



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:50 AM UTC

PDB ID : 7BK0 / pdb_00007bk0
EMDB ID : EMD-12195
Title : Salmonella FliF ring (34mer) in intact basal body - C1
Authors : Johnson, S.; Furlong, E.; Lea, S.M.
Deposited on : 2021-01-14
Resolution : 3.80 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

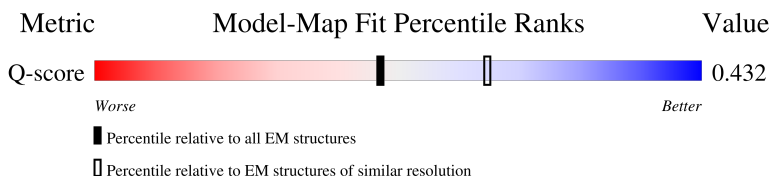
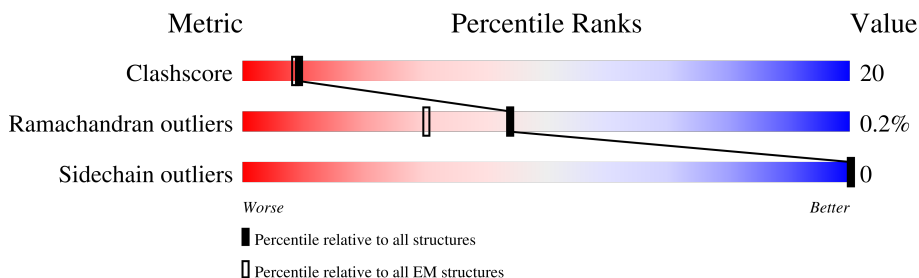
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	560	10% 19% 8% 73%
1	B	560	23% 28% 17% 55%
1	C	560	22% 27% 17% 55%
1	D	560	11% 18% 9% 73%

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Mol	Chain	Length	Quality of chain
1	E	560	
1	F	560	
1	G	560	
1	H	560	
1	I	560	
1	J	560	
1	K	560	
1	L	560	
1	M	560	
1	N	560	
1	O	560	
1	P	560	
1	Q	560	
1	R	560	
1	S	560	
1	T	560	
1	U	560	
1	V	560	
1	W	560	
1	X	560	
1	Y	560	
1	Z	560	
1	a	560	
1	b	560	
1	c	560	

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Mol	Chain	Length	Quality of chain
1	d	560	25%24%21%55%
1	e	560	9%18%9%73%
1	f	560	25%27%18%55%
1	g	560	23%25%19%55%
1	h	560	22%26%19%55%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 57536 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 Flagellar M-ring protein.

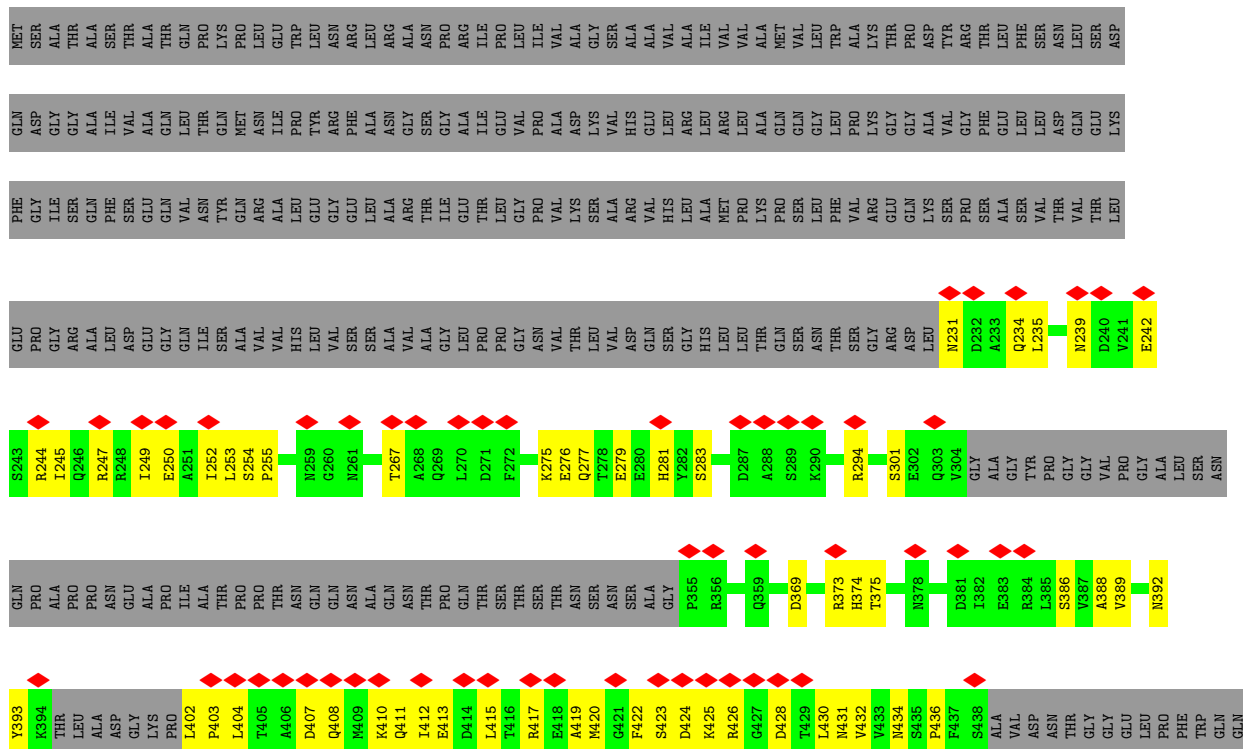
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	B	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	C	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	D	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	E	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	F	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	G	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	H	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	I	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	J	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	K	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	L	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	M	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	N	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	O	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	P	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	Q	250	Total 1931	C 1187	N 355	O 385	S 4	0	0

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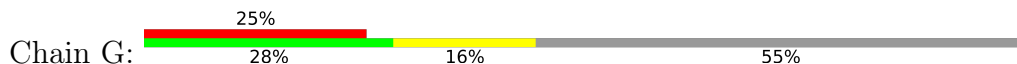
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	S	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	T	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	U	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	V	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	W	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	X	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	Y	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	Z	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	a	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	b	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	c	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	d	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	e	151	Total	C	N	O	S	0	0
			1193	726	223	241	3		
1	f	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	g	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		
1	h	250	Total	C	N	O	S	0	0
			1931	1187	355	385	4		





GLN	SER	ASP	GLN	LEU	LEU	ALA	GLY	ARG	TRP	LEU	VAL	VAL	ALA	ILE	TRP	ARG	LYS	VAL	ARG	PRO	GLN	LEU	THR	ARG	ARG	VAL	VAL	GLU	GLU	ALA	LYS	LYS	ALA	ALA	GLN	GLU	GLN	VAL	ARG	LEU		
SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ASN	GLN	ARG	GLY	VAL	VAL	MET	SER	GLN	ARG	ILE	ARG	GLU	MET	SER	VAL	ASP	ASN	ASP	PRO	ARG	VAL	VAL	ALA	ILE	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU

- Molecule 1: Flagellar M-ring protein

[illegible][illegible]

R184	R185	L186	D187	E188	G189	Q190	S192	A193		H196	L197	V198	S199	Z200	A201	V202	A203	G204	L205	P206	P207	G208	N209	V210	T211	L212	V213	D214	Q215	S216	G217	H218	L219	L220	L221	Q222	Q223	ASN	THR	SER	GLY	ARG	LEU	ASP	N231	D232	A233	Q234	L235	K236		N239	D240	V241	E242	S243	R244	T245
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	ASN	GLN	PRO	PRO	ALA	ALA	ASN	GLU	ALA	ALA	ILE	ALA	THR	PRO	PRO	TIR	ASN	GLN	GLN	ASN	GLN	GLN	ASN	ASN	TIR	TIR	GLN	TIR	SER	SER	SER	THR	ASN	SER	SER	ASN	ASN	ALA	ALA	GLY	P355	P356	P357	P358	Q359	R360	N361	E367	V368	D369	R370	R373	H374	M377	N378	V379	G380	D381	I382	F383
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◆ R384 ◆ L385 ◆ S386 ◆ V387 ◆ V388 ◆ A389 ◆ S390 ◆ S391 ◆ S392 ◆ Y393 ◆ Y394 ◆ THR ◆ LEU ◆ ALA ◆ ASP ◆ GLY ◆ LYS ◆ PRO ◆ L402 ◆ P403 ◆ L404 ◆ T405 ◆ A406 ◆ D407 ◆ Q408 ◆ M409 ◆ K410 ◆ Q411 ◆ T412 ◆ E413 ◆ D414 ◆ L415 ◆ T416 ◆ R417 ◆ E418 ◆ A419 ◆ M420 ◆ G421 ◆ F422 ◆ S423 ◆ D424 ◆ K425 ◆ R426 ◆ G427 ◆ D428 ◆ N431 ◆ V432 ◆ V433 ◆ A434 ◆ S435 ◆ P436 ◆ F437 ◆ S438 ◆ ALA ◆ VAL ◆ ASP ◆ ASN ◆ THR ◆ THR ◆ GLY

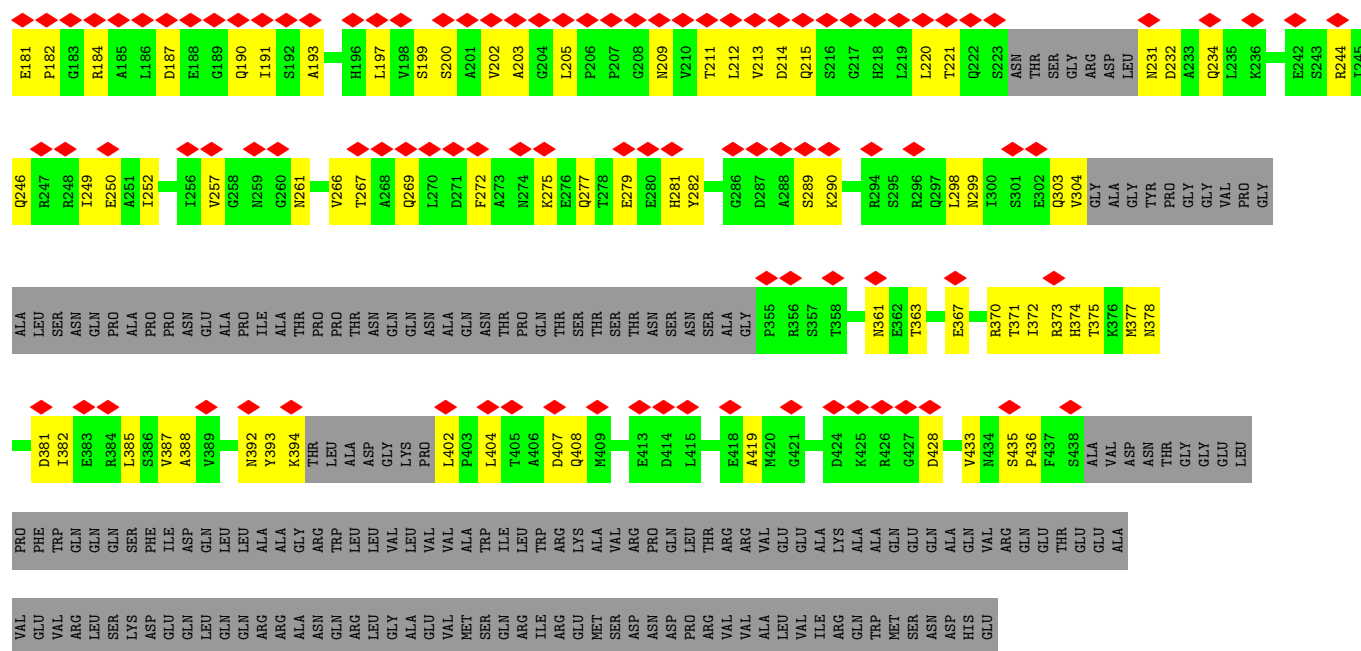
GLU LEU PRO PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL VAL VAL VAL ILE LEU TRP ARG LYS ALA ALA VAL ARG PRO GLN LEU LEU THR ARG ARG VAL GLU GLU ALA ALA LYS GLU GLN GLN ALA GLN VAL ARG GLU GLN THR

GLU	ALA	VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	ARG	ALA	ASN	GLN	ARG	LEU	GLY	ALA	GLU	VAL	MET	SER	GLN	ARG	ILE	ARG	GLU	MET	MET	SER	GLN	ASP	ASN	ASP	PRO	ARG	VAL	VAL	VAL	LEU	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU
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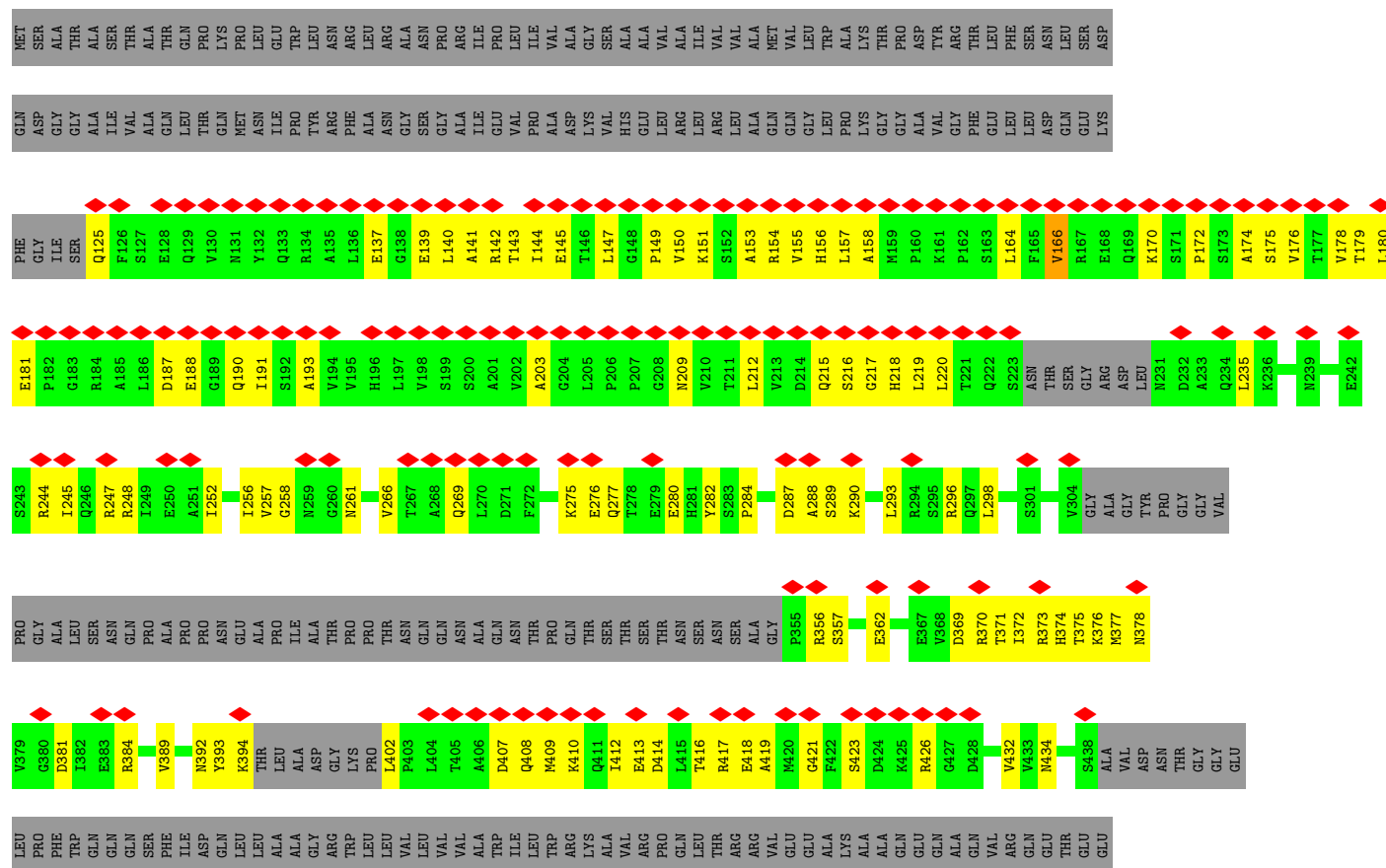
- Molecule 1: Flagellar M-ring protein

[illegible][illegible]

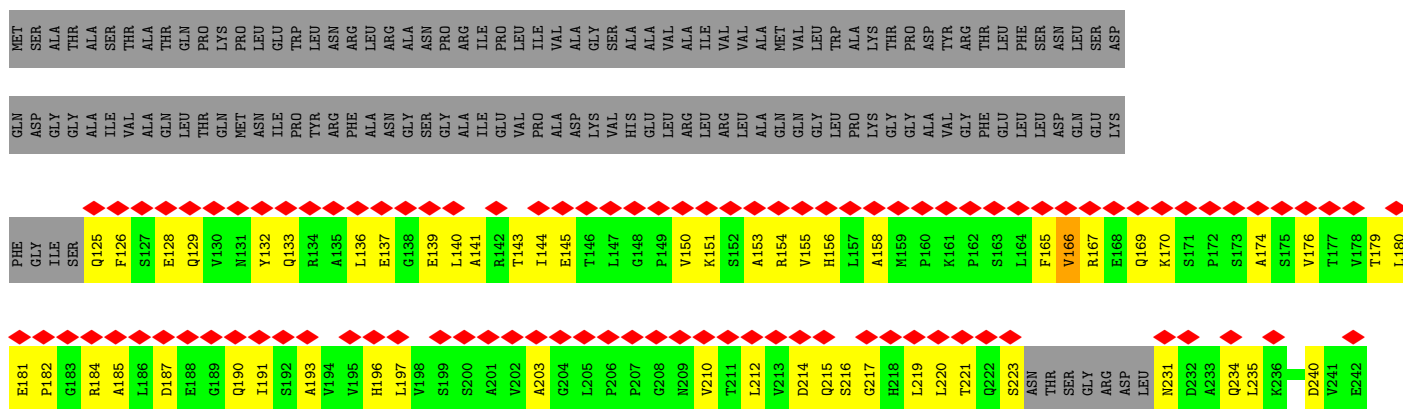


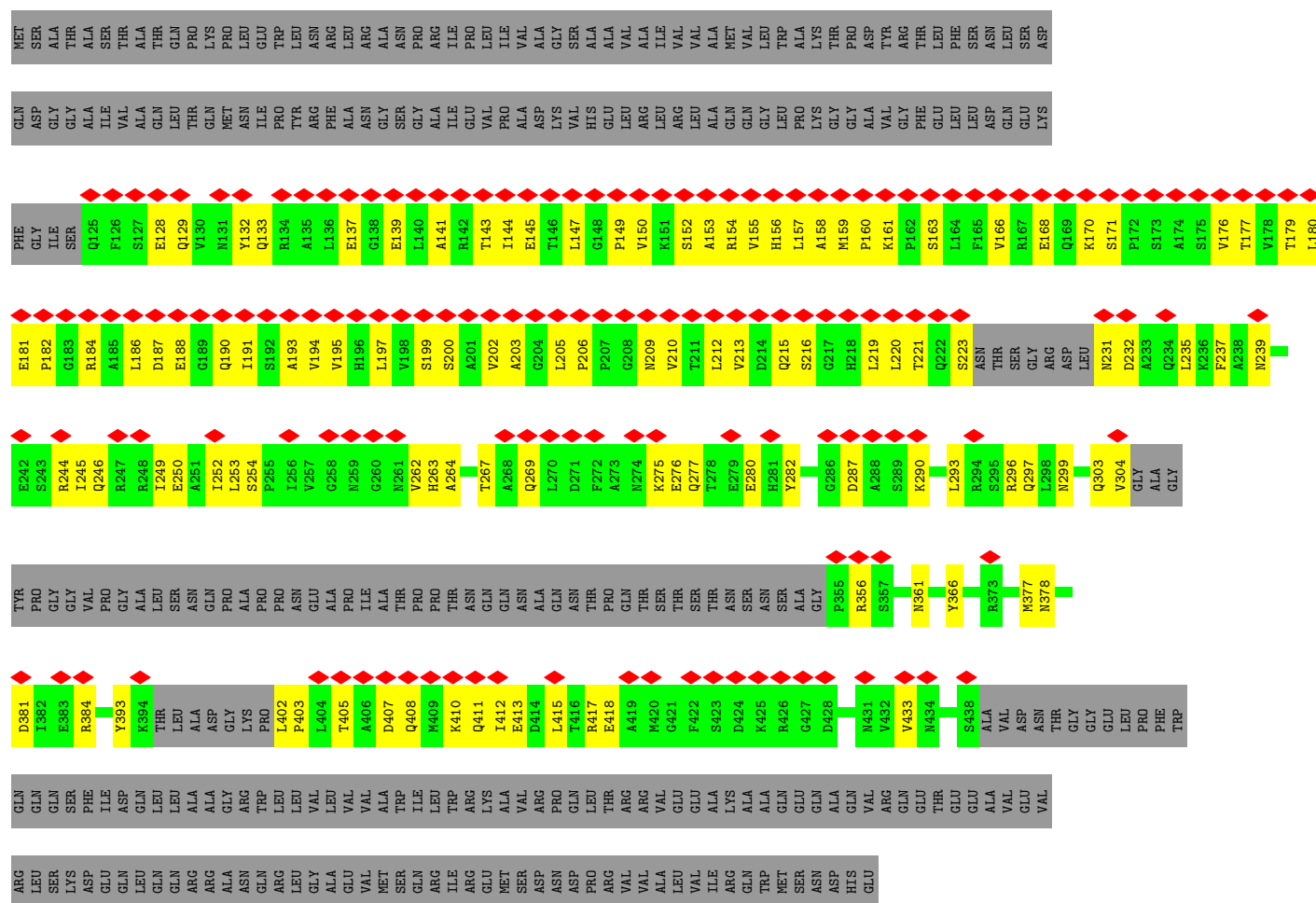


• Molecule 1: Flagellar M-ring protein

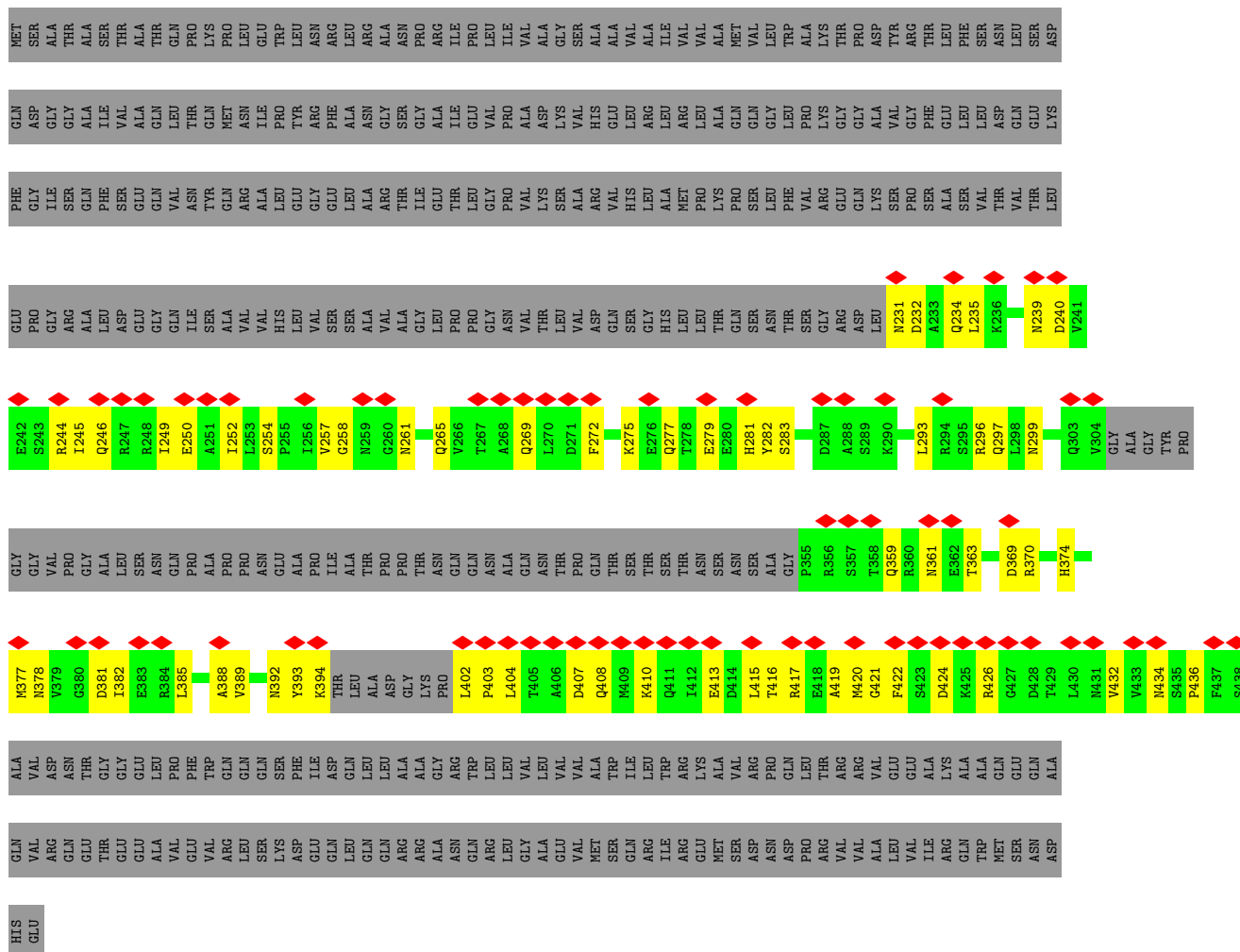


Chain M:

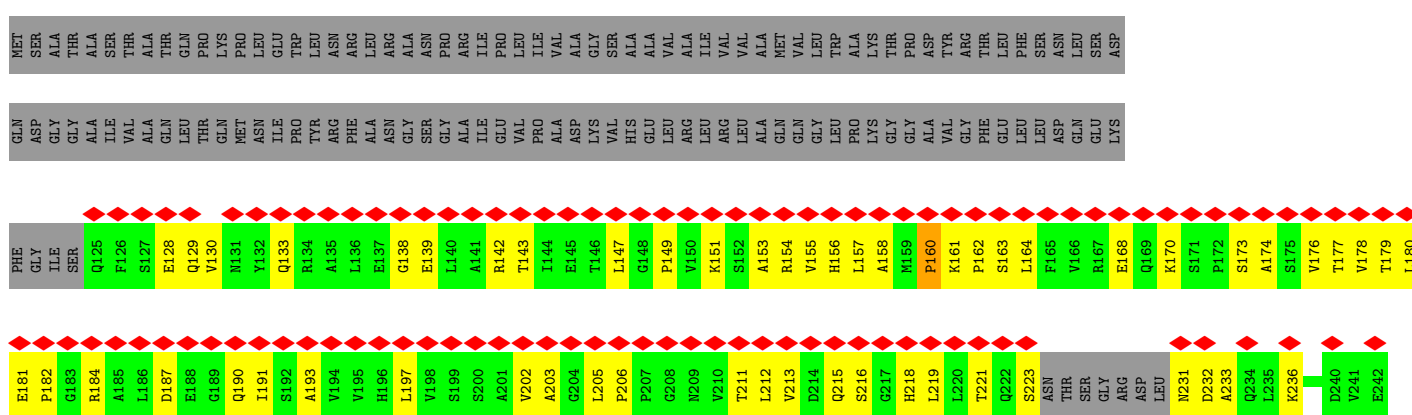




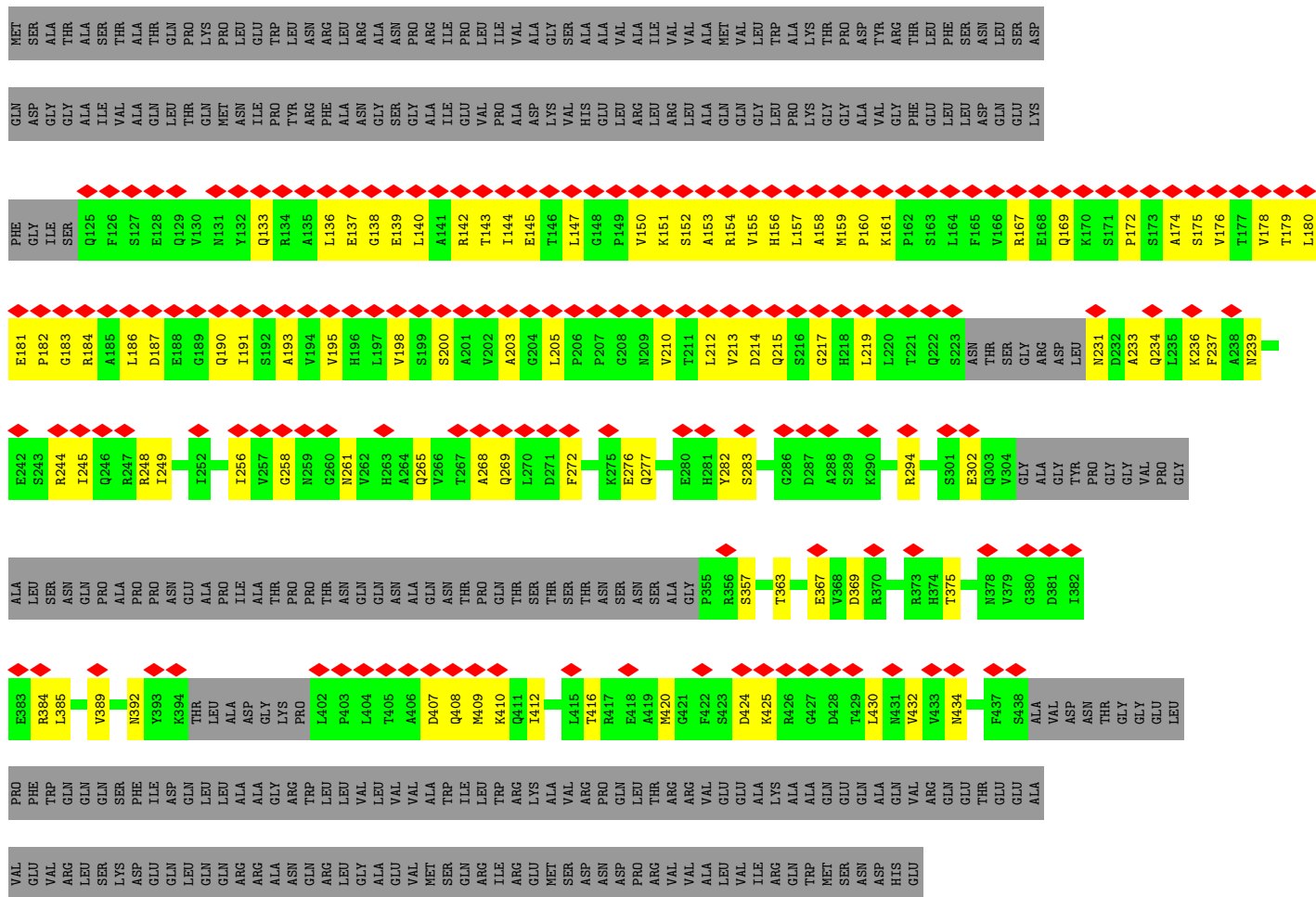
Chain P:



Chain Q:

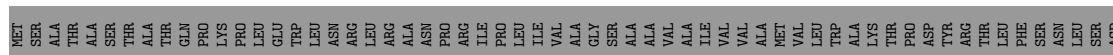


- Molecule 1: Flagellar M-ring protein



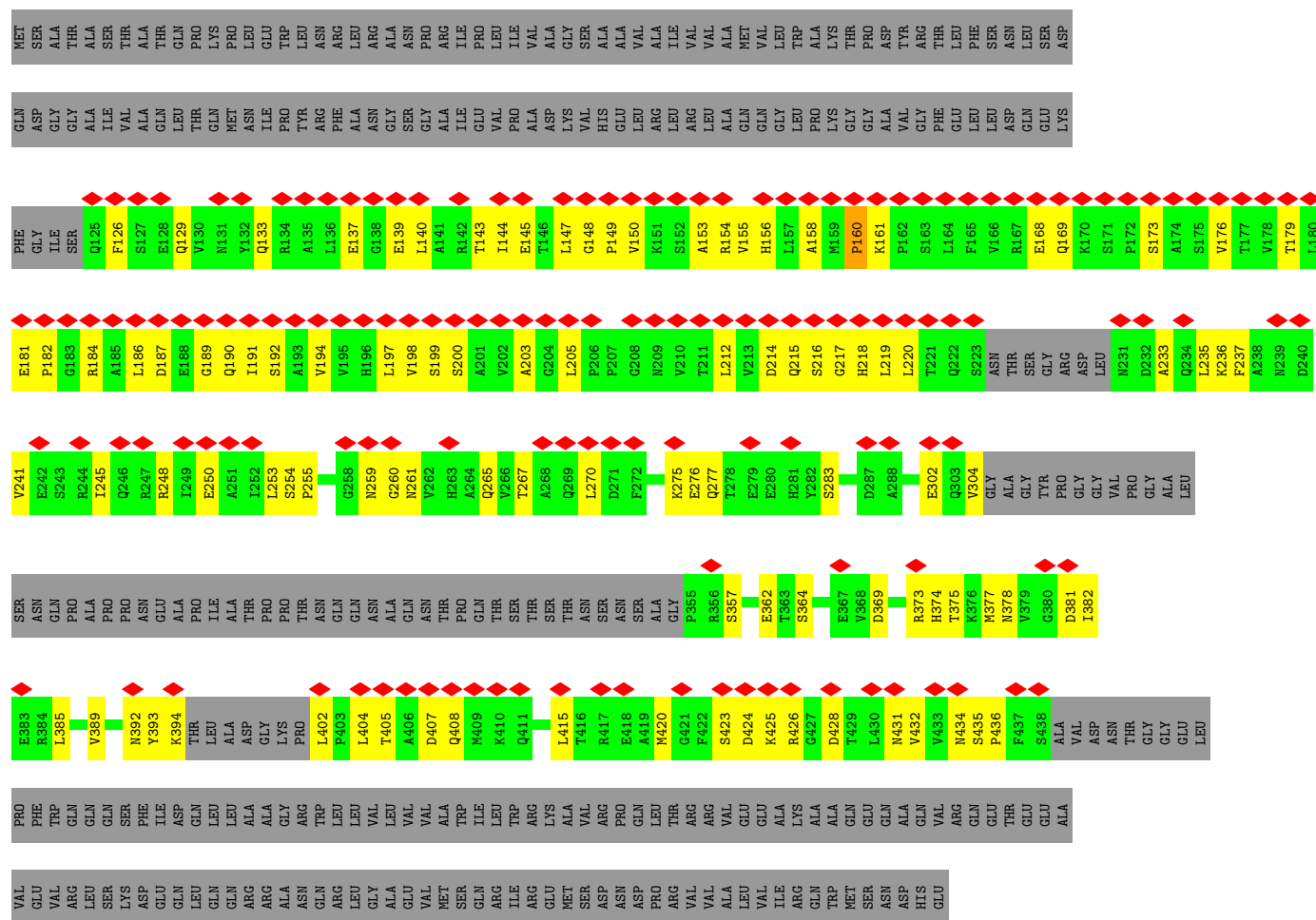
- Molecule 1: Flagellar M-ring protein



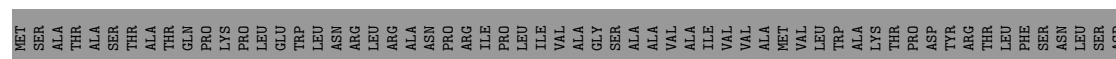




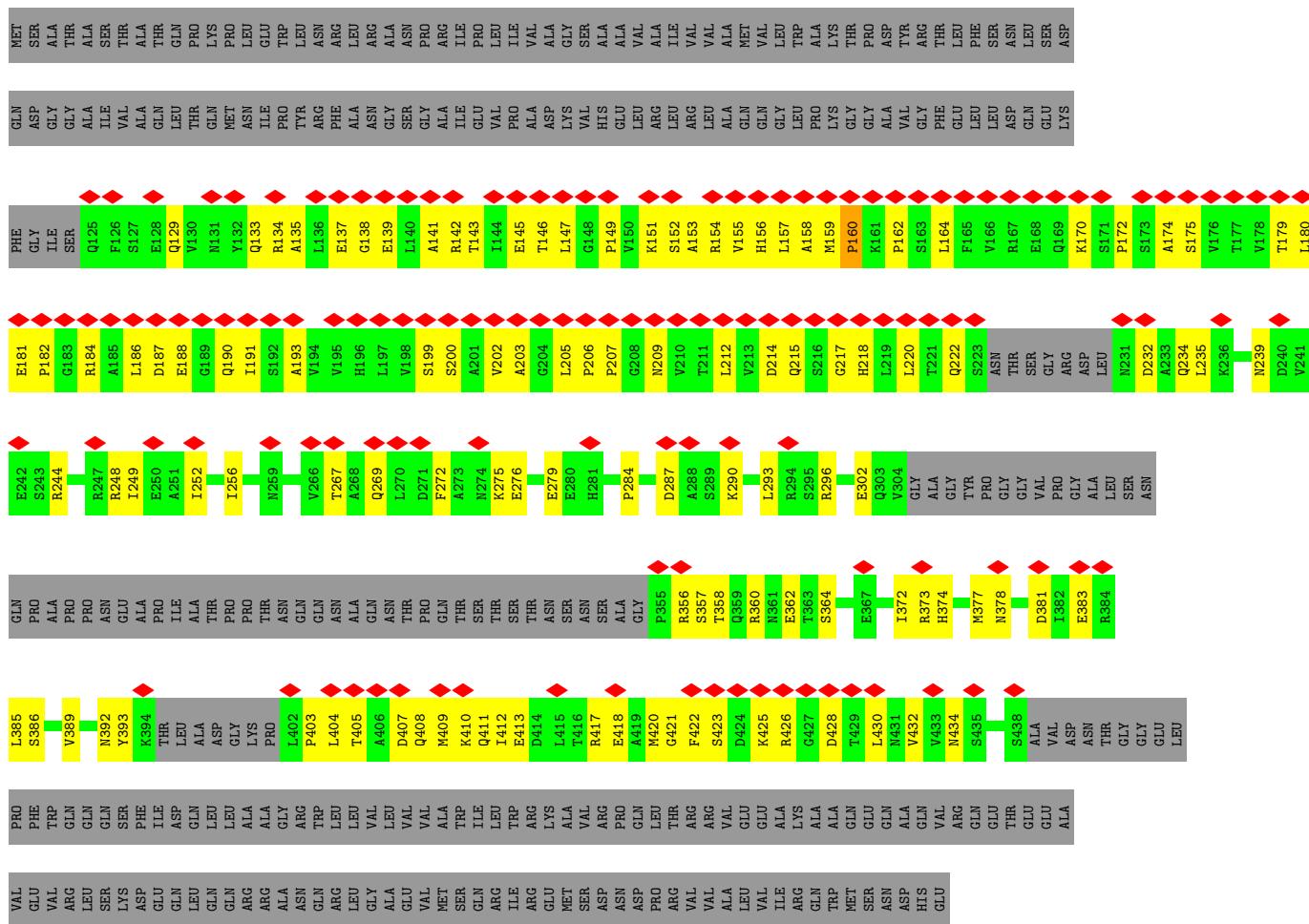
- Molecule 1: Flagellar M-ring protein



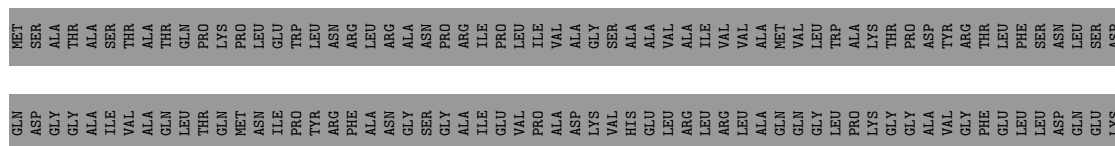
- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein



- Molecule 1: Flagellar M-ring protein





PRO	PHE	GLU	TRP	GLN	GLN	GLN	SER	PHE	ILE	GLN	ASP	GLN	LEU	LEU	ALA	ALA	GLY	ARG	GLN	TRP	LEU	LEU	VAL	VAL	VAL	VAL	ALA	TRP	ILE	LEU	TRP	ARG	GLY	LYS	ALA	VAL	GLU	GLU	LYS	ALA	ALA	GLN	GLU	GLN	ALA	GLN	ARG	GLN	GLU	THR	GLU	GLU	ALA
VAL	GLU	VAL	ARG	GLY	LEU	SER	LYS	ASP	GLU	GLN	LEU	LEU	GLN	GLN	ARG	ARG	ALA	ASN	GLN	ARG	LEU	LEU	GLY	ALA	GLU	VAL	VAL	MET	SER	GLN	ARG	ILE	TRP	ARG	VAL	VAL	ALA	LEU	LEU	VAL	ILE	ARG	GLN	TRP	MET	ASN	ASP	HIS	GLU				

● Molecule 1: Flagellar M-ring protein



ARG	LEU	SER	LYS	ASP	GLU	GLN	VAL	ARG	ALA	GLY	ALA	GLY	PRO	ASN	GLN	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
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● Molecule 1: Flagellar M-ring protein



PHE	GLY	ILE	SER	Q125	F126	S127	E128	M131	Y132	Q133	R134	A135	L136	E137	G138	E139	L140	A141	R142	T143	I144	E145	T146	L147	G148	P149	V150	K151	S152	A153	R154	V155	H156	L157	A158	M159	P160	K161	P162	S163	L164	F165	V166	R167	E168	Q169	K170	S171	P172	S173	A174	S175	V176	T177	V178	T179	L180	E181
MET	SER	THR	ALA	SER	ALA	ALA	THR	GLN	PRO	LYS	PRO	LEU	LEU	TRP	LEU	ASN	ARG	LEU	ARG	ALA	ASN	PRO	ARG	ILE	PRO	LEU	VAL	ALA	GLY	SER	ALA	VAL	VAL	VAL	MET	LEU	TRP	ALA	LYS	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	ASP						
GLN	ASP	GLY	GLY	ALA	ILE	VAL	ALA	GLN	GLN	MET	ASN	ILE	PRO	TYR	ARG	PHE	ASN	GLY	GLY	ILE	ILE	GLU	VAL	PRO	ALA	ASP	LYS	VAL	HIS	GLU	ARG	ILE	ARG	LEU	LEU	PRO	LYS	GLY	GLY	ALA	VAL	GLY	PHE	GLU	LEU	ASP	GLN	GLU	LYS									

VAL	GLU	VAL	ARG	LEU	SER	LYS	ASP	GLU	GLN	LEU	GLN	LEU	GLN	ARG	GLN	ARG	GLN	GLN	GLN	GLN	VAL	VAL	VAL	MET	SER	SER	ASP	ASN	PRO	ASP	PRO	ARG	VAL	VAL	ARG	VAL	VAL	LEU	LEU	VAL	VAL	ILE	ARG	GLN	TRP	MET	SER	ASN	HIS	GLU							
PHE	PHE	GLN	GLN	GLN	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	ALA	ALA	ARG	TRP	LEU	VAL	VAL	ALA	ALA	TRP	ILE	GLU	GLU	VAL	ARG	GLN	GLN	LEU	GLN	THR	ARG	VAL	VAL	VAL	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ALA									
S386	V387	A388	V389	V390	V391	N392	Y393	K394	THR	LEU	LEU	ALA	ASP	GLY	LYS	PRO	L402	P403	L404	T405	A406	D407	Q408	M409	K410	Q411	I412	E413	D414	L415	T416	R417	E418	A419	M420	S423	D424	K425	R426	G427	L430	N431	V432	V433	N434	S435	P436	F437	S438	ALA	VAL	ASP	ASN	THR	GLY	GLU	LEU
ALA	LEU	SER	ASN	GLN	PRO	ALA	PRO	ASN	GLU	ALA	ALA	PRO	THR	THR	ASN	GLN	GLN	ASN	GLN	GLN	ASN	GLN	GLN	ASN	THR	THR	SER	THR	SER	ASN	SER	ASN	SER	ALA	GLY	P355	R356	S357	E362	T363	S364	D369	R373	H374	M377	D381	I382	E383	R384	L385							
R247	R248	I249	E250	A251	I252	L253	S254	P255	I256	V257	G258	N259	G260	N261	H263	A264	Q265	V266	Q269	L270	D271	F272	A273	N274	K275	E279	E280	H281	Y282	S283	D287	A288	S289	K290	L293	R294	S295	R296	N299	E302	Q303	V304	GLY	ALA	GLY	TYR	PRO	GLY	GLY	VAL	PRO	GLY					
P182	G183	R184	A185	L186	D187	E188	G189	Q190	I191	S192	A193	V194	V195	H196	L197	V198	S199	V202	A203	G204	L205	N209	V210	T211	L212	V213	D214	Q215	S216	G217	H218	L219	L220	T221	Q222	S223	ASN	THR	SER	GLY	ARG	ASP	LEU	N231	Q234	F237	A238	N239	D240	V241	E242	S243	R244	I245	Q246		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60497	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.025	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	638.976, 638.976, 638.976	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/1205	0.48	0/1624
1	B	0.33	0/1955	0.53	0/2645
1	C	0.34	0/1955	0.52	2/2645 (0.1%)
1	D	0.36	0/1205	0.50	0/1624
1	E	0.32	0/1955	0.53	0/2645
1	F	0.35	0/1205	0.51	0/1624
1	G	0.33	0/1955	0.50	0/2645
1	H	0.34	0/1955	0.56	2/2645 (0.1%)
1	I	0.33	0/1955	0.48	0/2645
1	J	0.36	0/1205	0.50	0/1624
1	K	0.31	0/1955	0.53	2/2645 (0.1%)
1	L	0.32	0/1955	0.51	1/2645 (0.0%)
1	M	0.35	0/1205	0.51	0/1624
1	N	0.31	0/1955	0.54	1/2645 (0.0%)
1	O	0.30	0/1955	0.49	0/2645
1	P	0.32	0/1205	0.49	0/1624
1	Q	0.30	0/1955	0.48	0/2645
1	R	0.29	0/1955	0.47	0/2645
1	S	0.33	0/1205	0.47	0/1624
1	T	0.29	0/1955	0.50	0/2645
1	U	0.30	0/1955	0.56	2/2645 (0.1%)
1	V	0.33	0/1205	0.50	0/1624
1	W	0.29	0/1955	0.50	0/2645
1	X	0.30	0/1955	0.50	0/2645
1	Y	0.29	0/1955	0.49	0/2645
1	Z	0.35	0/1205	0.54	0/1624
1	a	0.30	0/1955	0.50	0/2645
1	b	0.35	0/1205	0.50	0/1624
1	c	0.31	0/1955	0.49	0/2645
1	d	0.32	0/1955	0.50	0/2645
1	e	0.35	0/1205	0.48	0/1624
1	f	0.32	0/1955	0.49	0/2645
1	g	0.32	0/1955	0.50	0/2645
1	h	0.32	0/1955	0.46	0/2645

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.32	0/58220	0.50	10/78699 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	G	0	1
1	H	0	1
1	L	0	1
1	N	0	1
All	All	0	6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	282	TYR	CA-C-N	-7.46	111.24	121.61
1	K	282	TYR	C-N-CA	-7.46	111.24	121.61
1	L	166	VAL	N-CA-C	-6.60	106.03	111.91
1	U	282	TYR	CA-C-N	-5.98	109.28	121.48
1	U	282	TYR	C-N-CA	-5.98	109.28	121.48
1	N	166	VAL	N-CA-C	-5.58	97.74	109.34
1	H	164	LEU	CA-C-N	5.56	132.16	121.54
1	H	164	LEU	C-N-CA	5.56	132.16	121.54
1	C	160	PRO	CA-C-N	5.11	134.27	121.80
1	C	160	PRO	C-N-CA	5.11	134.27	121.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	163	SER	Peptide
1	E	162	PRO	Peptide
1	G	165	PHE	Peptide
1	H	165	PHE	Peptide
1	L	125	GLN	Peptide
1	N	165	PHE	Peptide

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	1193	0	1173	46	0
1	B	1931	0	1925	85	0
1	C	1931	0	1925	84	0
1	D	1193	0	1173	41	0
1	E	1931	0	1925	102	0
1	F	1193	0	1173	53	0
1	G	1931	0	1925	79	0
1	H	1931	0	1925	102	0
1	I	1931	0	1925	97	0
1	J	1193	0	1173	56	0
1	K	1931	0	1925	86	0
1	L	1931	0	1925	111	0
1	M	1193	0	1173	72	0
1	N	1931	0	1925	111	0
1	O	1931	0	1925	101	0
1	P	1193	0	1173	50	0
1	Q	1931	0	1925	102	0
1	R	1931	0	1925	83	0
1	S	1193	0	1173	41	0
1	T	1931	0	1925	107	0
1	U	1931	0	1925	108	0
1	V	1193	0	1173	59	0
1	W	1931	0	1925	104	0
1	X	1931	0	1925	107	0
1	Y	1931	0	1925	108	0
1	Z	1193	0	1173	63	0
1	a	1931	0	1925	96	0
1	b	1193	0	1173	52	0
1	c	1931	0	1925	85	0
1	d	1931	0	1925	102	0
1	e	1193	0	1173	41	0
1	f	1931	0	1925	87	0
1	g	1931	0	1925	95	0
1	h	1931	0	1925	103	0
All	All	57536	0	57178	2329	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 20.

All (2329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:143:THR:HG23	1:h:154:ARG:HH21	1.30	0.95
1:R:143:THR:HG21	1:T:156:HIS:HE1	1.33	0.92
1:L:414:ASP:HB3	1:M:431:ASN:HD21	1.32	0.91
1:S:275:LYS:HB3	1:S:377:MET:HE2	1.55	0.89
1:S:387:VAL:HB	1:S:420:MET:HE2	1.55	0.88
1:h:275:LYS:HB2	1:h:377:MET:HB2	1.55	0.86
1:T:375:THR:HG23	1:U:275:LYS:HZ3	1.38	0.85
1:B:175:SER:HB2	1:h:197:LEU:HD12	1.56	0.85
1:X:301:SER:HB3	1:X:359:GLN:HB2	1.56	0.85
1:c:420:MET:HE1	1:c:430:LEU:HB2	1.56	0.85
1:M:416:THR:HG23	1:M:430:LEU:HD11	1.57	0.84
1:G:143:THR:HG22	1:H:154:ARG:HD2	1.58	0.84
1:A:267:THR:HG22	1:h:248:ARG:HH11	1.41	0.84
1:L:275:LYS:HB3	1:L:377:MET:HE2	1.60	0.84
1:g:191:ILE:HD13	1:g:220:LEU:HB3	1.60	0.84
1:H:275:LYS:HB2	1:H:377:MET:HB2	1.59	0.84
1:R:143:THR:HG23	1:T:154:ARG:HH21	1.42	0.83
1:c:214:ASP:HB3	1:c:218:HIS:HB2	1.60	0.83
1:a:179:THR:HA	1:a:215:GLN:HB3	1.60	0.83
1:H:420:MET:HE1	1:H:430:LEU:HD13	1.59	0.83
1:g:190:GLN:HG3	1:h:217:GLY:HA3	1.60	0.83
1:G:266:VAL:HG12	1:G:387:VAL:HG22	1.60	0.83
1:T:144:ILE:HG21	1:T:153:ALA:HB3	1.61	0.82
1:c:151:LYS:NZ	1:c:180:LEU:O	2.11	0.82
1:Z:275:LYS:HB3	1:Z:377:MET:HE2	1.62	0.82
1:B:151:LYS:HZ1	1:B:181:GLU:HA	1.42	0.81
1:g:151:LYS:NZ	1:g:180:LEU:O	2.13	0.81
1:A:277:GLN:OE1	1:h:373:ARG:NH1	2.12	0.81
1:O:203:ALA:HB1	1:Q:160:PRO:HA	1.60	0.81
1:J:277:GLN:HB3	1:J:375:THR:HB	1.61	0.81
1:E:139:GLU:HG2	1:G:154:ARG:HH11	1.45	0.80
1:Y:161:LYS:HD3	1:Y:162:PRO:HD2	1.63	0.80
1:K:190:GLN:HG2	1:L:217:GLY:HA3	1.62	0.80
1:O:275:LYS:HB2	1:O:377:MET:HB2	1.63	0.80
1:e:246:GLN:HE22	1:e:265:GLN:HA	1.46	0.80
1:G:275:LYS:HB2	1:G:377:MET:HB2	1.62	0.80
1:W:301:SER:HB3	1:W:359:GLN:HB3	1.64	0.80
1:L:244:ARG:HH22	1:M:239:ASN:HB2	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:417:ARG:HA	1:d:420:MET:HE2	1.65	0.79
1:f:275:LYS:HB2	1:f:377:MET:HB2	1.64	0.79
1:R:256:ILE:HG21	1:R:412:ILE:HD11	1.65	0.78
1:d:139:GLU:OE2	1:f:134:ARG:NH1	2.15	0.78
1:W:277:GLN:HB3	1:W:375:THR:HB	1.66	0.78
1:Y:151:LYS:NZ	1:Y:180:LEU:O	2.16	0.78
1:N:144:ILE:HG22	1:N:150:VAL:HG11	1.65	0.78
1:V:275:LYS:HB2	1:V:377:MET:HB2	1.65	0.78
1:X:246:GLN:NE2	1:X:250:GLU:OE2	2.17	0.78
1:W:139:GLU:OE2	1:X:154:ARG:NH1	2.13	0.78
1:N:245:ILE:HD11	1:N:420:MET:HA	1.66	0.77
1:H:166:VAL:O	1:H:167:ARG:NE	2.16	0.77
1:K:246:GLN:NE2	1:K:250:GLU:OE2	2.17	0.77
1:H:216:SER:O	1:H:218:HIS:ND1	2.11	0.77
1:O:149:PRO:HA	1:O:181:GLU:HG2	1.65	0.77
1:S:414:ASP:OD2	1:T:431:ASN:ND2	2.16	0.77
1:U:246:GLN:NE2	1:U:264:ALA:O	2.18	0.77
1:N:275:LYS:HB3	1:N:377:MET:HE2	1.66	0.77
1:X:161:LYS:HD2	1:X:162:PRO:HD2	1.64	0.77
1:N:126:PHE:HA	1:N:129:GLN:HE22	1.50	0.77
1:E:174:ALA:O	1:E:210:VAL:HA	1.84	0.76
1:f:151:LYS:NZ	1:f:180:LEU:O	2.17	0.76
1:g:414:ASP:OD2	1:h:431:ASN:ND2	2.18	0.76
1:G:242:GLU:HB2	1:G:266:VAL:HG23	1.67	0.76
1:T:413:GLU:OE2	1:T:417:ARG:NH1	2.18	0.76
1:W:275:LYS:HB2	1:W:377:MET:HB2	1.68	0.76
1:I:378:ASN:ND2	1:I:381:ASP:OD1	2.19	0.76
1:K:277:GLN:HB3	1:K:375:THR:HB	1.68	0.76
1:K:374:HIS:HB3	1:L:276:GLU:HB3	1.68	0.76
1:X:275:LYS:HB3	1:X:377:MET:HE2	1.68	0.76
1:R:193:ALA:HA	1:T:219:LEU:HG	1.66	0.76
1:J:275:LYS:HB2	1:J:377:MET:HB2	1.66	0.76
1:L:203:ALA:HA	1:N:158:ALA:HB1	1.67	0.76
1:U:416:THR:HG23	1:U:430:LEU:HD21	1.68	0.76
1:K:179:THR:HA	1:K:215:GLN:HB3	1.68	0.76
1:a:216:SER:O	1:a:218:HIS:ND1	2.18	0.76
1:Q:275:LYS:HB3	1:Q:377:MET:HE2	1.67	0.75
1:G:155:VAL:HG23	1:G:176:VAL:HG22	1.66	0.75
1:H:174:ALA:HB3	1:H:210:VAL:HG12	1.68	0.75
1:L:137:GLU:HG2	1:L:155:VAL:HG13	1.67	0.75
1:T:375:THR:HG23	1:U:275:LYS:NZ	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:129:GLN:O	1:K:133:GLN:NE2	2.20	0.75
1:L:172:PRO:O	1:L:209:ASN:ND2	2.20	0.75
1:Y:256:ILE:HG21	1:Y:412:ILE:HD11	1.68	0.75
1:Y:203:ALA:HB1	1:a:160:PRO:HA	1.69	0.75
1:N:257:VAL:O	1:N:261:ASN:ND2	2.20	0.75
1:F:244:ARG:HH22	1:G:239:ASN:HB2	1.52	0.74
1:L:421:GLY:O	1:L:426:ARG:NH2	2.20	0.74
1:U:139:GLU:HB3	1:W:156:HIS:HE1	1.52	0.74
1:d:235:LEU:O	1:d:239:ASN:ND2	2.20	0.74
1:Y:413:GLU:OE2	1:Y:417:ARG:NH1	2.20	0.74
1:e:275:LYS:HB2	1:e:377:MET:HB2	1.69	0.74
1:L:216:SER:O	1:L:218:HIS:ND1	2.18	0.74
1:Q:139:GLU:O	1:R:154:ARG:NH1	2.20	0.74
1:G:256:ILE:HG23	1:G:257:VAL:HG13	1.69	0.74
1:f:389:VAL:HB	1:f:432:VAL:HG12	1.70	0.74
1:g:420:MET:HE3	1:g:422:PHE:HB2	1.67	0.74
1:B:275:LYS:HB3	1:B:377:MET:HE2	1.69	0.74
1:E:161:LYS:O	1:E:169:GLN:NE2	2.21	0.74
1:b:374:HIS:HB3	1:c:276:GLU:HB3	1.69	0.74
1:K:257:VAL:O	1:K:261:ASN:ND2	2.20	0.73
1:a:168:GLU:HG2	1:a:169:GLN:H	1.52	0.73
1:d:244:ARG:HH11	1:e:235:LEU:HD13	1.53	0.73
1:I:180:LEU:HD11	1:I:186:LEU:HG	1.71	0.73
1:Q:153:ALA:HA	1:Q:177:THR:O	1.87	0.73
1:W:262:VAL:HG12	1:W:391:VAL:HG12	1.68	0.73
1:b:275:LYS:HB3	1:b:377:MET:HE2	1.68	0.73
1:d:373:ARG:NH2	1:e:277:GLN:HG2	2.03	0.73
1:L:149:PRO:HA	1:L:181:GLU:HG2	1.70	0.73
1:P:275:LYS:HB3	1:P:377:MET:HE2	1.70	0.73
1:E:179:THR:HA	1:E:215:GLN:HB3	1.71	0.73
1:X:197:LEU:HD12	1:Y:175:SER:HB2	1.70	0.73
1:C:420:MET:HE3	1:C:422:PHE:HB2	1.71	0.73
1:a:233:ALA:HA	1:a:236:LYS:HE2	1.70	0.73
1:U:248:ARG:HH11	1:V:267:THR:HG22	1.54	0.72
1:a:259:ASN:OD1	1:a:260:GLY:N	2.21	0.72
1:g:407:ASP:HA	1:g:410:LYS:HE3	1.71	0.72
1:E:375:THR:HG21	1:E:377:MET:HE2	1.71	0.72
1:Z:252:ILE:HD11	1:a:265:GLN:HB2	1.70	0.72
1:c:275:LYS:HB3	1:c:377:MET:HE2	1.70	0.72
1:N:296:ARG:NH2	1:O:366:TYR:OH	2.22	0.72
1:Y:405:THR:OG1	1:Y:407:ASP:OD1	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:253:LEU:HD11	1:Y:412:ILE:HG23	1.71	0.72
1:Z:233:ALA:HA	1:Z:236:LYS:HD3	1.70	0.72
1:L:151:LYS:NZ	1:L:180:LEU:O	2.22	0.72
1:O:378:ASN:ND2	1:O:381:ASP:OD1	2.22	0.72
1:X:142:ARG:HB2	1:Y:154:ARG:HH12	1.55	0.72
1:e:277:GLN:HE22	1:e:279:GLU:HB2	1.52	0.72
1:E:389:VAL:HB	1:E:432:VAL:HG22	1.71	0.72
1:F:373:ARG:NH2	1:G:277:GLN:OE1	2.23	0.72
1:H:197:LEU:HD12	1:I:175:SER:HB2	1.72	0.72
1:U:245:ILE:HG23	1:U:266:VAL:HG21	1.72	0.71
1:f:197:LEU:HD12	1:g:175:SER:HB2	1.71	0.71
1:O:180:LEU:HB2	1:O:215:GLN:HE22	1.55	0.71
1:Q:245:ILE:HD11	1:Q:420:MET:HA	1.71	0.71
1:R:375:THR:HG23	1:S:275:LYS:HZ3	1.54	0.71
1:b:360:ARG:NH1	1:b:362:GLU:OE2	2.23	0.71
1:f:257:VAL:O	1:f:261:ASN:ND2	2.19	0.71
1:E:277:GLN:HB3	1:E:375:THR:HB	1.73	0.71
1:H:143:THR:HG21	1:I:156:HIS:NE2	2.06	0.71
1:Q:151:LYS:HZ1	1:Q:182:PRO:HD3	1.54	0.71
1:V:250:GLU:O	1:V:254:SER:OG	2.09	0.71
1:X:203:ALA:HA	1:Y:158:ALA:HB1	1.73	0.71
1:g:139:GLU:O	1:h:154:ARG:NH2	2.24	0.71
1:S:404:LEU:HD23	1:S:408:GLN:HG2	1.71	0.71
1:M:360:ARG:NH1	1:M:362:GLU:OE1	2.24	0.70
1:F:231:ASN:O	1:F:234:GLN:NE2	2.24	0.70
1:Z:389:VAL:HB	1:Z:432:VAL:HG22	1.71	0.70
1:N:143:THR:HG23	1:O:154:ARG:HH21	1.55	0.70
1:Z:257:VAL:O	1:Z:261:ASN:ND2	2.24	0.70
1:d:181:GLU:HB3	1:d:184:ARG:HH21	1.55	0.70
1:E:143:THR:HG21	1:G:156:HIS:CE1	2.26	0.70
1:K:244:ARG:NH2	1:L:235:LEU:O	2.23	0.70
1:f:190:GLN:HG2	1:g:217:GLY:HA3	1.73	0.70
1:E:375:THR:OG1	1:F:275:LYS:NZ	2.24	0.70
1:H:248:ARG:HH11	1:I:267:THR:HG22	1.57	0.70
1:U:212:LEU:N	1:U:221:THR:OG1	2.24	0.70
1:L:275:LYS:HB2	1:L:377:MET:HB2	1.73	0.70
1:N:140:LEU:O	1:N:143:THR:OG1	2.08	0.70
1:U:160:PRO:HD3	1:U:172:PRO:HB3	1.72	0.70
1:G:378:ASN:ND2	1:G:381:ASP:OD1	2.20	0.70
1:I:244:ARG:NH1	1:J:239:ASN:OD1	2.24	0.70
1:L:414:ASP:HB3	1:M:431:ASN:ND2	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:362:GLU:OE2	1:X:364:SER:OG	2.10	0.70
1:g:195:VAL:HG13	1:g:210:VAL:HB	1.74	0.70
1:C:139:GLU:HG2	1:E:156:HIS:HE1	1.57	0.69
1:Q:213:VAL:HG22	1:Q:219:LEU:HD23	1.73	0.69
1:d:191:ILE:HG23	1:d:212:LEU:HD23	1.74	0.69
1:f:259:ASN:OD1	1:f:260:GLY:N	2.25	0.69
1:d:214:ASP:OD1	1:d:215:GLN:N	2.25	0.69
1:d:296:ARG:NH1	1:d:362:GLU:OE2	2.25	0.69
1:Q:190:GLN:HG2	1:R:217:GLY:HA3	1.74	0.69
1:X:139:GLU:OE2	1:Y:154:ARG:NH1	2.24	0.69
1:B:214:ASP:OD1	1:B:215:GLN:N	2.26	0.69
1:L:409:MET:HE1	1:L:434:ASN:HB2	1.74	0.69
1:Z:271:ASP:HB3	1:Z:383:GLU:OE2	1.92	0.69
1:h:394:LYS:HG2	1:h:402:LEU:HB2	1.74	0.69
1:E:373:ARG:NH1	1:F:277:GLN:OE1	2.24	0.69
1:E:378:ASN:ND2	1:E:381:ASP:OD1	2.24	0.69
1:I:182:PRO:O	1:I:184:ARG:NH1	2.25	0.69
1:Z:404:LEU:HD23	1:Z:408:GLN:HG2	1.74	0.69
1:d:179:THR:HA	1:d:215:GLN:HB3	1.74	0.69
1:g:244:ARG:HH11	1:h:239:ASN:HB2	1.57	0.69
1:Q:151:LYS:NZ	1:Q:180:LEU:O	2.25	0.69
1:Q:205:LEU:HD12	1:Q:206:PRO:HD2	1.73	0.69
1:U:139:GLU:HB3	1:W:156:HIS:CE1	2.27	0.69
1:W:413:GLU:OE2	1:W:417:ARG:NH1	2.26	0.69
1:a:200:SER:OG	1:c:173:SER:OG	2.11	0.69
1:c:214:ASP:OD1	1:c:215:GLN:N	2.26	0.69
1:c:275:LYS:HB2	1:c:377:MET:HB2	1.73	0.69
1:h:181:GLU:HB3	1:h:184:ARG:HH21	1.58	0.69
1:R:231:ASN:O	1:R:234:GLN:NE2	2.26	0.69
1:b:392:ASN:OD1	1:b:393:TYR:N	2.26	0.69
1:e:257:VAL:O	1:e:261:ASN:ND2	2.24	0.69
1:g:378:ASN:ND2	1:g:381:ASP:OD1	2.22	0.69
1:h:362:GLU:OE2	1:h:364:SER:OG	2.11	0.69
1:X:199:SER:OG	1:X:205:LEU:O	2.08	0.68
1:Q:143:THR:HG1	1:R:156:HIS:CE1	2.11	0.68
1:a:191:ILE:HG23	1:a:212:LEU:HD21	1.75	0.68
1:L:190:GLN:HG2	1:N:217:GLY:HA3	1.75	0.68
1:V:409:MET:HE1	1:V:434:ASN:HB2	1.74	0.68
1:H:155:VAL:HG23	1:H:176:VAL:HG22	1.75	0.68
1:X:416:THR:HG23	1:X:430:LEU:HD21	1.75	0.68
1:E:248:ARG:HH11	1:F:267:THR:HG22	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:LEU:HD11	1:O:177:THR:HG22	1.75	0.68
1:U:133:GLN:O	1:U:137:GLU:HG2	1.92	0.68
1:U:206:PRO:HG2	1:U:209:ASN:HB2	1.74	0.68
1:a:133:GLN:O	1:a:137:GLU:HG2	1.94	0.68
1:d:389:VAL:HB	1:d:432:VAL:HG12	1.75	0.68
1:I:203:ALA:HB1	1:K:160:PRO:HA	1.75	0.68
1:N:155:VAL:HG23	1:N:176:VAL:HG22	1.75	0.68
1:a:378:ASN:ND2	1:a:381:ASP:OD1	2.22	0.68
1:F:404:LEU:HD23	1:F:434:ASN:HD21	1.57	0.68
1:J:266:VAL:HG22	1:J:387:VAL:HG22	1.74	0.68
1:O:191:ILE:HG12	1:O:220:LEU:HD13	1.75	0.68
1:D:416:THR:HG23	1:D:430:LEU:HD11	1.76	0.68
1:M:414:ASP:OD2	1:N:431:ASN:ND2	2.27	0.68
1:Q:246:GLN:NE2	1:Q:250:GLU:OE2	2.27	0.68
1:H:190:GLN:HG2	1:I:217:GLY:HA3	1.75	0.67
1:C:275:LYS:HB2	1:C:377:MET:HB2	1.76	0.67
1:E:174:ALA:HB3	1:E:210:VAL:HG12	1.76	0.67
1:R:375:THR:HG23	1:S:275:LYS:NZ	2.09	0.67
1:W:233:ALA:HA	1:W:236:LYS:HE2	1.74	0.67
1:a:200:SER:HG	1:c:173:SER:HG	1.43	0.67
1:a:362:GLU:OE2	1:a:364:SER:OG	2.11	0.67
1:G:221:THR:HG22	1:G:223:SER:H	1.59	0.67
1:Q:179:THR:HA	1:Q:215:GLN:HB3	1.77	0.67
1:D:249:ILE:HD11	1:D:416:THR:HA	1.75	0.67
1:G:199:SER:HA	1:G:205:LEU:HD23	1.76	0.67
1:X:151:LYS:NZ	1:X:180:LEU:O	2.26	0.67
1:c:392:ASN:OD1	1:c:393:TYR:N	2.27	0.67
1:L:408:GLN:O	1:L:412:ILE:HG12	1.95	0.67
1:O:137:GLU:OE1	1:O:155:VAL:HG13	1.94	0.67
1:S:407:ASP:O	1:S:411:GLN:HG2	1.95	0.67
1:X:216:SER:HG	1:X:218:HIS:HE2	1.42	0.67
1:T:166:VAL:HG22	1:T:168:GLU:H	1.58	0.67
1:a:248:ARG:NH1	1:b:267:THR:OG1	2.26	0.67
1:C:155:VAL:HG23	1:C:176:VAL:HG22	1.75	0.67
1:I:253:LEU:HD11	1:I:412:ILE:HG23	1.75	0.67
1:Y:275:LYS:HB2	1:Y:377:MET:HB2	1.76	0.67
1:B:256:ILE:HG21	1:B:412:ILE:HD11	1.75	0.67
1:J:360:ARG:NH1	1:J:362:GLU:OE2	2.27	0.67
1:d:145:GLU:OE2	1:d:153:ALA:N	2.27	0.67
1:g:182:PRO:O	1:g:184:ARG:NH1	2.28	0.67
1:E:275:LYS:HB2	1:E:377:MET:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:181:GLU:HB3	1:g:184:ARG:HH21	1.60	0.66
1:C:362:GLU:OE2	1:C:364:SER:OG	2.14	0.66
1:D:253:LEU:HD11	1:D:412:ILE:HG23	1.77	0.66
1:I:151:LYS:NZ	1:I:180:LEU:O	2.28	0.66
1:E:203:ALA:HA	1:G:158:ALA:HB1	1.78	0.66
1:L:370:ARG:HB3	1:M:280:GLU:OE1	1.96	0.66
1:c:145:GLU:OE1	1:c:153:ALA:N	2.28	0.66
1:c:246:GLN:NE2	1:c:250:GLU:OE2	2.27	0.66
1:B:151:LYS:NZ	1:B:181:GLU:HA	2.10	0.66
1:B:203:ALA:HA	1:C:158:ALA:HB1	1.77	0.66
1:X:216:SER:OG	1:X:218:HIS:NE2	2.28	0.66
1:h:132:TYR:CZ	1:h:136:LEU:HD11	2.30	0.66
1:N:423:SER:OG	1:N:425:LYS:NZ	2.29	0.66
1:P:296:ARG:NH2	1:Q:366:TYR:OH	2.28	0.66
1:Q:157:LEU:HD11	1:Q:202:VAL:HG21	1.76	0.66
1:R:179:THR:HA	1:R:215:GLN:HB3	1.76	0.66
1:S:362:GLU:OE2	1:S:364:SER:OG	2.13	0.66
1:c:203:ALA:HA	1:d:158:ALA:HB1	1.76	0.66
1:g:203:ALA:HA	1:h:158:ALA:HB1	1.76	0.66
1:C:378:ASN:ND2	1:C:381:ASP:OD1	2.29	0.66
1:I:409:MET:HE3	1:I:434:ASN:HB2	1.78	0.66
1:N:394:LYS:HG2	1:N:402:LEU:HB2	1.77	0.66
1:Q:139:GLU:HG3	1:R:156:HIS:CE1	2.30	0.66
1:U:275:LYS:HB2	1:U:377:MET:HB2	1.78	0.66
1:Y:149:PRO:HA	1:Y:181:GLU:HG2	1.77	0.66
1:A:404:LEU:H	1:A:434:ASN:HD21	1.41	0.66
1:J:302:GLU:HG2	1:J:358:THR:HG22	1.78	0.66
1:R:174:ALA:HB3	1:R:210:VAL:HG22	1.77	0.66
1:B:195:VAL:HG13	1:B:210:VAL:HG21	1.78	0.66
1:T:199:SER:HA	1:T:205:LEU:HD23	1.77	0.66
1:J:250:GLU:O	1:J:254:SER:OG	2.11	0.66
1:M:279:GLU:OE1	1:M:281:HIS:ND1	2.29	0.66
1:R:277:GLN:HB3	1:R:375:THR:HB	1.77	0.66
1:g:187:ASP:O	1:g:191:ILE:HG13	1.96	0.66
1:Y:190:GLN:HG2	1:a:217:GLY:HA3	1.78	0.65
1:a:145:GLU:OE2	1:a:153:ALA:N	2.28	0.65
1:d:152:SER:HB3	1:d:179:THR:HB	1.77	0.65
1:N:181:GLU:OE1	1:N:184:ARG:NH2	2.29	0.65
1:U:144:ILE:HG22	1:U:150:VAL:HG11	1.78	0.65
1:V:420:MET:HE3	1:V:422:PHE:HB2	1.78	0.65
1:B:160:PRO:HA	1:h:203:ALA:HB1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:195:VAL:HG22	1:R:212:LEU:HD13	1.77	0.65
1:g:392:ASN:OD1	1:g:393:TYR:N	2.30	0.65
1:H:245:ILE:HD11	1:H:420:MET:HA	1.79	0.65
1:H:378:ASN:ND2	1:H:381:ASP:OD1	2.24	0.65
1:U:287:ASP:HB3	1:U:290:LYS:HE3	1.78	0.65
1:U:370:ARG:HB3	1:V:280:GLU:OE2	1.95	0.65
1:X:279:GLU:OE2	1:X:281:HIS:N	2.30	0.65
1:d:193:ALA:HA	1:f:219:LEU:HD12	1.78	0.65
1:N:137:GLU:HB2	1:N:155:VAL:HG13	1.78	0.65
1:X:214:ASP:HB2	1:X:218:HIS:HB2	1.77	0.65
1:f:416:THR:HG23	1:f:430:LEU:HD21	1.78	0.65
1:E:392:ASN:OD1	1:E:393:TYR:N	2.30	0.65
1:O:200:SER:OG	1:Q:174:ALA:O	2.13	0.65
1:b:245:ILE:HG23	1:b:266:VAL:HG21	1.77	0.65
1:b:275:LYS:HB2	1:b:377:MET:HB2	1.79	0.65
1:C:191:ILE:HG23	1:C:212:LEU:HD12	1.77	0.65
1:N:166:VAL:HG12	1:N:167:ARG:H	1.61	0.65
1:X:413:GLU:OE2	1:X:417:ARG:NH1	2.30	0.65
1:g:279:GLU:OE2	1:g:281:HIS:N	2.25	0.65
1:B:193:ALA:HA	1:C:219:LEU:HG	1.79	0.65
1:C:151:LYS:NZ	1:C:180:LEU:O	2.30	0.65
1:I:373:ARG:HH21	1:J:275:LYS:HE2	1.61	0.65
1:M:231:ASN:OD1	1:M:232:ASP:N	2.30	0.65
1:N:180:LEU:HD13	1:N:185:ALA:HA	1.78	0.65
1:U:244:ARG:HH11	1:V:239:ASN:HB2	1.62	0.65
1:W:139:GLU:O	1:W:143:THR:HG23	1.97	0.65
1:G:392:ASN:OD1	1:G:393:TYR:N	2.30	0.64
1:T:157:LEU:HD11	1:T:202:VAL:HG21	1.79	0.64
1:f:203:ALA:HB1	1:g:160:PRO:HA	1.77	0.64
1:L:145:GLU:OE2	1:L:153:ALA:N	2.29	0.64
1:R:153:ALA:HB2	1:R:178:VAL:HG23	1.80	0.64
1:h:293:LEU:HD13	1:h:296:ARG:HD2	1.80	0.64
1:G:142:ARG:O	1:H:154:ARG:NH1	2.30	0.64
1:K:140:LEU:O	1:K:144:ILE:HG13	1.97	0.64
1:Q:250:GLU:O	1:Q:254:SER:OG	2.14	0.64
1:R:151:LYS:HZ1	1:R:182:PRO:HD3	1.61	0.64
1:f:301:SER:OG	1:f:303:GLN:NE2	2.26	0.64
1:T:293:LEU:HD13	1:T:296:ARG:HH12	1.61	0.64
1:a:276:GLU:OE2	1:a:374:HIS:NE2	2.31	0.64
1:G:257:VAL:O	1:G:261:ASN:ND2	2.30	0.64
1:T:203:ALA:H	1:U:158:ALA:HB1	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:163:SER:H	1:I:169:GLN:HE22	1.42	0.64
1:J:271:ASP:OD2	1:J:381:ASP:N	2.30	0.64
1:L:248:ARG:NH2	1:M:242:GLU:OE1	2.31	0.64
1:P:257:VAL:O	1:P:261:ASN:ND2	2.29	0.64
1:F:393:TYR:HB3	1:F:402:LEU:N	2.12	0.64
1:f:407:ASP:HA	1:f:410:LYS:HG2	1.80	0.64
1:R:424:ASP:OD1	1:R:425:LYS:NZ	2.27	0.64
1:E:182:PRO:O	1:E:184:ARG:NH1	2.31	0.64
1:L:275:LYS:HE3	1:L:275:LYS:HA	1.80	0.64
1:V:266:VAL:HG22	1:V:387:VAL:HG22	1.80	0.64
1:V:296:ARG:NH2	1:V:362:GLU:OE2	2.31	0.64
1:d:256:ILE:HG21	1:d:412:ILE:HD11	1.78	0.64
1:d:293:LEU:HD11	1:d:296:ARG:HH21	1.63	0.64
1:E:151:LYS:NZ	1:E:181:GLU:HA	2.14	0.63
1:X:180:LEU:N	1:X:215:GLN:OE1	2.27	0.63
1:a:143:THR:HG21	1:c:156:HIS:NE2	2.13	0.63
1:f:231:ASN:OD1	1:f:232:ASP:N	2.31	0.63
1:C:392:ASN:OD1	1:C:393:TYR:N	2.32	0.63
1:I:373:ARG:NH1	1:J:277:GLN:OE1	2.31	0.63
1:f:283:SER:HB2	1:f:369:ASP:HB2	1.80	0.63
1:G:373:ARG:NH1	1:H:277:GLN:OE1	2.30	0.63
1:H:394:LYS:HG2	1:H:402:LEU:HB2	1.79	0.63
1:N:197:LEU:HD12	1:O:213:VAL:HG21	1.80	0.63
1:U:140:LEU:O	1:U:143:THR:OG1	2.15	0.63
1:f:304:VAL:HG22	1:f:356:ARG:HG2	1.78	0.63
1:H:151:LYS:HZ1	1:H:182:PRO:HD3	1.62	0.63
1:N:231:ASN:O	1:N:234:GLN:NE2	2.31	0.63
1:P:407:ASP:OD1	1:P:408:GLN:N	2.32	0.63
1:Q:138:GLY:O	1:Q:142:ARG:HG2	1.99	0.63
1:U:191:ILE:HG23	1:U:212:LEU:HD23	1.79	0.63
1:W:392:ASN:OD1	1:W:393:TYR:N	2.31	0.63
1:Y:216:SER:O	1:Y:218:HIS:ND1	2.32	0.63
1:Y:407:ASP:OD1	1:Y:408:GLN:N	2.32	0.63
1:Z:375:THR:HG23	1:a:275:LYS:NZ	2.13	0.63
1:b:231:ASN:O	1:b:234:GLN:NE2	2.31	0.63
1:C:140:LEU:O	1:C:143:THR:OG1	2.15	0.63
1:D:389:VAL:HB	1:D:432:VAL:HG22	1.81	0.63
1:Z:392:ASN:OD1	1:Z:393:TYR:N	2.30	0.63
1:A:279:GLU:OE2	1:A:281:HIS:N	2.32	0.63
1:B:161:LYS:NZ	1:B:163:SER:HA	2.13	0.63
1:W:197:LEU:HG	1:X:175:SER:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:133:GLN:O	1:T:137:GLU:HG2	1.99	0.63
1:V:385:LEU:N	1:V:428:ASP:OD2	2.31	0.63
1:G:246:GLN:NE2	1:G:250:GLU:OE2	2.32	0.63
1:d:133:GLN:HE21	1:d:157:LEU:HB2	1.62	0.63
1:N:275:LYS:HB2	1:N:377:MET:HB2	1.81	0.62
1:P:402:LEU:HD12	1:P:403:PRO:HD2	1.81	0.62
1:V:256:ILE:HG23	1:V:257:VAL:HG13	1.80	0.62
1:a:424:ASP:OD1	1:a:425:LYS:N	2.32	0.62
1:d:137:GLU:OE1	1:d:155:VAL:HG13	1.99	0.62
1:D:409:MET:HE2	1:D:409:MET:HA	1.81	0.62
1:F:244:ARG:NH2	1:G:239:ASN:HB2	2.15	0.62
1:F:415:LEU:HD22	1:G:388:ALA:HB1	1.81	0.62
1:H:140:LEU:O	1:H:143:THR:OG1	2.17	0.62
1:H:303:GLN:NE2	1:H:304:VAL:O	2.32	0.62
1:O:203:ALA:HA	1:Q:158:ALA:HB1	1.79	0.62
1:F:252:ILE:HG23	1:F:253:LEU:HD22	1.80	0.62
1:N:240:ASP:OD2	1:N:244:ARG:NH2	2.32	0.62
1:P:392:ASN:OD1	1:P:393:TYR:N	2.31	0.62
1:S:275:LYS:HB2	1:S:377:MET:HB2	1.81	0.62
1:X:176:VAL:HG13	1:X:212:LEU:HD13	1.82	0.62
1:A:404:LEU:HD23	1:A:408:GLN:HG2	1.81	0.62
1:M:248:ARG:NH1	1:N:267:THR:OG1	2.33	0.62
1:W:375:THR:HG23	1:X:275:LYS:NZ	2.14	0.62
1:c:190:GLN:HE21	1:d:218:HIS:CD2	2.17	0.62
1:S:408:GLN:HA	1:S:411:GLN:HE21	1.63	0.62
1:T:275:LYS:HB2	1:T:377:MET:HB2	1.81	0.62
1:a:214:ASP:OD1	1:a:215:GLN:N	2.32	0.62
1:H:404:LEU:HD13	1:H:434:ASN:HD21	1.64	0.62
1:a:140:LEU:O	1:a:144:ILE:HG12	1.99	0.62
1:D:374:HIS:HB3	1:E:276:GLU:HB3	1.82	0.62
1:H:373:ARG:HH21	1:I:275:LYS:HE2	1.65	0.62
1:B:231:ASN:OD1	1:B:232:ASP:N	2.31	0.62
1:I:199:SER:HA	1:I:205:LEU:HD23	1.82	0.62
1:U:143:THR:HG22	1:W:154:ARG:HE	1.63	0.62
1:Y:369:ASP:OD1	1:Z:282:TYR:N	2.31	0.62
1:Y:404:LEU:HB2	1:Y:409:MET:HE3	1.82	0.62
1:L:139:GLU:HG3	1:N:156:HIS:HE1	1.65	0.62
1:Y:158:ALA:HB3	1:Y:173:SER:HB3	1.81	0.62
1:Z:248:ARG:NH1	1:a:267:THR:OG1	2.32	0.62
1:d:275:LYS:HB2	1:d:377:MET:HB2	1.82	0.62
1:f:139:GLU:O	1:g:154:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:375:THR:HG23	1:L:275:LYS:NZ	2.15	0.61
1:g:181:GLU:HB3	1:g:184:ARG:NH2	2.15	0.61
1:G:216:SER:O	1:G:218:HIS:ND1	2.34	0.61
1:J:415:LEU:HD11	1:K:433:VAL:HG21	1.82	0.61
1:T:261:ASN:O	1:T:392:ASN:N	2.26	0.61
1:X:231:ASN:O	1:X:234:GLN:NE2	2.32	0.61
1:Y:143:THR:HG21	1:a:156:HIS:NE2	2.15	0.61
1:N:370:ARG:NH1	1:O:280:GLU:OE2	2.33	0.61
1:U:275:LYS:HA	1:U:275:LYS:HE3	1.82	0.61
1:U:279:GLU:OE2	1:U:281:HIS:N	2.28	0.61
1:Y:375:THR:HG23	1:Z:275:LYS:HE2	1.81	0.61
1:M:240:ASP:OD2	1:M:244:ARG:NH2	2.32	0.61
1:S:257:VAL:O	1:S:261:ASN:ND2	2.33	0.61
1:d:413:GLU:OE1	1:d:417:ARG:NH1	2.32	0.61
1:J:392:ASN:OD1	1:J:393:TYR:N	2.31	0.61
1:J:415:LEU:HD22	1:K:388:ALA:HB1	1.82	0.61
1:P:359:GLN:HE22	1:P:361:ASN:HB2	1.65	0.61
1:T:253:LEU:HD22	1:T:412:ILE:HG23	1.83	0.61
1:Y:246:GLN:NE2	1:Y:250:GLU:OE2	2.34	0.61
1:Y:360:ARG:NH1	1:Y:362:GLU:OE2	2.33	0.61
1:d:220:LEU:O	1:d:222:GLN:NE2	2.33	0.61
1:A:275:LYS:HE2	1:h:373:ARG:HH21	1.66	0.61
1:I:246:GLN:NE2	1:I:250:GLU:OE2	2.33	0.61
1:L:140:LEU:O	1:L:144:ILE:HG12	2.01	0.61
1:N:405:THR:OG1	1:N:407:ASP:OD1	2.13	0.61
1:V:374:HIS:HB3	1:W:276:GLU:HB3	1.82	0.61
1:X:275:LYS:HA	1:X:275:LYS:HE3	1.83	0.61
1:H:151:LYS:NZ	1:H:180:LEU:O	2.33	0.61
1:N:385:LEU:N	1:N:428:ASP:OD2	2.32	0.61
1:T:212:LEU:HG	1:T:220:LEU:HD12	1.80	0.61
1:U:272:PHE:HA	1:U:379:VAL:HG13	1.83	0.61
1:X:394:LYS:HG2	1:X:402:LEU:HB2	1.83	0.61
1:a:405:THR:OG1	1:a:407:ASP:OD1	2.17	0.61
1:A:276:GLU:OE2	1:A:374:HIS:NE2	2.33	0.61
1:E:300:ILE:HG12	1:E:360:ARG:HG2	1.83	0.61
1:Q:155:VAL:O	1:Q:156:HIS:ND1	2.34	0.61
1:Q:249:ILE:HD11	1:Q:416:THR:HG22	1.83	0.61
1:W:424:ASP:OD1	1:W:425:LYS:N	2.33	0.61
1:h:214:ASP:OD1	1:h:215:GLN:N	2.34	0.61
1:B:214:ASP:HB3	1:B:218:HIS:HB2	1.83	0.61
1:D:404:LEU:HD23	1:D:434:ASN:HD21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:280:GLU:OE1	1:Z:372:ILE:HG12	2.01	0.61
1:a:144:ILE:HA	1:a:147:LEU:HD13	1.83	0.61
1:d:284:PRO:O	1:d:290:LYS:NZ	2.32	0.61
1:G:193:ALA:HA	1:H:219:LEU:HG	1.83	0.60
1:Q:283:SER:HB2	1:Q:369:ASP:HB2	1.83	0.60
1:R:245:ILE:O	1:R:249:ILE:HG12	2.00	0.60
1:a:143:THR:HG23	1:c:154:ARG:HH21	1.66	0.60
1:d:135:ALA:O	1:d:139:GLU:HG2	2.00	0.60
1:g:268:ALA:HB1	1:g:382:ILE:HD11	1.83	0.60
1:A:378:ASN:ND2	1:A:381:ASP:OD2	2.33	0.60
1:I:256:ILE:HG21	1:I:412:ILE:HD11	1.83	0.60
1:K:275:LYS:HB3	1:K:377:MET:HE2	1.83	0.60
1:X:257:VAL:O	1:X:261:ASN:ND2	2.33	0.60
1:b:407:ASP:HA	1:b:410:LYS:HG2	1.83	0.60
1:d:157:LEU:HD11	1:d:202:VAL:HG21	1.83	0.60
1:d:420:MET:HE1	1:d:430:LEU:HB2	1.83	0.60
1:R:186:LEU:HD23	1:R:191:ILE:HD13	1.83	0.60
1:d:143:THR:HG21	1:f:156:HIS:NE2	2.17	0.60
1:e:362:GLU:OE2	1:e:364:SER:OG	2.17	0.60
1:f:404:LEU:H	1:f:434:ASN:ND2	1.99	0.60
1:g:143:THR:HG23	1:h:154:ARG:NH2	2.09	0.60
1:O:133:GLN:O	1:O:137:GLU:HG2	2.01	0.60
1:T:277:GLN:HB3	1:T:375:THR:HB	1.83	0.60
1:U:192:SER:O	1:U:196:HIS:ND1	2.28	0.60
1:c:301:SER:HB3	1:c:359:GLN:HB2	1.82	0.60
1:M:413:GLU:OE1	1:M:417:ARG:NH1	2.33	0.60
1:c:180:LEU:HD13	1:c:185:ALA:HA	1.82	0.60
1:E:259:ASN:OD1	1:E:260:GLY:N	2.34	0.60
1:H:299:ASN:HB2	1:H:361:ASN:HB2	1.83	0.60
1:a:275:LYS:HB2	1:a:377:MET:HB2	1.84	0.60
1:h:409:MET:HE1	1:h:434:ASN:HB2	1.83	0.60
1:B:413:GLU:OE2	1:B:417:ARG:NH1	2.35	0.60
1:C:266:VAL:HG22	1:C:387:VAL:HG22	1.83	0.60
1:R:151:LYS:NZ	1:R:182:PRO:HD3	2.17	0.60
1:W:378:ASN:ND2	1:W:381:ASP:OD1	2.31	0.60
1:K:407:ASP:OD1	1:K:408:GLN:N	2.35	0.60
1:N:245:ILE:HG23	1:N:266:VAL:HG21	1.84	0.60
1:W:144:ILE:HG22	1:W:150:VAL:HG11	1.83	0.60
1:b:424:ASP:OD1	1:b:425:LYS:N	2.35	0.60
1:C:157:LEU:HD11	1:C:202:VAL:HG21	1.83	0.60
1:I:128:GLU:N	1:I:128:GLU:OE2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:GLU:HA	1:I:150:VAL:HG12	1.83	0.60
1:P:404:LEU:H	1:P:434:ASN:ND2	2.00	0.60
1:T:248:ARG:NH1	1:U:267:THR:OG1	2.35	0.60
1:U:383:GLU:OE1	1:U:383:GLU:N	2.35	0.60
1:d:203:ALA:HA	1:f:158:ALA:HB1	1.84	0.60
1:V:287:ASP:HB2	1:V:290:LYS:NZ	2.16	0.60
1:a:407:ASP:OD1	1:a:408:GLN:N	2.35	0.60
1:c:407:ASP:OD1	1:c:408:GLN:N	2.35	0.60
1:I:143:THR:HG21	1:K:156:HIS:NE2	2.18	0.59
1:Q:392:ASN:OD1	1:Q:393:TYR:N	2.34	0.59
1:I:413:GLU:OE2	1:I:417:ARG:NH1	2.35	0.59
1:P:378:ASN:ND2	1:P:381:ASP:OD1	2.34	0.59
1:S:374:HIS:HB3	1:T:276:GLU:HB2	1.82	0.59
1:T:216:SER:O	1:T:218:HIS:ND1	2.35	0.59
1:W:143:THR:HG22	1:X:154:ARG:HD3	1.84	0.59
1:X:234:GLN:HB2	1:X:272:PHE:CZ	2.37	0.59
1:b:301:SER:HB3	1:b:359:GLN:HB3	1.83	0.59
1:h:393:TYR:CE2	1:h:436:PRO:HD3	2.38	0.59
1:B:142:ARG:HB3	1:C:154:ARG:HH22	1.67	0.59
1:B:158:ALA:HB1	1:h:203:ALA:HA	1.84	0.59
1:D:405:THR:HG23	1:D:408:GLN:H	1.67	0.59
1:I:140:LEU:O	1:I:144:ILE:HG12	2.01	0.59
1:N:378:ASN:ND2	1:N:381:ASP:OD1	2.36	0.59
1:P:245:ILE:O	1:P:249:ILE:HD12	2.02	0.59
1:Z:374:HIS:HB3	1:a:276:GLU:HB3	1.85	0.59
1:Z:388:ALA:HA	1:Z:431:ASN:O	2.03	0.59
1:g:256:ILE:HG21	1:g:412:ILE:HD11	1.83	0.59
1:G:139:GLU:HG3	1:H:156:HIS:HE1	1.67	0.59
1:K:138:GLY:O	1:K:142:ARG:HG2	2.02	0.59
1:Y:374:HIS:HB3	1:Z:276:GLU:HB3	1.85	0.59
1:B:404:LEU:H	1:B:434:ASN:HD21	1.51	0.59
1:J:298:LEU:HD13	1:J:362:GLU:HB3	1.84	0.59
1:N:203:ALA:HB2	1:O:158:ALA:HB1	1.84	0.59
1:S:413:GLU:HB3	1:S:432:VAL:HG21	1.83	0.59
1:a:155:VAL:HG23	1:a:176:VAL:HG22	1.82	0.59
1:b:248:ARG:NH1	1:c:267:THR:OG1	2.36	0.59
1:f:248:ARG:NH1	1:g:267:THR:OG1	2.36	0.59
1:C:143:THR:HG21	1:E:156:HIS:NE2	2.18	0.59
1:N:129:GLN:OE1	1:N:129:GLN:N	2.30	0.59
1:S:404:LEU:H	1:S:434:ASN:HD21	1.48	0.59
1:d:392:ASN:OD1	1:d:393:TYR:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:234:GLN:HB2	1:R:272:PHE:CZ	2.38	0.59
1:T:245:ILE:HD11	1:T:420:MET:HA	1.85	0.59
1:c:257:VAL:O	1:c:261:ASN:ND2	2.36	0.59
1:d:420:MET:HE3	1:d:422:PHE:HB2	1.84	0.59
1:e:408:GLN:HE22	1:e:412:ILE:HD11	1.68	0.59
1:I:139:GLU:OE2	1:K:154:ARG:NH1	2.35	0.59
1:L:293:LEU:HD13	1:L:296:ARG:HE	1.68	0.59
1:Q:197:LEU:HD12	1:R:175:SER:HB2	1.85	0.59
1:X:250:GLU:O	1:X:254:SER:OG	2.20	0.58
1:C:283:SER:HB2	1:C:369:ASP:HB2	1.86	0.58
1:D:411:GLN:O	1:D:415:LEU:HD23	2.03	0.58
1:K:392:ASN:OD1	1:K:393:TYR:N	2.30	0.58
1:L:269:GLN:HB2	1:L:384:ARG:HB3	1.85	0.58
1:O:143:THR:HG21	1:Q:156:HIS:NE2	2.18	0.58
1:T:284:PRO:O	1:T:290:LYS:NZ	2.32	0.58
1:U:150:VAL:HA	1:U:180:LEU:HA	1.84	0.58
1:U:187:ASP:OD1	1:U:190:GLN:NE2	2.36	0.58
1:W:186:LEU:HG	1:W:190:GLN:HB2	1.84	0.58
1:a:250:GLU:O	1:a:254:SER:OG	2.16	0.58
1:K:279:GLU:OE2	1:K:281:HIS:N	2.34	0.58
1:L:407:ASP:OD1	1:L:408:GLN:N	2.37	0.58
1:W:200:SER:HB3	1:X:175:SER:HB3	1.85	0.58
1:W:418:GLU:HB3	1:X:388:ALA:HB2	1.85	0.58
1:X:248:ARG:HH11	1:Y:267:THR:HG22	1.67	0.58
1:H:407:ASP:OD1	1:H:410:LYS:NZ	2.37	0.58
1:I:143:THR:HG22	1:K:154:ARG:HD3	1.86	0.58
1:I:407:ASP:HA	1:I:410:LYS:HG3	1.85	0.58
1:E:241:VAL:HG22	1:F:235:LEU:HD11	1.84	0.58
1:P:277:GLN:HB2	1:P:377:MET:HE1	1.84	0.58
1:c:233:ALA:HA	1:c:236:LYS:HD3	1.85	0.58
1:A:231:ASN:O	1:A:234:GLN:NE2	2.36	0.58
1:A:267:THR:HG21	1:h:419:ALA:O	2.04	0.58
1:D:297:GLN:HB3	1:D:363:THR:HB	1.85	0.58
1:K:203:ALA:HA	1:L:158:ALA:HB1	1.84	0.58
1:M:392:ASN:OD1	1:M:393:TYR:N	2.34	0.58
1:V:299:ASN:HB2	1:V:361:ASN:HB2	1.83	0.58
1:W:293:LEU:HD13	1:W:296:ARG:HE	1.69	0.58
1:B:275:LYS:HB2	1:B:377:MET:HB2	1.86	0.58
1:F:413:GLU:OE1	1:F:417:ARG:NH1	2.33	0.58
1:L:139:GLU:O	1:L:143:THR:HG23	2.03	0.58
1:L:375:THR:HG23	1:M:275:LYS:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:407:ASP:HA	1:L:410:LYS:HG2	1.84	0.58
1:O:197:LEU:HD22	1:Q:213:VAL:HG21	1.85	0.58
1:Q:405:THR:OG1	1:Q:407:ASP:OD1	2.22	0.58
1:V:244:ARG:NH2	1:W:235:LEU:HB3	2.19	0.58
1:V:392:ASN:OD1	1:V:393:TYR:N	2.36	0.58
1:W:205:LEU:HD11	1:W:209:ASN:HB2	1.85	0.58
1:Z:275:LYS:HB2	1:Z:377:MET:HB2	1.85	0.58
1:B:283:SER:HB2	1:B:369:ASP:HB2	1.84	0.58
1:K:299:ASN:HB2	1:K:361:ASN:HB2	1.86	0.58
1:L:413:GLU:OE1	1:L:417:ARG:NH1	2.34	0.58
1:J:407:ASP:OD1	1:J:408:GLN:N	2.37	0.58
1:K:155:VAL:HG23	1:K:176:VAL:HG22	1.86	0.58
1:N:392:ASN:OD1	1:N:393:TYR:N	2.35	0.58
1:O:297:GLN:HG2	1:P:363:THR:HG23	1.86	0.58
1:Q:404:LEU:HD13	1:Q:434:ASN:HD21	1.69	0.58
1:e:250:GLU:O	1:e:254:SER:OG	2.18	0.58
1:g:404:LEU:H	1:g:434:ASN:ND2	2.01	0.58
1:B:203:ALA:HB1	1:C:160:PRO:HA	1.86	0.57
1:C:187:ASP:OD1	1:C:190:GLN:HG2	2.04	0.57
1:M:252:ILE:HD11	1:N:265:GLN:HB2	1.86	0.57
1:N:407:ASP:OD1	1:N:408:GLN:N	2.37	0.57
1:T:407:ASP:HA	1:T:410:LYS:HG2	1.86	0.57
1:Y:214:ASP:OD1	1:Y:215:GLN:N	2.36	0.57
1:a:245:ILE:HD11	1:a:420:MET:HA	1.86	0.57
1:F:250:GLU:O	1:F:254:SER:OG	2.21	0.57
1:H:245:ILE:HG23	1:H:266:VAL:HG21	1.86	0.57
1:K:304:VAL:N	1:L:356:ARG:O	2.37	0.57
1:U:180:LEU:HD21	1:U:186:LEU:HB2	1.85	0.57
1:Y:389:VAL:HB	1:Y:432:VAL:HG22	1.85	0.57
1:g:413:GLU:OE2	1:g:417:ARG:NH1	2.38	0.57
1:C:160:PRO:HG2	1:C:170:LYS:O	2.05	0.57
1:H:374:HIS:HB3	1:I:276:GLU:HB3	1.84	0.57
1:R:176:VAL:HB	1:R:212:LEU:HG	1.86	0.57
1:f:261:ASN:O	1:f:392:ASN:N	2.31	0.57
1:h:157:LEU:HD11	1:h:202:VAL:HG21	1.86	0.57
1:Q:191:ILE:HG23	1:Q:212:LEU:HD23	1.85	0.57
1:V:293:LEU:HD22	1:V:296:ARG:HD2	1.87	0.57
1:Y:179:THR:HA	1:Y:215:GLN:HB3	1.86	0.57
1:D:250:GLU:O	1:D:254:SER:OG	2.16	0.57
1:E:180:LEU:HD11	1:E:186:LEU:HB2	1.86	0.57
1:E:193:ALA:HA	1:G:219:LEU:HG	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:392:ASN:OD1	1:T:393:TYR:N	2.37	0.57
1:V:389:VAL:HB	1:V:432:VAL:HG22	1.86	0.57
1:d:181:GLU:HB3	1:d:184:ARG:NH2	2.19	0.57
1:J:297:GLN:OE1	1:K:363:THR:OG1	2.10	0.57
1:K:266:VAL:HG22	1:K:387:VAL:HG22	1.87	0.57
1:L:244:ARG:NH2	1:M:239:ASN:HB2	2.19	0.57
1:N:193:ALA:HA	1:O:219:LEU:HG	1.84	0.57
1:X:300:ILE:O	1:Y:359:GLN:NE2	2.37	0.57
1:Y:245:ILE:HD11	1:Y:420:MET:HA	1.85	0.57
1:c:378:ASN:ND2	1:c:381:ASP:OD1	2.35	0.57
1:c:421:GLY:O	1:c:426:ARG:NH2	2.37	0.57
1:h:244:ARG:HH22	1:h:248:ARG:HH22	1.52	0.57
1:T:158:ALA:O	1:T:172:PRO:HA	2.04	0.57
1:W:140:LEU:O	1:W:144:ILE:HG12	2.05	0.57
1:X:144:ILE:HG22	1:X:150:VAL:HG11	1.87	0.57
1:d:129:GLN:OE1	1:d:129:GLN:N	2.30	0.57
1:C:145:GLU:OE2	1:C:153:ALA:N	2.38	0.57
1:I:133:GLN:O	1:I:137:GLU:HG2	2.04	0.57
1:K:394:LYS:HE3	1:K:402:LEU:HD13	1.87	0.57
1:N:141:ALA:O	1:N:144:ILE:N	2.37	0.57
1:O:407:ASP:OD1	1:O:408:GLN:N	2.38	0.57
1:U:214:ASP:HB3	1:U:218:HIS:HB2	1.86	0.57
1:Y:193:ALA:HA	1:a:219:LEU:HG	1.85	0.57
1:Z:297:GLN:O	1:Z:362:GLU:HA	2.05	0.57
1:d:200:SER:HB3	1:f:175:SER:HB3	1.87	0.57
1:g:275:LYS:HB2	1:g:377:MET:HB2	1.87	0.57
1:B:200:SER:HB3	1:C:175:SER:HB3	1.86	0.57
1:H:145:GLU:HG3	1:H:150:VAL:HG12	1.87	0.57
1:I:252:ILE:HB	1:J:265:GLN:HG3	1.87	0.57
1:K:214:ASP:OD1	1:K:215:GLN:N	2.38	0.57
1:L:191:ILE:HG23	1:L:212:LEU:HD23	1.87	0.57
1:O:199:SER:HA	1:O:205:LEU:HD23	1.86	0.57
1:U:140:LEU:O	1:U:144:ILE:HD12	2.05	0.57
1:g:408:GLN:O	1:g:412:ILE:HG12	2.05	0.57
1:C:214:ASP:OD1	1:C:215:GLN:N	2.38	0.56
1:M:273:ALA:O	1:M:275:LYS:NZ	2.35	0.56
1:P:250:GLU:O	1:P:254:SER:OG	2.20	0.56
1:Q:256:ILE:HG21	1:Q:412:ILE:HD11	1.87	0.56
1:U:283:SER:HB2	1:U:369:ASP:HB2	1.88	0.56
1:Y:420:MET:SD	1:Y:422:PHE:HB2	2.45	0.56
1:B:155:VAL:HG23	1:B:176:VAL:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:PRO:HA	1:H:181:GLU:HG2	1.85	0.56
1:J:404:LEU:H	1:J:434:ASN:ND2	2.03	0.56
1:R:133:GLN:OE1	1:R:161:LYS:NZ	2.37	0.56
1:T:394:LYS:HE2	1:T:402:LEU:HD12	1.86	0.56
1:X:414:ASP:HB3	1:Y:431:ASN:HD21	1.69	0.56
1:A:392:ASN:OD1	1:A:393:TYR:N	2.35	0.56
1:B:360:ARG:NH1	1:B:362:GLU:OE1	2.35	0.56
1:F:424:ASP:OD1	1:F:425:LYS:N	2.38	0.56
1:G:283:SER:HB2	1:G:369:ASP:HB2	1.86	0.56
1:H:143:THR:HG21	1:I:156:HIS:CE1	2.40	0.56
1:J:234:GLN:HB3	1:J:272:PHE:CE1	2.40	0.56
1:L:140:LEU:O	1:L:143:THR:OG1	2.16	0.56
1:V:277:GLN:HG2	1:V:377:MET:HE1	1.85	0.56
1:V:423:SER:HB2	1:W:384:ARG:NH1	2.19	0.56
1:W:203:ALA:HA	1:X:158:ALA:HB1	1.87	0.56
1:W:393:TYR:CZ	1:W:436:PRO:HD3	2.41	0.56
1:d:162:PRO:HB2	1:f:165:PHE:HD2	1.70	0.56
1:f:143:THR:HG23	1:g:154:ARG:HE	1.68	0.56
1:S:393:TYR:CE2	1:S:436:PRO:HD3	2.41	0.56
1:a:191:ILE:HD12	1:a:212:LEU:HD11	1.87	0.56
1:b:287:ASP:OD2	1:b:290:LYS:NZ	2.37	0.56
1:f:140:LEU:O	1:f:144:ILE:HG12	2.06	0.56
1:f:219:LEU:HD23	1:f:221:THR:H	1.69	0.56
1:W:140:LEU:O	1:W:143:THR:OG1	2.20	0.56
1:D:248:ARG:NH1	1:E:267:THR:OG1	2.39	0.56
1:E:256:ILE:HG23	1:E:257:VAL:HG13	1.87	0.56
1:J:271:ASP:HB3	1:J:383:GLU:OE2	2.06	0.56
1:J:388:ALA:HA	1:J:431:ASN:O	2.05	0.56
1:K:143:THR:HG21	1:L:156:HIS:NE2	2.20	0.56
1:M:378:ASN:ND2	1:M:381:ASP:OD1	2.33	0.56
1:M:404:LEU:H	1:M:434:ASN:ND2	2.04	0.56
1:O:262:VAL:O	1:O:263:HIS:ND1	2.39	0.56
1:X:245:ILE:O	1:X:249:ILE:HG12	2.06	0.56
1:d:407:ASP:OD1	1:d:408:GLN:N	2.39	0.56
1:L:413:GLU:HA	1:L:416:THR:HG22	1.87	0.56
1:M:303:GLN:HG3	1:N:357:SER:HA	1.87	0.56
1:T:173:SER:HA	1:T:209:ASN:HB3	1.88	0.56
1:T:280:GLU:HG2	1:T:282:TYR:HE2	1.71	0.56
1:X:423:SER:OG	1:X:425:LYS:NZ	2.29	0.56
1:Y:181:GLU:HB3	1:Y:184:ARG:HH21	1.70	0.56
1:E:416:THR:HG23	1:E:430:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:394:LYS:HG2	1:J:402:LEU:HB2	1.88	0.56
1:K:385:LEU:N	1:K:428:ASP:OD2	2.38	0.56
1:O:166:VAL:HG22	1:O:168:GLU:OE1	2.06	0.56
1:R:261:ASN:O	1:R:392:ASN:N	2.37	0.56
1:R:407:ASP:OD1	1:R:408:GLN:N	2.39	0.56
1:S:275:LYS:CB	1:S:377:MET:HB2	2.35	0.56
1:a:241:VAL:HG22	1:b:235:LEU:HD21	1.88	0.56
1:d:141:ALA:O	1:d:145:GLU:HG2	2.05	0.56
1:g:373:ARG:NH2	1:h:275:LYS:HD2	2.21	0.56
1:B:417:ARG:HG3	1:B:422:PHE:HB3	1.88	0.56
1:F:420:MET:HE3	1:F:422:PHE:HB2	1.87	0.56
1:H:140:LEU:O	1:H:144:ILE:HG12	2.05	0.56
1:M:293:LEU:HD21	1:M:296:ARG:HH21	1.71	0.56
1:Y:275:LYS:HB3	1:Y:377:MET:HE2	1.88	0.56
1:b:287:ASP:HB2	1:b:290:LYS:HG2	1.87	0.56
1:d:193:ALA:HA	1:f:219:LEU:CD1	2.36	0.56
1:h:164:LEU:C	1:h:167:ARG:HH22	2.14	0.56
1:D:360:ARG:NH1	1:D:362:GLU:OE2	2.38	0.56
1:E:140:LEU:O	1:E:144:ILE:HG12	2.06	0.56
1:K:199:SER:OG	1:K:205:LEU:O	2.19	0.56
1:X:369:ASP:OD1	1:Y:282:TYR:N	2.37	0.56
1:Y:172:PRO:HG2	1:Y:205:LEU:HA	1.88	0.56
1:Z:244:ARG:CZ	1:a:235:LEU:HB3	2.36	0.56
1:b:266:VAL:HG22	1:b:387:VAL:HG22	1.88	0.56
1:d:385:LEU:N	1:d:428:ASP:OD2	2.34	0.56
1:A:275:LYS:CE	1:h:373:ARG:HH21	2.19	0.55
1:B:150:VAL:C	1:B:151:LYS:HD3	2.30	0.55
1:E:284:PRO:O	1:E:290:LYS:NZ	2.31	0.55
1:O:299:ASN:HB2	1:O:361:ASN:HB2	1.88	0.55
1:V:373:ARG:HH21	1:W:275:LYS:HD2	1.70	0.55
1:Y:257:VAL:O	1:Y:261:ASN:ND2	2.19	0.55
1:d:138:GLY:O	1:d:142:ARG:HG2	2.05	0.55
1:d:267:THR:HB	1:d:386:SER:HB2	1.87	0.55
1:g:145:GLU:OE2	1:g:153:ALA:N	2.39	0.55
1:E:161:LYS:HD3	1:E:162:PRO:HD2	1.87	0.55
1:X:193:ALA:HA	1:Y:219:LEU:HG	1.86	0.55
1:X:275:LYS:CB	1:X:377:MET:HB2	2.37	0.55
1:a:189:GLY:O	1:a:192:SER:OG	2.19	0.55
1:c:203:ALA:HB1	1:d:160:PRO:HA	1.88	0.55
1:e:244:ARG:HH11	1:f:239:ASN:HB2	1.71	0.55
1:C:134:ARG:O	1:C:137:GLU:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:237:PHE:HE2	1:V:232:ASP:HA	1.70	0.55
1:V:373:ARG:NH1	1:W:277:GLN:OE1	2.39	0.55
1:A:248:ARG:HH11	1:B:267:THR:HG22	1.70	0.55
1:L:284:PRO:O	1:L:290:LYS:NZ	2.39	0.55
1:N:244:ARG:NH1	1:O:239:ASN:OD1	2.38	0.55
1:O:179:THR:HA	1:O:215:GLN:HB3	1.87	0.55
1:T:203:ALA:N	1:U:158:ALA:HB1	2.21	0.55
1:T:257:VAL:O	1:T:261:ASN:ND2	2.34	0.55
1:U:385:LEU:N	1:U:428:ASP:OD2	2.20	0.55
1:a:394:LYS:HE2	1:a:402:LEU:HD22	1.89	0.55
1:N:413:GLU:OE2	1:N:417:ARG:NH1	2.40	0.55
1:R:200:SER:HB3	1:T:175:SER:HB3	1.88	0.55
1:Z:375:THR:HG23	1:a:275:LYS:HZ3	1.71	0.55
1:a:393:TYR:CE2	1:a:436:PRO:HD3	2.41	0.55
1:h:219:LEU:HD12	1:h:219:LEU:H	1.70	0.55
1:G:143:THR:HA	1:H:154:ARG:HH11	1.71	0.55
1:K:151:LYS:NZ	1:K:180:LEU:O	2.40	0.55
1:Q:211:THR:HA	1:Q:221:THR:HG21	1.87	0.55
1:d:360:ARG:NH1	1:d:362:GLU:OE1	2.40	0.55
1:f:420:MET:HE2	1:f:422:PHE:HA	1.88	0.55
1:Q:275:LYS:HB2	1:Q:377:MET:HB2	1.87	0.55
1:R:143:THR:CG2	1:T:156:HIS:HE1	2.13	0.55
1:T:159:MET:HG3	1:T:172:PRO:HB3	1.89	0.55
1:g:197:LEU:HD12	1:h:213:VAL:HG21	1.89	0.55
1:T:244:ARG:HH11	1:U:239:ASN:HB2	1.72	0.55
1:W:133:GLN:O	1:W:137:GLU:HG2	2.06	0.55
1:Z:301:SER:O	1:Z:359:GLN:N	2.40	0.55
1:d:151:LYS:HE3	1:d:180:LEU:O	2.06	0.55
1:d:374:HIS:HB3	1:e:276:GLU:HB3	1.89	0.55
1:X:203:ALA:HB1	1:Y:160:PRO:HA	1.89	0.55
1:Z:244:ARG:HH22	1:a:235:LEU:C	2.14	0.55
1:a:168:GLU:O	1:a:169:GLN:HB2	2.07	0.55
1:H:407:ASP:HA	1:H:410:LYS:HG2	1.89	0.55
1:V:404:LEU:HD23	1:V:408:GLN:HG2	1.89	0.55
1:X:181:GLU:HB3	1:X:184:ARG:NH2	2.22	0.55
1:X:182:PRO:O	1:X:184:ARG:NH1	2.40	0.55
1:X:195:VAL:HG13	1:X:210:VAL:HB	1.89	0.55
1:d:147:LEU:O	1:d:149:PRO:HD2	2.06	0.55
1:d:248:ARG:HH11	1:e:267:THR:HG22	1.72	0.55
1:D:394:LYS:HG2	1:D:402:LEU:HB2	1.89	0.54
1:E:248:ARG:NH1	1:F:267:THR:HG22	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:MET:HE1	1:F:430:LEU:HB2	1.89	0.54
1:N:169:GLN:CD	1:N:170:LYS:H	2.15	0.54
1:c:393:TYR:CE2	1:c:436:PRO:HD3	2.42	0.54
1:O:147:LEU:O	1:O:149:PRO:HD2	2.08	0.54
1:Q:394:LYS:HE2	1:Q:402:LEU:HD22	1.89	0.54
1:W:186:LEU:HD23	1:W:191:ILE:HD13	1.89	0.54
1:W:287:ASP:HB3	1:W:290:LYS:HG2	1.88	0.54
1:Z:280:GLU:OE2	1:Z:370:ARG:HD2	2.07	0.54
1:c:191:ILE:HD13	1:c:220:LEU:HB3	1.89	0.54
1:f:375:THR:HG23	1:g:275:LYS:HZ2	1.71	0.54
1:Y:177:THR:HG22	1:Y:213:VAL:HB	1.89	0.54
1:a:270:LEU:HD23	1:a:382:ILE:HA	1.89	0.54
1:H:257:VAL:O	1:H:261:ASN:ND2	2.30	0.54
1:I:200:SER:OG	1:K:173:SER:OG	2.21	0.54
1:K:234:GLN:OE1	1:K:234:GLN:N	2.39	0.54
1:M:404:LEU:HD23	1:M:434:ASN:HD21	1.73	0.54
1:X:138:GLY:O	1:X:142:ARG:HG2	2.06	0.54
1:a:261:ASN:O	1:a:392:ASN:N	2.30	0.54
1:b:367:GLU:HG3	1:c:368:VAL:HG11	1.89	0.54
1:d:373:ARG:HH22	1:e:277:GLN:HG2	1.72	0.54
1:h:199:SER:OG	1:h:205:LEU:O	2.24	0.54
1:I:181:GLU:OE1	1:I:184:ARG:NH2	2.41	0.54
1:V:417:ARG:HA	1:V:420:MET:HE2	1.89	0.54
1:Z:283:SER:HB2	1:Z:369:ASP:HB2	1.89	0.54
1:A:424:ASP:OD2	1:A:425:LYS:N	2.40	0.54
1:B:375:THR:HG23	1:C:275:LYS:HE3	1.88	0.54
1:E:252:ILE:O	1:E:255:PRO:HD2	2.08	0.54
1:N:214:ASP:OD2	1:N:216:SER:N	2.40	0.54
1:Q:216:SER:O	1:Q:218:HIS:ND1	2.40	0.54
1:T:153:ALA:HA	1:T:177:THR:O	2.08	0.54
1:c:394:LYS:HG2	1:c:402:LEU:HB2	1.90	0.54
1:e:394:LYS:HG2	1:e:402:LEU:HB2	1.88	0.54
1:H:199:SER:HA	1:H:205:LEU:HD22	1.89	0.54
1:U:159:MET:HE2	1:U:172:PRO:HB2	1.90	0.54
1:V:287:ASP:HB2	1:V:290:LYS:HZ3	1.71	0.54
1:V:411:GLN:O	1:V:415:LEU:HD23	2.07	0.54
1:X:404:LEU:H	1:X:434:ASN:ND2	2.05	0.54
1:b:234:GLN:HB2	1:b:272:PHE:CZ	2.42	0.54
1:B:198:VAL:HG13	1:B:210:VAL:HG11	1.90	0.54
1:I:163:SER:N	1:I:169:GLN:HE22	2.06	0.54
1:J:378:ASN:ND2	1:J:381:ASP:OD1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:212:LEU:HG	1:K:220:LEU:HD12	1.89	0.54
1:Y:417:ARG:HA	1:Y:420:MET:SD	2.47	0.54
1:a:404:LEU:H	1:a:434:ASN:ND2	2.06	0.54
1:b:413:GLU:OE1	1:b:417:ARG:NH1	2.20	0.54
1:c:374:HIS:HB3	1:d:276:GLU:HB3	1.90	0.54
1:f:375:THR:HG23	1:g:275:LYS:NZ	2.23	0.54
1:H:276:GLU:OE2	1:H:374:HIS:NE2	2.34	0.54
1:I:275:LYS:HB3	1:I:377:MET:HE2	1.90	0.54
1:Q:394:LYS:HE3	1:Q:402:LEU:HD13	1.88	0.54
1:V:410:LYS:NZ	1:V:414:ASP:OD2	2.40	0.54
1:X:133:GLN:O	1:X:137:GLU:HG2	2.07	0.54
1:X:139:GLU:HG3	1:Y:156:HIS:HE1	1.73	0.54
1:Z:372:ILE:O	1:a:277:GLN:HA	2.07	0.54
1:B:156:HIS:CD2	1:h:143:THR:HG21	2.43	0.54
1:Q:407:ASP:HA	1:Q:410:LYS:HG3	1.89	0.54
1:g:194:VAL:HG21	1:g:212:LEU:HD22	1.90	0.54
1:K:197:LEU:HD12	1:L:175:SER:HB2	1.89	0.53
1:R:143:THR:HG21	1:T:156:HIS:CE1	2.26	0.53
1:S:411:GLN:O	1:S:415:LEU:HD23	2.07	0.53
1:U:248:ARG:NH1	1:V:267:THR:HG22	2.22	0.53
1:W:189:GLY:O	1:W:192:SER:OG	2.23	0.53
1:X:142:ARG:HB2	1:Y:154:ARG:NH1	2.22	0.53
1:Y:181:GLU:HB3	1:Y:184:ARG:NH2	2.23	0.53
1:A:266:VAL:HG22	1:A:387:VAL:HG22	1.89	0.53
1:G:279:GLU:OE2	1:G:281:HIS:HB2	2.08	0.53
1:L:188:GLU:HA	1:L:191:ILE:HD12	1.90	0.53
1:V:245:ILE:HG23	1:V:266:VAL:HG21	1.89	0.53
1:Z:245:ILE:HG23	1:Z:266:VAL:HG21	1.89	0.53
1:Z:304:VAL:HG22	1:Z:356:ARG:HG2	1.90	0.53
1:a:182:PRO:O	1:a:184:ARG:NH1	2.41	0.53
1:d:405:THR:OG1	1:d:407:ASP:OD1	2.23	0.53
1:e:392:ASN:OD1	1:e:393:TYR:N	2.36	0.53
1:f:155:VAL:HG23	1:f:176:VAL:HG22	1.90	0.53
1:g:283:SER:HB2	1:g:369:ASP:HB2	1.90	0.53
1:g:301:SER:HB3	1:g:359:GLN:HB2	1.90	0.53
1:h:182:PRO:O	1:h:184:ARG:NH1	2.42	0.53
1:A:404:LEU:H	1:A:434:ASN:ND2	2.07	0.53
1:R:137:GLU:OE2	1:R:157:LEU:N	2.31	0.53
1:S:392:ASN:OD1	1:S:393:TYR:N	2.42	0.53
1:T:140:LEU:O	1:U:154:ARG:NH1	2.41	0.53
1:X:297:GLN:HB3	1:X:363:THR:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLN:HB3	1:B:272:PHE:CE1	2.43	0.53
1:D:392:ASN:OD1	1:D:393:TYR:N	2.37	0.53
1:E:155:VAL:HG23	1:E:176:VAL:HG22	1.89	0.53
1:Q:416:THR:OG1	1:Q:430:LEU:HD21	2.09	0.53
1:R:147:LEU:HG	1:T:216:SER:HA	1.91	0.53
1:U:372:ILE:HG22	1:V:278:THR:HB	1.90	0.53
1:U:389:VAL:HB	1:U:432:VAL:HG13	1.90	0.53
1:a:199:SER:HA	1:a:205:LEU:HD23	1.89	0.53
1:c:141:ALA:O	1:c:145:GLU:HG2	2.09	0.53
1:h:179:THR:HA	1:h:215:GLN:HB3	1.90	0.53
1:h:231:ASN:O	1:h:234:GLN:NE2	2.39	0.53
1:C:203:ALA:HA	1:E:158:ALA:HB1	1.91	0.53
1:K:375:THR:HA	1:L:275:LYS:HZ2	1.73	0.53
1:L:245:ILE:HG23	1:L:266:VAL:HG21	1.90	0.53
1:N:145:GLU:OE2	1:N:153:ALA:N	2.40	0.53
1:a:126:PHE:HA	1:a:129:GLN:NE2	2.24	0.53
1:e:371:THR:HG22	1:f:279:GLU:HG2	1.89	0.53
1:L:280:GLU:HG2	1:L:282:TYR:HE2	1.74	0.53
1:R:283:SER:HB2	1:R:369:ASP:HB2	1.91	0.53
1:T:275:LYS:HG3	1:T:377:MET:HE2	1.91	0.53
1:d:420:MET:HE3	1:d:422:PHE:HD1	1.73	0.53
1:C:409:MET:HE2	1:C:434:ASN:HB2	1.91	0.53
1:D:298:LEU:HD13	1:D:362:GLU:HB3	1.89	0.53
1:O:253:LEU:HD22	1:O:412:ILE:HG23	1.91	0.53
1:U:142:ARG:HG3	1:W:154:ARG:HH12	1.74	0.53
1:U:420:MET:HE2	1:U:430:LEU:HD22	1.91	0.53
1:W:143:THR:HG21	1:X:156:HIS:NE2	2.24	0.53
1:H:250:GLU:O	1:H:254:SER:OG	2.23	0.53
1:Q:407:ASP:OD1	1:Q:408:GLN:N	2.41	0.53
1:X:266:VAL:HG22	1:X:387:VAL:HG22	1.90	0.53
1:Y:234:GLN:HG3	1:Y:272:PHE:CE1	2.44	0.53
1:c:259:ASN:OD1	1:c:260:GLY:N	2.41	0.53
1:g:304:VAL:HB	1:h:356:ARG:H	1.74	0.53
1:C:190:GLN:OE1	1:E:217:GLY:HA3	2.09	0.53
1:O:132:TYR:HE2	1:Q:130:VAL:HG13	1.74	0.53
1:U:151:LYS:NZ	1:U:180:LEU:O	2.28	0.53
1:U:189:GLY:O	1:U:192:SER:OG	2.23	0.53
1:Y:272:PHE:HA	1:Y:379:VAL:HG13	1.90	0.53
1:J:420:MET:HE1	1:J:429:THR:O	2.09	0.53
1:T:179:THR:HA	1:T:215:GLN:HB3	1.91	0.53
1:W:142:ARG:HG3	1:X:154:ARG:HH22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:151:LYS:NZ	1:W:180:LEU:O	2.43	0.53
1:W:163:SER:OG	1:W:164:LEU:N	2.41	0.53
1:g:253:LEU:HD11	1:g:412:ILE:HG23	1.90	0.53
1:h:279:GLU:OE2	1:h:281:HIS:N	2.41	0.53
1:B:143:THR:HG21	1:C:156:HIS:CD2	2.44	0.52
1:B:154:ARG:HH22	1:h:143:THR:N	2.06	0.52
1:L:287:ASP:OD1	1:L:289:SER:N	2.30	0.52
1:Q:181:GLU:OE1	1:Q:184:ARG:NH2	2.43	0.52
1:S:252:ILE:HD11	1:T:265:GLN:HB2	1.91	0.52
1:X:203:ALA:O	1:Y:170:LYS:NZ	2.42	0.52
1:c:155:VAL:HG23	1:c:176:VAL:HG22	1.90	0.52
1:c:409:MET:HE3	1:c:434:ASN:HB2	1.91	0.52
1:f:392:ASN:OD1	1:f:393:TYR:N	2.42	0.52
1:g:420:MET:HE1	1:g:430:LEU:HB2	1.91	0.52
1:h:188:GLU:OE2	1:h:188:GLU:N	2.39	0.52
1:L:193:ALA:HA	1:N:219:LEU:HG	1.91	0.52
1:N:139:GLU:O	1:O:154:ARG:NH2	2.43	0.52
1:a:186:LEU:HD23	1:a:191:ILE:HD13	1.91	0.52
1:a:197:LEU:HG	1:c:213:VAL:HG21	1.90	0.52
1:g:294:ARG:NE	1:g:367:GLU:OE1	2.42	0.52
1:B:217:GLY:HA3	1:h:190:GLN:HG2	1.91	0.52
1:R:151:LYS:NZ	1:R:180:LEU:O	2.42	0.52
1:S:404:LEU:H	1:S:434:ASN:ND2	2.07	0.52
1:U:139:GLU:O	1:U:143:THR:HG23	2.09	0.52
1:a:375:THR:HG23	1:b:275:LYS:HE3	1.90	0.52
1:G:294:ARG:NE	1:G:367:GLU:OE1	2.37	0.52
1:O:176:VAL:HB	1:O:212:LEU:HD13	1.91	0.52
1:Q:149:PRO:O	1:Q:180:LEU:HD13	2.09	0.52
1:U:360:ARG:NH1	1:U:362:GLU:OE1	2.42	0.52
1:U:392:ASN:OD1	1:U:393:TYR:N	2.40	0.52
1:Y:176:VAL:HB	1:Y:212:LEU:HD23	1.91	0.52
1:Y:393:TYR:HB3	1:Y:402:LEU:N	2.23	0.52
1:e:253:LEU:HD11	1:e:416:THR:HG22	1.91	0.52
1:g:148:GLY:O	1:g:150:VAL:N	2.41	0.52
1:h:144:ILE:HA	1:h:147:LEU:HD23	1.92	0.52
1:C:257:VAL:O	1:C:261:ASN:ND2	2.32	0.52
1:I:203:ALA:HA	1:K:158:ALA:HB1	1.91	0.52
1:I:393:TYR:CE2	1:I:436:PRO:HD3	2.45	0.52
1:J:413:GLU:OE1	1:J:432:VAL:HB	2.09	0.52
1:N:393:TYR:CE2	1:N:436:PRO:HD3	2.44	0.52
1:R:143:THR:HG23	1:T:154:ARG:NH2	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:267:THR:OG1	1:S:386:SER:HB2	2.09	0.52
1:Y:267:THR:OG1	1:Y:386:SER:HB2	2.10	0.52
1:K:375:THR:HG23	1:L:275:LYS:HZ1	1.75	0.52
1:L:369:ASP:OD1	1:M:282:TYR:N	2.43	0.52
1:W:256:ILE:HD11	1:X:390:VAL:HG21	1.92	0.52
1:Z:386:SER:HA	1:Z:429:THR:O	2.10	0.52
1:a:187:ASP:O	1:a:191:ILE:HG12	2.08	0.52
1:c:268:ALA:HB1	1:c:382:ILE:HD11	1.90	0.52
1:c:405:THR:OG1	1:c:407:ASP:OD1	2.24	0.52
1:d:420:MET:HE3	1:d:422:PHE:CD1	2.45	0.52
1:e:378:ASN:ND2	1:e:381:ASP:OD1	2.37	0.52
1:E:404:LEU:H	1:E:434:ASN:ND2	2.08	0.52
1:L:258:GLY:HA3	1:L:261:ASN:HD22	1.75	0.52
1:Q:297:GLN:OE1	1:R:363:THR:OG1	2.18	0.52
1:R:407:ASP:HA	1:R:410:LYS:HG2	1.92	0.52
1:U:195:VAL:HG13	1:U:210:VAL:HB	1.91	0.52
1:X:392:ASN:OD1	1:X:393:TYR:N	2.42	0.52
1:h:392:ASN:OD1	1:h:393:TYR:N	2.43	0.52
1:D:237:PHE:HE1	1:E:232:ASP:HA	1.75	0.52
1:G:169:GLN:HE22	1:H:161:LYS:NZ	2.06	0.52
1:J:385:LEU:N	1:J:428:ASP:OD2	2.42	0.52
1:Q:182:PRO:O	1:Q:184:ARG:NH1	2.42	0.52
1:T:187:ASP:O	1:T:191:ILE:HG12	2.10	0.52
1:W:129:GLN:O	1:W:133:GLN:HG2	2.09	0.52
1:B:237:PHE:HE1	1:C:232:ASP:HA	1.74	0.52
1:D:279:GLU:OE2	1:D:281:HIS:N	2.40	0.52
1:G:160:PRO:O	1:G:161:LYS:HG2	2.09	0.52
1:H:203:ALA:HA	1:I:158:ALA:HB1	1.92	0.52
1:S:389:VAL:HB	1:S:432:VAL:HG12	1.92	0.52
1:W:407:ASP:OD1	1:W:408:GLN:N	2.43	0.52
1:a:199:SER:OG	1:a:205:LEU:O	2.21	0.52
1:h:245:ILE:O	1:h:249:ILE:HG13	2.09	0.52
1:B:146:THR:O	1:B:147:LEU:HD23	2.10	0.52
1:D:416:THR:HG21	1:D:432:VAL:HG21	1.92	0.52
1:H:246:GLN:O	1:H:250:GLU:HG2	2.10	0.52
1:K:170:LYS:HD2	1:K:171:SER:O	2.10	0.52
1:K:187:ASP:O	1:K:191:ILE:HG12	2.10	0.52
1:M:415:LEU:HD22	1:N:431:ASN:ND2	2.25	0.52
1:T:125:GLN:N	1:T:128:GLU:OE1	2.43	0.52
1:T:195:VAL:HG13	1:T:210:VAL:HB	1.92	0.52
1:V:369:ASP:OD1	1:W:282:TYR:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:301:SER:HB2	1:Y:359:GLN:HE22	1.75	0.52
1:Y:283:SER:HB2	1:Y:369:ASP:HB2	1.92	0.52
1:b:250:GLU:O	1:b:254:SER:OG	2.26	0.52
1:g:248:ARG:NH2	1:h:242:GLU:OE1	2.42	0.52
1:O:153:ALA:HA	1:O:177:THR:O	2.09	0.51
1:Q:389:VAL:HB	1:Q:432:VAL:HG22	1.92	0.51
1:R:416:THR:HG23	1:R:430:LEU:HD21	1.92	0.51
1:b:301:SER:O	1:b:359:GLN:N	2.32	0.51
1:B:157:LEU:HD11	1:B:202:VAL:HG11	1.91	0.51
1:G:413:GLU:OE2	1:G:417:ARG:NH1	2.43	0.51
1:M:369:ASP:OD1	1:N:282:TYR:N	2.43	0.51
1:Q:297:GLN:HB3	1:Q:363:THR:HB	1.92	0.51
1:U:199:SER:OG	1:U:205:LEU:O	2.20	0.51
1:W:279:GLU:OE2	1:W:281:HIS:HB2	2.10	0.51
1:d:181:GLU:N	1:d:181:GLU:OE1	2.43	0.51
1:f:200:SER:HB3	1:g:175:SER:HB3	1.91	0.51
1:f:246:GLN:NE2	1:f:250:GLU:OE2	2.43	0.51
1:F:301:SER:HB2	1:G:359:GLN:OE1	2.10	0.51
1:I:369:ASP:OD1	1:J:282:TYR:N	2.42	0.51
1:K:303:GLN:HG3	1:L:357:SER:HB2	1.92	0.51
1:L:392:ASN:OD1	1:L:393:TYR:N	2.43	0.51
1:Q:147:LEU:O	1:Q:149:PRO:HD2	2.10	0.51
1:U:276:GLU:OE2	1:U:374:HIS:NE2	2.42	0.51
1:d:190:GLN:CD	1:f:217:GLY:HA2	2.36	0.51
1:A:283:SER:HB2	1:A:369:ASP:HB2	1.91	0.51
1:C:143:THR:O	1:C:146:THR:OG1	2.27	0.51
1:C:420:MET:HE1	1:C:430:LEU:HB2	1.92	0.51
1:F:294:ARG:NH1	1:G:368:VAL:HG22	2.26	0.51
1:G:173:SER:HA	1:G:209:ASN:HB3	1.91	0.51
1:M:374:HIS:HB3	1:N:276:GLU:HB3	1.92	0.51
1:U:214:ASP:OD1	1:U:216:SER:N	2.37	0.51
1:Y:195:VAL:HA	1:Y:210:VAL:HG11	1.93	0.51
1:g:188:GLU:HA	1:g:191:ILE:HD12	1.92	0.51
1:A:234:GLN:HG2	1:A:272:PHE:CD2	2.45	0.51
1:A:267:THR:OG1	1:A:386:SER:HB2	2.09	0.51
1:F:389:VAL:HB	1:F:432:VAL:HG13	1.93	0.51
1:P:283:SER:HB2	1:P:369:ASP:HB3	1.93	0.51
1:P:394:LYS:HG2	1:P:402:LEU:HB3	1.91	0.51
1:b:420:MET:SD	1:b:422:PHE:HD1	2.33	0.51
1:f:287:ASP:OD2	1:f:290:LYS:NZ	2.32	0.51
1:h:140:LEU:O	1:h:143:THR:OG1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:246:GLN:O	1:h:250:GLU:HG2	2.10	0.51
1:E:188:GLU:HA	1:E:191:ILE:HD12	1.92	0.51
1:E:253:LEU:HD11	1:E:412:ILE:HG23	1.92	0.51
1:H:205:LEU:HD21	1:H:210:VAL:HG13	1.91	0.51
1:H:294:ARG:NH1	1:I:366:TYR:O	2.44	0.51
1:L:376:LYS:C	1:L:376:LYS:HD3	2.36	0.51
1:M:410:LYS:O	1:M:413:GLU:HG3	2.10	0.51
1:T:152:SER:O	1:T:178:VAL:HA	2.09	0.51
1:X:414:ASP:HB3	1:Y:431:ASN:ND2	2.24	0.51
1:c:420:MET:HE3	1:c:422:PHE:HD1	1.76	0.51
1:C:163:SER:O	1:C:169:GLN:NE2	2.34	0.51
1:C:252:ILE:HG12	1:D:265:GLN:HG3	1.93	0.51
1:G:252:ILE:O	1:G:255:PRO:HD2	2.10	0.51
1:T:138:GLY:O	1:T:142:ARG:HG3	2.10	0.51
1:U:407:ASP:O	1:U:410:LYS:HG3	2.11	0.51
1:V:394:LYS:HG2	1:V:402:LEU:HB2	1.92	0.51
1:W:213:VAL:HG22	1:W:219:LEU:HD23	1.92	0.51
1:Y:214:ASP:HB3	1:Y:218:HIS:HB2	1.92	0.51
1:H:193:ALA:HA	1:I:219:LEU:HD21	1.93	0.51
1:L:378:ASN:ND2	1:L:381:ASP:OD1	2.38	0.51
1:M:394:LYS:HG2	1:M:402:LEU:HB3	1.93	0.51
1:P:299:ASN:HB2	1:P:361:ASN:HB3	1.93	0.51
1:c:388:ALA:HA	1:c:431:ASN:O	2.10	0.51
1:G:190:GLN:HG2	1:H:217:GLY:HA3	1.92	0.51
1:I:139:GLU:HG3	1:K:156:HIS:HE1	1.76	0.51
1:O:139:GLU:CD	1:Q:154:ARG:HH11	2.19	0.51
1:R:233:ALA:HA	1:R:236:LYS:HE2	1.92	0.51
1:S:420:MET:HE1	1:S:430:LEU:HB2	1.93	0.51
1:W:199:SER:HA	1:W:205:LEU:HD23	1.93	0.51
1:c:149:PRO:HA	1:c:181:GLU:HG2	1.93	0.51
1:g:407:ASP:OD1	1:g:408:GLN:N	2.44	0.51
1:A:275:LYS:HB2	1:A:377:MET:HB2	1.91	0.51
1:I:151:LYS:HZ3	1:I:182:PRO:HD3	1.76	0.51
1:I:281:HIS:CE1	1:I:282:TYR:O	2.64	0.51
1:L:287:ASP:OD1	1:L:288:ALA:N	2.44	0.51
1:N:393:TYR:CZ	1:N:436:PRO:HD3	2.46	0.51
1:P:389:VAL:HB	1:P:432:VAL:HG13	1.92	0.51
1:T:373:ARG:HH21	1:U:275:LYS:HE2	1.76	0.51
1:U:159:MET:CE	1:U:172:PRO:HB2	2.40	0.51
1:g:287:ASP:HB3	1:g:290:LYS:HG2	1.93	0.51
1:h:165:PHE:C	1:h:167:ARG:HH12	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:GLU:O	1:H:143:THR:HG23	2.11	0.50
1:I:301:SER:HB3	1:I:359:GLN:HB3	1.92	0.50
1:L:257:VAL:O	1:L:261:ASN:ND2	2.40	0.50
1:N:196:HIS:HB2	1:O:219:LEU:HD21	1.94	0.50
1:N:370:ARG:HG2	1:N:371:THR:N	2.26	0.50
1:e:240:ASP:OD2	1:e:244:ARG:NH2	2.44	0.50
1:h:194:VAL:HG21	1:h:212:LEU:HD22	1.93	0.50
1:h:271:ASP:OD1	1:h:381:ASP:N	2.40	0.50
1:H:252:ILE:HB	1:I:265:GLN:HG3	1.93	0.50
1:I:303:GLN:HB2	1:I:357:SER:H	1.76	0.50
1:O:155:VAL:HG23	1:O:176:VAL:HG22	1.93	0.50
1:R:269:GLN:HG3	1:R:384:ARG:CZ	2.40	0.50
1:S:385:LEU:HB2	1:S:428:ASP:OD2	2.10	0.50
1:T:282:TYR:CZ	1:T:370:ARG:HD3	2.45	0.50
1:Z:249:ILE:HD12	1:Z:416:THR:HG23	1.91	0.50
1:Z:276:GLU:OE2	1:Z:374:HIS:NE2	2.44	0.50
1:a:137:GLU:OE1	1:a:155:VAL:HG13	2.11	0.50
1:d:199:SER:HA	1:d:205:LEU:HD23	1.92	0.50
1:g:385:LEU:N	1:g:428:ASP:OD2	2.36	0.50
1:F:374:HIS:HB3	1:G:276:GLU:HB3	1.94	0.50
1:G:374:HIS:HB3	1:H:276:GLU:HB3	1.94	0.50
1:H:299:ASN:N	1:H:361:ASN:O	2.39	0.50
1:L:393:TYR:HB3	1:L:402:LEU:N	2.26	0.50
1:M:409:MET:CE	1:M:434:ASN:HB2	2.41	0.50
1:N:125:GLN:O	1:N:128:GLU:HG3	2.11	0.50
1:Y:404:LEU:H	1:Y:434:ASN:ND2	2.09	0.50
1:a:382:ILE:HD12	1:a:382:ILE:H	1.75	0.50
1:b:283:SER:HB2	1:b:369:ASP:HB2	1.93	0.50
1:f:418:GLU:HB3	1:g:388:ALA:HB2	1.93	0.50
1:f:424:ASP:OD2	1:f:424:ASP:N	2.41	0.50
1:B:126:PHE:HA	1:B:129:GLN:HE22	1.77	0.50
1:C:129:GLN:OE1	1:C:129:GLN:N	2.39	0.50
1:I:147:LEU:O	1:I:149:PRO:HD2	2.11	0.50
1:I:294:ARG:NE	1:I:367:GLU:OE1	2.36	0.50
1:Q:161:LYS:HD3	1:Q:162:PRO:C	2.37	0.50
1:Q:252:ILE:HD11	1:R:265:GLN:HB2	1.93	0.50
1:Q:393:TYR:HB3	1:Q:402:LEU:N	2.27	0.50
1:U:142:ARG:HG3	1:W:154:ARG:NH1	2.27	0.50
1:d:404:LEU:HB2	1:d:434:ASN:ND2	2.27	0.50
1:A:389:VAL:HB	1:A:432:VAL:HG22	1.94	0.50
1:C:394:LYS:HE3	1:C:402:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:GLN:OE1	1:D:234:GLN:N	2.38	0.50
1:K:142:ARG:O	1:K:146:THR:HG23	2.12	0.50
1:N:277:GLN:HB3	1:N:375:THR:HB	1.92	0.50
1:b:257:VAL:O	1:b:261:ASN:ND2	2.45	0.50
1:B:154:ARG:HH12	1:h:142:ARG:C	2.19	0.50
1:K:393:TYR:CE2	1:K:436:PRO:HD3	2.46	0.50
1:L:407:ASP:HA	1:L:410:LYS:HE3	1.94	0.50
1:V:393:TYR:CE2	1:V:436:PRO:HD3	2.46	0.50
1:X:256:ILE:HG22	1:X:257:VAL:HG13	1.93	0.50
1:a:176:VAL:O	1:a:212:LEU:HA	2.12	0.50
1:e:271:ASP:OD1	1:e:381:ASP:N	2.43	0.50
1:H:137:GLU:HB2	1:H:155:VAL:HG13	1.94	0.50
1:J:377:MET:HE3	1:J:377:MET:HA	1.93	0.50
1:K:161:LYS:HG2	1:K:162:PRO:HD2	1.93	0.50
1:R:248:ARG:NH1	1:S:267:THR:HG22	2.27	0.50
1:Y:203:ALA:HA	1:a:158:ALA:HB1	1.92	0.50
1:a:149:PRO:HA	1:a:181:GLU:HG2	1.92	0.50
1:f:170:LYS:HD2	1:f:171:SER:O	2.12	0.50
1:C:291:ALA:HB1	1:C:366:TYR:HE1	1.76	0.50
1:I:174:ALA:O	1:I:210:VAL:HA	2.12	0.50
1:M:276:GLU:OE2	1:M:374:HIS:NE2	2.38	0.50
1:T:233:ALA:HA	1:T:236:LYS:HD3	1.93	0.50
1:T:262:VAL:HG23	1:T:391:VAL:HG12	1.94	0.50
1:V:267:THR:OG1	1:V:386:SER:HB2	2.12	0.50
1:f:233:ALA:HA	1:f:236:LYS:HE2	1.94	0.50
1:B:161:LYS:HZ3	1:B:163:SER:HA	1.77	0.50
1:C:144:ILE:HG22	1:C:150:VAL:HG11	1.92	0.50
1:E:373:ARG:HH21	1:F:275:LYS:HE3	1.77	0.50
1:H:147:LEU:O	1:H:149:PRO:HD2	2.12	0.50
1:L:256:ILE:HG21	1:L:412:ILE:HD11	1.92	0.50
1:O:180:LEU:H	1:O:215:GLN:CD	2.20	0.50
1:X:140:LEU:O	1:X:143:THR:OG1	2.27	0.50
1:X:407:ASP:OD1	1:X:408:GLN:N	2.43	0.50
1:d:356:ARG:NH2	1:d:358:THR:OG1	2.45	0.50
1:g:213:VAL:HG22	1:g:219:LEU:HD23	1.93	0.50
1:C:161:LYS:HA	1:C:161:LYS:HE2	1.93	0.49
1:E:143:THR:HG21	1:G:156:HIS:NE2	2.26	0.49
1:E:191:ILE:HD13	1:E:220:LEU:HB3	1.93	0.49
1:E:393:TYR:CE2	1:E:436:PRO:HD3	2.47	0.49
1:F:407:ASP:OD1	1:F:408:GLN:N	2.44	0.49
1:J:417:ARG:O	1:J:422:PHE:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:422:PHE:HE2	1:P:424:ASP:HB3	1.76	0.49
1:U:161:LYS:HD3	1:U:162:PRO:C	2.37	0.49
1:W:242:GLU:OE2	1:W:268:ALA:N	2.39	0.49
1:c:200:SER:HB3	1:d:175:SER:HB3	1.93	0.49
1:f:302:GLU:HB3	1:f:358:THR:HG23	1.94	0.49
1:K:137:GLU:HB2	1:K:155:VAL:HG13	1.94	0.49
1:K:157:LEU:HD21	1:K:202:VAL:HG21	1.94	0.49
1:M:375:THR:HG23	1:N:275:LYS:HZ2	1.77	0.49
1:N:133:GLN:O	1:N:136:LEU:N	2.43	0.49
1:W:404:LEU:HD13	1:W:434:ASN:HD21	1.77	0.49
1:W:420:MET:HE1	1:W:430:LEU:HB2	1.93	0.49
1:a:283:SER:HB2	1:a:369:ASP:HB2	1.94	0.49
1:c:139:GLU:OE2	1:d:134:ARG:NH2	2.45	0.49
1:d:407:ASP:HA	1:d:410:LYS:HG3	1.94	0.49
1:d:426:ARG:NE	1:d:428:ASP:OD1	2.38	0.49
1:h:192:SER:O	1:h:196:HIS:ND1	2.39	0.49
1:A:231:ASN:OD1	1:A:232:ASP:N	2.45	0.49
1:N:244:ARG:CZ	1:O:235:LEU:HB3	2.42	0.49
1:O:304:VAL:HG22	1:O:356:ARG:HG2	1.93	0.49
1:c:236:LYS:H	1:c:236:LYS:HD2	1.77	0.49
1:f:275:LYS:HB3	1:f:377:MET:HE2	1.94	0.49
1:B:246:GLN:NE2	1:B:264:ALA:O	2.45	0.49
1:H:160:PRO:HD3	1:H:172:PRO:HA	1.93	0.49
1:I:216:SER:O	1:I:218:HIS:ND1	2.43	0.49
1:M:252:ILE:HG22	1:M:253:LEU:HD12	1.94	0.49
1:N:143:THR:HA	1:O:154:ARG:HD3	1.94	0.49
1:N:179:THR:HA	1:N:215:GLN:HB3	1.95	0.49
1:Q:369:ASP:OD1	1:R:282:TYR:N	2.44	0.49
1:f:143:THR:HG23	1:g:154:ARG:NE	2.27	0.49
1:g:234:GLN:HB3	1:g:272:PHE:CE2	2.47	0.49
1:h:287:ASP:HB3	1:h:290:LYS:HE2	1.94	0.49
1:h:407:ASP:HA	1:h:410:LYS:HG2	1.95	0.49
1:B:191:ILE:HG23	1:B:212:LEU:HD12	1.95	0.49
1:F:413:GLU:CD	1:F:417:ARG:HH12	2.18	0.49
1:G:239:ASN:HA	1:G:242:GLU:HG2	1.95	0.49
1:T:191:ILE:HD12	1:T:220:LEU:HD13	1.94	0.49
1:W:378:ASN:HB3	1:W:381:ASP:OD2	2.12	0.49
1:g:257:VAL:O	1:g:261:ASN:ND2	2.30	0.49
1:C:143:THR:HG22	1:E:154:ARG:HD3	1.94	0.49
1:C:195:VAL:HG13	1:C:210:VAL:HB	1.95	0.49
1:L:298:LEU:HG	1:L:362:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:147:LEU:HD23	1:T:150:VAL:HG21	1.94	0.49
1:U:161:LYS:HG2	1:U:162:PRO:HD2	1.95	0.49
1:e:373:ARG:NH2	1:f:377:MET:HE3	2.28	0.49
1:C:250:GLU:O	1:C:254:SER:OG	2.27	0.49
1:C:424:ASP:OD1	1:C:425:LYS:N	2.46	0.49
1:K:180:LEU:N	1:K:215:GLN:OE1	2.37	0.49
1:K:373:ARG:NH1	1:L:277:GLN:OE1	2.46	0.49
1:N:212:LEU:HB2	1:N:220:LEU:HB2	1.93	0.49
1:Y:187:ASP:O	1:Y:191:ILE:HG12	2.11	0.49
1:b:245:ILE:HG21	1:b:266:VAL:HG11	1.93	0.49
1:b:277:GLN:HB3	1:b:375:THR:HB	1.94	0.49
1:d:160:PRO:HD3	1:d:172:PRO:HA	1.95	0.49
1:C:389:VAL:HB	1:C:432:VAL:HG13	1.93	0.49
1:E:134:ARG:O	1:E:137:GLU:HB3	2.13	0.49
1:J:387:VAL:HB	1:J:420:MET:HE3	1.95	0.49
1:U:269:GLN:HB2	1:U:383:GLU:HG2	1.94	0.49
1:c:143:THR:HG22	1:d:154:ARG:HD3	1.95	0.49
1:d:421:GLY:O	1:d:426:ARG:NH2	2.45	0.49
1:f:189:GLY:O	1:f:192:SER:OG	2.25	0.49
1:L:142:ARG:HB3	1:N:154:ARG:HH22	1.78	0.49
1:P:279:GLU:OE2	1:P:281:HIS:HB2	2.13	0.49
1:b:239:ASN:O	1:b:242:GLU:HG2	2.13	0.49
1:c:420:MET:HE3	1:c:422:PHE:CD1	2.48	0.49
1:B:182:PRO:O	1:B:184:ARG:NH1	2.46	0.49
1:B:414:ASP:HB3	1:C:431:ASN:ND2	2.27	0.49
1:G:187:ASP:O	1:G:191:ILE:HG12	2.13	0.49
1:G:393:TYR:CE2	1:G:436:PRO:HD3	2.48	0.49
1:L:143:THR:HG21	1:N:156:HIS:NE2	2.27	0.49
1:L:282:TYR:OH	1:L:370:ARG:HD3	2.12	0.49
1:O:144:ILE:HG22	1:O:150:VAL:HG11	1.94	0.49
1:O:161:LYS:HZ2	1:O:163:SER:HA	1.78	0.49
1:Q:244:ARG:HH11	1:R:239:ASN:HB2	1.78	0.49
1:V:281:HIS:CE1	1:V:282:TYR:O	2.65	0.49
1:A:276:GLU:HB3	1:h:374:HIS:HB3	1.94	0.48
1:B:187:ASP:O	1:B:191:ILE:HG12	2.12	0.48
1:H:195:VAL:HG13	1:H:210:VAL:HG21	1.94	0.48
1:L:409:MET:CE	1:L:434:ASN:HB2	2.43	0.48
1:R:203:ALA:HB1	1:T:160:PRO:HG3	1.94	0.48
1:W:410:LYS:HD2	1:W:410:LYS:C	2.38	0.48
1:Z:252:ILE:O	1:Z:255:PRO:HD2	2.14	0.48
1:b:252:ILE:HB	1:c:265:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:187:ASP:O	1:d:191:ILE:HG12	2.13	0.48
1:h:256:ILE:HG21	1:h:412:ILE:HD11	1.95	0.48
1:G:267:THR:HB	1:G:386:SER:HB2	1.95	0.48
1:L:151:LYS:NZ	1:L:179:THR:HG22	2.28	0.48
1:L:244:ARG:NH1	1:M:235:LEU:O	2.46	0.48
1:Q:374:HIS:HB3	1:R:276:GLU:HB3	1.95	0.48
1:S:368:VAL:HG22	1:S:369:ASP:O	2.13	0.48
1:T:141:ALA:O	1:T:144:ILE:HG22	2.13	0.48
1:T:424:ASP:OD1	1:T:425:LYS:N	2.47	0.48
1:U:373:ARG:HG2	1:V:277:GLN:OE1	2.12	0.48
1:W:188:GLU:HA	1:W:191:ILE:HB	1.94	0.48
1:Y:182:PRO:O	1:Y:184:ARG:NH1	2.46	0.48
1:a:389:VAL:O	1:a:432:VAL:HA	2.12	0.48
1:b:404:LEU:H	1:b:434:ASN:ND2	2.11	0.48
1:C:404:LEU:H	1:C:434:ASN:ND2	2.11	0.48
1:I:193:ALA:HB1	1:K:213:VAL:HG13	1.94	0.48
1:P:293:LEU:O	1:Q:366:TYR:HD2	1.95	0.48
1:P:299:ASN:ND2	1:P:361:ASN:HD22	2.11	0.48
1:X:166:VAL:O	1:X:169:GLN:NE2	2.46	0.48
1:Z:266:VAL:HG22	1:Z:387:VAL:HG22	1.94	0.48
1:c:137:GLU:OE2	1:c:155:VAL:HG22	2.13	0.48
1:g:394:LYS:HG3	1:g:402:LEU:HB2	1.94	0.48
1:h:266:VAL:HG22	1:h:387:VAL:HG22	1.94	0.48
1:G:407:ASP:OD1	1:G:408:GLN:N	2.47	0.48
1:H:200:SER:HB3	1:I:175:SER:HB3	1.95	0.48
1:H:264:ALA:HB2	1:H:389:VAL:HG22	1.96	0.48
1:K:205:LEU:HD11	1:K:209:ASN:HB2	1.95	0.48
1:Q:275:LYS:CB	1:Q:377:MET:HB2	2.43	0.48
1:Q:410:LYS:HD2	1:Q:411:GLN:N	2.28	0.48
1:T:392:ASN:OD1	1:T:436:PRO:HA	2.14	0.48
1:U:419:ALA:O	1:V:267:THR:HG21	2.11	0.48
1:a:423:SER:HB3	1:a:426:ARG:HB2	1.96	0.48
1:h:133:GLN:O	1:h:137:GLU:HG2	2.14	0.48
1:B:187:ASP:OD1	1:B:190:GLN:HG3	2.13	0.48
1:L:142:ARG:HA	1:L:145:GLU:OE1	2.12	0.48
1:O:244:ARG:NE	1:P:239:ASN:HD21	2.10	0.48
1:P:240:ASP:O	1:P:244:ARG:HG3	2.14	0.48
1:R:138:GLY:O	1:R:142:ARG:HG2	2.13	0.48
1:U:143:THR:HG21	1:W:156:HIS:CD2	2.48	0.48
1:U:245:ILE:HG21	1:U:266:VAL:HG11	1.95	0.48
1:d:410:LYS:HD2	1:d:411:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:199:SER:OG	1:f:205:LEU:O	2.19	0.48
1:g:270:LEU:HD23	1:g:382:ILE:HA	1.96	0.48
1:A:405:THR:HG22	1:A:408:GLN:HB2	1.95	0.48
1:J:389:VAL:HB	1:J:432:VAL:HG22	1.95	0.48
1:P:374:HIS:HB3	1:Q:276:GLU:HB3	1.94	0.48
1:Q:160:PRO:HG2	1:Q:170:LYS:O	2.12	0.48
1:Q:187:ASP:OD1	1:Q:190:GLN:HG3	2.13	0.48
1:S:248:ARG:NH1	1:T:267:THR:OG1	2.46	0.48
1:T:203:ALA:HB3	1:U:160:PRO:HG3	1.95	0.48
1:T:281:HIS:HB3	1:T:371:THR:HB	1.96	0.48
1:W:154:ARG:HG3	1:W:177:THR:HG23	1.96	0.48
1:Y:407:ASP:HA	1:Y:410:LYS:HG3	1.94	0.48
1:c:283:SER:OG	1:c:369:ASP:HB2	2.14	0.48
1:d:139:GLU:HB3	1:f:156:HIS:HE1	1.79	0.48
1:B:417:ARG:HG3	1:B:422:PHE:CB	2.43	0.48
1:E:424:ASP:OD1	1:E:425:LYS:N	2.46	0.48
1:H:143:THR:HG22	1:I:154:ARG:CD	2.43	0.48
1:I:275:LYS:HB2	1:I:377:MET:HB2	1.96	0.48
1:J:267:THR:HB	1:J:386:SER:HB2	1.95	0.48
1:O:405:THR:OG1	1:O:407:ASP:OD1	2.20	0.48
1:R:187:ASP:O	1:R:191:ILE:HG12	2.14	0.48
1:Y:392:ASN:OD1	1:Y:393:TYR:N	2.44	0.48
1:Z:301:SER:OG	1:Z:303:GLN:NE2	2.46	0.48
1:a:203:ALA:HA	1:c:158:ALA:HB1	1.95	0.48
1:d:244:ARG:HH21	1:e:239:ASN:HD21	1.60	0.48
1:B:194:VAL:HG13	1:B:212:LEU:HD11	1.96	0.48
1:F:393:TYR:CE2	1:F:436:PRO:HD3	2.48	0.48
1:J:370:ARG:HG2	1:J:371:THR:N	2.29	0.48
1:N:374:HIS:HB3	1:O:276:GLU:HB2	1.95	0.48
1:T:250:GLU:O	1:T:254:SER:OG	2.25	0.48
1:Z:245:ILE:O	1:Z:249:ILE:HG12	2.14	0.48
1:c:391:VAL:HG21	1:c:409:MET:HE1	1.95	0.48
1:A:267:THR:HG22	1:h:248:ARG:HD2	1.95	0.48
1:B:408:GLN:O	1:B:412:ILE:HG12	2.14	0.48
1:E:197:LEU:HD12	1:G:175:SER:HB2	1.96	0.48
1:F:392:ASN:OD1	1:F:393:TYR:N	2.46	0.48
1:I:151:LYS:NZ	1:I:182:PRO:HD3	2.29	0.48
1:I:283:SER:HB2	1:I:369:ASP:HB2	1.96	0.48
1:L:245:ILE:HG21	1:L:266:VAL:HG11	1.96	0.48
1:N:415:LEU:HD11	1:O:433:VAL:HG21	1.95	0.48
1:Q:244:ARG:HG2	1:Q:247:ARG:HH22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:234:GLN:HB2	1:X:272:PHE:CE2	2.49	0.48
1:Y:298:LEU:HD13	1:Y:362:GLU:HB3	1.95	0.48
1:E:178:VAL:HG12	1:E:180:LEU:HD22	1.96	0.48
1:G:191:ILE:HD11	1:G:220:LEU:HD13	1.96	0.48
1:L:373:ARG:HH21	1:M:275:LYS:HD2	1.79	0.48
1:O:139:GLU:O	1:O:143:THR:HG23	2.14	0.48
1:Q:178:VAL:HG12	1:Q:213:VAL:O	2.13	0.48
1:Q:412:ILE:O	1:Q:416:THR:HG23	2.14	0.48
1:Y:266:VAL:HG22	1:Y:387:VAL:HG22	1.95	0.48
1:Y:393:TYR:CE2	1:Y:436:PRO:HD3	2.49	0.48
1:Z:404:LEU:H	1:Z:434:ASN:ND2	2.12	0.48
1:B:252:ILE:HD11	1:C:265:GLN:HB2	1.95	0.47
1:I:282:TYR:CZ	1:I:370:ARG:HD3	2.49	0.47
1:I:393:TYR:HB3	1:I:402:LEU:N	2.29	0.47
1:L:179:THR:HG23	1:L:215:GLN:HB3	1.96	0.47
1:N:275:LYS:CB	1:N:377:MET:HB2	2.44	0.47
1:O:244:ARG:NH1	1:P:235:LEU:O	2.47	0.47
1:T:417:ARG:HG3	1:T:422:PHE:HB3	1.96	0.47
1:Y:180:LEU:H	1:Y:215:GLN:CD	2.22	0.47
1:a:423:SER:HB3	1:a:426:ARG:HE	1.79	0.47
1:c:231:ASN:OD1	1:c:232:ASP:N	2.42	0.47
1:g:266:VAL:HG22	1:g:387:VAL:HG22	1.96	0.47
1:E:151:LYS:HZ1	1:E:181:GLU:HA	1.79	0.47
1:E:180:LEU:HD23	1:E:214:ASP:HB2	1.96	0.47
1:E:413:GLU:OE2	1:E:432:VAL:HB	2.14	0.47
1:G:140:LEU:HA	1:G:143:THR:OG1	2.14	0.47
1:H:189:GLY:O	1:H:192:SER:OG	2.25	0.47
1:I:139:GLU:O	1:I:143:THR:HG23	2.14	0.47
1:K:372:ILE:O	1:L:277:GLN:HA	2.14	0.47
1:M:279:GLU:OE2	1:M:281:HIS:N	2.46	0.47
1:R:203:ALA:HB2	1:T:158:ALA:HB1	1.95	0.47
1:h:165:PHE:CE1	1:h:166:VAL:HG23	2.50	0.47
1:M:293:LEU:HD21	1:M:296:ARG:NH2	2.29	0.47
1:O:182:PRO:O	1:O:184:ARG:NH1	2.47	0.47
1:W:404:LEU:H	1:W:434:ASN:ND2	2.12	0.47
1:X:190:GLN:CD	1:Y:217:GLY:HA3	2.39	0.47
1:X:206:PRO:HG2	1:X:209:ASN:OD1	2.14	0.47
1:X:241:VAL:HG22	1:Y:235:LEU:HD21	1.96	0.47
1:D:297:GLN:OE1	1:E:363:THR:HG22	2.14	0.47
1:K:257:VAL:C	1:K:261:ASN:HD22	2.23	0.47
1:L:143:THR:HG22	1:N:154:ARG:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:420:MET:HE3	1:U:422:PHE:HB2	1.96	0.47
1:W:378:ASN:HD22	1:W:381:ASP:CG	2.20	0.47
1:Y:231:ASN:OD1	1:Y:232:ASP:N	2.47	0.47
1:f:137:GLU:HB2	1:f:155:VAL:HG13	1.96	0.47
1:h:244:ARG:NH2	1:h:248:ARG:HH22	2.12	0.47
1:h:387:VAL:HB	1:h:420:MET:SD	2.54	0.47
1:B:409:MET:HE2	1:B:434:ASN:HB2	1.96	0.47
1:E:206:PRO:HG2	1:E:209:ASN:OD1	2.15	0.47
1:I:143:THR:HG22	1:K:154:ARG:CD	2.45	0.47
1:M:375:THR:HG23	1:N:275:LYS:NZ	2.29	0.47
1:R:302:GLU:HA	1:R:357:SER:O	2.15	0.47
1:U:126:PHE:O	1:U:129:GLN:HG2	2.15	0.47
1:W:404:LEU:HD23	1:W:408:GLN:HG2	1.96	0.47
1:Z:408:GLN:O	1:Z:412:ILE:HG12	2.14	0.47
1:a:254:SER:HB2	1:a:255:PRO:HD3	1.96	0.47
1:c:140:LEU:O	1:c:144:ILE:HG12	2.15	0.47
1:g:389:VAL:HB	1:g:432:VAL:HG13	1.96	0.47
1:h:263:HIS:HB2	1:h:390:VAL:HG22	1.97	0.47
1:F:267:THR:OG1	1:F:386:SER:HB2	2.14	0.47
1:I:145:GLU:HG2	1:I:152:SER:HA	1.96	0.47
1:I:174:ALA:HB3	1:I:210:VAL:HG22	1.95	0.47
1:K:128:GLU:HG2	1:K:129:GLN:N	2.28	0.47
1:Q:193:ALA:HA	1:R:219:LEU:HG	1.96	0.47
1:X:254:SER:HB2	1:X:255:PRO:HD3	1.96	0.47
1:b:412:ILE:O	1:b:416:THR:HG23	2.15	0.47
1:A:268:ALA:HB2	1:A:385:LEU:HD23	1.97	0.47
1:E:382:ILE:H	1:E:382:ILE:HD12	1.80	0.47
1:H:134:ARG:HA	1:H:137:GLU:OE2	2.15	0.47
1:O:128:GLU:HG2	1:O:129:GLN:N	2.30	0.47
1:O:152:SER:HG	1:O:179:THR:HG1	1.61	0.47
1:V:275:LYS:CB	1:V:377:MET:HE2	2.45	0.47
1:V:389:VAL:O	1:V:432:VAL:HA	2.14	0.47
1:Y:298:LEU:HD11	1:Y:300:ILE:HD11	1.95	0.47
1:a:190:GLN:NE2	1:c:216:SER:O	2.48	0.47
1:d:409:MET:CE	1:d:434:ASN:HB2	2.45	0.47
1:e:393:TYR:CE2	1:e:436:PRO:HD3	2.50	0.47
1:e:413:GLU:O	1:e:416:THR:OG1	2.27	0.47
1:D:378:ASN:ND2	1:D:381:ASP:OD1	2.38	0.47
1:E:166:VAL:HG22	1:E:168:GLU:HG3	1.96	0.47
1:E:261:ASN:HB3	1:E:392:ASN:HB3	1.96	0.47
1:H:133:GLN:O	1:H:136:LEU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:ALA:O	1:J:242:GLU:HG2	2.14	0.47
1:L:139:GLU:OE2	1:N:154:ARG:NH1	2.43	0.47
1:M:234:GLN:HB2	1:M:272:PHE:CE2	2.50	0.47
1:N:298:LEU:HD12	1:N:361:ASN:O	2.15	0.47
1:O:152:SER:OG	1:O:179:THR:OG1	2.30	0.47
1:T:197:LEU:HD11	1:U:154:ARG:HH21	1.79	0.47
1:W:142:ARG:HG3	1:X:154:ARG:HH12	1.80	0.47
1:X:244:ARG:NH2	1:Y:235:LEU:HB3	2.30	0.47
1:c:389:VAL:HB	1:c:432:VAL:HG22	1.95	0.47
1:e:420:MET:SD	1:e:422:PHE:HB2	2.55	0.47
1:H:150:VAL:HG22	1:H:178:VAL:HG21	1.96	0.47
1:I:408:GLN:O	1:I:412:ILE:HG12	2.15	0.47
1:N:280:GLU:HG2	1:N:282:TYR:HE2	1.80	0.47
1:O:197:LEU:CD2	1:Q:213:VAL:HG21	2.45	0.47
1:T:172:PRO:HG2	1:T:204:GLY:O	2.15	0.47
1:T:192:SER:HB2	1:T:196:HIS:CE1	2.50	0.47
1:U:302:GLU:HA	1:U:357:SER:O	2.15	0.47
1:U:393:TYR:CE2	1:U:436:PRO:HD3	2.49	0.47
1:W:374:HIS:HB3	1:X:276:GLU:HB3	1.96	0.47
1:Z:277:GLN:HB3	1:Z:375:THR:HB	1.96	0.47
1:d:287:ASP:HB3	1:d:290:LYS:HE3	1.97	0.47
1:d:408:GLN:HA	1:d:411:GLN:NE2	2.30	0.47
1:f:199:SER:HA	1:f:205:LEU:HD23	1.97	0.47
1:B:195:VAL:HG13	1:B:210:VAL:CG2	2.42	0.47
1:C:139:GLU:O	1:C:143:THR:HG23	2.14	0.47
1:E:244:ARG:HD2	1:F:235:LEU:HD12	1.97	0.47
1:I:257:VAL:O	1:I:261:ASN:ND2	2.39	0.47
1:O:144:ILE:HG22	1:O:150:VAL:HG21	1.97	0.47
1:R:172:PRO:HG2	1:R:205:LEU:HD13	1.96	0.47
1:T:236:LYS:H	1:T:236:LYS:HD2	1.80	0.47
1:d:296:ARG:NH1	1:d:364:SER:OG	2.48	0.47
1:g:423:SER:OG	1:g:425:LYS:HE2	2.15	0.47
1:D:254:SER:HB2	1:D:255:PRO:HD3	1.97	0.46
1:F:245:ILE:O	1:F:249:ILE:HG12	2.15	0.46
1:L:423:SER:HB2	1:M:384:ARG:NH1	2.29	0.46
1:O:237:PHE:HE1	1:P:232:ASP:HA	1.79	0.46
1:V:240:ASP:OD1	1:W:235:LEU:HD13	2.15	0.46
1:X:275:LYS:HB2	1:X:377:MET:HB2	1.96	0.46
1:Y:250:GLU:O	1:Y:254:SER:OG	2.32	0.46
1:Z:231:ASN:O	1:Z:234:GLN:NE2	2.48	0.46
1:a:237:PHE:HE2	1:b:232:ASP:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:155:VAL:HG22	1:d:156:HIS:N	2.30	0.46
1:G:187:ASP:N	1:G:187:ASP:OD1	2.35	0.46
1:H:245:ILE:HG21	1:H:266:VAL:HG11	1.98	0.46
1:I:416:THR:HG23	1:I:430:LEU:HD21	1.97	0.46
1:K:140:LEU:O	1:K:143:THR:OG1	2.30	0.46
1:L:157:LEU:HA	1:L:174:ALA:HA	1.97	0.46
1:L:374:HIS:HB3	1:M:276:GLU:HB3	1.96	0.46
1:N:245:ILE:O	1:N:249:ILE:HG12	2.15	0.46
1:S:276:GLU:HG2	1:S:374:HIS:HE1	1.79	0.46
1:U:173:SER:OG	1:U:174:ALA:N	2.46	0.46
1:U:408:GLN:O	1:U:411:GLN:HG2	2.14	0.46
1:Y:180:LEU:HB2	1:Y:215:GLN:HE22	1.80	0.46
1:a:140:LEU:O	1:a:143:THR:OG1	2.26	0.46
1:I:416:THR:O	1:I:420:MET:HG3	2.14	0.46
1:M:287:ASP:OD2	1:M:289:SER:HB3	2.15	0.46
1:O:193:ALA:HA	1:Q:219:LEU:HD21	1.96	0.46
1:P:422:PHE:CE2	1:P:424:ASP:HB3	2.50	0.46
1:Q:181:GLU:HB3	1:Q:184:ARG:NH2	2.31	0.46
1:Q:393:TYR:CE2	1:Q:436:PRO:HD3	2.50	0.46
1:U:164:LEU:HD12	1:U:164:LEU:HA	1.68	0.46
1:c:151:LYS:HD3	1:c:182:PRO:HD3	1.96	0.46
1:h:246:GLN:HB2	1:h:266:VAL:HG23	1.96	0.46
1:E:162:PRO:HA	1:E:169:GLN:HG3	1.98	0.46
1:M:360:ARG:HG2	1:M:362:GLU:OE2	2.15	0.46
1:T:414:ASP:HB3	1:U:431:ASN:ND2	2.31	0.46
1:U:393:TYR:HB3	1:U:402:LEU:N	2.31	0.46
1:U:415:LEU:HD21	1:V:433:VAL:HG22	1.97	0.46
1:W:293:LEU:HD11	1:W:296:ARG:HH21	1.80	0.46
1:Z:411:GLN:O	1:Z:415:LEU:HD23	2.16	0.46
1:e:417:ARG:HG3	1:e:422:PHE:HB3	1.98	0.46
1:f:214:ASP:HB2	1:f:220:LEU:HD11	1.97	0.46
1:g:360:ARG:NH1	1:g:362:GLU:OE1	2.47	0.46
1:B:181:GLU:CD	1:B:184:ARG:HH21	2.22	0.46
1:B:407:ASP:O	1:B:410:LYS:HG3	2.16	0.46
1:F:253:LEU:CD1	1:F:412:ILE:HG23	2.46	0.46
1:N:375:THR:HG23	1:O:275:LYS:NZ	2.31	0.46
1:Q:173:SER:OG	1:Q:174:ALA:N	2.48	0.46
1:Z:267:THR:OG1	1:Z:386:SER:HB2	2.15	0.46
1:e:283:SER:HB2	1:e:369:ASP:HB2	1.97	0.46
1:L:164:LEU:H	1:L:164:LEU:HD23	1.80	0.46
1:L:244:ARG:HH11	1:M:235:LEU:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:402:LEU:HD23	1:M:403:PRO:O	2.16	0.46
1:U:193:ALA:HA	1:W:219:LEU:HD21	1.97	0.46
1:X:203:ALA:C	1:Y:170:LYS:HZ3	2.23	0.46
1:e:244:ARG:NH2	1:f:235:LEU:HB3	2.30	0.46
1:f:416:THR:O	1:f:420:MET:HG2	2.15	0.46
1:g:404:LEU:H	1:g:434:ASN:HD21	1.63	0.46
1:E:140:LEU:HD23	1:E:140:LEU:HA	1.82	0.46
1:F:279:GLU:H	1:F:373:ARG:HB2	1.81	0.46
1:I:192:SER:O	1:I:196:HIS:ND1	2.49	0.46
1:N:190:GLN:NE2	1:O:216:SER:O	2.46	0.46
1:T:173:SER:OG	1:T:174:ALA:N	2.48	0.46
1:X:143:THR:HG21	1:Y:156:HIS:NE2	2.30	0.46
1:Y:404:LEU:HD23	1:Y:408:GLN:HG2	1.97	0.46
1:a:373:ARG:HH21	1:b:275:LYS:HE2	1.80	0.46
1:c:168:GLU:OE1	1:c:170:LYS:HB2	2.16	0.46
1:c:236:LYS:HD2	1:c:236:LYS:N	2.30	0.46
1:c:362:GLU:N	1:c:362:GLU:OE2	2.49	0.46
1:f:385:LEU:HD12	1:f:426:ARG:NH2	2.31	0.46
1:F:279:GLU:OE2	1:F:281:HIS:N	2.38	0.46
1:N:212:LEU:CB	1:N:220:LEU:HB2	2.46	0.46
1:O:195:VAL:HG13	1:O:210:VAL:HB	1.96	0.46
1:P:421:GLY:O	1:P:426:ARG:NH2	2.49	0.46
1:R:389:VAL:HB	1:R:432:VAL:HG13	1.97	0.46
1:S:279:GLU:OE1	1:S:281:HIS:HB2	2.16	0.46
1:X:404:LEU:HB2	1:X:434:ASN:ND2	2.30	0.46
1:a:304:VAL:HB	1:b:356:ARG:H	1.81	0.46
1:b:298:LEU:HD13	1:b:362:GLU:HB3	1.97	0.46
1:c:190:GLN:CD	1:d:217:GLY:HA3	2.41	0.46
1:e:237:PHE:HE1	1:f:232:ASP:HA	1.80	0.46
1:A:393:TYR:CE2	1:A:436:PRO:HD3	2.51	0.46
1:B:156:HIS:CE1	1:h:140:LEU:HD22	2.51	0.46
1:B:190:GLN:HG2	1:C:217:GLY:HA3	1.97	0.46
1:F:247:ARG:NH1	1:F:247:ARG:HB2	2.31	0.46
1:F:415:LEU:HD23	1:F:415:LEU:HA	1.78	0.46
1:H:187:ASP:OD1	1:H:187:ASP:N	2.49	0.46
1:H:191:ILE:HG23	1:H:212:LEU:HD12	1.97	0.46
1:H:413:GLU:OE1	1:H:417:ARG:NH1	2.49	0.46
1:O:245:ILE:O	1:O:249:ILE:HG12	2.16	0.46
1:S:382:ILE:HG21	1:S:385:LEU:HG	1.98	0.46
1:U:149:PRO:HA	1:U:181:GLU:HB2	1.97	0.46
1:h:257:VAL:HG23	1:h:261:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ILE:O	1:C:277:GLN:HA	2.16	0.46
1:B:393:TYR:HB3	1:B:402:LEU:N	2.31	0.46
1:C:180:LEU:H	1:C:215:GLN:CD	2.22	0.46
1:G:202:VAL:HB	1:G:205:LEU:HD22	1.97	0.46
1:H:174:ALA:O	1:H:210:VAL:HA	2.15	0.46
1:J:423:SER:OG	1:J:425:LYS:HG2	2.16	0.46
1:K:249:ILE:HD13	1:K:419:ALA:HB3	1.98	0.46
1:N:303:GLN:N	1:N:303:GLN:OE1	2.48	0.46
1:R:186:LEU:HD11	1:R:190:GLN:OE1	2.16	0.46
1:U:197:LEU:HD12	1:W:175:SER:HB2	1.97	0.46
1:Y:262:VAL:HG23	1:Y:391:VAL:HG12	1.98	0.46
1:h:165:PHE:O	1:h:167:ARG:NH1	2.49	0.46
1:C:246:GLN:HE22	1:C:250:GLU:CD	2.24	0.45
1:I:138:GLY:O	1:I:142:ARG:HG2	2.16	0.45
1:J:256:ILE:HD12	1:K:435:SER:OG	2.16	0.45
1:K:193:ALA:HA	1:L:219:LEU:HG	1.99	0.45
1:L:244:ARG:HH22	1:M:239:ASN:CB	2.20	0.45
1:M:411:GLN:O	1:M:415:LEU:HD23	2.16	0.45
1:P:258:GLY:HA3	1:P:261:ASN:HD22	1.82	0.45
1:P:419:ALA:O	1:Q:267:THR:OG1	2.28	0.45
1:W:382:ILE:HD13	1:W:385:LEU:HD21	1.98	0.45
1:g:212:LEU:HD23	1:g:220:LEU:HD12	1.97	0.45
1:I:181:GLU:HB3	1:I:184:ARG:NH2	2.32	0.45
1:J:253:LEU:O	1:J:257:VAL:HG22	2.16	0.45
1:L:166:VAL:O	1:L:166:VAL:HG12	2.16	0.45
1:O:141:ALA:O	1:O:145:GLU:HG2	2.16	0.45
1:d:199:SER:HB2	1:d:207:PRO:HA	1.97	0.45
1:f:143:THR:HG21	1:g:156:HIS:NE2	2.31	0.45
1:f:212:LEU:HG	1:f:220:LEU:HD13	1.98	0.45
1:g:302:GLU:HA	1:g:357:SER:O	2.16	0.45
1:B:151:LYS:HD3	1:B:151:LYS:N	2.31	0.45
1:D:267:THR:HB	1:D:386:SER:HB2	1.99	0.45
1:F:294:ARG:HD2	1:F:294:ARG:HA	1.81	0.45
1:G:245:ILE:O	1:G:249:ILE:HG12	2.16	0.45
1:J:246:GLN:HG2	1:J:264:ALA:HB3	1.98	0.45
1:L:377:MET:HA	1:M:273:ALA:HB1	1.98	0.45
1:N:411:GLN:O	1:N:415:LEU:HG	2.16	0.45
1:Q:243:SER:O	1:Q:247:ARG:HG3	2.16	0.45
1:R:160:PRO:HG3	1:R:169:GLN:HG3	1.98	0.45
1:W:186:LEU:HD12	1:W:186:LEU:HA	1.81	0.45
1:a:377:MET:HE3	1:a:377:MET:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:142:ARG:HB2	1:d:154:ARG:HH12	1.81	0.45
1:e:405:THR:HG23	1:e:408:GLN:H	1.81	0.45
1:g:147:LEU:HD12	1:g:149:PRO:HD2	1.98	0.45
1:h:252:ILE:O	1:h:255:PRO:HD2	2.16	0.45
1:B:424:ASP:OD2	1:B:425:LYS:HG3	2.16	0.45
1:N:419:ALA:O	1:O:267:THR:OG1	2.31	0.45
1:O:157:LEU:HD22	1:O:202:VAL:HG21	1.98	0.45
1:O:293:LEU:HA	1:O:293:LEU:HD23	1.71	0.45
1:P:231:ASN:O	1:P:234:GLN:HG3	2.16	0.45
1:T:149:PRO:HA	1:T:181:GLU:HG2	1.97	0.45
1:c:394:LYS:HE3	1:c:402:LEU:HD13	1.96	0.45
1:A:267:THR:HG22	1:h:248:ARG:NH1	2.20	0.45
1:C:125:GLN:O	1:C:128:GLU:HG2	2.16	0.45
1:F:253:LEU:HD11	1:F:412:ILE:HG23	1.97	0.45
1:K:187:ASP:OD2	1:K:190:GLN:HG3	2.17	0.45
1:L:150:VAL:HG13	1:L:178:VAL:HG23	1.97	0.45
1:L:244:ARG:HA	1:L:247:ARG:NH1	2.31	0.45
1:O:143:THR:HG22	1:Q:154:ARG:HD3	1.98	0.45
1:P:269:GLN:O	1:P:382:ILE:HD12	2.16	0.45
1:Q:151:LYS:NZ	1:Q:182:PRO:HD3	2.27	0.45
1:U:187:ASP:O	1:U:191:ILE:N	2.46	0.45
1:X:299:ASN:HB2	1:X:361:ASN:HB2	1.97	0.45
1:C:254:SER:HB2	1:C:255:PRO:HD3	1.99	0.45
1:C:404:LEU:HD13	1:C:434:ASN:HD21	1.81	0.45
1:D:409:MET:SD	1:D:434:ASN:HB2	2.57	0.45
1:E:191:ILE:HD11	1:E:220:LEU:HD22	1.98	0.45
1:H:143:THR:HG22	1:I:154:ARG:NE	2.32	0.45
1:H:191:ILE:HD11	1:H:220:LEU:HD13	1.99	0.45
1:H:404:LEU:HD23	1:H:408:GLN:HG2	1.98	0.45
1:H:417:ARG:HA	1:H:420:MET:HE3	1.99	0.45
1:I:280:GLU:HG3	1:I:372:ILE:CD1	2.47	0.45
1:P:404:LEU:H	1:P:434:ASN:HD21	1.63	0.45
1:Q:394:LYS:CG	1:Q:402:LEU:HB2	2.47	0.45
1:T:245:ILE:HG23	1:T:266:VAL:HG21	1.97	0.45
1:T:409:MET:HE1	1:T:434:ASN:HB2	1.97	0.45
1:X:218:HIS:O	1:X:220:LEU:N	2.49	0.45
1:X:252:ILE:O	1:X:255:PRO:HD2	2.17	0.45
1:Y:157:LEU:HD23	1:Y:157:LEU:HA	1.79	0.45
1:g:246:GLN:O	1:g:250:GLU:HG2	2.16	0.45
1:h:237:PHE:HA	1:h:240:ASP:OD1	2.17	0.45
1:A:377:MET:HA	1:A:377:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:VAL:HG22	1:B:178:VAL:HG21	1.99	0.45
1:E:160:PRO:HG2	1:E:170:LYS:O	2.17	0.45
1:E:287:ASP:OD1	1:E:289:SER:N	2.43	0.45
1:G:199:SER:OG	1:G:205:LEU:O	2.31	0.45
1:H:298:LEU:HD13	1:H:362:GLU:HB3	1.98	0.45
1:M:385:LEU:N	1:M:428:ASP:OD2	2.43	0.45
1:O:250:GLU:O	1:O:254:SER:OG	2.27	0.45
1:S:407:ASP:HA	1:S:410:LYS:HG2	1.99	0.45
1:W:420:MET:HG3	1:W:422:PHE:N	2.31	0.45
1:Y:435:SER:HB2	1:Y:436:PRO:HD2	1.99	0.45
1:c:237:PHE:HE1	1:d:232:ASP:HA	1.82	0.45
1:A:374:HIS:HB3	1:B:276:GLU:HB3	1.98	0.45
1:G:287:ASP:HB3	1:G:290:LYS:HG2	1.99	0.45
1:L:418:GLU:HB3	1:M:388:ALA:HB2	1.99	0.45
1:N:268:ALA:HB1	1:N:382:ILE:HD13	1.98	0.45
1:O:299:ASN:HD22	1:O:361:ASN:HD22	1.65	0.45
1:R:140:LEU:O	1:R:144:ILE:HG12	2.16	0.45
1:R:294:ARG:NE	1:R:367:GLU:OE1	2.47	0.45
1:S:423:SER:HB3	1:S:426:ARG:HB2	1.98	0.45
1:U:368:VAL:HG22	1:U:369:ASP:O	2.17	0.45
1:Y:410:LYS:HD2	1:Y:411:GLN:N	2.32	0.45
1:e:393:TYR:HB3	1:e:402:LEU:N	2.32	0.45
1:E:415:LEU:HD12	1:F:431:ASN:ND2	2.32	0.45
1:H:192:SER:O	1:H:196:HIS:ND1	2.41	0.45
1:K:147:LEU:O	1:K:149:PRO:HD2	2.17	0.45
1:M:235:LEU:HD23	1:M:235:LEU:HA	1.81	0.45
1:P:407:ASP:HA	1:P:410:LYS:HG3	1.99	0.45
1:T:266:VAL:HG22	1:T:387:VAL:HG22	1.98	0.45
1:W:250:GLU:O	1:W:254:SER:OG	2.27	0.45
1:X:142:ARG:HB2	1:Y:154:ARG:HH22	1.81	0.45
1:a:385:LEU:HB2	1:a:428:ASP:OD2	2.17	0.45
1:d:248:ARG:NH1	1:e:267:THR:HG22	2.32	0.45
1:C:166:VAL:HG13	1:C:169:GLN:H	1.81	0.45
1:E:246:GLN:O	1:E:250:GLU:HG3	2.17	0.45
1:F:283:SER:HB2	1:F:369:ASP:HB2	2.00	0.45
1:Q:128:GLU:HG2	1:Q:129:GLN:OE1	2.17	0.45
1:R:186:LEU:HB3	1:R:191:ILE:HD11	1.99	0.45
1:R:244:ARG:CZ	1:S:235:LEU:HB3	2.46	0.45
1:Z:244:ARG:NH2	1:a:235:LEU:O	2.33	0.45
1:Z:246:GLN:O	1:Z:250:GLU:OE1	2.35	0.45
1:h:242:GLU:HB3	1:h:266:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:252:ILE:HG22	1:h:253:LEU:HD23	1.98	0.45
1:A:267:THR:CG2	1:h:248:ARG:HD2	2.47	0.44
1:C:301:SER:HB3	1:C:359:GLN:NE2	2.32	0.44
1:C:404:LEU:HD23	1:C:408:GLN:HG2	1.99	0.44
1:G:200:SER:HB3	1:H:175:SER:HB3	1.98	0.44
1:H:248:ARG:HD2	1:I:267:THR:HG22	1.98	0.44
1:I:179:THR:HA	1:I:215:GLN:HB3	1.99	0.44
1:I:426:ARG:NE	1:I:428:ASP:OD1	2.45	0.44
1:J:261:ASN:HB3	1:J:392:ASN:HB3	1.97	0.44
1:O:200:SER:OG	1:Q:173:SER:OG	2.36	0.44
1:Q:160:PRO:O	1:Q:161:LYS:HB2	2.17	0.44
1:S:410:LYS:HA	1:S:413:GLU:HG3	2.00	0.44
1:T:137:GLU:OE1	1:T:155:VAL:HG13	2.17	0.44
1:V:245:ILE:HG21	1:V:266:VAL:HG11	1.99	0.44
1:Y:234:GLN:HG3	1:Y:272:PHE:CZ	2.52	0.44
1:f:279:GLU:OE1	1:f:281:HIS:HB2	2.17	0.44
1:h:133:GLN:NE2	1:h:137:GLU:OE2	2.50	0.44
1:E:126:PHE:HA	1:E:129:GLN:NE2	2.32	0.44
1:J:248:ARG:NH1	1:K:267:THR:OG1	2.49	0.44
1:K:393:TYR:HB3	1:K:402:LEU:N	2.32	0.44
1:P:413:GLU:HG3	1:P:417:ARG:HH12	1.82	0.44
1:U:389:VAL:HB	1:U:432:VAL:HG22	1.99	0.44
1:W:302:GLU:HB3	1:W:358:THR:HG23	1.99	0.44
1:c:393:TYR:HB3	1:c:402:LEU:N	2.33	0.44
1:h:416:THR:O	1:h:420:MET:HG3	2.17	0.44
1:D:387:VAL:HG21	1:D:420:MET:HG3	1.99	0.44
1:G:180:LEU:HD13	1:G:185:ALA:HA	1.98	0.44
1:K:211:THR:HA	1:K:221:THR:HG21	1.99	0.44
1:L:147:LEU:O	1:L:149:PRO:HD2	2.18	0.44
1:P:407:ASP:O	1:P:410:LYS:HG3	2.17	0.44
1:R:145:GLU:HG2	1:R:152:SER:HA	1.99	0.44
1:T:176:VAL:HG13	1:T:212:LEU:HD13	1.99	0.44
1:X:173:SER:HA	1:X:209:ASN:HB3	1.98	0.44
1:b:256:ILE:HG22	1:b:257:VAL:HG13	1.98	0.44
1:H:195:VAL:HG13	1:H:210:VAL:CG2	2.47	0.44
1:H:206:PRO:HG2	1:H:209:ASN:OD1	2.17	0.44
1:H:394:LYS:HE2	1:H:402:LEU:HD13	1.99	0.44
1:M:270:LEU:HD13	1:M:382:ILE:HA	1.99	0.44
1:P:275:LYS:HB2	1:P:275:LYS:HE3	1.64	0.44
1:Q:417:ARG:HG3	1:Q:422:PHE:HB3	2.00	0.44
1:T:161:LYS:HD2	1:T:163:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:139:GLU:O	1:U:142:ARG:HG2	2.18	0.44
1:Y:180:LEU:HD23	1:Y:185:ALA:HA	1.99	0.44
1:d:142:ARG:O	1:d:146:THR:HG23	2.16	0.44
1:e:418:GLU:HB3	1:f:388:ALA:HB2	1.99	0.44
1:g:157:LEU:HD12	1:g:173:SER:O	2.16	0.44
1:h:132:TYR:CE2	1:h:136:LEU:HD11	2.52	0.44
1:h:181:GLU:HB3	1:h:184:ARG:NH2	2.29	0.44
1:A:405:THR:HG23	1:A:408:GLN:H	1.82	0.44
1:C:252:ILE:O	1:C:255:PRO:HD2	2.17	0.44
1:E:151:LYS:HZ3	1:E:181:GLU:HA	1.82	0.44
1:F:407:ASP:HA	1:F:410:LYS:NZ	2.32	0.44
1:L:248:ARG:HH11	1:M:267:THR:HG22	1.83	0.44
1:O:159:MET:HE3	1:O:159:MET:HB3	1.92	0.44
1:U:231:ASN:OD1	1:U:232:ASP:N	2.51	0.44
1:Z:415:LEU:HD22	1:a:431:ASN:ND2	2.32	0.44
1:a:129:GLN:O	1:a:133:GLN:HG2	2.17	0.44
1:b:369:ASP:OD1	1:c:282:TYR:N	2.46	0.44
1:c:360:ARG:HG2	1:c:362:GLU:OE2	2.17	0.44
1:d:302:GLU:HA	1:d:357:SER:O	2.17	0.44
1:f:147:LEU:HB3	1:f:150:VAL:HG21	1.99	0.44
1:f:157:LEU:HB3	1:f:159:MET:HE3	1.99	0.44
1:f:216:SER:O	1:f:216:SER:OG	2.36	0.44
1:f:256:ILE:HD11	1:g:390:VAL:HG11	2.00	0.44
1:g:205:LEU:HD11	1:g:209:ASN:HB2	2.00	0.44
1:h:142:ARG:HA	1:h:145:GLU:OE2	2.18	0.44
1:B:280:GLU:HG3	1:B:372:ILE:CD1	2.48	0.44
1:B:385:LEU:N	1:B:428:ASP:OD2	2.27	0.44
1:B:393:TYR:CE2	1:B:436:PRO:HD3	2.52	0.44
1:C:188:GLU:H	1:C:188:GLU:CD	2.24	0.44
1:G:147:LEU:O	1:G:149:PRO:HD2	2.18	0.44
1:H:140:LEU:HD23	1:H:140:LEU:HA	1.83	0.44
1:H:283:SER:HB2	1:H:369:ASP:HB2	1.99	0.44
1:J:375:THR:HG23	1:K:275:LYS:NZ	2.33	0.44
1:K:404:LEU:HD23	1:K:408:GLN:HG2	2.00	0.44
1:M:269:GLN:OE1	1:M:384:ARG:NH1	2.49	0.44
1:O:413:GLU:CD	1:O:417:ARG:HH12	2.25	0.44
1:R:151:LYS:HZ1	1:R:181:GLU:HA	1.82	0.44
1:R:183:GLY:C	1:R:184:ARG:HD3	2.43	0.44
1:V:415:LEU:HD22	1:W:431:ASN:ND2	2.32	0.44
1:Y:141:ALA:O	1:Y:145:GLU:HG2	2.18	0.44
1:c:204:GLY:O	1:d:170:LYS:NZ	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.72	0.44
1:G:143:THR:HA	1:H:154:ARG:NH1	2.30	0.44
1:I:239:ASN:HA	1:I:242:GLU:HG2	1.98	0.44
1:K:200:SER:HB3	1:L:175:SER:HB3	2.00	0.44
1:O:246:GLN:O	1:O:250:GLU:HG2	2.18	0.44
1:Q:257:VAL:HG21	1:Q:262:VAL:HB	2.00	0.44
1:R:258:GLY:HA3	1:R:261:ASN:HD22	1.83	0.44
1:U:266:VAL:HG22	1:U:387:VAL:HG22	1.98	0.44
1:V:280:GLU:O	1:V:280:GLU:HG2	2.16	0.44
1:W:257:VAL:HG23	1:W:261:ASN:HB2	2.00	0.44
1:W:370:ARG:NH1	1:W:372:ILE:HD11	2.32	0.44
1:C:426:ARG:HH21	1:C:428:ASP:CG	2.26	0.44
1:E:297:GLN:HB3	1:E:363:THR:OG1	2.18	0.44
1:I:387:VAL:HB	1:I:420:MET:SD	2.58	0.44
1:K:143:THR:HG22	1:L:154:ARG:HD3	1.98	0.44
1:O:191:ILE:HD13	1:O:220:LEU:HB3	2.00	0.44
1:Q:272:PHE:HA	1:Q:379:VAL:HG13	2.00	0.44
1:R:145:GLU:HG3	1:R:153:ALA:HB3	2.00	0.44
1:T:188:GLU:O	1:T:191:ILE:HB	2.18	0.44
1:U:234:GLN:OE1	1:U:234:GLN:N	2.48	0.44
1:W:167:ARG:O	1:X:165:PHE:HB3	2.18	0.44
1:Z:302:GLU:HA	1:Z:357:SER:O	2.18	0.44
1:Z:413:GLU:OE1	1:Z:432:VAL:HB	2.17	0.44
1:c:244:ARG:NH2	1:c:248:ARG:HH22	2.15	0.44
1:d:151:LYS:NZ	1:d:182:PRO:HD3	2.32	0.44
1:D:420:MET:HE1	1:D:428:ASP:HB3	1.99	0.44
1:E:419:ALA:O	1:F:267:THR:HG21	2.18	0.44
1:G:203:ALA:HB1	1:H:160:PRO:HA	2.00	0.44
1:J:393:TYR:CE2	1:J:436:PRO:HD3	2.53	0.44
1:P:234:GLN:HB3	1:P:272:PHE:CE2	2.53	0.44
1:T:252:ILE:O	1:T:255:PRO:HD2	2.17	0.44
1:U:129:GLN:O	1:U:133:GLN:HG2	2.17	0.44
1:W:375:THR:HG23	1:X:275:LYS:HZ1	1.81	0.44
1:b:411:GLN:O	1:b:415:LEU:HD13	2.18	0.44
1:f:275:LYS:CB	1:f:377:MET:HE2	2.48	0.44
1:h:416:THR:HG23	1:h:430:LEU:HD21	1.98	0.44
1:A:431:ASN:HD21	1:h:414:ASP:HB3	1.82	0.43
1:E:125:GLN:O	1:E:128:GLU:HG3	2.18	0.43
1:G:231:ASN:OD1	1:G:232:ASP:N	2.45	0.43
1:M:279:GLU:CD	1:M:281:HIS:H	2.26	0.43
1:N:275:LYS:HA	1:N:275:LYS:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:407:ASP:O	1:O:410:LYS:HG3	2.17	0.43
1:V:303:GLN:HA	1:W:357:SER:HA	1.99	0.43
1:X:252:ILE:HD11	1:Y:265:GLN:HB2	2.00	0.43
1:b:407:ASP:O	1:b:410:LYS:HG2	2.18	0.43
1:c:420:MET:HE3	1:c:422:PHE:HB2	2.00	0.43
1:e:297:GLN:OE1	1:f:363:THR:OG1	2.27	0.43
1:h:252:ILE:HD13	1:h:252:ILE:HA	1.90	0.43
1:A:409:MET:HA	1:A:409:MET:HE2	1.99	0.43
1:B:197:LEU:HD11	1:C:177:THR:OG1	2.18	0.43
1:G:420:MET:SD	1:G:422:PHE:HD1	2.41	0.43
1:L:275:LYS:CB	1:L:377:MET:HB2	2.47	0.43
1:N:174:ALA:O	1:N:210:VAL:HA	2.17	0.43
1:T:409:MET:HE2	1:T:409:MET:HB2	1.90	0.43
1:W:167:ARG:HH11	1:X:165:PHE:HE1	1.66	0.43
1:X:147:LEU:O	1:X:149:PRO:HD2	2.17	0.43
1:X:304:VAL:HG22	1:X:356:ARG:HG2	1.99	0.43
1:d:188:GLU:HA	1:d:191:ILE:HG12	1.99	0.43
1:C:186:LEU:HD22	1:C:190:GLN:HB3	2.00	0.43
1:E:195:VAL:HG13	1:E:210:VAL:CG2	2.48	0.43
1:F:393:TYR:CE1	1:F:403:PRO:HA	2.53	0.43
1:H:372:ILE:O	1:I:277:GLN:HA	2.18	0.43
1:J:263:HIS:HB2	1:J:390:VAL:HG22	2.00	0.43
1:L:139:GLU:HG3	1:N:156:HIS:CE1	2.50	0.43
1:N:197:LEU:HD11	1:O:177:THR:CG2	2.47	0.43
1:O:170:LYS:HD2	1:O:170:LYS:C	2.43	0.43
1:O:231:ASN:OD1	1:O:232:ASP:N	2.51	0.43
1:Q:161:LYS:HD2	1:Q:163:SER:HA	2.01	0.43
1:W:191:ILE:O	1:W:195:VAL:HG23	2.18	0.43
1:X:393:TYR:HB3	1:X:402:LEU:N	2.33	0.43
1:d:186:LEU:HD12	1:d:186:LEU:HA	1.86	0.43
1:g:252:ILE:O	1:g:255:PRO:HD2	2.18	0.43
1:C:176:VAL:HB	1:C:212:LEU:HD23	2.00	0.43
1:E:160:PRO:HD3	1:E:172:PRO:HA	2.00	0.43
1:G:234:GLN:HB3	1:G:272:PHE:CZ	2.52	0.43
1:H:261:ASN:O	1:H:392:ASN:N	2.42	0.43
1:J:234:GLN:OE1	1:J:234:GLN:N	2.47	0.43
1:Q:231:ASN:OD1	1:Q:232:ASP:N	2.51	0.43
1:R:186:LEU:HD12	1:R:186:LEU:HA	1.73	0.43
1:T:280:GLU:HG2	1:T:282:TYR:CE2	2.53	0.43
1:e:267:THR:OG1	1:e:386:SER:HB2	2.19	0.43
1:g:125:GLN:O	1:g:128:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ALA:HA	1:G:178:VAL:HA	1.99	0.43
1:J:389:VAL:HB	1:J:432:VAL:HG13	2.01	0.43
1:O:202:VAL:HB	1:O:205:LEU:HD22	1.99	0.43
1:Q:252:ILE:O	1:Q:255:PRO:HD2	2.18	0.43
1:Q:269:GLN:HG3	1:Q:384:ARG:NH1	2.34	0.43
1:W:244:ARG:HH21	1:W:244:ARG:HG3	1.83	0.43
1:W:373:ARG:NH2	1:X:275:LYS:HE2	2.34	0.43
1:Y:142:ARG:HB3	1:a:154:ARG:HH22	1.83	0.43
1:a:148:GLY:O	1:a:150:VAL:N	2.44	0.43
1:f:191:ILE:HD11	1:f:220:LEU:HD23	2.00	0.43
1:D:249:ILE:CD1	1:D:416:THR:HA	2.47	0.43
1:E:420:MET:SD	1:E:422:PHE:HB2	2.58	0.43
1:N:191:ILE:HD11	1:N:220:LEU:HD13	2.00	0.43
1:c:256:ILE:HG21	1:c:412:ILE:HD11	2.01	0.43
1:f:203:ALA:HA	1:g:158:ALA:HB1	2.00	0.43
1:F:249:ILE:HD13	1:F:419:ALA:HB3	2.01	0.43
1:F:426:ARG:HH21	1:F:428:ASP:CG	2.27	0.43
1:G:304:VAL:N	1:H:356:ARG:O	2.48	0.43
1:K:181:GLU:HB3	1:K:184:ARG:NH2	2.34	0.43
1:K:298:LEU:O	1:L:362:GLU:N	2.50	0.43
1:L:139:GLU:OE2	1:N:154:ARG:NE	2.48	0.43
1:N:304:VAL:HG22	1:O:356:ARG:O	2.18	0.43
1:O:411:GLN:O	1:O:415:LEU:HD13	2.17	0.43
1:Q:129:GLN:O	1:Q:133:GLN:NE2	2.50	0.43
1:T:393:TYR:CE2	1:T:436:PRO:HD3	2.54	0.43
1:f:193:ALA:HA	1:g:219:LEU:HD21	2.01	0.43
1:h:283:SER:HB2	1:h:369:ASP:HB2	2.01	0.43
1:A:392:ASN:ND2	1:A:437:PHE:HB2	2.34	0.43
1:C:199:SER:HA	1:C:205:LEU:HD23	2.00	0.43
1:E:156:HIS:O	1:E:174:ALA:HA	2.19	0.43
1:F:239:ASN:HA	1:F:242:GLU:OE1	2.19	0.43
1:I:144:ILE:HG22	1:I:150:VAL:HG11	2.01	0.43
1:L:187:ASP:N	1:L:187:ASP:OD1	2.50	0.43
1:O:303:GLN:OE1	1:O:303:GLN:N	2.51	0.43
1:P:415:LEU:HD13	1:Q:388:ALA:HB1	2.01	0.43
1:Q:155:VAL:HG23	1:Q:176:VAL:HG22	2.01	0.43
1:Q:279:GLU:OE1	1:Q:281:HIS:HB2	2.18	0.43
1:S:420:MET:SD	1:S:422:PHE:HD1	2.42	0.43
1:W:166:VAL:O	1:W:167:ARG:HD3	2.18	0.43
1:X:187:ASP:OD1	1:X:190:GLN:HG3	2.19	0.43
1:Y:160:PRO:O	1:Y:161:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:267:THR:HG1	1:Y:386:SER:HB2	1.83	0.43
1:b:404:LEU:H	1:b:434:ASN:HD21	1.66	0.43
1:g:191:ILE:HG12	1:g:220:LEU:HD13	2.00	0.43
1:h:148:GLY:O	1:h:150:VAL:N	2.47	0.43
1:B:253:LEU:HD22	1:B:412:ILE:HD12	1.99	0.43
1:G:203:ALA:HA	1:H:158:ALA:HB1	2.01	0.43
1:M:267:THR:OG1	1:M:386:SER:HB2	2.19	0.43
1:T:246:GLN:O	1:T:250:GLU:HG3	2.19	0.43
1:X:420:MET:HE3	1:X:430:LEU:HD13	2.00	0.43
1:a:139:GLU:HB3	1:c:156:HIS:CE1	2.54	0.43
1:a:158:ALA:HB3	1:a:173:SER:HB3	2.00	0.43
1:b:240:ASP:OD2	1:b:244:ARG:NH2	2.51	0.43
1:c:408:GLN:O	1:c:412:ILE:HG12	2.18	0.43
1:g:211:THR:HA	1:g:221:THR:HG21	1.99	0.43
1:C:143:THR:HG22	1:E:154:ARG:CD	2.48	0.43
1:D:275:LYS:HB2	1:D:377:MET:HG2	2.01	0.43
1:I:302:GLU:HA	1:I:357:SER:O	2.19	0.43
1:I:426:ARG:NH2	1:I:428:ASP:OD1	2.52	0.43
1:N:196:HIS:ND1	1:O:219:LEU:HD11	2.34	0.43
1:R:268:ALA:HA	1:R:385:LEU:HD23	2.00	0.43
1:V:263:HIS:HB2	1:V:390:VAL:CG2	2.49	0.43
1:X:126:PHE:HA	1:X:129:GLN:NE2	2.33	0.43
1:Y:382:ILE:HD12	1:Y:382:ILE:H	1.84	0.43
1:Z:409:MET:HE2	1:Z:409:MET:HB3	1.78	0.43
1:c:235:LEU:HD23	1:c:235:LEU:HA	1.82	0.43
1:f:373:ARG:HH21	1:g:275:LYS:HE2	1.83	0.43
1:B:143:THR:HG21	1:C:156:HIS:NE2	2.33	0.42
1:B:152:SER:O	1:B:178:VAL:HA	2.19	0.42
1:D:417:ARG:HG3	1:D:422:PHE:CG	2.53	0.42
1:I:392:ASN:OD1	1:I:393:TYR:N	2.52	0.42
1:M:413:GLU:HA	1:M:416:THR:HG22	2.00	0.42
1:N:298:LEU:HD11	1:N:300:ILE:HD11	2.01	0.42
1:Q:163:SER:OG	1:Q:164:LEU:N	2.51	0.42
1:S:254:SER:HB2	1:S:255:PRO:HD3	2.02	0.42
1:S:408:GLN:HA	1:S:411:GLN:NE2	2.31	0.42
1:T:203:ALA:CB	1:U:160:PRO:HG3	2.49	0.42
1:V:372:ILE:HG23	1:V:372:ILE:O	2.19	0.42
1:W:151:LYS:HG2	1:W:179:THR:O	2.19	0.42
1:W:157:LEU:HD11	1:W:202:VAL:HG21	2.01	0.42
1:Y:128:GLU:HG2	1:Y:129:GLN:OE1	2.19	0.42
1:Y:213:VAL:HG12	1:Y:214:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:415:LEU:HG	1:b:388:ALA:HB1	2.01	0.42
1:d:157:LEU:HD13	1:d:174:ALA:HB2	2.00	0.42
1:f:248:ARG:HD2	1:g:267:THR:OG1	2.19	0.42
1:f:413:GLU:CD	1:f:417:ARG:HH12	2.27	0.42
1:g:141:ALA:O	1:g:145:GLU:HG2	2.19	0.42
1:B:389:VAL:O	1:B:432:VAL:HA	2.18	0.42
1:E:250:GLU:O	1:E:254:SER:OG	2.31	0.42
1:E:283:SER:HB2	1:E:369:ASP:HB2	1.99	0.42
1:K:159:MET:SD	1:K:172:PRO:HB3	2.59	0.42
1:L:141:ALA:HB1	1:L:153:ALA:O	2.19	0.42
1:L:276:GLU:OE2	1:L:374:HIS:NE2	2.52	0.42
1:N:132:TYR:O	1:N:136:LEU:HD23	2.18	0.42
1:O:250:GLU:OE2	1:O:264:ALA:N	2.52	0.42
1:P:258:GLY:HA3	1:P:261:ASN:ND2	2.34	0.42
1:T:290:LYS:O	1:T:290:LYS:HG2	2.20	0.42
1:U:287:ASP:OD1	1:U:288:ALA:N	2.52	0.42
1:W:142:ARG:HD2	1:X:154:ARG:HH12	1.84	0.42
1:a:191:ILE:HD11	1:a:220:LEU:HD12	2.01	0.42
1:g:256:ILE:HD13	1:g:256:ILE:HA	1.91	0.42
1:h:407:ASP:O	1:h:410:LYS:HG2	2.19	0.42
1:D:253:LEU:O	1:D:257:VAL:HG22	2.20	0.42
1:D:393:TYR:CZ	1:D:436:PRO:HD3	2.54	0.42
1:E:207:PRO:O	1:E:210:VAL:HG22	2.19	0.42
1:H:269:GLN:O	1:H:270:LEU:HD23	2.19	0.42
1:L:372:ILE:O	1:M:277:GLN:HA	2.19	0.42
1:N:266:VAL:HG22	1:N:387:VAL:HG22	2.01	0.42
1:P:297:GLN:HB3	1:P:363:THR:HB	2.00	0.42
1:Q:187:ASP:O	1:Q:191:ILE:HG12	2.19	0.42
1:Q:221:THR:HG23	1:Q:223:SER:H	1.84	0.42
1:Y:147:LEU:HD11	1:a:217:GLY:H	1.85	0.42
1:Y:367:GLU:HG3	1:Z:368:VAL:HG11	2.01	0.42
1:b:407:ASP:OD1	1:b:408:GLN:N	2.52	0.42
1:h:273:ALA:HB3	1:h:275:LYS:HE3	2.01	0.42
1:B:392:ASN:OD1	1:B:393:TYR:N	2.50	0.42
1:D:373:ARG:HH21	1:E:275:LYS:HZ2	1.67	0.42
1:E:393:TYR:HB3	1:E:402:LEU:N	2.35	0.42
1:E:416:THR:O	1:E:420:MET:HG3	2.18	0.42
1:G:405:THR:OG1	1:G:407:ASP:OD1	2.21	0.42
1:H:378:ASN:HB3	1:H:381:ASP:OD2	2.18	0.42
1:K:370:ARG:HG2	1:K:371:THR:N	2.33	0.42
1:O:293:LEU:HD13	1:O:296:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:231:ASN:CG	1:P:232:ASP:H	2.27	0.42
1:R:408:GLN:O	1:R:412:ILE:HG12	2.20	0.42
1:T:161:LYS:NZ	1:T:163:SER:HA	2.34	0.42
1:T:186:LEU:HD11	1:T:190:GLN:HB3	2.00	0.42
1:T:187:ASP:OD1	1:T:187:ASP:N	2.44	0.42
1:T:242:GLU:HA	1:T:245:ILE:HG22	2.00	0.42
1:V:382:ILE:HG21	1:V:385:LEU:HG	2.00	0.42
1:X:164:LEU:HD12	1:X:169:GLN:NE2	2.34	0.42
1:Z:271:ASP:O	1:Z:380:GLY:N	2.52	0.42
1:Z:280:GLU:OE1	1:Z:280:GLU:HA	2.19	0.42
1:b:381:ASP:OD1	1:b:382:ILE:N	2.52	0.42
1:f:151:LYS:NZ	1:f:182:PRO:HD3	2.35	0.42
1:A:415:LEU:CD1	1:B:388:ALA:HB1	2.49	0.42
1:H:141:ALA:O	1:H:144:ILE:N	2.52	0.42
1:H:241:VAL:HG22	1:I:235:LEU:HD21	2.00	0.42
1:J:408:GLN:O	1:J:411:GLN:HG2	2.20	0.42
1:K:393:TYR:CZ	1:K:436:PRO:HD3	2.54	0.42
1:L:394:LYS:HG2	1:L:402:LEU:HB2	2.01	0.42
1:N:293:LEU:HD13	1:N:296:ARG:HE	1.84	0.42
1:T:405:THR:OG1	1:T:408:GLN:HB2	2.19	0.42
1:W:287:ASP:H	1:W:290:LYS:NZ	2.17	0.42
1:Y:301:SER:O	1:Y:359:GLN:N	2.45	0.42
1:d:423:SER:HB2	1:e:384:ARG:NH1	2.35	0.42
1:e:249:ILE:HD13	1:e:419:ALA:HB3	2.01	0.42
1:e:417:ARG:HG3	1:e:422:PHE:CB	2.50	0.42
1:f:158:ALA:C	1:f:159:MET:HE2	2.44	0.42
1:f:420:MET:HE1	1:f:428:ASP:HB3	2.02	0.42
1:g:186:LEU:HA	1:g:186:LEU:HD12	1.78	0.42
1:g:252:ILE:HG22	1:g:253:LEU:HD22	2.02	0.42
1:A:294:ARG:NE	1:A:367:GLU:OE1	2.52	0.42
1:B:186:LEU:HD11	1:B:190:GLN:HB2	2.01	0.42
1:C:166:VAL:HG22	1:C:168:GLU:OE1	2.19	0.42
1:C:409:MET:CE	1:C:434:ASN:HB2	2.49	0.42
1:D:287:ASP:HB3	1:D:290:LYS:HG2	2.01	0.42
1:E:145:GLU:OE2	1:E:153:ALA:N	2.53	0.42
1:H:231:ASN:OD1	1:H:232:ASP:N	2.51	0.42
1:H:262:VAL:HG23	1:H:391:VAL:HG12	2.02	0.42
1:O:187:ASP:N	1:O:187:ASP:OD1	2.50	0.42
1:R:409:MET:HE1	1:R:434:ASN:HB2	1.99	0.42
1:S:268:ALA:HA	1:S:385:LEU:HD23	2.02	0.42
1:U:159:MET:HA	1:U:172:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:385:LEU:N	1:W:428:ASP:OD2	2.47	0.42
1:Z:247:ARG:HA	1:Z:250:GLU:CD	2.45	0.42
1:a:143:THR:HG23	1:c:154:ARG:NH2	2.34	0.42
1:a:186:LEU:HD11	1:a:190:GLN:OE1	2.20	0.42
1:c:411:GLN:O	1:c:415:LEU:HG	2.20	0.42
1:d:418:GLU:HB3	1:e:388:ALA:HB2	2.01	0.42
1:g:144:ILE:HD11	1:g:197:LEU:HD22	2.02	0.42
1:C:142:ARG:HB3	1:E:154:ARG:HH22	1.83	0.42
1:C:248:ARG:NH2	1:D:242:GLU:OE1	2.53	0.42
1:D:415:LEU:HD21	1:E:433:VAL:HG11	2.01	0.42
1:E:205:LEU:HD12	1:E:206:PRO:HD2	2.02	0.42
1:G:206:PRO:HG2	1:G:209:ASN:OD1	2.19	0.42
1:L:139:GLU:CD	1:N:154:ARG:HH11	2.27	0.42
1:M:387:VAL:HB	1:M:420:MET:HE1	2.01	0.42
1:N:261:ASN:O	1:N:392:ASN:N	2.43	0.42
1:O:393:TYR:HB3	1:O:402:LEU:N	2.35	0.42
1:Q:233:ALA:HA	1:Q:236:LYS:HE2	2.01	0.42
1:T:293:LEU:HD13	1:T:296:ARG:NH1	2.31	0.42
1:V:275:LYS:HB3	1:V:377:MET:HE2	2.00	0.42
1:X:372:ILE:HG23	1:X:372:ILE:O	2.20	0.42
1:Z:280:GLU:HG3	1:Z:282:TYR:HE2	1.85	0.42
1:d:206:PRO:HG2	1:d:209:ASN:OD1	2.19	0.42
1:g:236:LYS:HE3	1:g:236:LYS:HB3	1.75	0.42
1:g:252:ILE:CG1	1:h:265:GLN:HB2	2.49	0.42
1:A:382:ILE:HD12	1:A:382:ILE:H	1.85	0.42
1:C:369:ASP:OD1	1:D:282:TYR:HB2	2.19	0.42
1:E:134:ARG:HE	1:E:134:ARG:HB3	1.70	0.42
1:E:181:GLU:HG2	1:E:184:ARG:NH2	2.35	0.42
1:E:254:SER:HB2	1:E:255:PRO:HD3	2.02	0.42
1:K:269:GLN:O	1:K:382:ILE:HD12	2.19	0.42
1:N:234:GLN:HB2	1:N:272:PHE:CE2	2.55	0.42
1:P:282:TYR:CE1	1:P:370:ARG:HD3	2.55	0.42
1:Q:245:ILE:HG21	1:Q:266:VAL:HG11	2.00	0.42
1:R:407:ASP:HA	1:R:410:LYS:HE3	2.02	0.42
1:U:157:LEU:HD11	1:U:202:VAL:HG11	2.02	0.42
1:U:301:SER:HB3	1:U:359:GLN:HB3	2.01	0.42
1:W:257:VAL:HG21	1:W:262:VAL:HG13	2.02	0.42
1:X:232:ASP:OD2	1:X:233:ALA:N	2.53	0.42
1:Y:245:ILE:HD11	1:Y:420:MET:CA	2.50	0.42
1:a:214:ASP:HB3	1:a:217:GLY:O	2.20	0.42
1:a:253:LEU:HD23	1:a:253:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:181:GLU:HB3	1:c:184:ARG:HD3	2.02	0.42
1:d:164:LEU:HD21	1:f:165:PHE:HA	2.02	0.42
1:h:140:LEU:O	1:h:144:ILE:HG12	2.19	0.42
1:A:431:ASN:ND2	1:h:414:ASP:HB3	2.35	0.42
1:B:211:THR:HG21	1:h:196:HIS:HB3	2.02	0.42
1:D:393:TYR:HB3	1:D:402:LEU:N	2.35	0.42
1:F:388:ALA:HA	1:F:431:ASN:O	2.19	0.42
1:H:154:ARG:HB3	1:H:177:THR:OG1	2.19	0.42
1:I:176:VAL:HG12	1:I:178:VAL:HG23	2.02	0.42
1:T:128:GLU:OE2	1:T:128:GLU:N	2.39	0.42
1:U:204:GLY:H	1:W:170:LYS:HZ2	1.67	0.42
1:W:167:ARG:HB3	1:X:165:PHE:CD1	2.55	0.42
1:W:187:ASP:OD1	1:W:190:GLN:HG3	2.20	0.42
1:Z:239:ASN:HA	1:Z:242:GLU:OE1	2.20	0.42
1:d:146:THR:O	1:d:146:THR:OG1	2.38	0.42
1:h:147:LEU:O	1:h:149:PRO:HD2	2.20	0.42
1:B:301:SER:HA	1:C:359:GLN:HA	2.01	0.42
1:C:246:GLN:NE2	1:C:264:ALA:O	2.52	0.42
1:D:275:LYS:HB2	1:D:377:MET:CG	2.49	0.42
1:I:159:MET:SD	1:I:172:PRO:HB3	2.60	0.42
1:K:234:GLN:HB3	1:K:272:PHE:CE2	2.55	0.42
1:N:136:LEU:HD13	1:N:136:LEU:HA	1.88	0.42
1:N:394:LYS:CG	1:N:402:LEU:HB2	2.49	0.42
1:O:418:GLU:HB3	1:P:388:ALA:HB2	2.02	0.42
1:R:167:ARG:O	1:R:169:GLN:NE2	2.53	0.42
1:S:385:LEU:HD23	1:S:385:LEU:HA	1.82	0.42
1:U:142:ARG:HA	1:U:145:GLU:CD	2.45	0.42
1:W:182:PRO:O	1:W:184:ARG:NH1	2.53	0.42
1:Y:126:PHE:HA	1:Y:129:GLN:HE22	1.85	0.42
1:Y:245:ILE:HG23	1:Y:266:VAL:HG21	2.02	0.42
1:Y:407:ASP:O	1:Y:411:GLN:HG2	2.20	0.42
1:C:194:VAL:HG13	1:C:212:LEU:HD11	2.00	0.41
1:F:423:SER:HB2	1:G:384:ARG:NH1	2.34	0.41
1:G:190:GLN:CG	1:H:217:GLY:HA3	2.50	0.41
1:G:422:PHE:HE2	1:G:424:ASP:OD1	2.02	0.41
1:J:293:LEU:HD13	1:J:296:ARG:HE	1.85	0.41
1:K:367:GLU:C	1:K:367:GLU:CD	2.88	0.41
1:L:258:GLY:HA3	1:L:261:ASN:ND2	2.35	0.41
1:Q:293:LEU:CD1	1:Q:296:ARG:HE	2.33	0.41
1:T:274:ASN:C	1:T:275:LYS:HD3	2.45	0.41
1:U:186:LEU:HD11	1:U:190:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:237:PHE:HE2	1:X:232:ASP:HA	1.84	0.41
1:Z:245:ILE:HG21	1:Z:266:VAL:HG11	2.02	0.41
1:c:394:LYS:CG	1:c:402:LEU:HB2	2.48	0.41
1:g:140:LEU:HD22	1:h:156:HIS:NE2	2.35	0.41
1:g:268:ALA:HB1	1:g:382:ILE:CD1	2.49	0.41
1:h:423:SER:OG	1:h:425:LYS:HG2	2.20	0.41
1:B:269:GLN:O	1:B:270:LEU:HD23	2.19	0.41
1:E:162:PRO:HA	1:E:169:GLN:CD	2.45	0.41
1:G:191:ILE:CD1	1:G:220:LEU:HD13	2.50	0.41
1:H:369:ASP:OD1	1:I:282:TYR:N	2.43	0.41
1:J:242:GLU:HG3	1:J:243:SER:N	2.34	0.41
1:J:249:ILE:HD12	1:J:416:THR:OG1	2.20	0.41
1:N:249:ILE:O	1:N:252:ILE:HG22	2.21	0.41
1:N:254:SER:OG	1:N:255:PRO:HD3	2.20	0.41
1:O:128:GLU:OE2	1:O:128:GLU:N	2.35	0.41
1:O:144:ILE:HD12	1:O:194:VAL:HG23	2.02	0.41
1:O:186:LEU:HD22	1:O:190:GLN:CB	2.50	0.41
1:Q:266:VAL:HG22	1:Q:387:VAL:HG22	2.01	0.41
1:Z:378:ASN:HB3	1:Z:381:ASP:OD2	2.20	0.41
1:Z:415:LEU:HD22	1:a:431:ASN:HD21	1.84	0.41
1:a:392:ASN:OD1	1:a:393:TYR:N	2.52	0.41
1:b:408:GLN:O	1:b:412:ILE:HG13	2.19	0.41
1:d:393:TYR:CD1	1:d:403:PRO:HA	2.56	0.41
1:d:420:MET:HE1	1:d:430:LEU:CB	2.49	0.41
1:h:424:ASP:OD2	1:h:425:LYS:N	2.54	0.41
1:B:424:ASP:OD2	1:B:425:LYS:N	2.54	0.41
1:C:181:GLU:HB3	1:C:184:ARG:HH21	1.85	0.41
1:C:191:ILE:O	1:C:195:VAL:HG23	2.20	0.41
1:C:212:LEU:HB2	1:C:221:THR:HG23	2.01	0.41
1:E:139:GLU:O	1:E:143:THR:HG23	2.19	0.41
1:G:165:PHE:HB3	1:G:167:ARG:HH21	1.86	0.41
1:G:169:GLN:HE22	1:H:161:LYS:HZ3	1.67	0.41
1:I:408:GLN:O	1:I:411:GLN:HG2	2.20	0.41
1:I:417:ARG:HG3	1:I:422:PHE:HB3	2.02	0.41
1:L:389:VAL:O	1:L:432:VAL:HA	2.19	0.41
1:M:240:ASP:OD2	1:N:235:LEU:HD13	2.20	0.41
1:O:252:ILE:HG23	1:O:253:LEU:HG	2.02	0.41
1:Q:168:GLU:OE1	1:Q:170:LYS:HG2	2.21	0.41
1:T:282:TYR:OH	1:T:370:ARG:HD3	2.20	0.41
1:U:157:LEU:HD11	1:U:159:MET:HE3	2.02	0.41
1:U:256:ILE:HD11	1:V:390:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:282:TYR:CZ	1:U:370:ARG:HD3	2.55	0.41
1:U:420:MET:SD	1:U:430:LEU:HD13	2.61	0.41
1:W:167:ARG:HD2	1:X:165:PHE:CE1	2.55	0.41
1:W:389:VAL:O	1:W:432:VAL:HA	2.20	0.41
1:a:143:THR:HG22	1:c:154:ARG:HD3	2.01	0.41
1:f:282:TYR:CZ	1:f:370:ARG:HD3	2.56	0.41
1:I:423:SER:HB2	1:J:384:ARG:NH1	2.36	0.41
1:N:182:PRO:O	1:N:184:ARG:NH1	2.53	0.41
1:N:404:LEU:HD13	1:N:434:ASN:HD21	1.85	0.41
1:O:269:GLN:HG3	1:O:384:ARG:NH1	2.35	0.41
1:O:277:GLN:HB2	1:O:377:MET:HE1	2.02	0.41
1:Q:203:ALA:HA	1:R:158:ALA:HB1	2.03	0.41
1:T:407:ASP:HA	1:T:410:LYS:NZ	2.35	0.41
1:Y:279:GLU:OE2	1:Y:281:HIS:N	2.43	0.41
1:Y:287:ASP:HB3	1:Y:290:LYS:HG2	2.02	0.41
1:Y:418:GLU:HB3	1:Z:388:ALA:HB2	2.02	0.41
1:Z:302:GLU:HB3	1:Z:358:THR:HG23	2.03	0.41
1:a:160:PRO:O	1:a:161:LYS:HB2	2.20	0.41
1:g:373:ARG:HH21	1:h:275:LYS:HD2	1.84	0.41
1:A:391:VAL:HG21	1:A:409:MET:HE1	2.02	0.41
1:F:254:SER:HB2	1:F:255:PRO:HD3	2.02	0.41
1:H:126:PHE:HA	1:H:129:GLN:HE22	1.86	0.41
1:H:157:LEU:HD12	1:H:157:LEU:HA	1.85	0.41
1:I:372:ILE:O	1:J:277:GLN:HA	2.20	0.41
1:K:289:SER:O	1:K:290:LYS:HE2	2.20	0.41
1:L:212:LEU:HB3	1:L:220:LEU:HB2	2.03	0.41
1:L:244:ARG:HG3	1:L:247:ARG:HH22	1.85	0.41
1:L:371:THR:OG1	1:M:279:GLU:HG2	2.20	0.41
1:M:275:LYS:HB2	1:M:377:MET:HB2	2.01	0.41
1:N:143:THR:HG21	1:O:156:HIS:CD2	2.56	0.41
1:O:221:THR:HG22	1:O:223:SER:H	1.85	0.41
1:R:136:LEU:HD12	1:R:136:LEU:HA	1.89	0.41
1:R:213:VAL:HG12	1:R:214:ASP:O	2.20	0.41
1:T:159:MET:HA	1:T:172:PRO:HB3	2.02	0.41
1:W:159:MET:HB2	1:W:172:PRO:HB3	2.02	0.41
1:W:235:LEU:HD23	1:W:235:LEU:HA	1.87	0.41
1:X:142:ARG:O	1:X:146:THR:HG23	2.21	0.41
1:X:221:THR:HG22	1:X:223:SER:H	1.85	0.41
1:X:418:GLU:OE2	1:Y:387:VAL:N	2.53	0.41
1:Y:149:PRO:HB2	1:Y:186:LEU:HD21	2.01	0.41
1:Y:152:SER:N	1:Y:179:THR:OG1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:247:ARG:HA	1:Z:250:GLU:OE2	2.21	0.41
1:d:378:ASN:ND2	1:d:381:ASP:OD1	2.42	0.41
1:g:392:ASN:ND2	1:g:437:PHE:HB2	2.36	0.41
1:h:431:ASN:OD1	1:h:432:VAL:N	2.53	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.73	0.41
1:A:382:ILE:HG21	1:A:385:LEU:HG	2.03	0.41
1:I:410:LYS:HD2	1:I:411:GLN:N	2.35	0.41
1:J:297:GLN:O	1:J:362:GLU:HA	2.20	0.41
1:L:371:THR:HG1	1:M:279:GLU:HG2	1.86	0.41
1:M:280:GLU:O	1:M:280:GLU:HG2	2.21	0.41
1:M:298:LEU:HD13	1:M:362:GLU:HB3	2.03	0.41
1:O:170:LYS:HD2	1:O:171:SER:O	2.21	0.41
1:R:248:ARG:HH11	1:S:267:THR:HG22	1.85	0.41
1:V:248:ARG:HD3	1:W:265:GLN:HB3	2.01	0.41
1:W:145:GLU:HG2	1:W:152:SER:HA	2.02	0.41
1:W:205:LEU:HD12	1:W:206:PRO:HD2	2.02	0.41
1:c:204:GLY:HA3	1:d:160:PRO:HB3	2.01	0.41
1:f:170:LYS:HE3	1:f:170:LYS:HB3	1.84	0.41
1:f:277:GLN:HB3	1:f:375:THR:HB	2.02	0.41
1:g:160:PRO:HB3	1:g:170:LYS:NZ	2.36	0.41
1:h:221:THR:HG22	1:h:223:SER:H	1.85	0.41
1:B:150:VAL:O	1:B:151:LYS:HD3	2.21	0.41
1:C:190:GLN:CD	1:E:217:GLY:HA3	2.46	0.41
1:K:191:ILE:HG21	1:K:220:LEU:O	2.21	0.41
1:L:155:VAL:HG23	1:L:176:VAL:HG22	2.02	0.41
1:L:170:LYS:HE2	1:L:170:LYS:HB2	1.97	0.41
1:O:188:GLU:HA	1:O:191:ILE:HD12	2.02	0.41
1:O:212:LEU:HB2	1:O:220:LEU:HB2	2.03	0.41
1:T:153:ALA:HB2	1:T:178:VAL:HG23	2.02	0.41
1:U:137:GLU:HB3	1:U:155:VAL:HG13	2.03	0.41
1:g:256:ILE:HG22	1:g:257:VAL:HG13	2.02	0.41
1:h:244:ARG:NH2	1:h:244:ARG:HB3	2.35	0.41
1:E:180:LEU:H	1:E:215:GLN:CD	2.26	0.41
1:E:409:MET:O	1:E:413:GLU:HG2	2.20	0.41
1:E:410:LYS:HE3	1:E:410:LYS:HB3	1.89	0.41
1:H:239:ASN:HA	1:H:242:GLU:HG2	2.03	0.41
1:H:279:GLU:OE2	1:H:281:HIS:HB2	2.21	0.41
1:I:180:LEU:H	1:I:215:GLN:CD	2.29	0.41
1:N:133:GLN:O	1:N:137:GLU:OE1	2.38	0.41
1:N:221:THR:HG22	1:N:223:SER:H	1.85	0.41
1:N:393:TYR:HB3	1:N:402:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:246:GLN:O	1:Q:249:ILE:HG22	2.21	0.41
1:Q:389:VAL:O	1:Q:432:VAL:HA	2.21	0.41
1:R:140:LEU:HD12	1:R:198:VAL:HG12	2.03	0.41
1:U:394:LYS:HG3	1:U:402:LEU:N	2.36	0.41
1:V:254:SER:HB2	1:V:255:PRO:HD3	2.02	0.41
1:Y:268:ALA:HA	1:Y:385:LEU:HD23	2.02	0.41
1:Z:245:ILE:CG2	1:Z:266:VAL:HG11	2.51	0.41
1:Z:375:THR:HG22	1:Z:377:MET:SD	2.61	0.41
1:a:194:VAL:O	1:a:198:VAL:HG22	2.19	0.41
1:b:241:VAL:HG11	1:b:382:ILE:HD11	2.01	0.41
1:c:149:PRO:O	1:c:180:LEU:HD23	2.20	0.41
1:f:268:ALA:HB1	1:f:382:ILE:HD11	2.03	0.41
1:g:143:THR:HG21	1:h:156:HIS:CE1	2.55	0.41
1:h:167:ARG:HA	1:h:167:ARG:NE	2.36	0.41
1:A:418:GLU:HB3	1:B:388:ALA:HB2	2.03	0.41
1:E:193:ALA:HA	1:G:219:LEU:CG	2.51	0.41
1:E:253:LEU:O	1:E:257:VAL:HG22	2.21	0.41
1:E:374:HIS:HB3	1:F:276:GLU:HB3	2.03	0.41
1:E:404:LEU:H	1:E:434:ASN:HD21	1.68	0.41
1:G:180:LEU:HD21	1:G:186:LEU:HB2	2.01	0.41
1:G:378:ASN:HD22	1:G:381:ASP:CG	2.22	0.41
1:H:254:SER:HB2	1:H:255:PRO:HD3	2.03	0.41
1:J:283:SER:HB2	1:J:369:ASP:HB2	2.03	0.41
1:K:151:LYS:HZ3	1:K:182:PRO:HD3	1.86	0.41
1:L:252:ILE:HB	1:M:265:GLN:HG3	2.02	0.41
1:L:410:LYS:HA	1:L:413:GLU:HG3	2.02	0.41
1:L:419:ALA:O	1:M:267:THR:HG21	2.20	0.41
1:M:290:LYS:HE2	1:M:290:LYS:HB2	1.88	0.41
1:Q:394:LYS:HG3	1:Q:402:LEU:HB2	2.02	0.41
1:R:139:GLU:O	1:T:154:ARG:NH2	2.43	0.41
1:R:180:LEU:H	1:R:215:GLN:CD	2.28	0.41
1:T:133:GLN:HE22	1:T:159:MET:HE1	1.85	0.41
1:T:197:LEU:HD12	1:U:177:THR:OG1	2.21	0.41
1:T:244:ARG:NH2	1:U:235:LEU:HB3	2.36	0.41
1:U:155:VAL:HG23	1:U:176:VAL:HG22	2.01	0.41
1:X:163:SER:OG	1:X:164:LEU:N	2.54	0.41
1:X:166:VAL:HG13	1:X:169:GLN:H	1.85	0.41
1:b:298:LEU:HD12	1:b:361:ASN:O	2.20	0.41
1:b:410:LYS:O	1:b:413:GLU:HG3	2.21	0.41
1:d:162:PRO:HB2	1:f:165:PHE:CD2	2.54	0.41
1:d:279:GLU:O	1:d:372:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:412:ILE:O	1:e:416:THR:HG23	2.21	0.41
1:f:296:ARG:HA	1:f:363:THR:O	2.21	0.41
1:g:252:ILE:HG12	1:h:265:GLN:HB2	2.03	0.41
1:h:240:ASP:O	1:h:244:ARG:HG3	2.21	0.41
1:A:290:LYS:HE2	1:A:290:LYS:HB2	1.88	0.41
1:B:133:GLN:O	1:B:137:GLU:HG3	2.21	0.41
1:B:370:ARG:HE	1:B:370:ARG:HB3	1.69	0.41
1:C:139:GLU:HG2	1:E:156:HIS:CE1	2.47	0.41
1:C:372:ILE:HG23	1:C:372:ILE:O	2.21	0.41
1:F:247:ARG:HB2	1:F:247:ARG:CZ	2.51	0.41
1:G:404:LEU:H	1:G:434:ASN:ND2	2.18	0.41
1:M:246:GLN:O	1:M:250:GLU:HG2	2.20	0.41
1:P:249:ILE:HA	1:P:252:ILE:HG22	2.03	0.41
1:R:137:GLU:OE1	1:R:155:VAL:HG13	2.21	0.41
1:V:417:ARG:HA	1:V:420:MET:CE	2.49	0.41
1:Y:143:THR:HG22	1:a:154:ARG:CD	2.51	0.41
1:Z:256:ILE:HD12	1:a:435:SER:OG	2.21	0.41
1:d:423:SER:OG	1:d:425:LYS:NZ	2.41	0.41
1:f:147:LEU:O	1:f:149:PRO:HD2	2.20	0.41
1:f:253:LEU:HD23	1:f:253:LEU:HA	1.92	0.41
1:g:417:ARG:HG3	1:g:422:PHE:HB3	2.03	0.41
1:D:378:ASN:HB3	1:D:381:ASP:OD2	2.20	0.40
1:F:277:GLN:HB3	1:F:375:THR:HB	2.04	0.40
1:M:261:ASN:O	1:M:392:ASN:N	2.44	0.40
1:N:166:VAL:HG12	1:N:167:ARG:N	2.33	0.40
1:N:181:GLU:CB	1:N:184:ARG:HB2	2.51	0.40
1:O:206:PRO:HG2	1:O:209:ASN:OD1	2.21	0.40
1:P:246:GLN:OE1	1:P:265:GLN:HA	2.21	0.40
1:R:142:ARG:HB2	1:T:154:ARG:CZ	2.51	0.40
1:T:151:LYS:HG2	1:T:179:THR:O	2.21	0.40
1:W:234:GLN:HB3	1:W:272:PHE:CE2	2.57	0.40
1:X:163:SER:O	1:Y:165:PHE:HB3	2.20	0.40
1:Z:253:LEU:HD22	1:Z:412:ILE:HD12	2.03	0.40
1:Z:413:GLU:CD	1:Z:432:VAL:HB	2.45	0.40
1:b:246:GLN:HE22	1:b:265:GLN:NE2	2.19	0.40
1:c:187:ASP:OD1	1:c:190:GLN:HG3	2.21	0.40
1:d:404:LEU:H	1:d:434:ASN:ND2	2.19	0.40
1:g:157:LEU:HD21	1:g:159:MET:HE3	2.02	0.40
1:A:301:SER:HB2	1:B:359:GLN:OE1	2.22	0.40
1:B:245:ILE:O	1:B:249:ILE:HG13	2.21	0.40
1:C:269:GLN:O	1:C:270:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:GLN:O	1:E:270:LEU:HD23	2.21	0.40
1:G:188:GLU:O	1:G:191:ILE:HB	2.22	0.40
1:G:234:GLN:HB3	1:G:272:PHE:CE2	2.57	0.40
1:H:293:LEU:O	1:I:285:ASN:ND2	2.39	0.40
1:K:249:ILE:O	1:K:252:ILE:HG22	2.22	0.40
1:N:369:ASP:OD1	1:O:282:TYR:N	2.51	0.40
1:P:393:TYR:CZ	1:P:436:PRO:HD3	2.56	0.40
1:R:237:PHE:HE1	1:S:232:ASP:HA	1.87	0.40
1:U:126:PHE:HA	1:U:129:GLN:NE2	2.36	0.40
1:U:372:ILE:O	1:U:372:ILE:HG23	2.21	0.40
1:V:244:ARG:CZ	1:W:235:LEU:HB3	2.51	0.40
1:V:269:GLN:HB3	1:V:383:GLU:OE2	2.21	0.40
1:V:393:TYR:CE1	1:V:403:PRO:HB3	2.56	0.40
1:W:142:ARG:CG	1:X:154:ARG:HH12	2.33	0.40
1:a:168:GLU:CG	1:a:169:GLN:H	2.27	0.40
1:a:302:GLU:HA	1:a:357:SER:O	2.21	0.40
1:c:219:LEU:HD23	1:c:219:LEU:HA	1.90	0.40
1:d:234:GLN:HB3	1:d:272:PHE:CZ	2.56	0.40
1:f:394:LYS:HG2	1:f:402:LEU:HB2	2.03	0.40
1:h:263:HIS:HB2	1:h:390:VAL:CG2	2.50	0.40
1:C:212:LEU:HD23	1:C:212:LEU:HA	1.88	0.40
1:F:408:GLN:O	1:F:411:GLN:HG2	2.20	0.40
1:I:180:LEU:HB2	1:I:215:GLN:HE22	1.87	0.40
1:I:214:ASP:OD1	1:I:220:LEU:HD11	2.21	0.40
1:K:378:ASN:HB3	1:K:381:ASP:OD2	2.21	0.40
1:N:151:LYS:N	1:N:151:LYS:HD2	2.36	0.40
1:N:407:ASP:O	1:N:410:LYS:HG3	2.22	0.40
1:O:393:TYR:CD1	1:O:403:PRO:HA	2.55	0.40
1:Q:413:GLU:O	1:Q:416:THR:OG1	2.33	0.40
1:R:420:MET:SD	1:R:430:LEU:HB2	2.60	0.40
1:T:304:VAL:HG22	1:T:356:ARG:HG2	2.03	0.40
1:T:382:ILE:HG21	1:T:385:LEU:HG	2.03	0.40
1:U:172:PRO:HG2	1:U:204:GLY:O	2.21	0.40
1:X:252:ILE:HD13	1:X:252:ILE:HA	1.92	0.40
1:b:414:ASP:HB3	1:c:431:ASN:HD22	1.86	0.40
1:c:410:LYS:HB3	1:c:410:LYS:HE3	1.84	0.40
1:d:249:ILE:O	1:d:252:ILE:HG22	2.21	0.40
1:e:372:ILE:O	1:f:277:GLN:HA	2.21	0.40
1:h:137:GLU:OE2	1:h:157:LEU:N	2.54	0.40
1:A:246:GLN:OE1	1:A:265:GLN:HA	2.21	0.40
1:E:141:ALA:O	1:E:145:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:GLU:OE2	1:H:153:ALA:N	2.39	0.40
1:J:385:LEU:HB3	1:J:420:MET:HE2	2.03	0.40
1:J:393:TYR:HB3	1:J:402:LEU:N	2.37	0.40
1:K:231:ASN:OD1	1:K:232:ASP:N	2.54	0.40
1:N:187:ASP:O	1:N:191:ILE:HG12	2.22	0.40
1:O:287:ASP:HB3	1:O:290:LYS:HG2	2.03	0.40
1:R:145:GLU:HA	1:R:150:VAL:HG11	2.03	0.40
1:R:159:MET:SD	1:R:172:PRO:HB3	2.61	0.40
1:T:191:ILE:CD1	1:T:220:LEU:HD13	2.51	0.40
1:U:187:ASP:O	1:U:191:ILE:HG12	2.21	0.40
1:V:421:GLY:HA3	1:W:267:THR:HG21	2.04	0.40
1:Y:191:ILE:HG21	1:Y:220:LEU:O	2.21	0.40
1:b:239:ASN:HA	1:b:242:GLU:HG2	2.03	0.40
1:b:423:SER:HB3	1:b:426:ARG:HG3	2.03	0.40
1:c:144:ILE:HD12	1:c:194:VAL:HG23	2.03	0.40
1:c:184:ARG:N	1:c:184:ARG:HD2	2.36	0.40
1:d:269:GLN:O	1:d:383:GLU:HG2	2.22	0.40
1:B:269:GLN:HG3	1:B:384:ARG:NH1	2.35	0.40
1:B:370:ARG:HD2	1:B:372:ILE:HD11	2.04	0.40
1:F:404:LEU:HD23	1:F:434:ASN:ND2	2.29	0.40
1:G:143:THR:CB	1:H:156:HIS:HE2	2.34	0.40
1:I:142:ARG:CD	1:K:154:ARG:HH12	2.35	0.40
1:I:284:PRO:O	1:I:290:LYS:NZ	2.54	0.40
1:J:279:GLU:OE2	1:J:281:HIS:N	2.53	0.40
1:K:191:ILE:HD12	1:K:220:LEU:HB3	2.03	0.40
1:M:273:ALA:HB3	1:M:275:LYS:NZ	2.37	0.40
1:M:280:GLU:HA	1:M:371:THR:O	2.22	0.40
1:N:394:LYS:HE2	1:N:402:LEU:HD13	2.03	0.40
1:P:299:ASN:HD22	1:P:361:ASN:HD22	1.68	0.40
1:P:385:LEU:HD23	1:P:385:LEU:HA	1.80	0.40
1:P:416:THR:O	1:P:420:MET:HG3	2.22	0.40
1:Q:410:LYS:HD2	1:Q:410:LYS:C	2.47	0.40
1:V:279:GLU:OE2	1:V:373:ARG:HB2	2.22	0.40
1:X:199:SER:HA	1:X:205:LEU:HB3	2.04	0.40
1:d:158:ALA:O	1:d:159:MET:HE2	2.22	0.40
1:h:191:ILE:HG12	1:h:220:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	145/560 (26%)	143 (99%)	2 (1%)	0	100	100
1	B	242/560 (43%)	227 (94%)	15 (6%)	0	100	100
1	C	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	30	62
1	D	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	E	242/560 (43%)	226 (93%)	16 (7%)	0	100	100
1	F	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	G	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	30	62
1	H	242/560 (43%)	221 (91%)	19 (8%)	2 (1%)	16	48
1	I	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	30	62
1	J	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	K	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	30	62
1	L	242/560 (43%)	224 (93%)	18 (7%)	0	100	100
1	M	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	N	242/560 (43%)	223 (92%)	19 (8%)	0	100	100
1	O	242/560 (43%)	231 (96%)	10 (4%)	1 (0%)	30	62
1	P	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	Q	242/560 (43%)	224 (93%)	17 (7%)	1 (0%)	30	62
1	R	242/560 (43%)	229 (95%)	13 (5%)	0	100	100
1	S	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	T	242/560 (43%)	230 (95%)	12 (5%)	0	100	100
1	U	242/560 (43%)	231 (96%)	11 (4%)	0	100	100
1	V	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	W	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	30	62
1	X	242/560 (43%)	225 (93%)	17 (7%)	0	100	100
1	Y	242/560 (43%)	228 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	a	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	30	62
1	b	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	c	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	30	62
1	d	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	30	62
1	e	145/560 (26%)	144 (99%)	1 (1%)	0	100	100
1	f	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	30	62
1	g	242/560 (43%)	226 (93%)	15 (6%)	1 (0%)	30	62
1	h	242/560 (43%)	232 (96%)	10 (4%)	0	100	100
All	All	7161/19040 (38%)	6784 (95%)	363 (5%)	14 (0%)	44	73

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	160	PRO
1	O	160	PRO
1	g	160	PRO
1	K	160	PRO
1	a	160	PRO
1	C	160	PRO
1	H	166	VAL
1	Q	160	PRO
1	f	160	PRO
1	G	160	PRO
1	I	160	PRO
1	W	160	PRO
1	d	160	PRO
1	c	160	PRO

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	134/467 (29%)	134 (100%)	0	100	100
1	B	217/467 (46%)	217 (100%)	0	100	100
1	C	217/467 (46%)	217 (100%)	0	100	100
1	D	134/467 (29%)	134 (100%)	0	100	100
1	E	217/467 (46%)	217 (100%)	0	100	100
1	F	134/467 (29%)	134 (100%)	0	100	100
1	G	217/467 (46%)	217 (100%)	0	100	100
1	H	217/467 (46%)	217 (100%)	0	100	100
1	I	217/467 (46%)	217 (100%)	0	100	100
1	J	134/467 (29%)	134 (100%)	0	100	100
1	K	217/467 (46%)	217 (100%)	0	100	100
1	L	217/467 (46%)	217 (100%)	0	100	100
1	M	134/467 (29%)	134 (100%)	0	100	100
1	N	217/467 (46%)	217 (100%)	0	100	100
1	O	217/467 (46%)	217 (100%)	0	100	100
1	P	134/467 (29%)	134 (100%)	0	100	100
1	Q	217/467 (46%)	217 (100%)	0	100	100
1	R	217/467 (46%)	217 (100%)	0	100	100
1	S	134/467 (29%)	134 (100%)	0	100	100
1	T	217/467 (46%)	217 (100%)	0	100	100
1	U	217/467 (46%)	217 (100%)	0	100	100
1	V	134/467 (29%)	134 (100%)	0	100	100
1	W	217/467 (46%)	217 (100%)	0	100	100
1	X	217/467 (46%)	217 (100%)	0	100	100
1	Y	217/467 (46%)	217 (100%)	0	100	100
1	Z	134/467 (29%)	134 (100%)	0	100	100
1	a	217/467 (46%)	217 (100%)	0	100	100
1	b	134/467 (29%)	134 (100%)	0	100	100
1	c	217/467 (46%)	217 (100%)	0	100	100
1	d	217/467 (46%)	217 (100%)	0	100	100
1	e	134/467 (29%)	134 (100%)	0	100	100
1	f	217/467 (46%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	217/467 (46%)	217 (100%)	0	100	100
1	h	217/467 (46%)	217 (100%)	0	100	100
All	All	6465/15878 (41%)	6465 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	365	ASN
1	A	378	ASN
1	A	434	ASN
1	B	156	HIS
1	B	234	GLN
1	B	378	ASN
1	B	434	ASN
1	C	218	HIS
1	C	234	GLN
1	C	246	GLN
1	D	303	GLN
1	D	434	ASN
1	E	169	GLN
1	E	281	HIS
1	F	263	HIS
1	G	156	HIS
1	G	169	GLN
1	G	263	HIS
1	G	281	HIS
1	G	434	ASN
1	H	434	ASN
1	I	169	GLN
1	J	263	HIS
1	J	281	HIS
1	K	133	GLN
1	K	378	ASN
1	L	209	ASN
1	L	234	GLN
1	L	365	ASN
1	M	277	GLN
1	M	431	ASN

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Mol	Chain	Res	Type
1	M	434	ASN
1	N	156	HIS
1	N	277	GLN
1	O	156	HIS
1	O	361	ASN
1	P	299	ASN
1	P	359	GLN
1	P	365	ASN
1	P	374	HIS
1	P	431	ASN
1	Q	299	ASN
1	R	169	GLN
1	R	299	ASN
1	S	365	ASN
1	S	374	HIS
1	S	411	GLN
1	T	131	ASN
1	T	156	HIS
1	T	169	GLN
1	U	125	GLN
1	V	359	GLN
1	W	156	HIS
1	W	169	GLN
1	W	222	GLN
1	W	263	HIS
1	W	269	GLN
1	W	281	HIS
1	X	222	GLN
1	X	277	GLN
1	X	281	HIS
1	X	434	ASN
1	Y	169	GLN
1	Y	378	ASN
1	Z	234	GLN
1	Z	263	HIS
1	Z	281	HIS
1	a	299	ASN
1	b	265	GLN
1	b	374	HIS
1	c	277	GLN
1	d	133	GLN
1	d	218	HIS

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Mol	Chain	Res	Type
1	d	411	GLN
1	e	263	HIS
1	e	274	ASN
1	e	277	GLN
1	e	434	ASN
1	f	133	GLN
1	g	263	HIS
1	h	277	GLN
1	h	299	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

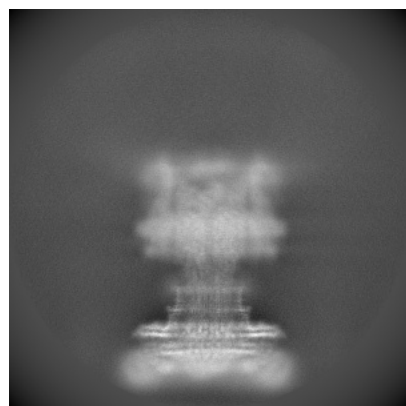
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12195. These allow visual inspection of the internal detail of the map and identification of artifacts.

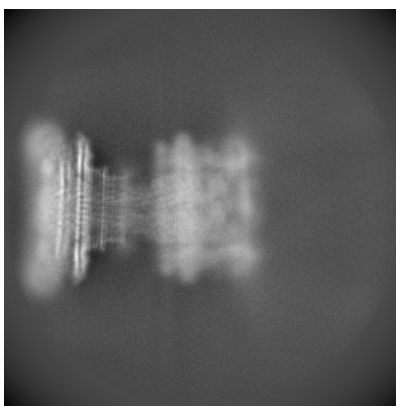
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

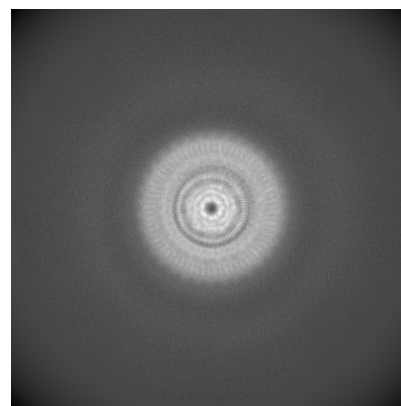
6.1.1 Primary map



X

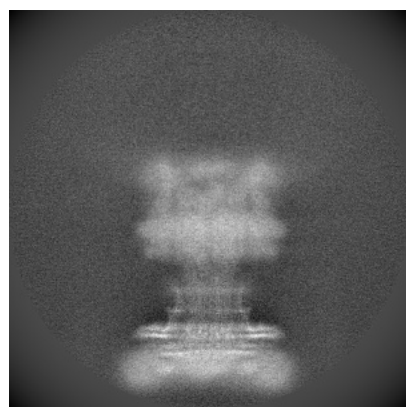


Y

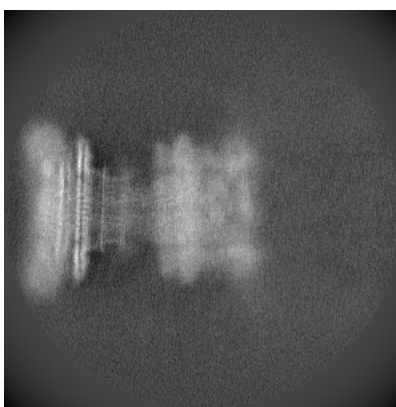


Z

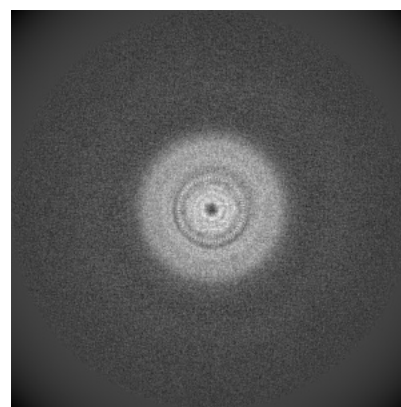
6.1.2 Raw map



X



Y

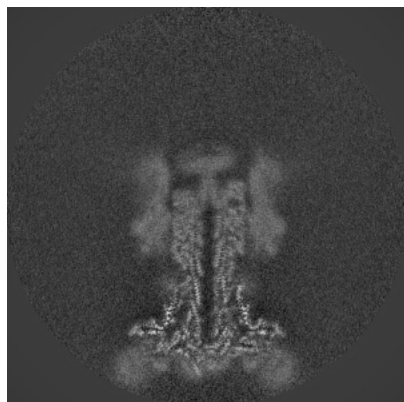


Z

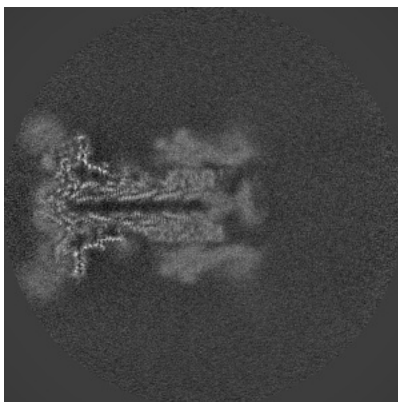
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

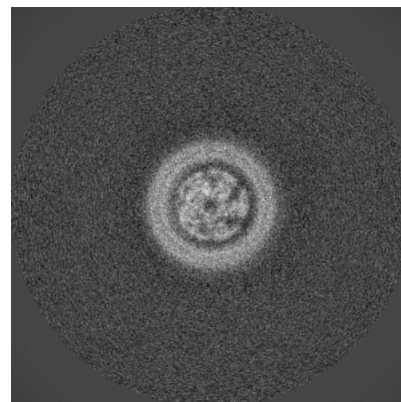
6.2.1 Primary map



X Index: 384

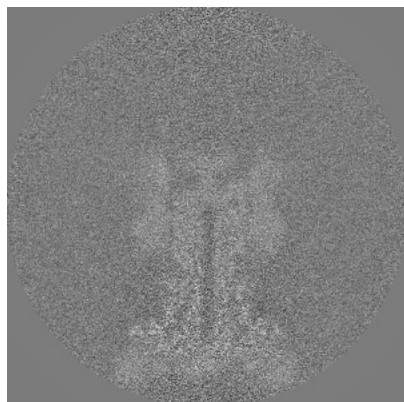


Y Index: 384

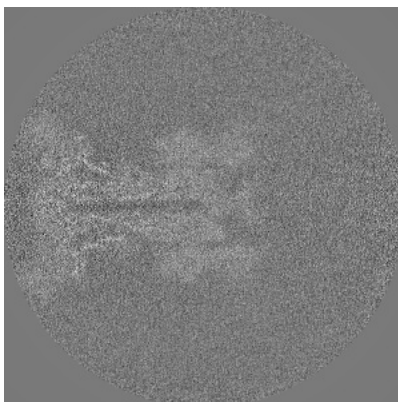


Z Index: 384

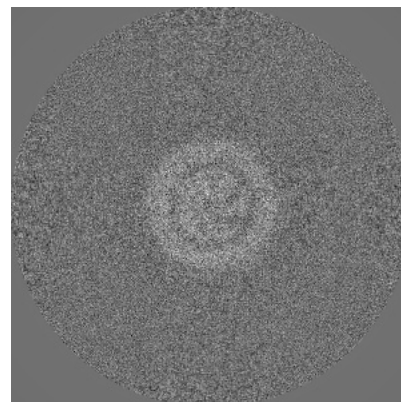
6.2.2 Raw map



X Index: 384



Y Index: 384

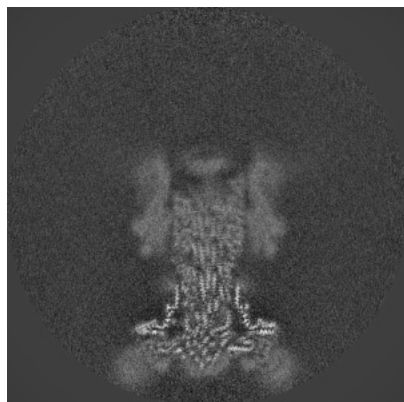


Z Index: 384

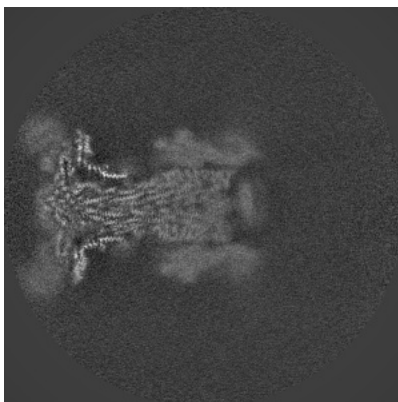
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

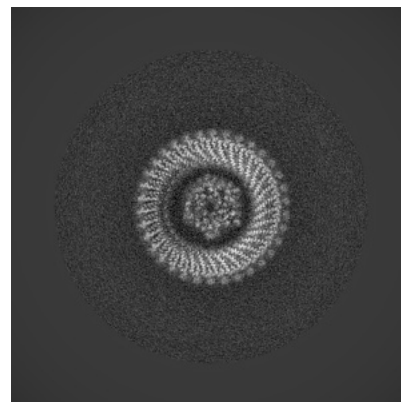
6.3.1 Primary map



X Index: 402

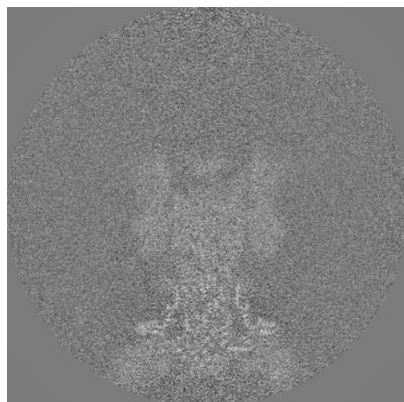


Y Index: 398

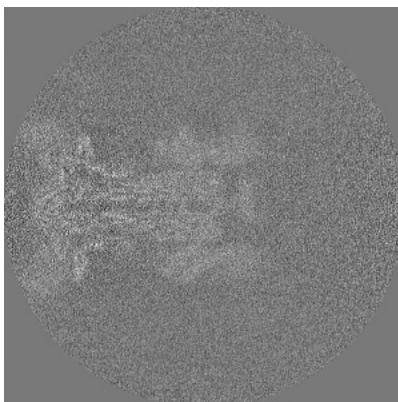


Z Index: 143

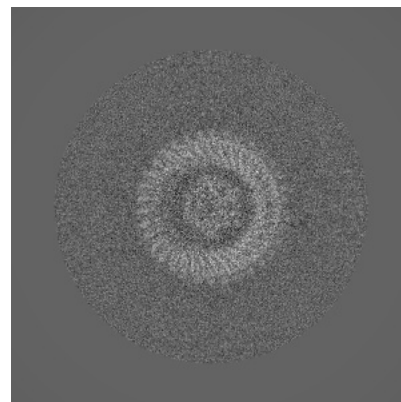
6.3.2 Raw map



X Index: 402



Y Index: 376

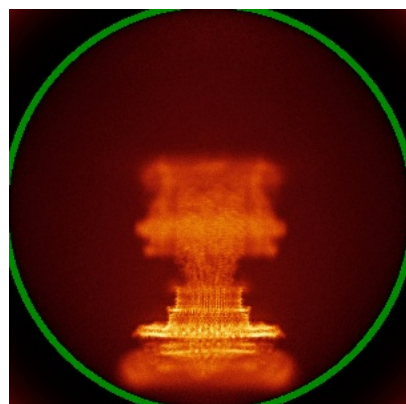


Z Index: 143

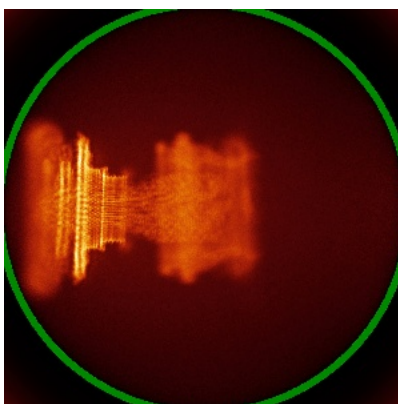
The images above show the largest variance slices of the map in three orthogonal directions.

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

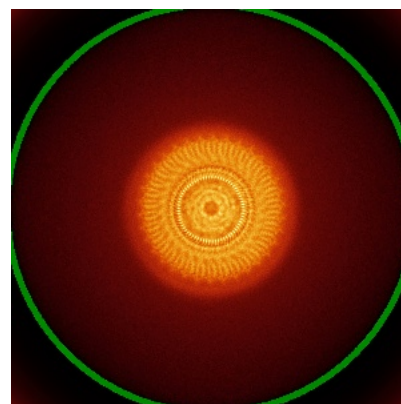
6.4.1 Primary map



X

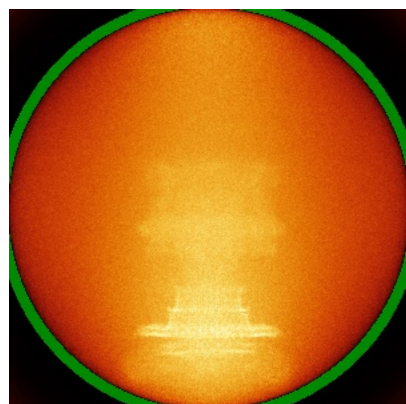


Y

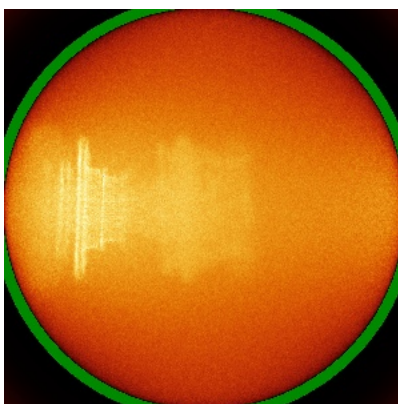


Z

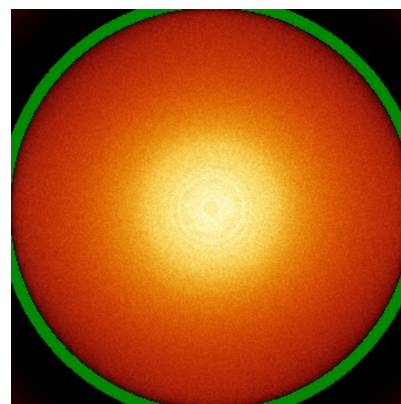
6.4.2 Raw map



X



Y

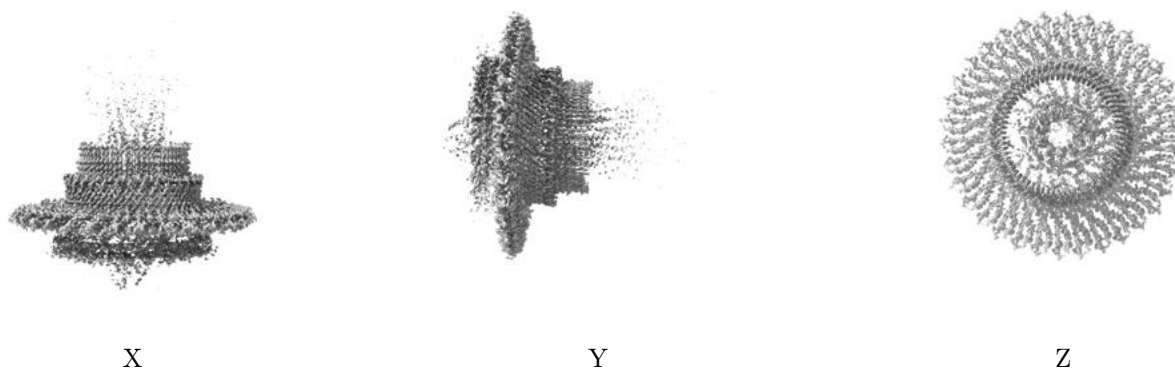


Z

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

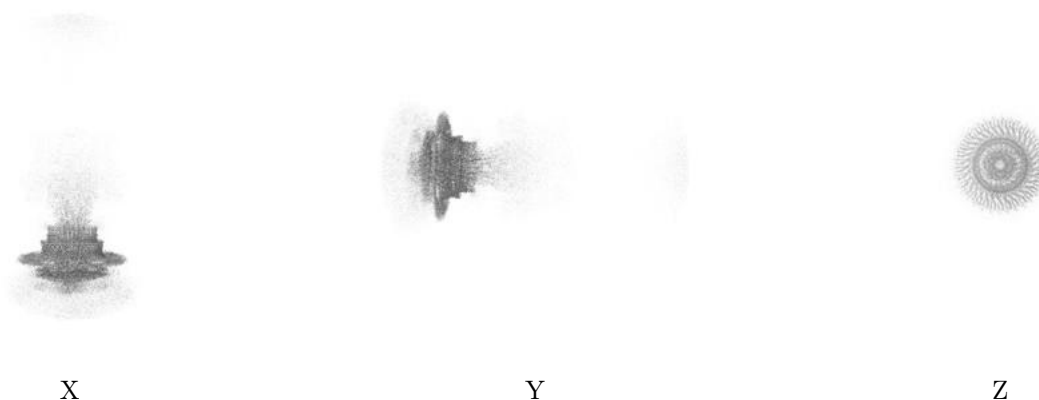
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

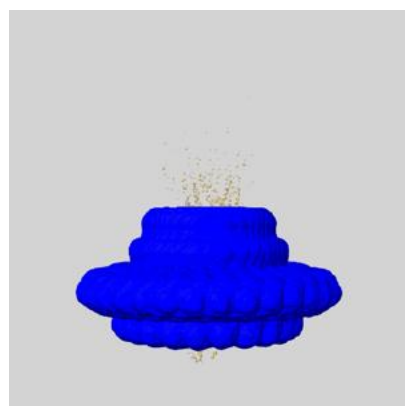
6.6 Mask visualisation [i](#)

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

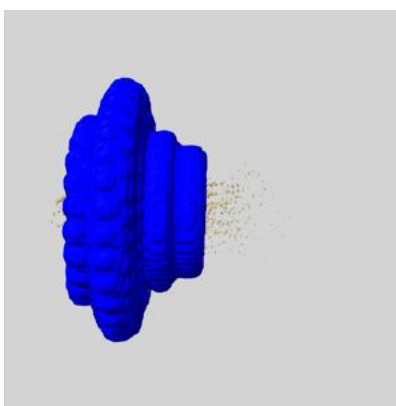
A mask typically either:

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

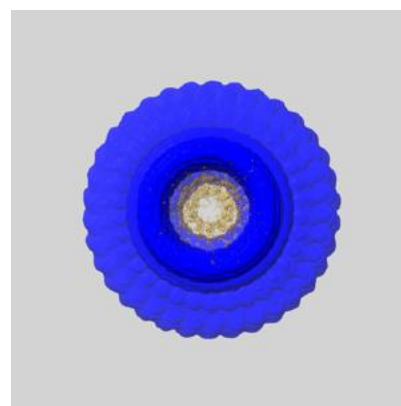
6.6.1 emd_12195_msk_1.map [i](#)



X



Y

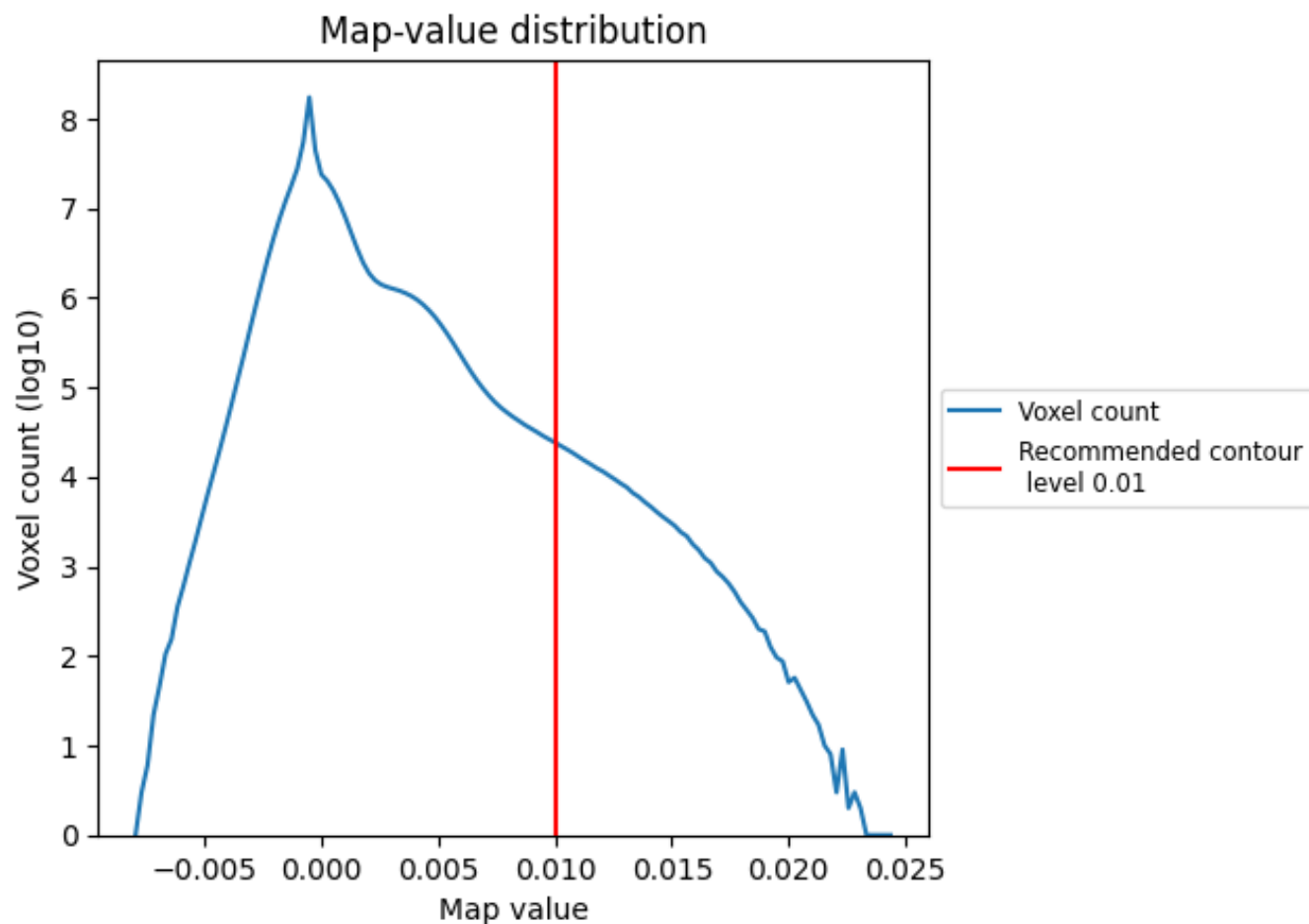


Z

7 Map analysis [i](#)

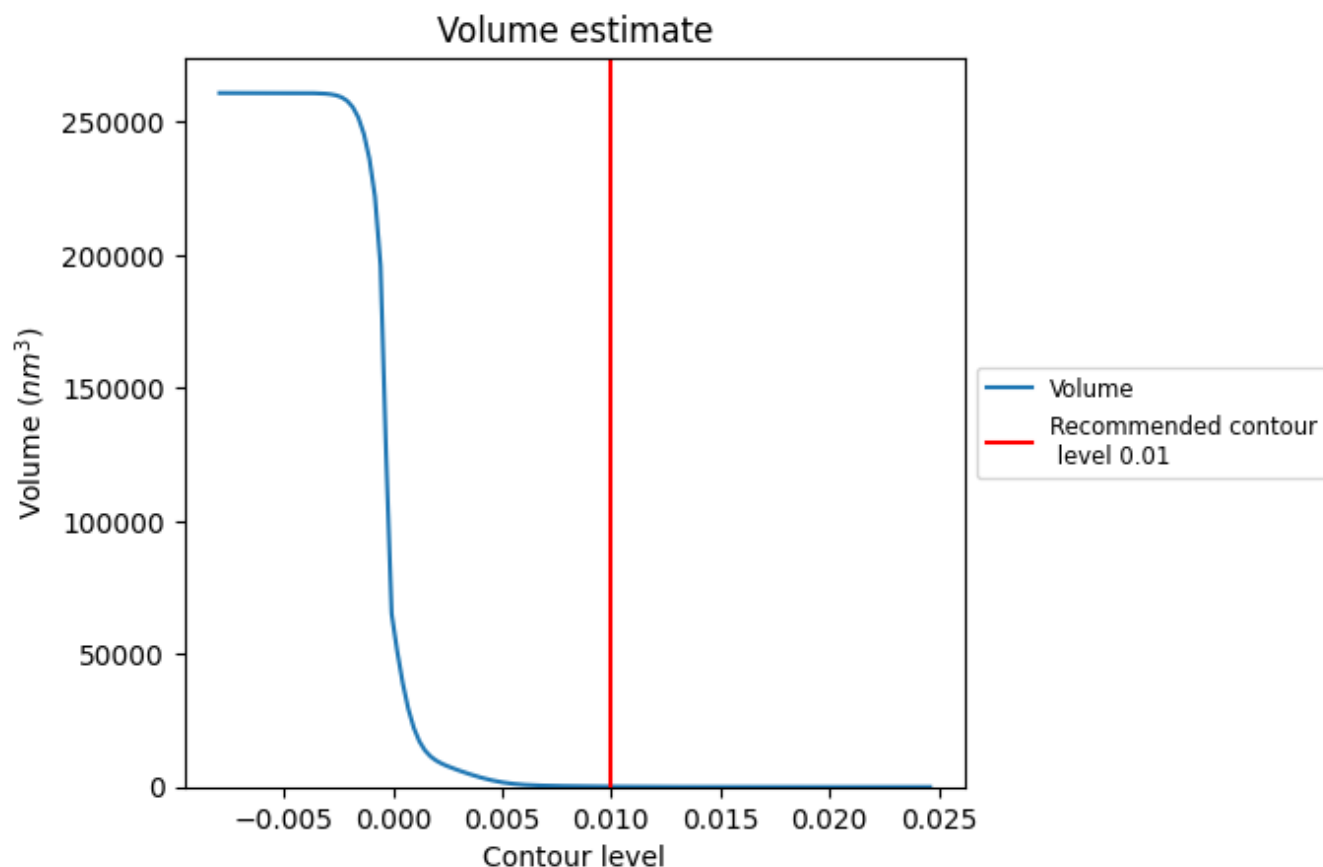
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

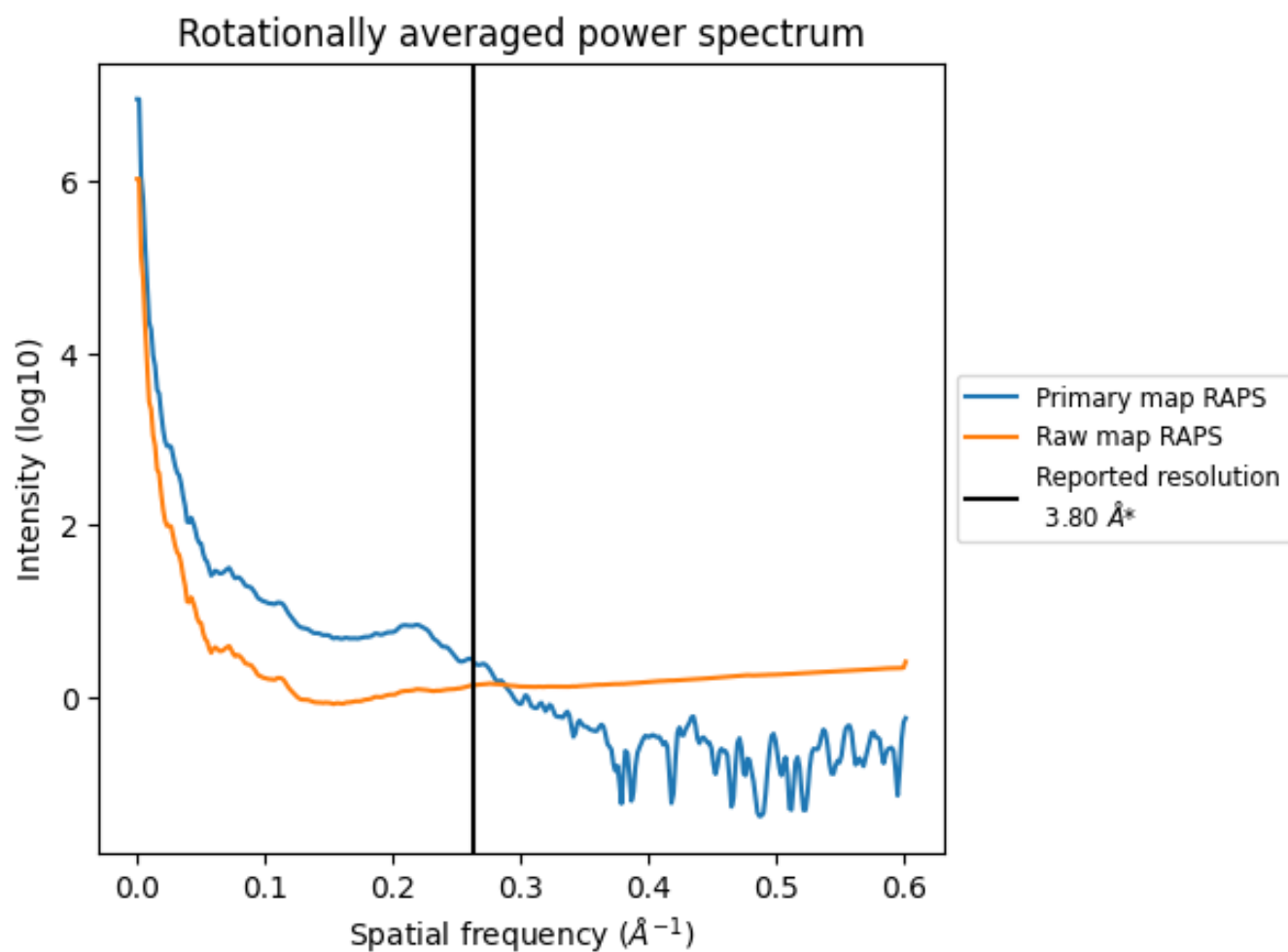
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm^3 ; this corresponds to an approximate mass of 125 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 ⓘ

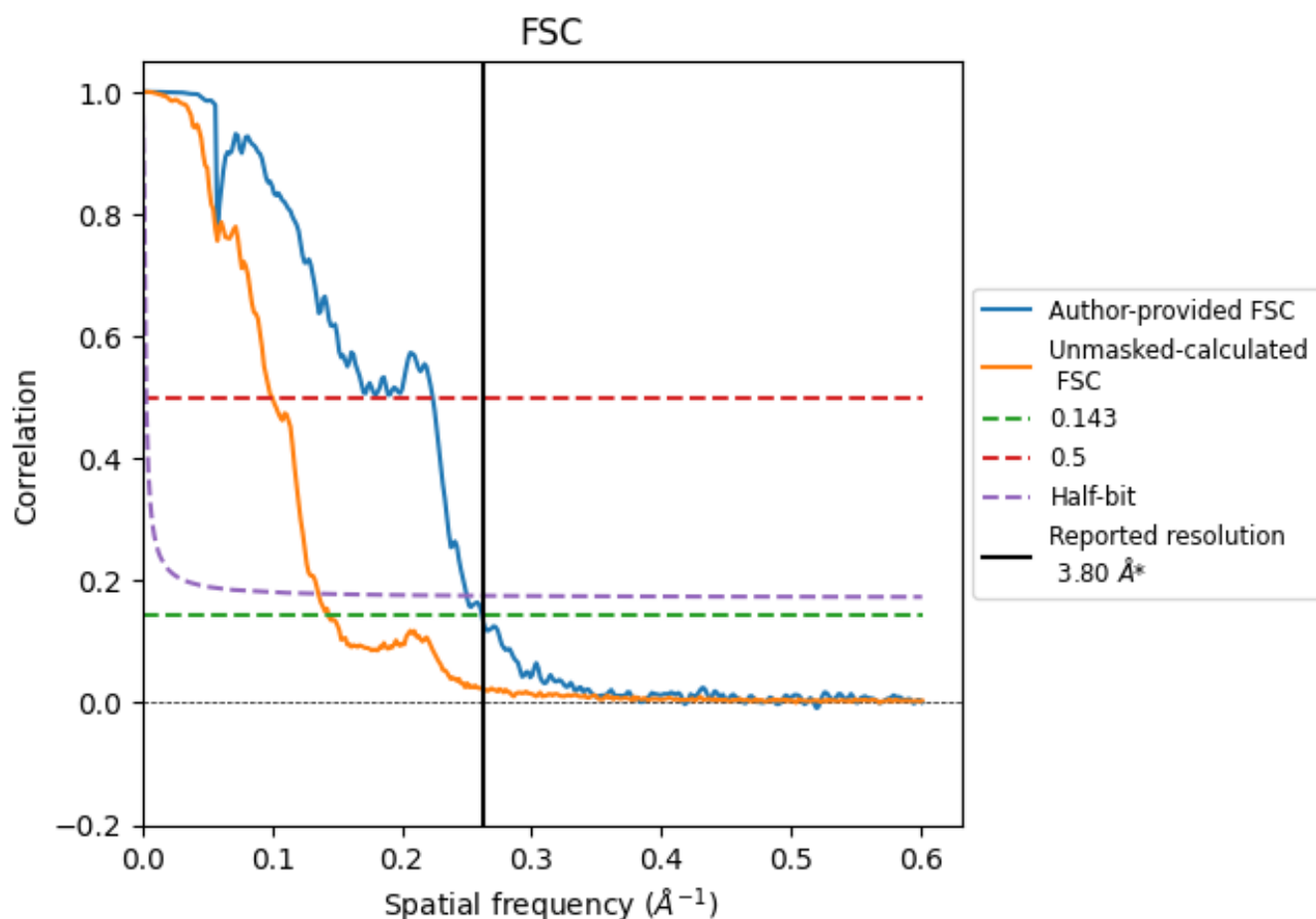


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

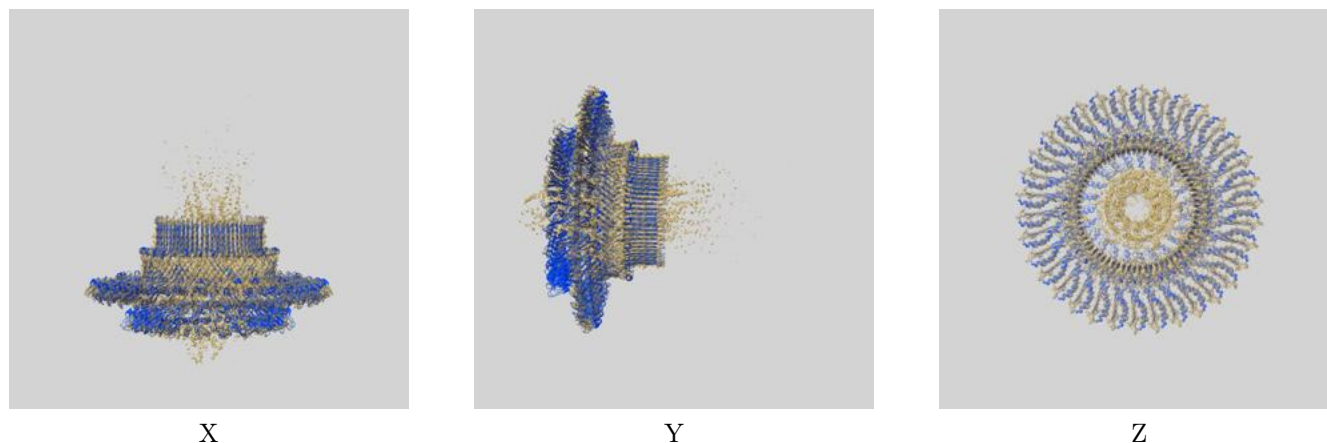
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.47	4.00
Unmasked-calculated*	6.96	9.98	7.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.96 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

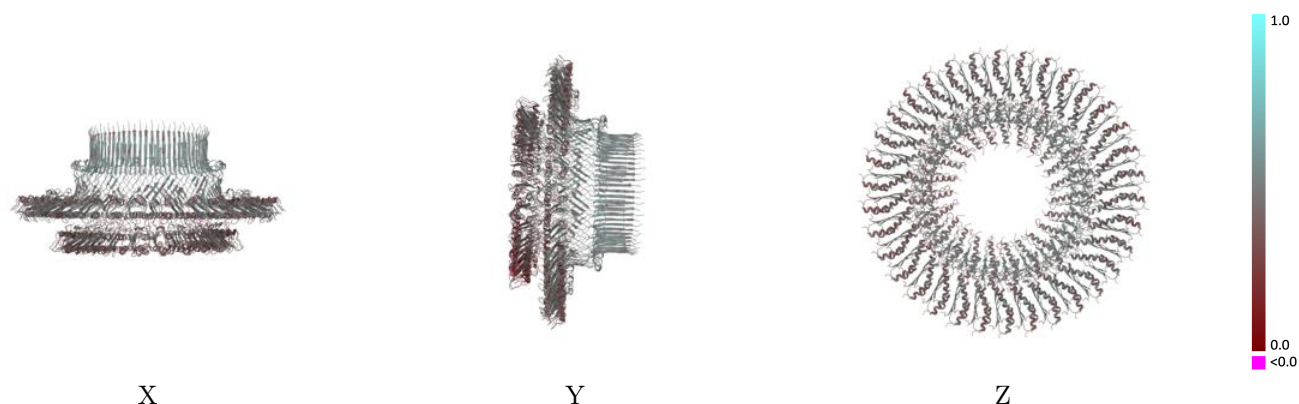
This section contains information regarding the fit between EMDB map EMD-12195 and PDB model 7BK0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



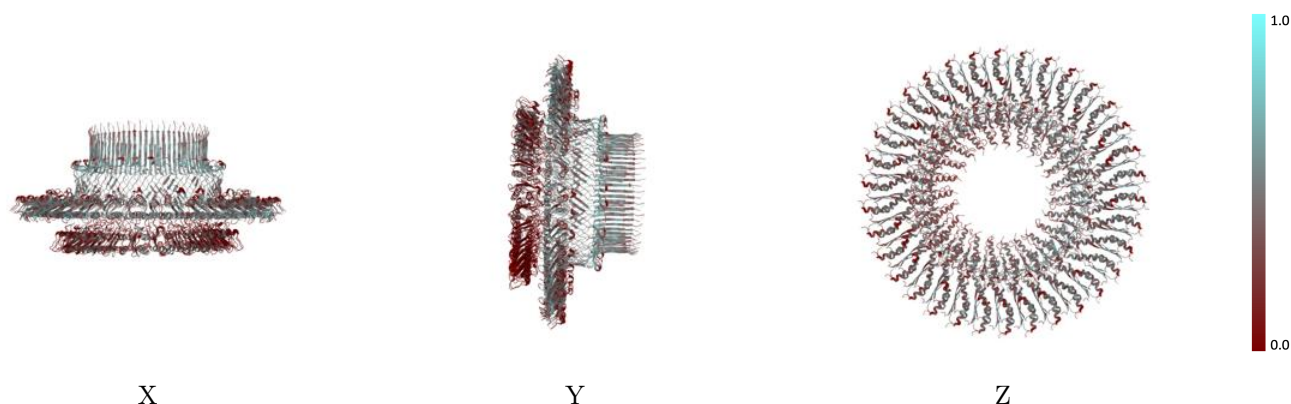
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



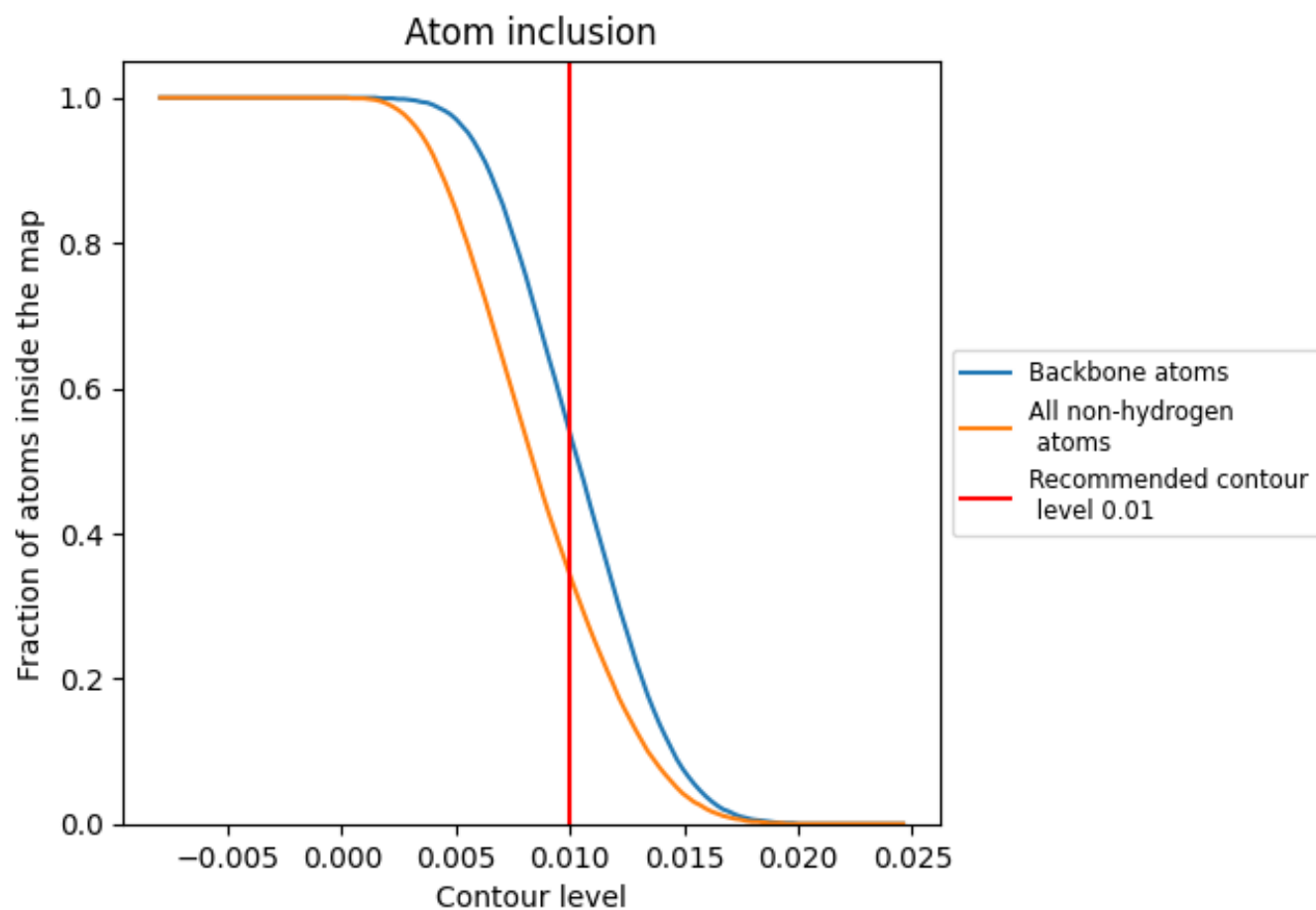
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3430	 0.4320
A	 0.4500	 0.4750
B	 0.3730	 0.4420
C	 0.3810	 0.4520
D	 0.4430	 0.4620
E	 0.3560	 0.4460
F	 0.4410	 0.4680
G	 0.3640	 0.4500
H	 0.3540	 0.4420
I	 0.3550	 0.4370
J	 0.4410	 0.4600
K	 0.3420	 0.4330
L	 0.3130	 0.4370
M	 0.4450	 0.4600
N	 0.3070	 0.4170
O	 0.2830	 0.4180
P	 0.4040	 0.4500
Q	 0.2670	 0.4070
R	 0.2670	 0.4030
S	 0.4090	 0.4570
T	 0.2430	 0.3790
U	 0.2500	 0.3740
V	 0.3770	 0.4360
W	 0.2360	 0.3850
X	 0.2570	 0.3930
Y	 0.2760	 0.4100
Z	 0.4180	 0.4510
a	 0.3120	 0.4260
b	 0.4390	 0.4550
c	 0.3240	 0.4320
d	 0.3490	 0.4350
e	 0.4480	 0.4670
f	 0.3490	 0.4350
g	 0.3620	 0.4430
h	 0.3740	 0.4520

