



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 09:08 AM JST

PDB ID : 23FU / pdb_000023fu
EMDB ID : EMD-68935
Title : Cryo-EM structure of Chaetomium thermophilum RSC bound to a nucleosome
Authors : Ma, S.S.; Liu, M.D.; Shen, Q.T.; Chen, Y.
Deposited on : 2026-02-05
Resolution : 4.45 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.50

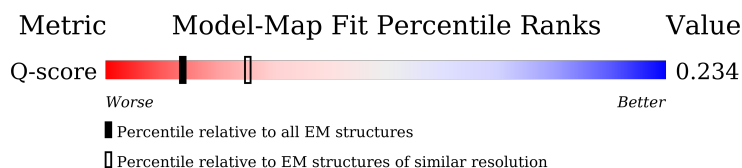
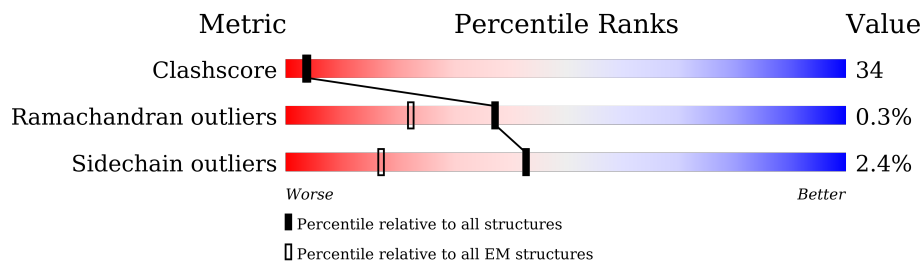
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.45 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.



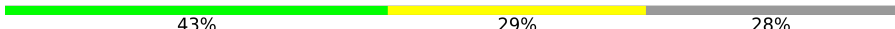
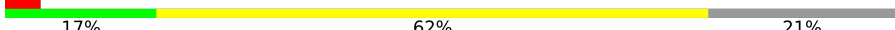
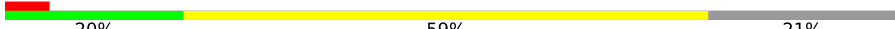
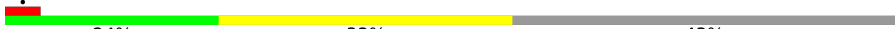
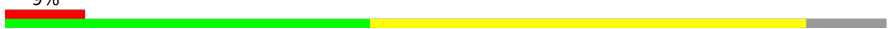
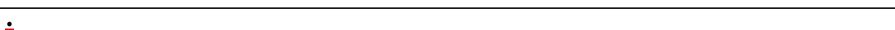
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3027 (3.95 - 4.95)

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	135	
1	E	135	
2	B	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	125	
4	H	125	
5	I	167	
6	J	167	
7	K	1595	
8	L	733	
9	M	476	
10	N	694	
10	O	694	
11	P	547	
12	Q	769	
13	R	763	
14	S	607	
15	T	534	
16	U	991	
17	V	990	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 46373 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			744	469	141	131	3		
1	E	91	Total	C	N	O	S	0	0
			744	469	141	131	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	F	77	Total	C	N	O	S	0	0
			614	389	119	105	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	95	Total	C	N	O	0	0
			733	459	145	129		
3	G	95	Total	C	N	O	0	0
			734	461	145	128		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	S	0	0
			685	433	121	129	2		
4	H	90	Total	C	N	O	S	0	0
			703	444	124	133	2		

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	132	Total	C	N	O	P	0	0
			2694	1277	493	792	132		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	132	Total	C	N	O	P	0	0
			2718	1285	509	792	132		

- Molecule 7 is a protein called WD40 repeat-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	826	Total	C	N	O	S	0	0
			6825	4307	1254	1229	35		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-60	GLY	-	expression tag	UNP G0SHD8
K	-59	SER	-	expression tag	UNP G0SHD8
K	-58	PRO	-	expression tag	UNP G0SHD8
K	-57	GLN	-	expression tag	UNP G0SHD8
K	-56	GLN	-	expression tag	UNP G0SHD8
K	-55	ASN	-	expression tag	UNP G0SHD8
K	-54	LYS	-	expression tag	UNP G0SHD8
K	-53	THR	-	expression tag	UNP G0SHD8
K	-52	ALA	-	expression tag	UNP G0SHD8
K	-51	ALA	-	expression tag	UNP G0SHD8
K	-50	LEU	-	expression tag	UNP G0SHD8
K	-49	ALA	-	expression tag	UNP G0SHD8
K	-48	GLN	-	expression tag	UNP G0SHD8
K	-47	HIS	-	expression tag	UNP G0SHD8
K	-46	ASP	-	expression tag	UNP G0SHD8
K	-45	GLU	-	expression tag	UNP G0SHD8
K	-44	ALA	-	expression tag	UNP G0SHD8
K	-43	ASP	-	expression tag	UNP G0SHD8
K	-42	TYR	-	expression tag	UNP G0SHD8
K	-41	LYS	-	expression tag	UNP G0SHD8
K	-40	ASP	-	expression tag	UNP G0SHD8
K	-39	HIS	-	expression tag	UNP G0SHD8
K	-38	ASP	-	expression tag	UNP G0SHD8
K	-37	GLY	-	expression tag	UNP G0SHD8
K	-36	ASP	-	expression tag	UNP G0SHD8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-35	TYR	-	expression tag	UNP G0SHD8
K	-34	LYS	-	expression tag	UNP G0SHD8
K	-33	ASP	-	expression tag	UNP G0SHD8
K	-32	HIS	-	expression tag	UNP G0SHD8
K	-31	ASP	-	expression tag	UNP G0SHD8
K	-30	ILE	-	expression tag	UNP G0SHD8
K	-29	ASP	-	expression tag	UNP G0SHD8
K	-28	TYR	-	expression tag	UNP G0SHD8
K	-27	LYS	-	expression tag	UNP G0SHD8
K	-26	ASP	-	expression tag	UNP G0SHD8
K	-25	ASP	-	expression tag	UNP G0SHD8
K	-24	ASP	-	expression tag	UNP G0SHD8
K	-23	ASP	-	expression tag	UNP G0SHD8
K	-22	LYS	-	expression tag	UNP G0SHD8
K	-21	GLY	-	expression tag	UNP G0SHD8
K	-20	GLY	-	expression tag	UNP G0SHD8
K	-19	SER	-	expression tag	UNP G0SHD8
K	-18	GLY	-	expression tag	UNP G0SHD8
K	-17	GLY	-	expression tag	UNP G0SHD8
K	-16	SER	-	expression tag	UNP G0SHD8
K	-15	LEU	-	expression tag	UNP G0SHD8
K	-14	GLU	-	expression tag	UNP G0SHD8
K	-13	VAL	-	expression tag	UNP G0SHD8
K	-12	LEU	-	expression tag	UNP G0SHD8
K	-11	PHE	-	expression tag	UNP G0SHD8
K	-10	GLN	-	expression tag	UNP G0SHD8
K	-9	GLY	-	expression tag	UNP G0SHD8
K	-8	PRO	-	expression tag	UNP G0SHD8
K	-7	GLY	-	expression tag	UNP G0SHD8
K	-6	GLY	-	expression tag	UNP G0SHD8
K	-5	SER	-	expression tag	UNP G0SHD8
K	-4	GLY	-	expression tag	UNP G0SHD8
K	-3	GLY	-	expression tag	UNP G0SHD8
K	-2	SER	-	expression tag	UNP G0SHD8
K	-1	GLY	-	expression tag	UNP G0SHD8
K	0	THR	-	expression tag	UNP G0SHD8
K	112	VAL	ILE	conflict	UNP G0SHD8
K	280	ILE	VAL	conflict	UNP G0SHD8
K	1511	THR	ALA	conflict	UNP G0SHD8

- Molecule 8 is a protein called Putative chromatin structure remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	415	Total	C	N	O	S	0	0
			3340	2121	587	614	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	374	PRO	ALA	conflict	UNP G0S882
L	375	ALA	THR	conflict	UNP G0S882
L	415	LYS	ARG	conflict	UNP G0S882
L	428	SER	PRO	conflict	UNP G0S882
L	712	GLU	-	expression tag	UNP G0S882
L	713	LEU	-	expression tag	UNP G0S882
L	714	GLY	-	expression tag	UNP G0S882
L	715	PRO	-	expression tag	UNP G0S882
L	716	LYS	-	expression tag	UNP G0S882
L	717	GLY	-	expression tag	UNP G0S882
L	718	ILE	-	expression tag	UNP G0S882
L	719	ARG	-	expression tag	UNP G0S882
L	720	SER	-	expression tag	UNP G0S882
L	721	HIS	-	expression tag	UNP G0S882
L	722	SER	-	expression tag	UNP G0S882
L	723	MET	-	expression tag	UNP G0S882
L	724	LEU	-	expression tag	UNP G0S882
L	725	ALA	-	expression tag	UNP G0S882
L	726	LEU	-	expression tag	UNP G0S882
L	727	GLU	-	expression tag	UNP G0S882
L	728	HIS	-	expression tag	UNP G0S882
L	729	HIS	-	expression tag	UNP G0S882
L	730	HIS	-	expression tag	UNP G0S882
L	731	HIS	-	expression tag	UNP G0S882
L	732	HIS	-	expression tag	UNP G0S882
L	733	HIS	-	expression tag	UNP G0S882

- Molecule 9 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	431	Total	C	N	O	S	0	0
			3371	2141	590	625	15		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	469	LEU	-	expression tag	UNP G0SBW4

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Chain	Residue	Modelled	Actual	Comment	Reference
M	470	GLU	-	expression tag	UNP G0SBW4
M	471	HIS	-	expression tag	UNP G0SBW4
M	472	HIS	-	expression tag	UNP G0SBW4
M	473	HIS	-	expression tag	UNP G0SBW4
M	474	HIS	-	expression tag	UNP G0SBW4
M	475	HIS	-	expression tag	UNP G0SBW4
M	476	HIS	-	expression tag	UNP G0SBW4

- Molecule 10 is a protein called Ssr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	471	Total	C	N	O	S	0	0
			3714	2319	662	713	20		
10	O	274	Total	C	N	O	S	0	0
			2245	1421	404	409	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	687	ASP	-	expression tag	UNP G0S647
N	688	TYR	-	expression tag	UNP G0S647
N	689	LYS	-	expression tag	UNP G0S647
N	690	ASP	-	expression tag	UNP G0S647
N	691	ASP	-	expression tag	UNP G0S647
N	692	ASP	-	expression tag	UNP G0S647
N	693	ASP	-	expression tag	UNP G0S647
N	694	LYS	-	expression tag	UNP G0S647
O	687	ASP	-	expression tag	UNP G0S647
O	688	TYR	-	expression tag	UNP G0S647
O	689	LYS	-	expression tag	UNP G0S647
O	690	ASP	-	expression tag	UNP G0S647
O	691	ASP	-	expression tag	UNP G0S647
O	692	ASP	-	expression tag	UNP G0S647
O	693	ASP	-	expression tag	UNP G0S647
O	694	LYS	-	expression tag	UNP G0S647

- Molecule 11 is a protein called DM2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	377	Total	C	N	O	S	0	0
			3089	1944	553	583	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	191	ASP	ASN	conflict	UNP G0RYN3
P	540	ASP	-	expression tag	UNP G0RYN3
P	541	TYR	-	expression tag	UNP G0RYN3
P	542	LYS	-	expression tag	UNP G0RYN3
P	543	ASP	-	expression tag	UNP G0RYN3
P	544	ASP	-	expression tag	UNP G0RYN3
P	545	ASP	-	expression tag	UNP G0RYN3
P	546	ASP	-	expression tag	UNP G0RYN3
P	547	LYS	-	expression tag	UNP G0RYN3

- Molecule 12 is a protein called DUF1750-domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	319	Total	C	N	O	S	0	0
			2620	1679	466	465	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	763	ASP	-	expression tag	UNP G0SEZ9
Q	764	TYR	-	expression tag	UNP G0SEZ9
Q	765	LYS	-	expression tag	UNP G0SEZ9
Q	766	ASP	-	expression tag	UNP G0SEZ9
Q	767	ASP	-	expression tag	UNP G0SEZ9
Q	768	ASP	-	expression tag	UNP G0SEZ9
Q	769	ASP	-	expression tag	UNP G0SEZ9
Q	770	LYS	-	expression tag	UNP G0SEZ9

- Molecule 13 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	415	Total	C	N	O	S	0	0
			3307	2103	569	620	15		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	269	MET	-	initiating methionine	UNP G0S909
R	444	ILE	ASN	conflict	UNP G0S909
R	601	GLU	ASP	conflict	UNP G0S909
R	741	THR	SER	conflict	UNP G0S909

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1026	HIS	-	expression tag	UNP G0S909
R	1027	HIS	-	expression tag	UNP G0S909
R	1028	HIS	-	expression tag	UNP G0S909
R	1029	HIS	-	expression tag	UNP G0S909
R	1030	HIS	-	expression tag	UNP G0S909
R	1031	HIS	-	expression tag	UNP G0S909

- Molecule 14 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	411	Total	C	N	O	S	0	0
			3276	2066	583	615	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	6	ASP	ASN	conflict	UNP G0S475
S	272	ILE	THR	conflict	UNP G0S475
S	600	ASP	-	expression tag	UNP G0S475
S	601	TYR	-	expression tag	UNP G0S475
S	602	LYS	-	expression tag	UNP G0S475
S	603	ASP	-	expression tag	UNP G0S475
S	604	ASP	-	expression tag	UNP G0S475
S	605	ASP	-	expression tag	UNP G0S475
S	606	ASP	-	expression tag	UNP G0S475
S	607	LYS	-	expression tag	UNP G0S475

- Molecule 15 is a protein called Rsc7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	197	Total	C	N	O	S	0	0
			1585	997	286	296	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	527	ASP	-	expression tag	UNP G0S6N5
T	528	TYR	-	expression tag	UNP G0S6N5
T	529	LYS	-	expression tag	UNP G0S6N5
T	530	ASP	-	expression tag	UNP G0S6N5
T	531	ASP	-	expression tag	UNP G0S6N5
T	532	ASP	-	expression tag	UNP G0S6N5

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Chain	Residue	Modelled	Actual	Comment	Reference
T	533	ASP	-	expression tag	UNP G0S6N5
T	534	LYS	-	expression tag	UNP G0S6N5

- Molecule 16 is a protein called Rsc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	105	Total	C	N	O	S	0	0
			844	517	161	165	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	294	GLY	ASP	conflict	UNP G0SB54
U	300	ASP	ASN	conflict	UNP G0SB54
U	363	HIS	TYR	conflict	UNP G0SB54
U	984	ASP	-	expression tag	UNP G0SB54
U	985	TYR	-	expression tag	UNP G0SB54
U	986	LYS	-	expression tag	UNP G0SB54
U	987	ASP	-	expression tag	UNP G0SB54
U	988	ASP	-	expression tag	UNP G0SB54
U	989	ASP	-	expression tag	UNP G0SB54
U	990	ASP	-	expression tag	UNP G0SB54
U	991	LYS	-	expression tag	UNP G0SB54

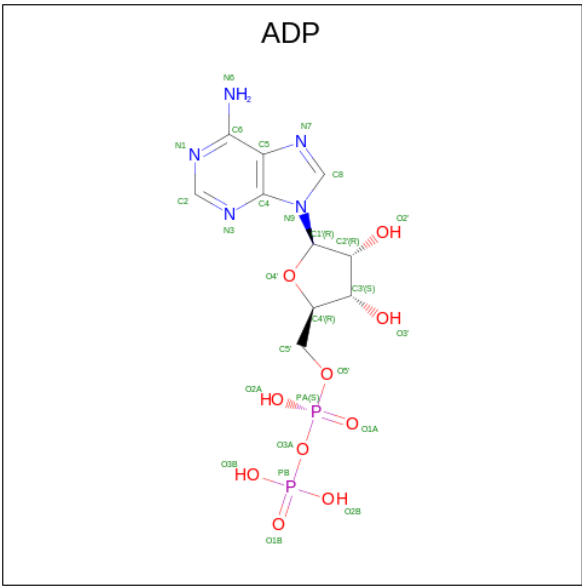
- Molecule 17 is a protein called Rsc58.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	143	Total	C	N	O	S	0	0
			1113	692	193	223	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	300	GLU	ASP	conflict	UNP G0S281
V	612	HIS	PRO	conflict	UNP G0S281
V	985	HIS	-	expression tag	UNP G0S281
V	986	HIS	-	expression tag	UNP G0S281
V	987	HIS	-	expression tag	UNP G0S281
V	988	HIS	-	expression tag	UNP G0S281
V	989	HIS	-	expression tag	UNP G0S281
V	990	HIS	-	expression tag	UNP G0S281

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

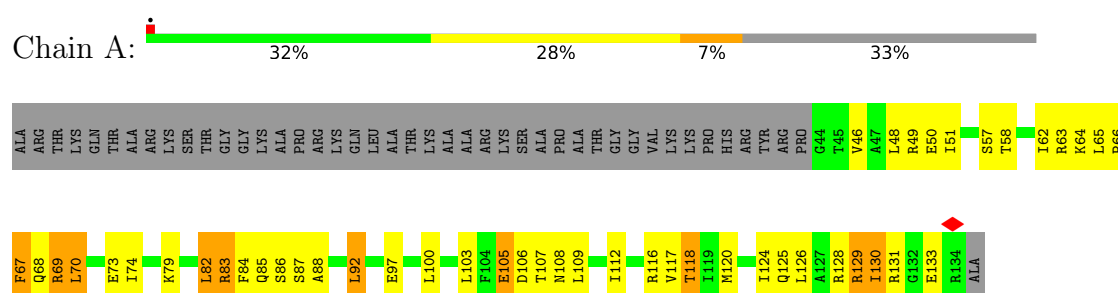


Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	C	N	O	P	0
			27	10	5	10	2	

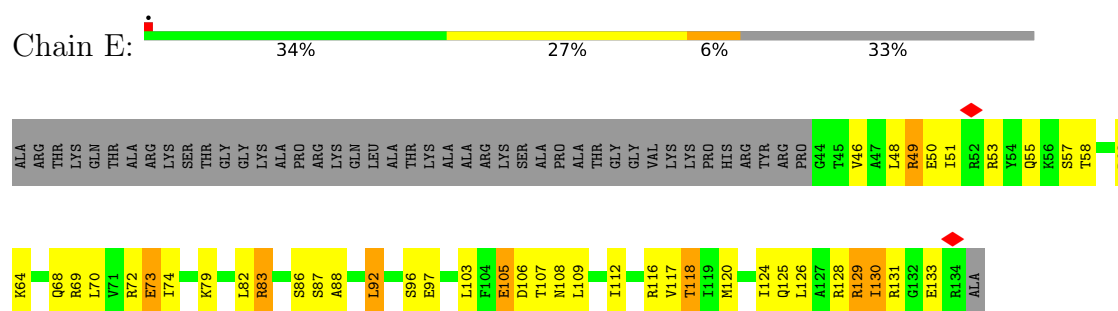
3 Residue-property plots [i](#)

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

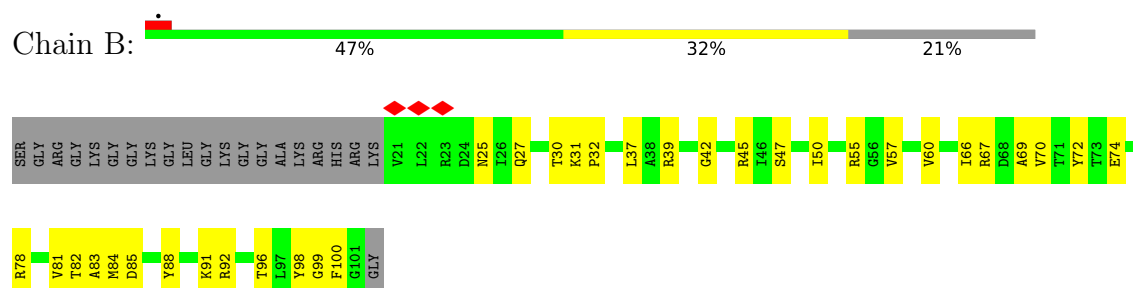
• Molecule 1: Histone H3



• Molecule 1: Histone H3



• Molecule 2: Histone H4



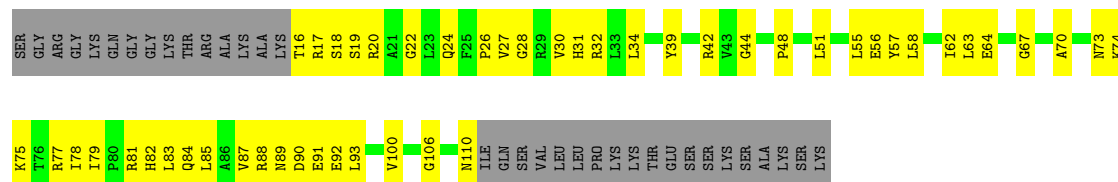
• Molecule 2: Histone H4





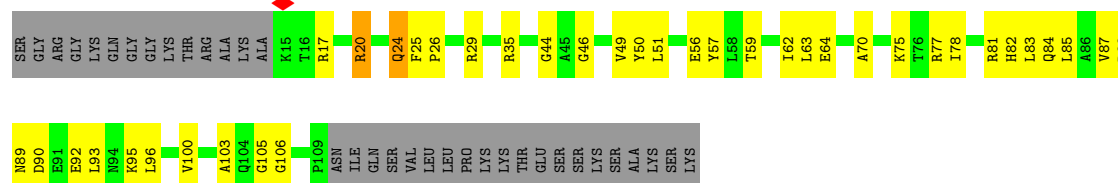
• Molecule 3: Histone H2A

Chain C: 36% 38% 26%



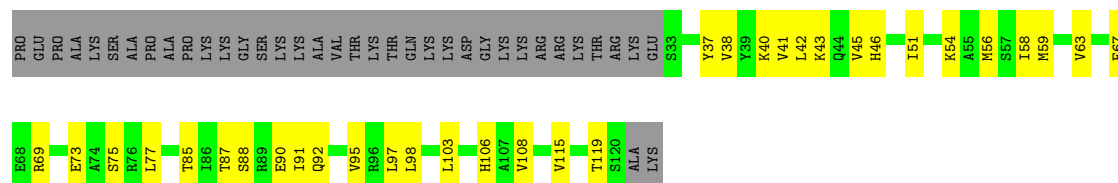
• Molecule 3: Histone H2A

Chain G: 43% 29% 26%



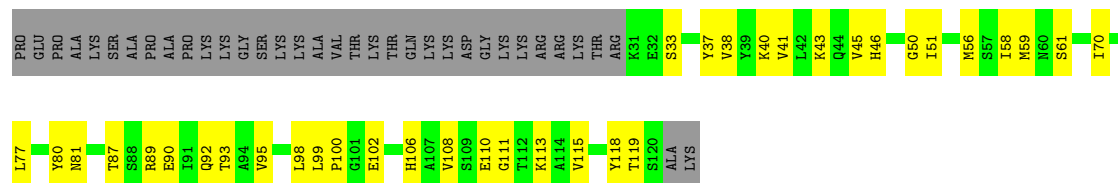
• Molecule 4: Histone H2B

Chain D: 44% 26% 30%



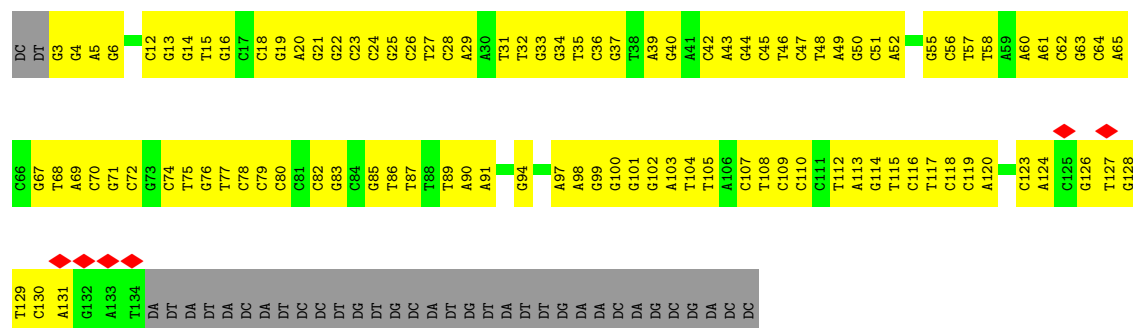
• Molecule 4: Histone H2B

Chain H: 43% 29% 28%

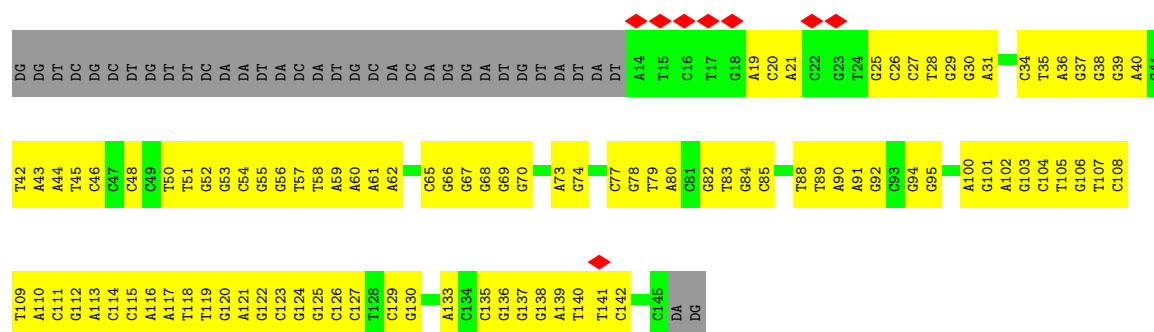


• Molecule 5: DNA (167-MER)

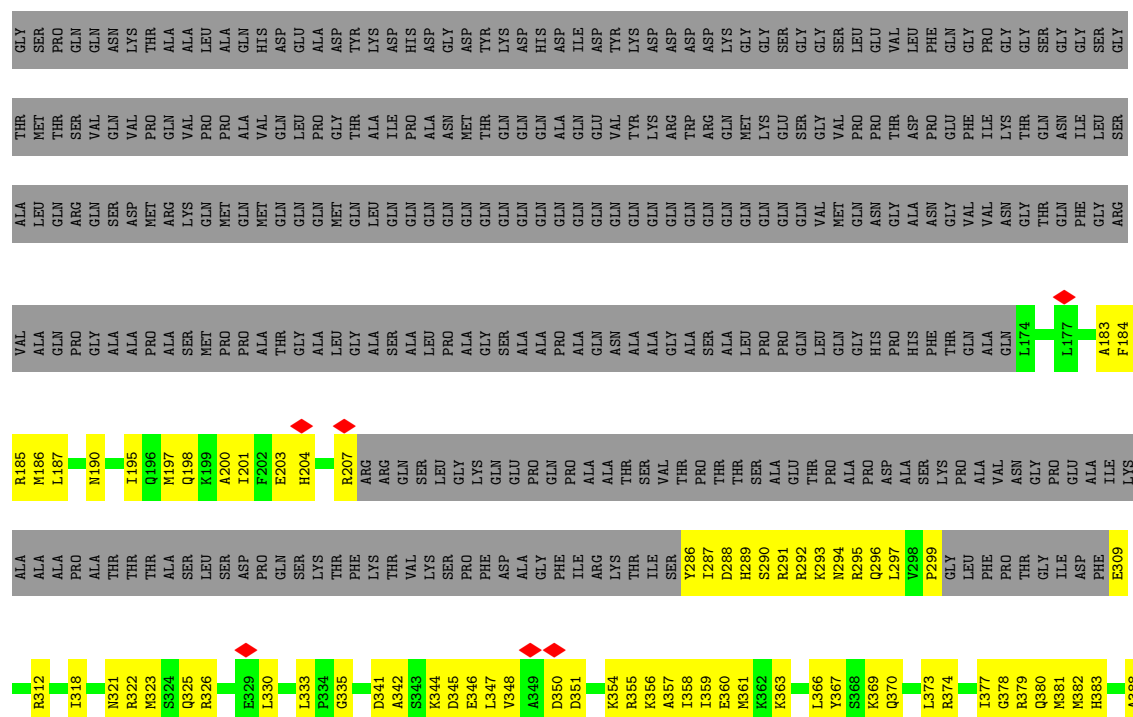
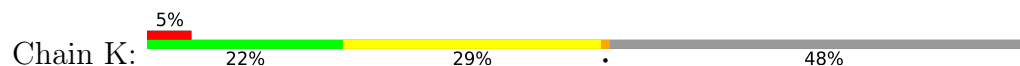
Chain I: 17% 62% 21%



• Molecule 6: DNA (167-MER)

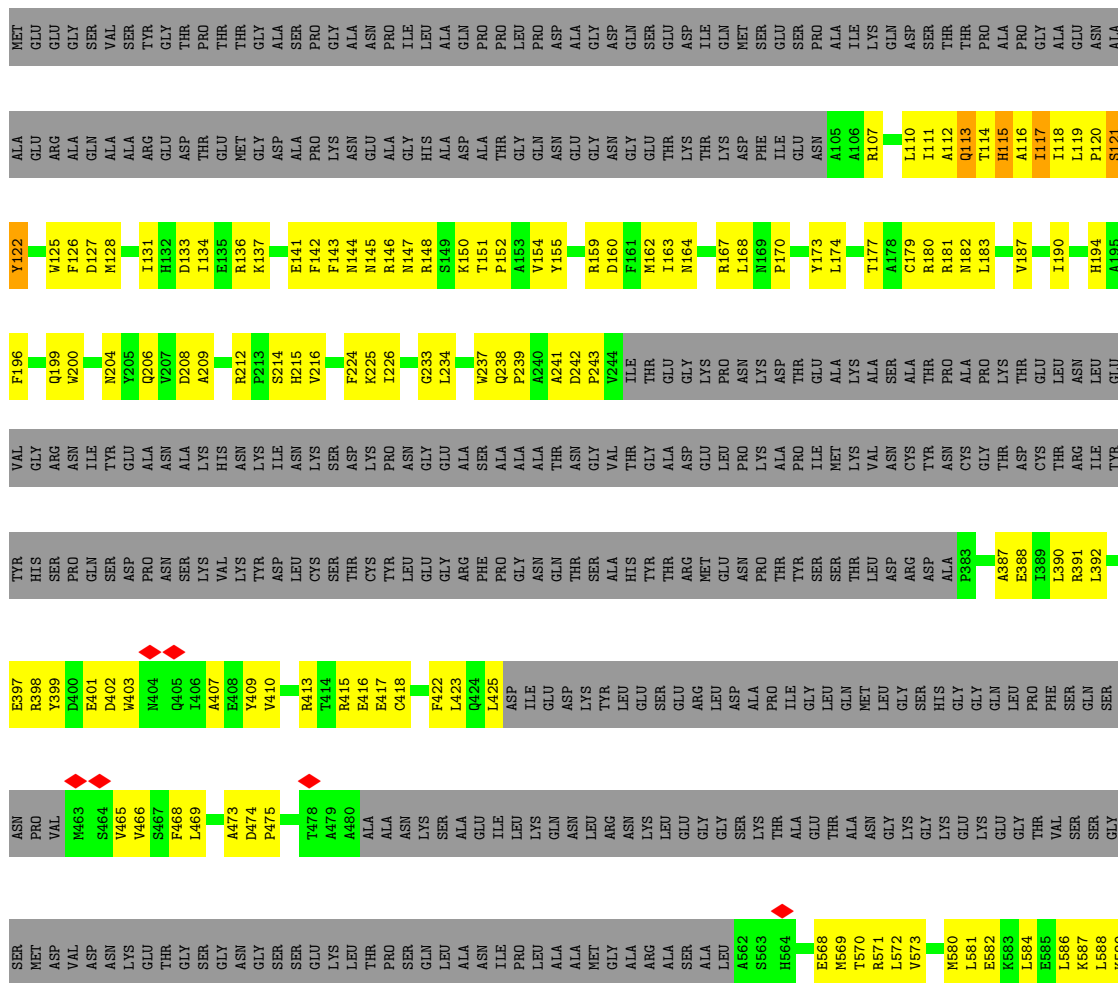


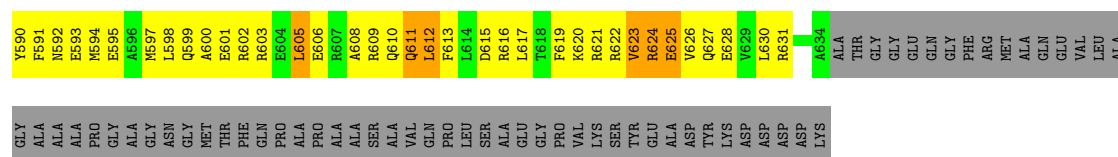
• Molecule 7: WD40 repeat-containing protein



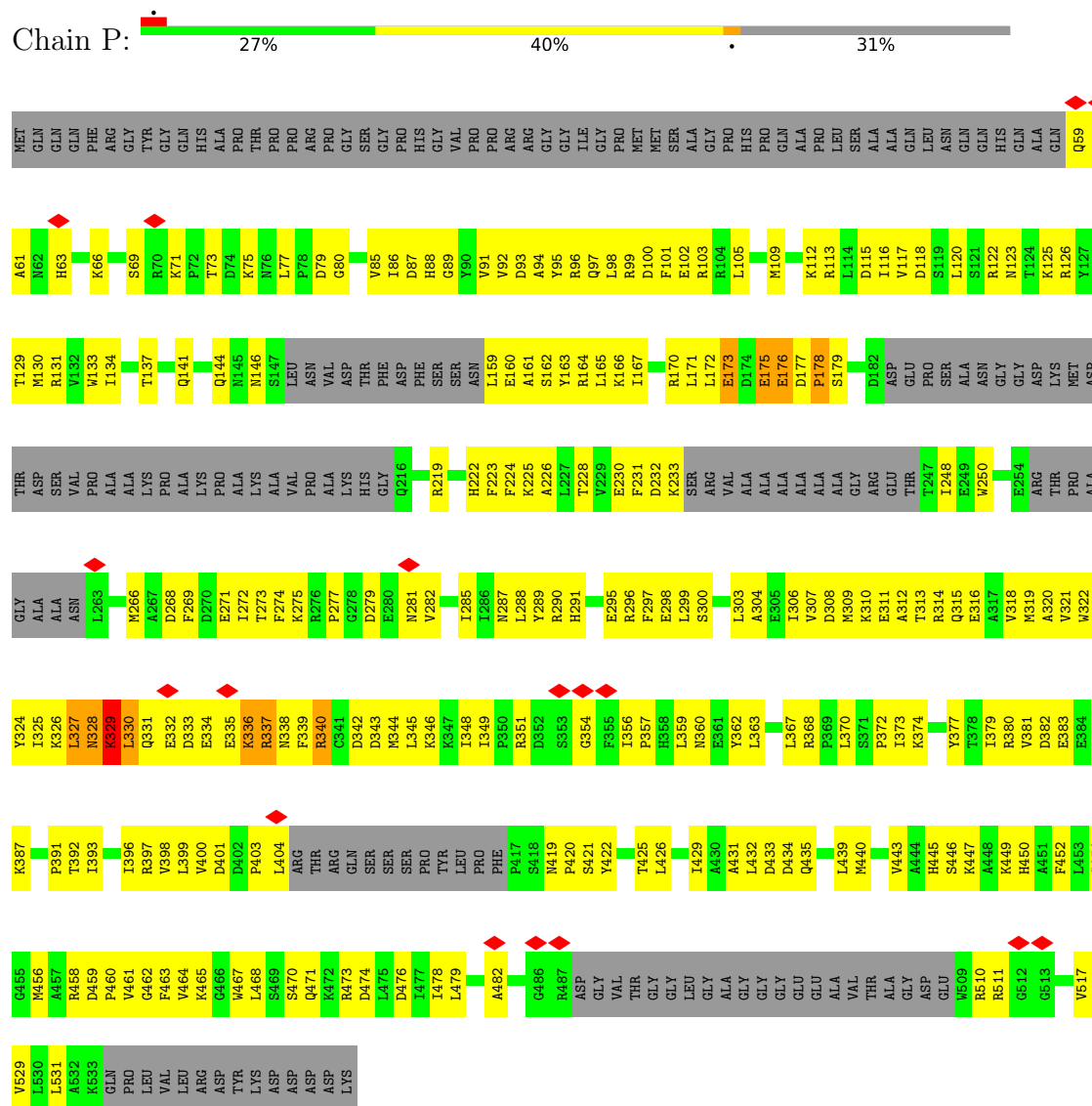


- Molecule 10: Ssr1

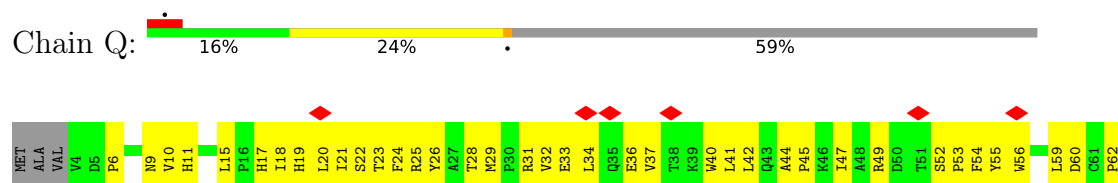


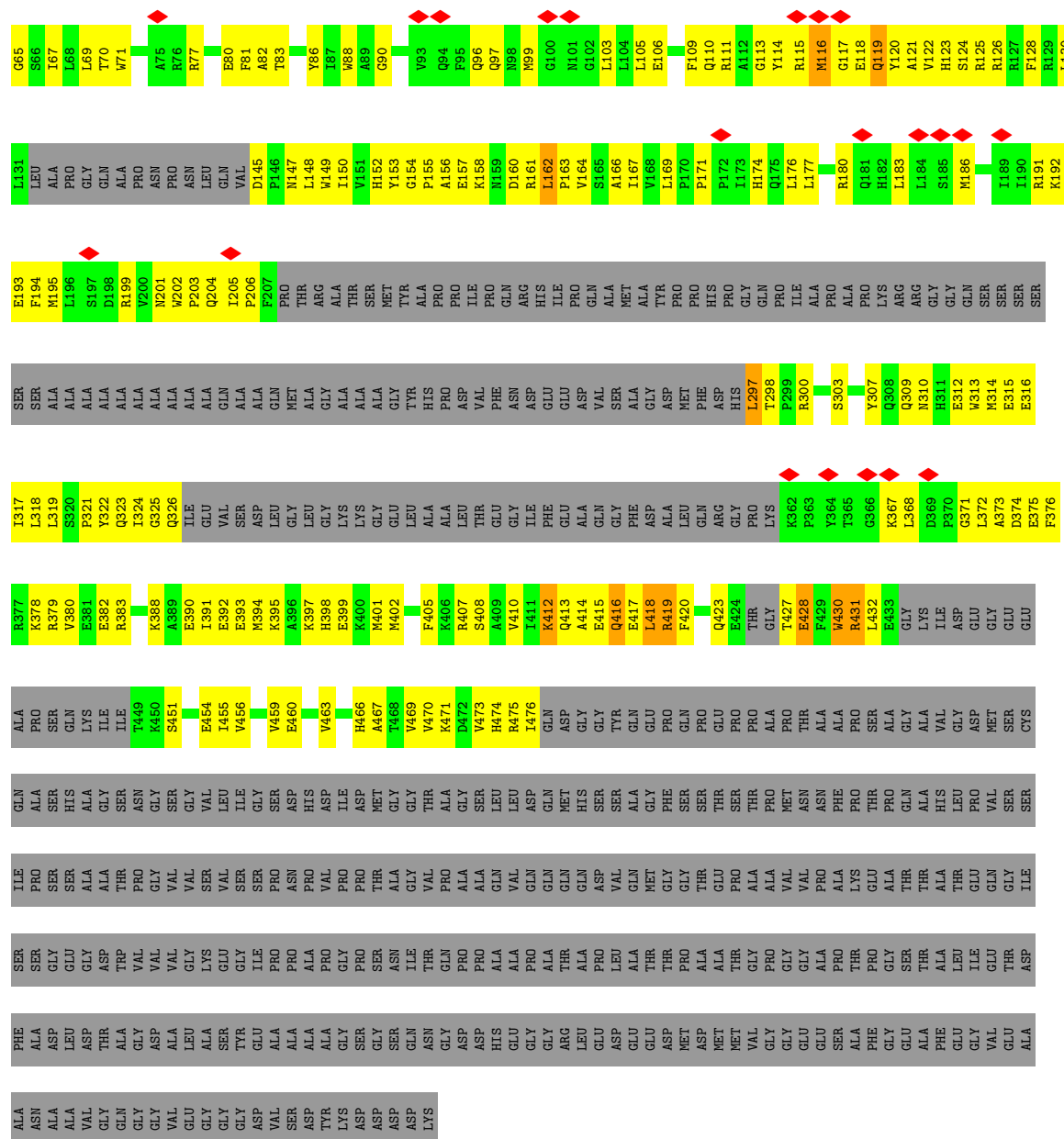


• Molecule 11: DM2 domain-containing protein



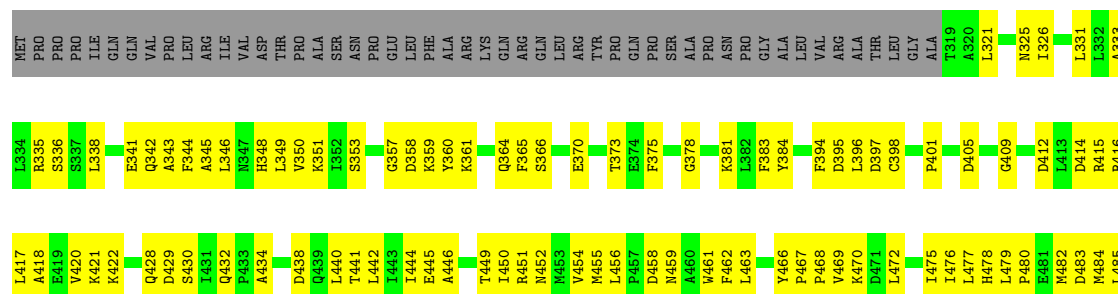
• Molecule 12: DUF1750-domain-containing protein

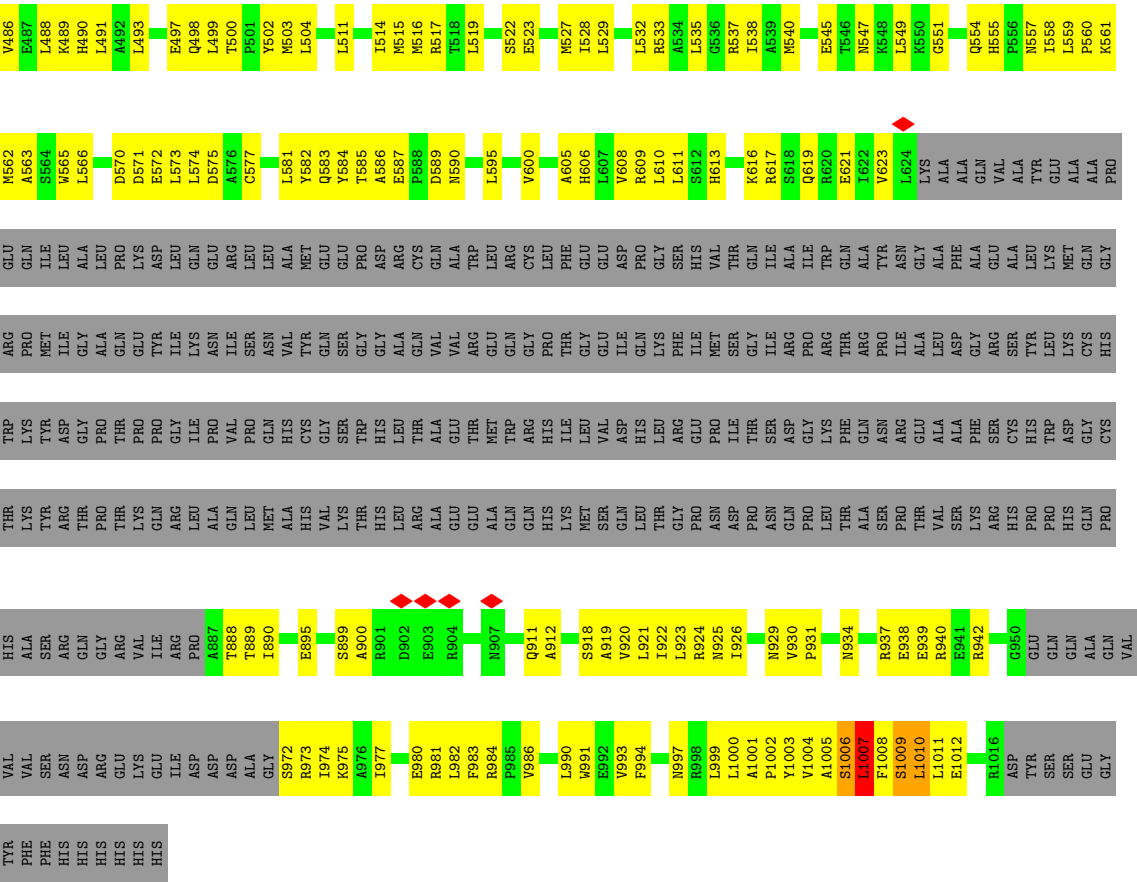




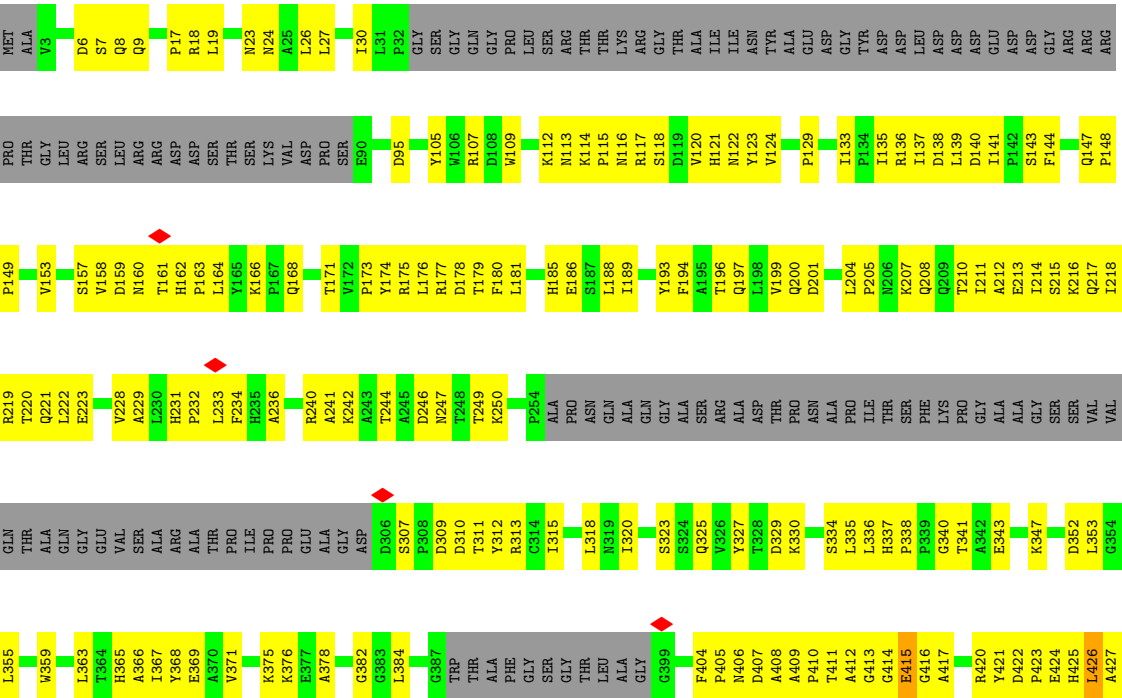
- Molecule 13: Putative chromatin structure-remodeling complex protein

Chain R: 25% 29% 46%





● Molecule 14: Putative chromatin structure-remodeling complex protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.472	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.47	0/752	0.92	4/1008 (0.4%)
1	E	0.42	0/752	0.75	2/1008 (0.2%)
2	B	0.37	0/655	0.58	0/878
2	F	0.38	0/621	0.59	0/832
3	C	0.32	0/742	0.56	0/1002
3	G	0.37	0/743	0.62	0/1002
4	D	0.34	0/696	0.44	0/939
4	H	0.33	0/714	0.48	0/962
5	I	0.35	0/3019	0.43	0/4654
6	J	0.36	0/3051	0.44	0/4710
7	K	0.25	0/6936	0.57	6/9302 (0.1%)
8	L	0.23	0/3418	0.51	0/4633
9	M	0.25	0/3459	0.48	1/4704 (0.0%)
10	N	0.33	0/3789	0.67	4/5135 (0.1%)
10	O	0.35	0/2292	0.70	3/3103 (0.1%)
11	P	0.32	0/3148	0.61	0/4244
12	Q	0.45	0/2683	0.69	0/3628
13	R	0.32	0/3369	0.56	0/4573
14	S	0.35	0/3363	0.61	2/4578 (0.0%)
15	T	0.33	0/1627	0.64	1/2214 (0.0%)
16	U	0.20	0/851	0.56	0/1140
17	V	0.29	0/1126	0.62	0/1515
All	All	0.33	0/47806	0.58	23/65764 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1016	ILE	N-CA-C	-10.25	94.88	109.63
7	K	620	ILE	N-CA-C	10.00	120.82	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	618	GLN	N-CA-C	-7.38	103.38	112.38
14	S	455	ARG	N-CA-C	6.35	119.02	111.33
10	N	427	ILE	N-CA-C	-6.19	107.26	113.20
7	K	620	ILE	N-CA-CB	-6.14	102.19	110.54
1	A	130	ILE	CA-C-N	-5.86	110.66	122.55
1	A	130	ILE	C-N-CA	-5.86	110.66	122.55
1	E	130	ILE	CA-C-N	-5.85	110.68	122.55
1	E	130	ILE	C-N-CA	-5.85	110.68	122.55
10	O	625	GLU	N-CA-C	5.80	118.35	111.33
10	O	623	VAL	N-CA-C	-5.38	105.29	110.72
7	K	1012	ARG	N-CA-C	-5.37	105.43	111.28
9	M	243	VAL	CA-C-O	-5.34	117.98	122.63
10	O	113	GLN	N-CA-C	-5.28	105.94	112.38
1	A	67	PHE	N-CA-C	-5.19	105.70	111.36
10	N	417	GLU	N-CA-C	-5.15	105.16	111.75
15	T	491	GLU	N-CA-CB	5.09	117.69	110.16
10	N	416	GLU	N-CA-C	-5.06	106.24	112.72
1	A	69	ARG	N-CA-C	5.03	116.77	111.28
7	K	1009	ALA	N-CA-C	-5.02	105.81	111.28
10	N	614	LEU	N-CA-C	-5.02	105.82	112.34
14	S	453	ILE	N-CA-C	-5.01	105.65	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	744	0	784	49	0
1	E	744	0	784	43	0
2	B	648	0	693	32	0
2	F	614	0	656	42	0
3	C	733	0	771	51	0
3	G	734	0	778	46	0
4	D	685	0	703	33	0
4	H	703	0	722	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2694	0	1480	117	0
6	J	2718	0	1480	134	0
7	K	6825	0	6974	499	0
8	L	3340	0	3316	252	0
9	M	3371	0	3303	228	0
10	N	3714	0	3619	391	0
10	O	2245	0	2217	225	0
11	P	3089	0	3054	288	0
12	Q	2620	0	2607	232	0
13	R	3307	0	3325	226	0
14	S	3276	0	3189	216	0
15	T	1585	0	1542	125	0
16	U	844	0	836	48	0
17	V	1113	0	1081	98	0
18	K	27	0	12	7	0
All	All	46373	0	43926	2974	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 34.

All (2974) 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)
7:K:1018:GLN:NE2	7:K:1020:ASN:HD22	1.31	1.24
10:N:320:CYS:SG	10:N:348:CYS:CB	2.29	1.21
7:K:1018:GLN:HE21	7:K:1020:ASN:ND2	1.41	1.17
10:N:320:CYS:SG	10:N:348:CYS:HB2	1.84	1.17
11:P:426:LEU:HD21	17:V:360:LEU:CB	1.76	1.15
8:L:248:TYR:HB2	8:L:547:ASN:OD1	1.48	1.14
11:P:426:LEU:CD2	17:V:360:LEU:HB3	1.83	1.09
10:N:257:LYS:HD2	10:O:117:ILE:HD11	1.11	1.06
7:K:374:ARG:HH22	10:N:423:LEU:HA	1.20	1.04
8:L:42:ARG:CG	8:L:90:TYR:HE1	1.71	1.03
10:N:569:MET:SD	11:P:447:LYS:HD3	1.99	1.03
7:K:1018:GLN:NE2	7:K:1020:ASN:ND2	2.03	1.02
11:P:281:ASN:HA	11:P:379:ILE:O	1.60	1.01
10:N:320:CYS:SG	10:N:348:CYS:N	2.34	1.00
10:N:367:THR:HG22	10:N:369:MET:SD	2.01	1.00
12:Q:41:LEU:HD13	12:Q:130:LEU:HB2	1.45	0.99
8:L:42:ARG:HG2	8:L:90:TYR:CE1	1.97	0.99
10:N:188:CYS:HA	10:N:191:MET:HE2	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:419:VAL:HG21	11:P:531:LEU:HD21	1.46	0.97
10:O:612:LEU:HB3	10:O:616:ARG:HH22	1.25	0.96
11:P:426:LEU:HD21	17:V:360:LEU:HB3	1.39	0.94
10:N:257:LYS:CD	10:O:117:ILE:HD11	1.97	0.94
3:C:42:ARG:HD3	4:D:85:THR:HG22	1.46	0.94
13:R:990:LEU:HB3	13:R:1008:PHE:HE1	1.30	0.94
9:M:245:VAL:HG11	9:M:283:GLU:HA	1.49	0.94
10:O:115:HIS:HB3	10:O:117:ILE:HG22	1.49	0.93
8:L:242:ILE:HD11	8:L:353:PHE:HE1	1.33	0.92
11:P:131:ARG:HG3	11:P:172:LEU:HD11	1.49	0.92
7:K:342:ALA:H	7:K:347:LEU:HD11	1.32	0.92
8:L:42:ARG:CG	8:L:90:TYR:CE1	2.51	0.92
10:N:254:THR:HG22	10:O:117:ILE:HD13	1.50	0.91
1:E:107:THR:HG21	1:E:124:ILE:HD13	1.50	0.91
8:L:256:MET:HE1	8:L:547:ASN:HD21	1.35	0.91
11:P:426:LEU:HD21	17:V:360:LEU:HB2	1.48	0.90
1:A:107:THR:HG21	1:A:124:ILE:HD13	1.50	0.90
9:M:446:HIS:HA	9:M:449:TRP:CD1	2.06	0.90
10:N:103:GLU:HB2	10:N:107:ARG:HH12	1.34	0.90
12:Q:418:LEU:C	12:Q:420:PHE:H	1.78	0.90
8:L:42:ARG:HG2	8:L:90:TYR:HE1	1.35	0.90
7:K:635:PRO:HB2	7:K:706:PHE:H	1.37	0.89
3:C:39:TYR:HB3	4:D:75:SER:OG	1.72	0.89
17:V:325:ALA:H	17:V:362:ARG:HH12	1.20	0.89
10:O:612:LEU:HB3	10:O:616:ARG:NH2	1.88	0.89
10:N:569:MET:HE1	11:P:447:LYS:HA	1.53	0.89
10:N:232:ARG:HH21	15:T:441:TYR:HB2	1.37	0.88
17:V:391:ARG:HG2	17:V:392:ILE:HD12	1.55	0.88
10:N:580:MET:HE2	11:P:98:LEU:HB3	1.54	0.88
7:K:876:ASN:HD21	7:K:931:ILE:HD13	1.40	0.87
8:L:348:ARG:HH11	8:L:351:ASN:HD21	1.22	0.87
10:N:572:LEU:HD13	11:P:443:VAL:HG22	1.56	0.87
11:P:461:VAL:HA	11:P:465:LYS:HZ3	1.39	0.87
2:F:92:ARG:HH21	4:H:98:LEU:HD13	1.40	0.86
7:K:929:THR:HA	7:K:932:MET:HE2	1.58	0.85
12:Q:28:THR:HG23	12:Q:65:GLY:HA3	1.58	0.85
11:P:356:ILE:HA	11:P:359:LEU:HG	1.58	0.85
10:N:320:CYS:SG	10:N:348:CYS:HB3	2.15	0.84
12:Q:164:VAL:HA	12:Q:167:ILE:HD12	1.59	0.84
10:N:621:ARG:HA	10:N:624:ARG:HE	1.41	0.84
11:P:426:LEU:CD2	17:V:360:LEU:CB	2.47	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:117:ILE:CG2	10:O:170:PRO:HG2	2.07	0.84
13:R:480:PRO:HG2	13:R:482:MET:HE1	1.59	0.84
12:Q:37:VAL:HA	12:Q:40:TRP:HE3	1.40	0.83
12:Q:114:TYR:HB3	12:Q:121:ALA:HA	1.58	0.83
8:L:61:ARG:HE	8:L:62:LYS:H	1.24	0.83
8:L:248:TYR:CB	8:L:547:ASN:OD1	2.26	0.83
17:V:527:LEU:HD13	17:V:530:ILE:HD12	1.59	0.83
12:Q:9:ASN:HB3	12:Q:204:GLN:HA	1.58	0.83
12:Q:123:HIS:CE1	12:Q:153:TYR:HB3	2.14	0.83
10:N:243:PRO:HB2	10:O:119:LEU:HD12	1.59	0.82
7:K:616:THR:O	7:K:619:THR:HB	1.80	0.82
8:L:526:PRO:HA	8:L:529:TRP:HE3	1.43	0.82
7:K:662:VAL:HG11	7:K:686:LEU:HD12	1.61	0.82
11:P:306:ILE:HG23	11:P:307:VAL:HG13	1.62	0.81
15:T:411:PHE:CZ	15:T:426:ASP:HB2	2.15	0.81
10:N:274:ARG:HH12	15:T:412:PRO:HD2	1.45	0.81
2:F:29:ILE:HD12	2:F:34:ILE:HD11	1.62	0.81
10:O:151:THR:HG22	10:O:154:VAL:HG23	1.62	0.81
9:M:148:MET:HE3	9:M:177:LEU:HD13	1.62	0.81
15:T:411:PHE:HZ	15:T:426:ASP:HB2	1.46	0.81
11:P:226:ALA:HB3	11:P:289:TYR:HB2	1.62	0.81
7:K:374:ARG:NH2	10:N:423:LEU:HA	1.96	0.80
8:L:242:ILE:HD11	8:L:353:PHE:CE1	2.15	0.80
10:O:118:ILE:HD11	10:O:167:ARG:HD3	1.64	0.80
13:R:563:ALA:HA	13:R:566:LEU:HD23	1.63	0.80
15:T:515:ASP:HB3	15:T:518:ILE:HD13	1.64	0.80
8:L:198:PRO:HG3	8:L:210:ILE:HG12	1.62	0.80
9:M:25:VAL:HG21	9:M:437:SER:HA	1.64	0.80
10:N:569:MET:CE	11:P:447:LYS:HA	2.12	0.80
14:S:30:ILE:HB	14:S:173:PRO:HB2	1.64	0.80
11:P:115:ASP:HA	13:R:609:ARG:HH12	1.47	0.79
1:A:130:ILE:HD11	1:E:109:LEU:HD11	1.62	0.79
10:O:613:PHE:HZ	11:P:320:ALA:HA	1.47	0.79
10:N:228:VAL:HG23	15:T:429:LEU:HD23	1.63	0.79
7:K:697:ARG:HH11	7:K:730:TYR:HB3	1.46	0.79
8:L:719:ARG:NH1	8:L:720:SER:OG	2.15	0.79
7:K:896:ASP:HB2	7:K:899:TRP:HE1	1.48	0.79
8:L:345:ASN:HD22	8:L:542:ARG:HH12	1.31	0.79
14:S:572:ASN:OD1	14:S:573:ASN:N	2.14	0.79
7:K:994:VAL:HG21	7:K:1013:ALA:HB2	1.64	0.79
9:M:44:LYS:HE3	9:M:101:LEU:HD13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:225:LYS:HE3	10:N:227:ILE:HD11	1.66	0.78
10:N:609:ARG:HD3	12:Q:412:LYS:HD3	1.64	0.78
8:L:18:PRO:HD2	8:L:126:MET:HB3	1.65	0.78
7:K:811:ARG:HH12	7:K:1057:PHE:HB2	1.49	0.78
10:N:362:THR:HG22	10:N:365:HIS:HB2	1.65	0.78
7:K:835:LEU:HD11	7:K:901:THR:HG23	1.66	0.77
14:S:408:ALA:HA	14:S:420:ARG:HG2	1.66	0.77
10:N:609:ARG:O	10:N:612:LEU:HB3	1.84	0.77
10:N:613:PHE:CZ	10:N:661:MET:HE1	2.20	0.77
7:K:456:LYS:HE3	8:L:692:LEU:HD11	1.65	0.77
8:L:43:MET:HG2	8:L:55:PRO:HA	1.66	0.77
9:M:148:MET:HE2	9:M:175:PHE:HZ	1.47	0.77
9:M:310:GLU:HG3	9:M:333:GLU:HG3	1.67	0.77
8:L:712:GLU:HG2	8:L:713:LEU:HG	1.67	0.77
10:N:380:ARG:HE	10:N:381:ASP:H	1.31	0.77
3:C:31:HIS:HD2	3:C:48:PRO:HG3	1.50	0.76
10:N:320:CYS:SG	10:N:348:CYS:CA	2.73	0.76
1:A:118:THR:HG23	2:B:45:ARG:HG3	1.65	0.76
7:K:940:ARG:HH22	7:K:945:HIS:HA	1.49	0.76
9:M:183:LEU:HD21	9:M:439:LEU:HD22	1.68	0.76
12:Q:145:ASP:HB3	12:Q:148:LEU:HB2	1.67	0.76
10:N:103:GLU:HB2	10:N:107:ARG:NH1	2.00	0.76
10:O:199:GLN:HG3	10:O:200:TRP:HD1	1.50	0.76
14:S:458:ARG:HG2	14:S:462:ARG:NE	2.01	0.76
7:K:330:LEU:HD13	7:K:356:LYS:HZ3	1.51	0.76
8:L:171:THR:HB	8:L:532:ILE:HA	1.66	0.76
9:M:240:ASP:HA	9:M:241:PRO:C	2.09	0.76
15:T:443:VAL:HG13	15:T:445:PHE:HD1	1.48	0.76
7:K:393:ARG:HH21	13:R:441:THR:HG23	1.50	0.76
7:K:615:LYS:HZ1	7:K:739:LEU:HG	1.51	0.76
10:O:118:ILE:HG22	10:O:120:PRO:HD3	1.68	0.76
8:L:52:LYS:HE3	8:L:54:ARG:HE	1.51	0.76
10:O:113:GLN:HB3	10:O:168:LEU:HD11	1.67	0.76
7:K:634:GLY:HA2	7:K:684:GLN:HA	1.69	0.75
10:O:588:LEU:HD21	11:P:105:LEU:HD12	1.68	0.75
13:R:582:TYR:HE1	13:R:921:LEU:HB3	1.50	0.75
3:C:63:LEU:HD12	4:D:42:LEU:HD13	1.67	0.75
7:K:736:ARG:HH22	7:K:760:PRO:HD3	1.52	0.75
10:O:603:ARG:HH12	13:R:981:ARG:HA	1.49	0.75
6:J:52:DG:H2'	6:J:53:DG:C8	2.22	0.75
8:L:42:ARG:CD	8:L:90:TYR:HE1	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1026:ARG:NH1	7:K:1027:LEU:O	2.19	0.75
10:N:621:ARG:HB3	10:N:624:ARG:HH21	1.52	0.75
7:K:333:LEU:HD11	7:K:356:LYS:HZ1	1.50	0.75
7:K:607:LEU:HG	7:K:737:LEU:HD11	1.66	0.75
8:L:246:LEU:HD11	8:L:497:PHE:HB3	1.69	0.75
11:P:77:LEU:HG	11:P:99:ARG:HH22	1.50	0.75
7:K:620:ILE:H	7:K:620:ILE:HD12	1.49	0.75
12:Q:20:LEU:HD23	12:Q:71:TRP:HB3	1.68	0.74
12:Q:126:ARG:HG2	12:Q:126:ARG:HH11	1.52	0.74
7:K:309:GLU:O	7:K:312:ARG:NH1	2.20	0.74
8:L:126:MET:HE3	8:L:127:ALA:H	1.51	0.74
8:L:192:SER:OG	8:L:194:LYS:NZ	2.20	0.74
7:K:989:GLN:HE22	7:K:1015:ARG:HG3	1.52	0.74
8:L:537:ASN:OD1	8:L:538:GLY:N	2.21	0.74
15:T:470:VAL:HG11	15:T:486:PHE:HZ	1.51	0.74
10:O:148:ARG:HH22	14:S:415:GLU:C	1.94	0.74
9:M:148:MET:HE2	9:M:175:PHE:CZ	2.22	0.74
13:R:429:ASP:HA	13:R:484:MET:HE1	1.70	0.74
14:S:19:LEU:HD22	14:S:24:ASN:HD22	1.51	0.74
9:M:86:TRP:HE1	9:M:165:VAL:HG21	1.53	0.74
12:Q:418:LEU:C	12:Q:420:PHE:N	2.40	0.74
14:S:546:ARG:HB2	14:S:551:ARG:HH11	1.52	0.74
14:S:573:ASN:OD1	14:S:574:CYS:N	2.21	0.74
10:N:569:MET:HE1	11:P:447:LYS:CA	2.17	0.74
8:L:259:PRO:HG2	8:L:347:LYS:HG2	1.69	0.74
9:M:311:ASP:HA	9:M:314:LYS:HD2	1.70	0.74
9:M:340:GLU:O	9:M:344:ASP:N	2.20	0.74
8:L:169:ASN:HD22	8:L:527:ALA:HB1	1.52	0.74
12:Q:319:LEU:O	12:Q:323:GLN:NE2	2.20	0.74
9:M:390:VAL:O	9:M:391:THR:HG23	1.87	0.73
17:V:517:MET:HA	17:V:520:TYR:HD2	1.51	0.73
10:N:257:LYS:HZ3	10:O:117:ILE:HG12	1.52	0.73
12:Q:416:GLN:HA	12:Q:419:ARG:HD2	1.69	0.73
7:K:299:PRO:HD3	17:V:394:ARG:HH22	1.53	0.73
7:K:440:ARG:HA	7:K:443:VAL:HG22	1.71	0.73
16:U:856:ILE:HB	16:U:857:PRO:HD3	1.70	0.73
7:K:744:LEU:O	7:K:1004:HIS:NE2	2.21	0.73
7:K:839:LEU:HA	7:K:842:GLN:HG3	1.71	0.73
9:M:257:VAL:HB	9:M:261:ALA:HB3	1.71	0.73
10:O:586:LEU:HA	10:O:589:LYS:HZ3	1.54	0.72
7:K:613:LEU:HD11	7:K:813:LYS:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:254:ASP:O	8:L:502:ARG:NH2	2.22	0.72
9:M:322:GLU:HA	9:M:328:ASN:HA	1.70	0.72
12:Q:45:PRO:HB2	12:Q:49:ARG:HH21	1.54	0.72
8:L:356:GLU:OE2	8:L:487:ARG:NE	2.22	0.72
8:L:506:ASP:HB3	8:L:507:ARG:HH21	1.55	0.72
10:N:602:ARG:HH12	10:O:597:MET:HE1	1.54	0.72
12:Q:195:MET:H	12:Q:201:ASN:HD21	1.37	0.72
11:P:383:GLU:HG2	11:P:387:LYS:HE3	1.71	0.72
14:S:107:ARG:HB2	14:S:109:TRP:HD1	1.55	0.72
10:N:583:LYS:HZ2	11:P:429:ILE:HA	1.55	0.72
12:Q:309:GLN:NE2	12:Q:312:GLU:OE2	2.21	0.72
11:P:473:ARG:HD2	13:R:434:ALA:HA	1.71	0.72
7:K:838:ARG:NH2	7:K:1144:HIS:O	2.21	0.72
11:P:300:SER:HB2	11:P:368:ARG:CZ	2.19	0.72
7:K:977:LEU:HD22	7:K:982:GLY:HA3	1.70	0.72
7:K:434:GLN:CD	9:M:442:LEU:HB2	2.15	0.72
8:L:362:GLU:HG2	8:L:481:ARG:HG2	1.70	0.72
8:L:223:LEU:HD22	8:L:495:GLU:HG3	1.71	0.71
8:L:17:CYS:HB3	8:L:675:MET:HE1	1.73	0.71
8:L:353:PHE:O	8:L:489:ASP:HA	1.90	0.71
9:M:72:GLU:OE1	9:M:74:ARG:NH2	2.21	0.71
15:T:346:TRP:HE3	15:T:350:HIS:CE1	2.08	0.71
14:S:18:ARG:NH1	15:T:375:ILE:O	2.23	0.71
7:K:287:ILE:HD12	12:Q:375:GLU:HB2	1.72	0.71
10:O:582:GLU:HB3	12:Q:391:ILE:HG21	1.72	0.71
8:L:255:LEU:O	8:L:256:MET:HE2	1.90	0.71
7:K:370:GLN:O	7:K:374:ARG:HG2	1.91	0.71
8:L:230:ASN:H	8:L:233:MET:HE2	1.54	0.71
9:M:102:GLN:HB2	9:M:105:ARG:HE	1.54	0.71
10:N:583:LYS:NZ	11:P:432:LEU:HB3	2.05	0.71
9:M:233:ARG:HH12	9:M:245:VAL:H	1.35	0.71
10:N:105:ALA:O	10:N:109:HIS:ND1	2.20	0.71
14:S:141:ILE:HB	14:S:174:TYR:HB2	1.71	0.71
8:L:141:ARG:HE	8:L:715:PRO:HG3	1.53	0.71
10:O:413:ARG:HB3	10:O:417:GLU:HB2	1.73	0.71
7:K:776:PRO:HB3	7:K:788:LEU:HD22	1.73	0.70
9:M:264:ASP:O	9:M:266:ARG:NH1	2.24	0.70
7:K:637:LEU:O	7:K:709:ILE:N	2.22	0.70
10:N:583:LYS:HZ3	11:P:432:LEU:HB3	1.56	0.70
7:K:524:SER:HB2	7:K:528:GLN:HE22	1.55	0.70
7:K:939:LEU:HD23	7:K:946:TYR:HD1	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:220:LEU:HD22	8:L:234:ALA:HA	1.72	0.70
8:L:358:LEU:HB3	8:L:483:THR:HB	1.73	0.70
14:S:133:ILE:HD11	14:S:222:LEU:HD13	1.73	0.70
1:E:68:GLN:HE22	1:E:72:ARG:NE	1.88	0.70
8:L:21:GLN:OE1	8:L:537:ASN:ND2	2.20	0.70
10:O:126:PHE:CE1	10:O:159:ARG:NH2	2.57	0.70
11:P:300:SER:O	11:P:304:ALA:N	2.24	0.70
13:R:582:TYR:CE1	13:R:921:LEU:HB3	2.25	0.70
8:L:256:MET:CE	8:L:547:ASN:HD21	2.04	0.70
13:R:504:LEU:HD11	13:R:545:GLU:HG3	1.74	0.70
11:P:130:MET:HA	11:P:172:LEU:HG	1.74	0.70
17:V:480:ARG:HA	17:V:483:ASN:HD22	1.57	0.70
9:M:235:MET:HE1	9:M:334:GLN:HG2	1.73	0.70
7:K:424:ARG:HD2	7:K:427:LYS:HZ1	1.57	0.70
10:O:117:ILE:O	10:O:118:ILE:HD13	1.91	0.70
10:O:624:ARG:O	10:O:627:GLN:HG3	1.91	0.70
13:R:412:ASP:HB2	13:R:415:ARG:HB2	1.72	0.70
14:S:199:VAL:HG23	14:S:204:LEU:HB2	1.73	0.70
5:I:103:DA:H2'	5:I:104:DT:H6	1.56	0.70
10:N:609:ARG:NE	10:N:609:ARG:HA	2.07	0.70
10:N:610:GLN:O	10:N:611:GLN:C	2.35	0.70
13:R:565:TRP:HE1	17:V:370:PRO:HD3	1.55	0.70
7:K:299:PRO:HB3	17:V:395:ARG:HH22	1.56	0.69
8:L:128:SER:HB3	8:L:131:TRP:CD1	2.26	0.69
10:N:348:CYS:SG	10:N:349:SER:N	2.65	0.69
9:M:253:ASN:OD1	9:M:254:LYS:N	2.25	0.69
3:C:32:ARG:HH12	6:J:29:DG:H3'	1.56	0.69
12:Q:183:LEU:HA	12:Q:186:MET:HE1	1.74	0.69
12:Q:324:ILE:HG22	12:Q:326:GLN:H	1.55	0.69
7:K:989:GLN:HE21	7:K:1017:GLY:HA3	1.57	0.69
9:M:147:LEU:HD13	9:M:440:ALA:HB2	1.75	0.69
15:T:459:ASP:HB3	15:T:462:ALA:HB2	1.73	0.69
10:N:384:TRP:HB3	10:N:388:GLU:HG3	1.75	0.69
11:P:126:ARG:NH1	11:P:401:ASP:O	2.20	0.69
13:R:973:ARG:HE	13:R:974:ILE:HG13	1.58	0.69
8:L:547:ASN:HA	8:L:550:GLN:OE1	1.93	0.69
10:N:128:MET:HE1	10:N:163:ILE:HG21	1.74	0.69
1:A:85:GLN:CD	2:B:82:THR:HA	2.17	0.69
7:K:652:PHE:O	7:K:656:ALA:N	2.22	0.69
10:N:566:GLU:HA	10:N:569:MET:HB2	1.75	0.69
10:N:678:GLU:HG2	11:P:272:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:128:LYS:HG2	11:P:129:THR:H	1.57	0.69
12:Q:158:LYS:HA	12:Q:161:ARG:HD2	1.74	0.69
14:S:148:PRO:HA	14:S:168:GLN:HE22	1.57	0.69
14:S:310:ASP:O	14:S:313:ARG:NH1	2.26	0.69
12:Q:114:TYR:HE1	12:Q:167:ILE:HG21	1.58	0.69
14:S:448:ASP:O	14:S:452:GLN:NE2	2.26	0.69
7:K:713:GLY:HA3	7:K:738:ILE:HG23	1.75	0.69
11:P:177:ASP:C	11:P:179:SER:N	2.50	0.69
10:N:188:CYS:HA	10:N:191:MET:CE	2.21	0.68
1:E:63:ARG:NH2	5:I:60:DA:O3'	2.26	0.68
9:M:393:SER:O	9:M:429:ARG:NH2	2.26	0.68
10:O:415:ARG:HH21	17:V:531:ILE:HG12	1.58	0.68
10:O:606:GLU:O	10:O:610:GLN:NE2	2.26	0.68
11:P:314:ARG:NH2	11:P:360:ASN:HD21	1.91	0.68
11:P:342:ASP:OD1	11:P:343:ASP:N	2.26	0.68
3:G:17:ARG:HA	3:G:20:ARG:HG3	1.74	0.68
7:K:366:LEU:O	7:K:370:GLN:HB3	1.93	0.68
15:T:475:ARG:HA	15:T:478:LEU:HD13	1.75	0.68
2:F:79:LYS:N	6:J:102:DA:OP1	2.26	0.68
14:S:338:PRO:HG2	14:S:341:THR:HG21	1.75	0.68
12:Q:103:LEU:HB3	12:Q:130:LEU:HD11	1.75	0.68
10:N:415:ARG:HG3	10:N:416:GLU:CD	2.19	0.68
11:P:377:TYR:HD2	11:P:379:ILE:HD13	1.57	0.68
12:Q:393:GLU:OE1	12:Q:397:LYS:NZ	2.20	0.68
10:N:605:LEU:HD11	12:Q:405:PHE:HE1	1.59	0.68
14:S:414:GLY:C	14:S:416:GLY:N	2.50	0.68
11:P:93:ASP:HA	11:P:96:ARG:HG3	1.76	0.68
8:L:545:LYS:HE2	8:L:549:ILE:HG13	1.75	0.68
7:K:921:ARG:HB2	7:K:991:ALA:HA	1.74	0.68
10:N:153:ALA:HB2	15:T:455:TRP:HD1	1.57	0.68
10:O:571:ARG:HD3	12:Q:380:VAL:HG11	1.74	0.68
12:Q:418:LEU:O	12:Q:420:PHE:N	2.27	0.67
13:R:1009:SER:O	13:R:1010:LEU:C	2.37	0.67
1:A:46:VAL:HG23	1:A:49:ARG:HH11	1.58	0.67
7:K:1056:ARG:HB2	7:K:1066:ARG:HE	1.59	0.67
8:L:248:TYR:HA	8:L:256:MET:HE1	1.75	0.67
8:L:492:VAL:O	8:L:496:ARG:NH1	2.27	0.67
10:N:568:GLU:OE1	10:N:568:GLU:N	2.27	0.67
5:I:70:DC:H42	6:J:78:DG:H1	1.40	0.67
7:K:637:LEU:HD11	7:K:693:ILE:HD11	1.76	0.67
7:K:899:TRP:CD1	7:K:938:TYR:HH	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:130:MET:SD	11:P:396:ILE:HG23	2.35	0.67
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.26	0.67
1:A:109:LEU:HD11	1:E:130:ILE:HD11	1.75	0.67
2:B:31:LYS:HG3	2:B:32:PRO:HD3	1.75	0.67
8:L:250:PRO:HA	8:L:255:LEU:HB3	1.76	0.67
10:O:387:ALA:HA	10:O:390:LEU:HD12	1.75	0.67
12:Q:382:GLU:OE2	12:Q:383:ARG:NH1	2.27	0.67
11:P:426:LEU:CG	17:V:360:LEU:HB3	2.24	0.67
7:K:190:ASN:HD21	17:V:482:ARG:HH22	1.43	0.67
13:R:412:ASP:O	13:R:416:ARG:N	2.25	0.67
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.28	0.67
13:R:938:GLU:O	13:R:942:ARG:HG2	1.96	0.67
16:U:900:HIS:HA	16:U:903:SER:HB3	1.77	0.67
5:I:97:DA:H61	6:J:51:DT:H3	1.43	0.66
7:K:913:PRO:HA	7:K:916:LYS:HE3	1.76	0.66
14:S:538:THR:HG23	14:S:541:GLU:H	1.60	0.66
14:S:590:MET:H	14:S:590:MET:HE2	1.59	0.66
7:K:366:LEU:O	7:K:370:GLN:CB	2.43	0.66
12:Q:123:HIS:HE1	12:Q:153:TYR:HB3	1.57	0.66
16:U:850:ASP:OD1	16:U:851:ASN:N	2.29	0.66
8:L:20:SER:HB3	8:L:176:GLY:HA3	1.78	0.66
12:Q:19:HIS:NE2	12:Q:83:THR:O	2.28	0.66
13:R:924:ARG:HH21	13:R:1003:TYR:HA	1.60	0.66
11:P:232:ASP:HB2	11:P:282:VAL:HG13	1.76	0.66
2:B:92:ARG:NH1	4:D:97:LEU:O	2.28	0.66
2:F:77:LYS:HE2	4:H:89:ARG:NH2	2.09	0.66
7:K:405:ARG:O	7:K:408:ARG:NH2	2.29	0.66
7:K:999:SER:OG	7:K:1026:ARG:NE	2.28	0.66
8:L:42:ARG:HG2	8:L:90:TYR:CD1	2.30	0.66
13:R:522:SER:HB3	13:R:528:ILE:HD11	1.78	0.66
17:V:460:GLN:HG2	17:V:464:ILE:HD13	1.78	0.66
3:C:57:TYR:HE1	7:K:1159:ARG:HB3	1.61	0.66
8:L:52:LYS:NZ	8:L:53:TRP:O	2.29	0.66
10:N:254:THR:HG22	10:O:117:ILE:CD1	2.24	0.66
8:L:20:SER:O	8:L:179:LYS:NZ	2.24	0.66
9:M:156:PRO:HA	9:M:159:ARG:HD2	1.78	0.66
10:N:367:THR:CG2	10:N:369:MET:SD	2.81	0.66
12:Q:192:LYS:HD3	12:Q:203:PRO:HB3	1.78	0.66
13:R:1006:SER:O	13:R:1010:LEU:HG	1.95	0.66
7:K:821:PRO:HD3	7:K:1019:LYS:HZ2	1.61	0.66
16:U:896:HIS:HB3	16:U:901:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:131:ARG:HB2	11:P:172:LEU:HD21	1.77	0.66
7:K:355:ARG:HA	7:K:358:ILE:HD12	1.77	0.65
7:K:745:GLN:N	7:K:750:GLU:OE1	2.29	0.65
8:L:248:TYR:N	8:L:547:ASN:CG	2.54	0.65
10:O:586:LEU:HA	10:O:589:LYS:NZ	2.11	0.65
13:R:900:ALA:N	13:R:911:GLN:O	2.29	0.65
14:S:24:ASN:HD21	14:S:27:LEU:HB2	1.60	0.65
14:S:426:LEU:HB3	15:T:353:GLU:HG2	1.79	0.65
15:T:443:VAL:HB	15:T:465:LYS:NZ	2.10	0.65
9:M:198:VAL:HG12	9:M:394:THR:HB	1.79	0.65
10:N:422:PHE:O	10:N:425:LEU:HB3	1.95	0.65
12:Q:171:PRO:HA	12:Q:174:HIS:CG	2.32	0.65
13:R:939:GLU:HG2	13:R:942:ARG:HH21	1.61	0.65
8:L:144:PHE:HD1	8:L:707:ARG:HH11	1.45	0.65
10:N:153:ALA:HB2	15:T:455:TRP:CD1	2.32	0.65
10:N:642:PHE:CE1	10:O:631:ARG:HA	2.31	0.65
13:R:924:ARG:NH2	13:R:1003:TYR:HA	2.11	0.65
13:R:990:LEU:HB3	13:R:1008:PHE:CE1	2.21	0.65
1:A:70:LEU:O	1:A:73:GLU:HG3	1.97	0.65
8:L:526:PRO:HA	8:L:529:TRP:CE3	2.31	0.65
9:M:440:ALA:HA	9:M:445:PHE:HE2	1.61	0.65
13:R:547:ASN:HB3	13:R:583:GLN:HE21	1.61	0.65
3:C:57:TYR:CE1	7:K:1159:ARG:HB3	2.32	0.65
7:K:578:ILE:HB	7:K:624:THR:HB	1.79	0.65
14:S:149:PRO:HG2	14:S:164:LEU:HB2	1.78	0.65
14:S:414:GLY:O	14:S:416:GLY:N	2.29	0.65
15:T:352:ARG:O	15:T:356:HIS:ND1	2.23	0.65
7:K:294:ASN:HD21	10:N:568:GLU:HB2	1.61	0.65
7:K:611:MET:HE1	7:K:615:LYS:NZ	2.12	0.65
9:M:150:GLU:HB3	9:M:177:LEU:HD11	1.79	0.65
9:M:255:LYS:HG3	9:M:266:ARG:HH22	1.62	0.65
2:F:34:ILE:HB	2:F:51:TYR:HE1	1.60	0.65
10:N:616:ARG:HD2	10:O:612:LEU:HD21	1.79	0.65
13:R:1009:SER:OG	13:R:1010:LEU:N	2.30	0.65
14:S:180:PHE:HE2	14:S:194:PHE:HE2	1.45	0.65
15:T:455:TRP:HH2	15:T:465:LYS:HE2	1.60	0.65
1:A:63:ARG:NH2	6:J:60:DA:O3'	2.30	0.65
5:I:68:DT:H3	6:J:80:DA:H61	1.41	0.65
7:K:794:ILE:HA	7:K:797:ILE:HG12	1.78	0.65
9:M:383:ASN:OD1	9:M:387:ASN:ND2	2.30	0.65
10:N:361:GLN:HB3	10:N:365:HIS:HB3	1.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:620:LYS:HD3	11:P:308:ASP:HB2	1.78	0.65
11:P:467:TRP:CD1	11:P:471:GLN:HE22	2.15	0.65
12:Q:37:VAL:HA	12:Q:40:TRP:CE3	2.30	0.65
14:S:17:PRO:HD3	14:S:105:TYR:HE1	1.61	0.65
14:S:219:ARG:NH1	14:S:554:GLY:O	2.29	0.65
9:M:192:THR:HA	9:M:208:ILE:O	1.96	0.64
11:P:230:GLU:HB2	11:P:285:ILE:HG22	1.78	0.64
13:R:364:GLN:O	14:S:116:ASN:ND2	2.30	0.64
3:G:84:GLN:OE1	3:G:106:GLY:N	2.31	0.64
7:K:289:HIS:H	12:Q:376:PHE:HZ	1.46	0.64
7:K:912:LEU:HA	7:K:915:TYR:CE1	2.32	0.64
12:Q:64:ASP:HB2	12:Q:155:PRO:HD3	1.77	0.64
13:R:490:HIS:CE1	13:R:527:MET:HB2	2.32	0.64
14:S:546:ARG:NH2	14:S:551:ARG:O	2.29	0.64
7:K:948:ARG:NH1	7:K:950:ASP:OD2	2.29	0.64
9:M:264:ASP:OD2	9:M:266:ARG:NH1	2.30	0.64
10:N:129:ASN:OD1	15:T:446:ARG:NH2	2.30	0.64
13:R:515:MET:HG3	13:R:535:LEU:HD21	1.78	0.64
1:E:70:LEU:O	1:E:73:GLU:HG3	1.97	0.64
10:N:253:ASP:OD1	10:N:257:LYS:NZ	2.29	0.64
10:O:117:ILE:HG23	10:O:170:PRO:HG2	1.79	0.64
11:P:510:ARG:O	11:P:511:ARG:NH1	2.28	0.64
14:S:365:HIS:ND1	14:S:369:GLU:OE1	2.30	0.64
7:K:288:ASP:O	7:K:291:ARG:N	2.25	0.64
11:P:162:SER:HA	11:P:277:PRO:HA	1.79	0.64
10:O:127:ASP:O	10:O:159:ARG:NH2	2.28	0.64
14:S:424:GLU:H	14:S:424:GLU:CD	2.06	0.64
3:C:17:ARG:NH1	6:J:31:DA:OP2	2.31	0.64
5:I:51:DC:H2''	5:I:52:DA:C8	2.33	0.64
12:Q:60:ASP:OD1	12:Q:180:ARG:NH2	2.30	0.64
7:K:471:GLU:O	7:K:474:LYS:HG3	1.98	0.64
7:K:830:CYS:N	7:K:1028:ILE:O	2.30	0.64
10:N:329:ARG:HH21	10:N:373:THR:HB	1.62	0.64
13:R:476:ILE:HD12	13:R:488:LEU:HD21	1.79	0.64
2:F:31:LYS:HA	2:F:51:TYR:CZ	2.32	0.64
7:K:351:ASP:O	7:K:355:ARG:NE	2.31	0.64
7:K:393:ARG:HB2	17:V:378:ILE:HD13	1.79	0.64
7:K:616:THR:HG23	18:K:1601:ADP:PB	2.38	0.64
9:M:253:ASN:HB3	9:M:266:ARG:HB2	1.79	0.64
16:U:908:ARG:HH21	16:U:909:GLU:HG2	1.63	0.64
6:J:34:DC:H2'	6:J:35:DT:C6	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:390:VAL:O	9:M:391:THR:CG2	2.46	0.63
10:N:145:ASN:OD1	15:T:454:ASN:ND2	2.31	0.63
1:A:79:LYS:HB3	1:A:82:LEU:HD21	1.79	0.63
7:K:1042:ARG:HH21	7:K:1045:LEU:HD12	1.62	0.63
10:N:569:MET:SD	11:P:447:LYS:CD	2.83	0.63
10:N:608:ALA:O	10:N:609:ARG:C	2.40	0.63
12:Q:15:LEU:HD23	12:Q:18:ILE:HD11	1.81	0.63
14:S:422:ASP:HB3	14:S:425:HIS:O	1.98	0.63
16:U:893:GLN:HE21	16:U:901:LEU:HD21	1.63	0.63
6:J:120:DG:H1'	6:J:121:DA:N7	2.14	0.63
7:K:989:GLN:NE2	7:K:1015:ARG:HG3	2.13	0.63
8:L:345:ASN:OD1	8:L:348:ARG:NH1	2.31	0.63
8:L:555:ARG:HG2	9:M:253:ASN:OD1	1.98	0.63
9:M:274:ILE:HG23	9:M:278:PHE:HD2	1.63	0.63
9:M:340:GLU:OE1	9:M:403:ARG:NH1	2.31	0.63
12:Q:310:ASN:HB3	12:Q:314:MET:HE1	1.79	0.63
9:M:165:VAL:HG12	9:M:170:TRP:HZ3	1.62	0.63
10:O:118:ILE:HD11	10:O:167:ARG:CD	2.28	0.63
10:O:613:PHE:CZ	11:P:320:ALA:HA	2.30	0.63
11:P:130:MET:HE1	11:P:398:VAL:HG22	1.79	0.63
13:R:429:ASP:O	13:R:432:GLN:NE2	2.24	0.63
13:R:1000:LEU:O	13:R:1001:ALA:C	2.42	0.63
3:C:17:ARG:HA	3:C:20:ARG:HB2	1.81	0.63
7:K:813:LYS:HD2	7:K:817:GLU:HB3	1.81	0.63
8:L:26:GLN:NE2	8:L:33:THR:OG1	2.32	0.63
10:O:113:GLN:HB3	10:O:168:LEU:CD1	2.27	0.63
3:C:67:GLY:HA3	4:D:46:HIS:CD2	2.33	0.63
4:D:87:THR:H	4:D:90:GLU:HG2	1.62	0.63
5:I:49:DA:H1'	5:I:50:DG:C8	2.33	0.63
8:L:550:GLN:O	8:L:554:HIS:HB2	1.98	0.63
12:Q:414:ALA:O	12:Q:418:LEU:N	2.26	0.63
14:S:214:ILE:HA	14:S:217:GLN:OE1	1.97	0.63
15:T:471:SER:H	15:T:474:ILE:HD12	1.64	0.63
3:G:95:LYS:NZ	4:H:100:PRO:HB2	2.14	0.63
8:L:349:TYR:O	8:L:350:LYS:NZ	2.28	0.63
8:L:514:ARG:O	8:L:518:SER:N	2.32	0.63
10:N:272:VAL:HG12	15:T:427:THR:O	1.98	0.63
10:O:117:ILE:HG21	10:O:170:PRO:HG2	1.81	0.63
16:U:912:ALA:O	16:U:916:LYS:NZ	2.31	0.63
7:K:613:LEU:HG	7:K:1016:ILE:HG13	1.79	0.63
10:N:177:THR:O	10:N:178:ALA:C	2.41	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:615:ASP:O	10:N:616:ARG:C	2.42	0.63
10:O:111:ILE:O	10:O:114:THR:HB	1.98	0.63
11:P:86:ILE:HG22	11:P:89:GLY:H	1.62	0.63
1:A:66:PRO:HG3	5:I:91:DA:H5''	1.79	0.63
7:K:472:GLU:O	7:K:475:ARG:HG3	1.98	0.63
10:O:127:ASP:OD1	10:O:128:MET:N	2.32	0.63
6:J:116:DA:H2''	6:J:117:DA:C8	2.33	0.62
7:K:906:GLU:O	7:K:910:ARG:HG2	1.99	0.62
10:N:417:GLU:HA	10:N:420:LEU:HB2	1.80	0.62
1:E:108:ASN:ND2	2:F:42:GLY:O	2.32	0.62
7:K:902:ALA:HB3	7:K:905:PHE:HD2	1.64	0.62
7:K:903:GLY:HA2	7:K:906:GLU:HG3	1.81	0.62
9:M:237:LYS:NZ	9:M:244:ASN:OD1	2.31	0.62
10:N:233:GLY:HA3	15:T:386:MET:HE1	1.80	0.62
10:N:566:GLU:HA	10:N:569:MET:CG	2.30	0.62
13:R:467:PRO:O	13:R:470:LYS:HG3	1.99	0.62
14:S:164:LEU:HD23	14:S:164:LEU:H	1.64	0.62
8:L:348:ARG:HH11	8:L:351:ASN:ND2	1.95	0.62
11:P:343:ASP:OD1	11:P:344:MET:N	2.32	0.62
13:R:608:VAL:HA	13:R:611:LEU:HD23	1.79	0.62
1:A:63:ARG:HD2	5:I:91:DA:H4'	1.81	0.62
7:K:599:TYR:HD2	7:K:630:LYS:HZ3	1.47	0.62
9:M:323:PHE:N	9:M:327:SER:O	2.30	0.62
10:O:113:GLN:HG2	15:T:348:LEU:HD11	1.81	0.62
12:Q:69:LEU:HD12	12:Q:149:TRP:O	2.00	0.62
14:S:228:VAL:O	14:S:375:LYS:NZ	2.29	0.62
7:K:616:THR:HG22	7:K:648:TRP:HE1	1.63	0.62
10:N:208:ASP:OD1	14:S:8:GLN:NE2	2.33	0.62
10:N:322:ASN:ND2	10:N:356:ARG:O	2.33	0.62
15:T:446:ARG:O	15:T:446:ARG:HD2	1.99	0.62
3:C:42:ARG:CD	4:D:85:THR:HG22	2.24	0.62
10:N:271:GLU:CD	15:T:428:HIS:HB3	2.25	0.62
10:O:469:LEU:HD21	16:U:966:ARG:HG3	1.81	0.62
12:Q:410:VAL:O	12:Q:413:GLN:HB3	1.99	0.62
7:K:611:MET:HE1	7:K:615:LYS:HZ3	1.65	0.62
8:L:43:MET:HE3	8:L:106:LEU:HA	1.80	0.62
10:N:213:PRO:HD2	10:O:233:GLY:HA2	1.80	0.62
10:N:254:THR:CG2	10:O:117:ILE:HB	2.30	0.62
14:S:586:ARG:NH2	14:S:589:LYS:HG3	2.15	0.62
7:K:437:GLN:O	7:K:440:ARG:HD3	2.00	0.62
10:N:147:ASN:OD1	10:N:150:LYS:N	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:368:ARG:NH1	10:N:370:GLU:OE1	2.32	0.62
11:P:296:ARG:NH2	11:P:316:GLU:OE2	2.33	0.62
11:P:429:ILE:HG21	17:V:364:ALA:HB1	1.80	0.62
7:K:323:MET:O	7:K:363:LYS:NZ	2.27	0.62
7:K:888:MET:HE1	7:K:1139:PRO:HG2	1.82	0.62
8:L:199:ARG:HB3	8:L:202:VAL:HB	1.82	0.62
7:K:632:GLN:NE2	7:K:635:PRO:HD2	2.15	0.62
9:M:105:ARG:HH11	9:M:140:PRO:HB2	1.64	0.62
10:N:590:TYR:CE2	11:P:109:MET:HE2	2.35	0.62
3:G:75:LYS:HZ1	3:G:77:ARG:HB3	1.65	0.61
8:L:175:ILE:HD12	8:L:539:ALA:HB2	1.82	0.61
10:N:248:GLY:C	10:O:116:ALA:HB2	2.24	0.61
17:V:395:ARG:HA	17:V:398:ASN:HD22	1.64	0.61
7:K:752:TRP:HE1	7:K:763:PHE:HB3	1.64	0.61
8:L:42:ARG:HD3	8:L:90:TYR:HE1	1.63	0.61
11:P:476:ASP:OD1	11:P:476:ASP:N	2.33	0.61
8:L:186:TYR:CD2	8:L:524:MET:HG2	2.34	0.61
10:N:230:THR:HA	15:T:429:LEU:HD22	1.81	0.61
10:N:274:ARG:HA	15:T:426:ASP:HB3	1.82	0.61
13:R:934:ASN:O	13:R:937:ARG:N	2.33	0.61
10:N:276:ILE:HG22	10:N:286:ILE:HD12	1.83	0.61
10:N:613:PHE:CE1	10:N:661:MET:HE1	2.35	0.61
10:O:465:VAL:HA	10:O:468:PHE:CE1	2.35	0.61
12:Q:114:TYR:HB3	12:Q:121:ALA:CA	2.30	0.61
14:S:107:ARG:HB2	14:S:109:TRP:CD1	2.35	0.61
7:K:616:THR:HG23	18:K:1601:ADP:O1B	1.99	0.61
7:K:638:VAL:HG22	7:K:709:ILE:HD13	1.82	0.61
8:L:19:GLY:N	8:L:22:THR:O	2.33	0.61
8:L:256:MET:HG2	8:L:502:ARG:NH2	2.14	0.61
10:N:548:ASN:O	10:N:552:ALA:N	2.31	0.61
11:P:323:GLU:HA	11:P:326:LYS:HE2	1.82	0.61
12:Q:115:ARG:HG2	12:Q:118:GLU:HG3	1.83	0.61
12:Q:156:ALA:HB1	12:Q:160:ASP:OD1	2.01	0.61
1:E:72:ARG:HH22	5:I:51:DC:P	2.24	0.61
7:K:528:GLN:HB3	7:K:531:GLN:HE21	1.65	0.61
9:M:75:ASN:OD1	9:M:76:TYR:N	2.34	0.61
11:P:288:LEU:HB2	11:P:373:ILE:HB	1.81	0.61
12:Q:171:PRO:HA	12:Q:174:HIS:CD2	2.36	0.61
7:K:185:ARG:NH2	10:O:422:PHE:O	2.23	0.61
7:K:326:ARG:CZ	7:K:330:LEU:HD11	2.31	0.61
10:N:221:THR:HG21	10:O:241:ALA:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:415:GLU:HB3	12:Q:416:GLN:NE2	2.15	0.61
14:S:244:THR:O	14:S:247:ASN:ND2	2.24	0.61
10:N:189:ALA:O	10:N:190:ILE:C	2.42	0.61
8:L:655:LYS:NZ	8:L:656:THR:O	2.29	0.61
10:N:562:ALA:HB2	11:P:454:SER:HB2	1.81	0.61
10:O:238:GLN:HB3	10:O:239:PRO:HD3	1.81	0.61
11:P:224:PHE:HE1	11:P:373:ILE:HD13	1.65	0.61
13:R:997:ASN:OD1	13:R:1000:LEU:N	2.33	0.61
4:H:38:VAL:HA	4:H:41:VAL:HG12	1.83	0.61
10:N:631:ARG:HG2	12:Q:428:GLU:HG3	1.83	0.61
1:E:63:ARG:HH21	5:I:60:DA:H4'	1.65	0.60
11:P:335:GLU:HB3	11:P:338:ASN:O	2.01	0.60
2:B:91:LYS:HG3	2:B:96:THR:HG22	1.84	0.60
9:M:276:ASP:OD2	9:M:279:ARG:NH2	2.34	0.60
11:P:113:ARG:HG2	17:V:361:PHE:CE2	2.36	0.60
12:Q:191:ARG:NE	12:Q:193:GLU:OE2	2.33	0.60
13:R:370:GLU:OE1	13:R:370:GLU:N	2.29	0.60
7:K:287:ILE:N	12:Q:375:GLU:OE2	2.29	0.60
8:L:241:ASN:O	8:L:542:ARG:NH1	2.29	0.60
13:R:1008:PHE:HA	13:R:1011:LEU:HD12	1.83	0.60
6:J:52:DG:H2'	6:J:53:DG:H8	1.64	0.60
7:K:528:GLN:HA	7:K:531:GLN:HG3	1.83	0.60
8:L:61:ARG:HH21	8:L:62:LYS:HG2	1.65	0.60
9:M:147:LEU:HD11	9:M:439:LEU:HD23	1.81	0.60
9:M:299:ARG:HD3	9:M:402:ASP:HB3	1.82	0.60
9:M:440:ALA:HA	9:M:445:PHE:CE2	2.35	0.60
10:N:319:ASN:HB2	10:N:324:GLY:HA2	1.83	0.60
13:R:325:ASN:OD1	13:R:326:ILE:N	2.34	0.60
1:A:85:GLN:NE2	2:B:83:ALA:H	1.99	0.60
4:D:54:LYS:O	4:D:58:ILE:HD12	2.01	0.60
7:K:899:TRP:CG	7:K:938:TYR:HH	2.19	0.60
10:N:130:THR:HB	15:T:446:ARG:HH12	1.66	0.60
10:N:211:GLN:OE1	15:T:523:MET:N	2.34	0.60
12:Q:6:PRO:HB2	12:Q:56:TRP:HZ2	1.65	0.60
17:V:479:GLN:HA	17:V:482:ARG:HD2	1.82	0.60
7:K:877:HIS:HD2	7:K:878:PRO:HD2	1.65	0.60
8:L:175:ILE:HD11	8:L:534:PHE:HB3	1.82	0.60
8:L:199:ARG:NH2	8:L:209:ASP:OD2	2.34	0.60
10:O:118:ILE:HG13	10:O:167:ARG:CZ	2.32	0.60
7:K:423:ASN:HB3	7:K:424:ARG:HH11	1.65	0.60
7:K:978:SER:HB3	7:K:981:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:583:LYS:HE3	11:P:433:ASP:OD1	2.01	0.60
12:Q:31:ARG:NH1	12:Q:33:GLU:OE2	2.35	0.60
14:S:246:ASP:O	14:S:250:LYS:NZ	2.35	0.60
3:G:64:GLU:HG3	4:H:46:HIS:HE1	1.67	0.60
10:N:280:ASN:OD1	10:N:281:ALA:N	2.34	0.60
11:P:116:ILE:HD12	11:P:120:LEU:HD21	1.84	0.60
15:T:455:TRP:CH2	15:T:465:LYS:HE2	2.36	0.60
1:E:125:GLN:O	1:E:129:ARG:HB2	2.01	0.60
7:K:1005:GLN:HA	7:K:1008:GLN:HB3	1.82	0.60
9:M:464:GLU:O	9:M:468:LYS:NZ	2.34	0.60
3:G:75:LYS:NZ	3:G:77:ARG:HB3	2.16	0.59
8:L:531:ASN:HA	8:L:657:ALA:HB2	1.83	0.59
9:M:233:ARG:NH2	9:M:283:GLU:OE1	2.35	0.59
10:N:569:MET:HE1	11:P:447:LYS:N	2.17	0.59
11:P:439:LEU:O	11:P:443:VAL:HG23	2.02	0.59
7:K:295:ARG:HH12	7:K:297:LEU:HD23	1.67	0.59
10:N:617:LEU:HG	12:Q:419:ARG:HH22	1.67	0.59
11:P:458:ARG:NE	11:P:459:ASP:OD1	2.27	0.59
5:I:100:DG:H4'	5:I:101:DG:H5'	1.84	0.59
10:O:403:TRP:HB2	10:O:415:ARG:CZ	2.33	0.59
10:O:584:LEU:HB3	11:P:101:PHE:CZ	2.37	0.59
1:E:48:LEU:HA	1:E:51:ILE:HG12	1.84	0.59
9:M:430:PHE:O	9:M:434:ILE:HG13	2.02	0.59
10:N:232:ARG:NH2	15:T:441:TYR:HB2	2.14	0.59
7:K:767:LYS:O	7:K:771:GLU:HB2	2.03	0.59
8:L:156:HIS:O	8:L:160:ALA:N	2.35	0.59
3:C:17:ARG:NH2	6:J:30:DG:H3'	2.17	0.59
7:K:345:ASP:OD1	7:K:346:GLU:N	2.34	0.59
10:N:610:GLN:O	10:N:612:LEU:N	2.35	0.59
10:N:670:SER:HB2	11:P:170:ARG:HD2	1.85	0.59
3:G:25:PHE:CZ	3:G:59:THR:HG21	2.37	0.59
7:K:752:TRP:NE1	7:K:763:PHE:HB3	2.18	0.59
7:K:924:MET:HB3	7:K:926:PHE:CE2	2.37	0.59
8:L:686:ALA:O	8:L:700:GLN:NE2	2.35	0.59
10:O:599:GLN:OE1	10:O:602:ARG:NH1	2.23	0.59
1:A:125:GLN:O	1:A:129:ARG:HB2	2.02	0.59
5:I:42:DC:H42	6:J:106:DG:H1	1.50	0.59
8:L:56:TYR:HB2	8:L:80:GLU:OE2	2.03	0.59
9:M:40:GLU:HB2	9:M:433:TRP:HH2	1.68	0.59
16:U:921:ALA:HA	16:U:924:ARG:HG2	1.85	0.59
16:U:956:GLU:O	16:U:960:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HG3	1:A:106:ASP:N	2.18	0.59
7:K:584:LEU:HB3	7:K:588:GLN:HB2	1.85	0.59
10:N:624:ARG:HG2	12:Q:423:GLN:HG3	1.85	0.59
12:Q:313:TRP:O	12:Q:317:ILE:HG12	2.03	0.59
7:K:711:ASP:HA	7:K:739:LEU:HB2	1.84	0.59
9:M:78:ASN:HD21	9:M:82:MET:HB2	1.68	0.59
9:M:176:TRP:HE1	9:M:178:SER:HB3	1.67	0.59
10:N:187:VAL:HG22	10:N:191:MET:HE1	1.85	0.59
10:N:254:THR:HA	10:N:257:LYS:HZ2	1.68	0.59
13:R:490:HIS:HE1	13:R:527:MET:HB2	1.68	0.59
17:V:526:GLN:O	17:V:530:ILE:HG13	2.02	0.59
1:A:48:LEU:HA	1:A:51:ILE:HG12	1.84	0.58
7:K:610:GLU:OE1	7:K:610:GLU:N	2.29	0.58
7:K:1159:ARG:HA	7:K:1162:ARG:HG2	1.84	0.58
10:N:403:TRP:CE3	10:N:419:VAL:HG22	2.38	0.58
10:N:584:LEU:HA	10:N:587:LYS:HG2	1.84	0.58
10:N:611:GLN:O	10:N:612:LEU:C	2.45	0.58
12:Q:158:LYS:HD3	12:Q:161:ARG:HD2	1.85	0.58
17:V:388:TRP:HA	17:V:391:ARG:HD3	1.83	0.58
5:I:103:DA:H2'	5:I:104:DT:C6	2.37	0.58
7:K:810:ARG:HH12	7:K:1053:GLN:HA	1.66	0.58
9:M:247:PRO:HD2	9:M:250:MET:HE2	1.85	0.58
10:N:221:THR:HB	10:N:224:PHE:CE1	2.38	0.58
10:N:277:TYR:HE1	10:N:285:LYS:HE3	1.68	0.58
10:N:278:GLU:OE2	10:N:286:ILE:HG12	2.02	0.58
10:N:320:CYS:HB3	10:N:351:CYS:SG	2.43	0.58
12:Q:29:MET:HE3	12:Q:32:VAL:HG22	1.84	0.58
13:R:450:ILE:O	13:R:454:VAL:HG23	2.03	0.58
13:R:571:ASP:OD1	13:R:572:GLU:N	2.36	0.58
13:R:940:ARG:HH12	13:R:977:ILE:HG23	1.68	0.58
14:S:136:ARG:NH1	14:S:136:ARG:HB2	2.18	0.58
2:B:82:THR:HG22	2:B:84:MET:H	1.68	0.58
3:C:58:LEU:HD11	4:D:103:LEU:HD21	1.85	0.58
7:K:821:PRO:HD3	7:K:1019:LYS:NZ	2.18	0.58
7:K:1003:PRO:O	7:K:1007:LEU:HG	2.04	0.58
14:S:180:PHE:CE2	14:S:194:PHE:HE2	2.22	0.58
2:B:27:GLN:OE1	2:B:55:ARG:NH1	2.37	0.58
8:L:532:ILE:HB	8:L:656:THR:HA	1.84	0.58
8:L:703:MET:HE1	8:L:723:MET:HE3	1.86	0.58
9:M:314:LYS:O	9:M:332:ARG:NH1	2.35	0.58
10:N:415:ARG:HG3	10:N:416:GLU:OE2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:623:VAL:HG22	13:R:889:THR:HA	1.86	0.58
16:U:959:GLU:HB3	16:U:963:LYS:NZ	2.19	0.58
17:V:396:ASN:HA	17:V:399:LYS:HE2	1.84	0.58
7:K:773:PHE:HB3	7:K:800:LEU:HD21	1.85	0.58
8:L:663:LEU:HD22	8:L:666:TRP:HB2	1.84	0.58
3:G:44:GLY:HA2	6:J:112:DG:H5''	1.84	0.58
7:K:614:GLY:HA2	18:K:1601:ADP:H1'	1.85	0.58
8:L:141:ARG:HB2	8:L:715:PRO:HB3	1.85	0.58
11:P:171:LEU:HD21	11:P:223:PHE:HZ	1.68	0.58
13:R:621:GLU:OE2	13:R:890:ILE:N	2.37	0.58
16:U:863:GLN:HE22	16:U:865:GLN:HB3	1.68	0.58
7:K:616:THR:O	7:K:619:THR:CB	2.50	0.58
10:N:590:TYR:HE2	11:P:109:MET:HE2	1.68	0.58
13:R:361:LYS:HB2	13:R:364:GLN:OE1	2.03	0.58
13:R:378:GLY:O	13:R:381:LYS:HG3	2.03	0.58
14:S:411:THR:O	14:S:412:ALA:C	2.47	0.58
9:M:406:HIS:CE1	9:M:410:ASN:HD21	2.21	0.58
8:L:41:THR:HG21	8:L:92:MET:HB3	1.86	0.58
9:M:96:LEU:HD12	9:M:100:ARG:HD3	1.84	0.58
9:M:159:ARG:HH22	9:M:179:ARG:HH21	1.51	0.58
10:N:251:ASN:HB3	10:N:254:THR:HG23	1.85	0.58
10:N:257:LYS:NZ	10:O:117:ILE:HG12	2.19	0.58
10:N:580:MET:SD	10:N:584:LEU:HD23	2.44	0.58
10:O:190:ILE:H	10:O:190:ILE:HD12	1.69	0.58
11:P:318:VAL:HA	11:P:321:VAL:HG22	1.84	0.58
6:J:37:DG:H2''	6:J:38:DG:C8	2.39	0.58
7:K:388:ALA:O	17:V:308:THR:OG1	2.22	0.58
7:K:467:ASN:HA	7:K:470:LYS:HE2	1.84	0.58
8:L:32:LEU:HD11	8:L:663:LEU:HD11	1.86	0.58
9:M:150:GLU:N	9:M:178:SER:O	2.36	0.58
11:P:112:LYS:NZ	11:P:115:ASP:OD2	2.34	0.58
1:E:105:GLU:HG3	1:E:106:ASP:N	2.19	0.57
10:N:403:TRP:CZ3	10:N:419:VAL:HG13	2.39	0.57
10:N:557:ARG:HH21	12:Q:321:PRO:HB2	1.68	0.57
12:Q:25:ARG:HH11	12:Q:26:TYR:H	1.51	0.57
4:H:40:LYS:O	4:H:43:LYS:HG3	2.04	0.57
7:K:992:ASP:O	7:K:1022:VAL:HA	2.04	0.57
8:L:223:LEU:HD11	8:L:498:GLN:HB3	1.85	0.57
9:M:89:ALA:O	9:M:92:VAL:HG22	2.03	0.57
13:R:899:SER:HA	13:R:912:ALA:HA	1.84	0.57
14:S:437:LEU:HD12	14:S:441:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:135:DC:H2''	6:J:136:DG:C8	2.39	0.57
7:K:1140:GLU:HA	7:K:1143:LEU:HG	1.86	0.57
7:K:1157:LEU:H	7:K:1157:LEU:HD22	1.69	0.57
8:L:132:THR:HB	8:L:134:PRO:HD2	1.85	0.57
11:P:75:LYS:O	11:P:75:LYS:HD3	2.04	0.57
1:A:50:GLU:HG3	2:B:39:ARG:HD3	1.86	0.57
7:K:200:ALA:O	7:K:203:GLU:HG2	2.03	0.57
8:L:61:ARG:HE	8:L:62:LYS:N	1.98	0.57
10:O:107:ARG:O	10:O:110:LEU:HG	2.03	0.57
11:P:125:LYS:HD2	11:P:399:LEU:HB2	1.85	0.57
13:R:581:LEU:O	13:R:585:THR:N	2.35	0.57
14:S:353:LEU:HD12	15:T:361:LEU:HD11	1.85	0.57
4:H:110:GLU:O	4:H:113:LYS:HG3	2.04	0.57
6:J:91:DA:H2'	6:J:92:DG:C8	2.40	0.57
7:K:409:ILE:O	7:K:412:LYS:HB3	2.03	0.57
9:M:233:ARG:NH2	9:M:283:GLU:HB3	2.20	0.57
10:O:603:ARG:NH1	13:R:981:ARG:HA	2.18	0.57
14:S:309:ASP:HB3	14:S:312:TYR:HD2	1.69	0.57
6:J:129:DC:H2''	6:J:130:DG:C5	2.40	0.57
9:M:78:ASN:OD1	9:M:82:MET:N	2.36	0.57
9:M:97:LEU:HD13	9:M:141:LEU:HD11	1.86	0.57
10:N:386:ASP:HA	10:N:389:ILE:HD13	1.85	0.57
10:N:545:GLN:O	10:N:549:ILE:HG12	2.04	0.57
11:P:426:LEU:HG	17:V:360:LEU:HB3	1.87	0.57
11:P:467:TRP:HE1	12:Q:314:MET:HB3	1.70	0.57
12:Q:23:THR:HG22	12:Q:55:TYR:HE2	1.70	0.57
13:R:547:ASN:HB3	13:R:583:GLN:NE2	2.20	0.57
14:S:179:THR:C	14:S:180:PHE:HD1	2.11	0.57
3:G:70:ALA:HB2	3:G:78:ILE:HG22	1.87	0.57
8:L:256:MET:HG2	8:L:502:ARG:HH22	1.68	0.57
10:N:654:ALA:HA	11:P:308:ASP:OD1	2.04	0.57
10:O:580:MET:SD	10:O:581:LEU:N	2.77	0.57
11:P:113:ARG:HE	11:P:117:VAL:HG23	1.70	0.57
13:R:497:GLU:OE2	13:R:537:ARG:NH1	2.37	0.57
14:S:548:SER:HA	14:S:551:ARG:NH2	2.20	0.57
3:G:77:ARG:HD3	4:H:50:GLY:C	2.28	0.57
6:J:89:DT:H2''	6:J:90:DA:C8	2.40	0.57
6:J:115:DC:H2''	6:J:116:DA:C8	2.39	0.57
12:Q:65:GLY:HA2	12:Q:152:HIS:CE1	2.38	0.57
5:I:126:DG:O6	6:J:21:DA:N6	2.37	0.57
7:K:184:PHE:HE1	17:V:468:ILE:HG12	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:244:VAL:O	10:O:119:LEU:HA	2.05	0.57
10:O:114:THR:HG23	10:O:167:ARG:HD2	1.86	0.57
11:P:128:LYS:HG2	11:P:129:THR:N	2.20	0.57
6:J:54:DC:OP1	7:K:929:THR:N	2.35	0.57
7:K:374:ARG:HD3	11:P:518:TRP:CZ3	2.39	0.57
8:L:132:THR:HG21	9:M:103:PRO:HD3	1.87	0.57
11:P:79:ASP:HA	11:P:440:MET:HE3	1.87	0.57
14:S:329:ASP:OD1	14:S:330:LYS:N	2.37	0.57
15:T:501:GLY:N	15:T:506:CYS:SG	2.77	0.57
8:L:156:HIS:HE1	8:L:183:THR:HG21	1.70	0.56
8:L:256:MET:HE3	8:L:502:ARG:HH12	1.69	0.56
8:L:354:HIS:ND1	8:L:489:ASP:OD1	2.38	0.56
10:N:538:SER:O	10:N:542:THR:HG23	2.04	0.56
10:N:554:MET:HA	10:N:557:ARG:HG2	1.87	0.56
10:O:133:ASP:OD1	10:O:134:ILE:N	2.38	0.56
12:Q:309:GLN:NE2	17:V:390:GLN:HG3	2.19	0.56
7:K:753:ALA:HA	7:K:756:ASN:HD22	1.69	0.56
7:K:1165:LYS:H	7:K:1165:LYS:NZ	2.03	0.56
8:L:242:ILE:HB	8:L:345:ASN:HB3	1.87	0.56
10:N:403:TRP:HE3	10:N:419:VAL:HG22	1.69	0.56
10:N:583:LYS:NZ	11:P:429:ILE:HA	2.20	0.56
10:O:584:LEU:HB3	11:P:101:PHE:CE2	2.40	0.56
11:P:289:TYR:CE2	11:P:372:PRO:HB3	2.40	0.56
12:Q:11:HIS:ND1	12:Q:206:PRO:HA	2.19	0.56
12:Q:416:GLN:O	12:Q:419:ARG:HB2	2.04	0.56
12:Q:431:ARG:NE	12:Q:431:ARG:HA	2.19	0.56
13:R:523:GLU:HB2	17:V:372:ARG:HH12	1.70	0.56
14:S:334:SER:HB3	14:S:337:HIS:HB2	1.88	0.56
17:V:531:ILE:O	17:V:534:LEU:HB2	2.05	0.56
3:C:26:PRO:HD3	4:D:37:TYR:HD1	1.70	0.56
5:I:27:DT:H2"	5:I:28:DC:C6	2.40	0.56
7:K:880:VAL:HG21	7:K:930:ALA:HB1	1.87	0.56
7:K:953:THR:OG1	7:K:957:ASP:OD2	2.23	0.56
7:K:1163:GLU:O	7:K:1164:ARG:C	2.48	0.56
8:L:345:ASN:HA	8:L:348:ARG:HD2	1.86	0.56
9:M:29:GLY:O	9:M:49:SER:OG	2.22	0.56
9:M:299:ARG:NH1	9:M:402:ASP:O	2.37	0.56
9:M:385:LEU:HB3	9:M:417:ILE:HD13	1.87	0.56
10:N:186:ASP:O	10:N:187:VAL:C	2.49	0.56
10:N:188:CYS:SG	10:N:192:ARG:NH1	2.78	0.56
10:N:266:THR:OG1	10:N:267:GLU:OE1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:100:ASP:OD2	11:P:101:PHE:N	2.38	0.56
13:R:1004:VAL:HG12	13:R:1008:PHE:CZ	2.41	0.56
14:S:121:HIS:O	14:S:124:VAL:HG12	2.06	0.56
14:S:414:GLY:C	14:S:416:GLY:H	2.11	0.56
14:S:537:LEU:HD23	14:S:542:ARG:HE	1.70	0.56
7:K:201:ILE:HD11	17:V:468:ILE:HD13	1.88	0.56
9:M:166:VAL:HG11	9:M:175:PHE:CZ	2.40	0.56
10:N:249:LYS:HB2	10:O:115:HIS:HA	1.88	0.56
11:P:224:PHE:CD1	11:P:288:LEU:HB3	2.40	0.56
13:R:479:LEU:O	13:R:489:LYS:NZ	2.31	0.56
13:R:608:VAL:HG11	13:R:986:VAL:HB	1.86	0.56
13:R:993:VAL:O	13:R:997:ASN:ND2	2.38	0.56
14:S:408:ALA:CA	14:S:420:ARG:HG2	2.35	0.56
14:S:458:ARG:HG2	14:S:462:ARG:CZ	2.35	0.56
17:V:479:GLN:O	17:V:483:ASN:ND2	2.38	0.56
7:K:842:GLN:HE22	7:K:843:MET:HE3	1.70	0.56
10:N:179:CYS:O	10:N:181:ARG:N	2.38	0.56
10:N:642:PHE:O	10:N:646:GLN:NE2	2.31	0.56
10:O:131:ILE:HD12	10:O:143:PHE:HZ	1.69	0.56
12:Q:21:ILE:HG23	12:Q:55:TYR:CE1	2.41	0.56
12:Q:312:GLU:O	12:Q:315:GLU:HG3	2.05	0.56
14:S:558:TRP:CD1	14:S:572:ASN:HD22	2.23	0.56
2:F:29:ILE:HD11	2:F:55:ARG:HG3	1.86	0.56
7:K:294:ASN:OD1	7:K:295:ARG:N	2.38	0.56
7:K:947:LEU:HD22	7:K:972:TYR:HD2	1.71	0.56
7:K:949:LEU:HB2	7:K:977:LEU:HD23	1.88	0.56
8:L:26:GLN:HG3	8:L:36:ALA:HB2	1.87	0.56
9:M:340:GLU:HA	9:M:343:TRP:HB2	1.87	0.56
10:O:142:PHE:CD2	10:O:155:TYR:HB2	2.41	0.56
11:P:79:ASP:OD1	11:P:80:GLY:N	2.38	0.56
14:S:447:GLY:O	14:S:450:GLU:HG3	2.06	0.56
14:S:453:ILE:HG22	14:S:457:ARG:HH21	1.70	0.56
14:S:210:THR:O	14:S:214:ILE:HG12	2.05	0.56
1:E:68:GLN:HE22	1:E:72:ARG:HE	1.52	0.56
5:I:47:DC:N3	6:J:100:DA:N6	2.52	0.56
7:K:1163:GLU:HB3	7:K:1165:LYS:HZ3	1.69	0.56
8:L:42:ARG:HD3	8:L:90:TYR:CE1	2.41	0.56
8:L:350:LYS:HA	8:L:493:GLY:HA2	1.87	0.56
9:M:294:VAL:HG11	9:M:331:TRP:HB2	1.86	0.56
10:O:588:LEU:HD23	11:P:101:PHE:HZ	1.70	0.56
14:S:378:ALA:O	14:S:382:GLY:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:55:DG:H2''	6:J:56:DG:OP2	2.06	0.56
7:K:369:LYS:HZ1	10:N:400:ASP:HA	1.70	0.56
7:K:607:LEU:O	7:K:615:LYS:NZ	2.38	0.56
10:N:567:ARG:NH1	10:N:571:ARG:HG3	2.21	0.56
10:N:675:LEU:O	11:P:219:ARG:NH2	2.39	0.56
13:R:519:LEU:HD12	13:R:528:ILE:HD12	1.88	0.56
13:R:973:ARG:HG3	13:R:974:ILE:H	1.71	0.56
1:A:63:ARG:HH22	6:J:61:DA:H5'	1.71	0.56
1:E:50:GLU:OE2	2:F:39:ARG:NH2	2.39	0.56
7:K:752:TRP:O	7:K:756:ASN:ND2	2.39	0.56
8:L:681:VAL:O	8:L:685:LEU:HG	2.06	0.56
11:P:367:LEU:HD23	13:R:890:ILE:HD12	1.88	0.56
13:R:566:LEU:HD22	13:R:577:CYS:SG	2.46	0.56
6:J:61:DA:H2''	6:J:62:DA:C8	2.41	0.55
9:M:97:LEU:HA	9:M:101:LEU:HB2	1.88	0.55
10:O:399:TYR:CE2	10:O:409:TYR:HB2	2.41	0.55
10:O:611:GLN:HG3	10:O:612:LEU:N	2.20	0.55
11:P:295:GLU:O	11:P:313:THR:HA	2.06	0.55
14:S:411:THR:O	14:S:414:GLY:N	2.39	0.55
3:C:17:ARG:HG3	3:C:27:VAL:HG23	1.87	0.55
3:C:100:VAL:HG23	2:F:96:THR:HG23	1.87	0.55
10:N:232:ARG:HB3	15:T:385:THR:HG23	1.89	0.55
13:R:1001:ALA:HB3	13:R:1002:PRO:HD3	1.87	0.55
14:S:175:ARG:NH1	14:S:176:LEU:O	2.38	0.55
16:U:849:ALA:HA	16:U:852:ILE:HD12	1.89	0.55
7:K:585:LYS:NZ	7:K:819:ASP:OD2	2.34	0.55
10:N:403:TRP:H	10:N:403:TRP:CD1	2.25	0.55
10:N:606:GLU:O	10:N:610:GLN:N	2.39	0.55
11:P:109:MET:HG2	17:V:365:PHE:CE1	2.41	0.55
11:P:165:LEU:O	11:P:273:THR:HA	2.05	0.55
11:P:303:LEU:HA	11:P:306:ILE:HG22	1.87	0.55
3:C:17:ARG:HH21	3:C:28:GLY:HA3	1.70	0.55
5:I:13:DG:H2''	5:I:14:DG:H5'	1.87	0.55
7:K:1041:ALA:HA	7:K:1044:LYS:HD2	1.88	0.55
10:N:185:GLY:O	10:N:186:ASP:C	2.49	0.55
10:N:566:GLU:HA	10:N:569:MET:CB	2.37	0.55
11:P:335:GLU:HA	11:P:337:ARG:NH2	2.21	0.55
12:Q:6:PRO:HB2	12:Q:56:TRP:CZ2	2.42	0.55
13:R:401:PRO:HA	13:R:416:ARG:HD2	1.88	0.55
13:R:484:MET:HG2	13:R:485:LEU:HD22	1.88	0.55
16:U:924:ARG:NH1	16:U:925:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:27:DT:H2''	5:I:28:DC:C5	2.42	0.55
6:J:36:DA:H2''	6:J:37:DG:C8	2.41	0.55
9:M:105:ARG:NH1	9:M:140:PRO:HB2	2.22	0.55
9:M:233:ARG:HH22	9:M:245:VAL:HB	1.70	0.55
9:M:298:TRP:O	9:M:403:ARG:HB2	2.07	0.55
10:N:188:CYS:O	10:N:189:ALA:C	2.49	0.55
11:P:166:LYS:HA	11:P:272:ILE:O	2.06	0.55
11:P:177:ASP:O	11:P:179:SER:N	2.40	0.55
12:Q:199:ARG:HA	12:Q:202:TRP:CD1	2.41	0.55
12:Q:451:SER:O	12:Q:454:GLU:HG3	2.07	0.55
13:R:420:VAL:HG13	13:R:421:LYS:H	1.71	0.55
14:S:406:ASN:OD1	14:S:407:ASP:N	2.40	0.55
15:T:414:LEU:HD12	15:T:418:ILE:HB	1.88	0.55
2:F:77:LYS:HE2	4:H:89:ARG:HH22	1.70	0.55
3:G:46:GLY:O	3:G:49:VAL:HG22	2.07	0.55
7:K:629:LYS:O	7:K:631:LYS:NZ	2.39	0.55
7:K:742:THR:HB	7:K:1004:HIS:HB3	1.87	0.55
11:P:222:HIS:NE2	11:P:268:ASP:OD1	2.32	0.55
13:R:358:ASP:OD1	13:R:359:LYS:N	2.39	0.55
13:R:977:ILE:C	13:R:981:ARG:HE	2.14	0.55
14:S:137:ILE:HB	14:S:178:ASP:OD1	2.06	0.55
14:S:228:VAL:HG21	14:S:376:LYS:HG2	1.87	0.55
14:S:309:ASP:HB3	14:S:312:TYR:CD2	2.41	0.55
17:V:308:THR:O	17:V:312:GLN:NE2	2.33	0.55
8:L:96:ARG:NH1	8:L:200:PRO:HB3	2.22	0.55
8:L:215:VAL:HG22	8:L:218:ARG:HH22	1.72	0.55
10:O:208:ASP:OD1	10:O:209:ALA:N	2.39	0.55
12:Q:99:MET:SD	12:Q:103:LEU:HB2	2.47	0.55
3:G:95:LYS:HZ2	4:H:100:PRO:HB2	1.70	0.55
5:I:34:DG:H3'	5:I:35:DT:H71	1.89	0.55
7:K:1163:GLU:HB3	7:K:1165:LYS:NZ	2.21	0.55
8:L:57:HIS:HB3	8:L:81:ASP:HB2	1.88	0.55
8:L:91:PRO:HB2	8:L:103:PHE:HB2	1.88	0.55
14:S:217:GLN:O	14:S:221:GLN:HG3	2.06	0.55
3:G:81:ARG:HE	3:G:85:LEU:HD11	1.71	0.55
4:H:110:GLU:HG3	4:H:113:LYS:HE3	1.89	0.55
8:L:24:LEU:HB3	8:L:35:PRO:HB3	1.89	0.55
9:M:88:ALA:O	9:M:92:VAL:HG13	2.06	0.55
10:O:603:ARG:NH2	13:R:981:ARG:HG3	2.21	0.55
11:P:71:LYS:HZ1	11:P:75:LYS:H	1.55	0.55
11:P:337:ARG:HE	11:P:338:ASN:N	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:476:ILE:HG23	13:R:488:LEU:HG	1.89	0.55
13:R:595:LEU:HD22	13:R:600:VAL:HG11	1.89	0.55
17:V:356:GLU:O	17:V:360:LEU:HG	2.06	0.55
5:I:47:DC:H2''	5:I:48:DT:H71	1.89	0.55
5:I:130:DC:H2''	5:I:131:DA:C8	2.42	0.55
7:K:666:GLY:O	7:K:671:ARG:NH1	2.39	0.55
7:K:1026:ARG:HH11	7:K:1027:LEU:H	1.54	0.55
8:L:186:TYR:CG	8:L:524:MET:HG2	2.41	0.55
10:N:232:ARG:HG2	10:O:209:ALA:HB1	1.88	0.55
16:U:966:ARG:NH1	16:U:967:ASP:HB3	2.22	0.55
17:V:383:GLN:O	17:V:387:ILE:HG12	2.07	0.55
3:C:64:GLU:HA	4:D:45:VAL:HG11	1.89	0.54
5:I:110:DC:N4	6:J:38:DG:O6	2.37	0.54
8:L:255:LEU:HB2	8:L:502:ARG:NH2	2.22	0.54
10:O:147:ASN:OD1	10:O:148:ARG:N	2.40	0.54
10:O:595:GLU:HA	10:O:598:LEU:HG	1.89	0.54
12:Q:114:TYR:CG	12:Q:164:VAL:HG22	2.42	0.54
1:E:83:ARG:O	2:F:80:THR:HA	2.07	0.54
2:F:34:ILE:HG21	2:F:54:THR:HG21	1.89	0.54
7:K:1029:THR:N	7:K:1034:GLU:OE2	2.37	0.54
9:M:86:TRP:NE1	9:M:165:VAL:HG21	2.21	0.54
10:N:380:ARG:NE	10:N:381:ASP:H	2.04	0.54
10:O:125:TRP:CD2	10:O:134:ILE:HD11	2.42	0.54
12:Q:118:GLU:O	12:Q:164:VAL:HG21	2.06	0.54
14:S:407:ASP:O	14:S:420:ARG:HB3	2.07	0.54
14:S:549:HIS:NE2	14:S:585:PRO:HD2	2.23	0.54
5:I:46:DT:H2''	5:I:47:DC:H6	1.73	0.54
6:J:50:DT:H2''	6:J:51:DT:C5	2.42	0.54
7:K:903:GLY:O	7:K:906:GLU:HG3	2.07	0.54
9:M:390:VAL:C	9:M:391:THR:HG23	2.31	0.54
9:M:444:THR:HA	9:M:447:GLN:CD	2.32	0.54
12:Q:25:ARG:NH1	12:Q:26:TYR:H	2.06	0.54
15:T:357:PHE:O	15:T:360:VAL:HG12	2.06	0.54
1:E:46:VAL:HA	1:E:49:ARG:HB2	1.89	0.54
4:H:87:THR:HG22	4:H:90:GLU:HG2	1.89	0.54
5:I:87:DT:O4	6:J:60:DA:N6	2.40	0.54
7:K:810:ARG:HH22	7:K:1053:GLN:HG2	1.72	0.54
10:N:180:ARG:HG2	10:N:190:ILE:HG21	1.88	0.54
10:N:583:LYS:C	10:N:587:LYS:HZ2	2.15	0.54
10:O:605:LEU:O	10:O:609:ARG:HG2	2.07	0.54
10:O:606:GLU:HA	10:O:609:ARG:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:443:GLU:O	14:S:446:GLU:HG3	2.06	0.54
8:L:15:VAL:HG21	8:L:680:LEU:HA	1.89	0.54
9:M:227:TRP:O	9:M:231:GLN:HG2	2.08	0.54
10:N:393:LEU:O	10:N:396:LEU:N	2.40	0.54
10:O:163:ILE:O	10:O:167:ARG:HG2	2.08	0.54
14:S:161:THR:HB	14:S:164:LEU:HD21	1.90	0.54
17:V:461:VAL:O	17:V:465:LEU:HG	2.07	0.54
6:J:19:DA:H2''	6:J:20:DC:H5'	1.89	0.54
7:K:594:TRP:HZ3	7:K:607:LEU:HD23	1.71	0.54
7:K:694:ILE:HD11	7:K:722:LYS:HD2	1.89	0.54
7:K:1002:ASN:OD1	7:K:1005:GLN:NE2	2.36	0.54
8:L:21:GLN:OE1	8:L:21:GLN:N	2.41	0.54
10:O:216:VAL:HG22	15:T:381:PHE:HB3	1.90	0.54
11:P:313:THR:H	11:P:316:GLU:CD	2.14	0.54
12:Q:313:TRP:HZ3	17:V:386:ARG:HD3	1.72	0.54
1:E:131:ARG:HG3	1:E:133:GLU:HG2	1.90	0.54
5:I:33:DG:H2''	5:I:34:DG:H5''	1.90	0.54
7:K:835:LEU:HB3	7:K:1138:LEU:HD11	1.89	0.54
7:K:928:MET:HB3	7:K:931:ILE:HG12	1.89	0.54
7:K:939:LEU:HD21	7:K:974:MET:HG3	1.89	0.54
9:M:301:PRO:HA	9:M:406:HIS:CE1	2.43	0.54
10:N:384:TRP:HE1	10:N:413:ARG:NH1	2.06	0.54
10:O:620:LYS:HB3	10:O:624:ARG:HH21	1.72	0.54
11:P:161:ALA:HB3	11:P:279:ASP:HB3	1.89	0.54
11:P:224:PHE:HA	11:P:290:ARG:HA	1.90	0.54
14:S:153:VAL:HG11	14:S:157:SER:HB3	1.89	0.54
3:C:18:SER:O	3:C:22:GLY:N	2.41	0.54
3:C:90:ASP:OD1	3:C:91:GLU:N	2.41	0.54
7:K:561:TYR:HB3	7:K:802:LYS:NZ	2.23	0.54
7:K:940:ARG:NH2	7:K:945:HIS:HA	2.22	0.54
7:K:947:LEU:HD13	7:K:972:TYR:CE2	2.42	0.54
10:O:115:HIS:C	10:O:117:ILE:H	2.16	0.54
11:P:231:PHE:H	11:P:233:LYS:NZ	2.06	0.54
14:S:162:HIS:N	14:S:163:PRO:HD2	2.23	0.54
15:T:503:GLU:OE1	15:T:509:ARG:NH1	2.41	0.54
4:D:51:ILE:HG21	4:D:56:MET:HE2	1.89	0.54
7:K:185:ARG:NH1	10:O:425:LEU:O	2.41	0.54
7:K:1120:TYR:O	7:K:1131:ARG:NH1	2.41	0.54
8:L:214:GLU:HG3	8:L:218:ARG:HH11	1.73	0.54
11:P:298:GLU:OE1	11:P:298:GLU:N	2.40	0.54
12:Q:388:LYS:O	12:Q:392:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:LEU:O	3:C:87:VAL:HG22	2.08	0.54
5:I:119:DC:H2''	5:I:120:DA:C8	2.42	0.54
8:L:114:MET:HA	8:L:114:MET:HE3	1.89	0.54
10:N:186:ASP:CG	10:N:188:CYS:HB3	2.31	0.54
10:N:245:ILE:HA	10:O:118:ILE:O	2.08	0.54
11:P:348:ILE:HG13	11:P:349:ILE:HD12	1.90	0.54
12:Q:77:ARG:NH2	12:Q:80:GLU:OE1	2.40	0.54
8:L:59:TYR:CZ	8:L:61:ARG:HB2	2.43	0.53
9:M:148:MET:O	9:M:178:SER:OG	2.22	0.53
10:N:468:PHE:HE2	10:O:473:ALA:HB1	1.73	0.53
10:N:565:GLU:HG3	11:P:450:HIS:HB3	1.89	0.53
10:O:597:MET:SD	10:O:598:LEU:N	2.82	0.53
11:P:308:ASP:O	11:P:310:LYS:N	2.40	0.53
12:Q:460:GLU:HA	12:Q:463:VAL:HG22	1.90	0.53
14:S:186:GLU:OE1	14:S:188:LEU:N	2.41	0.53
14:S:590:MET:HE2	14:S:590:MET:N	2.23	0.53
3:C:89:ASN:OD1	3:C:90:ASP:N	2.42	0.53
1:E:116:ARG:HB2	5:I:71:DG:OP1	2.08	0.53
7:K:675:GLN:HE22	7:K:699:LEU:HD21	1.73	0.53
9:M:263:PRO:HD3	9:M:327:SER:HB3	1.91	0.53
10:N:660:GLY:N	12:Q:467:ALA:O	2.41	0.53
11:P:125:LYS:HD3	11:P:400:VAL:O	2.07	0.53
12:Q:126:ARG:HH12	12:Q:154:GLY:N	2.06	0.53
12:Q:163:PRO:HG2	12:Q:166:ALA:HB2	1.90	0.53
14:S:309:ASP:OD1	14:S:311:THR:OG1	2.25	0.53
15:T:426:ASP:OD1	15:T:426:ASP:N	2.41	0.53
2:B:45:ARG:NH1	6:J:70:DG:H4'	2.24	0.53
6:J:88:DT:H2'	6:J:89:DT:C6	2.43	0.53
7:K:727:ILE:HA	7:K:731:TYR:HD1	1.73	0.53
7:K:1090:ASP:OD1	7:K:1090:ASP:N	2.40	0.53
8:L:169:ASN:ND2	8:L:527:ALA:HB1	2.22	0.53
11:P:482:ALA:HA	17:V:305:ARG:HG3	1.90	0.53
14:S:194:PHE:O	14:S:197:GLN:HG3	2.08	0.53
6:J:44:DA:C5	6:J:45:DT:C4	2.96	0.53
7:K:582:GLY:HA3	7:K:655:TRP:HH2	1.74	0.53
10:N:248:GLY:N	10:O:116:ALA:HB2	2.23	0.53
10:N:616:ARG:HB2	12:Q:419:ARG:HH11	1.74	0.53
10:O:118:ILE:CD1	10:O:167:ARG:HD3	2.37	0.53
11:P:461:VAL:HA	11:P:465:LYS:NZ	2.18	0.53
17:V:325:ALA:H	17:V:362:ARG:NH1	2.00	0.53
7:K:399:MET:O	7:K:401:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:712:GLU:HA	7:K:714:HIS:CE1	2.44	0.53
7:K:898:LEU:HG	7:K:899:TRP:N	2.23	0.53
7:K:939:LEU:HD23	7:K:946:TYR:CD1	2.41	0.53
10:N:201:GLY:O	10:N:205:TYR:HB2	2.08	0.53
10:N:417:GLU:O	10:N:421:GLN:N	2.37	0.53
14:S:438:SER:OG	14:S:439:LYS:N	2.42	0.53
15:T:385:THR:C	15:T:386:MET:HE2	2.34	0.53
15:T:480:PRO:HA	15:T:483:ARG:NH1	2.23	0.53
7:K:486:ALA:HB3	7:K:489:ALA:HA	1.89	0.53
7:K:810:ARG:HH11	7:K:1057:PHE:HE2	1.55	0.53
7:K:1034:GLU:O	7:K:1038:LEU:HG	2.09	0.53
9:M:71:PHE:N	9:M:275:HIS:HB2	2.24	0.53
12:Q:126:ARG:HG2	12:Q:126:ARG:NH1	2.20	0.53
14:S:17:PRO:HD3	14:S:105:TYR:CE1	2.42	0.53
15:T:430:GLU:HG2	15:T:496:TRP:HH2	1.74	0.53
17:V:517:MET:O	17:V:521:GLN:HG2	2.08	0.53
7:K:443:VAL:HA	7:K:446:ALA:HB3	1.91	0.53
8:L:177:TYR:H	8:L:537:ASN:HD21	1.55	0.53
8:L:248:TYR:CA	8:L:547:ASN:OD1	2.56	0.53
8:L:255:LEU:HB2	8:L:502:ARG:CZ	2.39	0.53
8:L:526:PRO:O	8:L:529:TRP:N	2.41	0.53
9:M:235:MET:HE1	9:M:334:GLN:CG	2.38	0.53
10:N:548:ASN:HA	10:N:551:LEU:HD12	1.90	0.53
10:O:117:ILE:CD1	10:O:119:LEU:HD23	2.39	0.53
14:S:411:THR:HG21	14:S:417:ALA:O	2.09	0.53
1:A:131:ARG:HG3	1:A:133:GLU:HG2	1.90	0.53
6:J:78:DG:H1'	6:J:79:DT:C2	2.44	0.53
7:K:639:ILE:HD11	7:K:710:ILE:HG23	1.91	0.53
8:L:514:ARG:HH11	9:M:285:ARG:NH2	2.06	0.53
10:N:163:ILE:HD13	10:N:203:ILE:HD11	1.91	0.53
10:N:583:LYS:NZ	11:P:429:ILE:O	2.41	0.53
10:O:142:PHE:CZ	10:O:150:LYS:HE2	2.44	0.53
13:R:997:ASN:OD1	13:R:999:LEU:N	2.42	0.53
17:V:465:LEU:HA	17:V:468:ILE:HD12	1.91	0.53
3:C:77:ARG:NH1	4:D:51:ILE:O	2.42	0.53
3:C:78:ILE:HB	4:D:51:ILE:HD12	1.91	0.53
4:D:69:ARG:HB3	4:D:98:LEU:HD11	1.91	0.53
6:J:56:DG:H4'	7:K:691:GLU:OE1	2.08	0.53
7:K:746:ASN:N	7:K:750:GLU:OE2	2.38	0.53
7:K:789:THR:N	7:K:792:GLU:OE2	2.39	0.53
7:K:1067:ASP:HA	7:K:1070:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:199:GLN:HG3	10:O:200:TRP:CD1	2.37	0.53
10:O:401:GLU:HG2	10:O:402:ASP:H	1.74	0.53
11:P:289:TYR:HE2	11:P:372:PRO:HB3	1.72	0.53
12:Q:367:LYS:HG3	12:Q:368:LEU:H	1.73	0.53
14:S:312:TYR:HD1	14:S:335:LEU:HD21	1.74	0.53
15:T:487:ASP:O	15:T:490:ARG:HB3	2.09	0.53
1:E:106:ASP:OD2	1:E:131:ARG:NH2	2.42	0.53
7:K:295:ARG:NH1	7:K:296:GLN:O	2.42	0.53
7:K:606:ILE:HG12	7:K:758:VAL:HG21	1.90	0.53
9:M:32:ASN:O	9:M:34:ARG:NH2	2.42	0.53
9:M:69:ALA:HB2	9:M:272:PHE:HB2	1.90	0.53
10:O:148:ARG:NH1	14:S:414:GLY:O	2.42	0.53
12:Q:163:PRO:HG2	12:Q:166:ALA:CB	2.39	0.53
12:Q:388:LYS:HA	12:Q:391:ILE:HG12	1.91	0.53
4:H:92:GLN:CD	4:H:108:VAL:HG23	2.33	0.52
5:I:39:DA:C6	5:I:40:DG:C6	2.96	0.52
7:K:926:PHE:HB2	7:K:932:MET:SD	2.49	0.52
8:L:177:TYR:N	8:L:537:ASN:OD1	2.42	0.52
10:N:609:ARG:HE	10:N:612:LEU:HD22	1.74	0.52
11:P:126:ARG:NH1	11:P:403:PRO:HD3	2.23	0.52
12:Q:10:VAL:HA	12:Q:205:ILE:HB	1.90	0.52
12:Q:126:ARG:HG3	12:Q:152:HIS:HB3	1.90	0.52
1:A:106:ASP:OD2	1:A:131:ARG:NH2	2.42	0.52
3:C:17:ARG:CZ	6:J:30:DG:H3'	2.39	0.52
6:J:110:DA:H1'	6:J:111:DC:H5'	1.92	0.52
7:K:318:ILE:O	7:K:322:ARG:HG2	2.09	0.52
7:K:344:LYS:NZ	7:K:346:GLU:O	2.42	0.52
7:K:811:ARG:NH2	7:K:1057:PHE:O	2.43	0.52
9:M:147:LEU:HG	9:M:176:TRP:HD1	1.74	0.52
9:M:235:MET:HE2	9:M:331:TRP:HZ3	1.73	0.52
10:N:215:HIS:CE1	10:N:219:PRO:HD3	2.45	0.52
10:N:222:GLY:O	10:N:224:PHE:HD1	1.92	0.52
11:P:419:ASN:HA	11:P:422:TYR:HD2	1.73	0.52
11:P:426:LEU:CD2	17:V:360:LEU:HB2	2.28	0.52
12:Q:25:ARG:NH1	12:Q:67:ILE:O	2.42	0.52
14:S:577:MET:HA	14:S:580:ARG:HG3	1.91	0.52
6:J:79:DT:H4'	6:J:80:DA:H5'	1.91	0.52
10:N:623:VAL:HG23	12:Q:423:GLN:HE22	1.75	0.52
11:P:95:TYR:HA	11:P:98:LEU:HD12	1.90	0.52
14:S:219:ARG:O	14:S:222:LEU:HB2	2.09	0.52
5:I:31:DT:H1'	5:I:32:DT:H5'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:663:VAL:C	7:K:674:GLN:HE22	2.16	0.52
7:K:876:ASN:O	7:K:997:TYR:OH	2.26	0.52
9:M:90:THR:HA	9:M:93:TRP:HE3	1.74	0.52
11:P:137:THR:HG21	11:P:164:ARG:HH21	1.75	0.52
13:R:366:SER:HB3	14:S:116:ASN:HB2	1.91	0.52
13:R:559:LEU:HA	13:R:562:MET:HB2	1.92	0.52
4:D:91:ILE:O	4:D:95:VAL:HG23	2.09	0.52
6:J:53:DG:H2''	6:J:54:DC:H5'	1.91	0.52
7:K:641:PRO:O	7:K:644:THR:OG1	2.27	0.52
7:K:736:ARG:NH2	7:K:760:PRO:HD3	2.22	0.52
8:L:555:ARG:HA	9:M:254:LYS:O	2.10	0.52
10:O:181:ARG:HH12	15:T:353:GLU:HG3	1.74	0.52
11:P:303:LEU:O	11:P:307:VAL:HG22	2.09	0.52
11:P:452:PHE:HB2	13:R:428:GLN:HE21	1.74	0.52
12:Q:44:ALA:HA	12:Q:47:ILE:HD12	1.92	0.52
12:Q:114:TYR:CE1	12:Q:167:ILE:HG21	2.41	0.52
13:R:463:LEU:HB2	13:R:499:LEU:HD21	1.90	0.52
3:G:63:LEU:HD11	4:H:38:VAL:HG23	1.92	0.52
7:K:562:TYR:CD2	7:K:806:PRO:HA	2.45	0.52
9:M:216:ARG:NH1	11:P:351:ARG:HH22	2.07	0.52
10:N:598:LEU:HA	10:N:601:GLU:OE1	2.09	0.52
10:O:117:ILE:HG23	10:O:170:PRO:CG	2.39	0.52
7:K:183:ALA:O	7:K:186:MET:HG2	2.10	0.52
7:K:373:LEU:HD23	10:N:422:PHE:CD2	2.45	0.52
7:K:876:ASN:ND2	7:K:931:ILE:HD13	2.17	0.52
9:M:72:GLU:HG2	9:M:275:HIS:NE2	2.25	0.52
10:N:322:ASN:ND2	10:N:351:CYS:SG	2.80	0.52
3:C:24:GLN:N	3:C:56:GLU:OE2	2.42	0.52
3:C:34:LEU:HD21	3:C:51:LEU:HD23	1.91	0.52
7:K:1004:HIS:O	7:K:1008:GLN:N	2.39	0.52
10:O:613:PHE:O	10:O:617:LEU:HG	2.10	0.52
12:Q:9:ASN:O	12:Q:205:ILE:N	2.29	0.52
12:Q:83:THR:HB	12:Q:180:ARG:HD2	1.91	0.52
13:R:344:PHE:CE1	13:R:348:HIS:CE1	2.97	0.52
13:R:1001:ALA:O	13:R:1002:PRO:C	2.52	0.52
14:S:426:LEU:N	14:S:428:GLU:OE1	2.42	0.52
7:K:595:MET:SD	7:K:607:LEU:HD21	2.50	0.52
7:K:877:HIS:CD2	7:K:878:PRO:HD2	2.43	0.52
8:L:666:TRP:HA	8:L:669:HIS:HB2	1.91	0.52
10:N:136:ARG:HA	10:N:143:PHE:CE2	2.45	0.52
11:P:103:ARG:HD3	17:V:368:PHE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:300:SER:HB3	11:P:303:LEU:HB3	1.91	0.52
12:Q:156:ALA:HB3	12:Q:161:ARG:HG2	1.92	0.52
14:S:231:HIS:CD2	14:S:384:LEU:HD23	2.45	0.52
14:S:318:LEU:HD11	14:S:366:ALA:HB1	1.92	0.52
15:T:414:LEU:HD23	15:T:414:LEU:H	1.75	0.52
6:J:102:DA:C6	6:J:103:DG:C6	2.98	0.52
9:M:53:HIS:HB2	9:M:74:ARG:HH12	1.74	0.52
9:M:168:GLU:HG2	9:M:169:ASN:N	2.25	0.52
10:N:566:GLU:HG2	11:P:86:ILE:HG12	1.91	0.52
10:N:613:PHE:HZ	10:N:661:MET:HE1	1.73	0.52
10:O:133:ASP:O	10:O:136:ARG:HG2	2.09	0.52
11:P:397:ARG:NH1	12:Q:469:VAL:O	2.43	0.52
9:M:219:GLN:HB3	9:M:368:LEU:HD22	1.91	0.51
10:N:221:THR:HB	10:N:224:PHE:HE1	1.74	0.51
12:Q:111:ARG:O	12:Q:124:SER:HB3	2.09	0.51
13:R:485:LEU:O	13:R:489:LYS:HG2	2.10	0.51
13:R:600:VAL:HG23	13:R:982:LEU:HD21	1.92	0.51
14:S:336:LEU:HD23	14:S:336:LEU:H	1.75	0.51
15:T:349:GLU:O	15:T:353:GLU:N	2.25	0.51
15:T:430:GLU:HG2	15:T:496:TRP:CH2	2.46	0.51
15:T:494:GLU:O	15:T:498:ALA:N	2.34	0.51
17:V:510:HIS:CE1	17:V:512:PRO:HD3	2.46	0.51
3:G:78:ILE:HG13	3:G:78:ILE:O	2.11	0.51
9:M:294:VAL:HG13	9:M:319:ARG:HB2	1.93	0.51
10:N:163:ILE:HA	10:N:203:ILE:HD11	1.92	0.51
10:N:175:THR:O	10:N:176:VAL:C	2.53	0.51
10:N:254:THR:HG22	10:O:117:ILE:HA	1.92	0.51
10:N:348:CYS:HB3	10:N:351:CYS:HB3	1.92	0.51
5:I:12:DC:H2"	5:I:13:DG:C8	2.45	0.51
7:K:341:ASP:HA	7:K:347:LEU:HD21	1.92	0.51
7:K:887:GLN:HG2	7:K:1142:TYR:OH	2.10	0.51
8:L:20:SER:HB2	8:L:537:ASN:ND2	2.25	0.51
9:M:304:TYR:HB3	9:M:340:GLU:HG2	1.92	0.51
10:N:271:GLU:OE2	15:T:428:HIS:HB3	2.11	0.51
10:N:592:ASN:HA	10:N:595:GLU:CD	2.35	0.51
10:N:609:ARG:CD	12:Q:412:LYS:HD3	2.36	0.51
11:P:445:HIS:O	11:P:449:LYS:HG2	2.10	0.51
11:P:529:VAL:HA	15:T:521:TYR:OH	2.10	0.51
12:Q:467:ALA:HB1	12:Q:469:VAL:HG23	1.92	0.51
13:R:451:ARG:NH2	13:R:452:ASN:HA	2.25	0.51
14:S:112:LYS:HE3	14:S:112:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:828:ILE:H	7:K:1028:ILE:HD13	1.76	0.51
7:K:898:LEU:O	7:K:901:THR:HB	2.10	0.51
8:L:217:THR:HG1	8:L:238:LYS:HZ3	1.56	0.51
8:L:348:ARG:NH1	8:L:351:ASN:HD21	2.00	0.51
8:L:355:TYR:HB2	8:L:488:ARG:HB3	1.93	0.51
8:L:503:ARG:HH21	8:L:507:ARG:HE	1.58	0.51
9:M:41:GLU:O	9:M:434:ILE:HG12	2.10	0.51
10:N:639:GLU:HA	10:N:642:PHE:CE2	2.46	0.51
12:Q:318:LEU:C	12:Q:321:PRO:HD2	2.34	0.51
13:R:353:SER:OG	13:R:452:ASN:ND2	2.42	0.51
15:T:355:SER:O	15:T:359:SER:N	2.34	0.51
8:L:544:LEU:O	8:L:548:ILE:HG12	2.10	0.51
9:M:25:VAL:O	9:M:433:TRP:NE1	2.42	0.51
13:R:346:LEU:HD12	13:R:442:LEU:HD12	1.93	0.51
13:R:361:LYS:H	13:R:364:GLN:HE22	1.58	0.51
1:A:84:PHE:CE2	2:B:81:VAL:HG21	2.46	0.51
5:I:15:DT:H2''	5:I:16:DG:C8	2.46	0.51
6:J:56:DG:C4	6:J:57:DT:C4	2.99	0.51
6:J:58:DT:H4'	6:J:59:DA:H5'	1.93	0.51
6:J:68:DG:H2''	6:J:69:DG:C8	2.46	0.51
7:K:873:LYS:O	7:K:876:ASN:HB3	2.10	0.51
7:K:914:LYS:HD2	7:K:1107:PHE:CD2	2.46	0.51
7:K:1035:GLU:HA	7:K:1038:LEU:HD12	1.93	0.51
7:K:1109:LYS:O	7:K:1113:GLU:HG2	2.11	0.51
9:M:53:HIS:HA	9:M:57:ARG:O	2.11	0.51
10:N:177:THR:OG1	14:S:201:ASP:OD2	2.28	0.51
10:O:204:ASN:HD21	10:O:212:ARG:NH1	2.08	0.51
10:O:214:SER:OG	15:T:384:ARG:N	2.44	0.51
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.46	0.51
2:F:92:ARG:NH2	4:H:98:LEU:HA	2.26	0.51
3:G:88:ARG:NH2	3:G:100:VAL:O	2.44	0.51
7:K:377:ILE:HG22	7:K:381:MET:HE1	1.93	0.51
9:M:333:GLU:OE2	9:M:334:GLN:NE2	2.44	0.51
9:M:441:SER:O	9:M:442:LEU:HB3	2.10	0.51
10:N:395:ALA:HB2	10:N:409:TYR:CD2	2.45	0.51
10:N:416:GLU:C	10:N:418:CYS:N	2.65	0.51
10:N:616:ARG:NH1	12:Q:419:ARG:HB2	2.25	0.51
11:P:177:ASP:O	11:P:178:PRO:C	2.53	0.51
12:Q:414:ALA:O	12:Q:415:GLU:C	2.54	0.51
13:R:558:ILE:HA	13:R:561:LYS:HE3	1.91	0.51
13:R:611:LEU:HD11	13:R:920:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:973:ARG:HH21	13:R:974:ILE:HD11	1.76	0.51
7:K:185:ARG:CZ	10:O:425:LEU:HB2	2.40	0.51
7:K:345:ASP:CG	16:U:895:GLY:H	2.19	0.51
7:K:369:LYS:HZ3	10:N:396:LEU:HD12	1.76	0.51
7:K:914:LYS:O	7:K:918:THR:HG23	2.11	0.51
10:N:254:THR:CG2	10:O:117:ILE:HD13	2.34	0.51
10:O:243:PRO:HD2	15:T:510:ARG:NH1	2.25	0.51
11:P:517:VAL:HG13	11:P:518:TRP:CD1	2.45	0.51
13:R:516:MET:HE2	13:R:516:MET:HA	1.92	0.51
7:K:456:LYS:HD2	8:L:685:LEU:HD13	1.92	0.51
8:L:150:PRO:O	8:L:707:ARG:N	2.43	0.51
8:L:506:ASP:HB3	8:L:507:ARG:NH2	2.25	0.51
9:M:235:MET:HE2	9:M:331:TRP:CZ3	2.45	0.51
10:N:331:TYR:CE2	10:N:369:MET:HB2	2.46	0.51
10:N:542:THR:O	10:N:545:GLN:N	2.44	0.51
10:O:617:LEU:O	10:O:621:ARG:HG2	2.10	0.51
11:P:464:VAL:HG22	11:P:465:LYS:NZ	2.26	0.51
11:P:517:VAL:HG13	11:P:518:TRP:HD1	1.75	0.51
12:Q:23:THR:HG23	12:Q:53:PRO:O	2.10	0.51
13:R:375:PHE:CZ	13:R:442:LEU:HB3	2.46	0.51
13:R:537:ARG:HB2	13:R:540:MET:HG2	1.93	0.51
13:R:1009:SER:O	13:R:1012:GLU:N	2.42	0.51
1:E:124:ILE:HG12	2:F:50:ILE:HD11	1.93	0.51
3:G:78:ILE:HG12	4:H:51:ILE:HA	1.94	0.51
8:L:44:PHE:HE2	8:L:57:HIS:HB2	1.75	0.51
8:L:129:PRO:HB3	8:L:193:GLN:CD	2.36	0.51
10:N:608:ALA:C	10:N:610:GLN:N	2.66	0.51
11:P:94:ALA:O	11:P:98:LEU:HG	2.10	0.51
11:P:219:ARG:H	11:P:222:HIS:CE1	2.29	0.51
11:P:356:ILE:HD12	11:P:356:ILE:H	1.75	0.51
11:P:467:TRP:O	11:P:470:SER:OG	2.28	0.51
13:R:417:LEU:O	13:R:421:LYS:HG2	2.11	0.51
9:M:284:GLU:HA	9:M:287:LEU:HD12	1.91	0.50
13:R:1007:LEU:O	13:R:1008:PHE:C	2.52	0.50
7:K:744:LEU:HD23	7:K:1048:ASP:HA	1.92	0.50
7:K:766:ALA:O	7:K:770:ASP:N	2.27	0.50
7:K:1023:ARG:H	7:K:1099:ARG:HH21	1.58	0.50
10:N:254:THR:HG22	10:O:117:ILE:CB	2.40	0.50
10:N:350:THR:HA	10:N:353:LEU:HD23	1.94	0.50
10:N:580:MET:O	10:N:583:LYS:HB2	2.10	0.50
13:R:570:ASP:O	13:R:574:LEU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:355:LEU:HD12	14:S:359:TRP:CD1	2.47	0.50
14:S:549:HIS:HB3	14:S:574:CYS:SG	2.51	0.50
14:S:550:CYS:HB3	14:S:574:CYS:SG	2.50	0.50
16:U:893:GLN:NE2	16:U:901:LEU:HD21	2.24	0.50
16:U:974:ARG:O	16:U:977:GLN:HG3	2.11	0.50
1:E:88:ALA:O	1:E:92:LEU:HD12	2.12	0.50
7:K:987:ASN:ND2	18:K:1601:ADP:H5'1	2.26	0.50
7:K:989:GLN:NE2	7:K:1017:GLY:HA3	2.25	0.50
7:K:1033:VAL:HA	7:K:1036:LYS:HG2	1.93	0.50
8:L:217:THR:HB	8:L:231:TYR:OH	2.11	0.50
9:M:48:PRO:HD2	9:M:61:GLY:HA2	1.94	0.50
10:N:175:THR:O	10:N:178:ALA:HB3	2.11	0.50
10:N:276:ILE:HD12	15:T:424:VAL:HG22	1.93	0.50
10:O:242:ASP:OD1	15:T:510:ARG:NH2	2.44	0.50
12:Q:36:GLU:HG2	12:Q:40:TRP:CZ3	2.46	0.50
13:R:373:THR:HG21	13:R:466:TYR:HE2	1.77	0.50
14:S:135:ILE:HB	14:S:180:PHE:HB2	1.93	0.50
14:S:180:PHE:CE2	14:S:194:PHE:CE2	2.99	0.50
6:J:116:DA:C5	6:J:117:DA:C6	3.00	0.50
8:L:216:PHE:HB2	8:L:238:LYS:HD2	1.93	0.50
10:N:179:CYS:O	10:N:180:ARG:C	2.55	0.50
10:N:392:LEU:O	10:N:396:LEU:HD23	2.10	0.50
11:P:99:ARG:O	11:P:102:GLU:HG3	2.10	0.50
12:Q:115:ARG:O	12:Q:118:GLU:HB2	2.10	0.50
12:Q:162:LEU:HD11	12:Q:167:ILE:HG13	1.93	0.50
13:R:338:LEU:HB2	13:R:341:GLU:OE2	2.12	0.50
1:A:100:LEU:HD23	2:B:37:LEU:HD13	1.92	0.50
2:F:34:ILE:HB	2:F:51:TYR:CE1	2.44	0.50
7:K:999:SER:H	7:K:1026:ARG:NH2	2.10	0.50
8:L:25:ALA:O	8:L:36:ALA:N	2.44	0.50
8:L:545:LYS:HE3	8:L:656:THR:HB	1.93	0.50
10:N:162:MET:HE1	10:N:194:HIS:HB2	1.93	0.50
10:N:243:PRO:HB2	10:O:119:LEU:CD1	2.36	0.50
10:N:609:ARG:HD3	12:Q:412:LYS:NZ	2.25	0.50
10:O:121:SER:O	10:O:122:TYR:C	2.54	0.50
10:O:597:MET:O	10:O:600:ALA:N	2.45	0.50
11:P:171:LEU:HD21	11:P:223:PHE:CZ	2.47	0.50
13:R:535:LEU:HD13	13:R:538:ILE:HD11	1.93	0.50
1:E:74:ILE:HG21	2:F:62:LEU:CD2	2.42	0.50
7:K:377:ILE:HG22	7:K:381:MET:SD	2.52	0.50
7:K:638:VAL:HG21	7:K:685:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1159:ARG:O	7:K:1162:ARG:HB2	2.12	0.50
8:L:57:HIS:O	8:L:80:GLU:HG2	2.11	0.50
9:M:24:LEU:N	9:M:145:PRO:O	2.43	0.50
9:M:183:LEU:HD13	9:M:436:GLY:CA	2.41	0.50
9:M:396:LEU:HD21	9:M:425:THR:HG23	1.93	0.50
10:N:189:ALA:O	10:N:192:ARG:N	2.44	0.50
10:N:270:LEU:HD12	10:N:270:LEU:O	2.12	0.50
12:Q:110:GLN:HG3	12:Q:125:ARG:NH2	2.27	0.50
14:S:189:ILE:HD11	14:S:193:TYR:HD2	1.76	0.50
14:S:421:TYR:CZ	14:S:423:PRO:HB3	2.47	0.50
4:H:38:VAL:HG21	4:H:59:MET:HG2	1.94	0.50
6:J:68:DG:H4'	6:J:69:DG:H5'	1.92	0.50
7:K:354:LYS:HD2	10:N:369:MET:HG3	1.94	0.50
7:K:457:LEU:HB3	8:L:166:LYS:HD3	1.93	0.50
7:K:736:ARG:HG2	7:K:757:PHE:O	2.11	0.50
9:M:298:TRP:CG	9:M:304:TYR:HB2	2.46	0.50
9:M:403:ARG:HE	9:M:406:HIS:CD2	2.29	0.50
10:N:206:GLN:HE22	13:R:321:LEU:HA	1.76	0.50
10:N:414:THR:O	10:N:415:ARG:HG2	2.11	0.50
10:N:639:GLU:HA	10:N:642:PHE:CD2	2.47	0.50
10:O:162:MET:HE1	10:O:194:HIS:HA	1.93	0.50
10:O:179:CYS:O	10:O:183:LEU:N	2.40	0.50
11:P:461:VAL:CA	11:P:465:LYS:HZ3	2.17	0.50
15:T:467:LEU:HD11	15:T:486:PHE:CE1	2.47	0.50
2:F:29:ILE:HG13	2:F:29:ILE:O	2.11	0.50
2:F:75:HIS:HD2	4:H:93:THR:HG21	1.75	0.50
3:G:59:THR:OG1	4:H:59:MET:HE2	2.12	0.50
5:I:15:DT:H2''	5:I:16:DG:N7	2.26	0.50
5:I:64:DC:H2''	5:I:65:DA:C8	2.47	0.50
6:J:65:DC:H2''	6:J:66:DG:C8	2.47	0.50
7:K:994:VAL:HG21	7:K:1013:ALA:CB	2.37	0.50
8:L:91:PRO:HB3	8:L:99:GLN:HB2	1.94	0.50
8:L:675:MET:SD	8:L:676:PHE:N	2.85	0.50
9:M:303:LYS:HA	9:M:403:ARG:NH2	2.27	0.50
11:P:69:SER:OG	17:V:321:ASP:N	2.45	0.50
12:Q:114:TYR:CD1	12:Q:167:ILE:HD13	2.47	0.50
14:S:242:LYS:NZ	14:S:580:ARG:O	2.37	0.50
1:A:88:ALA:O	1:A:92:LEU:HD12	2.12	0.50
2:F:75:HIS:NE2	4:H:90:GLU:OE1	2.44	0.50
5:I:60:DA:C6	5:I:61:DA:C6	2.99	0.50
7:K:459:ARG:HA	7:K:462:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:736:ARG:HH12	7:K:760:PRO:HD3	1.76	0.50
7:K:995:ILE:HD11	7:K:1027:LEU:HD11	1.94	0.50
8:L:252:HIS:O	8:L:255:LEU:HD23	2.11	0.50
9:M:107:THR:HA	9:M:138:GLU:HB2	1.92	0.50
10:N:535:ASN:OD1	10:N:536:GLY:N	2.45	0.50
10:O:117:ILE:C	10:O:117:ILE:HD12	2.36	0.50
10:O:187:VAL:HA	10:O:190:ILE:HD13	1.94	0.50
11:P:59:GLN:HG3	11:P:60:GLN:H	1.77	0.50
12:Q:96:GLN:HE22	12:Q:106:GLU:HG3	1.76	0.50
14:S:246:ASP:OD1	14:S:249:THR:OG1	2.26	0.50
15:T:392:ARG:HH22	15:T:499:LYS:HE2	1.77	0.50
17:V:348:SER:O	17:V:352:LEU:N	2.39	0.50
17:V:464:ILE:O	17:V:468:ILE:HG13	2.12	0.50
3:C:62:ILE:HD13	3:C:93:LEU:HD13	1.93	0.49
7:K:1002:ASN:O	7:K:1005:GLN:NE2	2.45	0.49
8:L:503:ARG:NE	8:L:503:ARG:HA	2.27	0.49
12:Q:62:PRO:O	12:Q:86:TYR:OH	2.30	0.49
15:T:400:GLU:OE1	15:T:400:GLU:N	2.45	0.49
3:G:35:ARG:HG2	3:G:35:ARG:HH11	1.77	0.49
5:I:22:DG:H1'	5:I:23:DC:H5'	1.94	0.49
7:K:521:LEU:O	7:K:524:SER:OG	2.27	0.49
7:K:801:HIS:CE1	7:K:805:ARG:HD3	2.47	0.49
8:L:56:TYR:CE2	8:L:82:VAL:HG13	2.47	0.49
10:N:181:ARG:HE	14:S:26:LEU:HD12	1.77	0.49
10:N:380:ARG:NH1	15:T:421:ASN:HB3	2.27	0.49
10:N:610:GLN:C	10:N:612:LEU:N	2.70	0.49
11:P:115:ASP:HA	13:R:609:ARG:NH1	2.21	0.49
11:P:445:HIS:CE1	11:P:449:LYS:HD2	2.47	0.49
12:Q:415:GLU:CD	12:Q:419:ARG:HE	2.19	0.49
13:R:1005:ALA:O	13:R:1006:SER:C	2.53	0.49
14:S:117:ARG:HG3	14:S:121:HIS:HB2	1.93	0.49
15:T:377:THR:O	15:T:379:THR:N	2.44	0.49
17:V:516:GLU:HG3	17:V:520:TYR:CE2	2.47	0.49
1:A:108:ASN:ND2	2:B:42:GLY:O	2.45	0.49
3:G:29:ARG:NH2	4:H:33:SER:O	2.30	0.49
5:I:67:DG:H2''	5:I:68:DT:OP2	2.12	0.49
8:L:239:ARG:HG2	8:L:540:ARG:HE	1.78	0.49
9:M:233:ARG:HH21	9:M:283:GLU:HB3	1.78	0.49
10:N:254:THR:HG23	10:O:117:ILE:HB	1.94	0.49
10:N:320:CYS:HB2	10:N:323:CYS:HB2	1.94	0.49
10:N:604:GLU:HG3	11:P:404:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:374:ASP:O	12:Q:378:LYS:HG2	2.12	0.49
14:S:420:ARG:HD3	14:S:430:TRP:CZ3	2.47	0.49
14:S:446:GLU:O	14:S:449:ARG:HG3	2.12	0.49
17:V:395:ARG:HA	17:V:398:ASN:ND2	2.26	0.49
7:K:374:ARG:HH22	10:N:423:LEU:CA	2.08	0.49
8:L:533:VAL:HA	8:L:656:THR:HG23	1.94	0.49
9:M:140:PRO:HD2	9:M:170:TRP:HA	1.95	0.49
9:M:166:VAL:HA	9:M:170:TRP:HE3	1.77	0.49
10:N:236:PRO:O	10:N:238:GLN:NE2	2.45	0.49
10:O:199:GLN:NE2	15:T:466:GLY:O	2.41	0.49
10:O:584:LEU:HD12	11:P:101:PHE:HE2	1.78	0.49
13:R:477:LEU:O	13:R:489:LYS:NZ	2.45	0.49
14:S:163:PRO:HA	14:S:166:LYS:HD3	1.95	0.49
14:S:414:GLY:O	14:S:415:GLU:C	2.54	0.49
3:C:106:GLY:HA3	1:E:58:THR:HG22	1.94	0.49
4:H:37:TYR:OH	6:J:122:DG:H5"	2.11	0.49
7:K:357:ALA:HA	7:K:360:GLU:HG2	1.95	0.49
8:L:547:ASN:O	8:L:551:THR:OG1	2.28	0.49
10:N:126:PHE:CE1	10:N:159:ARG:NH1	2.80	0.49
10:N:251:ASN:H	10:O:115:HIS:CE1	2.31	0.49
10:O:571:ARG:NH1	10:O:572:LEU:HD23	2.26	0.49
13:R:333:ALA:HB3	13:R:345:ALA:HB2	1.94	0.49
13:R:420:VAL:HG13	13:R:421:LYS:N	2.27	0.49
13:R:608:VAL:O	13:R:611:LEU:HB2	2.12	0.49
16:U:957:ALA:O	16:U:961:LEU:HB2	2.13	0.49
7:K:345:ASP:OD1	16:U:894:LEU:HB2	2.12	0.49
7:K:632:GLN:HE22	7:K:635:PRO:HD2	1.77	0.49
7:K:876:ASN:HA	7:K:997:TYR:HE2	1.77	0.49
8:L:134:PRO:HG2	9:M:103:PRO:HD2	1.95	0.49
9:M:78:ASN:ND2	9:M:82:MET:HB2	2.27	0.49
9:M:142:THR:HA	9:M:171:GLY:O	2.12	0.49
10:O:173:TYR:HE1	10:O:204:ASN:HD21	1.59	0.49
10:O:571:ARG:HD3	12:Q:380:VAL:CG1	2.41	0.49
11:P:281:ASN:CA	11:P:379:ILE:O	2.47	0.49
12:Q:319:LEU:C	12:Q:323:GLN:HE22	2.18	0.49
1:A:63:ARG:HH21	6:J:60:DA:H4'	1.76	0.49
2:B:57:VAL:O	2:B:60:VAL:HG22	2.12	0.49
1:E:96:SER:HB2	2:F:58:LEU:HD11	1.94	0.49
2:F:51:TYR:CE2	2:F:55:ARG:NH2	2.80	0.49
5:I:74:DC:H2"	5:I:75:DT:OP2	2.13	0.49
5:I:101:DG:C5	5:I:102:DG:C6	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:54:DC:H1'	6:J:55:DG:C8	2.47	0.49
7:K:776:PRO:HG3	7:K:796:VAL:HG11	1.95	0.49
8:L:34:PRO:HG2	8:L:669:HIS:NE2	2.27	0.49
9:M:174:ALA:HB1	9:M:449:TRP:HB3	1.95	0.49
9:M:196:ILE:HG23	9:M:205:VAL:HG22	1.94	0.49
9:M:298:TRP:HD1	9:M:403:ARG:CZ	2.25	0.49
10:N:232:ARG:O	10:N:235:GLN:HG2	2.13	0.49
10:N:678:GLU:HG2	11:P:272:ILE:HA	1.95	0.49
11:P:322:TRP:O	11:P:325:ILE:HG22	2.12	0.49
12:Q:312:GLU:HA	12:Q:315:GLU:HG3	1.95	0.49
12:Q:473:VAL:HG22	12:Q:475:ARG:HE	1.78	0.49
14:S:229:ALA:HA	14:S:375:LYS:HZ1	1.77	0.49
14:S:233:LEU:HD23	14:S:236:ALA:HB2	1.93	0.49
6:J:77:DC:H2''	6:J:78:DG:N7	2.27	0.49
6:J:123:DC:H2''	6:J:124:DG:C8	2.47	0.49
7:K:440:ARG:NH1	7:K:441:ASN:OD1	2.44	0.49
8:L:95:GLY:C	8:L:130:GLN:HB2	2.37	0.49
10:N:283:HIS:HD2	10:O:225:LYS:HE3	1.77	0.49
10:N:611:GLN:O	10:N:615:ASP:N	2.45	0.49
10:O:137:LYS:HZ3	15:T:473:GLU:HG3	1.77	0.49
10:O:174:LEU:HA	15:T:358:ASN:HD21	1.78	0.49
11:P:144:GLN:OE1	11:P:146:ASN:HB2	2.13	0.49
12:Q:83:THR:HG22	12:Q:176:LEU:HD21	1.94	0.49
14:S:427:ALA:O	14:S:428:GLU:C	2.55	0.49
15:T:443:VAL:HB	15:T:465:LYS:HZ3	1.77	0.49
7:K:712:GLU:HG2	7:K:984:LEU:HD22	1.93	0.49
7:K:1105:ALA:HA	7:K:1108:GLN:NE2	2.27	0.49
8:L:215:VAL:HA	8:L:218:ARG:CZ	2.43	0.49
9:M:95:TYR:O	9:M:99:GLN:HB3	2.13	0.49
10:N:646:GLN:HA	10:N:649:LEU:HG	1.95	0.49
11:P:118:ASP:HB2	13:R:609:ARG:NH2	2.28	0.49
11:P:122:ARG:NH1	11:P:123:ASN:O	2.45	0.49
12:Q:11:HIS:ND1	12:Q:205:ILE:O	2.36	0.49
12:Q:375:GLU:OE2	12:Q:379:ARG:HD2	2.12	0.49
15:T:392:ARG:HH12	15:T:499:LYS:HD2	1.77	0.49
15:T:491:GLU:HA	15:T:494:GLU:CD	2.38	0.49
3:G:56:GLU:HA	3:G:59:THR:HG22	1.95	0.49
7:K:840:TYR:OH	7:K:1033:VAL:HG23	2.13	0.49
9:M:263:PRO:HB3	9:M:327:SER:H	1.78	0.49
10:O:148:ARG:HH12	14:S:414:GLY:C	2.21	0.49
10:O:214:SER:HB2	15:T:384:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:410:VAL:HG12	10:O:413:ARG:H	1.77	0.49
11:P:315:GLN:O	11:P:319:MET:HG2	2.13	0.49
13:R:1010:LEU:O	13:R:1011:LEU:C	2.56	0.49
15:T:433:PRO:HD3	15:T:496:TRP:CE3	2.47	0.49
16:U:893:GLN:NE2	16:U:897:SER:O	2.46	0.49
5:I:82:DC:H2''	5:I:83:DG:C8	2.48	0.48
6:J:45:DT:H3'	6:J:46:DC:C6	2.48	0.48
7:K:803:VAL:O	7:K:806:PRO:HD2	2.13	0.48
7:K:945:HIS:HD2	7:K:972:TYR:CD1	2.31	0.48
9:M:147:LEU:HD11	9:M:439:LEU:CD2	2.42	0.48
9:M:304:TYR:H	9:M:340:GLU:CD	2.21	0.48
10:N:161:PHE:CD2	10:N:183:LEU:HD21	2.48	0.48
10:N:350:THR:HA	10:N:353:LEU:HB2	1.94	0.48
10:O:568:GLU:OE2	10:O:571:ARG:NH2	2.46	0.48
10:O:589:LYS:O	10:O:592:ASN:N	2.46	0.48
10:O:611:GLN:HG3	10:O:612:LEU:H	1.78	0.48
11:P:131:ARG:HH21	11:P:393:ILE:HG12	1.79	0.48
11:P:476:ASP:O	11:P:479:LEU:HB2	2.13	0.48
14:S:547:CYS:HB2	14:S:571:CYS:HB3	1.95	0.48
15:T:467:LEU:HB3	15:T:493:GLU:OE1	2.12	0.48
2:B:25:ASN:OD1	2:B:25:ASN:N	2.45	0.48
4:D:73:GLU:OE1	4:D:73:GLU:HA	2.13	0.48
2:F:32:PRO:O	2:F:36:ARG:HG3	2.13	0.48
7:K:664:TYR:HA	7:K:674:GLN:OE1	2.13	0.48
7:K:1026:ARG:C	7:K:1027:LEU:HD12	2.38	0.48
8:L:175:ILE:N	8:L:535:VAL:O	2.25	0.48
9:M:236:TRP:HZ3	9:M:245:VAL:HA	1.77	0.48
10:N:347:LEU:HD11	10:N:357:PHE:HB3	1.95	0.48
10:O:625:GLU:HA	10:O:628:GLU:HG3	1.94	0.48
11:P:175:GLU:CD	11:P:175:GLU:H	2.19	0.48
12:Q:318:LEU:O	12:Q:321:PRO:HD2	2.13	0.48
13:R:428:GLN:HG3	13:R:430:SER:H	1.77	0.48
13:R:500:THR:HA	13:R:503:MET:SD	2.53	0.48
13:R:1000:LEU:C	13:R:1004:VAL:HG23	2.37	0.48
14:S:413:GLY:C	14:S:415:GLU:N	2.71	0.48
14:S:426:LEU:C	14:S:428:GLU:N	2.69	0.48
16:U:845:VAL:C	16:U:847:THR:H	2.20	0.48
3:C:74:LYS:O	3:C:75:LYS:HD2	2.14	0.48
3:G:24:GLN:NE2	4:H:41:VAL:HA	2.28	0.48
7:K:370:GLN:HE22	10:N:425:LEU:HG	1.78	0.48
7:K:691:GLU:O	7:K:694:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:111:HIS:NE2	8:L:115:THR:HG21	2.29	0.48
10:N:176:VAL:O	10:N:177:THR:C	2.54	0.48
10:N:626:VAL:HG21	10:O:619:PHE:CZ	2.48	0.48
10:O:162:MET:HE3	10:O:179:CYS:SG	2.54	0.48
12:Q:474:HIS:HE1	12:Q:476:ILE:HB	1.79	0.48
13:R:994:PHE:HB2	13:R:1004:VAL:HG11	1.96	0.48
15:T:428:HIS:CD2	15:T:428:HIS:C	2.91	0.48
15:T:445:PHE:CZ	15:T:497:PHE:HB3	2.47	0.48
15:T:472:ASP:HA	15:T:475:ARG:HG2	1.95	0.48
16:U:963:LYS:HA	16:U:966:ARG:CD	2.43	0.48
3:C:16:THR:HG23	3:C:19:SER:H	1.78	0.48
5:I:114:DG:C2	5:I:115:DT:C2	3.02	0.48
6:J:27:DC:H2''	6:J:28:DT:C5	2.48	0.48
8:L:666:TRP:O	8:L:670:GLY:N	2.45	0.48
9:M:166:VAL:HA	9:M:170:TRP:CE3	2.49	0.48
9:M:396:LEU:HG	9:M:429:ARG:HD3	1.94	0.48
10:N:186:ASP:OD2	10:N:188:CYS:HB3	2.13	0.48
10:N:471:SER:O	10:N:475:PRO:HD2	2.13	0.48
10:O:226:ILE:HG12	10:O:238:GLN:HB2	1.95	0.48
12:Q:26:TYR:HB2	12:Q:67:ILE:HB	1.95	0.48
13:R:918:SER:O	13:R:922:ILE:HG12	2.13	0.48
13:R:922:ILE:O	13:R:926:ILE:HG12	2.12	0.48
13:R:983:PHE:HE2	13:R:1007:LEU:HD11	1.78	0.48
16:U:960:LEU:O	16:U:964:VAL:HG23	2.12	0.48
7:K:453:LYS:HD3	8:L:188:GLY:HA3	1.96	0.48
8:L:515:ALA:O	8:L:518:SER:OG	2.25	0.48
9:M:190:LYS:HB2	9:M:193:ALA:HB2	1.96	0.48
9:M:252:GLU:HB2	9:M:268:ARG:HB2	1.96	0.48
9:M:312:PHE:O	9:M:315:THR:OG1	2.24	0.48
10:N:212:ARG:HB3	10:O:234:LEU:HD23	1.96	0.48
10:N:616:ARG:HB2	12:Q:419:ARG:NH1	2.28	0.48
10:N:647:GLU:CD	10:N:648:VAL:HG13	2.38	0.48
10:O:117:ILE:C	10:O:118:ILE:HD13	2.39	0.48
14:S:179:THR:HB	14:S:365:HIS:ND1	2.29	0.48
16:U:964:VAL:HG13	16:U:968:TRP:CE3	2.49	0.48
7:K:689:THR:OG1	7:K:691:GLU:HG2	2.14	0.48
7:K:1162:ARG:O	7:K:1163:GLU:C	2.56	0.48
9:M:54:VAL:HB	9:M:71:PHE:HD1	1.78	0.48
9:M:397:LEU:HB2	9:M:400:PHE:CE2	2.49	0.48
10:N:572:LEU:HD13	11:P:443:VAL:CG2	2.37	0.48
12:Q:417:GLU:O	12:Q:420:PHE:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:587:TRP:CD1	14:S:588:THR:HG23	2.48	0.48
15:T:451:ASP:OD1	15:T:452:TYR:N	2.45	0.48
3:G:26:PRO:HG2	3:G:29:ARG:HB3	1.94	0.48
6:J:35:DT:H2''	6:J:36:DA:N7	2.28	0.48
7:K:615:LYS:NZ	7:K:739:LEU:HG	2.26	0.48
9:M:52:GLY:HA2	9:M:73:VAL:HA	1.94	0.48
9:M:234:SER:HA	9:M:352:LEU:HD11	1.96	0.48
9:M:236:TRP:HB3	9:M:243:VAL:O	2.13	0.48
10:N:186:ASP:OD1	10:N:188:CYS:HB3	2.13	0.48
10:N:222:GLY:HA2	15:T:419:SER:OG	2.12	0.48
10:N:371:ASN:O	10:N:373:THR:OG1	2.29	0.48
10:O:148:ARG:NH2	14:S:415:GLU:O	2.38	0.48
11:P:324:TYR:O	11:P:327:LEU:HB2	2.14	0.48
13:R:405:ASP:OD2	13:R:409:GLY:N	2.46	0.48
13:R:466:TYR:O	13:R:469:VAL:HG12	2.14	0.48
17:V:471:MET:HE1	17:V:519:ALA:C	2.39	0.48
5:I:118:DC:N4	6:J:29:DG:O6	2.46	0.48
5:I:128:DG:H2''	5:I:129:DT:H5'	1.95	0.48
6:J:43:DA:C5	6:J:44:DA:C5	3.01	0.48
7:K:645:LEU:HD21	7:K:958:ARG:HD2	1.96	0.48
7:K:903:GLY:HA2	7:K:906:GLU:CG	2.43	0.48
7:K:908:LEU:HD12	7:K:911:ILE:HD11	1.95	0.48
9:M:233:ARG:HD2	9:M:237:LYS:HE2	1.96	0.48
9:M:305:LEU:HG	9:M:347:ALA:HB2	1.95	0.48
10:N:254:THR:HA	10:O:117:ILE:HD13	1.95	0.48
10:N:592:ASN:HA	10:N:595:GLU:OE2	2.14	0.48
10:N:615:ASP:O	10:N:618:THR:N	2.42	0.48
10:O:410:VAL:HG11	10:O:413:ARG:HB2	1.95	0.48
13:R:565:TRP:CD1	13:R:573:LEU:HD21	2.48	0.48
14:S:450:GLU:O	14:S:454:ARG:HG3	2.13	0.48
14:S:456:LEU:O	14:S:460:THR:HG23	2.13	0.48
17:V:478:TYR:HE2	17:V:482:ARG:HH21	1.62	0.48
1:A:83:ARG:NH2	5:I:101:DG:H4'	2.28	0.48
4:H:58:ILE:O	4:H:61:SER:OG	2.28	0.48
7:K:383:HIS:HA	7:K:389:MET:CE	2.44	0.48
8:L:156:HIS:HB3	8:L:159:LEU:HB2	1.95	0.48
10:N:320:CYS:O	10:N:324:GLY:N	2.46	0.48
11:P:112:LYS:HA	11:P:112:LYS:HD2	1.63	0.48
11:P:279:ASP:HA	11:P:381:VAL:HG21	1.95	0.48
13:R:585:THR:O	13:R:925:ASN:HB3	2.13	0.48
16:U:893:GLN:HG2	16:U:896:HIS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:469:SER:OG	17:V:473:GLU:OE2	2.32	0.48
1:A:79:LYS:HB3	1:A:82:LEU:CD2	2.43	0.48
6:J:54:DC:OP1	7:K:929:THR:HG23	2.14	0.48
9:M:34:ARG:HB3	9:M:46:VAL:HG13	1.95	0.48
10:N:233:GLY:HA2	10:O:209:ALA:HB3	1.95	0.48
10:N:251:ASN:N	10:O:115:HIS:CE1	2.81	0.48
10:N:623:VAL:O	10:N:626:VAL:HG22	2.14	0.48
11:P:300:SER:HB3	11:P:303:LEU:CB	2.44	0.48
11:P:313:THR:HB	11:P:316:GLU:OE1	2.14	0.48
12:Q:157:GLU:O	12:Q:161:ARG:HG3	2.14	0.48
16:U:968:TRP:O	16:U:971:GLU:HG3	2.14	0.48
2:F:31:LYS:HB3	2:F:32:PRO:HD3	1.96	0.47
5:I:18:DC:C2	5:I:19:DG:C2	3.02	0.47
5:I:24:DC:H2''	5:I:25:DG:C8	2.49	0.47
7:K:427:LYS:O	7:K:431:ASP:N	2.46	0.47
7:K:455:SER:O	7:K:458:SER:HB2	2.14	0.47
7:K:1139:PRO:HD2	7:K:1142:TYR:HD2	1.79	0.47
8:L:92:MET:HE1	8:L:95:GLY:C	2.39	0.47
8:L:224:LEU:HB3	8:L:229:PHE:CD1	2.49	0.47
8:L:248:TYR:N	8:L:550:GLN:OE1	2.41	0.47
10:N:113:GLN:OE1	10:O:224:PHE:HA	2.14	0.47
10:O:125:TRP:CD1	10:O:125:TRP:H	2.32	0.47
11:P:449:LYS:HG3	11:P:450:HIS:N	2.29	0.47
12:Q:395:LYS:O	12:Q:399:GLU:HG2	2.14	0.47
13:R:586:ALA:O	13:R:929:ASN:ND2	2.37	0.47
14:S:426:LEU:HG	15:T:353:GLU:CD	2.39	0.47
15:T:471:SER:OG	15:T:473:GLU:OE1	2.28	0.47
3:C:73:ASN:OD1	3:C:75:LYS:HD3	2.14	0.47
6:J:106:DG:H5'	6:J:106:DG:C8	2.49	0.47
7:K:434:GLN:OE1	9:M:442:LEU:HB2	2.13	0.47
7:K:438:ASN:O	7:K:441:ASN:HB2	2.14	0.47
7:K:476:ILE:O	7:K:479:THR:OG1	2.26	0.47
7:K:584:LEU:HD22	7:K:588:GLN:HB3	1.97	0.47
7:K:1036:LYS:HA	7:K:1039:GLU:OE1	2.14	0.47
8:L:61:ARG:NE	8:L:62:LYS:H	2.02	0.47
8:L:242:ILE:HG22	8:L:345:ASN:CG	2.39	0.47
9:M:151:ALA:HB1	9:M:153:TRP:CZ3	2.49	0.47
10:N:417:GLU:CD	10:N:417:GLU:N	2.72	0.47
10:O:603:ARG:HH22	13:R:981:ARG:HA	1.79	0.47
10:O:612:LEU:HA	10:O:615:ASP:OD2	2.14	0.47
13:R:361:LYS:HA	13:R:459:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:413:GLY:O	14:S:415:GLU:N	2.46	0.47
14:S:586:ARG:HH21	14:S:589:LYS:HG3	1.80	0.47
3:C:81:ARG:HE	3:C:85:LEU:HD21	1.79	0.47
4:D:45:VAL:HG12	4:D:46:HIS:CE1	2.49	0.47
2:F:83:ALA:O	2:F:86:VAL:N	2.45	0.47
3:G:62:ILE:HG13	3:G:83:LEU:HD11	1.95	0.47
4:H:106:HIS:HA	14:S:455:ARG:HH12	1.79	0.47
5:I:26:DC:H2''	5:I:27:DT:H73	1.96	0.47
7:K:461:MET:HE3	7:K:462:TYR:CE1	2.49	0.47
7:K:910:ARG:HE	7:K:1114:ARG:HD2	1.79	0.47
12:Q:126:ARG:NH1	12:Q:152:HIS:HD2	2.12	0.47
13:R:466:TYR:CE2	13:R:468:PRO:HB2	2.48	0.47
14:S:577:MET:HG3	14:S:585:PRO:HG2	1.95	0.47
16:U:959:GLU:HB3	16:U:963:LYS:HZ1	1.80	0.47
3:C:74:LYS:C	3:C:75:LYS:HD2	2.39	0.47
5:I:36:DC:H2''	5:I:37:DG:C8	2.49	0.47
5:I:123:DC:H2''	5:I:124:DA:N7	2.30	0.47
7:K:185:ARG:NH1	10:O:423:LEU:O	2.48	0.47
7:K:361:MET:HG3	10:N:397:GLU:OE2	2.14	0.47
7:K:642:LEU:HB2	7:K:958:ARG:HH12	1.79	0.47
7:K:947:LEU:HD13	7:K:972:TYR:CD2	2.49	0.47
7:K:1049:GLY:HA2	7:K:1053:GLN:HB2	1.95	0.47
9:M:439:LEU:O	9:M:445:PHE:CD2	2.67	0.47
9:M:446:HIS:C	9:M:448:MET:H	2.23	0.47
13:R:1009:SER:O	13:R:1011:LEU:N	2.47	0.47
14:S:212:ALA:O	14:S:215:SER:OG	2.29	0.47
1:A:130:ILE:CD1	1:E:109:LEU:HD11	2.37	0.47
2:F:84:MET:HE1	2:F:101:GLY:HA3	1.95	0.47
5:I:29:DA:H61	6:J:118:DT:H3	1.62	0.47
5:I:68:DT:H3	6:J:80:DA:N6	2.11	0.47
6:J:42:DT:H2''	6:J:43:DA:H8	1.80	0.47
7:K:379:ARG:O	7:K:382:MET:HG3	2.14	0.47
7:K:535:LYS:NZ	7:K:734:ARG:HE	2.11	0.47
7:K:606:ILE:HG23	7:K:738:ILE:HB	1.97	0.47
8:L:34:PRO:HG2	8:L:669:HIS:CE1	2.49	0.47
8:L:44:PHE:CE2	8:L:57:HIS:HB2	2.50	0.47
8:L:143:ILE:O	8:L:147:THR:OG1	2.31	0.47
8:L:171:THR:O	8:L:533:VAL:HG22	2.14	0.47
8:L:522:ILE:O	8:L:526:PRO:HD3	2.14	0.47
10:N:176:VAL:C	10:N:180:ARG:HG3	2.40	0.47
10:N:254:THR:O	10:N:257:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:464:SER:O	10:N:467:SER:OG	2.29	0.47
11:P:87:ASP:OD1	11:P:88:HIS:N	2.47	0.47
11:P:432:LEU:HA	11:P:435:GLN:OE1	2.14	0.47
12:Q:34:LEU:HA	12:Q:37:VAL:HG22	1.95	0.47
13:R:535:LEU:O	13:R:538:ILE:HG12	2.15	0.47
14:S:355:LEU:HD21	14:S:434:LEU:HD22	1.97	0.47
14:S:404:PHE:CD1	14:S:405:PRO:HD2	2.49	0.47
1:A:108:ASN:O	1:A:112:ILE:HG12	2.14	0.47
4:H:92:GLN:OE1	4:H:108:VAL:HG23	2.15	0.47
6:J:56:DG:OP2	6:J:56:DG:H8	1.98	0.47
6:J:137:DG:C5	6:J:138:DG:C6	3.02	0.47
7:K:184:PHE:HA	7:K:187:LEU:HG	1.97	0.47
7:K:333:LEU:O	7:K:335:GLY:N	2.47	0.47
7:K:393:ARG:HB2	17:V:378:ILE:CD1	2.44	0.47
7:K:839:LEU:HA	7:K:842:GLN:CG	2.43	0.47
7:K:906:GLU:HG2	7:K:1132:LEU:HD21	1.96	0.47
9:M:60:PHE:O	9:M:100:ARG:NH2	2.47	0.47
10:N:179:CYS:O	10:N:182:ASN:N	2.42	0.47
10:O:469:LEU:HD13	12:Q:322:TYR:OH	2.15	0.47
14:S:118:SER:OG	14:S:120:VAL:HG22	2.15	0.47
15:T:446:ARG:C	15:T:449:ARG:HH22	2.22	0.47
1:A:128:ARG:CG	1:A:133:GLU:HB2	2.45	0.47
5:I:57:DT:H1'	5:I:58:DT:C2	2.49	0.47
6:J:109:DT:H2''	6:J:110:DA:C8	2.50	0.47
7:K:572:VAL:HG11	7:K:592:LEU:HG	1.96	0.47
7:K:612:GLY:N	18:K:1601:ADP:O2B	2.48	0.47
7:K:616:THR:N	18:K:1601:ADP:O1B	2.43	0.47
7:K:896:ASP:O	7:K:900:ARG:HG3	2.15	0.47
7:K:1023:ARG:HB3	7:K:1099:ARG:HH21	1.78	0.47
8:L:514:ARG:HH21	8:L:517:GLN:C	2.23	0.47
9:M:286:VAL:HA	9:M:289:GLU:CD	2.39	0.47
9:M:332:ARG:O	9:M:335:ARG:NE	2.44	0.47
10:N:209:ALA:HB2	14:S:9:GLN:HE22	1.80	0.47
10:N:414:THR:H	10:N:417:GLU:CD	2.23	0.47
10:N:554:MET:HG2	10:N:557:ARG:NH1	2.30	0.47
10:N:572:LEU:HD12	10:N:573:VAL:N	2.30	0.47
10:N:616:ARG:O	10:N:617:LEU:C	2.57	0.47
10:O:146:ARG:HH12	14:S:307:SER:H	1.63	0.47
11:P:339:PHE:CZ	11:P:354:GLY:HA3	2.50	0.47
12:Q:99:MET:SD	12:Q:99:MET:N	2.87	0.47
12:Q:122:VAL:HA	12:Q:161:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:412:LYS:HB2	12:Q:412:LYS:HE2	1.39	0.47
12:Q:430:TRP:CZ2	12:Q:431:ARG:HG2	2.50	0.47
15:T:365:ARG:O	15:T:368:ASN:HB3	2.15	0.47
16:U:967:ASP:OD1	16:U:968:TRP:N	2.47	0.47
2:B:70:VAL:O	2:B:74:GLU:N	2.33	0.47
4:D:106:HIS:HD2	7:K:1158:GLY:N	2.13	0.47
1:E:97:GLU:OE1	1:E:97:GLU:HA	2.15	0.47
2:F:76:ALA:HB3	2:F:78:ARG:HH11	1.80	0.47
4:H:45:VAL:HG12	4:H:46:HIS:ND1	2.29	0.47
6:J:84:DG:N7	6:J:85:DC:N4	2.63	0.47
7:K:354:LYS:HG3	7:K:355:ARG:HD3	1.97	0.47
7:K:752:TRP:HB2	7:K:769:PHE:CE2	2.49	0.47
8:L:521:ASP:HB2	8:L:524:MET:SD	2.54	0.47
9:M:310:GLU:CG	9:M:333:GLU:HG3	2.39	0.47
10:O:595:GLU:O	10:O:599:GLN:HG2	2.15	0.47
11:P:128:LYS:HZ2	11:P:173:GLU:HA	1.80	0.47
11:P:393:ILE:HB	12:Q:475:ARG:O	2.15	0.47
13:R:418:ALA:HA	13:R:421:LYS:HG2	1.96	0.47
13:R:616:LYS:O	13:R:895:GLU:HA	2.14	0.47
15:T:416:PRO:HG2	15:T:420:ARG:HH22	1.79	0.47
1:A:63:ARG:NH2	6:J:61:DA:H5'	2.29	0.47
5:I:61:DA:C2	5:I:62:DC:C2	3.02	0.47
7:K:626:LEU:O	7:K:632:GLN:N	2.41	0.47
8:L:10:GLU:O	8:L:28:GLY:HA2	2.14	0.47
8:L:21:GLN:HB3	8:L:177:TYR:HB3	1.97	0.47
8:L:159:LEU:HG	8:L:190:ILE:HD11	1.96	0.47
10:N:384:TRP:HB3	10:N:388:GLU:CG	2.42	0.47
10:N:542:THR:O	10:N:543:PRO:C	2.58	0.47
10:N:659:ASN:HB3	12:Q:466:HIS:HB2	1.96	0.47
11:P:224:PHE:CD1	11:P:290:ARG:HB2	2.50	0.47
11:P:452:PHE:CE1	13:R:428:GLN:HB2	2.49	0.47
11:P:476:ASP:HA	11:P:479:LEU:HD12	1.97	0.47
12:Q:19:HIS:CE1	12:Q:82:ALA:HB3	2.50	0.47
12:Q:77:ARG:HA	12:Q:77:ARG:HH11	1.79	0.47
12:Q:156:ALA:O	12:Q:161:ARG:NE	2.48	0.47
14:S:363:LEU:O	14:S:367:ILE:HG12	2.14	0.47
15:T:427:THR:OG1	15:T:428:HIS:N	2.48	0.47
16:U:910:GLU:HG2	16:U:913:ARG:HH22	1.79	0.47
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.15	0.47
4:D:115:VAL:O	4:D:119:THR:HG23	2.14	0.47
2:F:47:SER:OG	2:F:48:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:38:VAL:HG11	4:H:56:MET:HE1	1.97	0.47
5:I:16:DG:C6	6:J:133:DA:N1	2.83	0.47
7:K:460:HIS:ND1	8:L:166:LYS:HB2	2.30	0.47
7:K:636:TYR:HA	7:K:707:HIS:O	2.15	0.47
7:K:708:MET:HE3	7:K:736:ARG:HG3	1.97	0.47
9:M:165:VAL:HG13	9:M:169:ASN:OD1	2.15	0.47
9:M:277:SER:O	9:M:281:PHE:HD2	1.98	0.47
10:N:655:PRO:HD2	11:P:308:ASP:CG	2.40	0.47
10:O:242:ASP:HA	15:T:510:ARG:NH1	2.30	0.47
10:O:416:GLU:HG2	10:O:417:GLU:N	2.29	0.47
13:R:417:LEU:O	13:R:421:LYS:N	2.47	0.47
13:R:462:PHE:HD2	13:R:463:LEU:HD23	1.80	0.47
13:R:621:GLU:OE1	13:R:623:VAL:HG23	2.14	0.47
3:C:84:GLN:HE22	3:C:88:ARG:HH21	1.63	0.46
2:F:35:ARG:HE	2:F:46:ILE:HD12	1.81	0.46
6:J:82:DG:H2'	6:J:83:DT:H71	1.97	0.46
7:K:483:ARG:HD2	7:K:487:LEU:HD21	1.96	0.46
7:K:727:ILE:HG23	7:K:731:TYR:HB2	1.97	0.46
7:K:1105:ALA:HA	7:K:1108:GLN:HE21	1.79	0.46
9:M:431:GLY:HA2	9:M:434:ILE:HD12	1.97	0.46
10:N:591:PHE:O	10:N:594:MET:HB2	2.15	0.46
10:O:568:GLU:HG2	10:O:571:ARG:HH21	1.80	0.46
11:P:309:MET:O	11:P:312:ALA:HB2	2.16	0.46
11:P:397:ARG:HE	12:Q:471:LYS:HA	1.79	0.46
14:S:161:THR:CB	14:S:164:LEU:HD21	2.45	0.46
14:S:208:GLN:HB2	14:S:599:PHE:CD2	2.50	0.46
14:S:423:PRO:HA	15:T:341:VAL:HG11	1.96	0.46
1:A:62:ILE:HD11	2:B:37:LEU:HD11	1.96	0.46
1:E:108:ASN:O	1:E:112:ILE:HG12	2.14	0.46
1:E:128:ARG:CG	1:E:133:GLU:HB2	2.45	0.46
6:J:94:DG:C2	6:J:95:DG:C4	3.04	0.46
7:K:378:GLY:HA2	7:K:381:MET:HE2	1.97	0.46
7:K:987:ASN:HA	7:K:1015:ARG:NH1	2.30	0.46
7:K:1165:LYS:H	7:K:1165:LYS:HZ3	1.61	0.46
8:L:156:HIS:CE1	8:L:158:GLY:H	2.33	0.46
9:M:28:PRO:HA	9:M:33:THR:HA	1.96	0.46
9:M:279:ARG:HH11	9:M:283:GLU:CD	2.23	0.46
9:M:304:TYR:HB3	9:M:340:GLU:CG	2.45	0.46
10:N:117:ILE:HB	10:O:226:ILE:HG22	1.97	0.46
10:N:248:GLY:CA	10:O:116:ALA:HB2	2.45	0.46
10:N:254:THR:HG22	10:O:117:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:131:ILE:HD12	10:O:143:PHE:CZ	2.48	0.46
11:P:71:LYS:HB3	11:P:73:THR:O	2.14	0.46
3:C:26:PRO:HB3	4:D:37:TYR:HE1	1.80	0.46
7:K:1099:ARG:H	7:K:1103:GLU:CD	2.23	0.46
8:L:256:MET:HE1	8:L:547:ASN:ND2	2.16	0.46
9:M:263:PRO:HB3	9:M:327:SER:N	2.31	0.46
9:M:299:ARG:CD	9:M:402:ASP:HB3	2.44	0.46
9:M:311:ASP:O	9:M:315:THR:HG23	2.15	0.46
9:M:318:GLY:HA3	9:M:332:ARG:HA	1.97	0.46
10:N:187:VAL:HG12	14:S:181:LEU:O	2.15	0.46
10:N:251:ASN:HB2	10:O:115:HIS:CG	2.51	0.46
10:N:605:LEU:O	10:N:609:ARG:N	2.38	0.46
10:N:609:ARG:HH21	10:N:612:LEU:HD22	1.80	0.46
10:O:119:LEU:N	10:O:206:GLN:HE21	2.14	0.46
10:O:591:PHE:O	10:O:595:GLU:OE1	2.34	0.46
12:Q:42:LEU:O	12:Q:45:PRO:HD2	2.16	0.46
14:S:413:GLY:HA3	14:S:415:GLU:OE2	2.15	0.46
1:A:103:LEU:O	1:A:107:THR:HG23	2.15	0.46
6:J:55:DG:H5"	7:K:981:ALA:HB2	1.96	0.46
7:K:185:ARG:NH2	10:O:425:LEU:HB2	2.31	0.46
8:L:150:PRO:HA	8:L:707:ARG:HB2	1.97	0.46
8:L:358:LEU:HD22	8:L:483:THR:O	2.15	0.46
10:N:618:THR:HG22	10:N:621:ARG:HE	1.80	0.46
10:N:621:ARG:NH2	10:N:657:ALA:O	2.49	0.46
10:O:142:PHE:CG	10:O:155:TYR:HB2	2.50	0.46
12:Q:24:PHE:HA	17:V:480:ARG:NH2	2.30	0.46
12:Q:70:THR:O	12:Q:148:LEU:HA	2.15	0.46
14:S:409:ALA:O	14:S:410:PRO:C	2.58	0.46
1:E:51:ILE:CG2	2:F:39:ARG:HD2	2.45	0.46
7:K:647:ASN:O	7:K:650:LEU:HG	2.15	0.46
7:K:675:GLN:HA	7:K:678:ILE:HG12	1.97	0.46
8:L:31:GLU:HB3	8:L:33:THR:HG23	1.97	0.46
10:N:186:ASP:HB3	10:N:189:ALA:HB2	1.97	0.46
10:N:316:MET:SD	10:N:316:MET:N	2.89	0.46
11:P:279:ASP:O	11:P:381:VAL:HG11	2.15	0.46
11:P:340:ARG:H	11:P:340:ARG:HG3	1.51	0.46
12:Q:111:ARG:HB3	12:Q:160:ASP:OD2	2.16	0.46
12:Q:303:SER:HB3	12:Q:307:TYR:HE2	1.81	0.46
12:Q:415:GLU:HA	12:Q:418:LEU:HD23	1.96	0.46
13:R:331:LEU:O	13:R:335:ARG:HG2	2.15	0.46
15:T:456:LEU:HD13	15:T:462:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:465:LYS:HD2	15:T:465:LYS:C	2.40	0.46
17:V:357:LEU:HD12	17:V:358:GLU:N	2.30	0.46
4:D:85:THR:HG23	6:J:40:DA:OP1	2.16	0.46
7:K:965:PHE:CE1	7:K:975:PHE:HB2	2.51	0.46
7:K:1113:GLU:OE1	7:K:1116:ARG:NE	2.36	0.46
8:L:152:LEU:O	8:L:705:LEU:HD23	2.16	0.46
8:L:200:PRO:C	8:L:202:VAL:H	2.24	0.46
9:M:43:PRO:HB3	9:M:433:TRP:CG	2.51	0.46
10:N:598:LEU:HD21	10:O:594:MET:HB3	1.97	0.46
10:N:660:GLY:O	12:Q:467:ALA:N	2.42	0.46
11:P:59:GLN:HG2	11:P:63:HIS:HB2	1.97	0.46
13:R:397:ASP:OD1	13:R:397:ASP:N	2.49	0.46
15:T:389:THR:HG23	15:T:390:HIS:ND1	2.31	0.46
1:A:70:LEU:O	1:A:74:ILE:HG22	2.16	0.46
4:D:92:GLN:HG2	4:D:108:VAL:HG23	1.98	0.46
1:E:124:ILE:CG1	2:F:50:ILE:HD11	2.46	0.46
5:I:109:DC:O2	6:J:40:DA:H2	1.99	0.46
7:K:1062:SER:OG	7:K:1063:GLU:N	2.49	0.46
9:M:22:SER:O	9:M:144:ASN:HA	2.16	0.46
9:M:443:GLY:HA2	9:M:446:HIS:ND1	2.31	0.46
10:O:591:PHE:O	10:O:594:MET:HB2	2.16	0.46
11:P:115:ASP:CA	13:R:609:ARG:HH12	2.23	0.46
11:P:166:LYS:HG3	11:P:271:GLU:HG3	1.97	0.46
11:P:336:LYS:HG2	11:P:337:ARG:N	2.31	0.46
11:P:465:LYS:O	11:P:468:LEU:HG	2.16	0.46
12:Q:23:THR:OG1	12:Q:52:SER:HB3	2.16	0.46
13:R:983:PHE:HA	13:R:986:VAL:HG22	1.97	0.46
14:S:141:ILE:HD11	14:S:176:LEU:HB2	1.97	0.46
1:A:58:THR:HG21	3:G:81:ARG:HD3	1.98	0.46
3:C:55:LEU:HD11	4:D:67:PHE:HB2	1.97	0.46
1:E:103:LEU:O	1:E:107:THR:HG23	2.15	0.46
2:F:34:ILE:HD12	2:F:51:TYR:CE1	2.51	0.46
6:J:43:DA:H2''	6:J:44:DA:O4'	2.16	0.46
7:K:190:ASN:HD21	17:V:482:ARG:NH2	2.12	0.46
7:K:350:ASP:CG	10:N:368:ARG:HE	2.24	0.46
7:K:620:ILE:H	7:K:620:ILE:CD1	2.18	0.46
8:L:133:ARG:HA	8:L:136:HIS:ND1	2.31	0.46
9:M:185:ALA:HA	9:M:389:VAL:HG21	1.98	0.46
10:N:177:THR:HG22	10:N:180:ARG:HH21	1.81	0.46
10:N:345:TYR:CE1	10:N:358:PRO:HD2	2.51	0.46
10:N:352:TYR:C	10:N:355:GLY:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:415:ARG:HH21	17:V:531:ILE:CG1	2.26	0.46
10:O:608:ALA:O	10:O:611:GLN:HG3	2.16	0.46
10:O:628:GLU:HA	10:O:631:ARG:HE	1.81	0.46
11:P:296:ARG:HD2	11:P:311:GLU:HB3	1.97	0.46
12:Q:86:TYR:HE1	12:Q:115:ARG:CZ	2.29	0.46
13:R:350:VAL:HG22	13:R:449:THR:HB	1.97	0.46
13:R:990:LEU:HD22	13:R:1007:LEU:HD23	1.98	0.46
13:R:1007:LEU:O	13:R:1009:SER:N	2.48	0.46
15:T:456:LEU:HA	15:T:462:ALA:HB1	1.97	0.46
7:K:369:LYS:NZ	10:N:400:ASP:HA	2.31	0.46
7:K:568:ILE:O	7:K:601:ASN:ND2	2.45	0.46
10:N:181:ARG:HH21	14:S:26:LEU:HB2	1.80	0.46
10:O:162:MET:HE1	10:O:194:HIS:HB2	1.98	0.46
11:P:80:GLY:H	11:P:440:MET:HE3	1.80	0.46
12:Q:33:GLU:HB2	12:Q:36:GLU:HB3	1.97	0.46
13:R:934:ASN:O	13:R:937:ARG:HG2	2.16	0.46
14:S:144:PHE:CE1	14:S:205:PRO:HD3	2.51	0.46
3:G:50:TYR:CZ	4:H:111:GLY:HA3	2.51	0.46
4:H:115:VAL:O	4:H:119:THR:HG23	2.16	0.46
7:K:186:MET:HE1	7:K:197:MET:HE2	1.98	0.46
7:K:1004:HIS:HA	7:K:1007:LEU:HD12	1.97	0.46
7:K:1029:THR:O	7:K:1032:SER:OG	2.24	0.46
7:K:1162:ARG:NH1	7:K:1163:GLU:H	2.14	0.46
8:L:546:ASP:OD2	8:L:550:GLN:NE2	2.49	0.46
9:M:153:TRP:CZ3	9:M:220:ARG:HD3	2.51	0.46
10:N:269:ASN:HB2	15:T:428:HIS:CD2	2.51	0.46
10:N:566:GLU:HA	10:N:569:MET:HG3	1.98	0.46
10:N:643:ARG:HA	10:N:646:GLN:HG2	1.98	0.46
10:O:474:ASP:HB3	10:O:475:PRO:HD3	1.96	0.46
12:Q:303:SER:HB3	12:Q:307:TYR:CE2	2.51	0.46
13:R:1000:LEU:O	13:R:1004:VAL:HG23	2.15	0.46
14:S:211:ILE:HG13	14:S:212:ALA:N	2.31	0.46
1:A:84:PHE:CD2	2:B:81:VAL:HB	2.51	0.45
3:G:90:ASP:OD2	3:G:92:GLU:HG3	2.16	0.45
5:I:33:DG:H2"	5:I:34:DG:H8	1.81	0.45
7:K:412:LYS:O	7:K:416:GLN:HG2	2.16	0.45
7:K:528:GLN:HA	7:K:531:GLN:CG	2.46	0.45
7:K:601:ASN:HB3	7:K:603:LEU:HD12	1.98	0.45
7:K:746:ASN:H	7:K:750:GLU:CD	2.22	0.45
7:K:902:ALA:HB3	7:K:905:PHE:CD2	2.47	0.45
7:K:1088:MET:HB2	7:K:1092:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:56:TYR:CD2	8:L:82:VAL:HG13	2.50	0.45
10:O:117:ILE:HD12	10:O:119:LEU:HD23	1.97	0.45
10:O:141:GLU:HA	10:O:144:ASN:HB3	1.98	0.45
10:O:603:ARG:HH12	13:R:981:ARG:CA	2.24	0.45
14:S:138:ASP:HB2	14:S:175:ARG:HH12	1.80	0.45
6:J:55:DG:H2"	6:J:56:DG:C8	2.51	0.45
7:K:920:HIS:HB3	7:K:992:ASP:HB2	1.98	0.45
8:L:519:ILE:O	8:L:525:ARG:NE	2.50	0.45
9:M:163:ILE:HG13	9:M:175:PHE:CD2	2.51	0.45
10:N:190:ILE:O	10:N:191:MET:C	2.59	0.45
10:N:417:GLU:CA	10:N:420:LEU:HB2	2.45	0.45
10:N:602:ARG:HD3	10:N:602:ARG:HA	1.69	0.45
10:N:602:ARG:O	10:N:605:LEU:HG	2.15	0.45
10:N:660:GLY:HA3	12:Q:467:ALA:HB3	1.98	0.45
11:P:177:ASP:C	11:P:179:SER:H	2.23	0.45
14:S:117:ARG:HH11	14:S:122:ASN:HD21	1.65	0.45
14:S:147:GLN:O	14:S:168:GLN:NE2	2.50	0.45
15:T:485:ALA:O	15:T:488:ARG:HB2	2.16	0.45
1:E:49:ARG:NH1	1:E:53:ARG:HH21	2.13	0.45
5:I:77:DT:H2"	5:I:78:DC:C6	2.52	0.45
7:K:183:ALA:HA	7:K:186:MET:SD	2.56	0.45
7:K:184:PHE:CE1	17:V:468:ILE:HG12	2.51	0.45
7:K:355:ARG:O	7:K:359:ILE:HG23	2.16	0.45
7:K:456:LYS:NZ	8:L:685:LEU:HB3	2.32	0.45
7:K:652:PHE:HE1	7:K:687:LEU:HD21	1.80	0.45
7:K:677:LYS:HD3	7:K:677:LYS:HA	1.71	0.45
7:K:1023:ARG:H	7:K:1099:ARG:NH2	2.14	0.45
8:L:91:PRO:O	8:L:98:VAL:N	2.49	0.45
10:N:655:PRO:HD2	11:P:308:ASP:OD1	2.17	0.45
11:P:133:TRP:HD1	11:P:391:PRO:HB2	1.80	0.45
2:F:64:ASN:O	2:F:67:ARG:HB3	2.16	0.45
4:H:95:VAL:O	4:H:99:LEU:HB2	2.16	0.45
7:K:1100:ASN:OD1	7:K:1103:GLU:N	2.47	0.45
8:L:95:GLY:O	8:L:131:TRP:HD1	1.98	0.45
8:L:537:ASN:C	8:L:540:ARG:HH11	2.25	0.45
9:M:27:ASP:O	9:M:34:ARG:HG2	2.16	0.45
10:N:474:ASP:HB2	10:N:475:PRO:HD3	1.98	0.45
11:P:422:TYR:O	11:P:426:LEU:HB2	2.16	0.45
11:P:440:MET:O	11:P:443:VAL:HB	2.16	0.45
13:R:349:LEU:HD23	13:R:349:LEU:HA	1.79	0.45
14:S:138:ASP:O	14:S:139:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:521:GLN:HA	17:V:524:LYS:HE2	1.99	0.45
3:C:84:GLN:OE1	3:C:88:ARG:NE	2.48	0.45
5:I:43:DA:H2''	5:I:44:DG:C8	2.51	0.45
6:J:139:DA:H2'	6:J:140:DT:O4'	2.16	0.45
7:K:1108:GLN:HA	7:K:1111:ASP:OD2	2.17	0.45
9:M:319:ARG:HG3	9:M:335:ARG:HH11	1.82	0.45
10:O:144:ASN:OD1	10:O:145:ASN:N	2.49	0.45
10:O:148:ARG:HH12	14:S:415:GLU:CA	2.30	0.45
10:O:162:MET:HE1	10:O:194:HIS:CB	2.46	0.45
10:O:196:PHE:HA	15:T:464:PHE:HB3	1.98	0.45
11:P:176:GLU:CD	11:P:176:GLU:N	2.75	0.45
13:R:1007:LEU:C	13:R:1009:SER:N	2.72	0.45
14:S:197:GLN:HA	14:S:200:GLN:HE21	1.81	0.45
17:V:386:ARG:O	17:V:390:GLN:HG2	2.16	0.45
7:K:998:ASP:N	7:K:998:ASP:OD1	2.49	0.45
9:M:152:PRO:HA	9:M:179:ARG:CZ	2.47	0.45
11:P:429:ILE:CG2	17:V:364:ALA:HB1	2.46	0.45
13:R:394:PHE:O	13:R:398:CYS:N	2.49	0.45
13:R:440:LEU:O	13:R:444:ILE:HG12	2.17	0.45
13:R:980:GLU:HG2	13:R:984:ARG:HH22	1.82	0.45
14:S:113:ASN:OD1	14:S:114:LYS:N	2.50	0.45
14:S:538:THR:O	14:S:542:ARG:N	2.50	0.45
14:S:548:SER:HA	14:S:551:ARG:HH22	1.81	0.45
15:T:374:ASP:OD1	15:T:375:ILE:N	2.50	0.45
16:U:973:ASP:OD1	16:U:974:ARG:N	2.50	0.45
1:A:58:THR:CG2	3:G:81:ARG:HD3	2.47	0.45
3:C:62:ILE:HD12	3:C:62:ILE:HA	1.85	0.45
5:I:82:DC:O2	6:J:67:DG:N2	2.50	0.45
6:J:136:DG:H2''	6:J:137:DG:OP2	2.16	0.45
7:K:896:ASP:HB3	7:K:941:TYR:OH	2.17	0.45
7:K:921:ARG:HG3	7:K:990:THR:HG22	1.99	0.45
8:L:32:LEU:HD12	8:L:677:LEU:HD11	1.98	0.45
8:L:44:PHE:CE1	8:L:88:ALA:HA	2.52	0.45
10:N:124:THR:HG23	10:O:237:TRP:CZ2	2.51	0.45
10:O:466:VAL:HA	10:O:469:LEU:HB2	1.99	0.45
10:O:599:GLN:HE22	10:O:602:ARG:HH22	1.62	0.45
11:P:313:THR:N	11:P:316:GLU:OE2	2.33	0.45
12:Q:398:HIS:HA	12:Q:401:MET:HG3	1.98	0.45
13:R:1000:LEU:C	13:R:1002:PRO:HD2	2.41	0.45
14:S:107:ARG:NH1	14:S:107:ARG:HG2	2.31	0.45
17:V:308:THR:C	17:V:312:GLN:HE22	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:57:TYR:HB2	4:H:110:GLU:OE2	2.17	0.45
5:I:31:DT:C2	5:I:32:DT:C5	3.05	0.45
7:K:402:HIS:ND1	13:R:455:MET:SD	2.89	0.45
9:M:72:GLU:HA	9:M:275:HIS:ND1	2.32	0.45
9:M:445:PHE:HA	9:M:448:MET:HE2	1.97	0.45
10:N:228:VAL:O	15:T:430:GLU:N	2.36	0.45
10:N:551:LEU:HA	10:N:554:MET:HE3	1.99	0.45
10:N:611:GLN:O	10:N:614:LEU:N	2.50	0.45
10:O:611:GLN:HG3	10:O:612:LEU:HD22	1.99	0.45
11:P:328:ASN:HB2	11:P:340:ARG:NH2	2.32	0.45
11:P:377:TYR:OH	11:P:380:ARG:HG3	2.17	0.45
13:R:566:LEU:HB3	13:R:606:HIS:HD2	1.82	0.45
13:R:587:GLU:CD	13:R:589:ASP:H	2.24	0.45
13:R:983:PHE:CE2	13:R:1007:LEU:HD11	2.51	0.45
15:T:487:ASP:O	15:T:491:GLU:OE1	2.34	0.45
2:B:72:TYR:CE1	4:D:77:LEU:HD13	2.52	0.45
1:E:79:LYS:O	1:E:82:LEU:HD23	2.17	0.45
6:J:109:DT:H2"	6:J:110:DA:N7	2.32	0.45
7:K:287:ILE:HD13	12:Q:372:LEU:HD12	1.98	0.45
7:K:428:LYS:NZ	7:K:431:ASP:OD2	2.41	0.45
7:K:456:LYS:HD3	7:K:459:ARG:HD3	1.98	0.45
7:K:876:ASN:ND2	7:K:931:ILE:HG21	2.32	0.45
7:K:901:THR:HA	7:K:1133:MET:HE1	1.97	0.45
7:K:1100:ASN:HD21	7:K:1102:GLU:HB3	1.82	0.45
7:K:1119:ILE:O	7:K:1127:LYS:HB2	2.16	0.45
9:M:145:PRO:HG3	9:M:173:PRO:HG2	1.98	0.45
10:N:418:CYS:O	10:N:419:VAL:C	2.59	0.45
11:P:529:VAL:HA	15:T:521:TYR:CZ	2.52	0.45
13:R:344:PHE:CE1	13:R:348:HIS:HE1	2.35	0.45
14:S:6:ASP:OD1	14:S:7:SER:N	2.44	0.45
14:S:140:ASP:OD1	14:S:141:ILE:N	2.49	0.45
15:T:463:PRO:HG2	15:T:464:PHE:CD2	2.52	0.45
17:V:392:ILE:HG22	17:V:396:ASN:OD1	2.16	0.45
17:V:510:HIS:O	17:V:512:PRO:HD2	2.17	0.45
5:I:33:DG:C2	5:I:34:DG:C4	3.05	0.45
7:K:1018:GLN:HE21	7:K:1020:ASN:HD22	0.56	0.45
8:L:18:PRO:HA	8:L:23:THR:HA	1.99	0.45
8:L:156:HIS:CE1	8:L:183:THR:HG21	2.52	0.45
10:O:133:ASP:HA	10:O:136:ARG:NE	2.31	0.45
11:P:460:PRO:HA	11:P:463:PHE:HB3	1.99	0.45
12:Q:110:GLN:HG3	12:Q:125:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:395:ASP:OD1	13:R:396:LEU:N	2.49	0.45
13:R:451:ARG:HH21	13:R:452:ASN:HA	1.82	0.45
13:R:997:ASN:OD1	13:R:1001:ALA:N	2.42	0.45
14:S:193:TYR:O	14:S:196:THR:OG1	2.27	0.45
14:S:312:TYR:HB3	14:S:335:LEU:HG	1.98	0.45
4:D:38:VAL:HA	4:D:41:VAL:HG12	1.99	0.44
1:E:116:ARG:HH12	1:E:120:MET:HG2	1.82	0.44
5:I:79:DC:H2"	5:I:80:DC:C5	2.52	0.44
5:I:113:DA:C5	5:I:114:DG:C5	3.05	0.44
6:J:55:DG:C5	6:J:56:DG:C6	3.05	0.44
7:K:366:LEU:O	7:K:370:GLN:HB2	2.16	0.44
7:K:461:MET:O	7:K:465:HIS:ND1	2.50	0.44
7:K:896:ASP:HB2	7:K:899:TRP:NE1	2.25	0.44
7:K:1007:LEU:O	7:K:1010:GLN:HB3	2.17	0.44
9:M:254:LYS:HA	9:M:265:CYS:HA	1.98	0.44
10:N:414:THR:C	10:N:415:ARG:HG2	2.42	0.44
10:N:583:LYS:HD3	10:N:583:LYS:HA	1.59	0.44
10:N:613:PHE:HD2	12:Q:419:ARG:NH2	2.14	0.44
11:P:93:ASP:OD1	11:P:93:ASP:N	2.48	0.44
11:P:330:LEU:HB2	11:P:340:ARG:NE	2.31	0.44
12:Q:114:TYR:HD1	12:Q:121:ALA:HB2	1.81	0.44
13:R:351:LYS:HD3	13:R:351:LYS:HA	1.75	0.44
15:T:443:VAL:HG13	15:T:445:PHE:CD1	2.38	0.44
5:I:97:DA:H2"	5:I:98:DA:N7	2.31	0.44
6:J:107:DT:C2	6:J:108:DC:N3	2.85	0.44
7:K:759:LEU:HD12	7:K:760:PRO:HD2	1.99	0.44
7:K:873:LYS:C	7:K:873:LYS:HD3	2.43	0.44
7:K:945:HIS:NE2	7:K:971:PRO:HB2	2.32	0.44
7:K:1139:PRO:HB2	7:K:1141:ILE:HG12	1.99	0.44
8:L:699:ALA:O	8:L:703:MET:HG2	2.17	0.44
9:M:138:GLU:OE2	9:M:142:THR:HG21	2.18	0.44
10:N:211:GLN:OE1	15:T:522:SER:HB2	2.18	0.44
11:P:141:GLN:HA	11:P:161:ALA:HB2	1.98	0.44
12:Q:414:ALA:HA	12:Q:417:GLU:HB3	1.99	0.44
16:U:961:LEU:HD13	16:U:964:VAL:HG21	1.97	0.44
16:U:964:VAL:HG22	16:U:968:TRP:CZ3	2.51	0.44
17:V:476:ALA:O	17:V:479:GLN:NE2	2.50	0.44
2:F:76:ALA:HB2	4:H:81:ASN:HD21	1.81	0.44
4:H:95:VAL:HG13	4:H:99:LEU:HD23	2.00	0.44
6:J:53:DG:C2	6:J:54:DC:C2	3.05	0.44
7:K:454:MET:O	7:K:458:SER:N	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:691:GLU:HA	7:K:694:ILE:HG22	1.99	0.44
7:K:882:ASP:O	7:K:886:ASN:ND2	2.51	0.44
8:L:168:PRO:O	8:L:187:ASP:N	2.50	0.44
9:M:96:LEU:HA	9:M:100:ARG:HB2	1.97	0.44
10:N:161:PHE:CZ	10:N:182:ASN:HB2	2.53	0.44
10:O:141:GLU:HB2	10:O:150:LYS:NZ	2.33	0.44
14:S:207:LYS:O	14:S:211:ILE:HG12	2.17	0.44
14:S:210:THR:HA	14:S:213:GLU:OE1	2.18	0.44
14:S:415:GLU:H	14:S:415:GLU:CD	2.25	0.44
14:S:539:GLU:HA	14:S:542:ARG:HB2	2.00	0.44
4:D:40:LYS:HD3	4:D:43:LYS:HZ1	1.81	0.44
5:I:32:DT:H1'	5:I:33:DG:O4'	2.17	0.44
5:I:71:DG:C2	6:J:78:DG:N2	2.85	0.44
7:K:293:LYS:NZ	17:V:405:GLU:HA	2.33	0.44
9:M:190:LYS:HE3	9:M:420:HIS:CG	2.53	0.44
10:N:549:ILE:HG21	16:U:968:TRP:CH2	2.53	0.44
10:N:624:ARG:O	10:N:625:GLU:C	2.61	0.44
11:P:85:VAL:HG21	11:P:447:LYS:HD2	1.98	0.44
11:P:342:ASP:H	11:P:345:LEU:HD21	1.82	0.44
13:R:359:LYS:HD2	13:R:359:LYS:HA	1.69	0.44
13:R:939:GLU:HB3	13:R:977:ILE:HD11	1.98	0.44
13:R:975:LYS:HG3	13:R:1011:LEU:O	2.17	0.44
14:S:554:GLY:O	14:S:557:VAL:HG22	2.17	0.44
16:U:964:VAL:HA	16:U:968:TRP:CE3	2.52	0.44
6:J:116:DA:H2'	6:J:116:DA:OP2	2.18	0.44
7:K:607:LEU:HB3	7:K:615:LYS:NZ	2.32	0.44
7:K:793:GLN:O	7:K:797:ILE:HG23	2.17	0.44
7:K:954:LYS:O	7:K:958:ARG:HG2	2.17	0.44
7:K:1016:ILE:HB	18:K:1601:ADP:O2'	2.18	0.44
8:L:20:SER:HA	8:L:179:LYS:HD2	2.00	0.44
8:L:115:THR:HG22	8:L:121:THR:HG21	2.00	0.44
9:M:52:GLY:HA3	9:M:71:PHE:CZ	2.52	0.44
10:O:605:LEU:HG	10:O:606:GLU:N	2.32	0.44
10:O:622:ARG:O	10:O:626:VAL:HG23	2.18	0.44
11:P:322:TRP:O	11:P:326:LYS:NZ	2.42	0.44
11:P:331:GLN:H	11:P:331:GLN:CD	2.24	0.44
11:P:445:HIS:CD2	17:V:390:GLN:HE22	2.35	0.44
13:R:924:ARG:HH22	13:R:1003:TYR:HD1	1.66	0.44
15:T:491:GLU:HA	15:T:494:GLU:OE1	2.16	0.44
1:A:116:ARG:HH12	1:A:120:MET:HG2	1.82	0.44
5:I:57:DT:H6	5:I:57:DT:H2'	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:25:DG:H2''	6:J:26:DC:OP2	2.16	0.44
7:K:585:LYS:HB2	7:K:588:GLN:HG3	1.99	0.44
8:L:43:MET:HA	8:L:55:PRO:O	2.17	0.44
9:M:25:VAL:HG12	9:M:433:TRP:CD1	2.52	0.44
9:M:318:GLY:HA2	9:M:335:ARG:CZ	2.48	0.44
9:M:386:GLY:O	9:M:418:LYS:HB3	2.17	0.44
10:N:645:ALA:HB2	10:O:630:LEU:HD23	2.00	0.44
11:P:382:ASP:HB2	11:P:385:PHE:HB2	1.99	0.44
12:Q:65:GLY:HA2	12:Q:152:HIS:NE2	2.33	0.44
12:Q:88:TRP:HE3	12:Q:113:GLY:HA3	1.83	0.44
13:R:342:GLN:O	13:R:343:ALA:C	2.59	0.44
13:R:346:LEU:HB3	13:R:445:GLU:OE2	2.17	0.44
13:R:511:LEU:O	13:R:515:MET:HB2	2.17	0.44
14:S:105:TYR:HB2	14:S:107:ARG:HH22	1.82	0.44
14:S:137:ILE:O	14:S:177:ARG:HA	2.18	0.44
14:S:411:THR:O	14:S:413:GLY:N	2.51	0.44
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.50	0.44
3:G:85:LEU:O	3:G:89:ASN:HB2	2.17	0.44
6:J:73:DA:H2''	6:J:74:DG:C8	2.52	0.44
6:J:113:DA:C5	6:J:114:DC:C4	3.06	0.44
7:K:393:ARG:NH2	13:R:441:THR:HG23	2.24	0.44
7:K:420:ALA:O	7:K:424:ARG:HG2	2.17	0.44
7:K:577:SER:N	7:K:628:GLU:OE1	2.51	0.44
7:K:832:PHE:HD1	7:K:836:GLN:HB3	1.83	0.44
7:K:1055:GLY:HA3	7:K:1057:PHE:CZ	2.53	0.44
9:M:343:TRP:CZ2	9:M:404:LEU:HD22	2.53	0.44
9:M:393:SER:HA	9:M:429:ARG:HD2	1.99	0.44
10:N:176:VAL:O	10:N:179:CYS:N	2.50	0.44
10:O:151:THR:OG1	10:O:152:PRO:HD2	2.18	0.44
11:P:300:SER:HB3	11:P:303:LEU:H	1.83	0.44
12:Q:116:MET:HE3	12:Q:117:GLY:H	1.83	0.44
12:Q:467:ALA:C	12:Q:469:VAL:H	2.25	0.44
14:S:213:GLU:HA	14:S:216:LYS:HZ1	1.83	0.44
16:U:954:LYS:HB2	16:U:954:LYS:HE3	1.76	0.44
1:A:85:GLN:OE1	2:B:82:THR:HA	2.18	0.44
5:I:127:DT:H2''	5:I:128:DG:C8	2.52	0.44
6:J:42:DT:H2''	6:J:43:DA:C8	2.52	0.44
6:J:54:DC:OP2	6:J:54:DC:H2'	2.18	0.44
7:K:198:GLN:HA	7:K:201:ILE:HG22	2.00	0.44
7:K:366:LEU:O	7:K:367:TYR:C	2.59	0.44
7:K:435:ALA:O	7:K:438:ASN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:460:HIS:NE2	8:L:163:TYR:O	2.50	0.44
7:K:833:SER:OG	7:K:836:GLN:HG2	2.18	0.44
8:L:133:ARG:NH1	8:L:136:HIS:HB2	2.33	0.44
8:L:246:LEU:HB3	8:L:257:GLU:OE2	2.18	0.44
8:L:530:GLU:HA	8:L:655:LYS:HB3	2.00	0.44
10:N:221:THR:CG2	10:O:241:ALA:HA	2.47	0.44
10:N:416:GLU:O	10:N:417:GLU:C	2.60	0.44
11:P:226:ALA:HA	11:P:250:TRP:O	2.18	0.44
11:P:274:PHE:C	11:P:275:LYS:HD3	2.43	0.44
11:P:327:LEU:O	11:P:329:LYS:HD2	2.18	0.44
11:P:360:ASN:HA	11:P:363:LEU:HG	1.99	0.44
12:Q:119:GLN:HG3	12:Q:120:TYR:CZ	2.51	0.44
12:Q:415:GLU:HG3	12:Q:459:VAL:HG11	2.00	0.44
13:R:554:GLN:HE22	13:R:555:HIS:CE1	2.36	0.44
17:V:387:ILE:HG22	17:V:391:ARG:HH11	1.83	0.44
5:I:68:DT:H2"	5:I:69:DA:C8	2.53	0.44
7:K:578:ILE:O	7:K:580:VAL:HG23	2.17	0.44
7:K:699:LEU:HG	7:K:700:LEU:HD22	1.99	0.44
7:K:947:LEU:HD12	7:K:947:LEU:HA	1.87	0.44
10:N:104:ASN:OD1	10:N:105:ALA:N	2.51	0.44
10:N:186:ASP:CG	10:N:189:ALA:H	2.26	0.44
10:N:620:LYS:O	10:N:624:ARG:HG3	2.18	0.44
10:O:601:GLU:HG2	12:Q:405:PHE:HZ	1.83	0.44
11:P:69:SER:HB3	17:V:319:TRP:O	2.18	0.44
11:P:315:GLN:O	11:P:318:VAL:HG12	2.18	0.44
12:Q:379:ARG:O	12:Q:383:ARG:HG2	2.18	0.44
13:R:572:GLU:HA	13:R:575:ASP:OD2	2.18	0.44
15:T:373:TYR:OH	15:T:378:ASN:ND2	2.28	0.44
15:T:416:PRO:HB2	15:T:420:ARG:HH12	1.83	0.44
15:T:455:TRP:HE3	15:T:456:LEU:HD22	1.83	0.44
2:B:67:ARG:O	2:B:70:VAL:HG22	2.17	0.43
3:G:25:PHE:CD1	3:G:56:GLU:HG2	2.53	0.43
4:H:102:GLU:OE1	4:H:102:GLU:N	2.43	0.43
5:I:43:DA:C6	5:I:44:DG:C6	3.06	0.43
7:K:1033:VAL:O	7:K:1036:LYS:N	2.51	0.43
8:L:10:GLU:O	8:L:13:VAL:HG22	2.18	0.43
8:L:61:ARG:HB3	8:L:79:VAL:HG21	1.99	0.43
8:L:650:THR:C	8:L:652:THR:H	2.26	0.43
9:M:42:MET:HE2	9:M:42:MET:HA	1.99	0.43
10:N:602:ARG:HD2	12:Q:405:PHE:CD1	2.53	0.43
10:N:618:THR:HG22	10:N:621:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:90:GLY:O	12:Q:110:GLN:NE2	2.45	0.43
14:S:234:PHE:HB3	14:S:561:ARG:NH2	2.33	0.43
3:G:24:GLN:N	3:G:56:GLU:OE2	2.51	0.43
6:J:140:DT:H2'	6:J:141:DT:C6	2.53	0.43
7:K:289:HIS:HE1	7:K:292:ARG:HD2	1.83	0.43
7:K:1044:LYS:O	7:K:1047:MET:HG2	2.18	0.43
8:L:54:ARG:HB3	8:L:55:PRO:HD2	2.00	0.43
9:M:195:VAL:HG22	9:M:389:VAL:HB	2.00	0.43
10:N:127:ASP:CG	10:N:130:THR:HG22	2.43	0.43
10:N:186:ASP:O	10:N:189:ALA:N	2.51	0.43
11:P:419:ASN:HB3	11:P:422:TYR:HB2	2.00	0.43
12:Q:312:GLU:O	12:Q:316:GLU:OE1	2.36	0.43
12:Q:432:LEU:HD23	12:Q:432:LEU:H	1.84	0.43
13:R:364:GLN:HG2	13:R:365:PHE:N	2.33	0.43
13:R:451:ARG:HD3	13:R:491:LEU:HD13	2.00	0.43
14:S:241:ALA:O	14:S:244:THR:OG1	2.29	0.43
15:T:445:PHE:O	15:T:447:THR:HG23	2.17	0.43
3:G:62:ILE:HD11	3:G:87:VAL:HG12	1.99	0.43
5:I:19:DG:H1'	5:I:20:DA:C8	2.53	0.43
6:J:56:DG:OP2	6:J:56:DG:H2'	2.19	0.43
7:K:294:ASN:ND2	10:N:568:GLU:HB2	2.32	0.43
7:K:434:GLN:O	7:K:438:ASN:N	2.39	0.43
7:K:668:PRO:HA	7:K:671:ARG:HG3	2.00	0.43
7:K:869:MET:HE3	7:K:870:GLN:NE2	2.33	0.43
8:L:653:VAL:O	8:L:654:ILE:HG13	2.19	0.43
9:M:302:GLY:C	9:M:303:LYS:HG3	2.42	0.43
10:O:238:GLN:OE1	10:O:238:GLN:HA	2.18	0.43
11:P:128:LYS:HE2	11:P:171:LEU:HB3	2.00	0.43
11:P:134:ILE:CD1	11:P:167:ILE:HG12	2.48	0.43
11:P:297:PHE:CD2	11:P:367:LEU:HD21	2.54	0.43
12:Q:31:ARG:HG3	12:Q:33:GLU:OE2	2.17	0.43
13:R:483:ASP:O	17:V:380:PRO:HG3	2.18	0.43
15:T:446:ARG:CZ	15:T:502:ASP:HB3	2.48	0.43
2:F:75:HIS:CD2	4:H:93:THR:HG21	2.54	0.43
6:J:20:DC:H2''	6:J:21:DA:C8	2.53	0.43
6:J:94:DG:H4'	6:J:95:DG:OP1	2.16	0.43
6:J:106:DG:H2''	6:J:107:DT:OP2	2.18	0.43
7:K:899:TRP:HH2	7:K:1131:ARG:HG3	1.83	0.43
8:L:503:ARG:HH21	8:L:507:ARG:NE	2.17	0.43
9:M:75:ASN:OD1	9:M:77:MET:N	2.29	0.43
9:M:171:GLY:O	9:M:452:ARG:NE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:176:TRP:CE2	9:M:445:PHE:HE1	2.36	0.43
10:N:99:LYS:HB3	10:N:101:PHE:CE1	2.53	0.43
10:N:232:ARG:HG2	10:O:209:ALA:CB	2.48	0.43
10:O:589:LYS:O	10:O:593:GLU:OE1	2.36	0.43
12:Q:23:THR:HG22	12:Q:55:TYR:CE2	2.51	0.43
13:R:346:LEU:HA	13:R:346:LEU:HD23	1.71	0.43
13:R:493:LEU:CD2	13:R:515:MET:HE1	2.47	0.43
13:R:997:ASN:HB2	13:R:999:LEU:HD23	2.01	0.43
14:S:325:GLN:HG2	14:S:436:THR:HG23	2.00	0.43
14:S:413:GLY:C	14:S:415:GLU:H	2.26	0.43
14:S:547:CYS:SG	14:S:550:CYS:N	2.75	0.43
15:T:346:TRP:HA	15:T:349:GLU:OE1	2.18	0.43
17:V:464:ILE:HG13	17:V:526:GLN:OE1	2.18	0.43
5:I:71:DG:C2	5:I:72:DC:C2	3.06	0.43
5:I:82:DC:H2''	5:I:83:DG:H8	1.83	0.43
6:J:125:DG:C5	6:J:126:DC:C4	3.06	0.43
7:K:432:PHE:O	7:K:436:ILE:HG12	2.17	0.43
7:K:456:LYS:O	7:K:459:ARG:HG2	2.19	0.43
10:N:582:GLU:HA	10:N:585:GLU:OE2	2.18	0.43
10:O:125:TRP:CE2	10:O:134:ILE:HD11	2.54	0.43
11:P:330:LEU:O	11:P:330:LEU:HG	2.17	0.43
12:Q:413:GLN:HG3	12:Q:414:ALA:N	2.32	0.43
13:R:476:ILE:CG2	13:R:488:LEU:HG	2.47	0.43
13:R:566:LEU:O	13:R:606:HIS:NE2	2.50	0.43
13:R:623:VAL:HA	13:R:888:THR:O	2.18	0.43
14:S:136:ARG:HB2	14:S:136:ARG:HH11	1.82	0.43
16:U:902:ALA:O	16:U:905:LYS:N	2.50	0.43
1:A:48:LEU:O	1:A:51:ILE:HG12	2.18	0.43
5:I:57:DT:H2''	5:I:58:DT:OP2	2.18	0.43
6:J:38:DG:H2''	6:J:39:DG:N7	2.34	0.43
6:J:68:DG:H1'	6:J:69:DG:C4	2.54	0.43
7:K:840:TYR:HH	7:K:1033:VAL:H	1.66	0.43
8:L:516:ILE:HA	8:L:519:ILE:HD12	2.00	0.43
9:M:30:TYR:OH	9:M:79:ARG:NE	2.51	0.43
10:N:226:ILE:HG23	15:T:393:ILE:HG12	2.01	0.43
10:N:415:ARG:HG3	10:N:416:GLU:OE1	2.18	0.43
10:N:626:VAL:HA	10:N:629:VAL:HG12	2.01	0.43
11:P:160:GLU:HG3	11:P:161:ALA:N	2.34	0.43
12:Q:22:SER:HA	12:Q:54:PHE:HA	1.99	0.43
12:Q:28:THR:HB	17:V:473:GLU:OE1	2.18	0.43
12:Q:391:ILE:HA	12:Q:394:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:412:LYS:O	12:Q:416:GLN:HG2	2.18	0.43
14:S:107:ARG:HG2	14:S:107:ARG:HH11	1.83	0.43
14:S:240:ARG:O	14:S:244:THR:HG23	2.17	0.43
14:S:441:GLU:HA	14:S:444:LYS:HE2	1.99	0.43
2:B:84:MET:HE3	2:B:88:TYR:CE1	2.53	0.43
3:G:26:PRO:CG	3:G:29:ARG:HB3	2.49	0.43
3:G:77:ARG:NH1	5:I:20:DA:H4'	2.34	0.43
3:G:84:GLN:NE2	3:G:106:GLY:O	2.43	0.43
5:I:62:DC:H1'	5:I:63:DG:H5'	2.00	0.43
5:I:65:DA:H61	6:J:83:DT:H3	1.65	0.43
5:I:117:DT:H1'	5:I:118:DC:H5'	2.01	0.43
7:K:427:LYS:HG3	7:K:428:LYS:N	2.34	0.43
7:K:650:LEU:HA	7:K:653:GLU:HG3	2.00	0.43
7:K:795:LEU:O	7:K:799:ARG:HG2	2.17	0.43
8:L:126:MET:CE	8:L:127:ALA:H	2.24	0.43
8:L:248:TYR:CA	8:L:547:ASN:CG	2.92	0.43
8:L:355:TYR:O	8:L:487:ARG:HA	2.18	0.43
9:M:53:HIS:CG	9:M:74:ARG:HH22	2.36	0.43
10:N:584:LEU:HD13	10:O:584:LEU:HD21	2.01	0.43
10:O:407:ALA:HA	10:O:418:CYS:SG	2.58	0.43
10:O:611:GLN:CG	10:O:612:LEU:N	2.81	0.43
12:Q:114:TYR:CE1	12:Q:167:ILE:HD13	2.54	0.43
13:R:461:TRP:HE3	13:R:502:TYR:CE2	2.35	0.43
13:R:493:LEU:HD23	13:R:493:LEU:HA	1.83	0.43
2:B:98:TYR:CE2	3:G:100:VAL:HG21	2.54	0.43
3:C:70:ALA:HA	3:C:82:HIS:CD2	2.54	0.43
1:E:57:SER:OG	1:E:58:THR:N	2.52	0.43
2:F:75:HIS:O	4:H:89:ARG:NH2	2.51	0.43
5:I:48:DT:C4	5:I:49:DA:C6	3.07	0.43
5:I:60:DA:H2''	5:I:61:DA:H8	1.84	0.43
6:J:57:DT:H2''	6:J:58:DT:C6	2.54	0.43
6:J:104:DC:H2''	6:J:105:DT:O5'	2.18	0.43
7:K:607:LEU:HD23	7:K:607:LEU:HA	1.78	0.43
7:K:664:TYR:N	7:K:674:GLN:HE22	2.16	0.43
7:K:810:ARG:NH2	7:K:1053:GLN:HG2	2.34	0.43
7:K:820:LEU:HD23	7:K:1014:HIS:NE2	2.33	0.43
7:K:974:MET:HA	7:K:974:MET:HE3	2.01	0.43
7:K:994:VAL:HB	7:K:1024:ILE:HG13	2.01	0.43
7:K:1012:ARG:HA	7:K:1015:ARG:NH2	2.34	0.43
8:L:42:ARG:HG3	8:L:90:TYR:CE1	2.46	0.43
8:L:176:GLY:O	8:L:212:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:174:ALA:HA	9:M:451:SER:HA	2.01	0.43
10:N:392:LEU:HD22	10:N:421:GLN:HG2	2.00	0.43
10:N:569:MET:HE1	11:P:446:SER:C	2.43	0.43
10:O:569:MET:O	10:O:573:VAL:HG13	2.18	0.43
11:P:319:MET:HE1	13:R:991:TRP:CD2	2.54	0.43
11:P:465:LYS:N	11:P:465:LYS:HD3	2.33	0.43
14:S:143:SER:OG	14:S:171:THR:O	2.34	0.43
14:S:458:ARG:C	14:S:462:ARG:HE	2.26	0.43
14:S:583:LYS:O	14:S:585:PRO:HD3	2.19	0.43
15:T:377:THR:HG22	15:T:379:THR:HG23	2.00	0.43
17:V:362:ARG:O	17:V:366:SER:N	2.36	0.43
3:G:84:GLN:HA	3:G:87:VAL:HG22	2.01	0.43
3:G:103:ALA:C	3:G:105:GLY:H	2.26	0.43
4:H:77:LEU:HD23	4:H:77:LEU:O	2.19	0.43
4:H:77:LEU:O	4:H:80:TYR:HB2	2.19	0.43
5:I:56:DC:H2''	5:I:57:DT:O5'	2.18	0.43
7:K:321:ASN:ND2	17:V:479:GLN:O	2.51	0.43
7:K:393:ARG:HH11	17:V:378:ILE:HD11	1.83	0.43
7:K:604:ASN:CG	7:K:736:ARG:H	2.24	0.43
7:K:619:THR:HB	7:K:620:ILE:HD12	2.01	0.43
7:K:880:VAL:HB	7:K:934:ILE:HG13	2.00	0.43
7:K:908:LEU:HA	7:K:911:ILE:HG12	2.01	0.43
9:M:26:LEU:O	9:M:149:THR:HG23	2.19	0.43
10:N:215:HIS:HE1	10:N:218:PRO:HB2	1.84	0.43
10:N:330:ILE:HD11	10:N:368:ARG:HD2	2.01	0.43
10:N:356:ARG:O	10:N:356:ARG:HG3	2.19	0.43
11:P:134:ILE:HG23	11:P:392:THR:HB	2.00	0.43
12:Q:88:TRP:CE3	12:Q:113:GLY:HA3	2.53	0.43
12:Q:109:PHE:HB2	12:Q:111:ARG:NH1	2.33	0.43
12:Q:390:GLU:O	12:Q:393:GLU:HG3	2.19	0.43
12:Q:469:VAL:HG12	12:Q:470:VAL:O	2.18	0.43
14:S:231:HIS:CG	14:S:232:PRO:HD2	2.54	0.43
14:S:577:MET:O	14:S:580:ARG:HG3	2.19	0.43
1:A:67:PHE:CD1	1:A:70:LEU:HD23	2.54	0.43
3:C:81:ARG:O	3:C:81:ARG:HD2	2.18	0.43
6:J:77:DC:C2	6:J:78:DG:C6	3.07	0.43
7:K:197:MET:N	7:K:197:MET:SD	2.81	0.43
7:K:437:GLN:O	7:K:438:ASN:C	2.61	0.43
7:K:939:LEU:O	7:K:943:GLY:N	2.52	0.43
7:K:1012:ARG:HH11	7:K:1015:ARG:HH22	1.67	0.43
7:K:1012:ARG:NH1	7:K:1015:ARG:HH22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:228:LEU:HD22	9:M:338:VAL:HG12	2.00	0.43
10:N:613:PHE:C	10:N:615:ASP:N	2.74	0.43
11:P:79:ASP:HA	11:P:440:MET:CE	2.48	0.43
11:P:80:GLY:N	11:P:440:MET:HE3	2.34	0.43
11:P:163:TYR:O	11:P:275:LYS:HA	2.19	0.43
11:P:269:PHE:HE2	11:P:272:ILE:HB	1.84	0.43
11:P:339:PHE:CE1	11:P:359:LEU:HD23	2.53	0.43
11:P:420:PRO:HD2	11:P:422:TYR:CD2	2.53	0.43
12:Q:59:LEU:HD23	12:Q:59:LEU:H	1.83	0.43
12:Q:71:TRP:CE2	12:Q:147:ASN:HB2	2.54	0.43
12:Q:430:TRP:CE3	12:Q:431:ARG:HB2	2.52	0.43
13:R:498:GLN:OE1	13:R:498:GLN:HA	2.18	0.43
13:R:610:LEU:HD12	13:R:613:HIS:HB2	1.99	0.43
13:R:1010:LEU:HD12	13:R:1011:LEU:H	1.83	0.43
1:E:118:THR:HG23	2:F:45:ARG:HB3	2.02	0.42
3:G:17:ARG:HG3	4:H:118:TYR:CE1	2.54	0.42
7:K:524:SER:O	7:K:527:GLU:N	2.51	0.42
8:L:111:HIS:O	8:L:115:THR:OG1	2.37	0.42
8:L:247:PRO:HA	8:L:547:ASN:HB2	2.01	0.42
8:L:718:ILE:O	8:L:722:SER:OG	2.31	0.42
9:M:142:THR:HA	9:M:452:ARG:HH21	1.84	0.42
10:N:274:ARG:NH1	15:T:412:PRO:HD2	2.22	0.42
10:N:384:TRP:HB2	10:N:389:ILE:HD11	2.00	0.42
10:N:567:ARG:HH12	10:N:571:ARG:HG3	1.84	0.42
10:N:614:LEU:HD23	10:N:614:LEU:HA	1.88	0.42
10:N:616:ARG:CZ	12:Q:419:ARG:HB2	2.49	0.42
10:O:115:HIS:C	10:O:117:ILE:N	2.76	0.42
10:O:160:ASP:O	10:O:164:ASN:ND2	2.51	0.42
11:P:115:ASP:HA	13:R:609:ARG:HH22	1.84	0.42
11:P:128:LYS:HE3	11:P:129:THR:O	2.19	0.42
11:P:298:GLU:OE1	11:P:370:LEU:HA	2.19	0.42
13:R:517:ARG:HG2	13:R:555:HIS:NE2	2.33	0.42
13:R:584:TYR:CE2	13:R:590:ASN:HB3	2.54	0.42
13:R:937:ARG:O	13:R:940:ARG:HB2	2.19	0.42
14:S:219:ARG:O	14:S:223:GLU:OE1	2.37	0.42
4:D:87:THR:OG1	4:D:88:SER:N	2.53	0.42
7:K:326:ARG:HB2	7:K:363:LYS:HZ2	1.84	0.42
7:K:461:MET:HB3	8:L:166:LYS:HG2	2.01	0.42
7:K:977:LEU:HD21	7:K:986:LEU:HD13	2.01	0.42
7:K:1056:ARG:HH21	7:K:1069:MET:HG2	1.84	0.42
8:L:32:LEU:HD23	8:L:32:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:357:GLU:HB3	8:L:486:VAL:HB	2.00	0.42
9:M:83:VAL:HG11	9:M:86:TRP:HE3	1.85	0.42
10:O:164:ASN:HA	10:O:167:ARG:CG	2.49	0.42
10:O:590:TYR:O	10:O:594:MET:HG2	2.19	0.42
11:P:130:MET:SD	11:P:130:MET:N	2.92	0.42
11:P:285:ILE:HD11	11:P:374:LYS:HB3	2.01	0.42
11:P:421:SER:O	11:P:425:THR:HG22	2.18	0.42
11:P:426:LEU:HD11	17:V:360:LEU:O	2.19	0.42
11:P:467:TRP:NE1	12:Q:314:MET:HB3	2.32	0.42
12:Q:105:LEU:HD23	12:Q:130:LEU:HD13	2.01	0.42
13:R:357:GLY:HA2	13:R:360:TYR:HB3	2.01	0.42
13:R:529:LEU:HD23	13:R:533:ARG:HD2	2.00	0.42
13:R:532:LEU:HD23	13:R:532:LEU:HA	1.88	0.42
13:R:587:GLU:OE1	13:R:589:ASP:HB2	2.18	0.42
16:U:955:ALA:HA	16:U:959:GLU:OE1	2.18	0.42
3:C:92:GLU:CD	4:D:103:LEU:HB2	2.45	0.42
5:I:13:DG:C2	5:I:14:DG:C4	3.07	0.42
5:I:89:DT:H2"	5:I:90:DA:C8	2.55	0.42
6:J:43:DA:C6	6:J:44:DA:C6	3.07	0.42
7:K:369:LYS:C	10:N:422:PHE:HZ	2.26	0.42
7:K:519:LYS:NZ	7:K:559:ILE:HB	2.35	0.42
7:K:697:ARG:HB3	7:K:698:PRO:HD3	2.00	0.42
8:L:10:GLU:HB2	8:L:30:ASN:HB3	2.00	0.42
8:L:26:GLN:HA	8:L:36:ALA:HB3	2.00	0.42
9:M:267:LEU:HD23	9:M:268:ARG:C	2.45	0.42
10:N:348:CYS:HB3	10:N:351:CYS:CB	2.49	0.42
10:N:647:GLU:OE2	10:N:648:VAL:HG13	2.19	0.42
10:O:584:LEU:HD12	11:P:101:PHE:CE2	2.54	0.42
11:P:89:GLY:O	11:P:92:VAL:HG12	2.18	0.42
12:Q:415:GLU:C	12:Q:415:GLU:CD	2.86	0.42
13:R:482:MET:HB2	13:R:485:LEU:HD23	2.01	0.42
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.19	0.42
2:B:99:GLY:C	2:B:100:PHE:HD1	2.27	0.42
2:F:92:ARG:HH21	4:H:98:LEU:HA	1.83	0.42
5:I:44:DG:C2	5:I:45:DC:C2	3.07	0.42
5:I:75:DT:H2"	5:I:76:DG:N7	2.34	0.42
7:K:201:ILE:CG1	17:V:465:LEU:HD22	2.49	0.42
7:K:201:ILE:HD13	17:V:468:ILE:HG21	2.02	0.42
7:K:1023:ARG:N	7:K:1099:ARG:HH21	2.17	0.42
7:K:1033:VAL:O	7:K:1037:ILE:HD12	2.19	0.42
10:N:144:ASN:OD1	10:N:145:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:222:GLY:H	10:N:224:PHE:HE1	1.67	0.42
10:N:609:ARG:HE	10:N:612:LEU:CD2	2.32	0.42
10:N:660:GLY:H	12:Q:467:ALA:N	2.17	0.42
10:O:594:MET:HE1	12:Q:398:HIS:CD2	2.55	0.42
11:P:77:LEU:HG	11:P:77:LEU:O	2.19	0.42
11:P:231:PHE:H	11:P:233:LYS:HZ2	1.66	0.42
11:P:431:ALA:O	11:P:434:ASP:HB2	2.19	0.42
12:Q:113:GLY:N	12:Q:123:HIS:O	2.53	0.42
12:Q:194:PHE:HE2	12:Q:202:TRP:CZ3	2.38	0.42
13:R:438:ASP:O	13:R:442:LEU:HD23	2.20	0.42
14:S:375:LYS:HB3	14:S:375:LYS:HE3	1.82	0.42
17:V:303:LYS:HE3	17:V:304:TYR:CZ	2.53	0.42
1:A:65:LEU:O	1:A:68:GLN:HB3	2.19	0.42
1:A:79:LYS:HD2	1:A:82:LEU:CD2	2.49	0.42
1:A:105:GLU:HG3	1:A:106:ASP:H	1.83	0.42
5:I:5:DA:C5	5:I:6:DG:C6	3.06	0.42
5:I:104:DT:H3'	5:I:105:DT:H71	2.01	0.42
6:J:105:DT:H2''	6:J:106:DG:N7	2.34	0.42
6:J:110:DA:C2	6:J:111:DC:C2	3.08	0.42
7:K:443:VAL:O	7:K:447:GLY:N	2.26	0.42
7:K:459:ARG:HA	7:K:462:TYR:HD2	1.84	0.42
7:K:828:ILE:HD13	7:K:1026:ARG:O	2.20	0.42
7:K:915:TYR:CD2	7:K:922:VAL:HG21	2.54	0.42
8:L:46:ASP:HB2	8:L:49:ASP:O	2.20	0.42
8:L:248:TYR:OH	9:M:253:ASN:ND2	2.52	0.42
8:L:557:LEU:HB3	9:M:256:PRO:HG2	2.01	0.42
9:M:186:PHE:CD2	9:M:438:ILE:HG13	2.54	0.42
10:N:403:TRP:HZ3	10:N:419:VAL:HG13	1.84	0.42
10:N:404:ASN:O	10:N:407:ALA:HB3	2.20	0.42
11:P:146:ASN:HD22	11:P:159:LEU:HD23	1.84	0.42
12:Q:122:VAL:C	12:Q:156:ALA:H	2.27	0.42
12:Q:169:LEU:HD21	12:Q:177:LEU:HD12	2.01	0.42
13:R:921:LEU:HD23	13:R:921:LEU:HA	1.88	0.42
13:R:939:GLU:HG2	13:R:942:ARG:NH2	2.32	0.42
13:R:1004:VAL:O	13:R:1007:LEU:HB3	2.20	0.42
14:S:335:LEU:HD12	14:S:336:LEU:N	2.34	0.42
16:U:902:ALA:O	16:U:905:LYS:HG2	2.20	0.42
3:C:84:GLN:HG2	3:C:106:GLY:O	2.19	0.42
2:F:84:MET:HE2	2:F:84:MET:HA	2.02	0.42
7:K:198:GLN:O	7:K:201:ILE:HG22	2.18	0.42
7:K:391:THR:OG1	7:K:396:TYR:HD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:457:LEU:O	7:K:460:HIS:HB3	2.20	0.42
8:L:248:TYR:CE1	8:L:551:THR:HG23	2.55	0.42
9:M:370:LYS:HA	9:M:412:TYR:OH	2.20	0.42
10:N:181:ARG:NH2	14:S:26:LEU:HB2	2.34	0.42
10:N:213:PRO:HG3	15:T:523:MET:HE1	2.02	0.42
10:N:231:PRO:HG2	10:N:234:LEU:HD13	2.01	0.42
10:N:566:GLU:OE1	11:P:86:ILE:HG23	2.19	0.42
10:O:119:LEU:H	10:O:206:GLN:HE21	1.66	0.42
12:Q:17:HIS:CG	12:Q:183:LEU:HD12	2.55	0.42
12:Q:466:HIS:ND1	12:Q:466:HIS:O	2.52	0.42
13:R:977:ILE:HA	13:R:980:GLU:OE1	2.20	0.42
13:R:1010:LEU:HD12	13:R:1011:LEU:N	2.34	0.42
14:S:408:ALA:HA	14:S:420:ARG:CG	2.43	0.42
14:S:426:LEU:O	14:S:428:GLU:N	2.51	0.42
6:J:27:DC:H2''	6:J:28:DT:C6	2.55	0.42
6:J:68:DG:C8	6:J:69:DG:C6	3.08	0.42
7:K:195:ILE:O	7:K:198:GLN:HG2	2.20	0.42
7:K:294:ASN:HA	10:N:571:ARG:NH1	2.34	0.42
7:K:688:THR:HG23	7:K:692:TYR:HB2	2.00	0.42
7:K:1010:GLN:O	7:K:1013:ALA:HB3	2.19	0.42
7:K:1015:ARG:O	7:K:1016:ILE:C	2.59	0.42
10:N:540:LYS:HA	10:N:540:LYS:HD3	1.81	0.42
10:O:155:TYR:O	10:O:159:ARG:HG3	2.19	0.42
10:O:182:ASN:OD1	15:T:354:ALA:HB2	2.19	0.42
11:P:443:VAL:O	11:P:447:LYS:HG2	2.20	0.42
11:P:452:PHE:CD1	13:R:428:GLN:HB2	2.55	0.42
12:Q:415:GLU:O	12:Q:419:ARG:HG3	2.19	0.42
15:T:479:PRO:HD2	15:T:482:CYS:HB2	2.01	0.42
3:C:30:VAL:O	3:C:34:LEU:HD23	2.19	0.42
3:C:110:ASN:O	1:E:55:GLN:NE2	2.51	0.42
5:I:98:DA:H2''	5:I:99:DG:H2'	2.02	0.42
7:K:439:HIS:O	7:K:442:GLU:HB3	2.20	0.42
7:K:716:MET:HE2	7:K:716:MET:HB2	1.96	0.42
7:K:1162:ARG:HD2	7:K:1162:ARG:HA	1.42	0.42
8:L:684:ARG:HA	8:L:688:CYS:SG	2.60	0.42
8:L:716:LYS:O	8:L:719:ARG:HD2	2.20	0.42
10:N:100:ASP:OD1	10:N:100:ASP:N	2.51	0.42
10:N:117:ILE:HD13	10:N:167:ARG:HD3	2.02	0.42
10:N:629:VAL:O	10:N:632:GLN:HG3	2.20	0.42
10:O:593:GLU:O	10:O:597:MET:HG3	2.20	0.42
12:Q:44:ALA:HA	12:Q:47:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:297:LEU:HD12	17:V:391:ARG:HH21	1.85	0.42
14:S:19:LEU:HD13	14:S:27:LEU:HD23	2.00	0.42
15:T:488:ARG:NH2	15:T:492:GLN:NE2	2.68	0.42
15:T:521:TYR:CD2	15:T:521:TYR:O	2.72	0.42
1:A:120:MET:HE2	1:A:120:MET:HA	2.02	0.42
2:B:72:TYR:HE1	4:D:77:LEU:HD13	1.84	0.42
3:C:57:TYR:HD1	7:K:1159:ARG:HD2	1.85	0.42
5:I:26:DC:H4'	5:I:27:DT:OP2	2.17	0.42
5:I:85:DG:C2'	5:I:86:DT:H71	2.50	0.42
6:J:94:DG:C4	6:J:95:DG:C8	3.07	0.42
6:J:117:DA:H2''	6:J:118:DT:O5'	2.20	0.42
6:J:119:DT:H2''	6:J:120:DG:N7	2.35	0.42
7:K:407:ALA:HB3	7:K:408:ARG:NH1	2.35	0.42
8:L:239:ARG:CD	8:L:540:ARG:HE	2.33	0.42
8:L:257:GLU:OE1	8:L:257:GLU:N	2.53	0.42
8:L:354:HIS:HB3	8:L:487:ARG:HD2	2.00	0.42
9:M:299:ARG:NE	9:M:402:ASP:HB3	2.35	0.42
9:M:446:HIS:C	9:M:448:MET:N	2.77	0.42
10:N:177:THR:HA	10:N:180:ARG:HB2	2.02	0.42
10:N:249:LYS:HB3	10:O:115:HIS:CE1	2.55	0.42
10:N:569:MET:O	10:N:572:LEU:HG	2.20	0.42
10:N:570:THR:HA	10:N:573:VAL:HG12	2.01	0.42
10:N:617:LEU:HD11	12:Q:456:VAL:HG22	2.02	0.42
11:P:167:ILE:HB	11:P:272:ILE:HG22	2.02	0.42
11:P:452:PHE:CE1	11:P:456:MET:HG3	2.54	0.42
11:P:474:ASP:O	11:P:478:ILE:HG23	2.20	0.42
12:Q:41:LEU:O	12:Q:45:PRO:HD3	2.19	0.42
12:Q:418:LEU:HG	12:Q:419:ARG:N	2.35	0.42
13:R:605:ALA:O	13:R:608:VAL:HG12	2.20	0.42
13:R:991:TRP:HD1	13:R:1008:PHE:CZ	2.37	0.42
14:S:430:TRP:N	14:S:430:TRP:CD1	2.88	0.42
16:U:848:LEU:HG	16:U:849:ALA:H	1.85	0.42
16:U:961:LEU:HA	16:U:964:VAL:HB	2.01	0.42
1:A:57:SER:OG	1:A:58:THR:N	2.52	0.42
1:E:108:ASN:HB2	2:F:43:VAL:HG22	2.02	0.42
5:I:32:DT:N3	5:I:33:DG:C5	2.87	0.42
6:J:107:DT:H2''	6:J:108:DC:C5	2.55	0.42
7:K:287:ILE:O	7:K:291:ARG:HB2	2.19	0.42
7:K:287:ILE:HB	12:Q:375:GLU:CD	2.45	0.42
7:K:344:LYS:HE3	7:K:348:VAL:HG22	2.01	0.42
7:K:436:ILE:HG13	7:K:437:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:697:ARG:NH1	7:K:730:TYR:HB3	2.24	0.42
7:K:795:LEU:HA	7:K:798:ARG:HG2	2.02	0.42
7:K:898:LEU:H	7:K:898:LEU:HD23	1.85	0.42
7:K:923:LEU:CD1	7:K:975:PHE:HD2	2.33	0.42
7:K:945:HIS:NE2	7:K:971:PRO:O	2.53	0.42
7:K:1000:ASP:OD1	7:K:1001:TRP:N	2.48	0.42
8:L:208:THR:O	8:L:210:ILE:HG13	2.20	0.42
9:M:82:MET:HE3	9:M:153:TRP:NE1	2.35	0.42
9:M:94:GLU:O	9:M:98:VAL:HB	2.20	0.42
9:M:141:LEU:O	9:M:172:THR:HA	2.20	0.42
10:N:621:ARG:CB	10:N:624:ARG:HH21	2.28	0.42
10:N:622:ARG:O	10:N:626:VAL:HG13	2.19	0.42
11:P:328:ASN:HB2	11:P:340:ARG:HH22	1.84	0.42
11:P:330:LEU:HD12	11:P:340:ARG:HG3	2.02	0.42
12:Q:171:PRO:O	12:Q:174:HIS:HB2	2.19	0.42
14:S:23:ASN:HD21	14:S:95:ASP:HB3	1.84	0.42
14:S:218:ILE:O	14:S:222:LEU:HD23	2.20	0.42
15:T:468:MET:HG2	15:T:493:GLU:OE2	2.20	0.42
15:T:472:ASP:O	15:T:475:ARG:HG2	2.19	0.42
1:A:116:ARG:HH12	1:A:120:MET:CG	2.33	0.41
2:B:66:ILE:O	2:B:70:VAL:HG13	2.20	0.41
3:C:64:GLU:OE2	7:K:1164:ARG:HD2	2.20	0.41
7:K:357:ALA:HA	7:K:360:GLU:CD	2.44	0.41
7:K:727:ILE:HA	7:K:731:TYR:CD1	2.54	0.41
8:L:247:PRO:HB3	8:L:550:GLN:HE22	1.85	0.41
9:M:246:VAL:HG11	9:M:325:ASP:HB3	2.02	0.41
10:N:579:VAL:HG13	11:P:432:LEU:HG	2.02	0.41
10:N:615:ASP:O	10:N:617:LEU:N	2.52	0.41
10:O:387:ALA:O	10:O:391:ARG:HG3	2.20	0.41
10:O:388:GLU:O	10:O:392:LEU:HG	2.20	0.41
10:O:603:ARG:HH12	13:R:980:GLU:C	2.28	0.41
11:P:61:ALA:HB1	13:R:572:GLU:HG2	2.01	0.41
11:P:144:GLN:OE1	11:P:146:ASN:N	2.52	0.41
12:Q:69:LEU:HG	12:Q:148:LEU:HD22	2.02	0.41
3:G:92:GLU:OE2	3:G:93:LEU:HG	2.19	0.41
5:I:107:DC:C2	5:I:108:DT:C5	3.08	0.41
5:I:116:DC:H2'	5:I:117:DT:C6	2.55	0.41
6:J:89:DT:H2''	6:J:90:DA:N7	2.35	0.41
6:J:110:DA:C4	6:J:111:DC:C5	3.08	0.41
7:K:621:SER:O	7:K:624:THR:OG1	2.33	0.41
7:K:1034:GLU:HA	7:K:1037:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:1161:ALA:O	7:K:1162:ARG:C	2.63	0.41
8:L:132:THR:O	8:L:135:ASP:HB2	2.19	0.41
8:L:221:LEU:HD22	8:L:231:TYR:CD1	2.55	0.41
8:L:546:ASP:O	8:L:550:GLN:HG3	2.20	0.41
9:M:216:ARG:HH12	11:P:351:ARG:HH22	1.68	0.41
10:N:127:ASP:OD1	10:N:129:ASN:N	2.53	0.41
10:N:245:ILE:HG22	10:N:246:THR:O	2.20	0.41
10:O:586:LEU:HD21	12:Q:391:ILE:HG22	2.01	0.41
10:O:612:LEU:O	10:O:613:PHE:C	2.63	0.41
11:P:269:PHE:CZ	11:P:272:ILE:HD13	2.55	0.41
13:R:375:PHE:CE2	13:R:442:LEU:HB3	2.54	0.41
13:R:456:LEU:HB3	13:R:458:ASP:OD1	2.19	0.41
13:R:486:VAL:HG11	17:V:380:PRO:HB3	2.01	0.41
16:U:972:ILE:O	16:U:976:THR:HG23	2.20	0.41
2:B:92:ARG:HD2	2:B:92:ARG:C	2.44	0.41
4:D:59:MET:O	4:D:63:VAL:HG23	2.21	0.41
1:E:105:GLU:HG3	1:E:106:ASP:H	1.84	0.41
5:I:94:DG:C2	6:J:55:DG:C6	3.09	0.41
5:I:114:DG:C5	5:I:115:DT:C4	3.09	0.41
6:J:48:DC:H6	6:J:48:DC:H2'	1.60	0.41
7:K:442:GLU:OE2	7:K:446:ALA:HB2	2.20	0.41
7:K:449:ALA:HB1	8:L:189:ARG:NH2	2.35	0.41
7:K:610:GLU:HG2	7:K:613:LEU:HB3	2.02	0.41
7:K:736:ARG:HH22	7:K:760:PRO:CD	2.28	0.41
7:K:999:SER:H	7:K:1026:ARG:CZ	2.32	0.41
8:L:13:VAL:O	8:L:28:GLY:N	2.51	0.41
8:L:351:ASN:HB2	8:L:496:ARG:CZ	2.49	0.41
8:L:523:TYR:OH	8:L:524:MET:HE3	2.20	0.41
9:M:50:PHE:CD2	9:M:75:ASN:HB2	2.55	0.41
9:M:60:PHE:C	9:M:100:ARG:HH22	2.28	0.41
10:N:187:VAL:HG13	10:N:188:CYS:N	2.35	0.41
11:P:225:LYS:HD3	11:P:291:HIS:HB3	2.02	0.41
11:P:266:MET:SD	11:P:266:MET:N	2.91	0.41
12:Q:53:PRO:HB3	12:Q:195:MET:HE2	2.01	0.41
12:Q:371:GLY:C	12:Q:373:ALA:H	2.28	0.41
13:R:551:GLY:O	13:R:554:GLN:HG3	2.21	0.41
13:R:557:ASN:C	13:R:560:PRO:HD2	2.45	0.41
14:S:320:ILE:HG22	14:S:327:TYR:HB3	2.02	0.41
14:S:428:GLU:HA	14:S:431:GLU:CD	2.46	0.41
1:A:46:VAL:HG23	1:A:49:ARG:NH1	2.31	0.41
2:B:69:ALA:O	2:B:72:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:ARG:HG3	2:F:35:ARG:HH11	1.85	0.41
5:I:12:DC:H2''	5:I:13:DG:H8	1.84	0.41
5:I:69:DA:H8	5:I:69:DA:OP2	2.04	0.41
5:I:102:DG:C2	5:I:103:DA:C4	3.08	0.41
7:K:325:GLN:NE2	7:K:326:ARG:HG2	2.34	0.41
8:L:249:ALA:O	8:L:251:GLU:N	2.53	0.41
8:L:255:LEU:HD12	8:L:502:ARG:HD2	2.03	0.41
10:N:618:THR:HA	10:N:621:ARG:NE	2.35	0.41
11:P:137:THR:CG2	11:P:164:ARG:HH21	2.34	0.41
11:P:164:ARG:HG3	11:P:273:THR:HB	2.03	0.41
11:P:462:GLY:H	11:P:465:LYS:HG2	1.83	0.41
12:Q:312:GLU:O	12:Q:313:TRP:C	2.63	0.41
13:R:499:LEU:HD23	13:R:499:LEU:HA	1.83	0.41
14:S:116:ASN:OD1	14:S:116:ASN:N	2.53	0.41
14:S:330:LYS:HZ2	14:S:430:TRP:CD1	2.38	0.41
15:T:356:HIS:HD1	15:T:356:HIS:H	1.68	0.41
2:B:47:SER:O	2:B:50:ILE:HG22	2.21	0.41
5:I:3:DG:N2	5:I:4:DG:N3	2.69	0.41
6:J:53:DG:C5	6:J:54:DC:C4	3.08	0.41
6:J:122:DG:C2	6:J:123:DC:N3	2.89	0.41
7:K:1164:ARG:HE	7:K:1164:ARG:HB2	1.54	0.41
9:M:42:MET:HE1	9:M:434:ILE:HD11	2.01	0.41
9:M:43:PRO:HB3	9:M:433:TRP:CD1	2.55	0.41
9:M:232:ILE:HD11	9:M:295:VAL:HG21	2.03	0.41
9:M:392:GLY:O	9:M:395:SER:OG	2.29	0.41
10:N:327:CYS:O	10:N:328:THR:OG1	2.33	0.41
10:N:404:ASN:OD1	10:N:404:ASN:N	2.53	0.41
10:N:612:LEU:HA	10:N:615:ASP:OD2	2.19	0.41
10:O:623:VAL:HG23	10:O:624:ARG:N	2.36	0.41
11:P:79:ASP:OD2	11:P:96:ARG:NE	2.53	0.41
11:P:93:ASP:O	11:P:97:GLN:OE1	2.39	0.41
12:Q:407:ARG:HG3	12:Q:408:SER:N	2.35	0.41
13:R:412:ASP:HA	13:R:415:ARG:CZ	2.51	0.41
13:R:972:SER:OG	13:R:973:ARG:N	2.54	0.41
14:S:441:GLU:O	14:S:445:ARG:HG2	2.21	0.41
15:T:411:PHE:CZ	15:T:426:ASP:CB	2.98	0.41
1:E:73:GLU:HG3	1:E:74:ILE:N	2.35	0.41
1:E:120:MET:HE2	1:E:120:MET:HA	2.02	0.41
6:J:19:DA:C2'	6:J:20:DC:H5'	2.51	0.41
6:J:36:DA:C5	6:J:37:DG:C6	3.09	0.41
6:J:44:DA:C6	6:J:45:DT:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:55:DG:C6	6:J:56:DG:C6	3.08	0.41
6:J:100:DA:C6	6:J:101:DG:C6	3.08	0.41
7:K:398:ARG:HD2	7:K:398:ARG:HA	1.83	0.41
7:K:811:ARG:NH1	7:K:1057:PHE:HB2	2.27	0.41
7:K:904:LYS:HD2	7:K:997:TYR:CZ	2.55	0.41
7:K:1010:GLN:O	7:K:1014:HIS:N	2.49	0.41
7:K:1026:ARG:HG3	7:K:1027:LEU:N	2.35	0.41
8:L:248:TYR:CD2	8:L:551:THR:HA	2.55	0.41
9:M:234:SER:OG	9:M:350:PRO:O	2.35	0.41
9:M:236:TRP:CZ3	9:M:245:VAL:HA	2.54	0.41
9:M:440:ALA:O	9:M:446:HIS:NE2	2.51	0.41
10:N:113:GLN:NE2	10:O:224:PHE:HD1	2.17	0.41
10:N:232:ARG:HH11	10:N:232:ARG:HD2	1.73	0.41
10:N:244:VAL:O	10:O:120:PRO:HD2	2.20	0.41
10:N:584:LEU:HD12	10:N:585:GLU:N	2.36	0.41
10:N:599:GLN:HG3	10:N:603:ARG:NH1	2.36	0.41
10:O:173:TYR:O	15:T:358:ASN:ND2	2.44	0.41
10:O:177:THR:O	10:O:180:ARG:HG2	2.21	0.41
10:O:398:ARG:HD2	10:O:399:TYR:CE2	2.55	0.41
11:P:299:LEU:HD23	11:P:304:ALA:HA	2.03	0.41
11:P:383:GLU:HA	11:P:386:HIS:ND1	2.35	0.41
12:Q:126:ARG:CG	12:Q:152:HIS:HB3	2.51	0.41
13:R:472:LEU:O	13:R:476:ILE:HG12	2.20	0.41
13:R:478:HIS:CD2	13:R:514:ILE:HD12	2.56	0.41
14:S:587:TRP:HD1	14:S:588:THR:HG23	1.85	0.41
15:T:343:ASP:OD1	15:T:344:VAL:N	2.54	0.41
17:V:359:ALA:O	17:V:363:GLY:N	2.44	0.41
3:C:44:GLY:HA2	5:I:112:DT:OP1	2.21	0.41
3:C:57:TYR:OH	7:K:1162:ARG:HD3	2.21	0.41
1:E:116:ARG:HH12	1:E:120:MET:CG	2.33	0.41
3:G:87:VAL:HG23	3:G:88:ARG:HD3	2.02	0.41
3:G:96:LEU:HD23	3:G:96:LEU:O	2.20	0.41
5:I:37:DG:N2	6:J:112:DG:C2	2.89	0.41
5:I:44:DG:H2''	5:I:45:DC:O4'	2.21	0.41
5:I:85:DG:H2''	5:I:86:DT:H71	2.03	0.41
5:I:110:DC:O2	6:J:39:DG:N2	2.52	0.41
7:K:289:HIS:CE1	7:K:292:ARG:HD2	2.56	0.41
7:K:318:ILE:HG22	17:V:479:GLN:OE1	2.21	0.41
7:K:642:LEU:HG	7:K:643:SER:N	2.36	0.41
7:K:959:SER:O	7:K:962:LEU:HG	2.21	0.41
8:L:148:LYS:HA	8:L:707:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:503:ARG:O	8:L:507:ARG:HG2	2.21	0.41
10:N:645:ALA:O	10:N:649:LEU:HG	2.20	0.41
10:N:660:GLY:O	12:Q:466:HIS:HA	2.19	0.41
10:O:148:ARG:HB3	14:S:310:ASP:OD2	2.21	0.41
10:O:215:HIS:HB2	14:S:347:LYS:HE2	2.03	0.41
11:P:59:GLN:HG3	11:P:60:GLN:N	2.35	0.41
11:P:346:LYS:HA	11:P:349:ILE:O	2.21	0.41
11:P:356:ILE:N	11:P:357:PRO:HD2	2.35	0.41
12:Q:34:LEU:HD13	12:Q:97:GLN:NE2	2.36	0.41
12:Q:455:ILE:H	12:Q:455:ILE:HD12	1.86	0.41
12:Q:473:VAL:HG21	12:Q:475:ARG:HH21	1.86	0.41
13:R:486:VAL:HG22	13:R:490:HIS:CD2	2.55	0.41
4:D:37:TYR:N	4:D:37:TYR:CD2	2.88	0.41
5:I:45:DC:H2'	5:I:46:DT:H71	2.03	0.41
5:I:57:DT:H1'	5:I:58:DT:N1	2.36	0.41
7:K:423:ASN:HB3	7:K:424:ARG:NH1	2.35	0.41
7:K:971:PRO:HG2	7:K:972:TYR:CE1	2.56	0.41
8:L:348:ARG:O	8:L:496:ARG:NH2	2.54	0.41
8:L:490:ILE:HG22	8:L:491:GLU:H	1.85	0.41
9:M:164:GLU:O	9:M:167:MET:N	2.53	0.41
9:M:241:PRO:O	9:M:242:PRO:C	2.61	0.41
10:N:362:THR:HG23	10:N:364:ALA:H	1.85	0.41
10:N:405:GLN:HA	10:N:408:GLU:CD	2.45	0.41
10:N:565:GLU:C	10:N:567:ARG:H	2.28	0.41
10:N:617:LEU:HD23	10:N:617:LEU:HA	1.89	0.41
11:P:116:ILE:HA	11:P:120:LEU:HD21	2.03	0.41
11:P:128:LYS:HZ2	11:P:173:GLU:CA	2.34	0.41
11:P:391:PRO:O	11:P:393:ILE:HG13	2.21	0.41
13:R:326:ILE:HD13	15:T:520:PRO:HD3	2.01	0.41
13:R:383:PHE:CZ	13:R:485:LEU:HD21	2.56	0.41
13:R:617:ARG:HH11	13:R:619:GLN:H	1.69	0.41
14:S:368:TYR:HA	14:S:371:VAL:HG12	2.03	0.41
17:V:356:GLU:HG2	17:V:360:LEU:CD1	2.51	0.41
17:V:380:PRO:HG2	17:V:383:GLN:HG2	2.03	0.41
2:B:78:ARG:NH2	2:B:82:THR:H	2.18	0.41
3:G:17:ARG:HG3	4:H:118:TYR:HE1	1.85	0.41
5:I:98:DA:O5'	7:K:1001:TRP:NE1	2.54	0.41
5:I:113:DA:C6	5:I:114:DG:C6	3.08	0.41
6:J:37:DG:C4	6:J:38:DG:C6	3.09	0.41
6:J:125:DG:H2''	6:J:126:DC:O5'	2.21	0.41
7:K:204:HIS:O	7:K:207:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:374:ARG:HA	11:P:518:TRP:CH2	2.55	0.41
7:K:517:PHE:O	7:K:520:GLN:HG3	2.20	0.41
7:K:606:ILE:O	7:K:608:ALA:N	2.54	0.41
7:K:710:ILE:O	7:K:739:LEU:HD13	2.20	0.41
8:L:137:GLU:CD	8:L:716:LYS:HA	2.46	0.41
8:L:204:GLY:N	9:M:57:ARG:HH12	2.19	0.41
8:L:507:ARG:NH1	8:L:510:THR:OG1	2.54	0.41
8:L:547:ASN:OD1	8:L:547:ASN:O	2.39	0.41
8:L:552:LEU:HG	8:L:654:ILE:HD13	2.03	0.41
9:M:45:GLN:HG2	9:M:100:ARG:HB3	2.03	0.41
9:M:319:ARG:HG3	9:M:335:ARG:NH1	2.36	0.41
9:M:396:LEU:HD23	9:M:396:LEU:HA	1.87	0.41
9:M:444:THR:HA	9:M:447:GLN:NE2	2.36	0.41
10:N:387:ALA:O	10:N:391:ARG:HG2	2.21	0.41
10:N:584:LEU:O	10:N:588:LEU:HD23	2.20	0.41
10:N:612:LEU:O	10:N:615:ASP:HB2	2.21	0.41
10:N:618:THR:HA	10:N:621:ARG:HE	1.86	0.41
10:O:397:GLU:H	10:O:397:GLU:CD	2.29	0.41
11:P:128:LYS:NZ	11:P:173:GLU:N	2.69	0.41
11:P:224:PHE:CE1	11:P:373:ILE:HD13	2.51	0.41
12:Q:81:PHE:HD2	12:Q:125:ARG:NH1	2.19	0.41
12:Q:157:GLU:O	12:Q:161:ARG:N	2.50	0.41
12:Q:297:LEU:HA	12:Q:297:LEU:HD13	1.75	0.41
12:Q:455:ILE:O	12:Q:459:VAL:HG22	2.20	0.41
13:R:516:MET:HE1	13:R:535:LEU:HG	2.03	0.41
13:R:930:VAL:CG1	13:R:931:PRO:HD3	2.51	0.41
14:S:107:ARG:HH22	14:S:149:PRO:HA	1.86	0.41
14:S:113:ASN:O	14:S:115:PRO:HD3	2.21	0.41
14:S:352:ASP:OD1	14:S:352:ASP:N	2.51	0.41
14:S:427:ALA:C	14:S:429:GLU:N	2.76	0.41
14:S:563:GLY:C	14:S:565:PHE:H	2.28	0.41
14:S:584:LEU:HD12	14:S:585:PRO:HD2	2.02	0.41
16:U:963:LYS:HG3	16:U:966:ARG:CZ	2.50	0.41
17:V:528:ALA:O	17:V:531:ILE:HG22	2.21	0.41
1:E:83:ARG:HH11	1:E:83:ARG:HB2	1.86	0.41
3:G:78:ILE:HA	3:G:82:HIS:HD1	1.85	0.41
5:I:71:DG:H2''	5:I:72:DC:C5'	2.51	0.41
5:I:119:DC:H2''	5:I:120:DA:H8	1.86	0.41
6:J:38:DG:C4	6:J:39:DG:C6	3.08	0.41
6:J:48:DC:C6	6:J:48:DC:H5'	2.55	0.41
6:J:101:DG:C2	6:J:102:DA:C5	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:113:DA:H5'	6:J:113:DA:C8	2.56	0.41
7:K:292:ARG:NH2	12:Q:368:LEU:HA	2.36	0.41
7:K:380:GLN:NE2	11:P:529:VAL:HG11	2.36	0.41
7:K:678:ILE:HA	7:K:683:PHE:HE2	1.86	0.41
7:K:877:HIS:CE1	7:K:879:PHE:HB3	2.56	0.41
7:K:956:GLU:OE1	7:K:956:GLU:N	2.38	0.41
8:L:20:SER:CB	8:L:176:GLY:HA3	2.49	0.41
9:M:139:LYS:HD3	9:M:139:LYS:HA	1.71	0.41
10:N:227:ILE:HD12	15:T:428:HIS:CE1	2.56	0.41
10:N:384:TRP:CZ3	10:N:392:LEU:HD22	2.56	0.41
10:O:112:ALA:C	10:O:114:THR:N	2.77	0.41
10:O:570:THR:O	10:O:573:VAL:HG22	2.20	0.41
12:Q:29:MET:HE1	12:Q:32:VAL:HG13	2.03	0.41
12:Q:325:GLY:H	16:U:974:ARG:HH22	1.69	0.41
12:Q:391:ILE:O	12:Q:395:LYS:HG3	2.21	0.41
12:Q:412:LYS:O	12:Q:415:GLU:HB3	2.21	0.41
13:R:336:SER:OG	13:R:341:GLU:OE2	2.30	0.41
13:R:421:LYS:HD2	13:R:421:LYS:HA	1.90	0.41
15:T:484:ALA:O	15:T:488:ARG:HG2	2.21	0.41
17:V:303:LYS:HG2	17:V:304:TYR:CE1	2.55	0.41
17:V:324:ASN:HA	17:V:362:ARG:HH22	1.85	0.41
17:V:467:GLU:HB3	17:V:523:LEU:HD21	2.02	0.41
3:G:51:LEU:HD13	4:H:70:ILE:HG21	2.03	0.40
5:I:32:DT:C4	5:I:33:DG:C6	3.09	0.40
5:I:98:DA:C6	5:I:99:DG:C6	3.09	0.40
7:K:357:ALA:HA	7:K:360:GLU:CG	2.51	0.40
7:K:373:LEU:HD22	10:N:403:TRP:HH2	1.86	0.40
7:K:906:GLU:HB2	7:K:910:ARG:HH12	1.85	0.40
8:L:514:ARG:HD2	9:M:285:ARG:NH2	2.36	0.40
9:M:245:VAL:HG12	9:M:247:PRO:HD3	2.03	0.40
10:N:160:ASP:OD1	10:N:160:ASP:N	2.53	0.40
10:N:174:LEU:HD12	10:N:175:THR:H	1.86	0.40
10:N:608:ALA:O	10:N:610:GLN:N	2.54	0.40
10:N:676:SER:OG	11:P:271:GLU:HB3	2.22	0.40
10:O:590:TYR:HA	10:O:593:GLU:CD	2.46	0.40
11:P:63:HIS:O	11:P:66:LYS:HG2	2.20	0.40
11:P:248:ILE:HD13	11:P:274:PHE:CE1	2.56	0.40
11:P:303:LEU:HD12	11:P:306:ILE:CG2	2.51	0.40
11:P:354:GLY:HA2	11:P:362:TYR:OH	2.21	0.40
12:Q:399:GLU:HA	12:Q:402:MET:HE3	2.03	0.40
13:R:414:ASP:OD1	13:R:415:ARG:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:446:ALA:O	13:R:449:THR:HG22	2.21	0.40
13:R:523:GLU:HB2	17:V:372:ARG:NH1	2.34	0.40
14:S:129:PRO:O	14:S:185:HIS:ND1	2.53	0.40
14:S:315:ILE:CG2	14:S:330:LYS:HD3	2.51	0.40
15:T:468:MET:N	15:T:493:GLU:OE2	2.54	0.40
17:V:476:ALA:HA	17:V:479:GLN:HE21	1.86	0.40
5:I:50:DG:C2	5:I:51:DC:C2	3.09	0.40
6:J:30:DG:H2"	6:J:31:DA:H8	1.86	0.40
7:K:585:LYS:H	7:K:588:GLN:HB2	1.86	0.40
7:K:939:LEU:HD11	7:K:944:LEU:HB2	2.03	0.40
8:L:12:GLN:NE2	8:L:687:PHE:HE2	2.20	0.40
9:M:203:THR:OG1	9:M:223:ALA:O	2.37	0.40
9:M:221:SER:HB3	9:M:368:LEU:HD11	2.03	0.40
10:N:336:GLN:O	10:N:398:ARG:NH2	2.54	0.40
10:N:428:GLU:OE1	10:N:428:GLU:N	2.54	0.40
10:N:567:ARG:O	10:N:570:THR:OG1	2.29	0.40
11:P:130:MET:HA	11:P:172:LEU:H	1.86	0.40
11:P:134:ILE:HD13	11:P:167:ILE:HG12	2.02	0.40
12:Q:113:GLY:C	12:Q:121:ALA:HB1	2.46	0.40
14:S:233:LEU:HB3	14:S:236:ALA:HB2	2.02	0.40
14:S:340:GLY:O	14:S:343:GLU:HB3	2.21	0.40
17:V:395:ARG:O	17:V:398:ASN:HB2	2.21	0.40
1:A:128:ARG:HG2	1:A:133:GLU:HB2	2.03	0.40
5:I:104:DT:C2	5:I:105:DT:C5	3.10	0.40
6:J:60:DA:C4	6:J:61:DA:C5	3.09	0.40
7:K:286:TYR:N	12:Q:375:GLU:OE2	2.55	0.40
7:K:528:GLN:CB	7:K:531:GLN:HE21	2.31	0.40
9:M:140:PRO:HG2	9:M:170:TRP:CD1	2.57	0.40
10:N:199:GLN:NE2	10:N:200:TRP:CD1	2.90	0.40
10:N:385:SER:O	10:N:389:ILE:HD12	2.21	0.40
10:O:148:ARG:HH12	14:S:415:GLU:HA	1.87	0.40
10:O:586:LEU:HD12	10:O:587:LYS:N	2.37	0.40
11:P:91:VAL:HG23	11:P:92:VAL:N	2.36	0.40
11:P:380:ARG:HB3	11:P:382:ASP:OD2	2.21	0.40
11:P:419:ASN:HA	11:P:422:TYR:CD2	2.54	0.40
13:R:417:LEU:HD21	13:R:475:ILE:HD13	2.01	0.40
13:R:919:ALA:O	13:R:923:LEU:HG	2.21	0.40
13:R:973:ARG:HG2	13:R:975:LYS:HZ3	1.86	0.40
14:S:580:ARG:HD2	14:S:581:ASP:HB3	2.03	0.40
15:T:440:ALA:O	15:T:443:VAL:HG12	2.21	0.40
15:T:452:TYR:O	15:T:456:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:847:THR:OG1	16:U:851:ASN:HB3	2.21	0.40
16:U:911:ARG:HH22	16:U:914:LYS:NZ	2.20	0.40
16:U:958:ARG:HD2	16:U:958:ARG:HA	1.78	0.40
16:U:973:ASP:OD1	16:U:973:ASP:C	2.64	0.40
17:V:350:ILE:HA	17:V:353:GLU:HG3	2.03	0.40
5:I:98:DA:H4'	7:K:1001:TRP:CZ2	2.56	0.40
7:K:287:ILE:HB	12:Q:375:GLU:CG	2.51	0.40
7:K:361:MET:HA	7:K:361:MET:HE2	2.03	0.40
7:K:407:ALA:O	7:K:410:THR:OG1	2.28	0.40
7:K:440:ARG:O	7:K:441:ASN:C	2.64	0.40
7:K:519:LYS:HA	7:K:519:LYS:HD3	1.70	0.40
7:K:680:GLN:HB3	7:K:682:LYS:HE3	2.02	0.40
8:L:46:ASP:H	8:L:50:PRO:HA	1.85	0.40
9:M:275:HIS:HB3	9:M:278:PHE:HB2	2.04	0.40
10:N:206:GLN:NE2	13:R:321:LEU:HD13	2.36	0.40
11:P:330:LEU:HD13	11:P:339:PHE:HA	2.03	0.40
11:P:511:ARG:NH1	17:V:304:TYR:OH	2.44	0.40
12:Q:148:LEU:HA	12:Q:148:LEU:HD23	1.92	0.40
13:R:384:TYR:O	13:R:422:LYS:HB2	2.21	0.40
13:R:547:ASN:ND2	13:R:549:LEU:HG	2.36	0.40
14:S:113:ASN:C	14:S:115:PRO:HD3	2.47	0.40
14:S:220:THR:HA	14:S:223:GLU:OE1	2.20	0.40
14:S:347:LYS:HD3	14:S:347:LYS:C	2.46	0.40
14:S:426:LEU:HB2	14:S:428:GLU:OE2	2.21	0.40
17:V:391:ARG:HG2	17:V:392:ILE:CD1	2.38	0.40
17:V:467:GLU:HG2	17:V:523:LEU:HG	2.04	0.40
5:I:21:DG:H1	6:J:127:DC:H42	1.69	0.40
5:I:55:DG:C5	5:I:56:DC:C4	3.10	0.40
6:J:141:DT:H2''	6:J:142:DC:H6	1.85	0.40
7:K:288:ASP:O	7:K:290:SER:N	2.54	0.40
7:K:635:PRO:CB	7:K:706:PHE:H	2.19	0.40
7:K:638:VAL:HA	7:K:709:ILE:HB	2.04	0.40
7:K:1032:SER:OG	7:K:1034:GLU:OE2	2.40	0.40
7:K:1065:ASP:O	7:K:1069:MET:HG3	2.21	0.40
10:N:181:ARG:HE	14:S:26:LEU:CD1	2.34	0.40
10:N:197:LEU:HD23	10:N:197:LEU:HA	1.88	0.40
10:O:597:MET:O	10:O:601:GLU:OE1	2.39	0.40
11:P:130:MET:HE3	11:P:130:MET:HB3	1.90	0.40
11:P:228:THR:OG1	11:P:287:ASN:HB2	2.22	0.40
11:P:429:ILE:HA	11:P:429:ILE:HD13	1.97	0.40
13:R:477:LEU:HD23	13:R:477:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:24:ASN:C	14:S:323:SER:HG	2.28	0.40
14:S:107:ARG:NH2	14:S:148:PRO:O	2.54	0.40
14:S:179:THR:O	14:S:180:PHE:HD1	2.05	0.40
15:T:346:TRP:HE3	15:T:350:HIS:HE1	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/135 (66%)	85 (96%)	4 (4%)	0	100	100
1	E	89/135 (66%)	85 (96%)	4 (4%)	0	100	100
2	B	79/102 (78%)	72 (91%)	7 (9%)	0	100	100
2	F	75/102 (74%)	70 (93%)	5 (7%)	0	100	100
3	C	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
3	G	93/129 (72%)	88 (95%)	5 (5%)	0	100	100
4	D	86/125 (69%)	81 (94%)	5 (6%)	0	100	100
4	H	88/125 (70%)	83 (94%)	5 (6%)	0	100	100
7	K	810/1595 (51%)	735 (91%)	75 (9%)	0	100	100
8	L	405/733 (55%)	364 (90%)	41 (10%)	0	100	100
9	M	427/476 (90%)	394 (92%)	33 (8%)	0	100	100
10	N	463/694 (67%)	392 (85%)	65 (14%)	6 (1%)	9	41
10	O	266/694 (38%)	239 (90%)	26 (10%)	1 (0%)	30	67
11	P	363/547 (66%)	318 (88%)	43 (12%)	2 (1%)	21	59
12	Q	307/769 (40%)	287 (94%)	19 (6%)	1 (0%)	36	71
13	R	409/763 (54%)	385 (94%)	22 (5%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	S	401/607 (66%)	356 (89%)	44 (11%)	1 (0%)	43	77
15	T	195/534 (36%)	177 (91%)	18 (9%)	0	100	100
16	U	99/991 (10%)	87 (88%)	12 (12%)	0	100	100
17	V	135/990 (14%)	125 (93%)	10 (7%)	0	100	100
All	All	4972/10375 (48%)	4510 (91%)	449 (9%)	13 (0%)	37	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	Q	419	ARG
10	N	180	ARG
10	N	610	GLN
13	R	1009	SER
14	S	415	GLU
10	N	186	ASP
10	N	615	ASP
10	O	122	TYR
13	R	1007	LEU
10	N	611	GLN
11	P	178	PRO
11	P	329	LYS
10	N	190	ILE

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	79/110 (72%)	66 (84%)	13 (16%)	2	12
1	E	79/110 (72%)	66 (84%)	13 (16%)	2	12
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	63/78 (81%)	63 (100%)	0	100	100
3	C	74/101 (73%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	74/101 (73%)	72 (97%)	2 (3%)	39	59
4	D	75/105 (71%)	75 (100%)	0	100	100
4	H	77/105 (73%)	77 (100%)	0	100	100
7	K	736/1356 (54%)	718 (98%)	18 (2%)	43	63
8	L	363/605 (60%)	362 (100%)	1 (0%)	86	84
9	M	354/395 (90%)	352 (99%)	2 (1%)	78	80
10	N	393/562 (70%)	381 (97%)	12 (3%)	35	56
10	O	238/562 (42%)	231 (97%)	7 (3%)	37	58
11	P	337/462 (73%)	324 (96%)	13 (4%)	28	50
12	Q	279/598 (47%)	264 (95%)	15 (5%)	20	42
13	R	360/655 (55%)	357 (99%)	3 (1%)	73	77
14	S	353/493 (72%)	348 (99%)	5 (1%)	59	71
15	T	173/457 (38%)	171 (99%)	2 (1%)	63	73
16	U	85/861 (10%)	85 (100%)	0	100	100
17	V	121/836 (14%)	121 (100%)	0	100	100
All	All	4380/8630 (51%)	4274 (98%)	106 (2%)	43	63

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
1	A	69	ARG
1	A	70	LEU
1	A	82	LEU
1	A	83	ARG
1	A	86	SER
1	A	87	SER
1	A	92	LEU
1	A	105	GLU
1	A	117	VAL
1	A	118	THR
1	A	126	LEU
1	A	129	ARG
1	E	49	ARG
1	E	64	LYS
1	E	69	ARG
1	E	73	GLU

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Mol	Chain	Res	Type
1	E	83	ARG
1	E	86	SER
1	E	87	SER
1	E	92	LEU
1	E	105	GLU
1	E	117	VAL
1	E	118	THR
1	E	126	LEU
1	E	129	ARG
3	G	20	ARG
3	G	24	GLN
7	K	715	ARG
7	K	717	LYS
7	K	901	THR
7	K	1008	GLN
7	K	1010	GLN
7	K	1012	ARG
7	K	1015	ARG
7	K	1018	GLN
7	K	1020	ASN
7	K	1021	GLU
7	K	1156	HIS
7	K	1157	LEU
7	K	1159	ARG
7	K	1162	ARG
7	K	1163	GLU
7	K	1165	LYS
7	K	1166	GLN
7	K	1167	ILE
8	L	178	GLU
9	M	239	GLN
9	M	439	LEU
10	N	175	THR
10	N	176	VAL
10	N	177	THR
10	N	179	CYS
10	N	182	ASN
10	N	224	PHE
10	N	226	ILE
10	N	420	LEU
10	N	424	GLN
10	N	610	GLN

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Mol	Chain	Res	Type
10	N	614	LEU
10	N	616	ARG
10	O	115	HIS
10	O	117	ILE
10	O	121	SER
10	O	605	LEU
10	O	611	GLN
10	O	612	LEU
10	O	624	ARG
11	P	173	GLU
11	P	175	GLU
11	P	176	GLU
11	P	327	LEU
11	P	328	ASN
11	P	329	LYS
11	P	330	LEU
11	P	332	GLU
11	P	333	ASP
11	P	334	GLU
11	P	336	LYS
11	P	337	ARG
11	P	340	ARG
12	Q	116	MET
12	Q	119	GLN
12	Q	128	PHE
12	Q	150	ILE
12	Q	162	LEU
12	Q	297	LEU
12	Q	298	THR
12	Q	300	ARG
12	Q	412	LYS
12	Q	416	GLN
12	Q	418	LEU
12	Q	427	THR
12	Q	428	GLU
12	Q	430	TRP
12	Q	431	ARG
13	R	1006	SER
13	R	1007	LEU
13	R	1010	LEU
14	S	123	TYR
14	S	158	VAL

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Mol	Chain	Res	Type
14	S	159	ASP
14	S	160	ASN
14	S	426	LEU
15	T	426	ASP
15	T	427	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	108	ASN
3	C	31	HIS
4	D	106	HIS
1	E	68	GLN
3	G	24	GLN
4	H	46	HIS
4	H	79	HIS
4	H	81	ASN
4	H	106	HIS
7	K	190	ASN
7	K	321	ASN
7	K	392	ASN
7	K	445	ASN
7	K	531	GLN
7	K	674	GLN
7	K	746	ASN
7	K	756	ASN
7	K	836	GLN
7	K	876	ASN
7	K	877	HIS
7	K	886	ASN
7	K	892	ASN
7	K	1008	GLN
7	K	1018	GLN
7	K	1108	GLN
7	K	1166	GLN
8	L	12	GLN
8	L	547	ASN
8	L	554	HIS
8	L	700	GLN
9	M	169	ASN
9	M	405	ASN

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Mol	Chain	Res	Type
9	M	406	HIS
9	M	410	ASN
10	N	206	GLN
10	N	235	GLN
10	N	284	ASN
10	N	405	GLN
10	N	610	GLN
10	N	627	GLN
10	O	164	ASN
10	O	204	ASN
10	O	206	GLN
10	O	592	ASN
10	O	610	GLN
11	P	63	HIS
11	P	88	HIS
11	P	360	ASN
12	Q	174	HIS
12	Q	309	GLN
13	R	348	HIS
13	R	490	HIS
13	R	554	GLN
13	R	583	GLN
13	R	602	HIS
14	S	8	GLN
14	S	24	ASN
14	S	121	HIS
14	S	122	ASN
14	S	168	GLN
14	S	206	ASN
14	S	337	HIS
14	S	348	GLN
15	T	347	GLN
15	T	376	HIS
15	T	428	HIS
15	T	454	ASN
15	T	495	ASN
16	U	863	GLN
17	V	383	GLN
17	V	390	GLN
17	V	460	GLN
17	V	479	GLN
17	V	483	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	ADP	K	1601	-	27,29,29	1.36	4 (14%)	42,45,45	2.10	15 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	K	1601	-	-	7/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	1601	ADP	C5-C4	3.99	1.46	1.39
18	K	1601	ADP	C4-N9	-2.52	1.32	1.37
18	K	1601	ADP	C5-N7	-2.47	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	1601	ADP	C5-C6	2.44	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1601	ADP	C5-C4-N3	-5.55	119.50	126.75
18	K	1601	ADP	N3-C4-N9	4.60	134.66	127.08
18	K	1601	ADP	PA-O3A-PB	-4.56	117.19	132.83
18	K	1601	ADP	C2-N3-C4	3.73	120.56	111.75
18	K	1601	ADP	N3-C2-N1	-3.20	123.60	128.60
18	K	1601	ADP	C4-N9-C8	3.18	109.18	105.73
18	K	1601	ADP	C2'-C3'-C4'	-2.84	97.13	102.64
18	K	1601	ADP	C4-C5-N7	-2.82	107.19	110.62
18	K	1601	ADP	C4'-O4'-C1'	-2.46	104.05	109.47
18	K	1601	ADP	C5-N7-C8	2.41	106.93	103.51
18	K	1601	ADP	O5'-C5'-C4'	-2.26	101.23	108.99
18	K	1601	ADP	N9-C8-N7	-2.23	110.87	113.91
18	K	1601	ADP	C3'-C2'-C1'	2.16	105.52	101.43
18	K	1601	ADP	C6-C5-N7	2.09	135.91	132.02
18	K	1601	ADP	O3B-PB-O1B	2.06	118.75	110.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	K	1601	ADP	PA-O3A-PB-O3B
18	K	1601	ADP	C5'-O5'-PA-O2A
18	K	1601	ADP	C5'-O5'-PA-O3A
18	K	1601	ADP	C4'-C5'-O5'-PA
18	K	1601	ADP	C3'-C4'-C5'-O5'
18	K	1601	ADP	O4'-C4'-C5'-O5'
18	K	1601	ADP	O4'-C1'-N9-C8

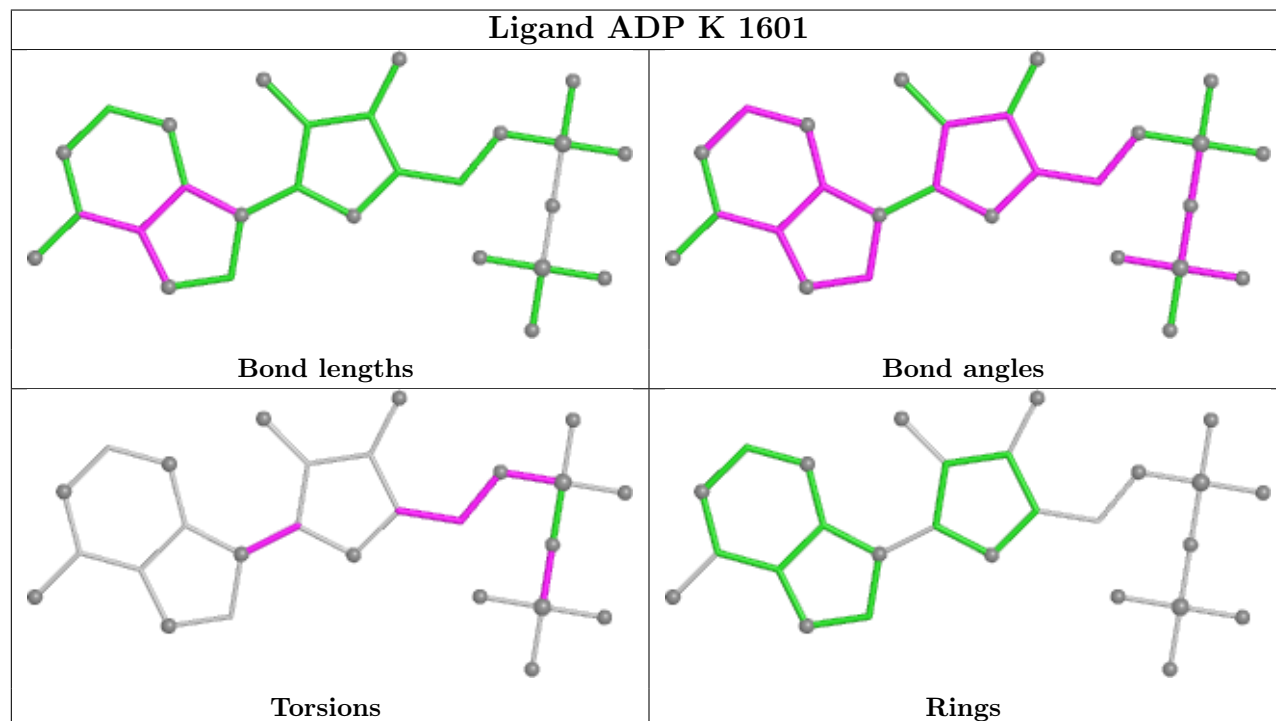
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	1601	ADP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



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.

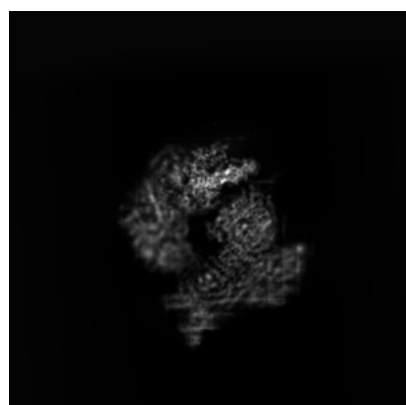
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68935. These allow visual inspection of the internal detail of the map and identification of artifacts.

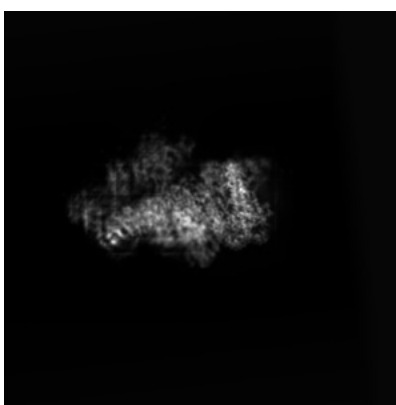
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

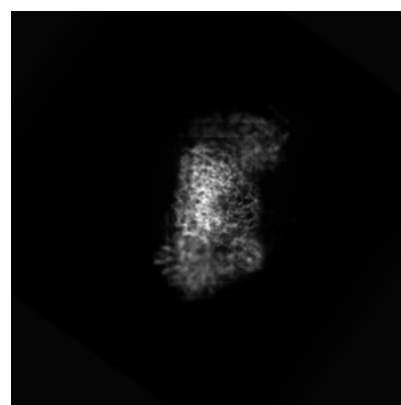
6.1.1 Primary map



X



Y



Z

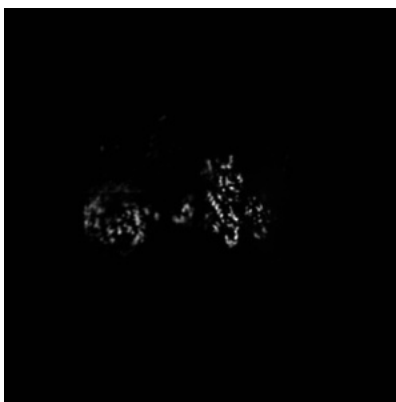
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

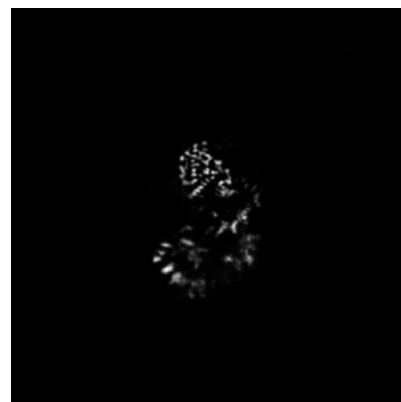
6.2.1 Primary map



X Index: 210



Y Index: 210

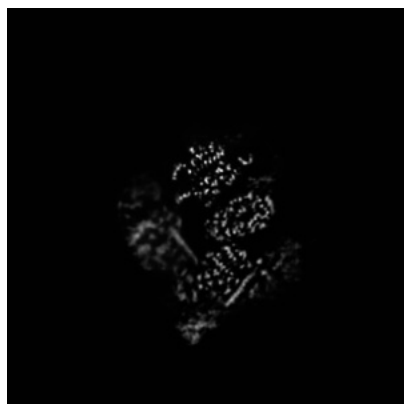


Z Index: 210

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

6.3 Largest variance slices [i](#)

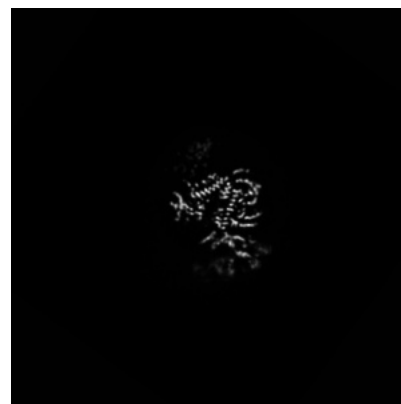
6.3.1 Primary map



X Index: 202



Y Index: 208



Z Index: 242

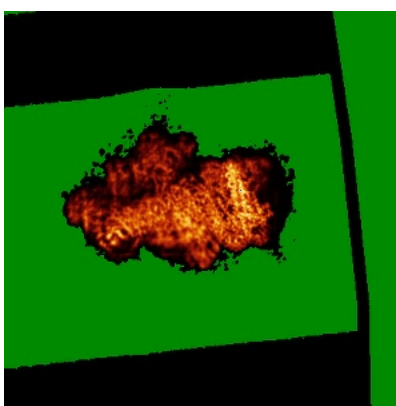
The images above show the largest variance slices of the map in three orthogonal directions.

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

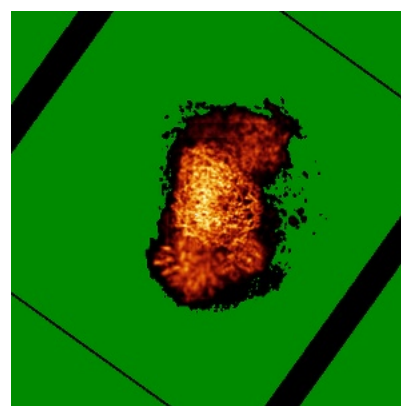
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

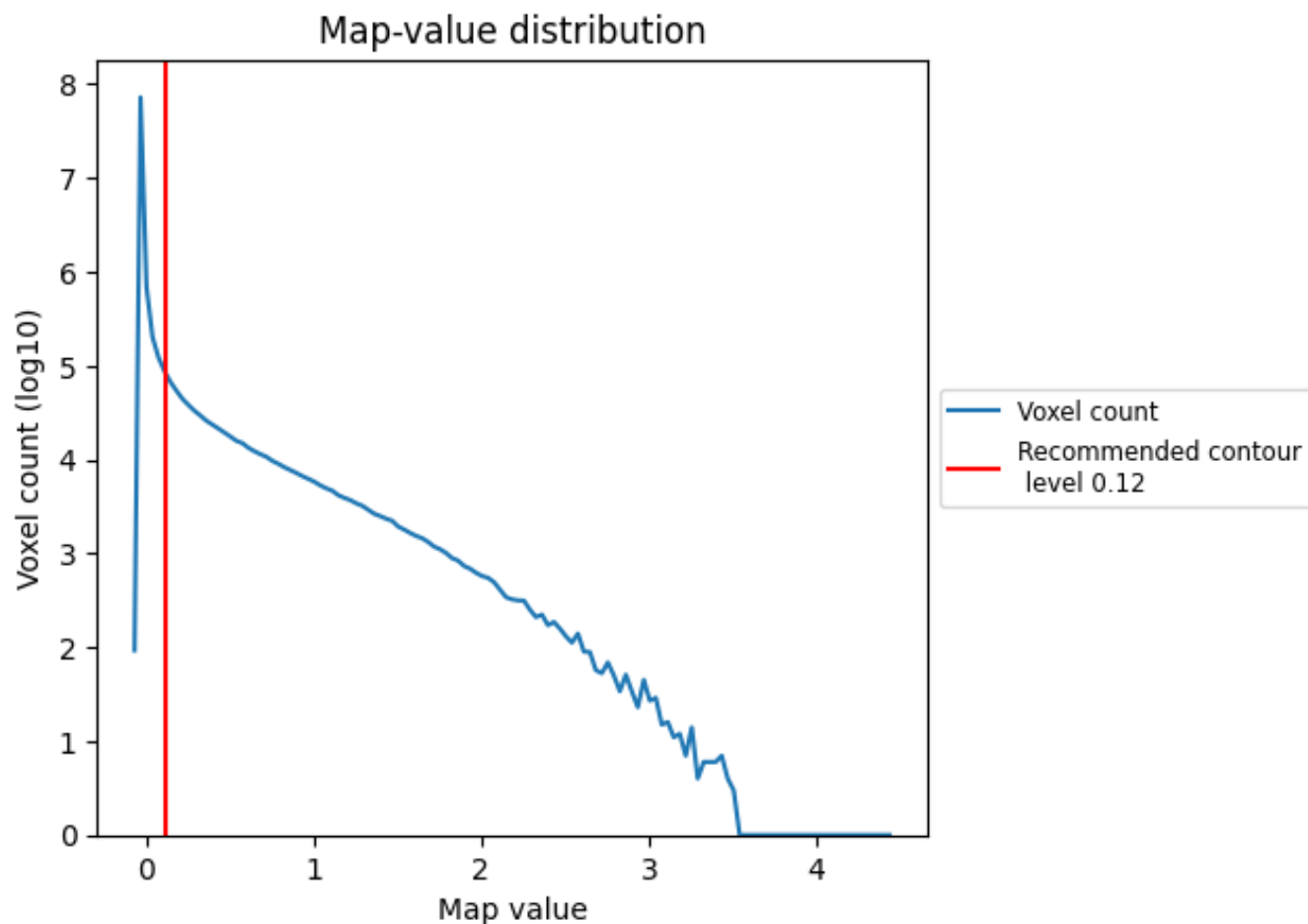
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

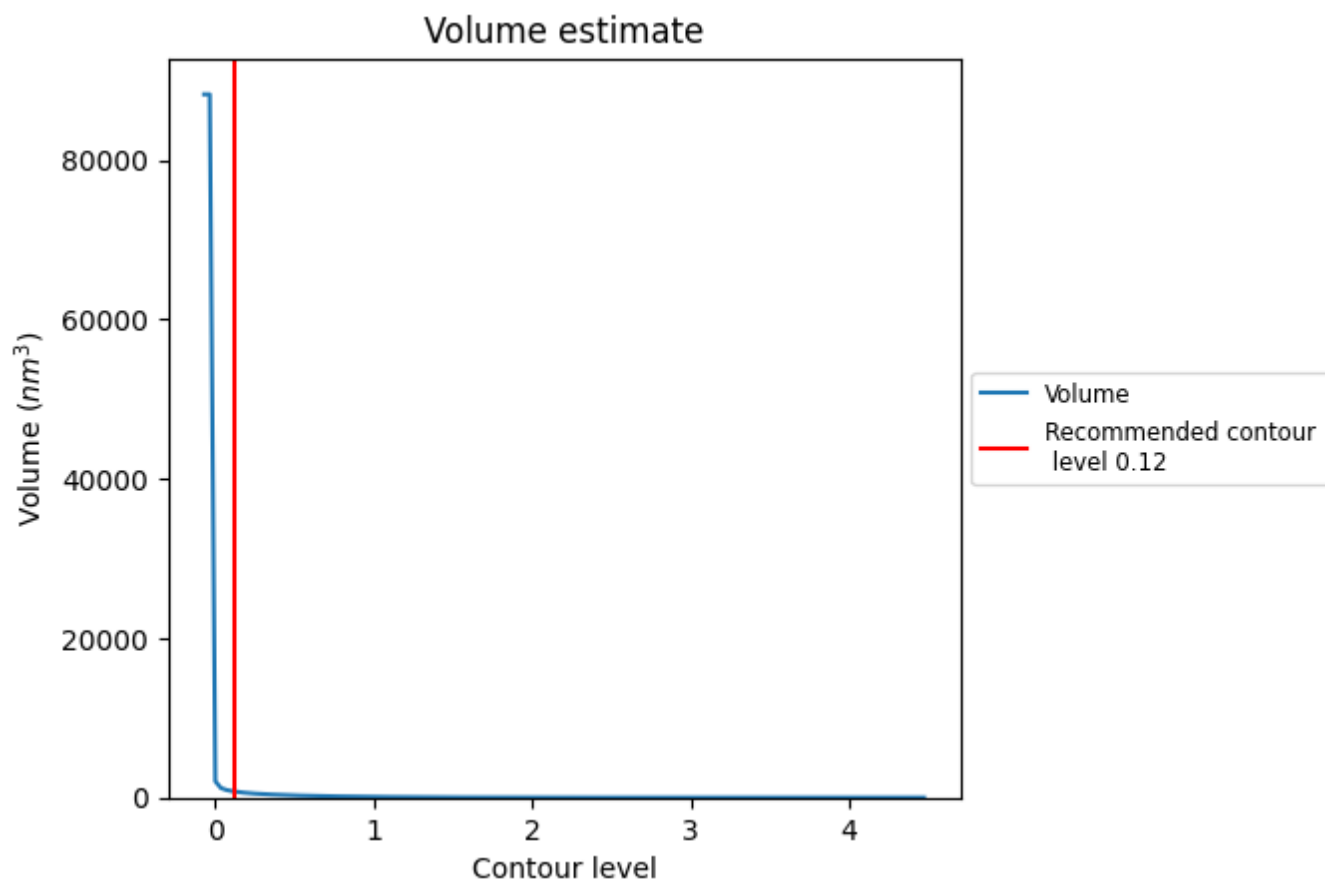
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

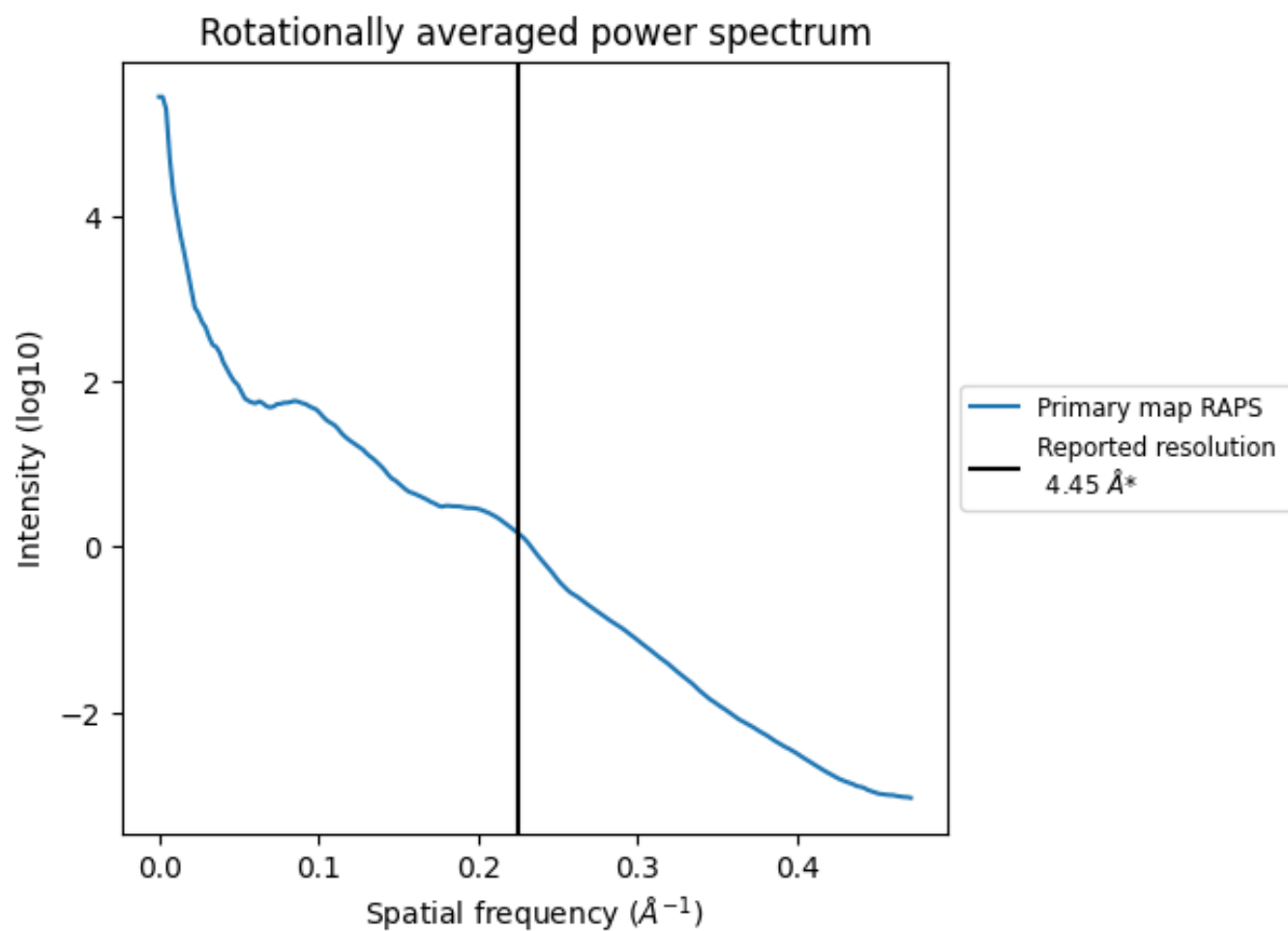
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 773 nm^3 ; this corresponds to an approximate mass of 698 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 0.225 $\text{\AA}^{-1}$

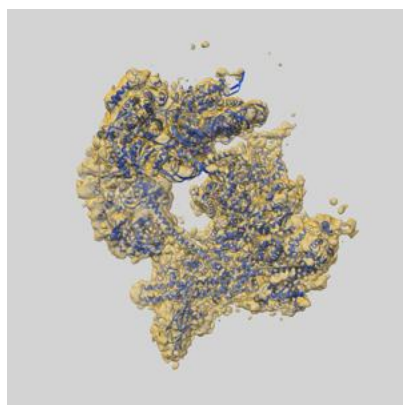
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

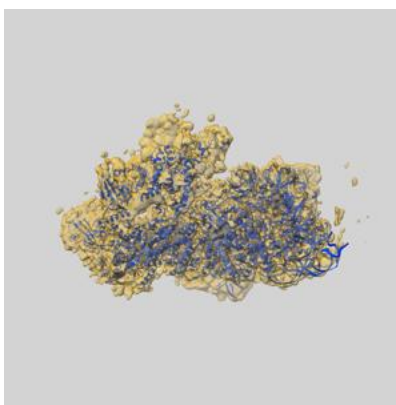
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68935 and PDB model 23FU. Per-residue inclusion information can be found in section [3](#) on page [13](#).

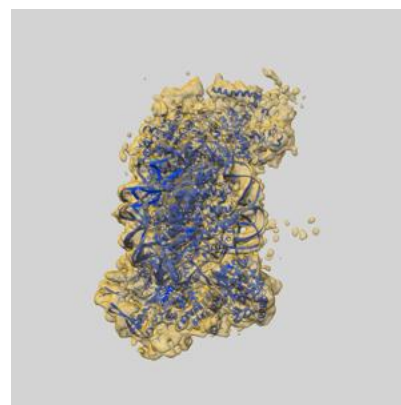
9.1 Map-model overlay [i](#)



X



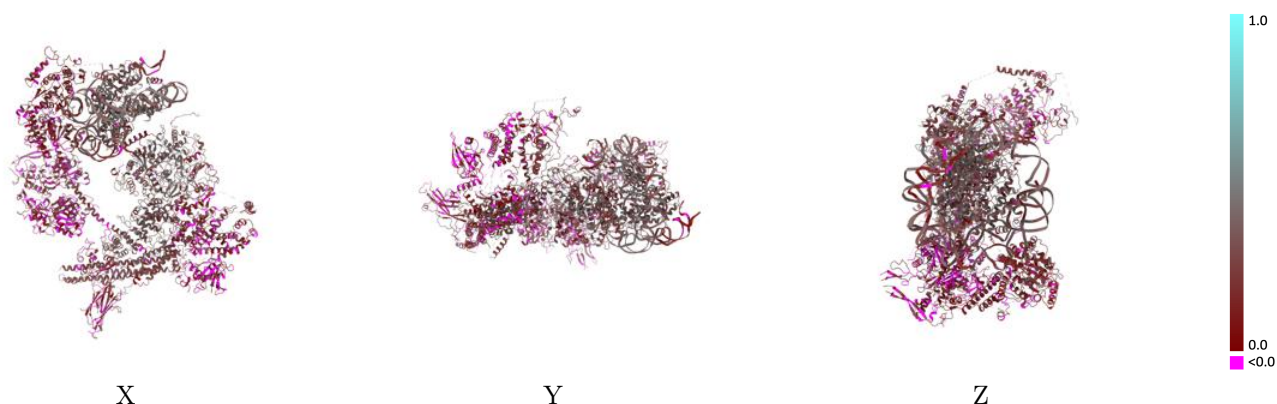
Y



Z

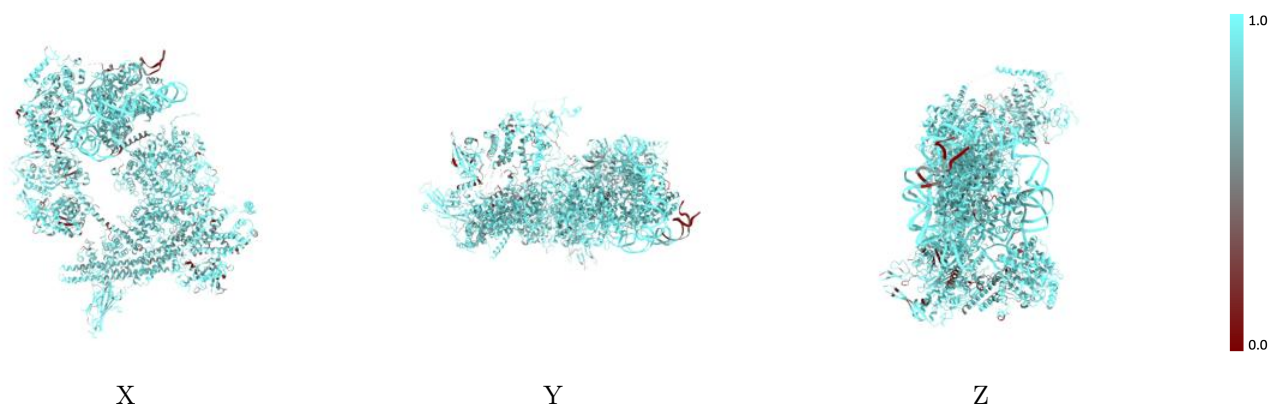
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



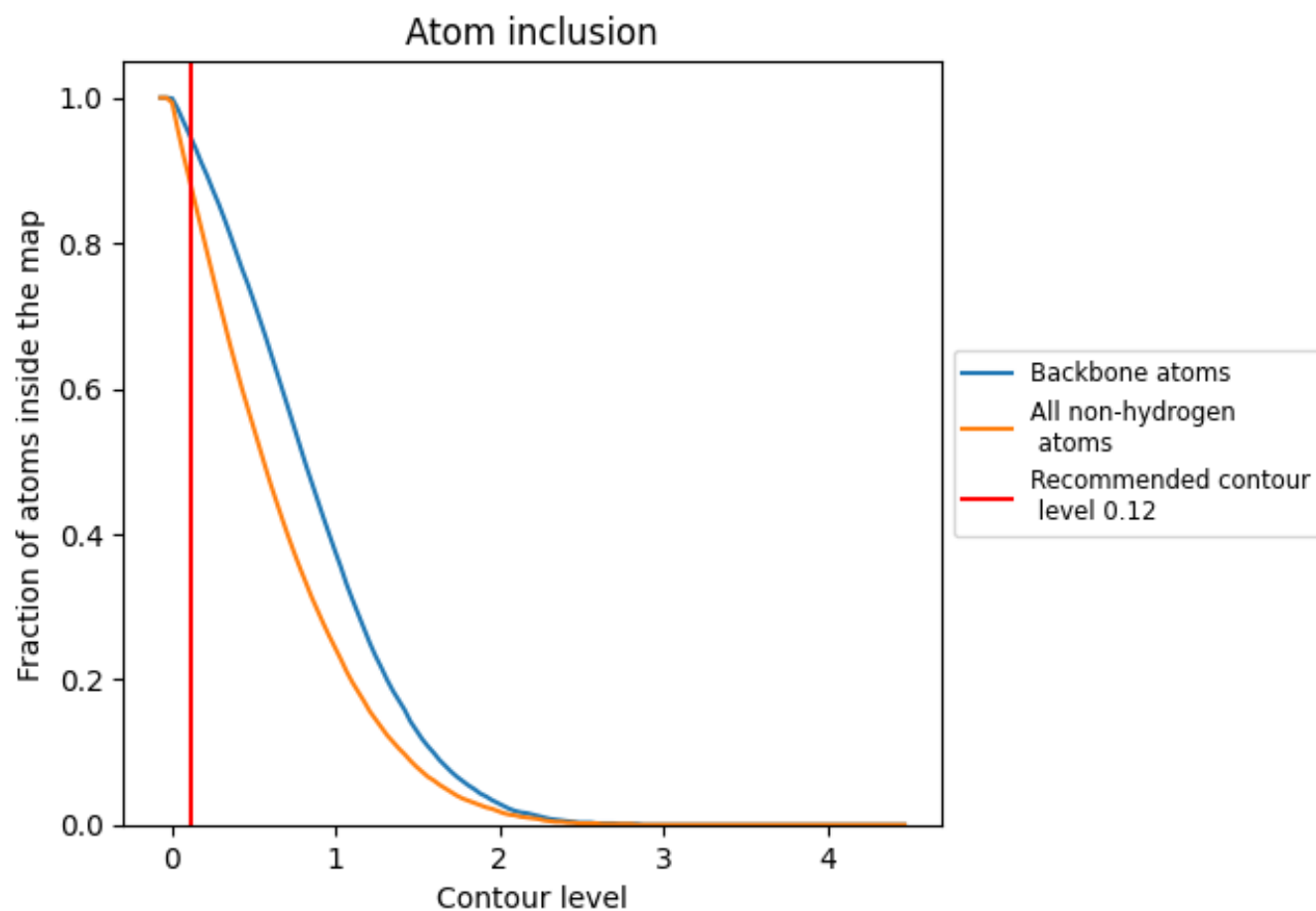
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.2340
A	 0.9050	 0.3230
B	 0.9000	 0.3850
C	 0.9280	 0.3570
D	 0.9370	 0.3670
E	 0.8900	 0.3340
F	 0.9320	 0.3960
G	 0.8930	 0.3440
H	 0.9110	 0.3510
I	 0.9160	 0.3150
J	 0.9100	 0.3050
K	 0.8070	 0.1630
L	 0.8730	 0.1100
M	 0.8710	 0.0770
N	 0.8890	 0.2610
O	 0.8990	 0.2570
P	 0.8610	 0.1840
Q	 0.8200	 0.1300
R	 0.9150	 0.3060
S	 0.8880	 0.3070
T	 0.9110	 0.3260
U	 0.9040	 0.2290
V	 0.8560	 0.2100

