	2.23	0.69
1:O:24:TYR:HD2	1:O:288:THR:O	1.74	0.69
3:K:159:LYS:CE	4:G:432:LEU:CD1	2.53	0.69
5:R:349:HIS:CE1	5:R:357:LEU:HD12	2.27	0.69
5:R:418:VAL:HA	5:R:419:ARG:C	2.17	0.69
5:T:351:HIS:O	5:T:355:ILE:HD12	1.92	0.69
1:M:41:THR:CB	1:N:125:HIS:HE1	2.01	0.69
3:K:160:TYR:HD2	5:S:397:ILE:HG22	0.73	0.69
5:Q:411:LEU:N	5:Q:413:SER:CB	2.54	0.69
5:Q:418:VAL:HA	5:Q:419:ARG:C	2.17	0.69
5:Q:417:CYS:O	5:Q:420:THR:HG21	1.92	0.69
4:F:434:VAL:O	4:F:438:ARG:HG3	1.92	0.69
5:R:345:ASN:HD22	5:R:345:ASN:C	2.01	0.69
5:S:406:ALA:CB	5:S:408:VAL:HB	2.21	0.69
5:T:417:CYS:O	5:T:420:THR:HG21	1.92	0.69
1:M:41:THR:HA	1:N:43:SER:HG	1.53	0.69
1:O:16:LYS:HZ1	1:O:340:ARG:C	1.99	0.69
3:K:159:LYS:NZ	4:G:432:LEU:HD21	2.07	0.69
4:E:434:VAL:O	4:E:438:ARG:HG3	1.92	0.69
3:I:157:SER:OG	5:Q:397:ILE:HG21	1.88	0.69
3:J:157:SER:CA	5:R:397:ILE:CD1	2.66	0.69
5:R:349:HIS:HE1	5:R:357:LEU:HB2	0.91	0.69
5:R:410:PHE:CA	5:R:413:SER:HB3	2.22	0.69
5:T:348:ALA:O	5:T:354:GLU:CD	2.35	0.69
5:T:363:TYR:CB	5:T:364:PRO:HD2	2.22	0.69
5:T:410:PHE:HA	5:T:413:SER:CB	2.23	0.69
1:M:293:ALA:HB1	1:M:294:PRO:HD2	1.75	0.69
1:O:23:GLY:CA	1:O:290:VAL:HG23	2.22	0.69
4:F:399:VAL:CG1	5:R:362:LEU:HD11	2.23	0.69
4:G:402:ILE:CG2	4:G:407:MET:HE1	2.17	0.69
5:S:349:HIS:HA	5:S:354:GLU:CB	2.23	0.69
5:S:410:PHE:HA	5:S:413:SER:CB	2.23	0.69
5:T:406:ALA:CB	5:T:408:VAL:HB	2.21	0.69
5:T:410:PHE:CA	5:T:413:SER:HB3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:356:ILE:C	5:T:359:TYR:CD2	2.62	0.69
3:K:130:VAL:HG11	5:S:401:GLU:OE1	1.93	0.68
3:I:157:SER:HA	5:Q:397:ILE:CD1	2.23	0.68
5:Q:354:GLU:HA	5:Q:357:LEU:HD12	1.74	0.68
5:S:417:CYS:O	5:S:420:THR:HG21	1.92	0.68
4:F:402:ILE:CG2	4:F:407:MET:HE1	2.18	0.68
5:R:354:GLU:HA	5:R:357:LEU:HD12	1.74	0.68
4:G:434:VAL:O	4:G:438:ARG:HG3	1.92	0.68
5:S:349:HIS:HA	5:S:354:GLU:HB2	1.72	0.68
5:S:354:GLU:HA	5:S:357:LEU:HD12	1.74	0.68
5:S:418:VAL:HA	5:S:419:ARG:C	2.17	0.68
1:O:28:VAL:CG1	1:O:342:ALA:HA	2.23	0.68
1:P:18:LEU:HB2	1:P:331:HIS:ND1	2.06	0.68
3:I:249:ILE:CG2	4:E:439:HIS:HE1	2.06	0.68
3:L:252:LYS:H	4:H:439:HIS:HB3	1.55	0.68
5:Q:410:PHE:HA	5:Q:413:SER:CB	2.23	0.68
5:T:349:HIS:HA	5:T:354:GLU:OE1	1.93	0.68
1:M:147:TYR:H	1:M:152:HIS:HD1	1.42	0.68
1:M:291:VAL:CB	1:O:304:PRO:HB2	2.23	0.68
1:P:382:PRO:CG	5:T:345:ASN:CB	2.70	0.68
5:S:407:THR:HG22	5:S:421:THR:HG1	1.58	0.68
5:T:354:GLU:HA	5:T:357:LEU:HD12	1.74	0.68
3:J:160:TYR:CE1	4:F:436:PHE:CE1	2.81	0.68
3:K:157:SER:HA	5:S:397:ILE:HD11	1.74	0.68
3:K:160:TYR:OH	5:S:398:THR:CG2	2.40	0.68
3:I:251:THR:CG2	4:E:439:HIS:HB2	2.04	0.68
3:L:160:TYR:CD2	5:T:398:THR:HA	2.28	0.68
5:S:352:PRO:O	5:S:353:HIS:C	2.36	0.68
1:N:359:ALA:O	5:R:345:ASN:OD1	2.12	0.68
3:I:159:LYS:NZ	4:E:432:LEU:HD13	2.09	0.68
4:H:434:VAL:O	4:H:438:ARG:HG3	1.92	0.68
1:M:149:ASN:HD22	1:N:191:PRO:HG3	1.59	0.68
3:L:221:LYS:HB2	3:L:221:LYS:HZ2	1.56	0.68
1:O:21:ARG:HH11	1:O:287:PHE:CB	2.07	0.67
3:K:159:LYS:HD3	4:G:432:LEU:HB3	1.76	0.67
5:Q:405:GLY:O	5:Q:406:ALA:CB	2.42	0.67
5:T:405:GLY:O	5:T:406:ALA:CB	2.42	0.67
3:L:159:LYS:HE2	4:H:432:LEU:HD13	1.74	0.67
5:R:405:GLY:O	5:R:406:ALA:CB	2.42	0.67
5:R:410:PHE:HA	5:R:413:SER:CB	2.23	0.67
5:T:349:HIS:NE2	5:T:355:ILE:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:410:PHE:C	5:T:413:SER:OG	2.38	0.67
3:I:234:GLU:CA	3:K:169:VAL:O	2.41	0.67
3:J:160:TYR:HE2	5:R:398:THR:OG1	1.78	0.67
1:C:109:GLU:HB2	1:D:142:HIS:NE2	2.01	0.67
1:O:24:TYR:HA	1:O:288:THR:O	1.95	0.67
1:O:24:TYR:CD2	1:O:288:THR:C	2.73	0.67
3:K:221:LYS:HB2	3:K:221:LYS:HZ2	1.59	0.67
5:Q:352:PRO:O	5:Q:353:HIS:C	2.37	0.67
5:Q:365:THR:O	5:Q:367:THR:N	2.28	0.67
5:R:417:CYS:O	5:R:420:THR:HG21	1.92	0.67
5:S:411:LEU:N	5:S:413:SER:CB	2.54	0.67
1:A:280:LYS:HG3	5:Q:343:SER:OG	1.95	0.67
1:P:26:PRO:HB2	1:P:329:ALA:HB3	1.76	0.67
5:R:406:ALA:CB	5:R:409:PRO:CD	2.34	0.67
4:E:403:SER:O	4:E:407:MET:N	2.26	0.67
3:K:159:LYS:NZ	4:G:432:LEU:HD22	2.09	0.66
5:S:407:THR:H	5:S:421:THR:CB	2.08	0.66
1:O:236:ALA:N	1:D:272:ARG:HH12	1.93	0.66
5:Q:407:THR:H	5:Q:421:THR:CB	2.08	0.66
4:G:403:SER:O	4:G:407:MET:N	2.26	0.66
1:M:147:TYR:HE2	1:N:192:PHE:CB	2.07	0.66
3:J:157:SER:HA	5:R:397:ILE:CD1	2.24	0.66
5:S:405:GLY:O	5:S:406:ALA:CB	2.42	0.66
5:S:410:PHE:C	5:S:413:SER:OG	2.38	0.66
1:O:235:GLN:C	1:D:272:ARG:HH12	2.02	0.66
5:R:410:PHE:C	5:R:413:SER:OG	2.38	0.66
4:H:403:SER:O	4:H:407:MET:N	2.26	0.66
1:M:126:THR:HG21	1:N:175:ASN:HD21	1.60	0.66
1:M:18:LEU:HB2	1:M:331:HIS:CE1	2.30	0.66
1:M:152:HIS:CE1	1:N:192:PHE:O	2.49	0.66
1:P:23:GLY:CA	1:P:290:VAL:HG23	2.26	0.66
3:J:160:TYR:CD1	4:F:436:PHE:CE1	2.83	0.66
1:M:125:HIS:CE1	1:N:41:THR:CB	2.71	0.66
3:L:133:LYS:CE	5:T:402:LEU:CD2	2.73	0.66
5:T:419:ARG:C	5:T:420:THR:HG23	2.20	0.66
3:I:234:GLU:O	3:K:173:SER:CB	2.42	0.66
4:E:432:LEU:HD21	5:Q:395:ARG:HA	1.76	0.66
5:S:419:ARG:C	5:S:420:THR:HG23	2.20	0.66
4:G:432:LEU:HD21	5:S:395:ARG:HA	1.76	0.66
5:Q:410:PHE:C	5:Q:413:SER:OG	2.38	0.65
4:F:432:LEU:HD21	5:R:395:ARG:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:349:HIS:CE1	5:S:355:ILE:N	2.62	0.65
5:Q:419:ARG:C	5:Q:420:THR:HG23	2.20	0.65
1:O:16:LYS:NZ	1:O:340:ARG:CA	2.58	0.65
1:M:294:PRO:HG2	1:M:328:CYS:SG	2.36	0.65
3:J:157:SER:OG	5:R:397:ILE:HD12	1.96	0.65
3:K:160:TYR:HH	5:S:398:THR:CB	2.08	0.65
4:E:403:SER:OG	4:E:403:SER:O	2.14	0.65
5:Q:406:ALA:CB	5:Q:409:PRO:CD	2.34	0.65
5:Q:416:CYS:N	5:Q:418:VAL:O	2.30	0.65
5:S:407:THR:O	5:S:410:PHE:N	2.30	0.65
4:H:432:LEU:HD21	5:T:395:ARG:HA	1.76	0.65
4:E:403:SER:O	4:E:407:MET:HB2	1.97	0.65
5:R:407:THR:H	5:R:421:THR:CB	2.08	0.65
5:S:416:CYS:N	5:S:418:VAL:O	2.30	0.65
5:T:345:ASN:C	5:T:345:ASN:HD22	2.01	0.65
3:J:162:LEU:HB3	5:R:400:TYR:OH	1.94	0.65
3:K:159:LYS:CD	4:G:432:LEU:CD1	2.62	0.65
5:S:352:PRO:O	5:S:355:ILE:CB	2.45	0.65
5:S:414:LEU:O	5:S:416:CYS:N	2.30	0.65
5:T:406:ALA:CB	5:T:409:PRO:CD	2.34	0.65
5:R:419:ARG:C	5:R:420:THR:HG23	2.20	0.65
5:R:397:ILE:O	5:R:400:TYR:N	2.30	0.65
5:S:365:THR:C	5:S:366:MET:HG2	2.18	0.65
4:H:402:ILE:CG2	4:H:407:MET:HE1	2.18	0.65
3:I:251:THR:HG1	4:E:439:HIS:HD1	1.43	0.65
5:R:349:HIS:CA	5:R:354:GLU:CB	2.21	0.65
5:R:352:PRO:O	5:R:353:HIS:C	2.40	0.65
5:T:407:THR:C	5:T:410:PHE:HD2	2.05	0.65
1:O:16:LYS:HZ3	1:O:340:ARG:HA	1.62	0.64
3:I:160:TYR:CD2	5:Q:397:ILE:CG2	2.80	0.64
3:K:251:THR:HA	4:G:439:HIS:NE2	2.12	0.64
5:S:407:THR:C	5:S:410:PHE:HD2	2.05	0.64
1:M:41:THR:OG1	1:N:123:ARG:HB2	1.97	0.64
3:K:162:LEU:HD23	5:S:400:TYR:HE1	0.90	0.64
5:R:416:CYS:N	5:R:418:VAL:O	2.30	0.64
5:T:407:THR:H	5:T:421:THR:CB	2.08	0.64
5:T:414:LEU:O	5:T:416:CYS:N	2.30	0.64
3:J:178:PHE:HA	3:J:224:VAL:HB	1.80	0.64
3:L:133:LYS:CE	5:T:402:LEU:HD21	2.28	0.64
5:R:414:LEU:O	5:R:416:CYS:N	2.30	0.64
5:S:397:ILE:O	5:S:400:TYR:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:361:ALA:HB1	5:S:345:ASN:CB	2.21	0.64
5:Q:411:LEU:N	5:Q:412:LEU:O	2.31	0.64
5:R:349:HIS:HE1	5:R:357:LEU:CG	2.10	0.64
5:S:402:LEU:C	5:S:403:THR:CG2	2.64	0.64
5:T:416:CYS:N	5:T:418:VAL:O	2.30	0.64
5:Q:397:ILE:O	5:Q:400:TYR:N	2.30	0.64
4:F:403:SER:O	4:F:407:MET:HB2	1.97	0.64
5:R:407:THR:C	5:R:410:PHE:HD2	2.05	0.64
5:S:351:HIS:HB3	5:S:352:PRO:CD	2.23	0.64
5:S:397:ILE:HG22	5:S:398:THR:H	1.62	0.64
5:T:397:ILE:HG22	5:T:398:THR:H	1.62	0.64
3:K:160:TYR:CE2	5:S:397:ILE:CG2	2.73	0.64
5:Q:345:ASN:C	5:Q:345:ASN:HD22	2.01	0.64
4:G:403:SER:OG	4:G:403:SER:O	2.14	0.64
4:G:404:THR:O	4:G:407:MET:N	2.31	0.64
5:S:363:TYR:CD2	5:S:364:PRO:HD2	2.30	0.64
4:H:403:SER:O	4:H:407:MET:HB2	1.97	0.64
4:H:421:VAL:HG11	5:T:388:MET:CG	2.27	0.64
5:T:397:ILE:O	5:T:400:TYR:N	2.30	0.64
5:T:416:CYS:HA	5:T:418:VAL:N	2.10	0.64
5:Q:363:TYR:O	5:Q:365:THR:N	2.30	0.64
5:Q:414:LEU:O	5:Q:416:CYS:N	2.30	0.64
5:R:411:LEU:N	5:R:412:LEU:O	2.31	0.64
4:G:421:VAL:HG11	5:S:388:MET:CG	2.28	0.64
1:P:18:LEU:HD22	1:P:331:HIS:CB	2.28	0.64
3:K:178:PHE:HA	3:K:224:VAL:HB	1.80	0.64
3:L:178:PHE:HA	3:L:224:VAL:HB	1.79	0.64
1:M:28:VAL:HG21	1:M:330:VAL:O	1.97	0.64
1:O:16:LYS:HG3	1:O:339:ILE:O	1.98	0.64
5:Q:407:THR:C	5:Q:410:PHE:HD2	2.05	0.64
5:Q:418:VAL:CG1	5:Q:419:ARG:N	2.57	0.64
5:S:351:HIS:HB2	5:S:352:PRO:HD2	1.79	0.64
1:C:27:SER:HB3	1:D:146:GLN:HG3	1.80	0.64
5:Q:413:SER:HB2	5:Q:417:CYS:HB3	1.79	0.64
4:F:403:SER:OG	4:F:403:SER:O	2.14	0.64
1:C:27:SER:CB	1:D:146:GLN:NE2	2.61	0.63
4:H:404:THR:O	4:H:407:MET:N	2.31	0.63
1:M:147:TYR:CE2	1:N:192:PHE:O	2.51	0.63
3:I:157:SER:CB	5:Q:400:TYR:CE2	2.80	0.63
4:G:403:SER:O	4:G:407:MET:HB2	1.97	0.63
1:P:18:LEU:HD22	1:P:331:HIS:CG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:421:VAL:HG11	5:Q:388:MET:CG	2.28	0.63
5:Q:349:HIS:CE1	5:Q:354:GLU:O	2.51	0.63
5:R:384:THR:O	5:R:388:MET:HG2	1.98	0.63
5:R:418:VAL:CG1	5:R:419:ARG:N	2.57	0.63
5:S:407:THR:HG22	5:S:421:THR:CB	2.27	0.63
5:S:394:ARG:HA	5:S:397:ILE:HG13	1.80	0.63
1:A:280:LYS:CG	5:Q:343:SER:OG	2.46	0.63
1:O:28:VAL:HG21	1:O:330:VAL:C	2.22	0.63
4:F:404:THR:O	4:F:407:MET:N	2.31	0.63
5:S:416:CYS:HA	5:S:418:VAL:N	2.10	0.63
5:T:352:PRO:CA	5:T:355:ILE:HD12	2.26	0.63
5:T:402:LEU:C	5:T:403:THR:CG2	2.64	0.63
5:T:418:VAL:CG1	5:T:419:ARG:N	2.57	0.63
1:M:125:HIS:HE1	1:N:41:THR:HG22	1.63	0.63
1:B:272:ARG:NH1	1:P:237:PRO:HD3	2.14	0.63
4:F:396:THR:C	4:F:397:LEU:HD13	2.24	0.63
5:R:407:THR:O	5:R:410:PHE:N	2.30	0.63
5:S:384:THR:O	5:S:388:MET:HG2	1.98	0.63
5:Q:351:HIS:H	5:Q:352:PRO:HD2	1.64	0.63
5:Q:397:ILE:HG22	5:Q:398:THR:H	1.62	0.63
5:R:394:ARG:HA	5:R:397:ILE:HG13	1.81	0.63
5:T:384:THR:O	5:T:388:MET:HG2	1.98	0.63
4:E:396:THR:C	4:E:397:LEU:HD13	2.24	0.63
4:E:404:THR:O	4:E:407:MET:N	2.31	0.63
5:R:407:THR:HG22	5:R:421:THR:CB	2.28	0.63
4:G:396:THR:C	4:G:397:LEU:HD13	2.24	0.63
3:I:137:PRO:HG2	3:I:213:SER:HB3	1.81	0.62
5:R:351:HIS:O	5:R:355:ILE:HD11	1.99	0.62
5:T:394:ARG:HA	5:T:397:ILE:HG13	1.80	0.62
5:T:411:LEU:N	5:T:412:LEU:O	2.31	0.62
3:I:178:PHE:HA	3:I:224:VAL:HB	1.79	0.62
3:K:159:LYS:NZ	5:S:394:ARG:CA	2.59	0.62
4:E:395:THR:HG23	4:E:395:THR:O	2.00	0.62
4:E:399:VAL:O	4:E:399:VAL:HG12	1.99	0.62
5:R:352:PRO:O	5:R:355:ILE:CB	2.44	0.62
5:R:397:ILE:HG22	5:R:398:THR:H	1.62	0.62
4:H:395:THR:O	4:H:395:THR:HG23	1.99	0.62
4:E:403:SER:CB	4:E:407:MET:CG	2.66	0.62
1:O:237:PRO:HD2	1:D:272:ARG:HH21	1.55	0.62
3:I:133:LYS:CB	5:Q:402:LEU:HG	2.01	0.62
5:Q:416:CYS:HA	5:Q:418:VAL:N	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:403:SER:O	4:F:407:MET:N	2.26	0.62
3:L:157:SER:CB	5:T:397:ILE:CD1	2.75	0.62
5:Q:407:THR:HG22	5:Q:421:THR:CB	2.28	0.62
4:H:399:VAL:O	4:H:399:VAL:HG12	1.99	0.62
3:K:137:PRO:HG2	3:K:213:SER:HB3	1.81	0.62
4:H:396:THR:C	4:H:397:LEU:HD13	2.24	0.62
5:T:407:THR:HG22	5:T:421:THR:CB	2.28	0.62
1:C:109:GLU:CB	1:D:142:HIS:CD2	2.80	0.62
1:O:26:PRO:HD2	1:O:370:CYS:HA	1.80	0.62
3:L:137:PRO:HG2	3:L:213:SER:HB3	1.81	0.62
4:F:406:ALA:HA	4:F:409:TRP:HD1	1.65	0.62
3:K:122:LYS:HG3	3:L:170:HIS:CB	2.30	0.62
4:F:421:VAL:HG11	5:R:388:MET:CG	2.27	0.62
4:G:396:THR:OG1	4:G:397:LEU:N	2.32	0.62
5:S:411:LEU:N	5:S:412:LEU:O	2.31	0.62
1:O:26:PRO:C	1:O:329:ALA:CB	2.73	0.62
1:P:18:LEU:HB2	1:P:331:HIS:NE2	2.13	0.62
5:R:367:THR:O	5:R:368:VAL:C	2.42	0.62
4:H:403:SER:OG	4:H:403:SER:O	2.14	0.62
3:I:251:THR:HG1	4:E:439:HIS:CG	2.18	0.62
5:R:410:PHE:HD1	5:R:417:CYS:CA	2.13	0.62
1:M:291:VAL:CG2	1:O:305:ALA:N	2.63	0.61
4:E:432:LEU:HB3	4:E:436:PHE:HE2	1.65	0.61
5:Q:407:THR:O	5:Q:410:PHE:N	2.30	0.61
4:F:396:THR:OG1	4:F:397:LEU:N	2.32	0.61
4:G:406:ALA:HA	4:G:409:TRP:HD1	1.65	0.61
3:I:178:PHE:HA	3:I:224:VAL:C	2.25	0.61
3:J:178:PHE:CZ	5:R:403:THR:HG22	2.31	0.61
5:Q:384:THR:O	5:Q:388:MET:HG2	1.98	0.61
4:G:432:LEU:HB3	4:G:436:PHE:HE2	1.65	0.61
5:T:410:PHE:HD1	5:T:417:CYS:CA	2.13	0.61
4:G:403:SER:CB	4:G:407:MET:CG	2.66	0.61
3:J:137:PRO:HG2	3:J:213:SER:HB3	1.81	0.61
3:K:160:TYR:CE2	5:S:398:THR:HA	2.28	0.61
5:Q:349:HIS:HE1	5:Q:358:TYR:CD2	2.11	0.61
4:F:403:SER:CB	4:F:407:MET:CG	2.66	0.61
5:R:407:THR:CA	5:R:410:PHE:HD2	2.13	0.61
4:H:399:VAL:HG12	5:T:366:MET:CE	2.30	0.61
1:O:16:LYS:NZ	1:O:340:ARG:C	2.57	0.61
3:K:133:LYS:HD3	5:S:401:GLU:O	2.00	0.61
4:E:396:THR:OG1	4:E:397:LEU:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:416:CYS:HA	5:R:418:VAL:N	2.10	0.61
3:J:130:VAL:HG13	5:R:401:GLU:CD	2.24	0.61
3:K:159:LYS:HZ3	4:G:432:LEU:HD21	1.59	0.61
5:S:410:PHE:HD1	5:S:417:CYS:CA	2.13	0.61
4:E:406:ALA:HA	4:E:409:TRP:HD1	1.65	0.61
5:Q:394:ARG:HA	5:Q:397:ILE:HG13	1.80	0.61
4:F:395:THR:HG23	4:F:395:THR:O	2.00	0.61
4:G:395:THR:HG23	4:G:395:THR:O	1.99	0.61
1:O:21:ARG:HH11	1:O:287:PHE:HB3	1.64	0.61
5:S:413:SER:CB	5:S:417:CYS:HB3	2.31	0.61
5:Q:411:LEU:HG	5:Q:413:SER:OG	2.01	0.61
5:T:407:THR:CA	5:T:410:PHE:HD2	2.13	0.61
3:J:170:HIS:CB	3:L:122:LYS:HD3	2.31	0.61
4:F:399:VAL:HG12	4:F:399:VAL:O	1.99	0.61
5:S:407:THR:CA	5:S:410:PHE:HD2	2.13	0.61
5:S:411:LEU:HG	5:S:413:SER:OG	2.01	0.61
5:T:349:HIS:CA	5:T:354:GLU:OE1	2.49	0.61
1:B:27:SER:N	1:C:146:GLN:HE21	1.98	0.60
1:B:143:SER:HB3	1:D:110:THR:CG2	2.31	0.60
3:J:178:PHE:HA	3:J:224:VAL:C	2.25	0.60
3:L:157:SER:HB2	5:T:397:ILE:HD12	1.82	0.60
4:G:399:VAL:O	4:G:399:VAL:HG12	1.99	0.60
5:S:345:ASN:HD22	5:S:345:ASN:C	2.01	0.60
1:P:27:MET:HE2	1:P:286:ALA:O	2.00	0.60
3:J:157:SER:HB2	5:R:397:ILE:CG2	2.16	0.60
5:R:413:SER:CB	5:R:417:CYS:HB3	2.31	0.60
3:K:178:PHE:CE1	3:K:245:TRP:CD1	2.89	0.60
5:R:411:LEU:HG	5:R:413:SER:OG	2.01	0.60
5:R:413:SER:HB2	5:R:417:CYS:HB3	1.79	0.60
4:H:432:LEU:HB3	4:H:436:PHE:HE2	1.65	0.60
1:N:237:PRO:CG	1:C:314:LYS:HZ3	2.12	0.60
3:J:133:LYS:HD2	5:R:402:LEU:HD21	1.83	0.60
5:Q:347:THR:O	5:Q:348:ALA:O	2.20	0.60
5:S:402:LEU:O	5:S:403:THR:CB	2.50	0.60
1:O:16:LYS:CE	1:O:340:ARG:O	2.49	0.60
1:P:26:PRO:HD2	1:P:370:CYS:HA	1.82	0.60
3:K:130:VAL:HG13	5:S:401:GLU:OE1	2.00	0.60
5:R:402:LEU:O	5:R:403:THR:CB	2.49	0.60
1:B:272:ARG:HH22	1:P:237:PRO:CD	2.00	0.60
3:K:178:PHE:HA	3:K:224:VAL:C	2.25	0.60
3:K:250:VAL:O	4:G:439:HIS:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:406:ALA:HA	4:H:409:TRP:HD1	1.65	0.60
5:T:410:PHE:CA	5:T:413:SER:CB	2.80	0.60
3:J:250:VAL:CG1	5:R:398:THR:HG22	2.18	0.60
3:L:178:PHE:HA	3:L:224:VAL:C	2.25	0.60
5:S:410:PHE:CA	5:S:413:SER:CB	2.80	0.60
3:L:251:THR:C	4:H:439:HIS:HB3	2.27	0.60
5:Q:410:PHE:HD1	5:Q:417:CYS:CA	2.13	0.60
4:F:399:VAL:CB	5:R:362:LEU:HD11	2.30	0.60
4:F:432:LEU:HB3	4:F:436:PHE:HE2	1.65	0.60
5:S:418:VAL:CG2	5:S:421:THR:H	2.15	0.60
1:O:18:LEU:HB2	1:O:331:HIS:CE1	2.37	0.60
3:I:178:PHE:CE1	3:I:245:TRP:CD1	2.89	0.60
3:J:160:TYR:CE2	5:R:398:THR:OG1	2.54	0.60
3:J:178:PHE:CE1	3:J:245:TRP:CD1	2.89	0.60
5:Q:402:LEU:O	5:Q:403:THR:CB	2.49	0.60
3:L:178:PHE:CE1	3:L:245:TRP:CD1	2.90	0.60
5:Q:407:THR:CA	5:Q:410:PHE:HD2	2.13	0.60
5:R:349:HIS:HE1	5:R:357:LEU:CD1	2.15	0.60
5:R:352:PRO:O	5:R:355:ILE:N	2.35	0.60
5:T:411:LEU:HG	5:T:413:SER:OG	2.01	0.60
4:F:399:VAL:HG23	5:R:362:LEU:HD21	1.81	0.59
4:H:403:SER:CB	4:H:407:MET:CG	2.66	0.59
1:O:24:TYR:CE2	1:O:287:PHE:O	2.55	0.59
1:P:282:ILE:HB	1:P:287:PHE:CZ	2.36	0.59
1:M:291:VAL:HG23	1:O:304:PRO:O	2.01	0.59
1:C:27:SER:HB3	1:D:146:GLN:CG	2.32	0.59
5:Q:351:HIS:HB2	5:Q:352:PRO:CD	2.32	0.59
5:R:407:THR:H	5:R:421:THR:HG22	1.64	0.59
5:S:363:TYR:CB	5:S:364:PRO:CD	2.75	0.59
5:T:402:LEU:O	5:T:403:THR:CB	2.49	0.59
3:I:157:SER:OG	5:Q:397:ILE:CD1	2.47	0.59
5:R:410:PHE:CA	5:R:413:SER:CB	2.80	0.59
4:G:428:LEU:O	4:G:432:LEU:HG	2.02	0.59
5:S:418:VAL:CG1	5:S:419:ARG:N	2.57	0.59
4:H:396:THR:OG1	4:H:397:LEU:N	2.32	0.59
4:H:428:LEU:O	4:H:432:LEU:HG	2.03	0.59
5:T:407:THR:O	5:T:410:PHE:N	2.30	0.59
5:T:418:VAL:CG2	5:T:421:THR:H	2.15	0.59
1:P:26:PRO:C	1:P:329:ALA:CB	2.76	0.59
5:Q:415:LEU:O	5:Q:416:CYS:CB	2.51	0.59
5:T:410:PHE:CD2	5:T:421:THR:CG2	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLN:NE2	1:D:27:SER:HB3	2.17	0.59
1:O:24:TYR:CA	1:O:288:THR:O	2.51	0.59
3:I:221:LYS:HB2	3:I:221:LYS:HZ3	1.68	0.59
3:J:160:TYR:HD2	5:R:397:ILE:HG22	1.67	0.59
5:T:421:THR:O	5:T:422:LYS:HB2	2.02	0.59
1:M:147:TYR:HD2	1:N:192:PHE:O	1.85	0.59
3:I:249:ILE:CG2	4:E:439:HIS:CE1	2.82	0.59
3:L:157:SER:HB2	5:T:397:ILE:CD1	2.32	0.59
5:R:410:PHE:CD2	5:R:421:THR:CG2	2.86	0.59
5:T:373:VAL:O	5:T:377:VAL:HG23	2.03	0.59
1:N:237:PRO:HD2	1:C:314:LYS:HZ3	1.66	0.59
5:Q:349:HIS:CG	5:Q:354:GLU:OE1	2.55	0.59
5:S:410:PHE:O	5:S:411:LEU:HB2	2.03	0.59
4:H:421:VAL:HG11	5:T:388:MET:HG2	1.85	0.59
3:J:117:VAL:HG11	3:J:140:VAL:HG12	1.85	0.59
3:I:159:LYS:CG	4:E:436:PHE:HZ	2.15	0.58
3:I:256:GLU:OE1	3:K:166:GLN:NE2	2.36	0.58
4:E:428:LEU:O	4:E:432:LEU:HG	2.03	0.58
5:S:373:VAL:O	5:S:377:VAL:HG23	2.03	0.58
5:S:410:PHE:CD2	5:S:421:THR:CG2	2.86	0.58
5:T:413:SER:CB	5:T:417:CYS:HB3	2.31	0.58
5:Q:373:VAL:O	5:Q:377:VAL:HG23	2.03	0.58
1:P:18:LEU:CB	1:P:331:HIS:ND1	2.65	0.58
5:Q:418:VAL:HG23	5:Q:421:THR:HG23	1.85	0.58
5:R:373:VAL:O	5:R:377:VAL:HG23	2.03	0.58
5:R:411:LEU:HA	5:R:413:SER:N	2.18	0.58
4:H:403:SER:CA	4:H:407:MET:HG3	2.17	0.58
1:O:26:PRO:HB2	1:O:329:ALA:HB3	1.85	0.58
3:K:250:VAL:C	4:G:439:HIS:CE1	2.81	0.58
3:I:117:VAL:HG11	3:I:140:VAL:HG12	1.85	0.58
3:K:159:LYS:HD3	4:G:432:LEU:CB	2.34	0.58
3:L:117:VAL:HG11	3:L:140:VAL:HG12	1.85	0.58
5:Q:418:VAL:CG2	5:Q:421:THR:H	2.15	0.58
5:R:410:PHE:O	5:R:411:LEU:HB2	2.03	0.58
5:S:421:THR:O	5:S:422:LYS:HB2	2.02	0.58
5:T:411:LEU:HA	5:T:413:SER:N	2.18	0.58
5:S:411:LEU:HA	5:S:413:SER:N	2.19	0.58
1:P:18:LEU:HB3	1:P:331:HIS:CE1	2.39	0.58
3:K:133:LYS:HD3	5:S:402:LEU:CD2	2.33	0.58
5:R:418:VAL:CG2	5:R:421:THR:H	2.15	0.58
5:Q:406:ALA:HB2	5:Q:409:PRO:CG	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:SER:HB2	1:O:293:ALA:HB2	1.86	0.58
3:I:250:VAL:HG21	5:Q:401:GLU:HG3	1.86	0.58
4:E:421:VAL:HG11	5:Q:388:MET:HG2	1.85	0.58
5:Q:410:PHE:CA	5:Q:413:SER:CB	2.80	0.58
4:F:428:LEU:O	4:F:432:LEU:HG	2.03	0.58
5:S:418:VAL:HG23	5:S:421:THR:HG23	1.85	0.58
5:S:418:VAL:HG12	5:S:419:ARG:N	2.19	0.58
4:H:408:SER:O	4:H:412:LYS:HG3	2.04	0.58
4:E:403:SER:CA	4:E:407:MET:HG3	2.17	0.58
5:Q:413:SER:CB	5:Q:417:CYS:HB3	2.31	0.58
4:F:403:SER:CA	4:F:407:MET:HG3	2.17	0.58
5:S:413:SER:HB2	5:S:417:CYS:HB3	1.79	0.58
1:M:41:THR:O	1:N:125:HIS:NE2	2.37	0.57
1:M:125:HIS:CE1	1:N:41:THR:HG22	2.38	0.57
3:K:133:LYS:CD	5:S:402:LEU:CD2	2.80	0.57
3:K:250:VAL:CG2	5:S:401:GLU:CB	2.79	0.57
3:L:159:LYS:HD3	4:H:432:LEU:CB	2.29	0.57
5:Q:410:PHE:CD2	5:Q:421:THR:CG2	2.86	0.57
3:K:117:VAL:HG11	3:K:140:VAL:HG12	1.85	0.57
5:Q:357:LEU:C	5:Q:359:TYR:H	2.11	0.57
4:F:421:VAL:HG11	5:R:388:MET:HG2	1.85	0.57
5:R:349:HIS:HE1	5:R:357:LEU:HD12	1.69	0.57
5:R:418:VAL:HG23	5:R:421:THR:HG23	1.85	0.57
5:R:421:THR:O	5:R:422:LYS:HB2	2.02	0.57
4:G:421:VAL:HG11	5:S:388:MET:HG2	1.85	0.57
5:S:369:VAL:O	5:S:373:VAL:HG23	2.04	0.57
1:O:16:LYS:HE2	1:O:340:ARG:O	2.04	0.57
3:J:160:TYR:HE2	5:R:398:THR:CB	2.08	0.57
4:F:399:VAL:CG2	5:R:362:LEU:CG	2.78	0.57
5:R:410:PHE:HA	5:R:413:SER:HB3	1.85	0.57
5:S:397:ILE:C	5:S:399:PRO:HD2	2.29	0.57
5:T:418:VAL:HG12	5:T:419:ARG:N	2.19	0.57
3:I:159:LYS:HZ3	4:E:432:LEU:HD13	1.69	0.57
3:I:160:TYR:CE2	5:Q:398:THR:CB	2.87	0.57
3:J:162:LEU:CD2	5:R:400:TYR:OH	2.52	0.57
3:K:159:LYS:CD	4:G:432:LEU:HB3	2.35	0.57
4:E:406:ALA:HA	4:E:409:TRP:CD1	2.40	0.57
5:S:415:LEU:O	5:S:416:CYS:CB	2.51	0.57
4:H:406:ALA:HA	4:H:409:TRP:CD1	2.39	0.57
1:M:125:HIS:CE1	1:N:41:THR:CG2	2.81	0.57
1:O:28:VAL:CG2	1:O:330:VAL:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:251:THR:CG2	4:E:439:HIS:CG	2.76	0.57
4:E:408:SER:O	4:E:412:LYS:HG3	2.04	0.57
5:R:418:VAL:HG22	5:R:420:THR:N	2.19	0.57
1:M:206:ARG:HG3	1:M:206:ARG:HH11	1.69	0.57
3:J:162:LEU:HD23	5:R:400:TYR:CE1	2.40	0.57
3:J:202:THR:HG22	3:J:239:ALA:HA	1.87	0.57
3:L:159:LYS:NZ	5:T:394:ARG:O	2.27	0.57
5:Q:418:VAL:HG12	5:Q:419:ARG:N	2.19	0.57
5:T:369:VAL:O	5:T:373:VAL:HG23	2.04	0.57
5:T:418:VAL:HG23	5:T:421:THR:HG23	1.85	0.57
1:N:237:PRO:CB	1:C:314:LYS:HZ1	2.17	0.57
1:P:206:ARG:HG3	1:P:206:ARG:HH11	1.69	0.57
3:L:162:LEU:HD23	5:T:400:TYR:CE1	2.39	0.57
5:Q:410:PHE:O	5:Q:411:LEU:HB2	2.03	0.57
5:R:411:LEU:N	5:R:412:LEU:C	2.63	0.57
5:R:418:VAL:HG12	5:R:419:ARG:N	2.19	0.57
5:T:415:LEU:O	5:T:416:CYS:CB	2.51	0.57
1:M:291:VAL:O	1:M:324:LYS:CE	2.53	0.57
3:I:157:SER:CB	5:Q:397:ILE:CD1	2.83	0.57
5:Q:421:THR:O	5:Q:422:LYS:HB2	2.03	0.57
4:F:405:THR:O	4:F:408:SER:N	2.38	0.57
4:F:408:SER:O	4:F:412:LYS:HG3	2.04	0.57
5:R:397:ILE:C	5:R:399:PRO:HD2	2.29	0.57
5:T:410:PHE:O	5:T:411:LEU:HB2	2.03	0.57
3:K:151:LYS:HA	3:K:151:LYS:CE	2.30	0.57
3:K:202:THR:HG22	3:K:239:ALA:HA	1.86	0.57
5:Q:411:LEU:HA	5:Q:413:SER:N	2.18	0.57
5:R:369:VAL:O	5:R:373:VAL:HG23	2.04	0.57
4:G:406:ALA:HA	4:G:409:TRP:CD1	2.39	0.57
1:N:206:ARG:HH11	1:N:206:ARG:HG3	1.69	0.57
3:L:202:THR:HG22	3:L:239:ALA:HA	1.86	0.57
5:Q:406:ALA:CA	5:Q:407:THR:O	2.53	0.57
4:F:406:ALA:HA	4:F:409:TRP:CD1	2.40	0.57
5:T:363:TYR:CD1	5:T:364:PRO:HD3	2.40	0.57
5:T:397:ILE:C	5:T:399:PRO:HD2	2.29	0.57
1:B:21:ASP:OD2	1:C:143:SER:HB2	2.04	0.56
3:K:182:LYS:HE3	3:K:244:THR:HG21	1.87	0.56
5:S:411:LEU:N	5:S:412:LEU:C	2.63	0.56
5:T:406:ALA:CA	5:T:407:THR:O	2.53	0.56
1:B:142:HIS:CD2	1:D:109:GLU:CG	2.81	0.56
1:O:18:LEU:CB	1:O:331:HIS:ND1	2.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:28:VAL:HG23	1:O:329:ALA:HB1	1.86	0.56
5:Q:418:VAL:HG22	5:Q:420:THR:N	2.19	0.56
1:M:291:VAL:CG1	1:O:304:PRO:HG2	2.35	0.56
1:N:237:PRO:CD	1:C:314:LYS:HZ3	2.19	0.56
1:O:18:LEU:CB	1:O:331:HIS:CE1	2.88	0.56
3:J:182:LYS:HE3	3:J:244:THR:HG21	1.87	0.56
5:Q:407:THR:H	5:Q:421:THR:HG22	1.64	0.56
5:R:407:THR:HG22	5:R:421:THR:HG1	1.70	0.56
5:S:406:ALA:HB2	5:S:409:PRO:CG	2.30	0.56
4:H:405:THR:O	4:H:408:SER:N	2.38	0.56
5:T:406:ALA:HB2	5:T:409:PRO:CG	2.30	0.56
5:T:411:LEU:N	5:T:412:LEU:C	2.63	0.56
3:K:130:VAL:C	5:S:402:LEU:HD12	2.29	0.56
4:E:405:THR:O	4:E:408:SER:N	2.38	0.56
5:Q:397:ILE:C	5:Q:399:PRO:HD2	2.29	0.56
4:G:408:SER:O	4:G:412:LYS:HG3	2.04	0.56
1:M:293:ALA:HB1	1:M:294:PRO:HD3	1.85	0.56
1:B:52:LEU:HD22	1:B:67:LEU:HD21	1.87	0.56
1:D:52:LEU:HD22	1:D:67:LEU:HD21	1.87	0.56
3:L:133:LYS:CE	5:T:402:LEU:HD23	2.35	0.56
5:R:406:ALA:CB	5:R:409:PRO:CG	2.84	0.56
5:T:410:PHE:HA	5:T:413:SER:HB3	1.85	0.56
5:Q:411:LEU:N	5:Q:412:LEU:C	2.63	0.56
4:F:399:VAL:CB	5:R:362:LEU:CD1	2.84	0.56
5:S:406:ALA:CA	5:S:407:THR:O	2.53	0.56
4:H:421:VAL:HG12	5:T:388:MET:SD	2.40	0.56
1:O:206:ARG:HH11	1:O:206:ARG:HG3	1.69	0.56
5:Q:410:PHE:HA	5:Q:413:SER:HB3	1.85	0.56
5:R:408:VAL:HB	5:R:409:PRO:HD3	1.65	0.56
3:J:247:LYS:HG3	3:J:248:ASP:N	2.21	0.56
3:J:248:ASP:CG	3:J:249:ILE:HG13	2.31	0.56
3:K:247:LYS:HG3	3:K:248:ASP:N	2.21	0.56
3:L:248:ASP:CG	3:L:249:ILE:HG13	2.31	0.56
4:G:405:THR:O	4:G:408:SER:N	2.38	0.56
5:T:406:ALA:CB	5:T:409:PRO:CG	2.84	0.56
1:A:52:LEU:HD22	1:A:67:LEU:HD21	1.87	0.56
3:L:162:LEU:CG	5:T:400:TYR:HH	1.99	0.56
3:L:252:LYS:N	4:H:439:HIS:CB	2.59	0.56
5:Q:369:VAL:O	5:Q:373:VAL:HG23	2.04	0.56
5:R:402:LEU:C	5:R:403:THR:CG2	2.64	0.56
5:S:406:ALA:CB	5:S:409:PRO:CG	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:418:VAL:HG22	5:S:420:THR:N	2.19	0.56
3:I:182:LYS:HE3	3:I:244:THR:HG21	1.87	0.56
3:I:247:LYS:HG3	3:I:248:ASP:N	2.21	0.56
3:K:250:VAL:HB	5:S:398:THR:O	2.05	0.56
3:L:182:LYS:HE3	3:L:244:THR:HG21	1.87	0.56
5:S:408:VAL:HB	5:S:409:PRO:HD3	1.65	0.56
5:T:378:LEU:O	5:T:382:VAL:HG23	2.06	0.56
3:K:159:LYS:HG2	4:G:436:PHE:CE2	2.41	0.55
3:L:247:LYS:HG3	3:L:248:ASP:N	2.20	0.55
3:I:248:ASP:CG	3:I:249:ILE:HG13	2.31	0.55
3:K:178:PHE:CD1	3:K:245:TRP:CD2	2.95	0.55
5:Q:406:ALA:CB	5:Q:410:PHE:CE2	2.89	0.55
3:I:202:THR:HG22	3:I:239:ALA:HA	1.87	0.55
5:T:408:VAL:C	5:T:410:PHE:H	2.14	0.55
5:T:418:VAL:HG22	5:T:420:THR:N	2.19	0.55
3:J:178:PHE:CD1	3:J:245:TRP:CD2	2.95	0.55
3:J:248:ASP:OD2	5:R:405:GLY:HA3	2.05	0.55
5:Q:378:LEU:O	5:Q:382:VAL:HG23	2.06	0.55
5:R:406:ALA:CB	5:R:410:PHE:CE2	2.89	0.55
5:S:406:ALA:CB	5:S:410:PHE:CE2	2.89	0.55
1:O:24:TYR:HB3	1:O:288:THR:O	2.06	0.55
4:H:403:SER:HG	4:H:407:MET:CG	2.20	0.55
3:L:133:LYS:CB	5:T:402:LEU:HG	2.35	0.55
5:R:378:LEU:O	5:R:382:VAL:HG23	2.06	0.55
5:S:378:LEU:O	5:S:382:VAL:HG23	2.06	0.55
5:R:406:ALA:HB2	5:R:409:PRO:CG	2.30	0.55
5:S:407:THR:H	5:S:421:THR:HG22	1.64	0.55
4:F:399:VAL:HG22	5:R:362:LEU:CD1	2.08	0.55
5:T:362:LEU:HD12	5:T:366:MET:HE2	1.87	0.55
1:A:280:LYS:HG3	5:Q:343:SER:CB	2.37	0.55
3:K:248:ASP:CG	3:K:249:ILE:HG13	2.31	0.55
1:O:16:LYS:HZ1	1:O:340:ARG:HA	1.67	0.54
5:Q:406:ALA:CB	5:Q:409:PRO:CG	2.84	0.54
5:T:413:SER:HB2	5:T:417:CYS:HB3	1.79	0.54
3:J:160:TYR:CE1	4:F:436:PHE:CD1	2.95	0.54
3:J:170:HIS:HB3	3:L:122:LYS:HD3	1.89	0.54
3:L:178:PHE:CD1	3:L:245:TRP:CD2	2.95	0.54
3:I:178:PHE:CD1	3:I:245:TRP:CD2	2.95	0.54
5:Q:408:VAL:C	5:Q:410:PHE:H	2.14	0.54
1:O:16:LYS:HZ1	1:O:340:ARG:CA	2.19	0.54
1:C:52:LEU:HD22	1:C:67:LEU:HD21	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:406:ALA:CB	5:T:410:PHE:CE2	2.89	0.54
1:P:282:ILE:HB	1:P:287:PHE:HZ	1.72	0.54
3:J:133:LYS:N	5:R:402:LEU:HD11	1.91	0.54
4:E:405:THR:O	4:E:406:ALA:C	2.51	0.54
4:E:432:LEU:C	4:E:436:PHE:CD2	2.86	0.54
4:F:405:THR:O	4:F:406:ALA:C	2.51	0.54
5:R:408:VAL:C	5:R:410:PHE:H	2.15	0.54
3:J:159:LYS:HD3	4:F:432:LEU:HB2	1.79	0.54
4:E:421:VAL:CG1	5:Q:388:MET:HG2	2.38	0.54
5:S:406:ALA:CB	5:S:409:PRO:CD	2.34	0.54
3:I:159:LYS:NZ	4:E:432:LEU:HD22	2.22	0.54
4:F:406:ALA:CA	4:F:409:TRP:HD1	2.21	0.54
5:S:410:PHE:HA	5:S:413:SER:HB3	1.85	0.54
1:M:291:VAL:CG1	1:O:304:PRO:CG	2.86	0.54
5:T:349:HIS:N	5:T:354:GLU:OE1	2.40	0.54
1:P:18:LEU:CD2	1:P:331:HIS:ND1	2.71	0.53
4:E:406:ALA:CA	4:E:409:TRP:HD1	2.21	0.53
1:O:25:SER:HB2	1:O:293:ALA:CB	2.38	0.53
1:P:24:TYR:HA	1:P:288:THR:O	2.08	0.53
3:I:160:TYR:OH	5:Q:398:THR:HG21	2.03	0.53
3:J:248:ASP:OD1	3:J:249:ILE:HG13	2.08	0.53
4:F:432:LEU:C	4:F:436:PHE:CD2	2.86	0.53
5:S:408:VAL:C	5:S:410:PHE:H	2.14	0.53
3:I:248:ASP:OD1	3:I:249:ILE:HG13	2.09	0.53
3:L:251:THR:HA	4:H:439:HIS:CD2	2.03	0.53
4:F:421:VAL:HG12	5:R:388:MET:SD	2.40	0.53
5:S:406:ALA:CB	5:S:407:THR:C	2.79	0.53
4:H:432:LEU:C	4:H:436:PHE:CD2	2.86	0.53
5:T:351:HIS:C	5:T:355:ILE:HD12	2.34	0.53
1:A:280:LYS:CG	5:Q:343:SER:HB3	2.37	0.53
1:P:28:VAL:HB	1:P:342:ALA:HB1	1.90	0.53
5:T:351:HIS:CB	5:T:352:PRO:CD	2.67	0.53
3:K:130:VAL:CG1	5:S:401:GLU:CD	2.82	0.53
3:K:159:LYS:NZ	5:S:394:ARG:CB	2.44	0.53
3:I:157:SER:CB	5:Q:397:ILE:HD12	2.38	0.53
5:R:349:HIS:CD2	5:R:354:GLU:C	2.62	0.53
1:M:41:THR:HG21	1:N:123:ARG:O	2.09	0.53
3:L:159:LYS:C	4:H:436:PHE:CE1	2.82	0.53
4:G:421:VAL:HG12	5:S:388:MET:SD	2.40	0.53
5:Q:398:THR:CB	5:Q:399:PRO:CD	2.87	0.53
4:G:432:LEU:C	4:G:436:PHE:CD2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:HIS:N	1:N:125:HIS:CD2	2.76	0.53
3:I:221:LYS:HB2	3:I:221:LYS:HZ2	1.72	0.53
5:T:398:THR:CB	5:T:399:PRO:CD	2.87	0.53
1:M:125:HIS:CD2	1:N:125:HIS:N	2.76	0.52
3:J:252:LYS:H	4:F:439:HIS:HB2	1.74	0.52
3:K:159:LYS:CE	5:S:394:ARG:CB	2.79	0.52
5:R:398:THR:CB	5:R:399:PRO:CD	2.87	0.52
4:G:406:ALA:CA	4:G:409:TRP:HD1	2.21	0.52
5:T:398:THR:C	5:T:400:TYR:H	2.16	0.52
3:L:248:ASP:OD1	3:L:249:ILE:HG13	2.09	0.52
5:Q:400:TYR:CD1	5:Q:401:GLU:N	2.78	0.52
5:R:403:THR:HB	5:R:404:PRO:HD2	1.91	0.52
4:H:406:ALA:CA	4:H:409:TRP:HD1	2.21	0.52
5:T:358:TYR:O	5:T:361:GLU:N	2.32	0.52
5:T:400:TYR:CD1	5:T:401:GLU:N	2.78	0.52
1:O:28:VAL:HB	1:O:342:ALA:C	2.34	0.52
5:Q:400:TYR:CD1	5:Q:400:TYR:C	2.87	0.52
5:R:400:TYR:CD1	5:R:401:GLU:N	2.78	0.52
1:B:94:THR:HG22	1:D:24:GLU:CD	2.24	0.52
5:Q:403:THR:HB	5:Q:404:PRO:HD2	1.91	0.52
3:I:130:VAL:O	5:Q:402:LEU:CD1	2.42	0.52
5:R:349:HIS:C	5:R:354:GLU:HB2	2.31	0.52
5:T:407:THR:H	5:T:421:THR:HG22	1.64	0.52
3:I:151:LYS:HA	3:I:151:LYS:CE	2.30	0.52
3:I:221:LYS:HZ1	3:I:223:ARG:CZ	2.22	0.52
3:K:159:LYS:HE2	4:G:432:LEU:HD13	1.81	0.52
3:K:160:TYR:HE2	5:S:398:THR:H	0.58	0.52
3:K:248:ASP:OD1	3:K:249:ILE:HG13	2.09	0.52
5:Q:398:THR:C	5:Q:400:TYR:H	2.16	0.52
5:S:406:ALA:HB2	5:S:409:PRO:HD2	0.61	0.52
4:E:432:LEU:C	4:E:436:PHE:HD2	2.18	0.52
5:S:398:THR:C	5:S:400:TYR:H	2.16	0.52
1:M:147:TYR:CE2	1:N:192:PHE:CB	2.87	0.52
3:L:160:TYR:CE2	5:T:398:THR:N	2.76	0.52
3:L:246:ASN:HB2	3:L:249:ILE:O	2.10	0.52
5:R:351:HIS:CB	5:R:352:PRO:HD3	2.20	0.52
5:S:400:TYR:CD1	5:S:401:GLU:N	2.78	0.52
4:H:432:LEU:C	4:H:436:PHE:HD2	2.18	0.52
5:T:407:THR:CA	5:T:410:PHE:CD2	2.92	0.52
1:A:280:LYS:CG	5:Q:343:SER:CB	2.88	0.52
3:J:130:VAL:HG12	3:J:135:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:160:TYR:CE2	5:R:398:THR:CA	2.93	0.52
3:J:251:THR:HG22	3:J:252:LYS:H	1.75	0.52
4:E:396:THR:OG1	4:E:397:LEU:CD2	2.46	0.52
5:R:356:ILE:HG23	5:R:359:TYR:CE2	2.45	0.52
5:S:398:THR:CB	5:S:399:PRO:CD	2.87	0.52
5:S:400:TYR:CD1	5:S:400:TYR:C	2.87	0.52
5:S:403:THR:HB	5:S:404:PRO:HD2	1.91	0.52
4:H:405:THR:O	4:H:406:ALA:C	2.51	0.52
5:T:397:ILE:O	5:T:399:PRO:N	2.43	0.52
5:T:401:GLU:C	5:T:402:LEU:HG	2.34	0.52
1:M:18:LEU:HD21	1:M:368:GLN:HE22	1.72	0.52
5:R:397:ILE:O	5:R:399:PRO:N	2.43	0.52
5:R:400:TYR:CD1	5:R:400:TYR:C	2.87	0.52
4:G:432:LEU:C	4:G:436:PHE:HD2	2.18	0.52
3:I:234:GLU:O	3:K:173:SER:N	2.42	0.51
5:Q:407:THR:O	5:Q:408:VAL:C	2.54	0.51
5:R:407:THR:CA	5:R:410:PHE:CD2	2.92	0.51
1:O:26:PRO:C	1:O:329:ALA:HB2	2.34	0.51
3:I:246:ASN:HB2	3:I:249:ILE:O	2.10	0.51
3:I:251:THR:HG22	3:I:252:LYS:H	1.75	0.51
3:J:160:TYR:CE1	5:R:398:THR:HG23	2.30	0.51
4:F:432:LEU:C	4:F:436:PHE:HD2	2.18	0.51
3:K:157:SER:HA	5:S:397:ILE:HD12	1.76	0.51
5:Q:397:ILE:O	5:Q:399:PRO:N	2.43	0.51
4:G:403:SER:CA	4:G:407:MET:HG3	2.17	0.51
4:G:405:THR:O	4:G:406:ALA:C	2.51	0.51
1:M:38:LEU:HB2	1:M:268:ALA:HB3	1.93	0.51
1:A:276:VAL:HG22	1:A:285:MET:HG2	1.93	0.51
3:J:133:LYS:HD2	5:R:402:LEU:CD2	2.40	0.51
3:J:252:LYS:H	4:F:439:HIS:CB	2.23	0.51
3:K:130:VAL:HG12	3:K:135:MET:HG3	1.92	0.51
5:R:398:THR:C	5:R:400:TYR:H	2.16	0.51
5:S:349:HIS:CG	5:S:355:ILE:N	2.78	0.51
1:M:291:VAL:HG21	1:O:304:PRO:CG	2.22	0.51
3:I:160:TYR:HD2	5:Q:397:ILE:HG22	1.72	0.51
3:I:164:CYS:SG	5:Q:400:TYR:CD2	3.04	0.51
3:J:246:ASN:HB2	3:J:249:ILE:O	2.10	0.51
5:Q:407:THR:CA	5:Q:410:PHE:CD2	2.92	0.51
4:H:399:VAL:HB	5:T:366:MET:CE	2.39	0.51
3:J:124:MET:O	3:J:211:GLY:HA2	2.11	0.51
5:R:349:HIS:HA	5:R:354:GLU:HB2	1.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:397:ILE:O	5:S:399:PRO:N	2.43	0.51
3:J:252:LYS:N	4:F:439:HIS:HB3	2.25	0.51
3:L:130:VAL:HG12	3:L:135:MET:HG3	1.92	0.51
5:Q:408:VAL:HG11	5:Q:409:PRO:HD3	1.83	0.51
5:T:403:THR:HB	5:T:404:PRO:HD2	1.91	0.51
5:T:406:ALA:HB2	5:T:409:PRO:HD2	0.61	0.51
1:O:24:TYR:CG	1:O:288:THR:O	2.64	0.51
3:I:251:THR:OG1	4:E:439:HIS:CG	2.63	0.51
3:K:246:ASN:HB2	3:K:249:ILE:O	2.10	0.51
3:K:251:THR:HG22	3:K:252:LYS:H	1.75	0.51
3:L:124:MET:O	3:L:211:GLY:HA2	2.11	0.51
3:L:221:LYS:NZ	3:L:221:LYS:CB	2.71	0.51
3:L:252:LYS:H	4:H:439:HIS:HB2	1.73	0.51
5:R:406:ALA:CA	5:R:407:THR:O	2.53	0.51
5:R:418:VAL:HA	5:R:420:THR:N	2.26	0.51
5:T:356:ILE:HG23	5:T:359:TYR:CE2	2.45	0.51
1:O:21:ARG:HB2	1:O:287:PHE:CE1	2.45	0.51
3:I:124:MET:O	3:I:211:GLY:HA2	2.11	0.51
3:J:244:THR:HG22	3:J:245:TRP:N	2.26	0.51
3:K:178:PHE:HB2	3:K:245:TRP:CZ3	2.46	0.51
5:S:354:GLU:HA	5:S:357:LEU:CD1	2.41	0.51
5:T:400:TYR:CD1	5:T:400:TYR:C	2.87	0.51
1:M:110:LYS:HG3	1:M:213:VAL:HG11	1.93	0.50
1:O:38:LEU:HB2	1:O:268:ALA:HB3	1.93	0.50
3:J:221:LYS:NZ	3:J:221:LYS:CB	2.71	0.50
3:L:178:PHE:C	3:L:179:THR:HG22	2.37	0.50
4:G:399:VAL:HG13	5:S:362:LEU:HD12	1.87	0.50
1:O:16:LYS:HZ3	1:O:340:ARG:CA	2.22	0.50
1:O:28:VAL:O	1:O:342:ALA:HB1	2.10	0.50
5:R:354:GLU:HA	5:R:357:LEU:CD1	2.41	0.50
1:P:38:LEU:HB2	1:P:268:ALA:HB3	1.93	0.50
5:T:394:ARG:HA	5:T:397:ILE:CG1	2.41	0.50
5:T:418:VAL:HA	5:T:420:THR:N	2.26	0.50
1:M:291:VAL:HG13	1:O:304:PRO:CG	2.42	0.50
1:P:282:ILE:HG22	1:P:287:PHE:CE2	2.47	0.50
3:K:122:LYS:CG	3:L:170:HIS:CB	2.89	0.50
3:L:182:LYS:CE	3:L:244:THR:HG21	2.42	0.50
3:L:244:THR:HG22	3:L:245:TRP:N	2.26	0.50
1:C:27:SER:CB	1:D:146:GLN:CD	2.84	0.50
1:O:110:LYS:HG3	1:O:213:VAL:HG11	1.93	0.50
3:I:130:VAL:HG12	3:I:135:MET:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:178:PHE:HB2	3:I:245:TRP:CZ3	2.46	0.50
3:I:182:LYS:CE	3:I:244:THR:HG21	2.42	0.50
3:J:178:PHE:HB2	3:J:245:TRP:CZ3	2.46	0.50
3:K:124:MET:O	3:K:211:GLY:HA2	2.11	0.50
3:K:159:LYS:HZ1	4:G:432:LEU:HD11	1.74	0.50
5:Q:418:VAL:HA	5:Q:420:THR:N	2.26	0.50
1:P:110:LYS:HG3	1:P:213:VAL:HG11	1.93	0.50
3:I:178:PHE:HA	3:I:224:VAL:CA	2.42	0.50
5:Q:394:ARG:HA	5:Q:397:ILE:CG1	2.41	0.50
5:Q:402:LEU:O	5:Q:403:THR:OG1	2.30	0.50
4:F:421:VAL:CG1	5:R:388:MET:HG2	2.38	0.50
5:R:407:THR:HA	5:R:421:THR:CG2	2.37	0.50
5:S:394:ARG:HA	5:S:397:ILE:CG1	2.41	0.50
5:T:407:THR:O	5:T:408:VAL:C	2.54	0.50
1:B:276:VAL:HG22	1:B:285:MET:HG2	1.93	0.50
1:N:38:LEU:HB2	1:N:268:ALA:HB3	1.93	0.50
1:O:1:TYR:HB3	1:O:287:PHE:CZ	2.47	0.50
3:I:178:PHE:C	3:I:179:THR:HG22	2.37	0.50
3:L:159:LYS:HZ2	4:H:432:LEU:CB	2.22	0.50
3:L:160:TYR:HE2	5:T:398:THR:N	2.04	0.50
4:E:421:VAL:HG12	5:Q:388:MET:SD	2.40	0.50
5:S:413:SER:OG	5:S:417:CYS:HB3	2.12	0.50
5:S:418:VAL:HA	5:S:420:THR:N	2.26	0.50
5:T:417:CYS:O	5:T:420:THR:OG1	2.30	0.50
3:K:178:PHE:HA	3:K:224:VAL:CA	2.42	0.50
3:K:178:PHE:HD1	3:K:179:THR:H	1.59	0.50
3:L:160:TYR:HE2	5:T:398:THR:H	1.59	0.50
3:L:178:PHE:HA	3:L:224:VAL:CA	2.42	0.50
5:Q:401:GLU:C	5:Q:402:LEU:HG	2.34	0.50
5:S:417:CYS:C	5:S:420:THR:HG1	2.19	0.50
5:T:410:PHE:HA	5:T:413:SER:HB2	1.93	0.50
5:T:413:SER:OG	5:T:417:CYS:HB3	2.12	0.50
1:D:276:VAL:HG22	1:D:285:MET:HG2	1.93	0.50
3:I:159:LYS:NZ	5:Q:394:ARG:C	2.69	0.50
3:K:178:PHE:C	3:K:179:THR:HG22	2.36	0.50
3:L:178:PHE:HB2	3:L:245:TRP:CZ3	2.46	0.50
4:E:403:SER:HG	4:E:407:MET:CG	2.25	0.50
5:Q:413:SER:OG	5:Q:417:CYS:HB3	2.12	0.50
5:Q:417:CYS:O	5:Q:420:THR:HG23	2.11	0.50
5:S:407:THR:O	5:S:408:VAL:C	2.54	0.50
3:K:182:LYS:CE	3:K:244:THR:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:244:THR:HG22	3:K:245:TRP:N	2.26	0.49
3:L:178:PHE:HD1	3:L:179:THR:H	1.59	0.49
5:Q:396:CYS:O	5:Q:397:ILE:O	2.30	0.49
5:Q:410:PHE:HA	5:Q:413:SER:HB2	1.93	0.49
5:T:408:VAL:HG11	5:T:409:PRO:HD3	1.84	0.49
1:C:276:VAL:HG22	1:C:285:MET:HG2	1.93	0.49
3:J:178:PHE:C	3:J:179:THR:HG22	2.37	0.49
3:L:162:LEU:HB3	5:T:400:TYR:CZ	2.37	0.49
5:R:406:ALA:CA	5:R:410:PHE:HD2	2.25	0.49
1:M:126:THR:CG2	1:N:175:ASN:HD21	2.25	0.49
5:Q:406:ALA:HB2	5:Q:409:PRO:HD2	0.61	0.49
5:R:410:PHE:HA	5:R:413:SER:HB2	1.93	0.49
4:G:397:LEU:N	4:G:397:LEU:CD2	2.74	0.49
5:S:407:THR:CA	5:S:410:PHE:CD2	2.92	0.49
5:S:410:PHE:CG	5:S:421:THR:HG21	2.48	0.49
1:N:110:LYS:HG3	1:N:213:VAL:HG11	1.93	0.49
3:I:244:THR:HG22	3:I:245:TRP:N	2.26	0.49
5:Q:407:THR:H	5:Q:421:THR:HB	1.77	0.49
5:R:396:CYS:O	5:R:397:ILE:O	2.30	0.49
5:R:417:CYS:O	5:R:420:THR:OG1	2.30	0.49
5:T:418:VAL:HG13	5:T:419:ARG:HA	0.60	0.49
1:O:28:VAL:HB	1:O:342:ALA:CA	2.42	0.49
3:I:157:SER:CA	5:Q:397:ILE:HD12	2.43	0.49
3:I:159:LYS:CG	4:E:436:PHE:CZ	2.94	0.49
3:J:133:LYS:HB2	5:R:401:GLU:OE2	2.12	0.49
3:J:178:PHE:HA	3:J:224:VAL:CA	2.42	0.49
5:R:407:THR:O	5:R:408:VAL:C	2.54	0.49
1:O:18:LEU:HD22	1:O:331:HIS:CB	2.43	0.49
3:J:182:LYS:CE	3:J:244:THR:HG21	2.42	0.49
5:R:409:PRO:O	5:R:412:LEU:O	2.31	0.49
5:S:396:CYS:O	5:S:397:ILE:O	2.30	0.49
5:T:402:LEU:O	5:T:403:THR:OG1	2.30	0.49
1:B:21:ASP:OD2	1:C:143:SER:HB3	2.11	0.49
1:O:18:LEU:HD21	1:O:368:GLN:NE2	2.27	0.49
1:P:23:GLY:HA2	1:P:290:VAL:CG2	2.42	0.49
3:K:122:LYS:HZ1	3:L:169:VAL:CG2	2.11	0.49
5:Q:406:ALA:CA	5:Q:410:PHE:HD2	2.25	0.49
5:R:410:PHE:CG	5:R:421:THR:HG21	2.48	0.49
1:B:142:HIS:HE1	1:D:109:GLU:CD	2.17	0.49
3:I:157:SER:HA	5:Q:397:ILE:HD12	1.95	0.49
5:T:356:ILE:CB	5:T:359:TYR:HE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:396:CYS:O	5:T:397:ILE:O	2.30	0.49
3:J:151:LYS:HE2	3:J:151:LYS:CA	2.33	0.49
3:J:252:LYS:N	4:F:439:HIS:CB	2.76	0.49
3:L:178:PHE:HZ	5:T:403:THR:CB	2.18	0.49
5:Q:407:THR:HA	5:Q:421:THR:CG2	2.37	0.49
5:R:413:SER:OG	5:R:417:CYS:HB3	2.12	0.49
5:T:409:PRO:O	5:T:412:LEU:O	2.31	0.49
5:T:410:PHE:CG	5:T:421:THR:HG21	2.48	0.49
1:M:291:VAL:O	1:M:324:LYS:HE3	2.13	0.49
1:M:293:ALA:CB	1:M:294:PRO:CD	2.78	0.49
3:K:248:ASP:CG	5:S:405:GLY:CA	2.73	0.49
3:L:137:PRO:HB2	3:L:140:VAL:HG23	1.95	0.49
5:R:394:ARG:HA	5:R:397:ILE:CG1	2.41	0.49
5:R:406:ALA:HB2	5:R:409:PRO:HD2	0.61	0.49
5:S:407:THR:HA	5:S:421:THR:CG2	2.37	0.49
5:S:409:PRO:O	5:S:412:LEU:O	2.31	0.49
1:M:291:VAL:HG21	1:O:305:ALA:N	2.28	0.48
3:J:133:LYS:H	5:R:402:LEU:CD1	2.26	0.48
5:Q:409:PRO:O	5:Q:412:LEU:O	2.31	0.48
5:Q:410:PHE:CG	5:Q:421:THR:HG21	2.48	0.48
1:O:24:TYR:N	1:O:290:VAL:HG23	2.24	0.48
5:T:406:ALA:CA	5:T:410:PHE:HD2	2.25	0.48
1:M:152:HIS:CA	1:N:194:ALA:CB	2.59	0.48
3:I:160:TYR:CD2	5:Q:398:THR:HA	2.46	0.48
4:E:397:LEU:N	4:E:397:LEU:CD2	2.74	0.48
1:M:41:THR:O	1:N:125:HIS:CE1	2.66	0.48
1:N:28:VAL:HG23	1:N:329:ALA:HB1	1.95	0.48
3:I:157:SER:CB	5:Q:397:ILE:HD13	2.43	0.48
3:I:250:VAL:HG21	5:Q:401:GLU:HB2	1.94	0.48
3:J:162:LEU:HD23	5:R:400:TYR:HE1	1.78	0.48
3:L:178:PHE:HE2	5:T:403:THR:HG22	1.74	0.48
5:R:402:LEU:O	5:R:403:THR:OG1	2.30	0.48
5:R:408:VAL:HG11	5:R:409:PRO:HD3	1.84	0.48
5:R:410:PHE:CG	5:R:421:THR:CG2	2.97	0.48
3:I:159:LYS:HZ3	4:E:432:LEU:CD1	2.27	0.48
3:J:137:PRO:HB2	3:J:140:VAL:HG23	1.95	0.48
5:R:367:THR:C	5:R:369:VAL:N	2.72	0.48
5:S:407:THR:H	5:S:421:THR:HB	1.77	0.48
5:T:416:CYS:SG	5:T:418:VAL:C	2.97	0.48
3:L:133:LYS:HE2	5:T:402:LEU:HD23	1.95	0.48
3:L:160:TYR:CD2	5:T:398:THR:CA	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:361:GLU:H	5:Q:361:GLU:HG3	1.51	0.48
5:Q:416:CYS:SG	5:Q:418:VAL:C	2.97	0.48
5:Q:417:CYS:O	5:Q:420:THR:OG1	2.30	0.48
5:R:367:THR:HA	5:R:370:ILE:HD12	1.94	0.48
5:R:416:CYS:SG	5:R:418:VAL:C	2.97	0.48
5:S:410:PHE:CG	5:S:421:THR:CG2	2.97	0.48
3:I:157:SER:CA	5:Q:397:ILE:CD1	2.91	0.48
3:K:137:PRO:HB2	3:K:140:VAL:HG23	1.95	0.48
5:Q:352:PRO:HG2	5:Q:353:HIS:H	1.78	0.48
5:Q:406:ALA:CB	5:Q:407:THR:C	2.79	0.48
5:R:397:ILE:CG2	5:R:398:THR:N	2.64	0.48
5:R:407:THR:H	5:R:421:THR:HB	1.77	0.48
4:G:396:THR:OG1	4:G:397:LEU:CD2	2.46	0.48
5:T:406:ALA:CA	5:T:410:PHE:CD2	2.97	0.48
5:R:358:TYR:O	5:R:361:GLU:N	2.46	0.48
5:S:402:LEU:O	5:S:403:THR:OG1	2.30	0.48
5:S:406:ALA:CA	5:S:410:PHE:CD2	2.97	0.48
1:M:41:THR:C	1:N:43:SER:HB2	2.29	0.48
1:B:25:GLY:O	1:C:144:ARG:O	2.30	0.48
1:M:28:VAL:HG23	1:M:329:ALA:HB1	1.96	0.48
3:J:133:LYS:CD	5:R:402:LEU:CD2	2.92	0.48
5:S:416:CYS:SG	5:S:418:VAL:C	2.97	0.48
1:M:293:ALA:C	1:M:324:LYS:HE2	2.34	0.47
5:Q:350:GLY:HA2	5:Q:351:HIS:HA	1.69	0.47
4:F:396:THR:OG1	4:F:397:LEU:CD2	2.46	0.47
4:F:426:LEU:O	4:F:430:VAL:HG23	2.14	0.47
5:R:417:CYS:O	5:R:420:THR:HG23	2.12	0.47
5:S:397:ILE:CG2	5:S:398:THR:H	2.24	0.47
5:S:406:ALA:CA	5:S:410:PHE:HD2	2.25	0.47
5:S:410:PHE:HA	5:S:413:SER:HB2	1.93	0.47
5:T:417:CYS:O	5:T:420:THR:HG23	2.12	0.47
3:J:178:PHE:HZ	5:R:403:THR:HG22	1.54	0.47
5:Q:354:GLU:HA	5:Q:357:LEU:CD1	2.41	0.47
5:T:410:PHE:CG	5:T:421:THR:CG2	2.97	0.47
1:O:196:ARG:HH21	1:D:275:THR:HG21	1.79	0.47
3:I:137:PRO:HB2	3:I:140:VAL:HG23	1.95	0.47
3:I:151:LYS:HE2	3:I:151:LYS:CA	2.33	0.47
3:J:133:LYS:N	5:R:402:LEU:CD1	2.69	0.47
4:H:396:THR:OG1	4:H:397:LEU:CD2	2.46	0.47
3:L:135:MET:HG2	5:T:401:GLU:OE2	2.13	0.47
5:Q:410:PHE:CG	5:Q:421:THR:CG2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:362:LEU:HB3	5:T:363:TYR:H	1.58	0.47
3:J:178:PHE:O	3:J:179:THR:HG22	2.15	0.47
3:K:221:LYS:NZ	3:K:221:LYS:CB	2.71	0.47
5:S:418:VAL:HG22	5:S:421:THR:N	2.27	0.47
4:E:426:LEU:O	4:E:430:VAL:HG23	2.14	0.47
5:Q:407:THR:CA	5:Q:421:THR:CG2	2.82	0.47
4:F:405:THR:OG1	4:F:406:ALA:N	2.46	0.47
5:T:354:GLU:HA	5:T:357:LEU:CD1	2.41	0.47
5:T:363:TYR:CB	5:T:364:PRO:CD	2.92	0.47
1:P:28:VAL:HG11	1:P:342:ALA:HA	1.96	0.47
3:I:250:VAL:HG21	5:Q:401:GLU:CB	2.44	0.47
3:L:151:LYS:HE2	3:L:151:LYS:CA	2.33	0.47
3:L:184:GLU:HG2	3:L:197:SER:HA	1.97	0.47
4:F:433:CYS:HA	4:F:436:PHE:HD2	1.79	0.47
5:R:363:TYR:CB	5:R:364:PRO:CD	2.83	0.47
5:S:365:THR:C	5:S:366:MET:CG	2.84	0.47
1:O:23:GLY:HA2	1:O:290:VAL:HG23	1.96	0.47
3:K:159:LYS:HD2	4:G:432:LEU:HD22	1.95	0.47
3:K:184:GLU:HG2	3:K:197:SER:HA	1.97	0.47
3:K:250:VAL:O	4:G:439:HIS:NE2	2.45	0.47
4:E:435:SER:O	4:E:439:HIS:CD2	2.68	0.47
4:G:399:VAL:HG22	5:S:362:LEU:CG	2.40	0.47
4:G:403:SER:C	4:G:407:MET:HG3	2.36	0.47
4:G:435:SER:O	4:G:439:HIS:CD2	2.68	0.47
4:H:403:SER:C	4:H:407:MET:HG3	2.36	0.47
4:H:426:LEU:O	4:H:430:VAL:HG23	2.14	0.47
3:J:160:TYR:OH	5:R:398:THR:HG21	2.14	0.47
3:J:184:GLU:HG2	3:J:197:SER:HA	1.97	0.47
4:F:435:SER:O	4:F:439:HIS:CD2	2.68	0.47
5:R:356:ILE:CB	5:R:359:TYR:CE2	2.98	0.47
5:S:407:THR:HA	5:S:410:PHE:HB2	1.96	0.47
5:S:417:CYS:O	5:S:420:THR:OG1	2.30	0.47
3:I:178:PHE:CZ	5:Q:403:THR:HG22	2.49	0.47
3:I:178:PHE:O	3:I:179:THR:HG22	2.14	0.47
5:Q:407:THR:HA	5:Q:410:PHE:HB2	1.96	0.47
5:R:344:THR:O	5:R:344:THR:HG22	2.15	0.47
5:R:354:GLU:O	5:R:357:LEU:N	2.48	0.47
5:R:356:ILE:CB	5:R:359:TYR:HE2	2.26	0.47
5:R:406:ALA:CA	5:R:410:PHE:CD2	2.97	0.47
4:G:433:CYS:HA	4:G:436:PHE:HD2	1.79	0.47
5:T:354:GLU:O	5:T:357:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:28:VAL:HG12	1:O:342:ALA:CB	2.45	0.46
3:J:251:THR:HG22	3:J:252:LYS:N	2.30	0.46
3:L:178:PHE:O	3:L:179:THR:HG22	2.14	0.46
4:G:405:THR:OG1	4:G:406:ALA:N	2.46	0.46
4:H:435:SER:O	4:H:439:HIS:CD2	2.68	0.46
3:L:162:LEU:C	5:T:400:TYR:OH	2.58	0.46
5:Q:417:CYS:C	5:Q:420:THR:HG1	2.22	0.46
5:R:407:THR:HA	5:R:410:PHE:HB2	1.96	0.46
3:K:251:THR:HG22	3:K:252:LYS:N	2.30	0.46
4:G:426:LEU:O	4:G:430:VAL:HG23	2.15	0.46
5:S:365:THR:O	5:S:366:MET:SD	2.74	0.46
4:H:433:CYS:HA	4:H:436:PHE:HD2	1.79	0.46
5:T:407:THR:HA	5:T:410:PHE:HB2	1.96	0.46
1:C:25:GLY:CA	1:D:144:ARG:HB3	2.45	0.46
1:O:18:LEU:HB3	1:O:331:HIS:CE1	2.51	0.46
3:K:178:PHE:O	3:K:179:THR:HG22	2.14	0.46
4:F:397:LEU:N	4:F:397:LEU:CD2	2.74	0.46
5:R:418:VAL:CA	5:R:419:ARG:C	2.87	0.46
5:S:418:VAL:HG13	5:S:419:ARG:HA	0.60	0.46
5:T:397:ILE:CG2	5:T:398:THR:H	2.24	0.46
3:J:199:GLY:O	3:J:200:ARG:HG3	2.16	0.46
5:Q:354:GLU:O	5:Q:357:LEU:N	2.48	0.46
5:Q:406:ALA:CA	5:Q:410:PHE:CD2	2.97	0.46
3:I:251:THR:OG1	4:E:439:HIS:HB3	2.16	0.46
5:R:401:GLU:C	5:R:402:LEU:HG	2.34	0.46
5:T:356:ILE:HG23	5:T:359:TYR:CD2	2.51	0.46
1:B:146:GLN:CD	1:D:27:SER:HB3	2.40	0.46
3:I:160:TYR:CE2	5:Q:397:ILE:CG2	2.95	0.46
3:I:199:GLY:O	3:I:200:ARG:HG3	2.15	0.46
3:I:251:THR:HG22	3:I:252:LYS:N	2.31	0.46
3:J:151:LYS:HA	3:J:151:LYS:CE	2.30	0.46
3:K:122:LYS:HZ3	3:L:169:VAL:CG2	2.25	0.46
3:K:151:LYS:HE2	3:K:151:LYS:CA	2.33	0.46
4:E:433:CYS:HA	4:E:436:PHE:HD2	1.79	0.46
5:Q:411:LEU:H	5:Q:413:SER:HB3	1.75	0.46
5:R:356:ILE:HG23	5:R:359:TYR:CD2	2.51	0.46
5:R:415:LEU:O	5:R:416:CYS:CB	2.51	0.46
5:T:356:ILE:CB	5:T:359:TYR:CE2	2.98	0.46
5:T:419:ARG:C	5:T:420:THR:CG2	2.86	0.46
3:J:170:HIS:CG	3:L:122:LYS:HD3	2.51	0.46
5:R:372:SER:O	5:R:376:PHE:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:418:VAL:HG13	5:R:419:ARG:HA	0.61	0.46
5:S:401:GLU:C	5:S:402:LEU:HG	2.33	0.46
5:S:417:CYS:O	5:S:420:THR:HG23	2.12	0.46
1:M:152:HIS:HB2	1:N:194:ALA:HB2	1.87	0.46
1:B:142:HIS:CD2	1:D:109:GLU:HB2	2.50	0.46
3:L:160:TYR:HD2	5:T:397:ILE:HG22	1.81	0.46
3:L:199:GLY:O	3:L:200:ARG:HG3	2.15	0.46
5:Q:416:CYS:SG	5:Q:420:THR:HG23	2.56	0.46
4:F:403:SER:HG	4:F:407:MET:CG	2.27	0.46
5:R:351:HIS:C	5:R:355:ILE:CD1	2.87	0.46
5:T:407:THR:H	5:T:421:THR:HB	1.77	0.46
1:M:125:HIS:CE1	1:N:41:THR:O	2.68	0.45
3:I:178:PHE:HA	3:I:224:VAL:CB	2.45	0.45
3:L:135:MET:CG	5:T:401:GLU:OE2	2.64	0.45
3:L:159:LYS:HZ1	4:H:432:LEU:CD2	2.05	0.45
1:B:24:GLU:O	1:C:144:ARG:NE	2.49	0.45
1:O:21:ARG:HH12	1:O:284:GLU:HG2	1.80	0.45
5:R:407:THR:CG2	5:R:421:THR:OG1	2.48	0.45
5:T:408:VAL:C	5:T:410:PHE:N	2.74	0.45
1:O:26:PRO:C	1:O:329:ALA:HB3	2.40	0.45
3:I:184:GLU:HG2	3:I:197:SER:HA	1.97	0.45
3:K:250:VAL:HG12	5:S:398:THR:CG2	2.44	0.45
4:G:399:VAL:CG1	5:S:362:LEU:HD12	2.24	0.45
5:T:349:HIS:HB3	5:T:350:GLY:H	1.50	0.45
1:M:126:THR:O	1:N:123:ARG:HD3	2.16	0.45
1:O:24:TYR:CD2	1:O:287:PHE:C	2.94	0.45
3:K:130:VAL:HG22	3:K:178:PHE:HD2	1.82	0.45
5:Q:408:VAL:C	5:Q:410:PHE:N	2.74	0.45
4:F:399:VAL:HG13	5:R:362:LEU:HD11	1.90	0.45
5:R:416:CYS:SG	5:R:420:THR:HG23	2.56	0.45
1:P:23:GLY:O	1:P:290:VAL:N	2.32	0.45
3:I:130:VAL:HG22	3:I:178:PHE:HD2	1.82	0.45
3:J:141:LYS:N	3:J:141:LYS:HD2	2.32	0.45
3:K:141:LYS:HD2	3:K:141:LYS:N	2.32	0.45
3:L:247:LYS:HD2	3:L:248:ASP:OD1	2.17	0.45
5:Q:344:THR:O	5:Q:344:THR:HG22	2.15	0.45
5:Q:418:VAL:HG13	5:Q:419:ARG:HA	0.61	0.45
5:Q:418:VAL:CA	5:Q:419:ARG:C	2.87	0.45
5:R:406:ALA:HB1	5:R:410:PHE:HD2	1.75	0.45
5:R:416:CYS:HG	5:R:420:THR:HG23	1.82	0.45
5:R:417:CYS:C	5:R:420:THR:HG1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:408:VAL:HG11	5:S:409:PRO:HD3	1.83	0.45
5:T:416:CYS:SG	5:T:420:THR:HG23	2.56	0.45
3:I:178:PHE:CA	3:I:224:VAL:HB	2.46	0.45
5:R:419:ARG:C	5:R:420:THR:CG2	2.86	0.45
5:S:344:THR:O	5:S:344:THR:HG22	2.15	0.45
5:T:407:THR:HA	5:T:421:THR:CG2	2.37	0.45
1:N:192:PHE:CE2	1:N:206:ARG:HG2	2.52	0.45
3:J:130:VAL:HG22	3:J:178:PHE:HD2	1.82	0.45
3:K:199:GLY:O	3:K:200:ARG:HG3	2.16	0.45
5:S:354:GLU:O	5:S:357:LEU:N	2.48	0.45
5:S:411:LEU:H	5:S:413:SER:HB3	1.75	0.45
5:T:344:THR:O	5:T:344:THR:HG22	2.15	0.45
3:J:178:PHE:HD1	3:J:179:THR:H	1.59	0.45
3:K:159:LYS:HD3	4:G:432:LEU:CG	2.46	0.45
5:R:407:THR:CA	5:R:421:THR:CG2	2.82	0.45
1:P:192:PHE:CE2	1:P:206:ARG:HG2	2.52	0.45
3:I:141:LYS:N	3:I:141:LYS:HD2	2.32	0.45
3:I:221:LYS:NZ	3:I:221:LYS:CB	2.71	0.45
3:L:141:LYS:N	3:L:141:LYS:HD2	2.32	0.45
5:Q:398:THR:CB	5:Q:399:PRO:HD3	2.47	0.45
5:Q:416:CYS:SG	5:Q:419:ARG:O	2.75	0.45
5:S:363:TYR:HB3	5:S:364:PRO:HD2	1.93	0.45
5:S:408:VAL:C	5:S:410:PHE:N	2.74	0.45
4:H:421:VAL:CG1	5:T:388:MET:HG2	2.38	0.45
3:I:162:LEU:HD23	5:Q:400:TYR:CZ	2.37	0.45
3:J:247:LYS:HD2	3:J:248:ASP:OD1	2.17	0.45
3:K:221:LYS:HZ1	3:K:223:ARG:CZ	2.29	0.45
5:R:406:ALA:CA	5:R:408:VAL:HB	2.47	0.45
5:R:413:SER:O	5:R:414:LEU:C	2.60	0.45
4:E:405:THR:OG1	4:E:406:ALA:N	2.46	0.44
5:R:375:SER:HA	5:R:378:LEU:HD12	1.99	0.44
5:R:407:THR:O	5:R:410:PHE:HB2	2.17	0.44
5:R:408:VAL:C	5:R:410:PHE:N	2.74	0.44
5:S:398:THR:CB	5:S:399:PRO:HD3	2.47	0.44
5:S:416:CYS:SG	5:S:419:ARG:O	2.75	0.44
4:H:405:THR:OG1	4:H:406:ALA:N	2.46	0.44
5:T:375:SER:HA	5:T:378:LEU:HD12	1.99	0.44
3:I:160:TYR:HE2	5:Q:398:THR:CB	2.29	0.44
3:I:225:VAL:O	3:I:244:THR:HG23	2.18	0.44
3:K:245:TRP:CZ2	5:S:401:GLU:OE1	2.62	0.44
5:R:416:CYS:SG	5:R:419:ARG:O	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:375:SER:HA	5:S:378:LEU:HD12	1.99	0.44
5:S:406:ALA:CA	5:S:408:VAL:HB	2.47	0.44
3:I:118:LYS:HD2	3:I:145:ASP:HB2	2.00	0.44
3:L:118:LYS:HD2	3:L:145:ASP:HB2	2.00	0.44
5:S:407:THR:O	5:S:410:PHE:HB2	2.17	0.44
5:T:406:ALA:CA	5:T:408:VAL:HB	2.47	0.44
1:P:23:GLY:CA	1:P:290:VAL:CG2	2.91	0.44
3:K:247:LYS:HD2	3:K:248:ASP:OD1	2.17	0.44
3:L:178:PHE:HA	3:L:224:VAL:CB	2.45	0.44
5:Q:351:HIS:N	5:Q:352:PRO:HD2	2.32	0.44
5:Q:353:HIS:O	5:Q:354:GLU:C	2.61	0.44
5:Q:375:SER:HA	5:Q:378:LEU:HD12	1.99	0.44
1:M:192:PHE:CE2	1:M:206:ARG:HG2	2.51	0.44
1:B:142:HIS:CD2	1:D:109:GLU:CB	3.01	0.44
1:O:192:PHE:CE2	1:O:206:ARG:HG2	2.52	0.44
3:J:249:ILE:HG22	4:F:439:HIS:HE1	1.82	0.44
3:L:133:LYS:HG2	5:T:401:GLU:O	2.09	0.44
5:Q:406:ALA:N	5:Q:408:VAL:HG23	2.33	0.44
5:R:352:PRO:HG2	5:R:353:HIS:H	1.83	0.44
5:T:398:THR:CB	5:T:399:PRO:HD3	2.47	0.44
1:P:28:VAL:HB	1:P:342:ALA:O	2.17	0.44
3:L:130:VAL:HG22	3:L:178:PHE:HD2	1.82	0.44
5:T:407:THR:O	5:T:410:PHE:HB2	2.17	0.44
3:I:247:LYS:HD2	3:I:248:ASP:OD1	2.17	0.44
3:L:221:LYS:HZ1	3:L:223:ARG:CZ	2.31	0.44
5:R:353:HIS:O	5:R:354:GLU:C	2.60	0.44
5:S:413:SER:O	5:S:414:LEU:C	2.61	0.44
5:S:416:CYS:SG	5:S:420:THR:HG23	2.56	0.44
5:T:406:ALA:N	5:T:408:VAL:HG23	2.33	0.44
1:C:248:LEU:HD13	1:C:251:ARG:HB2	2.00	0.44
1:O:361:ALA:HB1	5:S:345:ASN:HB2	1.87	0.44
3:L:248:ASP:OD2	5:T:405:GLY:CA	2.63	0.44
5:Q:372:SER:O	5:Q:376:PHE:HD2	1.97	0.44
5:Q:407:THR:O	5:Q:410:PHE:HB2	2.17	0.44
5:R:363:TYR:CD2	5:R:364:PRO:HD2	2.39	0.44
5:S:351:HIS:HB2	5:S:352:PRO:HD3	1.90	0.44
1:A:248:LEU:HD13	1:A:251:ARG:HB2	2.00	0.44
1:O:23:GLY:HA2	1:O:290:VAL:CG2	2.48	0.44
1:O:24:TYR:HD2	1:O:287:PHE:C	2.26	0.44
3:J:118:LYS:HD2	3:J:145:ASP:HB2	2.00	0.44
5:Q:406:ALA:CA	5:Q:408:VAL:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:419:ARG:C	5:Q:420:THR:CG2	2.86	0.44
5:R:398:THR:CB	5:R:399:PRO:HD3	2.47	0.44
5:T:413:SER:O	5:T:414:LEU:C	2.61	0.44
5:T:417:CYS:C	5:T:420:THR:HG1	2.24	0.44
3:I:178:PHE:CD1	3:I:245:TRP:CG	3.06	0.43
3:J:225:VAL:O	3:J:244:THR:HG23	2.18	0.43
3:K:118:LYS:HD2	3:K:145:ASP:HB2	2.00	0.43
5:R:407:THR:O	5:R:410:PHE:CB	2.66	0.43
3:J:178:PHE:HA	3:J:224:VAL:CB	2.45	0.43
3:K:178:PHE:CD1	3:K:245:TRP:CG	3.06	0.43
3:L:247:LYS:HG3	3:L:248:ASP:H	1.83	0.43
5:R:349:HIS:HA	5:R:354:GLU:CB	1.59	0.43
5:T:349:HIS:ND1	5:T:354:GLU:CB	2.82	0.43
5:T:353:HIS:O	5:T:354:GLU:C	2.61	0.43
1:M:294:PRO:HD2	1:M:370:CYS:SG	2.59	0.43
1:O:26:PRO:O	1:O:329:ALA:HB3	2.17	0.43
3:L:182:LYS:NZ	3:L:244:THR:HG21	2.34	0.43
4:E:402:ILE:C	4:E:407:MET:SD	3.02	0.43
5:S:398:THR:OG1	5:S:399:PRO:HD3	2.18	0.43
5:S:406:ALA:N	5:S:408:VAL:HG23	2.33	0.43
3:I:250:VAL:HG21	5:Q:401:GLU:CG	2.47	0.43
3:J:178:PHE:CD1	3:J:245:TRP:CG	3.06	0.43
4:E:399:VAL:CG1	5:Q:366:MET:HE1	2.48	0.43
5:Q:418:VAL:HG22	5:Q:421:THR:N	2.27	0.43
5:R:398:THR:OG1	5:R:399:PRO:HD3	2.18	0.43
5:R:406:ALA:N	5:R:408:VAL:HG23	2.33	0.43
4:G:421:VAL:CG1	5:S:388:MET:HG2	2.38	0.43
5:T:418:VAL:HG22	5:T:421:THR:N	2.27	0.43
1:M:28:VAL:CG2	1:M:331:HIS:HB2	2.48	0.43
1:B:248:LEU:HD13	1:B:251:ARG:HB2	1.99	0.43
1:D:280:LYS:HA	5:T:343:SER:OG	2.18	0.43
3:I:164:CYS:SG	5:Q:400:TYR:CG	3.11	0.43
5:T:372:SER:O	5:T:376:PHE:HD2	1.97	0.43
5:T:398:THR:OG1	5:T:399:PRO:HD3	2.18	0.43
3:I:162:LEU:HD21	5:Q:401:GLU:HG2	2.00	0.43
3:I:221:LYS:HZ3	3:I:221:LYS:CB	2.32	0.43
3:I:248:ASP:OD2	3:I:249:ILE:HG13	2.19	0.43
3:K:182:LYS:NZ	3:K:244:THR:HG21	2.34	0.43
5:Q:398:THR:OG1	5:Q:399:PRO:HD3	2.18	0.43
5:R:358:TYR:O	5:R:359:TYR:C	2.61	0.43
1:M:291:VAL:CA	1:O:304:PRO:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:157:SER:HB3	5:Q:400:TYR:HE2	1.81	0.43
3:J:232:ALA:HB2	3:J:258:ALA:HA	2.01	0.43
3:K:225:VAL:O	3:K:244:THR:HG23	2.18	0.43
3:L:178:PHE:CD1	3:L:245:TRP:CG	3.06	0.43
5:T:416:CYS:SG	5:T:419:ARG:O	2.75	0.43
3:I:161:ASP:CB	3:I:252:LYS:NZ	2.82	0.43
3:I:232:ALA:HB2	3:I:258:ALA:HA	2.01	0.43
3:J:182:LYS:NZ	3:J:244:THR:HG21	2.34	0.43
3:J:248:ASP:OD2	3:J:249:ILE:HG13	2.19	0.43
3:K:178:PHE:HA	3:K:224:VAL:CB	2.45	0.43
3:K:249:ILE:CG2	3:K:250:VAL:N	2.82	0.43
5:Q:364:PRO:C	5:Q:365:THR:CG2	2.55	0.43
5:Q:390:VAL:O	5:Q:394:ARG:HG3	2.19	0.43
5:Q:400:TYR:HD1	5:Q:401:GLU:N	2.17	0.43
4:G:399:VAL:CG1	5:S:366:MET:HE1	2.48	0.43
3:I:178:PHE:HD1	3:I:179:THR:H	1.59	0.43
3:J:161:ASP:CB	3:J:252:LYS:NZ	2.82	0.43
3:J:247:LYS:HG3	3:J:248:ASP:H	1.84	0.43
3:K:161:ASP:CB	3:K:252:LYS:NZ	2.82	0.43
3:L:161:ASP:CB	3:L:252:LYS:NZ	2.82	0.43
5:S:407:THR:O	5:S:410:PHE:CB	2.66	0.43
5:T:397:ILE:O	5:T:400:TYR:HB3	2.19	0.43
5:T:411:LEU:H	5:T:413:SER:HB3	1.75	0.43
1:O:21:ARG:NH1	1:O:287:PHE:CB	2.80	0.43
3:J:178:PHE:CA	3:J:224:VAL:HB	2.46	0.43
5:Q:407:THR:O	5:Q:410:PHE:CB	2.66	0.43
4:F:403:SER:OG	4:F:406:ALA:HB3	2.19	0.43
5:S:400:TYR:HD1	5:S:401:GLU:N	2.17	0.43
5:T:366:MET:O	5:T:370:ILE:HG13	2.19	0.43
5:T:407:THR:O	5:T:410:PHE:CB	2.66	0.43
1:B:272:ARG:CZ	1:P:237:PRO:CD	2.62	0.42
3:K:122:LYS:CD	3:L:170:HIS:HB3	2.48	0.42
3:L:160:TYR:CD2	5:T:397:ILE:HG22	2.53	0.42
5:R:362:LEU:HB3	5:R:363:TYR:H	1.58	0.42
1:M:18:LEU:HD13	1:M:331:HIS:CB	2.49	0.42
1:N:237:PRO:HG2	1:C:314:LYS:HZ3	1.61	0.42
3:I:247:LYS:HG3	3:I:248:ASP:H	1.84	0.42
3:J:156:ARG:O	5:R:397:ILE:HD11	2.19	0.42
3:J:249:ILE:CG2	3:J:250:VAL:N	2.82	0.42
3:K:132:ASP:CA	5:S:402:LEU:HD11	2.43	0.42
3:K:161:ASP:HB3	3:K:252:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:248:ASP:OD2	5:S:404:PRO:O	2.37	0.42
3:L:225:VAL:O	3:L:244:THR:HG23	2.18	0.42
4:F:399:VAL:CB	5:R:366:MET:HE2	2.38	0.42
5:R:381:MET:O	5:R:384:THR:OG1	2.36	0.42
5:R:390:VAL:O	5:R:394:ARG:HG3	2.19	0.42
5:R:397:ILE:CG2	5:R:398:THR:H	2.24	0.42
5:S:407:THR:CG2	5:S:421:THR:OG1	2.48	0.42
5:S:416:CYS:HG	5:S:420:THR:HG23	1.83	0.42
5:T:400:TYR:HD1	5:T:401:GLU:N	2.16	0.42
3:I:161:ASP:HB3	3:I:252:LYS:NZ	2.35	0.42
3:K:248:ASP:OD2	3:K:249:ILE:HG13	2.19	0.42
5:R:349:HIS:CG	5:R:355:ILE:N	2.72	0.42
5:S:382:VAL:O	5:S:386:VAL:HG23	2.20	0.42
5:T:358:TYR:O	5:T:359:TYR:C	2.61	0.42
5:T:416:CYS:HG	5:T:420:THR:HG23	1.83	0.42
1:M:291:VAL:HG13	1:O:304:PRO:HG3	2.01	0.42
1:D:248:LEU:HD13	1:D:251:ARG:HB2	2.00	0.42
1:P:26:PRO:CD	1:P:370:CYS:O	2.65	0.42
3:I:159:LYS:NZ	4:E:432:LEU:CD1	2.78	0.42
3:J:221:LYS:HZ1	3:J:223:ARG:CZ	2.32	0.42
3:J:247:LYS:HD2	3:J:248:ASP:HB3	2.01	0.42
3:K:159:LYS:HZ2	4:G:432:LEU:CD2	2.25	0.42
4:E:424:ALA:O	4:E:428:LEU:HG	2.20	0.42
4:F:402:ILE:C	4:F:407:MET:SD	3.02	0.42
5:R:418:VAL:CB	5:R:419:ARG:HA	2.35	0.42
4:G:403:SER:OG	4:G:406:ALA:HB3	2.19	0.42
5:T:382:VAL:O	5:T:386:VAL:HG23	2.20	0.42
3:L:247:LYS:HD2	3:L:248:ASP:HB3	2.01	0.42
5:Q:382:VAL:O	5:Q:386:VAL:HG23	2.20	0.42
1:M:28:VAL:HG22	1:M:331:HIS:HB2	2.01	0.42
3:I:182:LYS:NZ	3:I:244:THR:HG21	2.34	0.42
3:J:160:TYR:CD2	5:R:397:ILE:HG22	2.50	0.42
3:K:232:ALA:HB2	3:K:258:ALA:HA	2.01	0.42
5:Q:406:ALA:HB1	5:Q:410:PHE:CE2	2.53	0.42
5:R:410:PHE:O	5:R:413:SER:OG	2.38	0.42
5:S:353:HIS:O	5:S:354:GLU:C	2.61	0.42
5:S:397:ILE:O	5:S:400:TYR:HB3	2.19	0.42
5:S:410:PHE:O	5:S:413:SER:OG	2.38	0.42
4:H:399:VAL:HG11	5:T:362:LEU:HD12	1.34	0.42
5:T:390:VAL:O	5:T:394:ARG:HG3	2.19	0.42
5:T:413:SER:OG	5:T:417:CYS:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:23:GLY:O	1:O:289:ARG:HA	2.20	0.42
3:K:159:LYS:CE	5:S:394:ARG:O	2.61	0.42
3:L:161:ASP:HB3	3:L:252:LYS:NZ	2.35	0.42
3:L:232:ALA:HB2	3:L:258:ALA:HA	2.01	0.42
5:Q:413:SER:O	5:Q:414:LEU:C	2.61	0.42
5:S:398:THR:O	5:S:400:TYR:N	2.50	0.42
4:H:424:ALA:O	4:H:428:LEU:HG	2.20	0.42
3:K:247:LYS:HD2	3:K:248:ASP:HB3	2.01	0.42
3:L:178:PHE:CA	3:L:224:VAL:HB	2.46	0.42
5:Q:397:ILE:O	5:Q:400:TYR:HB3	2.19	0.42
4:G:402:ILE:C	4:G:407:MET:SD	3.01	0.42
4:H:397:LEU:N	4:H:397:LEU:CD2	2.74	0.42
4:H:403:SER:OG	4:H:406:ALA:HB3	2.19	0.42
3:J:156:ARG:O	5:R:397:ILE:CD1	2.68	0.42
3:K:178:PHE:CA	3:K:224:VAL:HB	2.46	0.42
3:L:179:THR:CG2	3:L:223:ARG:HB3	2.46	0.42
3:L:249:ILE:CG2	3:L:250:VAL:N	2.82	0.42
4:E:403:SER:OG	4:E:406:ALA:HB3	2.19	0.42
4:F:403:SER:OG	4:F:407:MET:CA	2.68	0.42
5:R:352:PRO:O	5:R:353:HIS:O	2.38	0.42
5:S:390:VAL:O	5:S:394:ARG:HG3	2.19	0.42
1:P:283:PRO:O	1:P:286:ALA:HB3	2.20	0.42
3:I:249:ILE:CG2	3:I:250:VAL:N	2.82	0.42
3:J:249:ILE:HG22	4:F:439:HIS:CE1	2.55	0.42
4:F:424:ALA:O	4:F:428:LEU:HG	2.20	0.42
5:R:397:ILE:O	5:R:400:TYR:HB3	2.19	0.42
5:T:418:VAL:CA	5:T:419:ARG:C	2.87	0.42
3:I:247:LYS:HD2	3:I:248:ASP:HB3	2.01	0.41
3:L:248:ASP:OD2	3:L:249:ILE:HG13	2.19	0.41
5:R:382:VAL:O	5:R:386:VAL:HG23	2.20	0.41
5:R:400:TYR:HD1	5:R:401:GLU:N	2.17	0.41
4:G:424:ALA:O	4:G:428:LEU:HG	2.20	0.41
5:S:358:TYR:C	5:S:360:TYR:N	2.78	0.41
5:T:406:ALA:CB	5:T:409:PRO:HG2	2.50	0.41
3:J:161:ASP:HB3	3:J:252:LYS:NZ	2.35	0.41
3:K:247:LYS:HG3	3:K:248:ASP:H	1.84	0.41
5:S:406:ALA:CB	5:S:409:PRO:HG2	2.50	0.41
3:L:133:LYS:HE2	5:T:402:LEU:CD2	2.47	0.41
4:E:434:VAL:HG12	4:E:438:ARG:NE	2.36	0.41
5:Q:357:LEU:C	5:Q:359:TYR:N	2.76	0.41
5:Q:413:SER:OG	5:Q:417:CYS:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:406:ALA:CB	5:R:409:PRO:HG2	2.50	0.41
5:T:410:PHE:O	5:T:413:SER:OG	2.38	0.41
1:P:23:GLY:HA2	1:P:290:VAL:HG21	2.02	0.41
5:Q:406:ALA:CB	5:Q:409:PRO:HG2	2.50	0.41
1:M:123:ARG:HB2	1:N:41:THR:HG21	2.02	0.41
1:O:236:ALA:CA	1:D:272:ARG:NH1	2.71	0.41
5:S:362:LEU:HB3	5:S:363:TYR:H	1.58	0.41
4:H:403:SER:OG	4:H:407:MET:CA	2.68	0.41
1:B:25:GLY:HA3	1:C:144:ARG:CA	2.51	0.41
1:O:24:TYR:HD2	1:O:287:PHE:O	2.00	0.41
3:I:164:CYS:SG	5:Q:400:TYR:CE2	3.14	0.41
3:K:159:LYS:CD	4:G:432:LEU:HD22	2.51	0.41
3:L:221:LYS:HB2	3:L:221:LYS:HZ3	1.84	0.41
5:Q:410:PHE:O	5:Q:413:SER:OG	2.38	0.41
3:J:133:LYS:CD	5:R:402:LEU:HG	2.51	0.41
3:K:250:VAL:CG1	5:S:398:THR:HA	2.51	0.41
4:G:430:VAL:O	4:G:434:VAL:HG23	2.21	0.41
1:N:330:VAL:HG11	1:N:354:ILE:HG21	2.03	0.41
3:I:159:LYS:HZ2	4:E:432:LEU:CD2	2.26	0.41
4:F:434:VAL:HG12	4:F:438:ARG:NE	2.36	0.41
4:H:434:VAL:HG12	4:H:438:ARG:NE	2.36	0.41
1:O:19:VAL:HB	1:O:27:MET:HB3	2.03	0.41
1:D:42:THR:HB	1:D:136:ILE:HD11	2.03	0.41
3:J:131:GLY:HA3	5:R:402:LEU:HD12	1.64	0.41
3:K:130:VAL:CG1	5:S:401:GLU:OE2	2.69	0.41
3:L:182:LYS:HA	3:L:183:PRO:HD2	1.96	0.41
4:E:403:SER:OG	4:E:407:MET:CA	2.68	0.41
5:R:413:SER:OG	5:R:417:CYS:CB	2.67	0.41
4:G:403:SER:OG	4:G:407:MET:CA	2.68	0.41
4:G:419:LEU:O	4:G:423:VAL:HG23	2.21	0.41
5:S:372:SER:O	5:S:376:PHE:HD2	1.96	0.41
5:S:413:SER:OG	5:S:417:CYS:CB	2.68	0.41
4:H:414:THR:HA	4:H:416:GLY:H	1.86	0.41
1:A:280:LYS:HG3	5:Q:343:SER:HB3	2.02	0.41
1:N:19:VAL:HB	1:N:27:MET:HB3	2.03	0.41
1:O:23:GLY:CA	1:O:290:VAL:CG2	2.96	0.41
1:P:282:ILE:HG22	1:P:286:ALA:HB3	2.03	0.41
3:K:248:ASP:CG	3:K:249:ILE:N	2.79	0.41
5:Q:363:TYR:H	5:Q:364:PRO:CD	2.25	0.41
4:F:430:VAL:O	4:F:434:VAL:HG23	2.21	0.41
5:R:406:ALA:C	5:R:410:PHE:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:350:GLY:HA2	5:S:351:HIS:HA	1.65	0.41
4:H:397:LEU:HB2	4:H:398:GLY:H	1.74	0.41
1:M:330:VAL:HG11	1:M:354:ILE:HG21	2.03	0.40
1:P:282:ILE:CG2	1:P:287:PHE:CE2	3.05	0.40
1:P:330:VAL:HG11	1:P:354:ILE:HG21	2.03	0.40
3:K:160:TYR:CZ	5:S:398:THR:HG21	2.31	0.40
4:E:430:VAL:O	4:E:434:VAL:HG23	2.21	0.40
5:T:408:VAL:CG1	5:T:409:PRO:N	2.68	0.40
1:C:42:THR:HB	1:C:136:ILE:HD11	2.03	0.40
3:L:130:VAL:HG13	3:L:130:VAL:O	2.22	0.40
4:G:434:VAL:HG12	4:G:438:ARG:NE	2.36	0.40
3:I:130:VAL:O	3:I:130:VAL:HG13	2.22	0.40
3:J:130:VAL:HG13	3:J:130:VAL:O	2.22	0.40
5:T:381:MET:O	5:T:384:THR:OG1	2.36	0.40
1:N:359:ALA:O	5:R:345:ASN:CG	2.65	0.40
1:O:60:VAL:HG22	1:O:102:GLN:HG3	2.04	0.40
1:O:330:VAL:HG11	1:O:354:ILE:HG21	2.03	0.40
3:I:179:THR:CG2	3:I:223:ARG:HB3	2.46	0.40
3:J:130:VAL:CG1	5:R:401:GLU:CD	2.89	0.40
3:K:135:MET:HE2	5:S:401:GLU:HA	1.91	0.40
3:L:130:VAL:HG11	5:T:401:GLU:OE1	2.14	0.40
5:Q:351:HIS:CB	5:Q:352:PRO:CD	2.98	0.40
4:G:414:THR:HA	4:G:416:GLY:H	1.86	0.40
1:C:27:SER:CB	1:D:146:GLN:CG	2.98	0.40
4:F:399:VAL:HB	5:R:366:MET:SD	2.61	0.40
5:R:356:ILE:CG1	5:R:359:TYR:HE2	2.34	0.40
5:S:381:MET:O	5:S:384:THR:OG1	2.36	0.40
5:T:406:ALA:CB	5:T:410:PHE:HD2	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	36	72
1	B	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	36	72
1	C	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	36	72
1	D	339/866 (39%)	320 (94%)	18 (5%)	1 (0%)	36	72
1	M	381/866 (44%)	370 (97%)	8 (2%)	3 (1%)	16	54
1	N	381/866 (44%)	372 (98%)	8 (2%)	1 (0%)	36	72
1	O	381/866 (44%)	370 (97%)	10 (3%)	1 (0%)	36	72
1	P	381/866 (44%)	370 (97%)	10 (3%)	1 (0%)	36	72
2	U	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	V	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	W	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
2	X	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
3	I	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	31
3	J	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	31
3	K	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	31
3	L	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	6	31
4	E	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	3
4	F	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	3
4	G	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	3
4	H	44/46 (96%)	33 (75%)	5 (11%)	6 (14%)	0	3
5	Q	79/81 (98%)	40 (51%)	15 (19%)	24 (30%)	0	0
5	R	79/81 (98%)	40 (51%)	15 (19%)	24 (30%)	0	0
5	S	79/81 (98%)	41 (52%)	17 (22%)	21 (27%)	0	0
5	T	79/81 (98%)	41 (52%)	20 (25%)	18 (23%)	0	1
All	All	4192/8272 (51%)	3808 (91%)	251 (6%)	133 (3%)	5	21

All (133) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	126	THR
1	N	126	THR
1	O	126	THR
1	P	126	THR
3	I	177	LYS
3	I	178	PHE

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Mol	Chain	Res	Type
3	I	179	THR
3	J	177	LYS
3	J	178	PHE
3	J	179	THR
3	K	177	LYS
3	K	178	PHE
3	K	179	THR
3	L	177	LYS
3	L	178	PHE
3	L	179	THR
4	E	396	THR
4	E	399	VAL
4	E	404	THR
4	E	405	THR
5	Q	348	ALA
5	Q	352	PRO
5	Q	353	HIS
5	Q	365	THR
5	Q	366	MET
5	Q	397	ILE
5	Q	398	THR
5	Q	408	VAL
5	Q	411	LEU
5	Q	415	LEU
5	Q	417	CYS
5	Q	422	LYS
4	F	396	THR
4	F	399	VAL
4	F	404	THR
4	F	405	THR
5	R	348	ALA
5	R	351	HIS
5	R	353	HIS
5	R	368	VAL
5	R	397	ILE
5	R	398	THR
5	R	408	VAL
5	R	411	LEU
5	R	415	LEU
5	R	417	CYS
5	R	422	LYS
4	G	396	THR

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Mol	Chain	Res	Type
4	G	399	VAL
4	G	404	THR
4	G	405	THR
5	S	353	HIS
5	S	366	MET
5	S	397	ILE
5	S	398	THR
5	S	408	VAL
5	S	411	LEU
5	S	415	LEU
5	S	417	CYS
5	S	422	LYS
4	H	396	THR
4	H	399	VAL
4	H	404	THR
4	H	405	THR
5	T	353	HIS
5	T	397	ILE
5	T	398	THR
5	T	408	VAL
5	T	411	LEU
5	T	415	LEU
5	T	417	CYS
5	T	422	LYS
4	E	402	ILE
5	Q	406	ALA
4	F	402	ILE
5	R	350	GLY
5	R	406	ALA
4	G	402	ILE
5	S	351	HIS
5	S	406	ALA
4	H	402	ILE
5	T	406	ALA
5	Q	344	THR
5	Q	358	TYR
5	Q	364	PRO
5	Q	407	THR
5	Q	414	LEU
5	Q	416	CYS
5	Q	420	THR
5	R	344	THR

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Mol	Chain	Res	Type
5	R	366	MET
5	R	407	THR
5	R	414	LEU
5	R	416	CYS
5	R	420	THR
5	S	344	THR
5	S	407	THR
5	S	414	LEU
5	S	416	CYS
5	S	420	THR
5	T	344	THR
5	T	407	THR
5	T	414	LEU
5	T	416	CYS
5	T	420	THR
5	Q	401	GLU
5	R	364	PRO
5	R	401	GLU
5	S	347	THR
5	S	364	PRO
5	S	401	GLU
5	T	364	PRO
5	T	401	GLU
5	Q	403	THR
5	R	352	PRO
5	R	403	THR
5	S	403	THR
5	T	403	THR
4	E	401	ASP
5	Q	351	HIS
4	F	401	ASP
4	G	401	ASP
4	H	401	ASP
1	M	293	ALA
1	A	249	GLY
1	B	249	GLY
1	C	249	GLY
1	D	249	GLY
1	M	294	PRO
5	Q	405	GLY
5	R	405	GLY
5	S	405	GLY

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Mol	Chain	Res	Type
5	T	405	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/741 (41%)	293 (97%)	10 (3%)	33	55
1	B	303/741 (41%)	293 (97%)	10 (3%)	33	55
1	C	303/741 (41%)	293 (97%)	10 (3%)	33	55
1	D	303/741 (41%)	293 (97%)	10 (3%)	33	55
1	M	320/741 (43%)	318 (99%)	2 (1%)	78	83
1	N	320/741 (43%)	318 (99%)	2 (1%)	78	83
1	O	320/741 (43%)	317 (99%)	3 (1%)	70	79
1	P	320/741 (43%)	318 (99%)	2 (1%)	78	83
2	U	57/57 (100%)	56 (98%)	1 (2%)	51	68
2	V	57/57 (100%)	56 (98%)	1 (2%)	51	68
2	W	57/57 (100%)	56 (98%)	1 (2%)	51	68
2	X	57/57 (100%)	56 (98%)	1 (2%)	51	68
3	I	118/118 (100%)	102 (86%)	16 (14%)	3	14
3	J	118/118 (100%)	102 (86%)	16 (14%)	3	14
3	K	118/118 (100%)	102 (86%)	16 (14%)	3	14
3	L	118/118 (100%)	102 (86%)	16 (14%)	3	14
4	E	38/38 (100%)	36 (95%)	2 (5%)	20	41
4	F	38/38 (100%)	36 (95%)	2 (5%)	20	41
4	G	38/38 (100%)	36 (95%)	2 (5%)	20	41
4	H	38/38 (100%)	36 (95%)	2 (5%)	20	41
5	Q	70/70 (100%)	62 (89%)	8 (11%)	5	18
5	R	70/70 (100%)	61 (87%)	9 (13%)	4	15
5	S	70/70 (100%)	63 (90%)	7 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	70/70 (100%)	61 (87%)	9 (13%)	4	15
All	All	3624/7060 (51%)	3466 (96%)	158 (4%)	27	47

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	89	TRP
1	M	370	CYS
1	A	40	GLU
1	A	54	ILE
1	A	73	HIS
1	A	158	GLN
1	A	183	GLN
1	A	207	ASN
1	A	222	VAL
1	A	248	LEU
1	A	265	THR
1	A	313	HIS
2	U	9	LEU
2	V	9	LEU
1	B	40	GLU
1	B	54	ILE
1	B	73	HIS
1	B	158	GLN
1	B	183	GLN
1	B	207	ASN
1	B	222	VAL
1	B	248	LEU
1	B	265	THR
1	B	313	HIS
1	N	89	TRP
1	N	370	CYS
2	W	9	LEU
1	C	40	GLU
1	C	54	ILE
1	C	73	HIS
1	C	158	GLN
1	C	183	GLN
1	C	207	ASN
1	C	222	VAL
1	C	248	LEU
1	C	265	THR

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Mol	Chain	Res	Type
1	C	313	HIS
1	O	89	TRP
1	O	288	THR
1	O	370	CYS
2	X	9	LEU
1	D	40	GLU
1	D	54	ILE
1	D	73	HIS
1	D	158	GLN
1	D	183	GLN
1	D	207	ASN
1	D	222	VAL
1	D	248	LEU
1	D	265	THR
1	D	313	HIS
1	P	89	TRP
1	P	370	CYS
3	I	133	LYS
3	I	149	LEU
3	I	151	LYS
3	I	164	CYS
3	I	166	GLN
3	I	169	VAL
3	I	179	THR
3	I	189	TRP
3	I	210	PRO
3	I	221	LYS
3	I	223	ARG
3	I	238	THR
3	I	243	VAL
3	I	246	ASN
3	I	247	LYS
3	I	250	VAL
3	J	133	LYS
3	J	149	LEU
3	J	151	LYS
3	J	164	CYS
3	J	166	GLN
3	J	169	VAL
3	J	179	THR
3	J	189	TRP
3	J	210	PRO

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Mol	Chain	Res	Type
3	J	221	LYS
3	J	223	ARG
3	J	238	THR
3	J	243	VAL
3	J	246	ASN
3	J	247	LYS
3	J	250	VAL
3	K	133	LYS
3	K	149	LEU
3	K	151	LYS
3	K	164	CYS
3	K	166	GLN
3	K	169	VAL
3	K	179	THR
3	K	189	TRP
3	K	210	PRO
3	K	221	LYS
3	K	223	ARG
3	K	238	THR
3	K	243	VAL
3	K	246	ASN
3	K	247	LYS
3	K	250	VAL
3	L	133	LYS
3	L	149	LEU
3	L	151	LYS
3	L	164	CYS
3	L	166	GLN
3	L	169	VAL
3	L	179	THR
3	L	189	TRP
3	L	210	PRO
3	L	221	LYS
3	L	223	ARG
3	L	238	THR
3	L	243	VAL
3	L	246	ASN
3	L	247	LYS
3	L	250	VAL
4	E	394	HIS
4	E	397	LEU
5	Q	344	THR

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Mol	Chain	Res	Type
5	Q	345	ASN
5	Q	349	HIS
5	Q	361	GLU
5	Q	363	TYR
5	Q	398	THR
5	Q	400	TYR
5	Q	401	GLU
4	F	394	HIS
4	F	397	LEU
5	R	344	THR
5	R	345	ASN
5	R	351	HIS
5	R	362	LEU
5	R	363	TYR
5	R	366	MET
5	R	398	THR
5	R	400	TYR
5	R	401	GLU
4	G	394	HIS
4	G	397	LEU
5	S	344	THR
5	S	345	ASN
5	S	362	LEU
5	S	363	TYR
5	S	398	THR
5	S	400	TYR
5	S	401	GLU
4	H	394	HIS
4	H	397	LEU
5	T	344	THR
5	T	345	ASN
5	T	349	HIS
5	T	362	LEU
5	T	363	TYR
5	T	366	MET
5	T	398	THR
5	T	400	TYR
5	T	401	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	125	HIS
1	M	149	ASN
1	M	175	ASN
1	M	218	GLN
1	M	351	GLN
1	A	29	HIS
1	A	245	ASN
1	B	29	HIS
1	B	142	HIS
1	B	146	GLN
1	B	245	ASN
1	N	218	GLN
1	N	331	HIS
1	N	351	GLN
2	W	62	GLN
1	C	18	HIS
1	C	29	HIS
1	C	146	GLN
1	C	184	GLN
1	C	245	ASN
1	O	138	GLN
1	O	175	ASN
1	O	218	GLN
1	O	368	GLN
1	D	18	HIS
1	D	29	HIS
1	D	184	GLN
1	D	245	ASN
1	P	138	GLN
1	P	175	ASN
1	P	199	GLN
1	P	218	GLN
1	P	351	GLN
3	J	246	ASN
3	K	246	ASN
3	L	246	ASN
5	Q	351	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

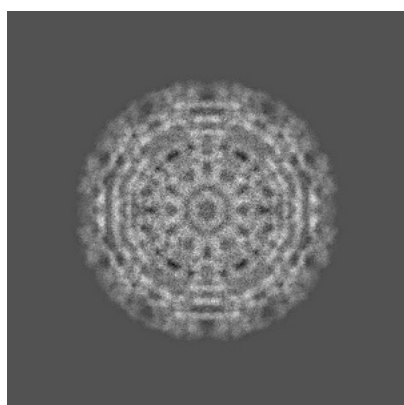
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8734. These allow visual inspection of the internal detail of the map and identification of artifacts.

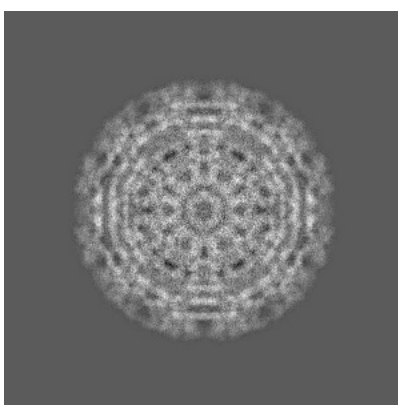
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

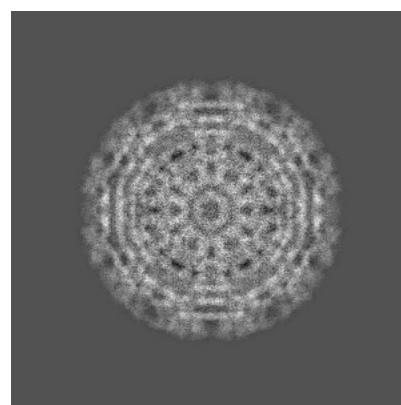
6.1.1 Primary map



X



Y

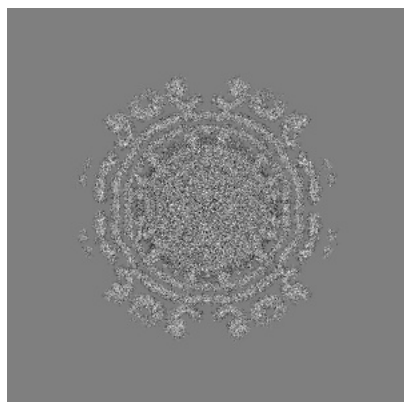


Z

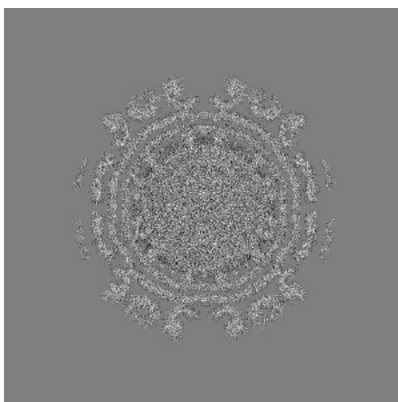
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

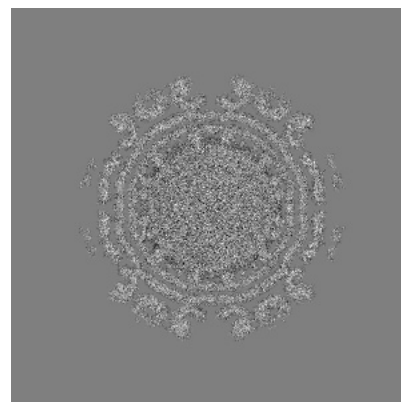
6.2.1 Primary map



X Index: 384



Y Index: 384

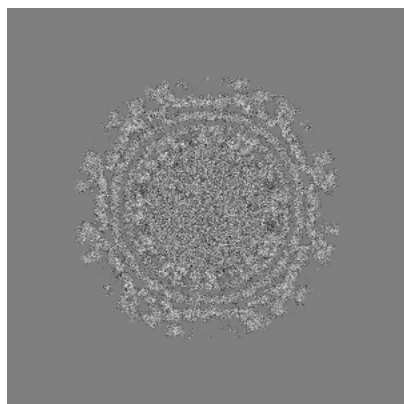


Z Index: 384

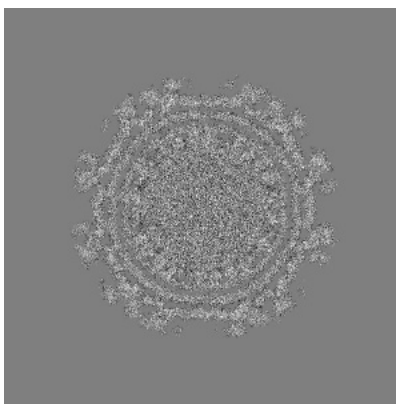
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

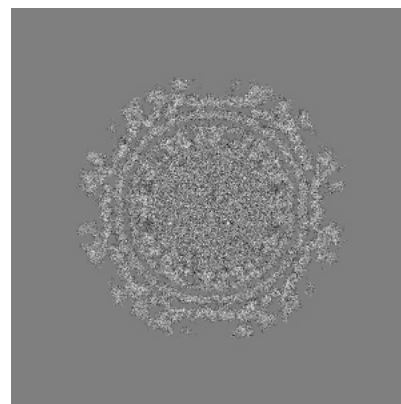
6.3.1 Primary map



X Index: 362



Y Index: 405

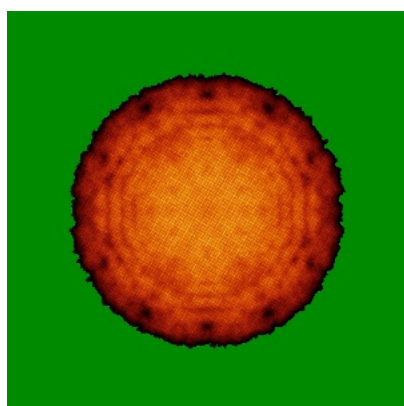


Z Index: 406

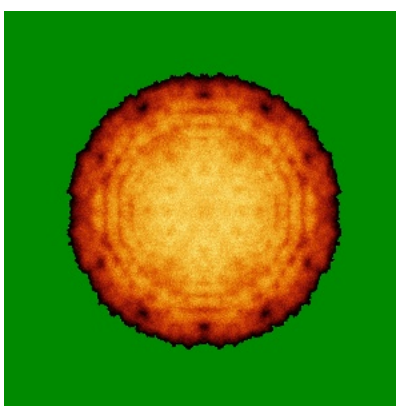
The images above show the largest variance slices of the map in three orthogonal directions.

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

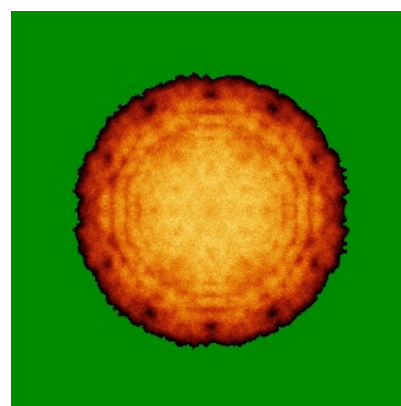
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

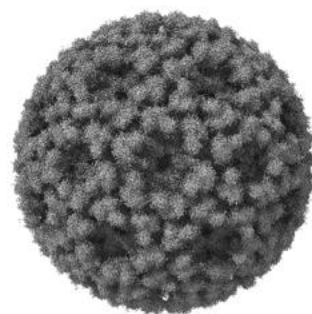
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

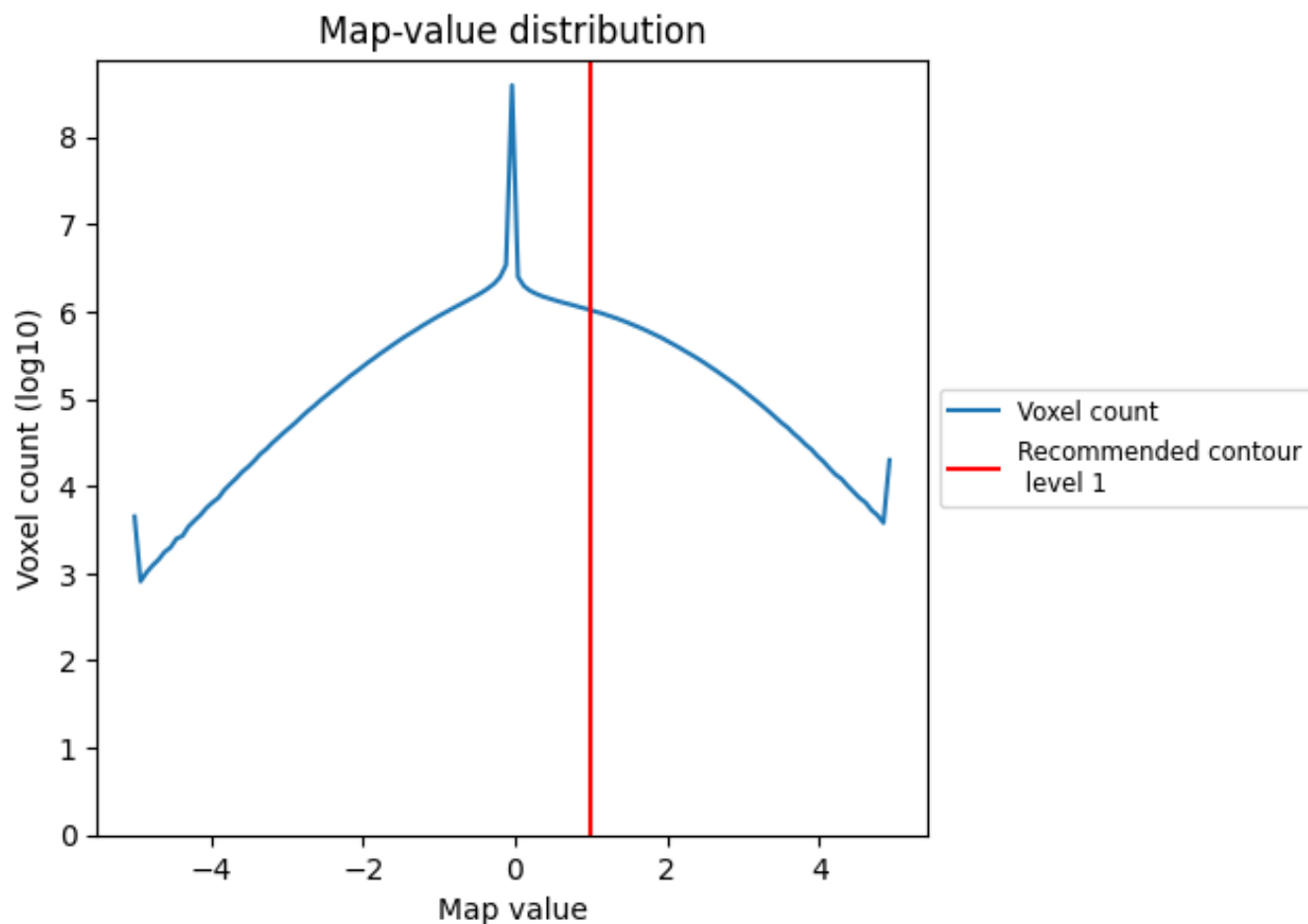
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

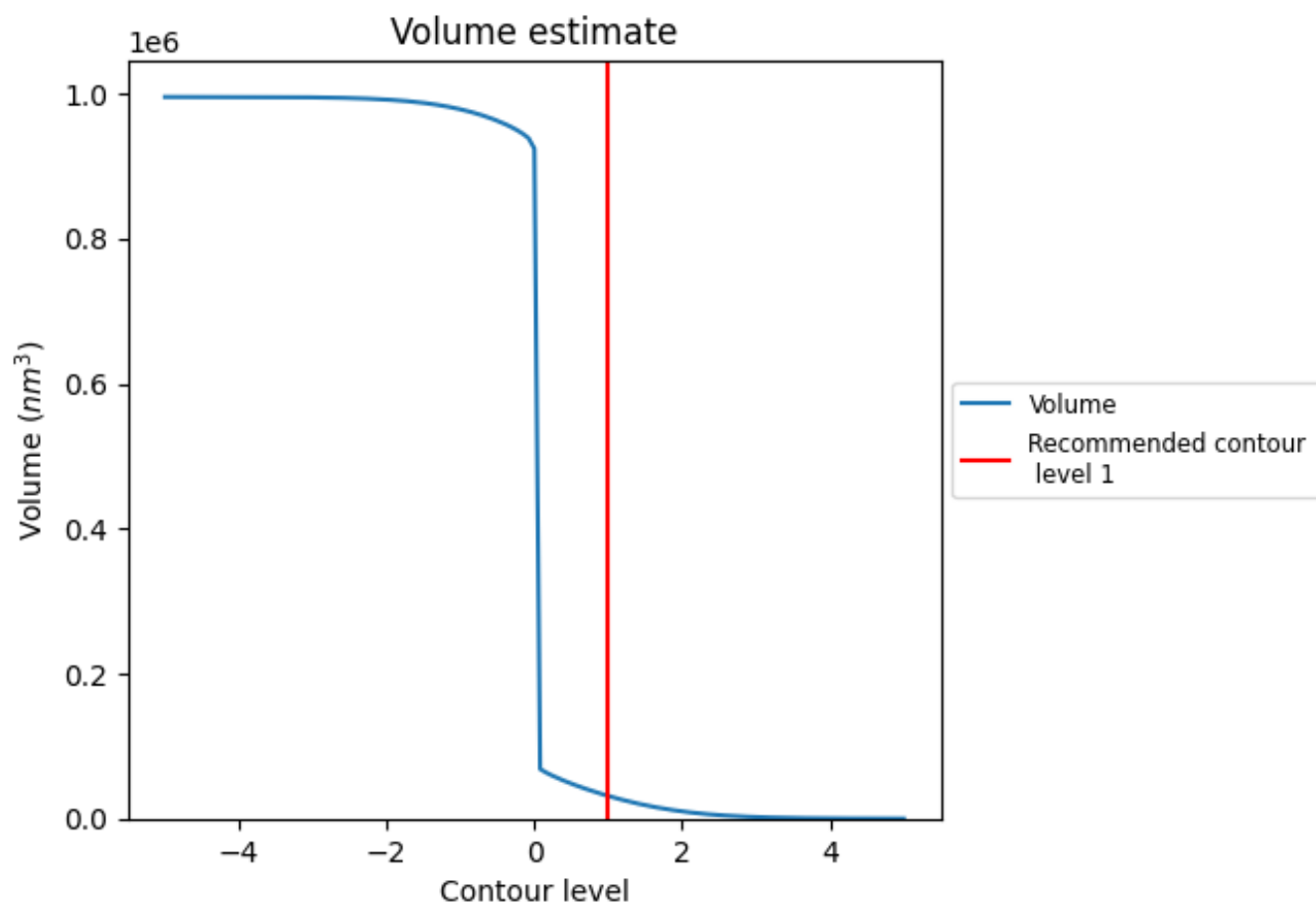
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

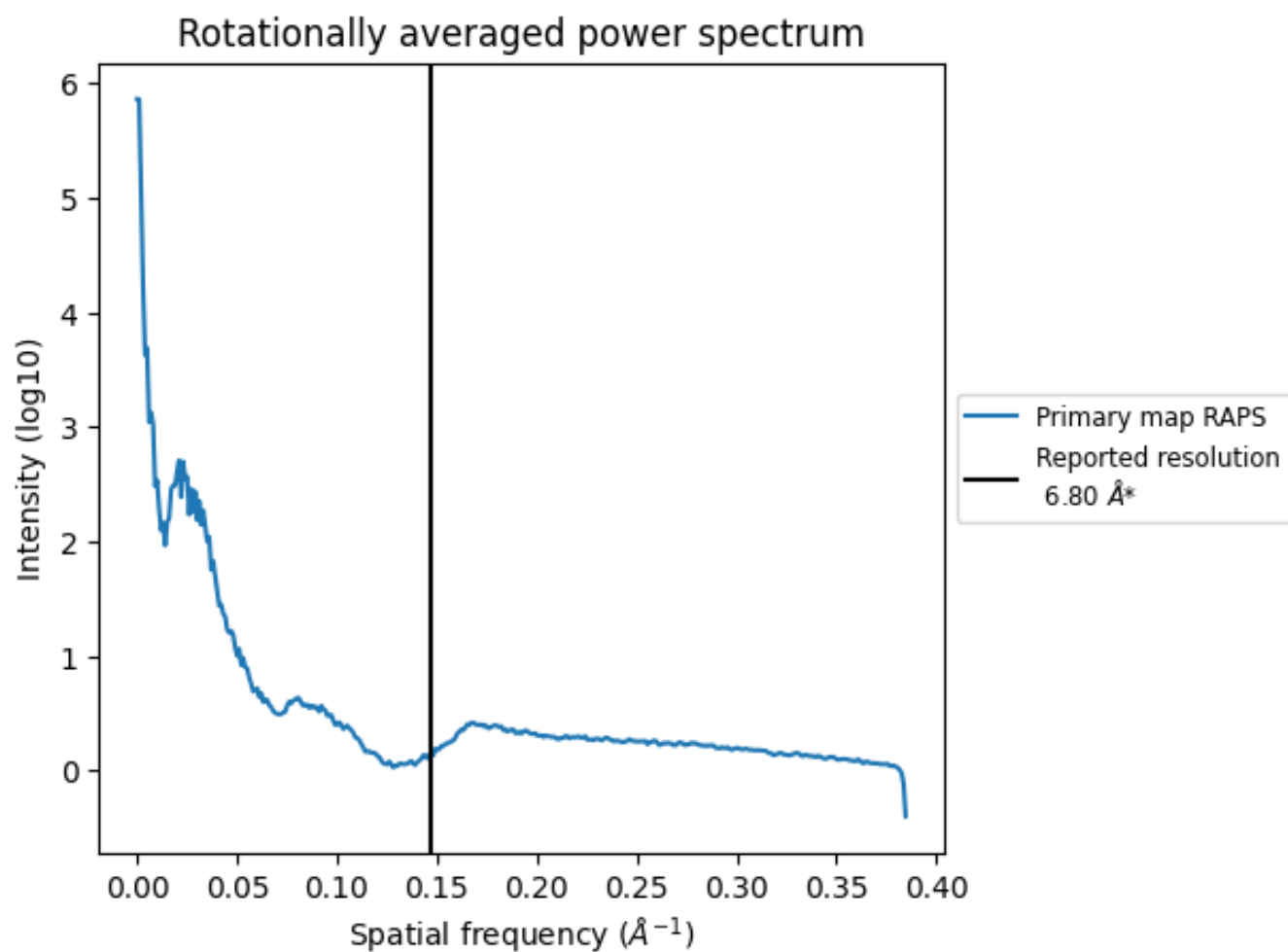
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31225 nm³; this corresponds to an approximate mass of 28206 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 ⓘ

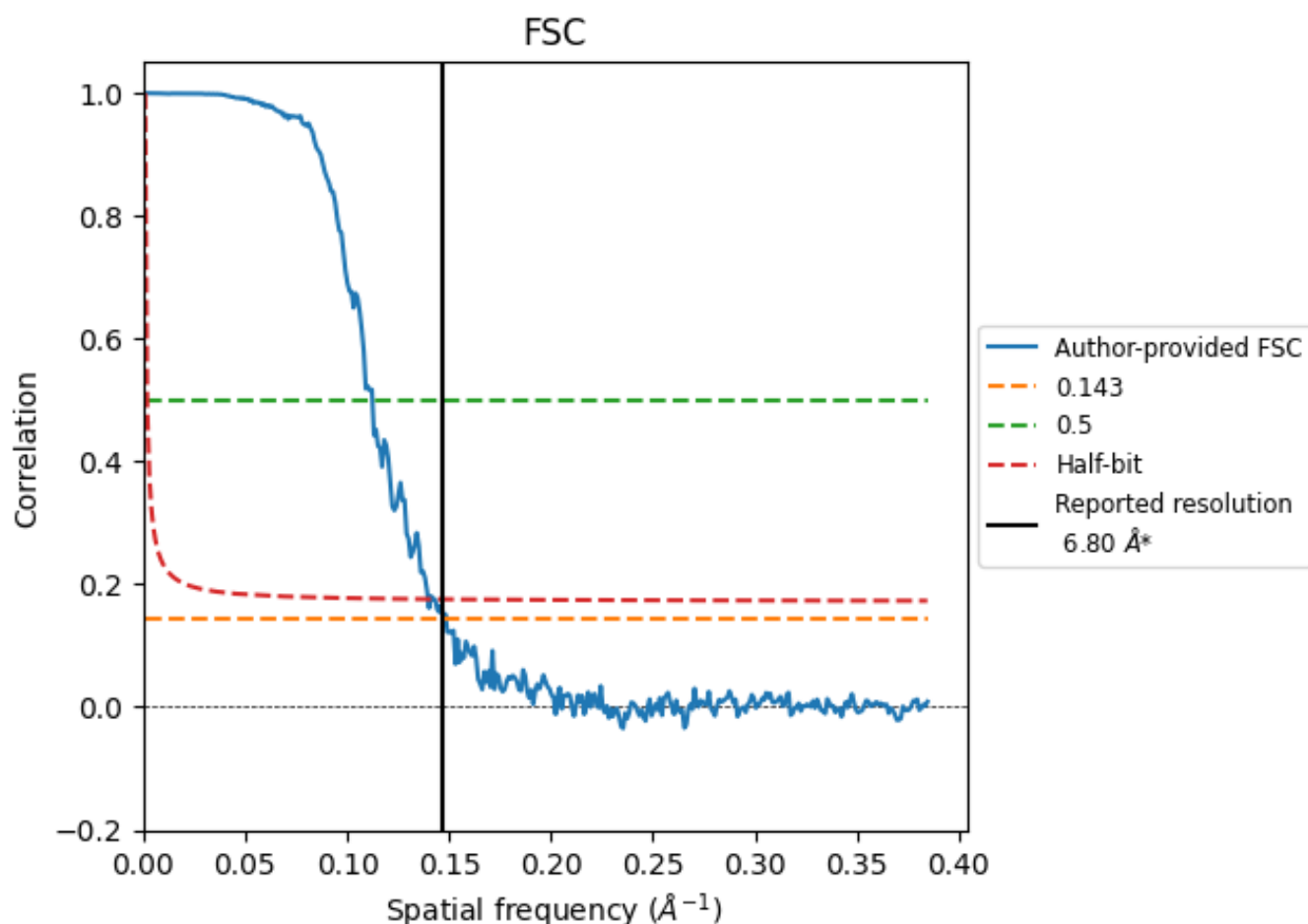


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.79	8.90	7.16
Unmasked-calculated*	-	-	-

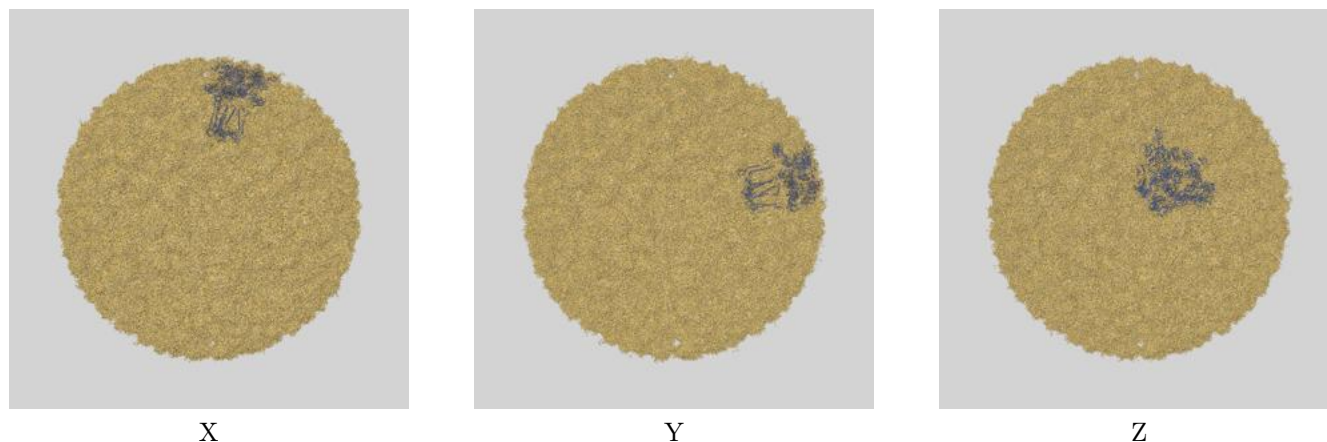
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

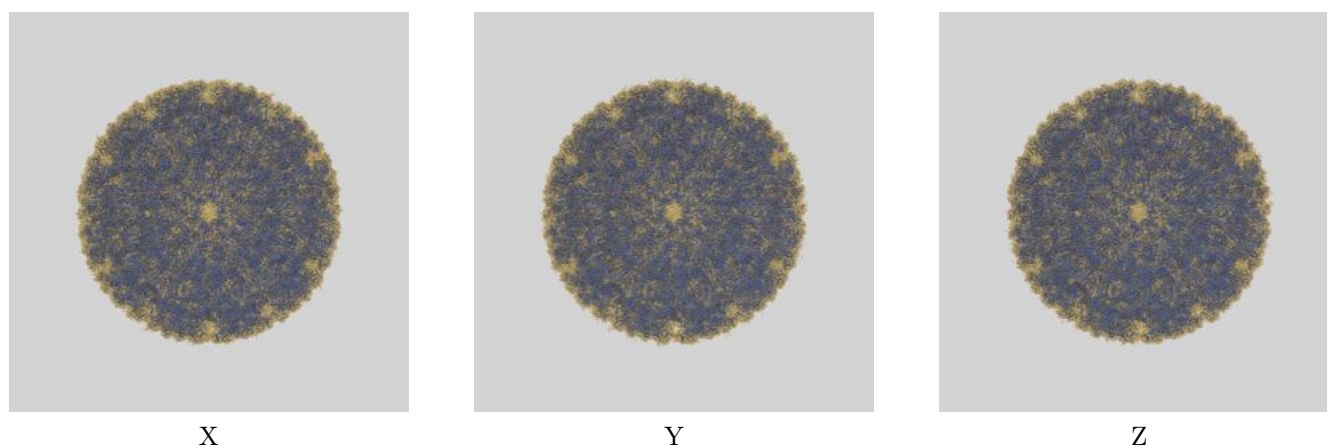
This section contains information regarding the fit between EMDB map EMD-8734 and PDB model 5VU2. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

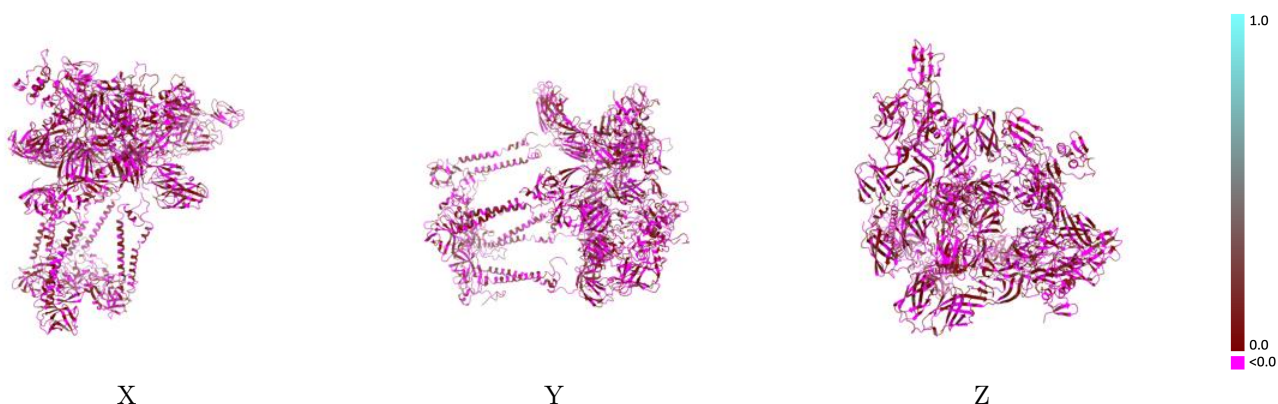


9.1.2 Map-model assembly overlay [i](#)



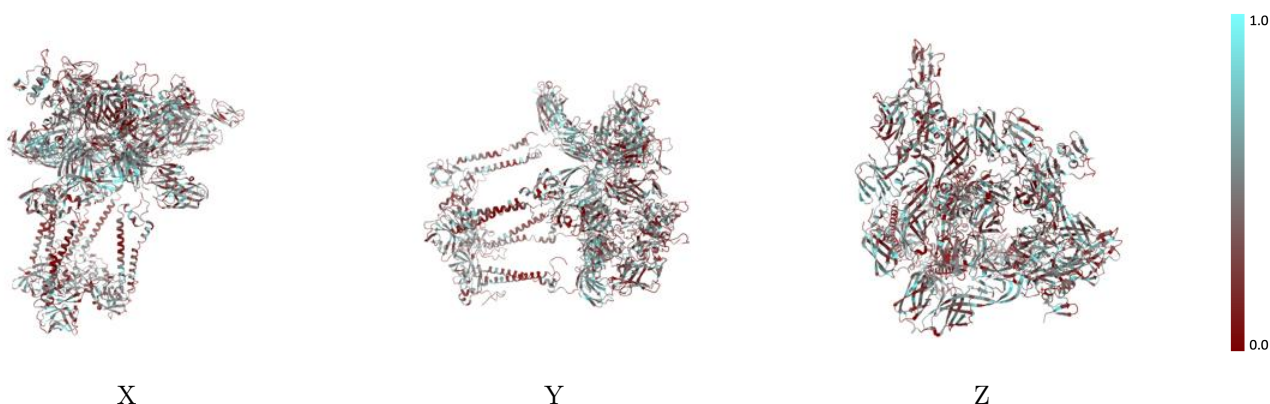
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



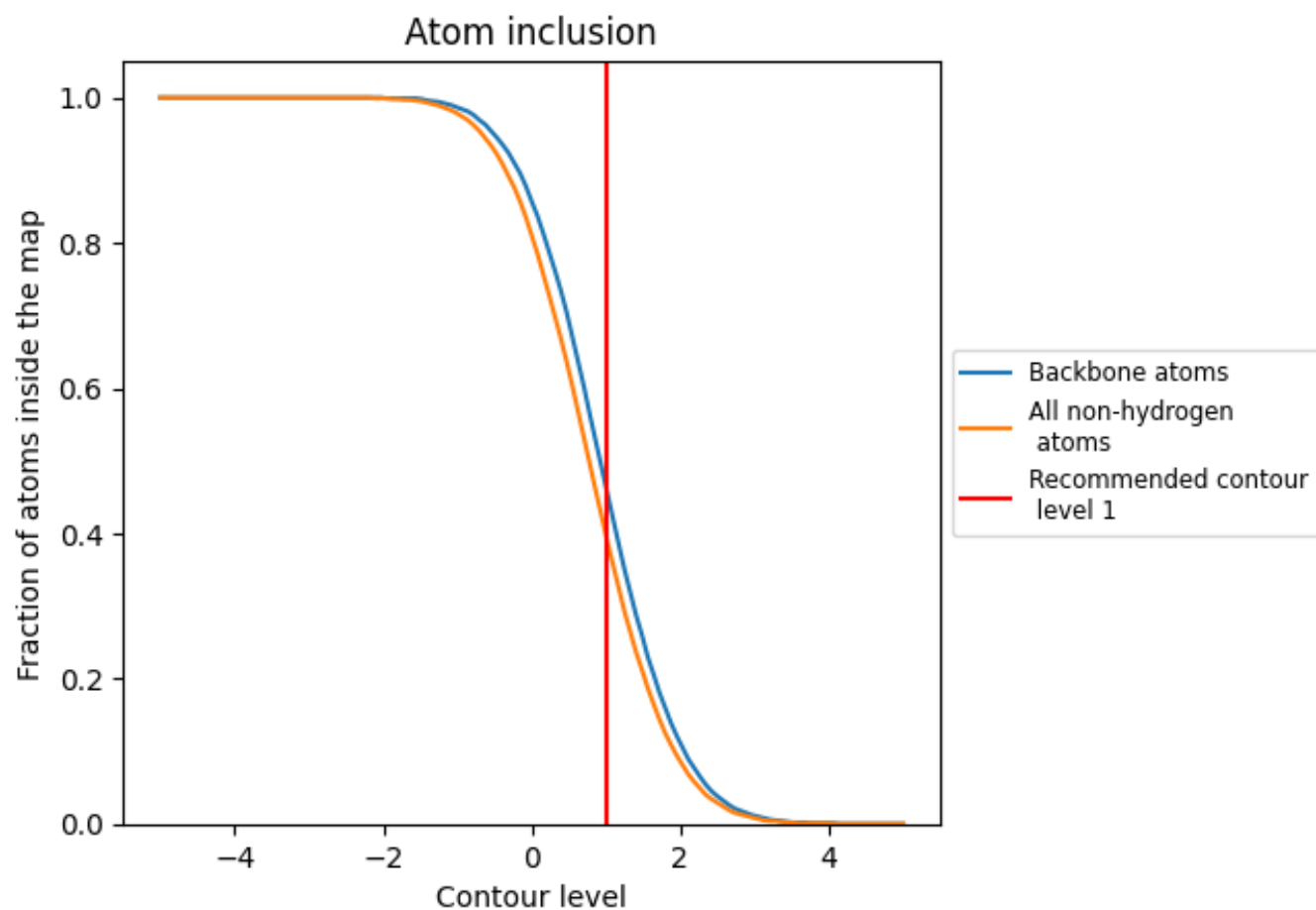
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 40% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3960	 0.0260
A	 0.4020	 0.0200
B	 0.3780	 0.0280
C	 0.3990	 0.0320
D	 0.3970	 0.0170
E	 0.2340	 0.0110
F	 0.2700	 -0.0000
G	 0.2550	 0.0270
H	 0.2670	 0.0410
I	 0.4030	 0.0230
J	 0.3990	 0.0310
K	 0.4060	 0.0420
L	 0.4090	 0.0280
M	 0.4430	 0.0360
N	 0.3780	 0.0180
O	 0.4520	 0.0360
P	 0.4680	 0.0290
Q	 0.3030	 0.0130
R	 0.3100	 0.0250
S	 0.2800	 0.0230
T	 0.3500	 0.0540
U	 0.3600	 -0.0090
V	 0.2730	 -0.0140
W	 0.3910	 -0.0000
X	 0.4210	 0.0210

