Full wwPDB EM Validation Report

Mar 10, 2026 – 01:00 PM UTC

PDB ID	:	8WW7 / pdb_00008ww7
EMDB ID	:	EMD-37883
Title	:	Structure of AMPPNP-Form AsfvPrimPol Dodecamer
Authors	:	Shi, T.H.; Guo, Y.Y.; Yan, R.H.
Deposited on	:	2023-10-25
Resolution	:	3.28 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

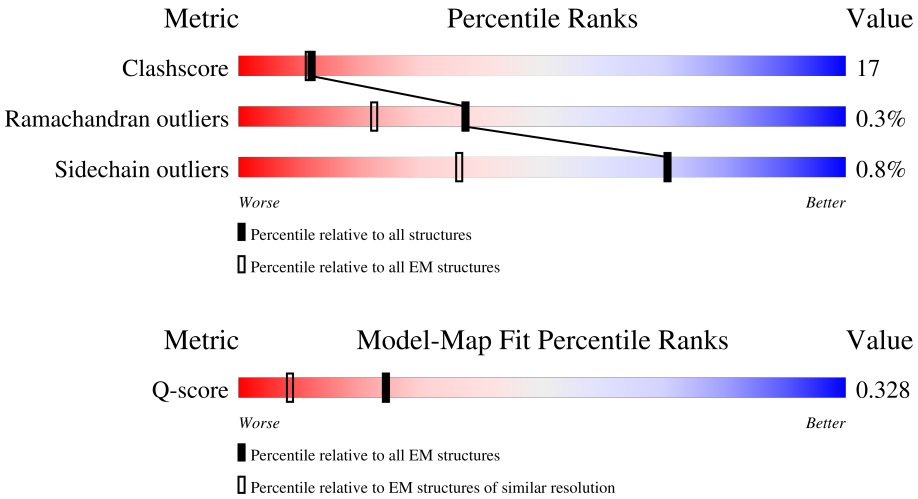
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.28 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	14492 (2.78 - 3.78)

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 <=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	M	26	85% 35% 65%
1	O	26	12% 19% 81%
2	N	4	100% 100%
3	A	972	59% 32% 9%

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Mol	Chain	Length	Quality of chain
3	B	972	7% 61% 30% 9%
3	C	972	9% 56% 34% 8%
3	D	972	10% 57% 33% 9%
3	E	972	6% 58% 34% 8%
3	F	972	62% 30% 9%
3	G	972	20% 59% 33% 8%
3	H	972	18% 54% 36% 9%
3	I	972	16% 54% 36% 9%
3	J	972	17% 56% 34% 9%
3	K	972	21% 56% 34% 9%
3	L	972	23% 58% 32% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ANP	J	1001	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 88330 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 DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	26	Total	C	N	O	P	0	0
			520	260	52	182	26		
1	O	5	Total	C	N	O	P	0	0
			100	50	10	35	5		

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	4	Total	C	N	O	P	0	0
			84	40	20	20	4		

- Molecule 3 is a protein called Putative primase C962R.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	887	Total	C	N	O	S	0	0
			7270	4688	1236	1315	31		
3	B	889	Total	C	N	O	S	0	0
			7284	4697	1238	1318	31		
3	C	892	Total	C	N	O	S	0	0
			7307	4712	1242	1322	31		
3	D	889	Total	C	N	O	S	0	0
			7284	4698	1238	1317	31		
3	E	898	Total	C	N	O	S	0	0
			7349	4736	1248	1334	31		
3	F	888	Total	C	N	O	S	0	0
			7275	4692	1235	1317	31		
3	G	898	Total	C	N	O	S	0	0
			7349	4736	1248	1334	31		
3	L	880	Total	C	N	O	S	0	0
			7209	4647	1224	1307	31		
3	K	881	Total	C	N	O	S	0	0
			7219	4655	1227	1306	31		
3	J	884	Total	C	N	O	S	0	0
			7242	4670	1230	1311	31		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	882	Total	C	N	O	S	0	0
			7226	4659	1228	1308	31		
3	H	883	Total	C	N	O	S	0	0
			7234	4664	1229	1310	31		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	963	LEU	-	expression tag	UNP A0A2X0TKI6
A	964	GLU	-	expression tag	UNP A0A2X0TKI6
A	965	ASP	-	expression tag	UNP A0A2X0TKI6
A	966	TYR	-	expression tag	UNP A0A2X0TKI6
A	967	LYS	-	expression tag	UNP A0A2X0TKI6
A	968	ASP	-	expression tag	UNP A0A2X0TKI6
A	969	ASP	-	expression tag	UNP A0A2X0TKI6
A	970	ASP	-	expression tag	UNP A0A2X0TKI6
A	971	ASP	-	expression tag	UNP A0A2X0TKI6
A	972	LYS	-	expression tag	UNP A0A2X0TKI6
B	963	LEU	-	expression tag	UNP A0A2X0TKI6
B	964	GLU	-	expression tag	UNP A0A2X0TKI6
B	965	ASP	-	expression tag	UNP A0A2X0TKI6
B	966	TYR	-	expression tag	UNP A0A2X0TKI6
B	967	LYS	-	expression tag	UNP A0A2X0TKI6
B	968	ASP	-	expression tag	UNP A0A2X0TKI6
B	969	ASP	-	expression tag	UNP A0A2X0TKI6
B	970	ASP	-	expression tag	UNP A0A2X0TKI6
B	971	ASP	-	expression tag	UNP A0A2X0TKI6
B	972	LYS	-	expression tag	UNP A0A2X0TKI6
C	963	LEU	-	expression tag	UNP A0A2X0TKI6
C	964	GLU	-	expression tag	UNP A0A2X0TKI6
C	965	ASP	-	expression tag	UNP A0A2X0TKI6
C	966	TYR	-	expression tag	UNP A0A2X0TKI6
C	967	LYS	-	expression tag	UNP A0A2X0TKI6
C	968	ASP	-	expression tag	UNP A0A2X0TKI6
C	969	ASP	-	expression tag	UNP A0A2X0TKI6
C	970	ASP	-	expression tag	UNP A0A2X0TKI6
C	971	ASP	-	expression tag	UNP A0A2X0TKI6
C	972	LYS	-	expression tag	UNP A0A2X0TKI6
D	963	LEU	-	expression tag	UNP A0A2X0TKI6
D	964	GLU	-	expression tag	UNP A0A2X0TKI6
D	965	ASP	-	expression tag	UNP A0A2X0TKI6
D	966	TYR	-	expression tag	UNP A0A2X0TKI6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	967	LYS	-	expression tag	UNP A0A2X0TKI6
D	968	ASP	-	expression tag	UNP A0A2X0TKI6
D	969	ASP	-	expression tag	UNP A0A2X0TKI6
D	970	ASP	-	expression tag	UNP A0A2X0TKI6
D	971	ASP	-	expression tag	UNP A0A2X0TKI6
D	972	LYS	-	expression tag	UNP A0A2X0TKI6
E	963	LEU	-	expression tag	UNP A0A2X0TKI6
E	964	GLU	-	expression tag	UNP A0A2X0TKI6
E	965	ASP	-	expression tag	UNP A0A2X0TKI6
E	966	TYR	-	expression tag	UNP A0A2X0TKI6
E	967	LYS	-	expression tag	UNP A0A2X0TKI6
E	968	ASP	-	expression tag	UNP A0A2X0TKI6
E	969	ASP	-	expression tag	UNP A0A2X0TKI6
E	970	ASP	-	expression tag	UNP A0A2X0TKI6
E	971	ASP	-	expression tag	UNP A0A2X0TKI6
E	972	LYS	-	expression tag	UNP A0A2X0TKI6
F	963	LEU	-	expression tag	UNP A0A2X0TKI6
F	964	GLU	-	expression tag	UNP A0A2X0TKI6
F	965	ASP	-	expression tag	UNP A0A2X0TKI6
F	966	TYR	-	expression tag	UNP A0A2X0TKI6
F	967	LYS	-	expression tag	UNP A0A2X0TKI6
F	968	ASP	-	expression tag	UNP A0A2X0TKI6
F	969	ASP	-	expression tag	UNP A0A2X0TKI6
F	970	ASP	-	expression tag	UNP A0A2X0TKI6
F	971	ASP	-	expression tag	UNP A0A2X0TKI6
F	972	LYS	-	expression tag	UNP A0A2X0TKI6
G	963	LEU	-	expression tag	UNP A0A2X0TKI6
G	964	GLU	-	expression tag	UNP A0A2X0TKI6
G	965	ASP	-	expression tag	UNP A0A2X0TKI6
G	966	TYR	-	expression tag	UNP A0A2X0TKI6
G	967	LYS	-	expression tag	UNP A0A2X0TKI6
G	968	ASP	-	expression tag	UNP A0A2X0TKI6
G	969	ASP	-	expression tag	UNP A0A2X0TKI6
G	970	ASP	-	expression tag	UNP A0A2X0TKI6
G	971	ASP	-	expression tag	UNP A0A2X0TKI6
G	972	LYS	-	expression tag	UNP A0A2X0TKI6
L	963	LEU	-	expression tag	UNP A0A2X0TKI6
L	964	GLU	-	expression tag	UNP A0A2X0TKI6
L	965	ASP	-	expression tag	UNP A0A2X0TKI6
L	966	TYR	-	expression tag	UNP A0A2X0TKI6
L	967	LYS	-	expression tag	UNP A0A2X0TKI6
L	968	ASP	-	expression tag	UNP A0A2X0TKI6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	969	ASP	-	expression tag	UNP A0A2X0TKI6
L	970	ASP	-	expression tag	UNP A0A2X0TKI6
L	971	ASP	-	expression tag	UNP A0A2X0TKI6
L	972	LYS	-	expression tag	UNP A0A2X0TKI6
K	963	LEU	-	expression tag	UNP A0A2X0TKI6
K	964	GLU	-	expression tag	UNP A0A2X0TKI6
K	965	ASP	-	expression tag	UNP A0A2X0TKI6
K	966	TYR	-	expression tag	UNP A0A2X0TKI6
K	967	LYS	-	expression tag	UNP A0A2X0TKI6
K	968	ASP	-	expression tag	UNP A0A2X0TKI6
K	969	ASP	-	expression tag	UNP A0A2X0TKI6
K	970	ASP	-	expression tag	UNP A0A2X0TKI6
K	971	ASP	-	expression tag	UNP A0A2X0TKI6
K	972	LYS	-	expression tag	UNP A0A2X0TKI6
J	963	LEU	-	expression tag	UNP A0A2X0TKI6
J	964	GLU	-	expression tag	UNP A0A2X0TKI6
J	965	ASP	-	expression tag	UNP A0A2X0TKI6
J	966	TYR	-	expression tag	UNP A0A2X0TKI6
J	967	LYS	-	expression tag	UNP A0A2X0TKI6
J	968	ASP	-	expression tag	UNP A0A2X0TKI6
J	969	ASP	-	expression tag	UNP A0A2X0TKI6
J	970	ASP	-	expression tag	UNP A0A2X0TKI6
J	971	ASP	-	expression tag	UNP A0A2X0TKI6
J	972	LYS	-	expression tag	UNP A0A2X0TKI6
I	963	LEU	-	expression tag	UNP A0A2X0TKI6
I	964	GLU	-	expression tag	UNP A0A2X0TKI6
I	965	ASP	-	expression tag	UNP A0A2X0TKI6
I	966	TYR	-	expression tag	UNP A0A2X0TKI6
I	967	LYS	-	expression tag	UNP A0A2X0TKI6
I	968	ASP	-	expression tag	UNP A0A2X0TKI6
I	969	ASP	-	expression tag	UNP A0A2X0TKI6
I	970	ASP	-	expression tag	UNP A0A2X0TKI6
I	971	ASP	-	expression tag	UNP A0A2X0TKI6
I	972	LYS	-	expression tag	UNP A0A2X0TKI6
H	963	LEU	-	expression tag	UNP A0A2X0TKI6
H	964	GLU	-	expression tag	UNP A0A2X0TKI6
H	965	ASP	-	expression tag	UNP A0A2X0TKI6
H	966	TYR	-	expression tag	UNP A0A2X0TKI6
H	967	LYS	-	expression tag	UNP A0A2X0TKI6
H	968	ASP	-	expression tag	UNP A0A2X0TKI6
H	969	ASP	-	expression tag	UNP A0A2X0TKI6
H	970	ASP	-	expression tag	UNP A0A2X0TKI6

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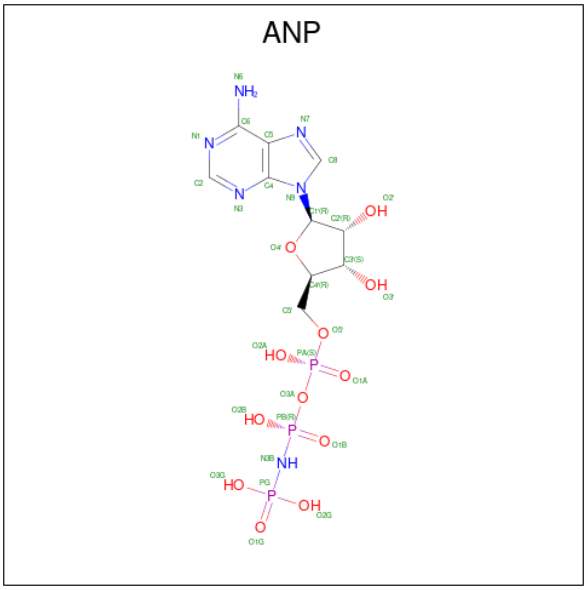
Chain	Residue	Modelled	Actual	Comment	Reference
H	971	ASP	-	expression tag	UNP A0A2X0TKI6
H	972	LYS	-	expression tag	UNP A0A2X0TKI6

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	C	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	G	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	L	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

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Mol	Chain	Residues	Atoms					AltConf
4	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
4	H	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

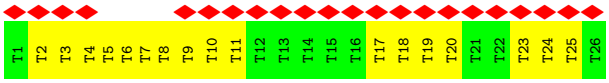
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

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.

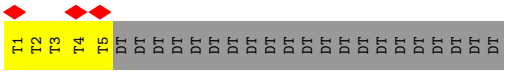
• Molecule 1: DNA (26-MER)

Chain M:



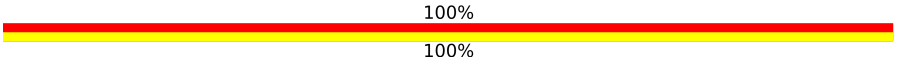
• Molecule 1: DNA (26-MER)

Chain O:



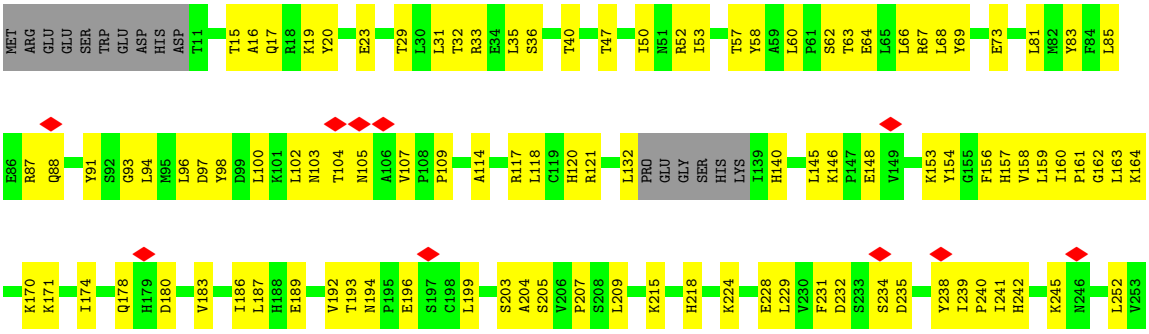
• Molecule 2: DNA (5'-D(P*AP*AP*AP*A)-3')

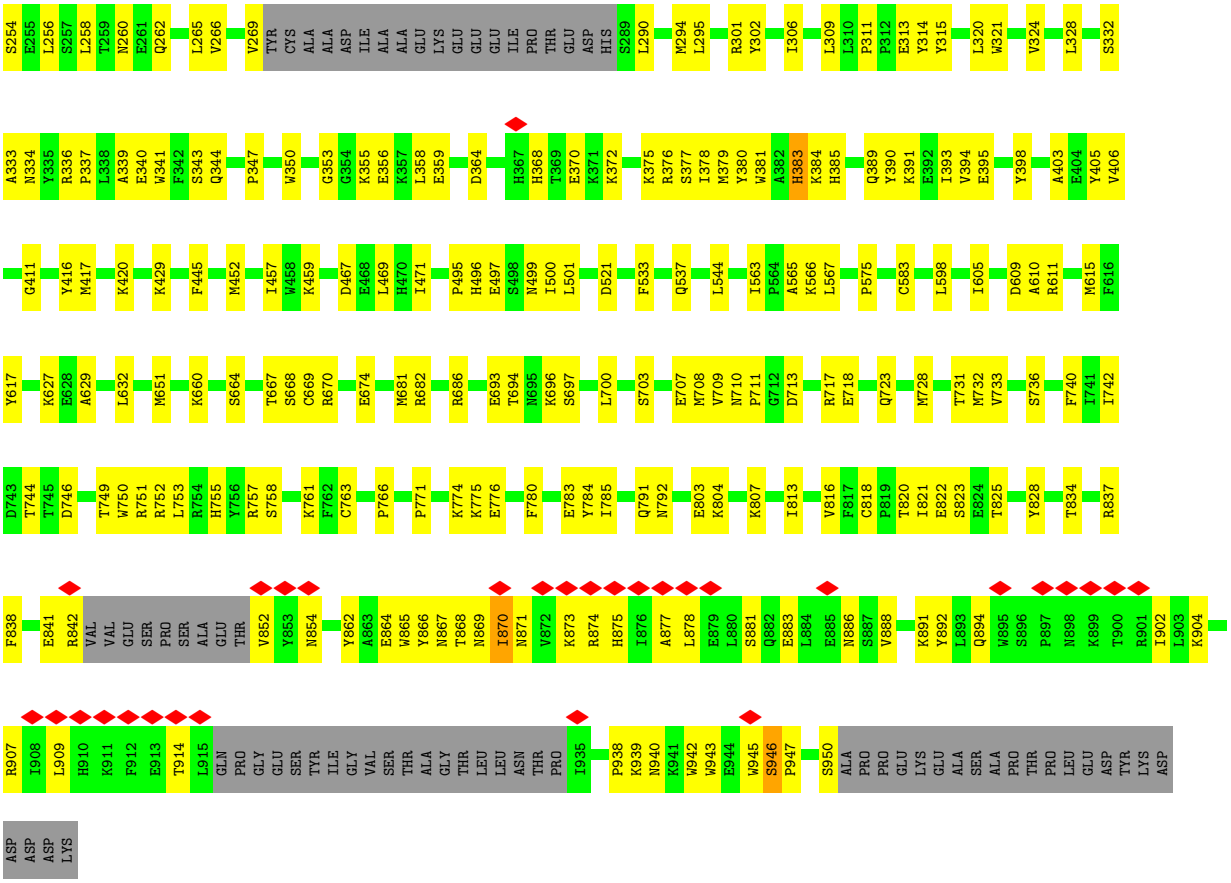
Chain N:



• Molecule 3: Putative primase C962R

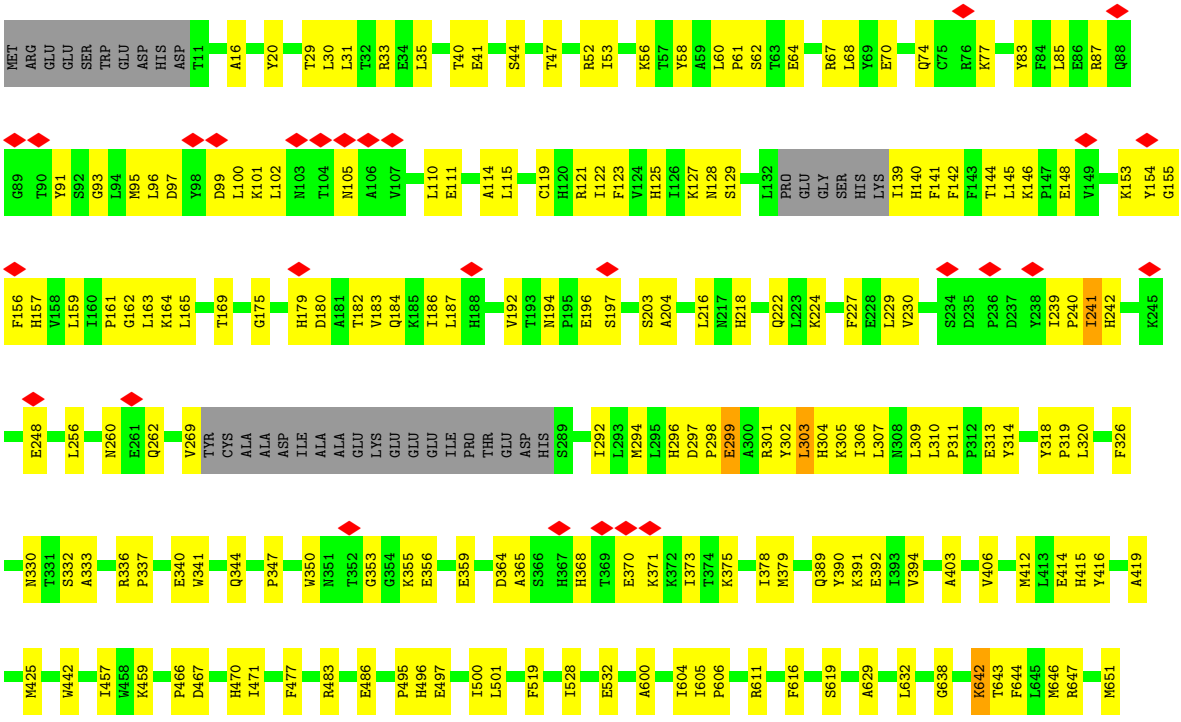
Chain A:

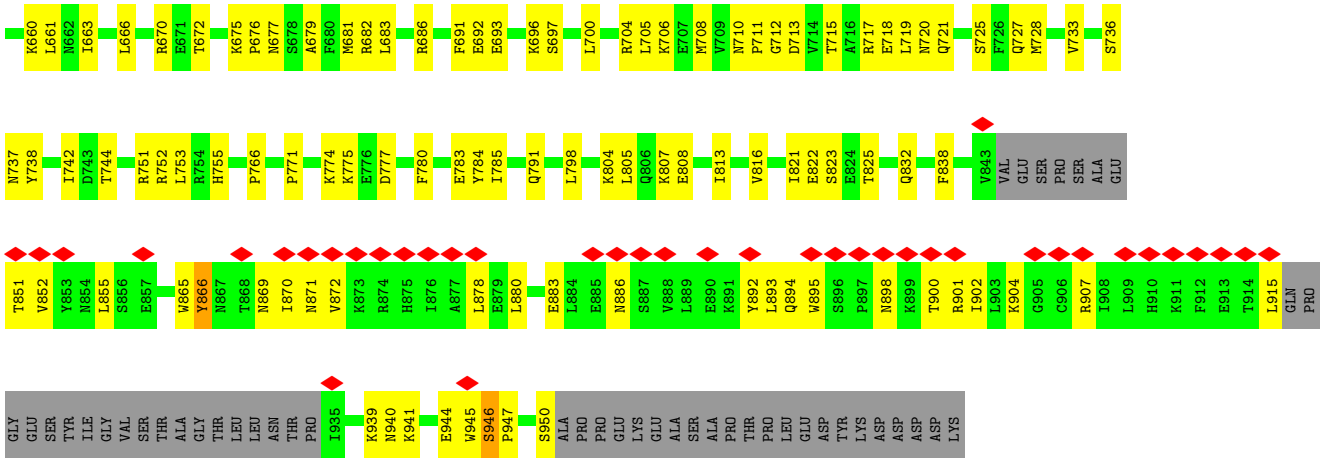




• Molecule 3: Putative primase C962R

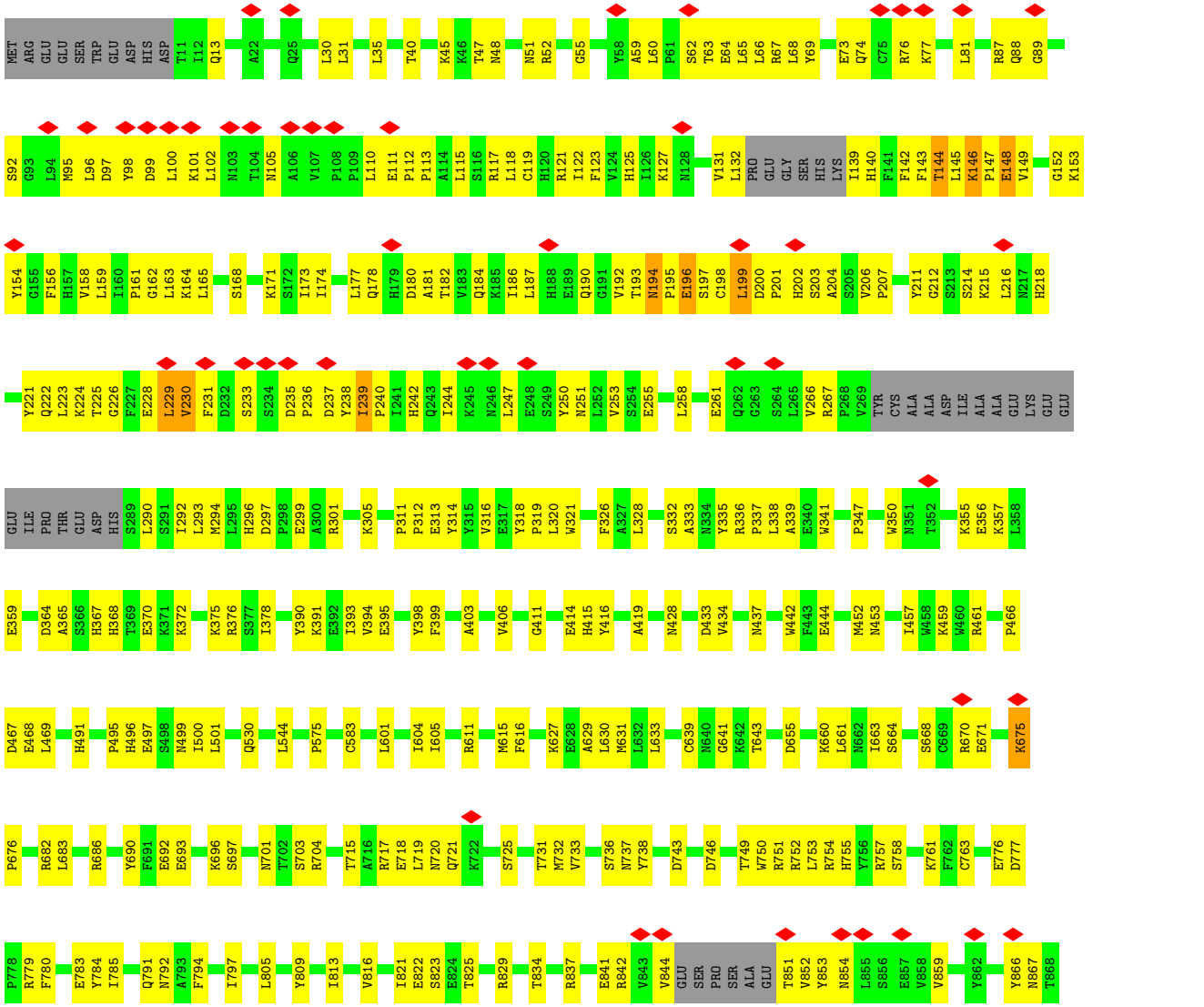
Chain B:

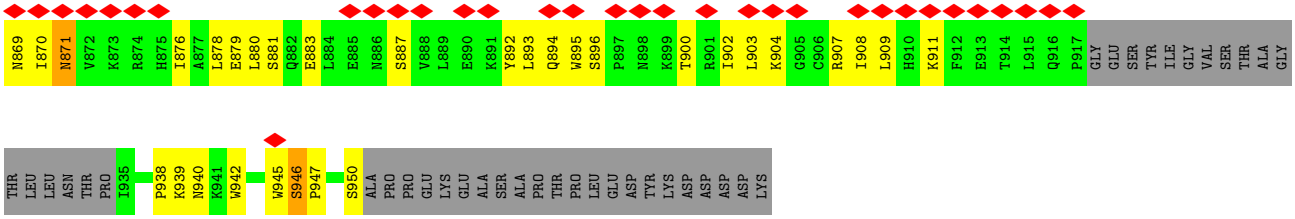




• Molecule 3: Putative primase C962R

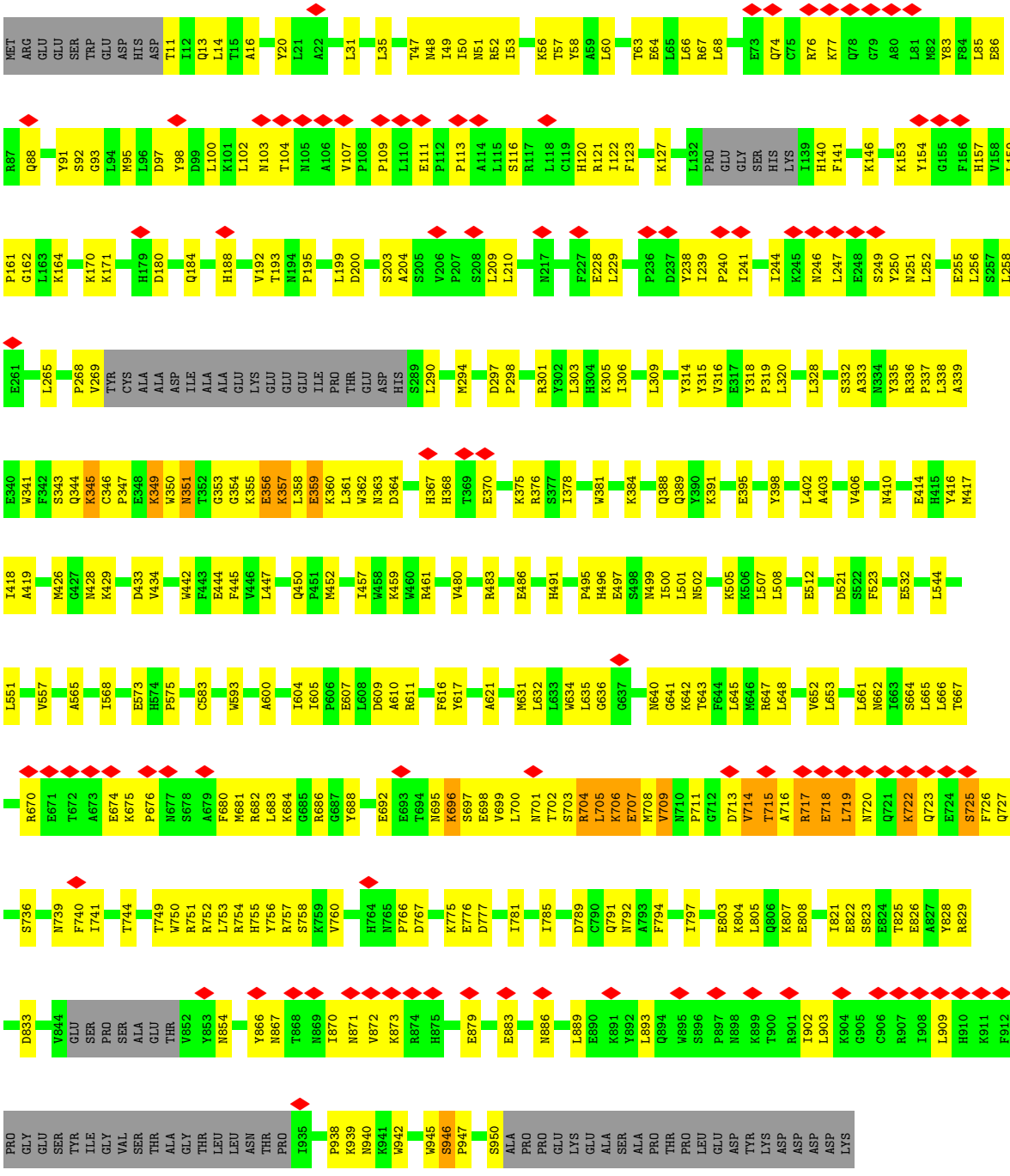
Chain C:





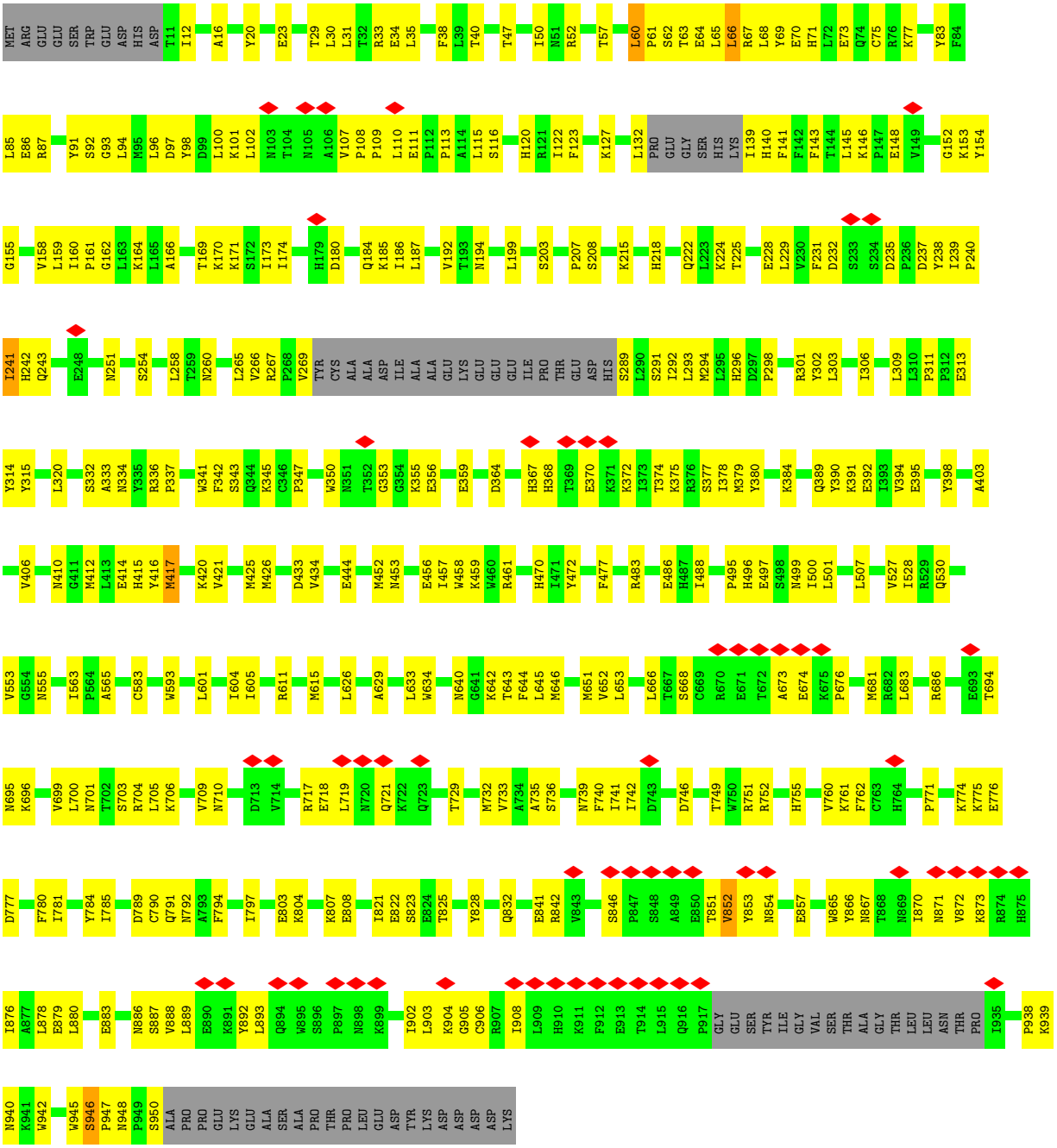
• Molecule 3: Putative primase C962R

Chain D:



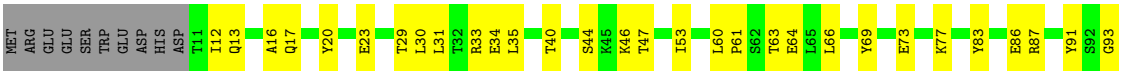
• Molecule 3: Putative primase C962R

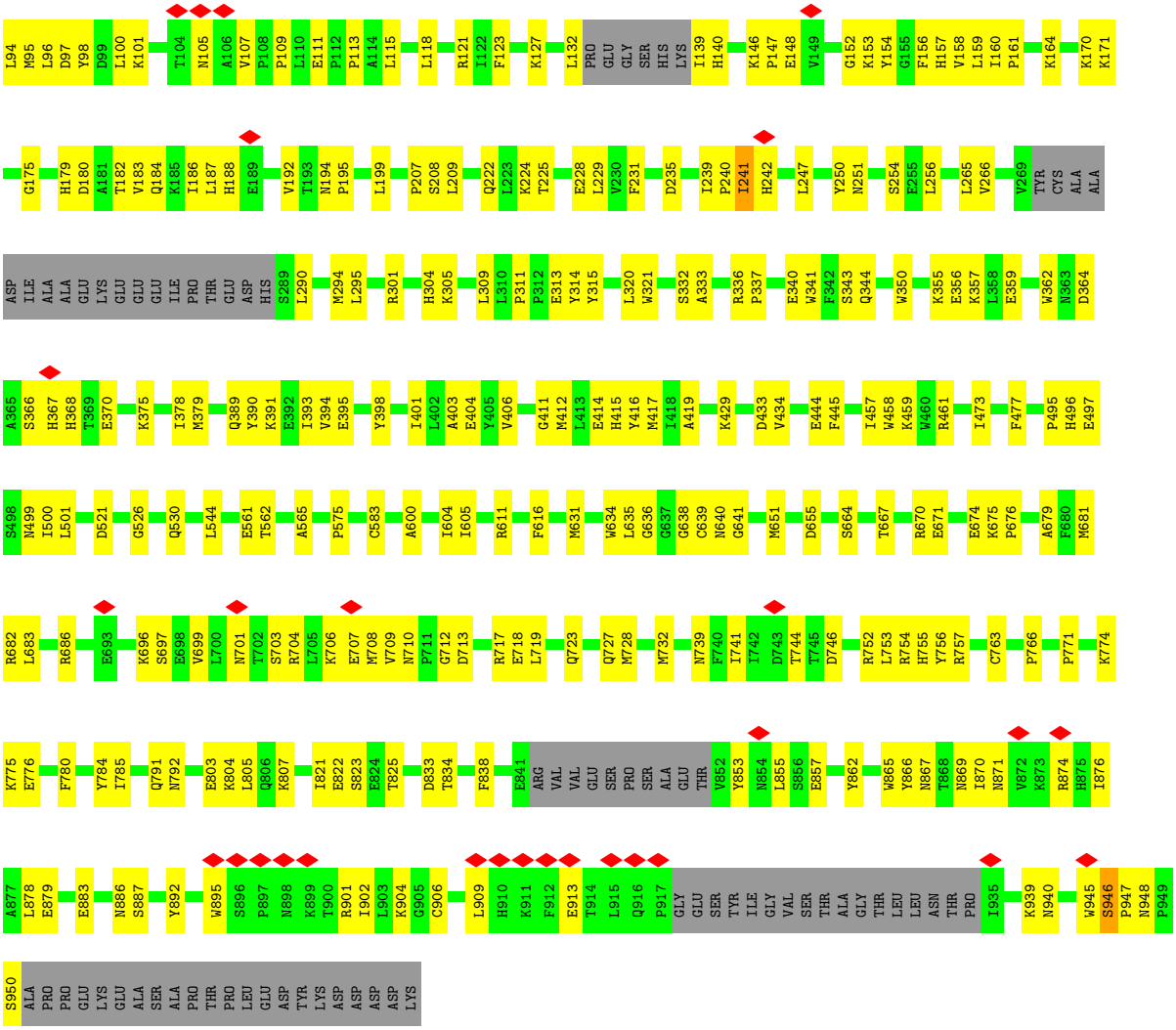
Chain E:



• Molecule 3: Putative primase C962R

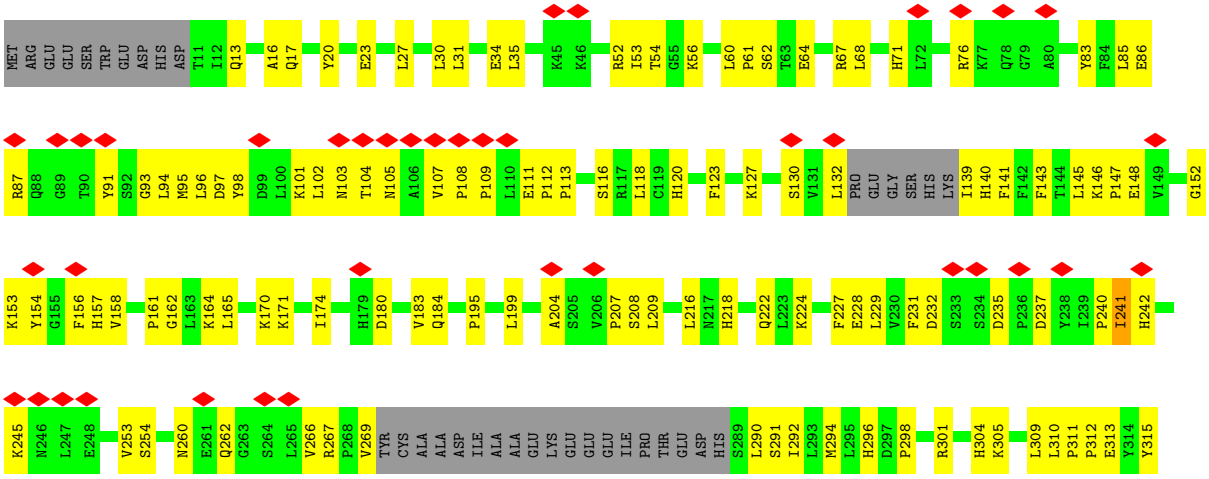
Chain F:

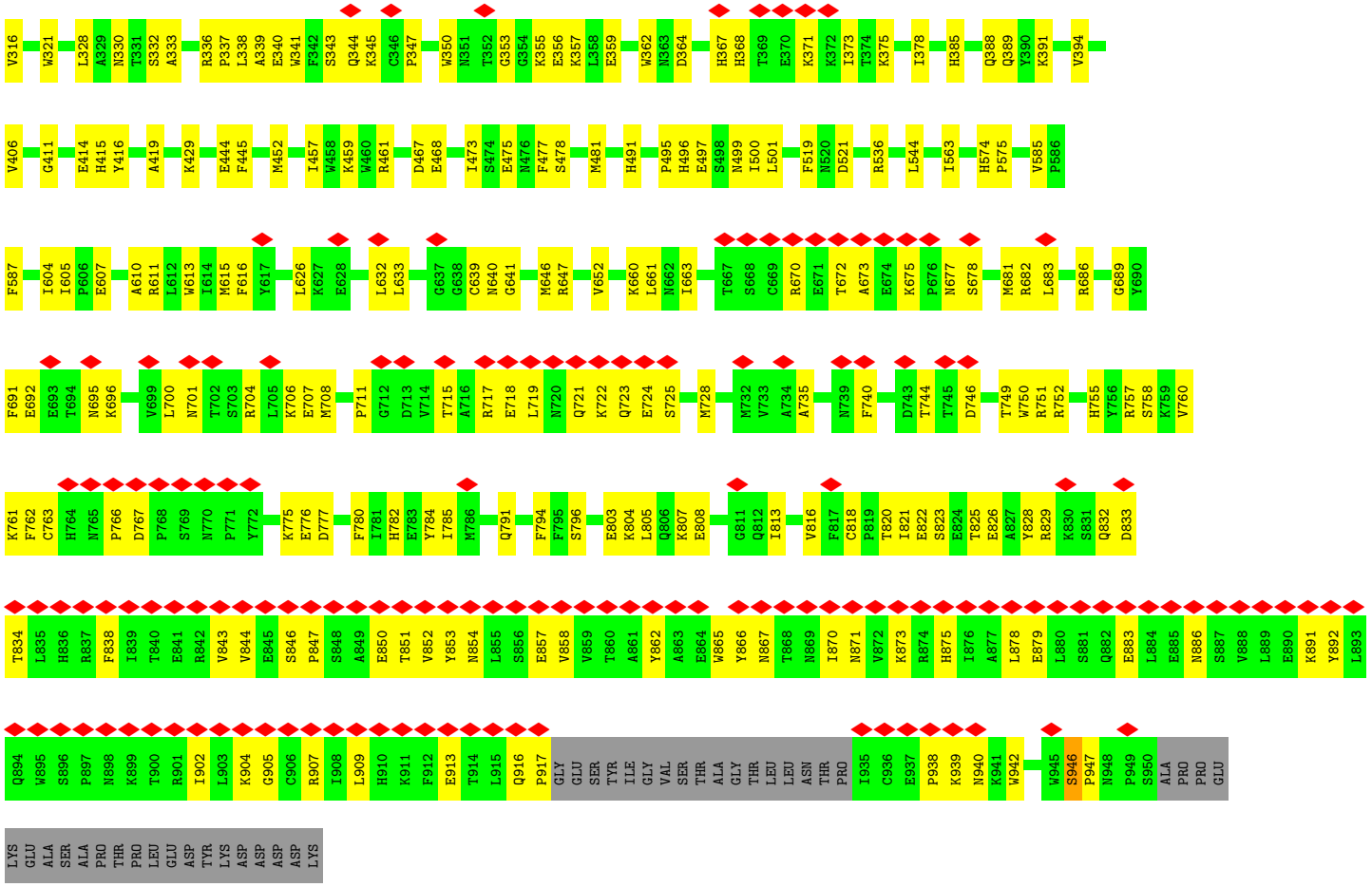




• Molecule 3: Putative primase C962R

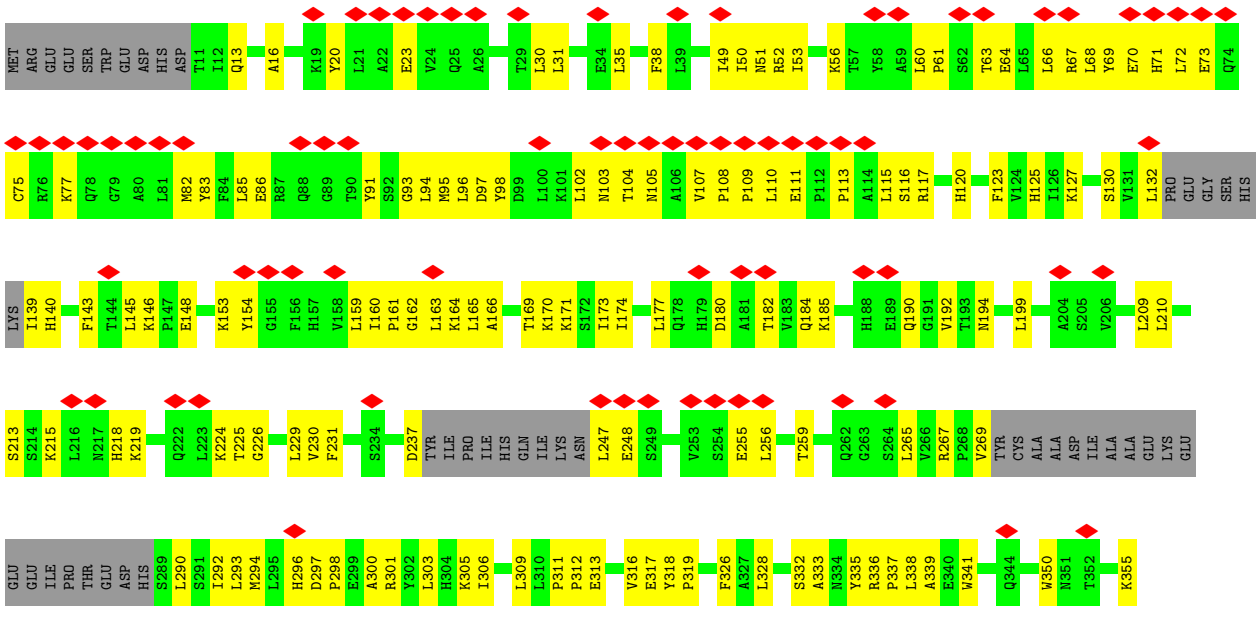
Chain G:

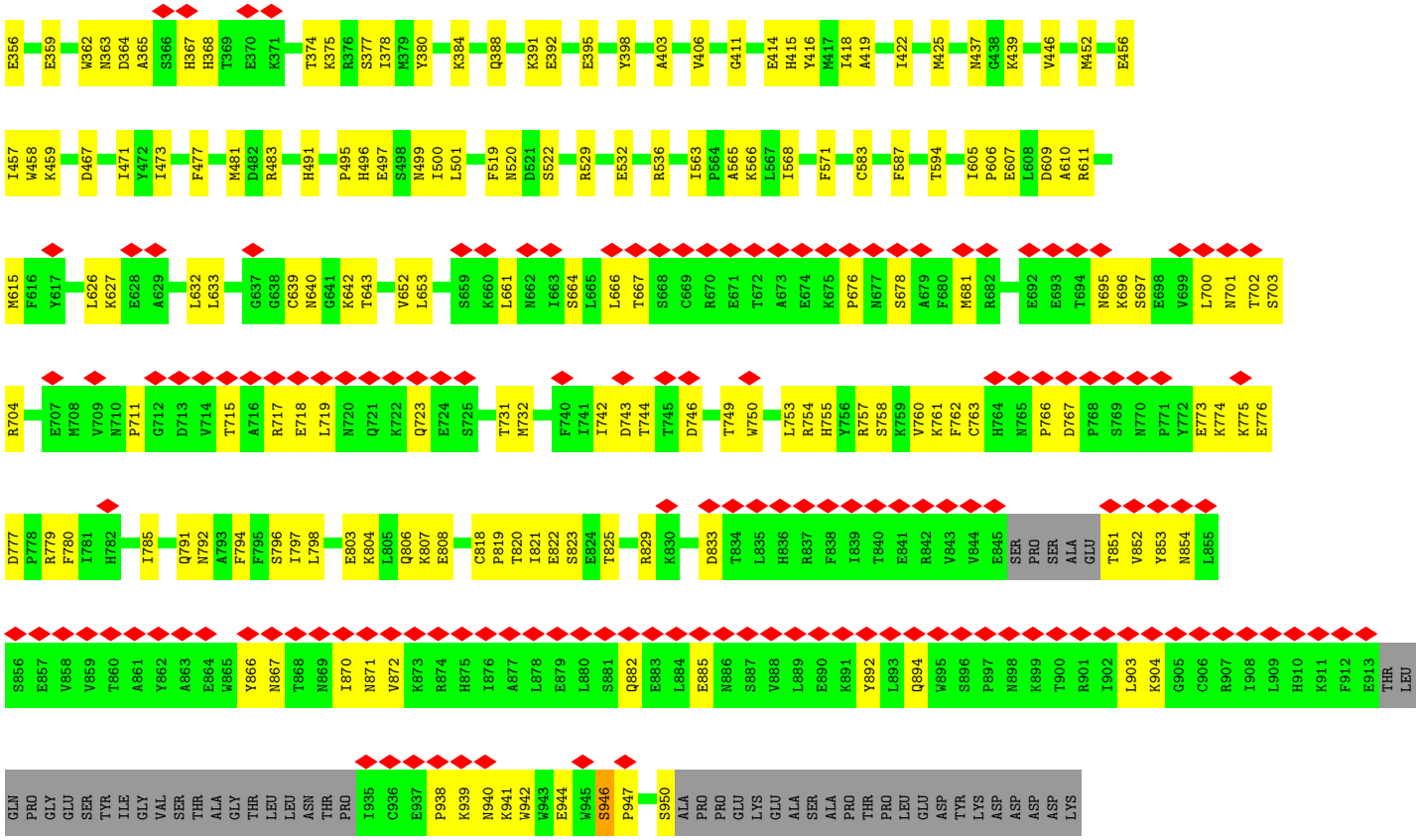




• Molecule 3: Putative primase C962R

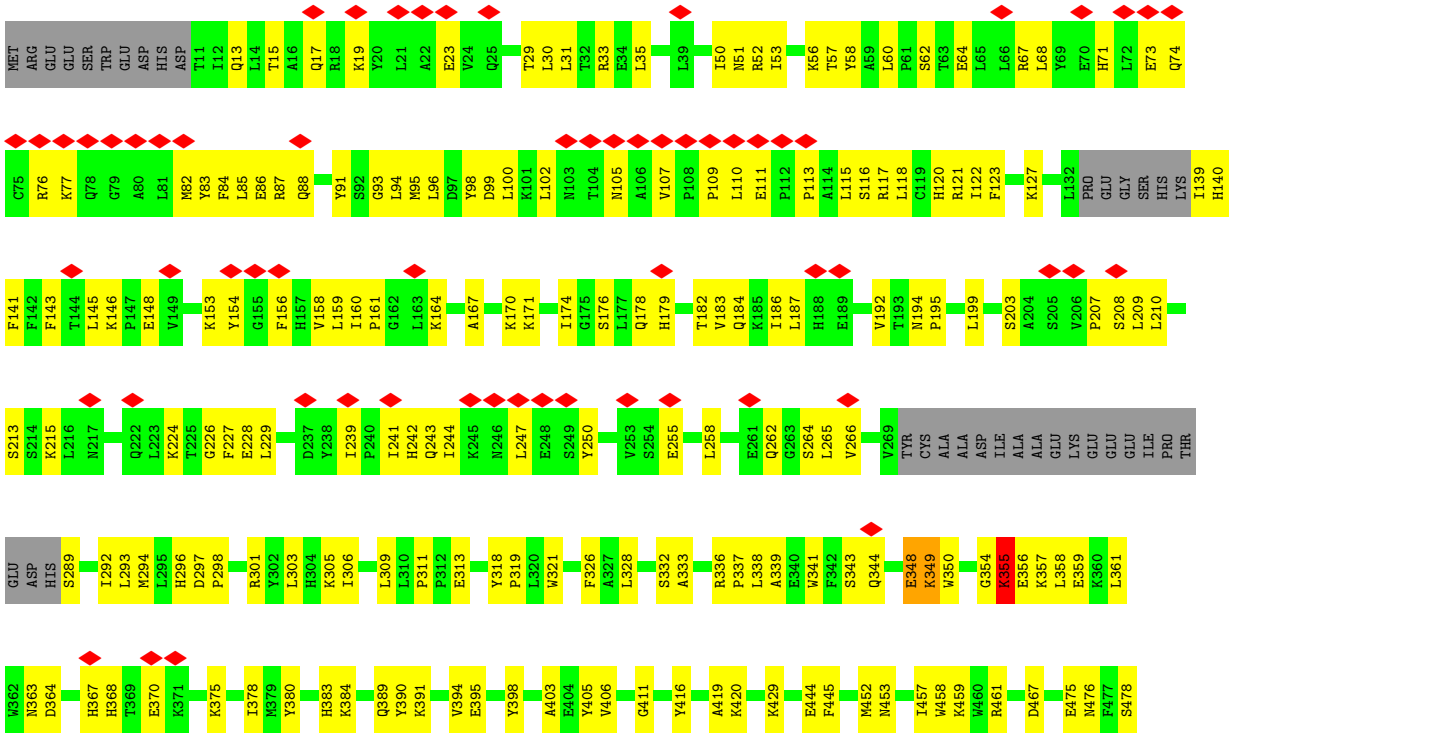
Chain L:

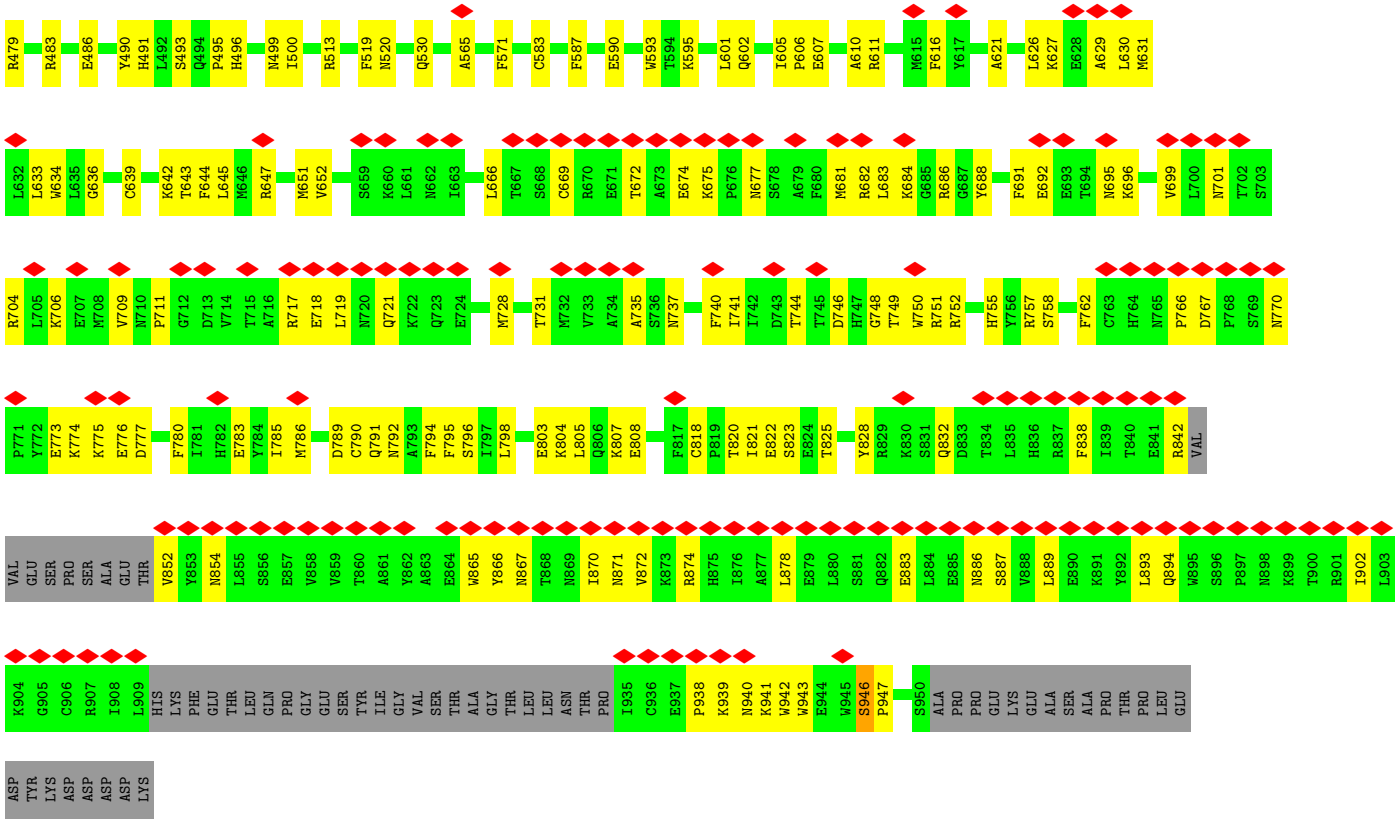




• Molecule 3: Putative primase C962R

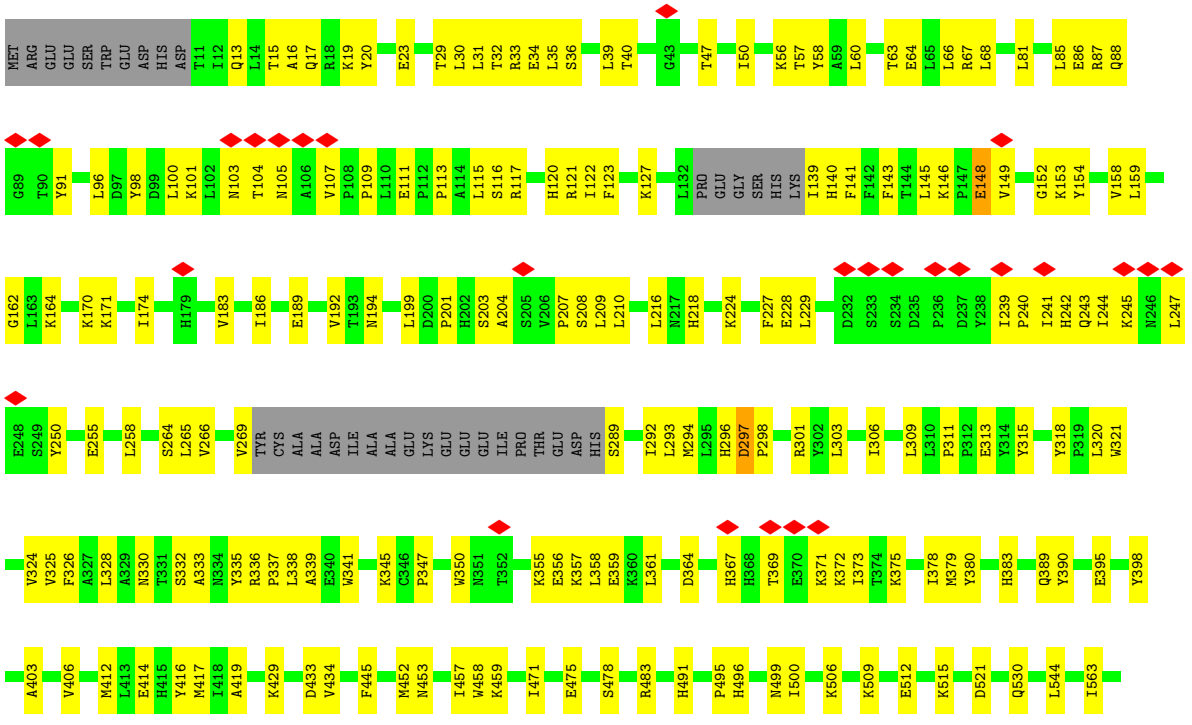
Chain K:

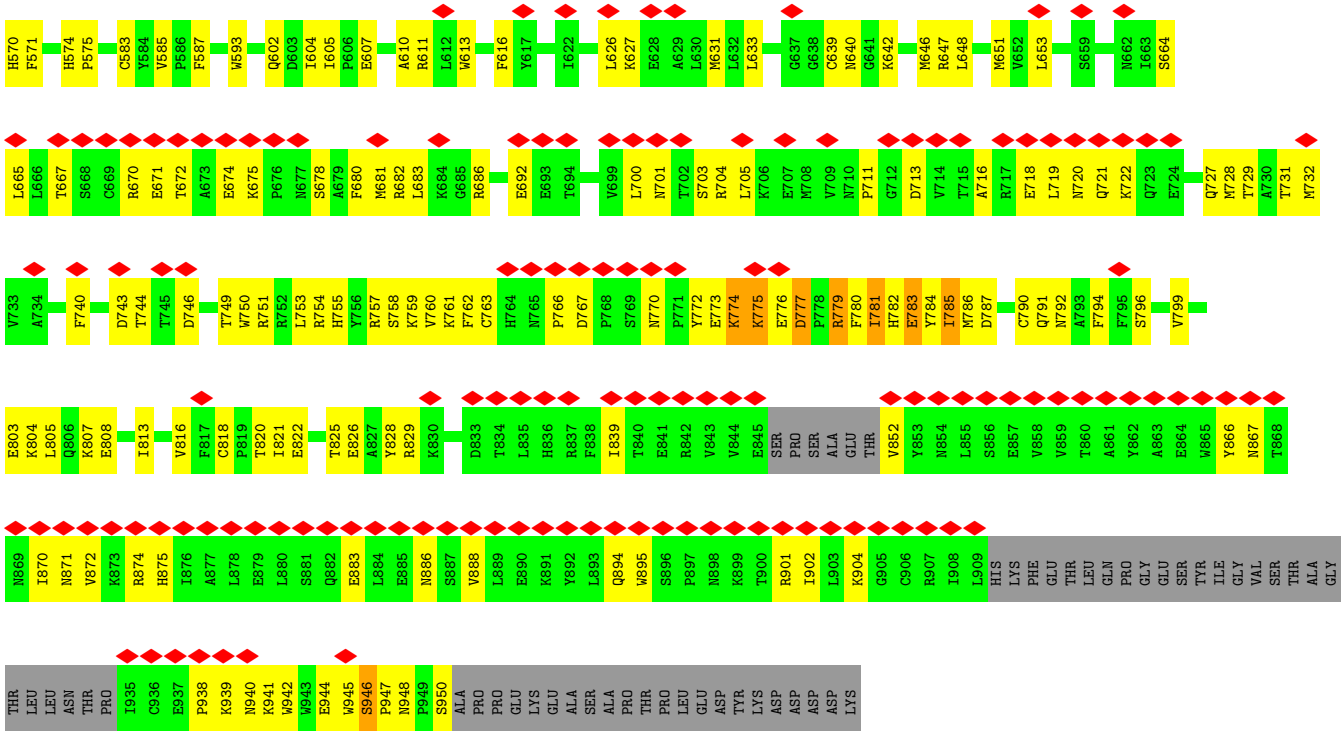




• Molecule 3: Putative primase C962R

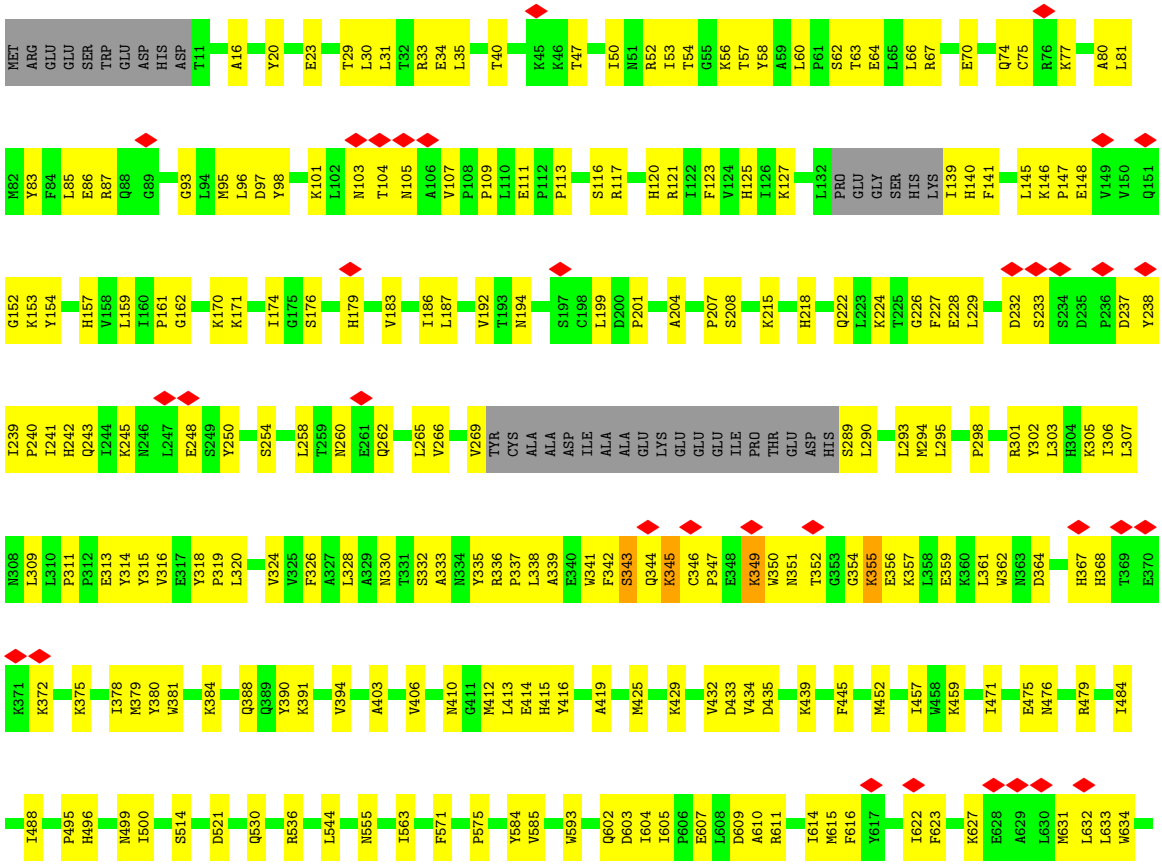
Chain J:

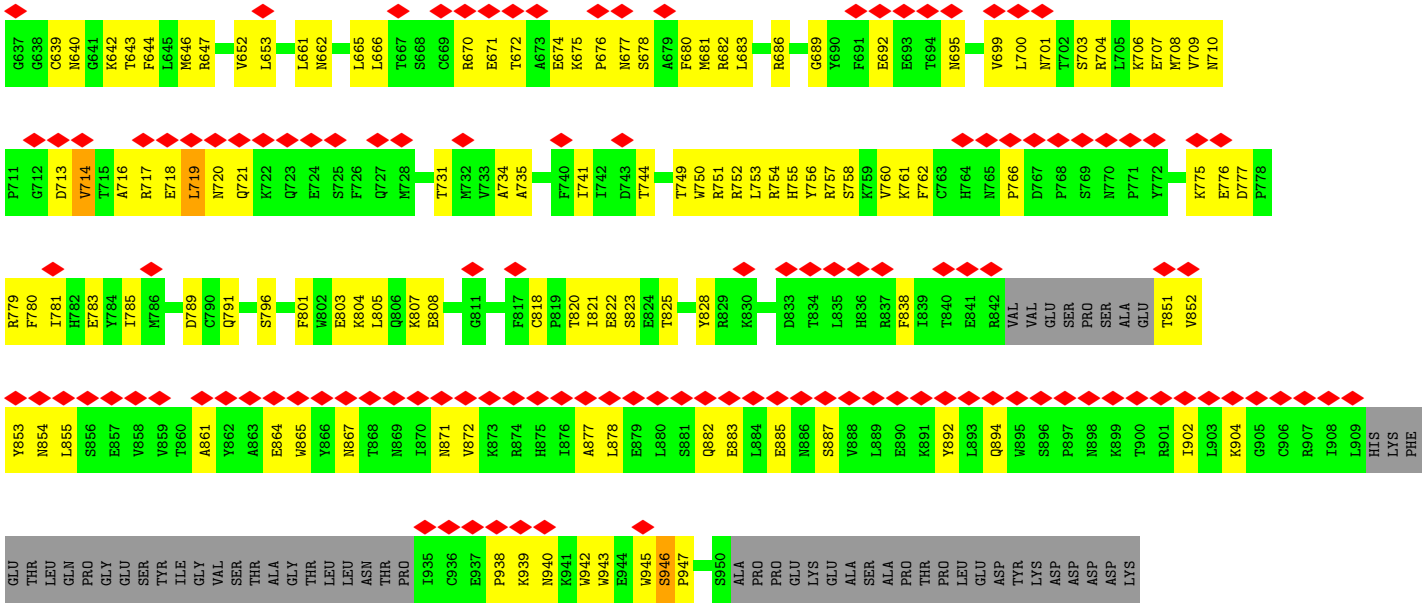




• Molecule 3: Putative primase C962R

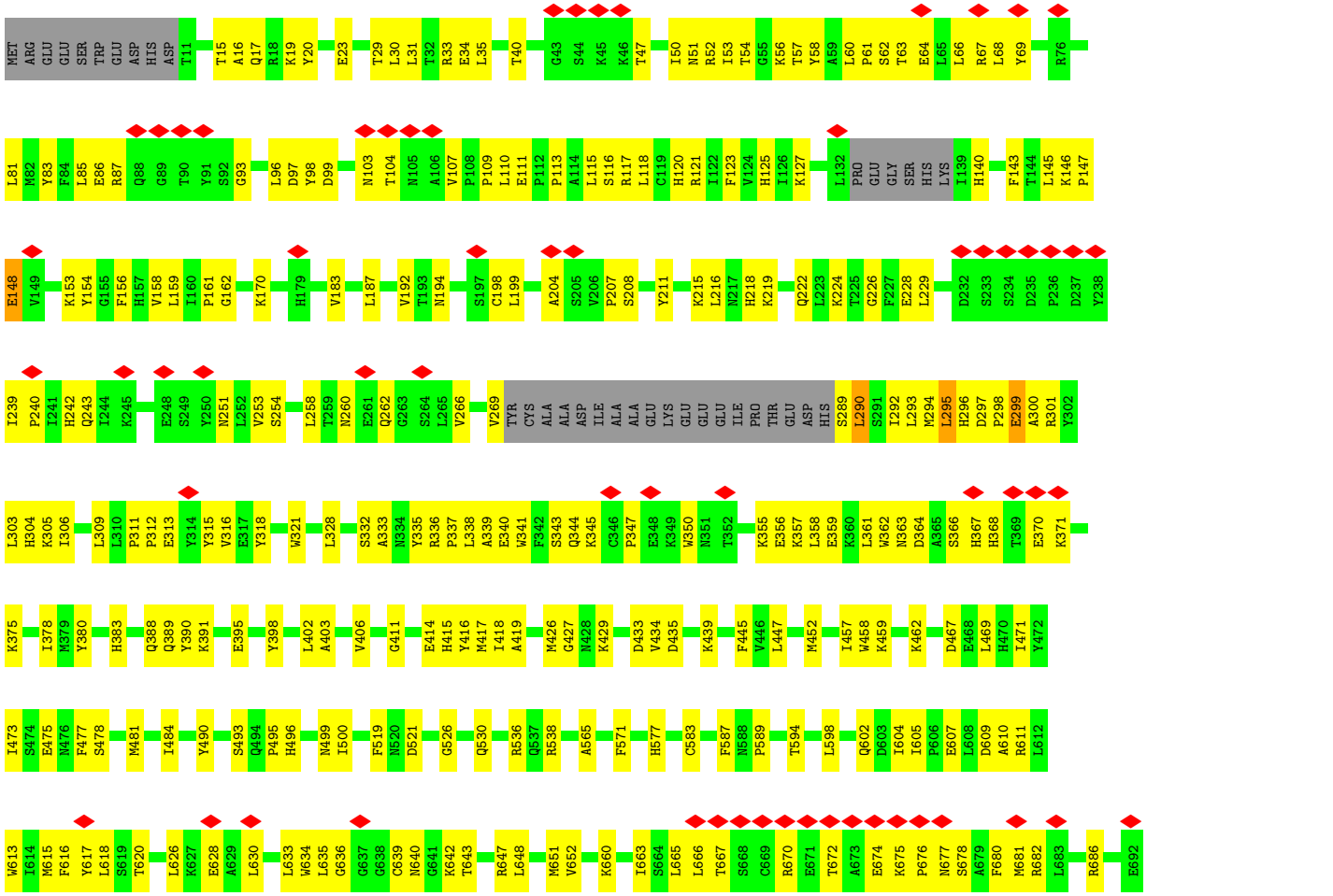
Chain I:

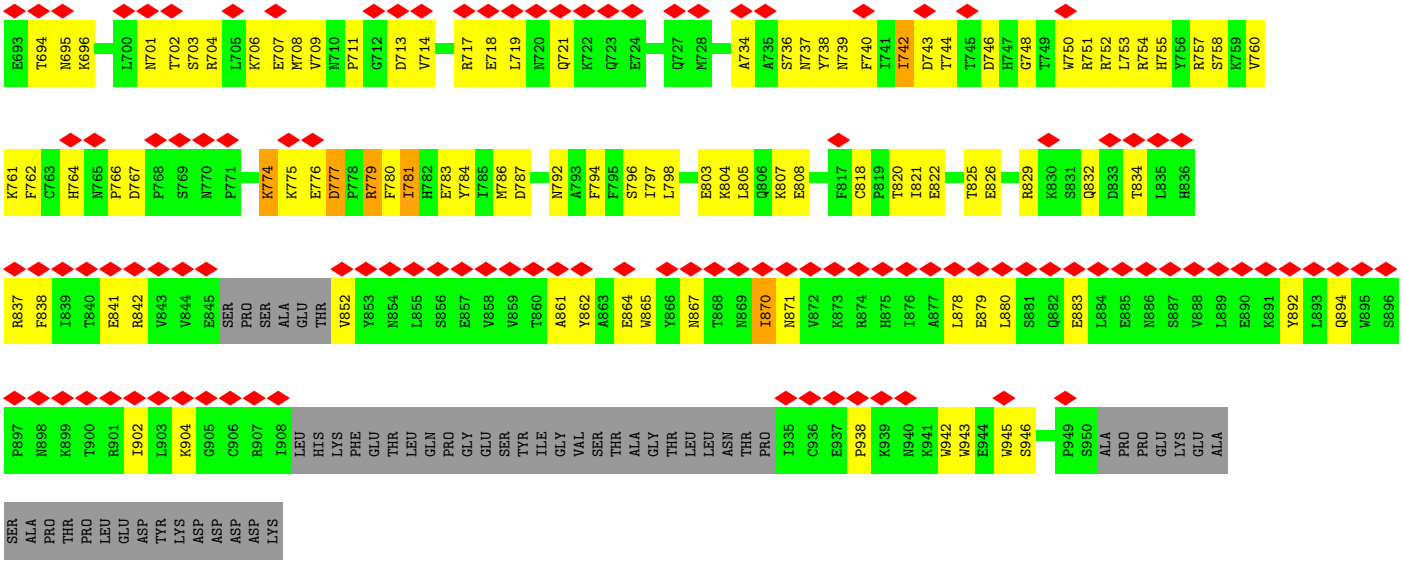




• Molecule 3: Putative primase C962R

Chain H:




E693 T694 N695 K696 L700 N701 T702 S703 R704 L705 K706 E707 M708 V709 N710 P711 G712 D713 V714 R717 E718 L719 N720 Q721 K722 Q723 E724 Q727 M728 A734 A735 S736 N737 Y738 N739 F740 I741 I742 D743 T744 T745 D746 H747 G748 T749 W750 R751 R752 L753 R754 H755 Y756 R757 S758 K759 V760
K761 F762 C763 H764 N765 P766 D767 P768 S769 N770 P771 K774 K775 E776 D777 P778 R779 F780 I781 H782 E783 Y784 I785 M786 D787 N792 A793 F794 F795 S796 I797 L798 E803 K804 L805 Q806 K807 E808 F817 C818 P819 T820 I821 E822 T825 E826 R829 K830 S831 Q832 D833 T834 L835 H836
R837 F838 I839 T840 E841 R842 V843 V844 E845 SER PRO SER ALA GLU THR V852 Y853 N854 L855 S856 E857 V858 V859 T860 A861 Y862 A863 E864 W865 Y866 N867 T868 N869 I870 N871 V872 K873 R874 H875 I876 A877 L878 E879 L880 S881 Q882 E883 L884 E885 N886 S887 V888 L889 E890 K891 Y892 L893 Q894 W895 S896
P897 N898 K899 T900 R901 I902 L903 K904 G905 C906 R907 I908 LEU HIS LYS PHE GLU THR LEU GLN PRO GLY GLU SER TYR ILE GLY VAL SER THR ALA GLY THR LEU LEU ASN THR PRO I935 C936 E937 P938 K939 N940 K941 W942 W943 E944 W945 S946 P949 S950 ALA PRO PRO GLU LYS GLU ALA
SER ALA PRO THR PRO LEU GLU ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210641	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.223	Depositor
Minimum map value	-0.444	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.258	Depositor
Map size (Å)	420.48, 420.48, 420.48	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality

5.1 Standard geometry

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

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	M	0.21	0/571	0.53	0/880
1	O	0.21	0/109	0.60	0/166
2	N	0.15	0/95	0.25	0/144
3	A	0.16	0/7466	0.34	0/10116
3	B	0.16	0/7480	0.37	0/10136
3	C	0.17	0/7504	0.40	0/10170
3	D	0.17	0/7480	0.39	0/10136
3	E	0.16	0/7548	0.37	0/10232
3	F	0.15	0/7472	0.36	0/10126
3	G	0.12	0/7548	0.31	0/10232
3	H	0.14	0/7428	0.36	2/10066 (0.0%)
3	I	0.14	0/7420	0.35	0/10055
3	J	0.13	0/7436	0.34	1/10077 (0.0%)
3	K	0.13	0/7413	0.34	0/10045
3	L	0.12	0/7401	0.32	1/10026 (0.0%)
All	All	0.15	0/90371	0.36	4/122607 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	418	ILE	N-CA-C	-6.06	106.33	113.42
3	H	418	ILE	N-CA-C	-5.99	106.97	112.96
3	H	148	GLU	CB-CA-C	-5.20	109.06	116.34
3	J	148	GLU	CB-CA-C	-5.09	109.17	115.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	M	520	0	313	18	0
1	O	100	0	61	7	0
2	N	84	0	45	5	0
3	A	7270	0	7192	240	0
3	B	7284	0	7209	231	0
3	C	7307	0	7233	290	0
3	D	7284	0	7211	273	0
3	E	7349	0	7267	260	0
3	F	7275	0	7194	209	0
3	G	7349	0	7268	257	0
3	H	7234	0	7162	292	0
3	I	7226	0	7156	290	0
3	J	7242	0	7173	268	0
3	K	7219	0	7149	263	0
3	L	7209	0	7131	234	0
4	A	31	0	13	1	0
4	B	31	0	13	5	0
4	C	31	0	13	8	0
4	D	31	0	13	2	0
4	E	31	0	13	2	0
4	F	31	0	13	3	0
4	G	31	0	13	3	0
4	H	31	0	13	5	0
4	I	31	0	13	4	0
4	J	31	0	13	11	0
4	K	31	0	13	3	0
4	L	31	0	13	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	88330	0	86920	3036	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 17.

All (3036) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:777:ASP:H	4:H:1001:ANP:H1'	1.27	0.97
3:G:846:SER:HB3	3:G:905:GLY:HA2	1.51	0.92
3:B:681:MET:HG3	3:B:718:GLU:HB3	1.53	0.90
3:G:847:PRO:HG3	3:G:916:GLN:HB3	1.53	0.90
3:L:776:GLU:HA	4:L:1001:ANP:H8	1.55	0.88
3:G:755:HIS:H	3:G:825:THR:HG22	1.38	0.87
3:D:414:GLU:H	3:D:417:MET:HE2	1.40	0.87
3:H:766:PRO:HG3	3:H:775:LYS:HB2	1.54	0.87
3:H:290:LEU:HD12	3:H:338:LEU:HG	1.59	0.85
3:D:701:ASN:HB3	3:D:704:ARG:HH12	1.42	0.84
3:B:661:LEU:HB2	3:B:691:PHE:HE1	1.43	0.83
3:G:146:LYS:HB3	3:G:154:TYR:HB2	1.61	0.83
3:D:350:TRP:HE1	3:D:355:LYS:HD3	1.43	0.82
3:L:153:LYS:HG3	3:L:154:TYR:H	1.44	0.82
3:C:776:GLU:HA	4:C:1001:ANP:H8	1.60	0.81
3:I:681:MET:HE3	3:I:716:ALA:HB3	1.60	0.81
3:I:713:ASP:H	3:H:647:ARG:HH12	1.26	0.81
3:K:717:ARG:NH1	3:K:718:GLU:O	2.14	0.80
3:A:681:MET:HG3	3:A:718:GLU:HB3	1.63	0.80
3:D:631:MET:HE3	3:D:632:LEU:H	1.47	0.80
3:J:681:MET:HE3	3:J:716:ALA:HB3	1.63	0.79
3:J:228:GLU:HB2	3:J:244:ILE:HG23	1.65	0.78
3:K:755:HIS:H	3:K:825:THR:HG22	1.47	0.78
3:H:780:PHE:HA	3:H:784:TYR:HD2	1.49	0.78
3:D:315:TYR:HE2	3:D:345:LYS:HB2	1.47	0.78
3:E:866:TYR:HE2	3:E:873:LYS:HB2	1.49	0.78
3:E:30:LEU:HD21	3:E:67:ARG:HE	1.47	0.78
3:G:683:LEU:HA	3:G:686:ARG:HB2	1.66	0.78
3:D:755:HIS:H	3:D:825:THR:HG22	1.48	0.77
3:I:701:ASN:HB2	3:I:704:ARG:HH12	1.50	0.77
3:I:146:LYS:HB3	3:I:154:TYR:HB2	1.67	0.77
3:C:102:LEU:HD11	3:C:192:VAL:HG13	1.64	0.77
3:E:63:THR:HA	3:E:66:LEU:HD23	1.67	0.77
3:L:60:LEU:HB3	3:L:64:GLU:HB2	1.66	0.77
3:F:701:ASN:HB3	3:F:704:ARG:HH12	1.48	0.77
3:G:846:SER:HB2	3:G:850:GLU:HG3	1.65	0.77
3:I:452:MET:HE1	3:I:457:ILE:HG13	1.67	0.77
3:L:701:ASN:HB2	3:L:704:ARG:HH12	1.50	0.77
3:B:642:LYS:HG3	3:B:643:THR:HG23	1.67	0.76
3:L:146:LYS:HB3	3:L:154:TYR:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:354:GLY:HA2	3:D:357:LYS:HD2	1.68	0.76
3:L:755:HIS:H	3:L:825:THR:HG22	1.49	0.76
3:I:755:HIS:H	3:I:825:THR:HG22	1.50	0.76
3:K:35:LEU:HD11	3:K:68:LEU:HD21	1.67	0.76
3:B:706:LYS:O	3:B:710:ASN:ND2	2.20	0.75
3:B:638:GLY:HA2	4:B:1001:ANP:HNB1	1.50	0.75
3:C:859:VAL:HG12	3:C:880:LEU:HD22	1.68	0.75
3:L:293:LEU:HD11	3:L:337:PRO:HB2	1.68	0.75
3:I:388:GLN:H	3:I:391:LYS:HZ3	1.34	0.75
3:H:52:ARG:HH22	3:H:215:LYS:HA	1.51	0.75
3:B:60:LEU:HB3	3:B:64:GLU:HB2	1.69	0.75
3:B:696:LYS:HG3	3:B:697:SER:H	1.52	0.75
3:K:605:ILE:O	3:K:611:ARG:NH1	2.20	0.75
3:K:111:GLU:HG3	3:K:113:PRO:HD2	1.68	0.75
3:I:170:LYS:HE3	3:I:204:ALA:HB1	1.69	0.75
3:D:35:LEU:HD11	3:D:68:LEU:HD21	1.67	0.74
3:C:145:LEU:HB3	3:C:222:GLN:HG2	1.67	0.74
3:H:298:PRO:O	3:H:301:ARG:HG2	1.87	0.74
3:F:681:MET:HG3	3:F:718:GLU:HB3	1.67	0.74
3:L:350:TRP:O	3:L:355:LYS:N	2.20	0.74
3:J:350:TRP:O	3:J:355:LYS:N	2.20	0.74
3:E:35:LEU:HD22	3:E:60:LEU:HD22	1.70	0.73
3:E:452:MET:HE1	3:E:457:ILE:HG13	1.70	0.73
3:E:350:TRP:O	3:E:355:LYS:N	2.20	0.73
3:D:736:SER:HB3	3:D:740:PHE:HE1	1.50	0.73
3:G:852:VAL:HG11	3:G:902:ILE:HD12	1.71	0.73
3:A:60:LEU:HB3	3:A:64:GLU:HB2	1.69	0.73
3:C:215:LYS:HG3	3:C:218:HIS:HB2	1.71	0.73
3:B:644:PHE:HZ	3:B:780:PHE:HB3	1.53	0.73
3:F:892:TYR:HB3	3:F:904:LYS:H	1.52	0.73
3:B:717:ARG:HH21	3:C:719:LEU:HD11	1.54	0.73
3:D:315:TYR:CE2	3:D:345:LYS:HB2	2.23	0.73
3:C:224:LYS:HG3	3:C:225:THR:HG23	1.70	0.73
3:L:892:TYR:HB3	3:L:904:LYS:H	1.53	0.73
3:G:60:LEU:HB3	3:G:64:GLU:HB2	1.69	0.73
3:H:452:MET:HE1	3:H:457:ILE:HG13	1.70	0.73
3:I:293:LEU:HD11	3:I:337:PRO:HB2	1.69	0.73
3:D:146:LYS:HB3	3:D:154:TYR:HB2	1.69	0.72
3:G:91:TYR:HB3	3:G:164:LYS:HB2	1.71	0.72
3:A:311:PRO:HB2	3:A:313:GLU:HG2	1.71	0.72
3:B:683:LEU:HA	3:B:686:ARG:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:OG1	3:C:221:TYR:HB3	1.89	0.72
3:D:343:SER:HB3	3:D:350:TRP:CD1	2.24	0.72
3:F:350:TRP:O	3:F:355:LYS:N	2.22	0.72
3:C:452:MET:HE1	3:C:457:ILE:HG13	1.70	0.72
3:E:148:GLU:HG3	3:E:154:TYR:HB3	1.70	0.72
3:I:605:ILE:O	3:I:611:ARG:NH1	2.23	0.72
3:D:31:LEU:HD23	3:D:35:LEU:HD12	1.70	0.72
3:A:324:VAL:HG12	3:A:381:TRP:CZ3	2.25	0.72
3:G:96:LEU:HD22	3:G:158:VAL:HG12	1.72	0.72
3:G:452:MET:HE1	3:G:457:ILE:HG13	1.70	0.72
3:C:102:LEU:HG	3:C:193:THR:H	1.54	0.72
3:F:771:PRO:O	3:F:774:LYS:NZ	2.23	0.71
3:K:146:LYS:HB3	3:K:154:TYR:HB2	1.72	0.71
3:H:718:GLU:HG2	3:H:719:LEU:H	1.54	0.71
3:I:364:ASP:C	3:I:368:HIS:HD1	1.97	0.71
3:C:139:ILE:HG23	3:C:162:GLY:HA3	1.73	0.71
3:D:699:VAL:HA	3:D:741:ILE:HB	1.73	0.71
3:J:146:LYS:HB3	3:J:154:TYR:HB2	1.70	0.71
3:H:605:ILE:O	3:H:611:ARG:NH1	2.23	0.71
3:L:388:GLN:H	3:L:391:LYS:HZ2	1.39	0.71
3:B:350:TRP:O	3:B:355:LYS:N	2.23	0.71
3:D:180:ASP:O	3:D:184:GLN:NE2	2.23	0.71
3:I:777:ASP:H	4:I:1001:ANP:H1'	1.55	0.71
3:K:752:ARG:NH2	4:J:1001:ANP:O1G	2.24	0.71
3:J:670:ARG:NH1	3:J:671:GLU:O	2.24	0.71
3:F:605:ILE:O	3:F:611:ARG:NH1	2.24	0.71
3:J:633:LEU:O	3:J:755:HIS:ND1	2.24	0.71
3:G:722:LYS:NZ	3:G:724:GLU:OE1	2.23	0.70
3:L:867:ASN:HB3	3:L:872:VAL:HG12	1.71	0.70
3:F:309:LEU:HD22	3:F:389:GLN:HE22	1.56	0.70
3:J:116:SER:O	3:J:120:HIS:ND1	2.24	0.70
3:D:670:ARG:HH12	3:D:704:ARG:HB3	1.56	0.70
3:D:702:THR:HG21	3:D:744:THR:HB	1.73	0.70
3:E:852:VAL:HG13	3:E:853:TYR:H	1.56	0.70
3:A:350:TRP:O	3:A:355:LYS:N	2.23	0.70
3:B:301:ARG:HB2	3:B:305:LYS:HZ1	1.55	0.70
3:B:632:LEU:HB3	3:B:733:VAL:HG12	1.71	0.70
3:D:350:TRP:HA	3:D:354:GLY:HA3	1.73	0.70
3:B:35:LEU:HD11	3:B:68:LEU:HD21	1.73	0.70
3:D:91:TYR:HB3	3:D:164:LYS:HB2	1.74	0.70
3:I:717:ARG:HH21	3:I:720:ASN:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:719:LEU:HD23	3:J:720:ASN:HB2	1.73	0.69
3:C:96:LEU:HA	3:C:203:SER:CA	2.22	0.69
3:D:102:LEU:HG	3:D:192:VAL:HA	1.73	0.69
3:I:780:PHE:HB2	4:I:1001:ANP:O2'	1.92	0.69
3:D:60:LEU:HB3	3:D:64:GLU:HB2	1.75	0.69
3:H:350:TRP:O	3:H:355:LYS:N	2.21	0.69
3:C:81:LEU:HD22	3:C:214:SER:HB2	1.75	0.69
3:F:94:LEU:HB2	3:F:160:ILE:HB	1.74	0.69
3:K:183:VAL:HA	3:K:186:ILE:HD12	1.74	0.69
3:A:311:PRO:HD3	3:A:385:HIS:HB3	1.75	0.69
3:D:680:PHE:O	3:D:684:LYS:NZ	2.26	0.69
3:E:605:ILE:O	3:E:611:ARG:NH1	2.25	0.69
3:H:719:LEU:O	3:H:721:GLN:NE2	2.25	0.69
3:D:452:MET:HE1	3:D:457:ILE:HG13	1.73	0.69
3:C:350:TRP:O	3:C:355:LYS:N	2.25	0.69
3:G:35:LEU:HD11	3:G:68:LEU:HD21	1.73	0.69
3:L:775:LYS:NZ	3:L:776:GLU:O	2.24	0.69
3:A:670:ARG:NH1	3:A:707:GLU:OE1	2.26	0.68
3:G:701:ASN:HB2	3:G:704:ARG:HH12	1.58	0.68
3:L:785:ILE:O	3:L:791:GLN:NE2	2.26	0.68
3:H:294:MET:HE2	3:H:300:ALA:HB1	1.75	0.68
3:E:666:LEU:O	3:E:704:ARG:NH2	2.26	0.68
3:K:139:ILE:N	3:K:229:LEU:O	2.27	0.68
3:A:664:SER:HA	3:A:667:THR:HG22	1.75	0.68
3:A:907:ARG:NH1	3:A:914:THR:O	2.27	0.68
3:L:395:GLU:OE1	3:L:483:ARG:NH1	2.20	0.68
3:K:93:GLY:HA3	3:K:161:PRO:HA	1.75	0.68
3:D:703:SER:HB3	3:D:704:ARG:HH11	1.58	0.68
3:G:719:LEU:O	3:G:721:GLN:NE2	2.27	0.68
3:K:110:LEU:HD23	3:K:115:LEU:HD21	1.75	0.68
3:H:616:PHE:HB3	3:H:805:LEU:HD12	1.75	0.68
3:D:703:SER:C	3:D:704:ARG:HD3	2.19	0.68
3:C:87:ARG:HD3	3:C:89:GLY:H	1.58	0.68
3:J:605:ILE:O	3:J:611:ARG:NH1	2.26	0.68
3:J:895:TRP:HA	3:J:901:ARG:HA	1.76	0.68
3:I:96:LEU:HD21	3:I:98:TYR:CE1	2.29	0.68
3:C:842:ARG:HD2	3:C:909:LEU:HD22	1.76	0.68
3:E:683:LEU:HA	3:E:686:ARG:HB2	1.75	0.68
3:L:718:GLU:HG2	3:L:719:LEU:H	1.58	0.68
3:G:785:ILE:O	3:G:791:GLN:NE2	2.27	0.67
3:G:938:PRO:HG3	3:G:942:TRP:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:110:LEU:HB2	3:L:224:LYS:HG2	1.76	0.67
3:K:683:LEU:HA	3:K:686:ARG:HB2	1.76	0.67
3:C:238:TYR:HB2	3:C:240:PRO:HD3	1.75	0.67
3:D:395:GLU:OE1	3:D:483:ARG:NH1	2.27	0.67
3:I:311:PRO:HB2	3:I:313:GLU:HG2	1.77	0.67
3:B:121:ARG:HE	3:B:182:THR:HB	1.58	0.67
3:C:187:LEU:HB3	3:C:192:VAL:HB	1.75	0.67
3:K:717:ARG:HH21	3:J:719:LEU:HD13	1.60	0.67
3:C:96:LEU:HA	3:C:203:SER:HA	1.75	0.67
3:G:718:GLU:HG2	3:G:719:LEU:H	1.59	0.67
3:G:31:LEU:HD23	3:G:35:LEU:HD12	1.75	0.67
3:J:429:LYS:NZ	3:J:445:PHE:O	2.27	0.67
3:I:364:ASP:O	3:I:368:HIS:ND1	2.27	0.67
3:B:883:GLU:HA	3:B:886:ASN:HB2	1.77	0.67
3:L:457:ILE:O	3:L:459:LYS:NZ	2.27	0.67
3:F:98:TYR:HE1	3:F:199:LEU:HD12	1.58	0.67
3:F:718:GLU:HG2	3:F:719:LEU:H	1.60	0.67
3:L:583:CYS:O	3:L:792:ASN:ND2	2.27	0.67
3:H:457:ILE:O	3:H:459:LYS:NZ	2.27	0.67
3:G:350:TRP:O	3:G:355:LYS:N	2.23	0.67
3:K:148:GLU:HG3	3:K:154:TYR:HB3	1.77	0.67
3:I:54:THR:OG1	3:I:56:LYS:NZ	2.28	0.67
3:H:290:LEU:O	3:H:294:MET:HG2	1.94	0.67
3:A:605:ILE:O	3:A:611:ARG:NH1	2.27	0.66
3:A:755:HIS:H	3:A:825:THR:HG22	1.60	0.66
3:C:140:HIS:HA	3:C:228:GLU:HA	1.77	0.66
3:K:115:LEU:HA	3:K:118:LEU:HD12	1.77	0.66
3:I:226:GLY:O	3:I:243:GLN:NE2	2.28	0.66
3:D:51:ASN:HB3	3:D:56:LYS:HZ2	1.59	0.66
3:D:102:LEU:HB2	3:D:153:LYS:HG2	1.77	0.66
3:D:309:LEU:HD22	3:D:389:GLN:HE22	1.61	0.66
3:E:583:CYS:O	3:E:792:ASN:ND2	2.28	0.66
3:E:852:VAL:HG22	3:E:854:ASN:H	1.58	0.66
3:E:883:GLU:HA	3:E:886:ASN:HB2	1.78	0.66
3:L:31:LEU:HD23	3:L:35:LEU:HD12	1.75	0.66
3:K:717:ARG:NH1	3:K:721:GLN:O	2.28	0.66
3:H:290:LEU:HD22	3:H:341:TRP:CD1	2.30	0.66
3:D:775:LYS:NZ	3:D:776:GLU:O	2.27	0.66
3:B:99:ASP:HA	3:B:155:GLY:HA3	1.76	0.66
3:B:718:GLU:OE1	3:B:718:GLU:N	2.29	0.66
3:B:718:GLU:HG2	3:B:719:LEU:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:851:THR:HG23	3:G:853:TYR:H	1.60	0.66
4:L:1001:ANP:O2G	4:L:1001:ANP:O3A	2.12	0.66
3:D:229:LEU:HG	3:D:240:PRO:HD2	1.76	0.66
1:M:7:DT:OP1	3:A:717:ARG:NH2	2.24	0.66
3:B:340:GLU:OE2	3:B:344:GLN:NE2	2.29	0.66
3:K:60:LEU:HB3	3:K:64:GLU:HB2	1.76	0.66
3:I:681:MET:HG3	3:I:718:GLU:HB3	1.77	0.66
3:A:406:VAL:HG23	3:A:411:GLY:HA2	1.76	0.66
3:G:867:ASN:HA	3:G:871:ASN:O	1.95	0.66
3:K:938:PRO:HG3	3:K:942:TRP:HB3	1.77	0.66
3:H:60:LEU:HB3	3:H:64:GLU:HB2	1.78	0.66
3:K:457:ILE:O	3:K:459:LYS:NZ	2.29	0.66
3:K:775:LYS:NZ	3:K:776:GLU:O	2.28	0.66
3:H:818:CYS:SG	3:H:820:THR:OG1	2.53	0.66
3:B:755:HIS:H	3:B:825:THR:HG22	1.59	0.66
3:C:495:PRO:O	3:C:496:HIS:ND1	2.29	0.66
3:K:105:ASN:HA	3:K:153:LYS:HD3	1.77	0.66
3:E:785:ILE:O	3:E:791:GLN:NE2	2.30	0.65
3:C:64:GLU:HG3	3:C:67:ARG:HH21	1.61	0.65
3:J:148:GLU:HG3	3:J:154:TYR:HB3	1.76	0.65
3:B:751:ARG:HH22	4:C:1001:ANP:HNB1	1.44	0.65
3:E:62:SER:HA	3:E:65:LEU:HD12	1.76	0.65
3:G:678:SER:N	3:H:674:GLU:OE1	2.28	0.65
3:L:336:ARG:HH12	3:L:359:GLU:HA	1.61	0.65
3:J:700:LEU:O	3:J:704:ARG:NH2	2.30	0.65
3:I:243:GLN:HB3	3:I:245:LYS:HZ2	1.61	0.65
3:D:93:GLY:HA3	3:D:161:PRO:HA	1.77	0.65
3:G:93:GLY:HA3	3:G:161:PRO:HA	1.76	0.65
3:J:874:ARG:NH1	3:J:875:HIS:O	2.29	0.65
3:D:757:ARG:NH1	3:D:758:SER:O	2.30	0.65
3:J:293:LEU:HD11	3:J:337:PRO:HB2	1.77	0.65
3:B:153:LYS:HG3	3:B:154:TYR:HD1	1.61	0.65
3:D:343:SER:HB3	3:D:350:TRP:NE1	2.11	0.65
3:D:716:ALA:O	3:D:723:GLN:HB3	1.97	0.65
3:E:495:PRO:O	3:E:496:HIS:ND1	2.30	0.65
3:J:682:ARG:HH21	3:J:686:ARG:HH22	1.42	0.65
3:H:867:ASN:HA	3:H:871:ASN:O	1.97	0.65
3:A:834:THR:HG21	3:A:870:ILE:HG21	1.79	0.65
3:E:40:THR:HG21	3:E:47:THR:HB	1.79	0.65
3:C:675:LYS:HB3	3:C:676:PRO:HD3	1.79	0.65
3:F:414:GLU:H	3:F:417:MET:HE3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:706:LYS:O	3:F:710:ASN:ND2	2.29	0.65
3:G:457:ILE:O	3:G:459:LYS:NZ	2.30	0.65
3:J:98:TYR:HE1	3:J:199:LEU:HD12	1.62	0.65
3:I:62:SER:OG	3:I:262:GLN:NE2	2.29	0.65
3:H:145:LEU:HD22	3:H:224:LYS:HB2	1.78	0.65
3:G:254:SER:OG	3:G:260:ASN:ND2	2.30	0.64
3:J:780:PHE:HA	3:J:784:TYR:HD2	1.62	0.64
3:E:336:ARG:HH12	3:E:359:GLU:HA	1.62	0.64
3:I:60:LEU:HB3	3:I:64:GLU:HB2	1.80	0.64
3:I:867:ASN:HA	3:I:871:ASN:O	1.96	0.64
3:H:495:PRO:O	3:H:496:HIS:ND1	2.31	0.64
3:C:146:LYS:HE3	3:C:147:PRO:HD2	1.79	0.64
3:E:146:LYS:HB3	3:E:154:TYR:HB2	1.78	0.64
3:L:139:ILE:N	3:L:229:LEU:O	2.31	0.64
3:L:145:LEU:HD22	3:L:224:LYS:HB2	1.79	0.64
3:K:94:LEU:HB2	3:K:160:ILE:HB	1.80	0.64
3:J:96:LEU:HD22	3:J:158:VAL:HG12	1.77	0.64
3:C:45:LYS:HB3	3:C:87:ARG:HH21	1.63	0.64
3:F:785:ILE:O	3:F:791:GLN:NE2	2.30	0.64
3:I:457:ILE:O	3:I:459:LYS:NZ	2.29	0.64
3:B:894:GLN:HB2	3:B:904:LYS:HG3	1.79	0.64
3:C:250:TYR:HB3	3:C:255:GLU:HG3	1.78	0.64
3:D:337:PRO:O	3:D:341:TRP:N	2.25	0.64
3:L:536:ARG:NH1	3:K:467:ASP:OD2	2.29	0.64
3:H:93:GLY:HA3	3:H:161:PRO:HA	1.79	0.64
3:A:145:LEU:HD22	3:A:224:LYS:HB2	1.79	0.64
3:A:377:SER:HB2	3:A:381:TRP:CZ2	2.33	0.64
3:E:35:LEU:HD11	3:E:68:LEU:HD21	1.79	0.64
3:L:700:LEU:O	3:L:704:ARG:NH1	2.31	0.64
3:J:818:CYS:SG	3:J:820:THR:OG1	2.55	0.64
3:I:892:TYR:HB3	3:I:904:LYS:H	1.62	0.64
3:H:426:MET:HE2	3:H:429:LYS:HB2	1.78	0.64
3:E:116:SER:O	3:E:120:HIS:ND1	2.31	0.64
3:G:852:VAL:HG23	3:G:854:ASN:H	1.63	0.64
3:L:609:ASP:OD1	3:L:610:ALA:N	2.30	0.64
3:I:316:VAL:HA	3:I:349:LYS:HD2	1.79	0.64
3:B:53:ILE:HG13	3:B:83:TYR:HB2	1.80	0.64
3:I:343:SER:HB3	3:I:350:TRP:CE2	2.32	0.64
3:H:290:LEU:HG	3:H:294:MET:HE3	1.80	0.64
3:E:94:LEU:HD13	3:E:170:LYS:HE3	1.80	0.64
3:F:682:ARG:HE	3:F:686:ARG:HH12	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:703:SER:O	3:F:704:ARG:HG2	1.98	0.64
3:G:866:TYR:CD2	3:G:875:HIS:HE1	2.15	0.64
3:I:290:LEU:HD12	3:I:293:LEU:HD12	1.78	0.64
3:D:642:LYS:HG3	3:D:643:THR:HG23	1.80	0.63
3:A:381:TRP:HB3	3:A:385:HIS:CE1	2.33	0.63
3:G:429:LYS:NZ	3:G:445:PHE:O	2.31	0.63
3:H:402:LEU:HD22	3:H:484:ILE:HG13	1.80	0.63
3:B:70:GLU:OE2	3:B:74:GLN:NE2	2.31	0.63
3:E:425:MET:HE1	3:E:477:PHE:HD1	1.64	0.63
3:F:495:PRO:O	3:F:496:HIS:ND1	2.31	0.63
3:L:294:MET:O	3:L:301:ARG:NH2	2.30	0.63
3:K:583:CYS:O	3:K:792:ASN:ND2	2.31	0.63
3:J:495:PRO:O	3:J:496:HIS:ND1	2.32	0.63
3:I:674:GLU:OE1	3:H:678:SER:N	2.30	0.63
3:A:821:ILE:O	3:A:822:GLU:HG3	1.99	0.63
3:C:96:LEU:HD11	3:C:199:LEU:HG	1.80	0.63
3:F:98:TYR:HB2	3:F:156:PHE:HB3	1.79	0.63
3:A:429:LYS:NZ	3:A:445:PHE:O	2.31	0.63
3:B:705:LEU:HD21	3:B:753:LEU:HD21	1.81	0.63
3:D:674:GLU:HG3	3:D:719:LEU:HD22	1.80	0.63
3:E:192:VAL:HG12	3:E:194:ASN:H	1.63	0.63
3:G:495:PRO:O	3:G:496:HIS:ND1	2.32	0.63
3:L:110:LEU:HD23	3:L:115:LEU:HD21	1.80	0.63
3:B:175:GLY:O	3:B:179:HIS:ND1	2.30	0.63
3:D:328:LEU:HD11	3:D:339:ALA:HB2	1.81	0.63
3:E:228:GLU:N	3:E:242:HIS:O	2.31	0.63
3:G:663:ILE:HG22	3:G:691:PHE:HB3	1.79	0.63
3:L:495:PRO:O	3:L:496:HIS:ND1	2.31	0.63
3:H:107:VAL:HA	3:H:153:LYS:HZ1	1.63	0.63
3:A:883:GLU:HA	3:A:886:ASN:HB2	1.81	0.63
3:B:62:SER:OG	3:B:262:GLN:NE2	2.32	0.63
3:B:93:GLY:HA3	3:B:161:PRO:HA	1.81	0.63
3:B:605:ILE:O	3:B:611:ARG:NH1	2.31	0.63
3:D:184:GLN:O	3:D:188:HIS:ND1	2.30	0.63
3:F:364:ASP:HA	3:F:367:HIS:CE1	2.34	0.63
3:L:13:GLN:OE1	3:L:491:HIS:NE2	2.32	0.63
3:J:88:GLN:OE1	3:J:170:LYS:NZ	2.26	0.63
3:J:457:ILE:O	3:J:459:LYS:NZ	2.31	0.63
3:I:93:GLY:HA3	3:I:161:PRO:HA	1.80	0.63
3:A:91:TYR:HB3	3:A:164:LYS:HB2	1.79	0.63
3:B:229:LEU:HB2	3:B:240:PRO:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:938:PRO:HG3	3:D:942:TRP:HB3	1.80	0.63
3:L:666:LEU:HA	3:L:704:ARG:HE	1.63	0.63
3:K:429:LYS:NZ	3:K:445:PHE:O	2.32	0.63
3:C:174:ILE:HD13	3:C:177:LEU:HD12	1.81	0.62
3:E:94:LEU:HB2	3:E:160:ILE:HB	1.80	0.62
3:K:31:LEU:HD23	3:K:35:LEU:HD12	1.81	0.62
3:F:616:PHE:HB3	3:F:805:LEU:HD12	1.80	0.62
3:C:31:LEU:HD23	3:C:35:LEU:HD12	1.82	0.62
3:E:457:ILE:O	3:E:459:LYS:NZ	2.31	0.62
3:K:883:GLU:HA	3:K:886:ASN:HB2	1.81	0.62
3:J:31:LEU:HD23	3:J:35:LEU:HD12	1.81	0.62
3:A:35:LEU:HD11	3:A:68:LEU:HD21	1.80	0.62
3:A:52:ARG:HE	3:A:83:TYR:HB3	1.63	0.62
3:J:672:THR:HB	3:J:675:LYS:HG3	1.80	0.62
3:I:878:LEU:HG	3:H:870:ILE:HG23	1.80	0.62
3:H:148:GLU:HG2	3:H:153:LYS:HZ3	1.63	0.62
3:C:717:ARG:NE	3:C:721:GLN:O	2.32	0.62
3:D:715:THR:HA	3:D:725:SER:HA	1.82	0.62
3:L:23:GLU:HG3	3:L:75:CYS:HA	1.82	0.62
3:L:50:ILE:O	3:L:85:LEU:N	2.27	0.62
3:L:192:VAL:HG12	3:L:194:ASN:H	1.65	0.62
3:L:804:LYS:HD2	3:L:807:LYS:HE3	1.80	0.62
3:E:771:PRO:O	3:E:774:LYS:NZ	2.32	0.62
3:G:111:GLU:HB3	3:G:113:PRO:HD2	1.82	0.62
3:H:98:TYR:HE1	3:H:199:LEU:HD12	1.64	0.62
3:A:380:TYR:CE1	3:A:384:LYS:HD3	2.34	0.62
3:C:785:ILE:O	3:C:791:GLN:NE2	2.33	0.62
3:D:495:PRO:O	3:D:496:HIS:ND1	2.32	0.62
3:E:364:ASP:HB3	3:E:368:HIS:CE1	2.34	0.62
3:G:143:PHE:HE2	3:G:227:PHE:HD1	1.46	0.62
3:J:719:LEU:O	3:J:721:GLN:NE2	2.32	0.62
3:F:565:ALA:N	3:F:803:GLU:OE2	2.33	0.62
3:G:821:ILE:O	3:G:822:GLU:HG3	2.00	0.62
3:J:294:MET:O	3:J:301:ARG:NH2	2.33	0.62
3:J:718:GLU:OE2	3:J:721:GLN:NE2	2.27	0.62
3:H:121:ARG:HG2	3:H:183:VAL:HG13	1.82	0.62
3:B:495:PRO:O	3:B:496:HIS:ND1	2.33	0.62
3:C:261:GLU:HG2	3:C:266:VAL:HG13	1.82	0.62
3:G:311:PRO:HB2	3:G:313:GLU:HG2	1.81	0.62
3:G:364:ASP:O	3:G:368:HIS:ND1	2.30	0.62
3:J:139:ILE:N	3:J:229:LEU:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:93:GLY:O	3:I:170:LYS:NZ	2.33	0.62
3:H:682:ARG:HE	3:H:686:ARG:HH12	1.47	0.62
3:A:315:TYR:OH	3:A:343:SER:HA	2.00	0.61
3:B:139:ILE:N	3:B:229:LEU:O	2.33	0.61
3:C:132:LEU:HG	3:C:233:SER:HA	1.80	0.61
3:F:294:MET:HE1	3:F:304:HIS:CG	2.35	0.61
3:G:761:LYS:HZ2	3:G:763:CYS:HB3	1.65	0.61
3:K:123:PHE:O	3:K:127:LYS:HG2	1.99	0.61
3:D:123:PHE:O	3:D:127:LYS:HG2	1.99	0.61
3:E:755:HIS:H	3:E:825:THR:HG22	1.65	0.61
3:L:761:LYS:HZ2	3:L:763:CYS:HB3	1.63	0.61
3:K:828:TYR:OH	3:K:832:GLN:NE2	2.31	0.61
3:I:298:PRO:HB3	3:I:301:ARG:HH11	1.65	0.61
3:H:40:THR:HG21	3:H:47:THR:HB	1.82	0.61
3:B:866:TYR:HA	3:B:870:ILE:HD13	1.83	0.61
3:F:148:GLU:HG3	3:F:154:TYR:HB3	1.82	0.61
3:I:215:LYS:HB2	3:I:218:HIS:HB2	1.82	0.61
3:E:159:LEU:HD11	3:E:258:LEU:HD21	1.80	0.61
3:F:29:THR:O	3:F:33:ARG:HG2	2.01	0.61
3:J:777:ASP:H	4:J:1001:ANP:H1'	1.64	0.61
3:A:632:LEU:HB3	3:A:733:VAL:HG12	1.81	0.61
3:A:838:PHE:HB2	3:A:865:TRP:CH2	2.36	0.61
3:B:298:PRO:HA	3:B:301:ARG:NE	2.16	0.61
3:C:146:LYS:HG3	3:C:148:GLU:HG2	1.82	0.61
3:E:50:ILE:HG12	3:E:57:THR:HG22	1.83	0.61
3:J:755:HIS:H	3:J:825:THR:HG22	1.65	0.61
3:H:96:LEU:HD21	3:H:98:TYR:CE1	2.35	0.61
3:A:31:LEU:HD23	3:A:35:LEU:HD12	1.83	0.61
3:C:228:GLU:O	3:C:240:PRO:HG2	2.00	0.61
3:F:340:GLU:OE2	3:F:344:GLN:NE2	2.33	0.61
3:K:228:GLU:O	3:K:242:HIS:N	2.34	0.61
3:J:616:PHE:HB3	3:J:805:LEU:HD12	1.83	0.61
3:A:98:TYR:HE1	3:A:199:LEU:HD12	1.66	0.61
3:C:605:ILE:O	3:C:611:ARG:NH1	2.32	0.61
3:C:879:GLU:OE1	3:C:879:GLU:N	2.32	0.61
3:E:892:TYR:HB3	3:E:904:LYS:H	1.64	0.61
3:F:866:TYR:CD1	3:F:870:ILE:HD13	2.36	0.61
3:K:88:GLN:OE1	3:K:170:LYS:NZ	2.28	0.61
3:I:642:LYS:HG3	3:I:643:THR:HG23	1.81	0.61
3:A:40:THR:HG21	3:A:47:THR:HB	1.83	0.61
3:C:127:LYS:HE2	3:C:131:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:311:PRO:HB2	3:F:313:GLU:HG2	1.83	0.61
3:K:311:PRO:HB2	3:K:313:GLU:HG2	1.82	0.61
3:C:204:ALA:C	3:C:206:VAL:H	2.08	0.61
3:D:666:LEU:HD13	3:D:704:ARG:HG2	1.83	0.61
3:F:95:MET:HE2	3:F:208:SER:HB2	1.83	0.61
3:I:52:ARG:HE	3:I:83:TYR:HB3	1.66	0.61
3:I:530:GLN:NE2	3:H:521:ASP:OD1	2.32	0.61
3:H:96:LEU:HD22	3:H:158:VAL:HG12	1.83	0.61
3:C:238:TYR:C	3:C:240:PRO:HD3	2.25	0.61
3:D:866:TYR:CD1	3:D:870:ILE:HD13	2.36	0.61
3:K:64:GLU:OE1	3:K:67:ARG:NH2	2.34	0.61
3:K:102:LEU:HG	3:K:192:VAL:HA	1.82	0.61
3:K:383:HIS:ND1	3:K:390:TYR:OH	2.25	0.61
3:H:429:LYS:NZ	3:H:445:PHE:O	2.25	0.61
3:A:583:CYS:O	3:A:792:ASN:ND2	2.34	0.60
3:K:852:VAL:HG23	3:K:854:ASN:H	1.65	0.60
3:I:495:PRO:O	3:I:496:HIS:ND1	2.34	0.60
3:A:873:LYS:NZ	3:A:874:ARG:O	2.33	0.60
3:A:939:LYS:HG3	3:A:940:ASN:H	1.65	0.60
3:C:87:ARG:NH1	3:C:89:GLY:O	2.33	0.60
3:D:111:GLU:HB3	3:D:113:PRO:HD2	1.84	0.60
3:D:170:LYS:HE3	3:D:204:ALA:HB1	1.83	0.60
3:E:180:ASP:O	3:E:184:GLN:NE2	2.30	0.60
3:G:892:TYR:HB3	3:G:904:LYS:H	1.66	0.60
3:L:93:GLY:HA3	3:L:161:PRO:HA	1.83	0.60
3:J:804:LYS:HD2	3:J:807:LYS:HE3	1.83	0.60
3:I:148:GLU:HG3	3:I:154:TYR:HB3	1.81	0.60
3:K:495:PRO:O	3:K:496:HIS:ND1	2.34	0.60
3:J:807:LYS:NZ	3:J:808:GLU:OE2	2.34	0.60
3:E:239:ILE:HD11	3:K:239:ILE:H	1.66	0.60
3:K:227:PHE:HB3	3:K:241:ILE:HG22	1.83	0.60
3:C:149:VAL:H	3:C:153:LYS:HZ2	1.47	0.60
3:L:818:CYS:SG	3:L:820:THR:OG1	2.58	0.60
3:I:703:SER:O	3:I:704:ARG:HG2	2.02	0.60
3:H:254:SER:OG	3:H:260:ASN:ND2	2.35	0.60
3:D:88:GLN:OE1	3:D:170:LYS:NZ	2.27	0.60
3:E:120:HIS:HE1	3:E:241:ILE:HD11	1.66	0.60
3:G:605:ILE:O	3:G:611:ARG:NH1	2.35	0.60
3:H:677:ASN:N	3:H:717:ARG:O	2.33	0.60
3:C:336:ARG:HH12	3:C:359:GLU:HA	1.66	0.60
3:E:593:TRP:NE1	3:E:789:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:701:ASN:O	3:E:701:ASN:ND2	2.34	0.60
3:F:718:GLU:OE1	3:F:718:GLU:N	2.34	0.60
3:L:82:MET:HG3	3:L:213:SER:HA	1.83	0.60
3:K:348:GLU:HG2	3:K:349:LYS:H	1.67	0.60
3:K:706:LYS:HD3	3:K:749:THR:HG22	1.84	0.60
3:I:375:LYS:HA	3:I:378:ILE:HD13	1.84	0.60
3:G:95:MET:HE2	3:G:208:SER:HB2	1.82	0.60
3:J:87:ARG:HG3	3:J:207:PRO:HG3	1.83	0.60
3:A:378:ILE:HG13	3:A:381:TRP:CZ3	2.37	0.60
3:B:330:ASN:ND2	3:B:373:ILE:O	2.34	0.60
3:C:757:ARG:NH1	3:C:758:SER:O	2.35	0.60
3:K:86:GLU:O	3:K:208:SER:N	2.33	0.60
3:J:583:CYS:O	3:J:792:ASN:ND2	2.35	0.60
3:J:874:ARG:NH2	3:I:871:ASN:OD1	2.24	0.60
3:I:31:LEU:HD23	3:I:35:LEU:HD12	1.84	0.60
3:I:718:GLU:HG2	3:I:719:LEU:H	1.67	0.60
3:I:821:ILE:O	3:I:822:GLU:HG3	2.02	0.60
3:H:760:VAL:HB	3:H:774:LYS:HZ1	1.66	0.60
3:D:664:SER:HA	3:D:667:THR:HG22	1.84	0.60
3:G:30:LEU:HD21	3:G:68:LEU:HD22	1.84	0.60
3:K:140:HIS:ND1	3:K:228:GLU:OE1	2.35	0.60
3:A:375:LYS:HA	3:A:378:ILE:HD13	1.83	0.59
3:D:102:LEU:HD11	3:D:192:VAL:HG22	1.84	0.59
3:D:701:ASN:HB3	3:D:704:ARG:NH1	2.14	0.59
3:F:683:LEU:HA	3:F:686:ARG:HB2	1.83	0.59
3:K:719:LEU:O	3:K:721:GLN:NE2	2.35	0.59
3:H:406:VAL:HG23	3:H:411:GLY:HA2	1.83	0.59
3:A:347:PRO:HA	3:A:350:TRP:HB3	1.83	0.59
3:B:47:THR:O	3:B:87:ARG:NH2	2.35	0.59
3:E:866:TYR:CD1	3:E:870:ILE:HD13	2.37	0.59
3:L:35:LEU:HD11	3:L:68:LEU:HD21	1.82	0.59
3:K:50:ILE:O	3:K:85:LEU:N	2.28	0.59
3:J:29:THR:O	3:J:33:ARG:HG2	2.02	0.59
3:H:111:GLU:HB3	3:H:113:PRO:HD2	1.84	0.59
3:H:583:CYS:O	3:H:792:ASN:ND2	2.35	0.59
3:A:894:GLN:HB3	3:A:902:ILE:HG13	1.84	0.59
3:B:230:VAL:H	3:B:240:PRO:HG2	1.67	0.59
3:D:122:ILE:HD11	3:D:141:PHE:HE2	1.67	0.59
3:E:254:SER:OG	3:E:260:ASN:ND2	2.35	0.59
3:K:706:LYS:NZ	3:K:748:GLY:O	2.31	0.59
3:J:762:PHE:CE1	3:J:774:LYS:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:770:ASN:ND2	3:J:773:GLU:HB2	2.17	0.59
3:G:406:VAL:HG23	3:G:411:GLY:HA2	1.85	0.59
3:I:229:LEU:HA	3:I:242:HIS:HD2	1.67	0.59
3:H:123:PHE:O	3:H:127:LYS:HG2	2.02	0.59
3:H:429:LYS:HD2	3:H:447:LEU:HD13	1.83	0.59
3:H:663:ILE:HG13	3:H:667:THR:HG23	1.84	0.59
3:B:771:PRO:O	3:B:774:LYS:NZ	2.31	0.59
3:C:229:LEU:HA	3:C:240:PRO:HG2	1.84	0.59
3:C:853:TYR:HE2	3:C:908:ILE:HB	1.67	0.59
3:D:64:GLU:OE1	3:D:67:ARG:NH2	2.35	0.59
3:L:123:PHE:O	3:L:127:LYS:HG2	2.01	0.59
3:L:130:SER:HB2	3:L:165:LEU:HD21	1.85	0.59
3:A:53:ILE:HG13	3:A:83:TYR:HB2	1.85	0.59
3:C:105:ASN:HA	3:C:153:LYS:HD3	1.83	0.59
3:G:116:SER:O	3:G:120:HIS:ND1	2.36	0.59
3:G:145:LEU:HD22	3:G:224:LYS:HB2	1.83	0.59
3:L:715:THR:OG1	3:L:723:GLN:NE2	2.36	0.59
3:K:62:SER:OG	3:K:262:GLN:NE2	2.36	0.59
3:H:670:ARG:NH1	3:H:703:SER:OG	2.35	0.59
3:A:682:ARG:O	3:A:686:ARG:NH1	2.36	0.59
3:B:41:GLU:HB2	3:B:44:SER:HB3	1.85	0.59
3:B:604:ILE:HG22	3:B:605:ILE:HG23	1.83	0.59
3:B:710:ASN:OD1	3:B:752:ARG:NH2	2.34	0.59
3:B:878:LEU:HD22	3:C:870:ILE:HG23	1.84	0.59
3:D:457:ILE:O	3:D:459:LYS:NZ	2.33	0.59
3:K:29:THR:O	3:K:33:ARG:HG2	2.03	0.59
3:J:60:LEU:HB3	3:J:64:GLU:HB2	1.85	0.59
3:H:292:ILE:HG23	3:H:296:HIS:CE1	2.38	0.59
3:L:64:GLU:OE1	3:L:67:ARG:NH2	2.30	0.59
3:I:683:LEU:HA	3:I:686:ARG:HB2	1.85	0.59
3:A:750:TRP:H	3:A:753:LEU:HD13	1.67	0.59
3:E:666:LEU:HB3	3:E:700:LEU:HD22	1.85	0.59
3:F:123:PHE:O	3:F:127:LYS:HG2	2.02	0.59
3:E:311:PRO:HB2	3:E:313:GLU:HG2	1.85	0.58
3:J:412:MET:N	3:J:412:MET:SD	2.74	0.58
3:B:192:VAL:HG12	3:B:194:ASN:H	1.68	0.58
3:B:229:LEU:HB3	3:B:241:ILE:H	1.68	0.58
3:D:683:LEU:HA	3:D:686:ARG:HB2	1.86	0.58
3:I:98:TYR:HE1	3:I:199:LEU:HD12	1.68	0.58
3:A:785:ILE:O	3:A:791:GLN:NE2	2.36	0.58
3:E:123:PHE:O	3:E:127:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:775:LYS:NZ	3:E:776:GLU:O	2.36	0.58
3:F:53:ILE:HG13	3:F:83:TYR:HB2	1.85	0.58
3:G:587:PHE:HA	3:G:796:SER:HB3	1.86	0.58
3:L:209:LEU:HB2	3:L:213:SER:HB2	1.85	0.58
3:K:683:LEU:HD13	3:K:728:MET:HE1	1.84	0.58
3:H:294:MET:HE1	3:H:338:LEU:HD21	1.84	0.58
1:M:24:DT:O4	2:N:2:DA:N6	2.37	0.58
3:B:314:TYR:HB3	3:B:320:LEU:HD22	1.84	0.58
3:E:60:LEU:HB2	3:E:64:GLU:HB2	1.85	0.58
3:F:13:GLN:O	3:F:17:GLN:HG2	2.04	0.58
3:G:757:ARG:NH1	3:G:758:SER:O	2.36	0.58
3:L:98:TYR:HE1	3:L:199:LEU:HD12	1.67	0.58
3:K:804:LYS:HD2	3:K:807:LYS:HE3	1.85	0.58
3:H:226:GLY:O	3:H:243:GLN:NE2	2.36	0.58
3:A:629:ALA:HB2	3:A:711:PRO:HD3	1.84	0.58
3:A:682:ARG:HD3	3:F:723:GLN:HB3	1.85	0.58
3:G:647:ARG:HH12	3:H:713:ASP:H	1.50	0.58
3:J:383:HIS:HD1	3:J:390:TYR:HH	1.49	0.58
3:I:603:ASP:HB2	4:I:1001:ANP:HN62	1.69	0.58
3:B:696:LYS:HA	3:B:738:TYR:HD2	1.68	0.58
3:L:633:LEU:O	3:L:755:HIS:ND1	2.28	0.58
3:L:807:LYS:NZ	3:L:808:GLU:OE2	2.36	0.58
3:K:239:ILE:HG22	3:K:241:ILE:HD11	1.85	0.58
3:I:852:VAL:HG23	3:I:854:ASN:H	1.68	0.58
3:A:356:GLU:O	3:A:359:GLU:HG2	2.04	0.58
3:B:821:ILE:O	3:B:822:GLU:HG3	2.04	0.58
3:C:76:ARG:NH2	3:C:212:GLY:O	2.36	0.58
3:D:713:ASP:HB2	3:D:727:GLN:NE2	2.19	0.58
3:F:869:ASN:HB3	3:F:870:ILE:HD12	1.86	0.58
3:K:228:GLU:N	3:K:242:HIS:O	2.34	0.58
3:A:609:ASP:OD1	3:A:610:ALA:N	2.36	0.58
3:C:939:LYS:HG3	3:C:940:ASN:H	1.68	0.58
3:D:294:MET:O	3:D:301:ARG:NH2	2.37	0.58
3:E:668:SER:O	3:E:704:ARG:NH2	2.37	0.58
3:G:852:VAL:HB	3:G:902:ILE:HB	1.84	0.58
3:I:123:PHE:O	3:I:127:LYS:HG2	2.03	0.58
3:I:801:PHE:HZ	3:I:943:TRP:HB2	1.67	0.58
3:A:148:GLU:HG3	3:A:154:TYR:HB3	1.84	0.58
3:B:855:LEU:HG	3:B:902:ILE:HG22	1.85	0.58
3:E:60:LEU:HD12	3:E:65:LEU:HD23	1.86	0.58
3:E:391:LYS:HA	3:E:394:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:710:ASN:OD1	3:E:752:ARG:NH1	2.37	0.58
3:F:356:GLU:O	3:F:359:GLU:HG2	2.04	0.58
3:G:818:CYS:SG	3:G:820:THR:OG1	2.60	0.58
3:L:406:VAL:HG23	3:L:411:GLY:HA2	1.85	0.58
3:C:117:ARG:NH1	3:I:237:ASP:O	2.37	0.58
3:D:604:ILE:HG23	3:D:641:GLY:HA3	1.86	0.58
3:E:642:LYS:HE3	3:E:735:ALA:HB1	1.85	0.58
3:J:171:LYS:NZ	3:J:201:PRO:O	2.37	0.58
3:D:755:HIS:HD2	3:D:828:TYR:HB2	1.68	0.57
3:E:52:ARG:HE	3:E:83:TYR:HB3	1.69	0.57
3:E:237:ASP:O	3:K:117:ARG:NH2	2.37	0.57
3:F:775:LYS:NZ	3:F:776:GLU:O	2.32	0.57
3:G:340:GLU:OE2	3:G:344:GLN:NE2	2.37	0.57
3:K:674:GLU:OE1	3:J:678:SER:N	2.37	0.57
3:J:120:HIS:HD2	3:J:239:ILE:HB	1.69	0.57
3:J:757:ARG:NH1	3:J:758:SER:O	2.37	0.57
3:I:40:THR:HG21	3:I:47:THR:HB	1.86	0.57
3:H:298:PRO:HA	3:H:301:ARG:NE	2.19	0.57
3:H:640:ASN:ND2	3:H:760:VAL:O	2.37	0.57
3:A:660:LYS:NZ	3:F:713:ASP:O	2.36	0.57
3:C:682:ARG:HE	3:C:686:ARG:HH12	1.51	0.57
3:D:939:LYS:HG3	3:D:940:ASN:H	1.69	0.57
3:E:291:SER:HA	3:E:294:MET:HG2	1.86	0.57
3:F:664:SER:HA	3:F:667:THR:HG22	1.85	0.57
3:G:62:SER:OG	3:G:262:GLN:NE2	2.37	0.57
3:K:807:LYS:NZ	3:K:808:GLU:OE2	2.36	0.57
3:I:785:ILE:O	3:I:791:GLN:NE2	2.29	0.57
3:H:52:ARG:HE	3:H:83:TYR:HB3	1.68	0.57
3:D:86:GLU:OE1	3:D:210:LEU:HD12	2.04	0.57
3:G:52:ARG:HE	3:G:83:TYR:HB3	1.70	0.57
3:I:640:ASN:ND2	3:I:760:VAL:O	2.37	0.57
3:H:309:LEU:HD22	3:H:389:GLN:HE22	1.69	0.57
3:C:337:PRO:O	3:C:341:TRP:N	2.29	0.57
3:D:794:PHE:HA	3:D:797:ILE:HD12	1.86	0.57
3:G:826:GLU:HA	3:G:829:ARG:HB2	1.85	0.57
3:J:40:THR:HG21	3:J:47:THR:HB	1.84	0.57
3:J:867:ASN:HA	3:J:871:ASN:O	2.04	0.57
3:A:495:PRO:O	3:A:496:HIS:ND1	2.38	0.57
3:A:740:PHE:O	3:A:828:TYR:OH	2.22	0.57
3:A:854:ASN:HA	3:A:902:ILE:HG22	1.85	0.57
3:B:676:PRO:HB2	3:B:718:GLU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:941:LYS:HE3	3:B:944:GLU:HG3	1.85	0.57
3:C:144:THR:HG1	3:C:221:TYR:HB3	1.69	0.57
3:L:395:GLU:HA	3:L:398:TYR:CE2	2.39	0.57
3:K:255:GLU:OE2	3:K:264:SER:N	2.37	0.57
3:J:91:TYR:HB3	3:J:164:LYS:HB2	1.86	0.57
1:O:2:DT:H2"	1:O:3:DT:C6	2.40	0.57
3:A:146:LYS:HB3	3:A:154:TYR:HB2	1.86	0.57
3:B:156:PHE:O	3:B:157:HIS:ND1	2.38	0.57
3:E:939:LYS:HG3	3:E:940:ASN:H	1.69	0.57
3:F:939:LYS:HG3	3:F:940:ASN:H	1.69	0.57
3:L:681:MET:HE2	3:L:718:GLU:HB2	1.87	0.57
3:L:757:ARG:NH1	3:L:758:SER:O	2.37	0.57
3:K:99:ASP:O	3:K:194:ASN:ND2	2.37	0.57
3:K:375:LYS:HA	3:K:378:ILE:HD13	1.87	0.57
3:F:229:LEU:HD12	3:F:241:ILE:HG13	1.86	0.57
3:F:321:TRP:HH2	3:F:357:LYS:HG3	1.70	0.57
3:G:13:GLN:OE1	3:G:491:HIS:NE2	2.34	0.57
3:K:350:TRP:HE1	3:K:355:LYS:HD2	1.69	0.57
3:K:683:LEU:H	3:K:686:ARG:HH11	1.51	0.57
3:K:821:ILE:O	3:K:822:GLU:HG3	2.05	0.57
3:J:777:ASP:N	4:J:1001:ANP:H1'	2.20	0.57
3:I:665:LEU:HD11	3:I:680:PHE:HB2	1.86	0.57
3:H:852:VAL:HB	3:H:902:ILE:HB	1.85	0.57
3:B:751:ARG:NH1	3:C:639:CYS:SG	2.78	0.57
3:C:64:GLU:HA	3:C:67:ARG:HG2	1.87	0.57
3:C:852:VAL:HG23	3:C:854:ASN:H	1.70	0.57
3:E:740:PHE:O	3:E:832:GLN:NE2	2.38	0.57
3:F:96:LEU:HB3	3:F:158:VAL:HG12	1.87	0.57
3:J:395:GLU:OE2	3:J:483:ARG:NH1	2.37	0.57
3:H:375:LYS:HA	3:H:378:ILE:HD13	1.87	0.57
3:A:379:MET:O	3:A:383:HIS:HB3	2.05	0.57
3:B:239:ILE:H	3:H:117:ARG:HH12	1.52	0.57
3:D:316:VAL:O	3:D:349:LYS:HD3	2.05	0.57
3:E:139:ILE:N	3:E:229:LEU:O	2.38	0.57
3:E:878:LEU:HD11	3:F:870:ILE:HG23	1.87	0.57
3:I:116:SER:HB3	3:I:241:ILE:HD13	1.85	0.57
3:H:162:GLY:O	3:H:269:VAL:N	2.37	0.57
3:H:311:PRO:HB2	3:H:313:GLU:HG2	1.87	0.57
3:C:311:PRO:HB2	3:C:313:GLU:HG2	1.86	0.57
3:E:946:SER:HB3	3:E:947:PRO:HD2	1.87	0.57
3:A:700:LEU:HD11	3:A:740:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:350:TRP:NE1	3:D:355:LYS:HD3	2.14	0.56
3:D:736:SER:HB3	3:D:740:PHE:CE1	2.37	0.56
3:E:91:TYR:HB3	3:E:164:LYS:HB2	1.85	0.56
3:E:98:TYR:HB3	3:E:100:LEU:HG	1.86	0.56
3:K:140:HIS:NE2	3:K:266:VAL:HA	2.20	0.56
3:K:785:ILE:O	3:K:791:GLN:NE2	2.25	0.56
3:J:938:PRO:HG3	3:J:942:TRP:HB3	1.87	0.56
3:A:874:ARG:NH1	3:A:875:HIS:O	2.38	0.56
3:C:364:ASP:C	3:C:368:HIS:HD1	2.13	0.56
3:L:753:LEU:O	3:L:754:ARG:NH1	2.35	0.56
3:L:821:ILE:O	3:L:822:GLU:HG3	2.05	0.56
3:L:866:TYR:CD1	3:L:870:ILE:HD13	2.40	0.56
3:K:740:PHE:O	3:K:832:GLN:NE2	2.38	0.56
3:J:153:LYS:HG3	3:J:154:TYR:HD1	1.70	0.56
3:I:666:LEU:HD12	3:I:700:LEU:HD12	1.87	0.56
3:C:100:LEU:HD23	3:C:198:CYS:SG	2.45	0.56
3:C:457:ILE:O	3:C:459:LYS:NZ	2.35	0.56
3:E:108:PRO:HD3	3:E:153:LYS:HE2	1.88	0.56
3:F:336:ARG:HH12	3:F:359:GLU:HA	1.70	0.56
3:F:391:LYS:O	3:F:394:VAL:HG22	2.06	0.56
3:F:707:GLU:OE1	3:F:707:GLU:N	2.35	0.56
3:G:336:ARG:HH12	3:G:359:GLU:HA	1.70	0.56
3:G:347:PRO:HA	3:G:350:TRP:HB3	1.86	0.56
3:G:673:ALA:O	3:L:678:SER:OG	2.21	0.56
3:G:706:LYS:HD3	3:G:749:THR:HG22	1.87	0.56
3:H:116:SER:O	3:H:120:HIS:ND1	2.38	0.56
3:H:676:PRO:HB3	3:H:717:ARG:HG2	1.87	0.56
3:C:187:LEU:HD22	3:C:192:VAL:HG21	1.87	0.56
3:E:314:TYR:HB3	3:E:320:LEU:HD22	1.87	0.56
3:E:646:MET:HE2	3:E:733:VAL:HG23	1.87	0.56
4:E:1001:ANP:N3B	4:E:1001:ANP:O2A	2.39	0.56
3:G:294:MET:HA	3:G:294:MET:HE3	1.87	0.56
3:L:337:PRO:O	3:L:341:TRP:N	2.30	0.56
3:H:30:LEU:HA	3:H:34:GLU:OE1	2.05	0.56
3:H:634:TRP:HZ3	3:H:758:SER:HB3	1.70	0.56
3:F:146:LYS:HB3	3:F:154:TYR:HB2	1.86	0.56
3:L:375:LYS:HA	3:L:378:ILE:HD13	1.88	0.56
3:J:227:PHE:HA	3:J:243:GLN:HA	1.87	0.56
3:A:337:PRO:O	3:A:341:TRP:N	2.25	0.56
3:D:826:GLU:HA	3:D:829:ARG:HB2	1.87	0.56
3:F:429:LYS:NZ	3:F:445:PHE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:561:GLU:HG3	3:F:562:THR:HG23	1.86	0.56
3:K:682:ARG:HH21	3:K:686:ARG:HH22	1.53	0.56
3:A:88:GLN:NE2	3:A:204:ALA:O	2.38	0.56
3:E:243:GLN:HB2	3:K:242:HIS:HE1	1.71	0.56
3:F:712:GLY:O	3:F:727:GLN:NE2	2.39	0.56
3:F:834:THR:OG1	3:F:862:TYR:OH	2.22	0.56
3:L:111:GLU:HB3	3:L:113:PRO:HD2	1.86	0.56
3:J:311:PRO:HB2	3:J:313:GLU:HG2	1.88	0.56
3:I:86:GLU:O	3:I:208:SER:N	2.38	0.56
3:B:644:PHE:CZ	3:B:780:PHE:HB3	2.39	0.56
3:B:661:LEU:HB2	3:B:691:PHE:CE1	2.32	0.56
3:C:395:GLU:HA	3:C:398:TYR:CE1	2.41	0.56
3:E:38:PHE:HB2	3:E:60:LEU:HD23	1.88	0.56
3:F:945:TRP:O	3:F:950:SER:OG	2.23	0.56
3:G:468:GLU:OE2	3:H:538:ARG:NH2	2.37	0.56
3:L:297:ASP:OD2	3:L:335:TYR:OH	2.22	0.56
3:L:946:SER:HB2	3:L:950:SER:HA	1.87	0.56
3:J:244:ILE:HD12	3:J:247:LEU:HD21	1.88	0.56
3:I:314:TYR:HB3	3:I:320:LEU:HD22	1.87	0.56
3:I:672:THR:HG22	3:I:674:GLU:H	1.69	0.56
3:H:53:ILE:HG13	3:H:83:TYR:HB2	1.86	0.56
3:H:701:ASN:HB2	3:H:704:ARG:HH12	1.71	0.56
3:B:777:ASP:O	4:B:1001:ANP:O2'	2.22	0.56
3:C:96:LEU:HA	3:C:203:SER:HB3	1.88	0.56
3:H:29:THR:O	3:H:33:ARG:HG2	2.05	0.56
3:H:170:LYS:HE3	3:H:204:ALA:HB1	1.87	0.56
3:C:96:LEU:HA	3:C:203:SER:CB	2.36	0.56
3:D:375:LYS:HA	3:D:378:ILE:HD13	1.87	0.56
3:L:701:ASN:HB2	3:L:704:ARG:NH1	2.20	0.56
3:K:53:ILE:HG13	3:K:83:TYR:HB2	1.87	0.56
3:K:348:GLU:H	3:K:348:GLU:CD	2.14	0.56
3:K:647:ARG:O	3:K:651:MET:HG2	2.06	0.56
3:J:499:ASN:OD1	3:J:500:ILE:N	2.38	0.56
1:M:23:DT:O4	2:N:3:DA:N6	2.39	0.55
3:C:894:GLN:HG3	3:C:895:TRP:H	1.71	0.55
3:G:544:LEU:HD23	3:G:575:PRO:HB2	1.87	0.55
3:L:326:PHE:HD1	3:L:365:ALA:HB2	1.71	0.55
3:L:938:PRO:HG3	3:L:942:TRP:HB3	1.88	0.55
3:I:87:ARG:HG3	3:I:207:PRO:HG3	1.87	0.55
3:I:666:LEU:O	3:I:704:ARG:NH2	2.39	0.55
3:I:680:PHE:HZ	3:I:714:VAL:HG21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:804:LYS:HD2	3:H:807:LYS:HE3	1.87	0.55
3:A:314:TYR:HB3	3:A:320:LEU:HD22	1.88	0.55
3:K:52:ARG:HH22	3:K:215:LYS:HA	1.72	0.55
3:I:140:HIS:ND1	3:I:228:GLU:OE1	2.39	0.55
3:H:86:GLU:O	3:H:208:SER:N	2.38	0.55
3:H:761:LYS:NZ	3:H:762:PHE:O	2.39	0.55
3:A:834:THR:OG1	3:A:862:TYR:OH	2.24	0.55
3:B:302:TYR:O	3:B:306:ILE:HG12	2.07	0.55
3:B:670:ARG:HA	3:B:704:ARG:HH12	1.71	0.55
3:D:314:TYR:HB3	3:D:320:LEU:HD22	1.87	0.55
3:B:302:TYR:CZ	3:B:306:ILE:HD11	2.42	0.55
3:C:894:GLN:N	3:C:902:ILE:O	2.34	0.55
3:D:682:ARG:HE	3:D:686:ARG:HH12	1.53	0.55
3:F:682:ARG:HH21	3:F:686:ARG:HH22	1.53	0.55
3:L:105:ASN:HA	3:L:153:LYS:HD3	1.88	0.55
3:L:851:THR:HG23	3:L:853:TYR:H	1.71	0.55
3:J:337:PRO:O	3:J:341:TRP:N	2.34	0.55
3:I:105:ASN:HA	3:I:153:LYS:HD3	1.87	0.55
3:B:643:THR:HG22	3:B:692:GLU:HB2	1.87	0.55
3:C:102:LEU:HD13	3:C:153:LYS:HB2	1.89	0.55
3:C:328:LEU:HD11	3:C:339:ALA:HB2	1.89	0.55
3:C:670:ARG:HA	3:C:704:ARG:HD3	1.87	0.55
3:C:683:LEU:HA	3:C:686:ARG:HB2	1.87	0.55
3:E:739:ASN:OD1	3:E:828:TYR:OH	2.21	0.55
3:E:761:LYS:NZ	3:E:762:PHE:O	2.38	0.55
3:F:153:LYS:HG3	3:F:154:TYR:CD2	2.42	0.55
3:F:821:ILE:O	3:F:822:GLU:HG3	2.06	0.55
3:L:718:GLU:HG2	3:L:719:LEU:N	2.21	0.55
3:K:395:GLU:HG3	3:K:398:TYR:OH	2.07	0.55
3:J:123:PHE:O	3:J:127:LYS:HG2	2.07	0.55
3:J:761:LYS:H	3:J:774:LYS:NZ	2.03	0.55
3:A:693:GLU:N	3:A:693:GLU:OE1	2.40	0.55
3:A:946:SER:HB3	3:A:947:PRO:HD2	1.88	0.55
3:D:116:SER:O	3:D:120:HIS:ND1	2.40	0.55
3:D:867:ASN:HB3	3:D:872:VAL:HG12	1.89	0.55
3:F:47:THR:HG23	3:F:87:ARG:HH12	1.71	0.55
3:F:457:ILE:O	3:F:459:LYS:NZ	2.39	0.55
3:F:674:GLU:O	3:F:717:ARG:NH1	2.39	0.55
3:G:633:LEU:O	3:G:755:HIS:ND1	2.32	0.55
3:A:156:PHE:HE1	3:A:158:VAL:HB	1.72	0.55
3:B:693:GLU:OE1	3:B:693:GLU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:777:ASP:O	3:C:779:ARG:N	2.35	0.55
3:D:718:GLU:HB2	3:D:723:GLN:N	2.22	0.55
3:E:410:ASN:HB2	3:E:507:LEU:HD13	1.89	0.55
3:A:93:GLY:O	3:A:170:LYS:NZ	2.40	0.55
3:D:356:GLU:H	3:D:356:GLU:CD	2.13	0.55
3:D:363:ASN:O	3:D:367:HIS:ND1	2.40	0.55
3:L:229:LEU:HG	3:L:230:VAL:H	1.72	0.55
3:J:297:ASP:O	3:J:301:ARG:NH2	2.39	0.55
3:I:183:VAL:HA	3:I:186:ILE:HD12	1.88	0.55
3:H:834:THR:OG1	3:H:862:TYR:OH	2.24	0.55
3:K:71:HIS:CD2	3:K:74:GLN:HE22	2.24	0.55
3:J:332:SER:OG	3:J:333:ALA:N	2.37	0.55
3:I:153:LYS:HG3	3:I:154:TYR:HD1	1.72	0.55
3:C:892:TYR:HB3	3:C:904:LYS:H	1.72	0.55
3:E:347:PRO:HA	3:E:350:TRP:HB3	1.88	0.55
3:E:530:GLN:NE2	3:F:521:ASP:OD1	2.36	0.55
3:F:69:TYR:HB3	3:F:254:SER:HB2	1.87	0.55
3:F:87:ARG:HG3	3:F:207:PRO:HG3	1.89	0.55
3:F:315:TYR:OH	3:F:343:SER:HA	2.07	0.55
3:G:228:GLU:HB3	3:G:242:HIS:HB2	1.89	0.55
3:J:159:LEU:HD11	3:J:258:LEU:HD21	1.89	0.55
3:I:775:LYS:HZ2	3:I:776:GLU:HG2	1.72	0.55
3:H:748:GLY:O	3:H:752:ARG:NH2	2.40	0.55
1:M:4:DT:H4'	1:M:5:DT:OP1	2.07	0.54
3:B:370:GLU:CD	3:B:371:LYS:H	2.14	0.54
3:C:244:ILE:HG22	3:C:247:LEU:HD21	1.88	0.54
3:C:701:ASN:C	3:C:703:SER:H	2.15	0.54
3:E:98:TYR:HE1	3:E:199:LEU:HD12	1.71	0.54
3:E:332:SER:OG	3:E:334:ASN:OD1	2.20	0.54
3:J:336:ARG:HH12	3:J:359:GLU:HA	1.72	0.54
3:A:391:LYS:O	3:A:394:VAL:HG22	2.07	0.54
3:A:544:LEU:HD23	3:A:575:PRO:HB2	1.89	0.54
3:B:61:PRO:HD2	3:B:64:GLU:HG3	1.89	0.54
3:B:111:GLU:HG2	3:B:114:ALA:H	1.71	0.54
3:D:640:ASN:ND2	3:D:760:VAL:O	2.40	0.54
3:E:694:THR:HG21	3:E:736:SER:HA	1.88	0.54
3:F:946:SER:HB3	3:F:947:PRO:HD2	1.89	0.54
3:I:29:THR:O	3:I:33:ARG:HG2	2.06	0.54
3:A:565:ALA:N	3:A:803:GLU:OE2	2.40	0.54
3:B:391:LYS:O	3:B:394:VAL:HG22	2.07	0.54
3:C:139:ILE:N	3:C:267:ARG:HH12	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:GLN:OE1	3:C:199:LEU:HB3	2.07	0.54
3:D:229:LEU:HD12	3:D:241:ILE:HG13	1.89	0.54
3:D:583:CYS:O	3:D:792:ASN:ND2	2.41	0.54
3:D:695:ASN:O	3:D:696:LYS:HG2	2.07	0.54
3:D:753:LEU:O	3:D:754:ARG:NH1	2.34	0.54
3:G:174:ILE:HD12	3:G:199:LEU:HD21	1.89	0.54
3:G:640:ASN:ND2	3:G:760:VAL:O	2.41	0.54
3:L:892:TYR:HB2	3:L:903:LEU:HD22	1.88	0.54
3:G:672:THR:HB	3:G:675:LYS:HB2	1.90	0.54
3:G:807:LYS:NZ	3:G:808:GLU:OE2	2.34	0.54
3:K:866:TYR:CD1	3:K:870:ILE:HD13	2.43	0.54
3:K:939:LYS:HG3	3:K:940:ASN:H	1.73	0.54
3:J:512:GLU:HA	3:J:515:LYS:HB2	1.89	0.54
3:J:779:ARG:O	3:J:783:GLU:HG3	2.06	0.54
3:I:766:PRO:HG3	3:I:775:LYS:HB2	1.89	0.54
3:H:148:GLU:HG2	3:H:153:LYS:NZ	2.21	0.54
3:H:499:ASN:OD1	3:H:500:ILE:N	2.41	0.54
3:H:757:ARG:NH1	3:H:758:SER:O	2.40	0.54
3:H:807:LYS:NZ	3:H:808:GLU:OE2	2.41	0.54
3:A:336:ARG:HH12	3:A:359:GLU:HA	1.72	0.54
3:C:13:GLN:OE1	3:C:491:HIS:NE2	2.41	0.54
3:D:246:ASN:OD1	3:D:249:SER:OG	2.23	0.54
3:D:642:LYS:NZ	3:D:736:SER:O	2.40	0.54
3:F:40:THR:HG21	3:F:47:THR:HB	1.89	0.54
3:F:321:TRP:CH2	3:F:357:LYS:HG3	2.42	0.54
3:H:146:LYS:HG2	3:H:148:GLU:H	1.72	0.54
3:H:602:GLN:HB2	3:H:942:TRP:NE1	2.22	0.54
3:A:383:HIS:HB2	3:A:390:TYR:CZ	2.43	0.54
3:B:337:PRO:O	3:B:341:TRP:N	2.34	0.54
3:E:945:TRP:O	3:E:950:SER:OG	2.25	0.54
3:K:878:LEU:HD11	3:J:870:ILE:HG23	1.90	0.54
3:I:713:ASP:O	3:H:660:LYS:HE3	2.07	0.54
3:A:452:MET:HE1	3:A:457:ILE:HG13	1.90	0.54
3:B:712:GLY:O	3:B:727:GLN:NE2	2.39	0.54
3:C:364:ASP:O	3:C:368:HIS:ND1	2.28	0.54
3:K:643:THR:HG22	3:K:692:GLU:HG2	1.90	0.54
3:K:777:ASP:H	4:K:1001:ANP:H1'	1.72	0.54
3:J:740:PHE:O	3:J:828:TYR:OH	2.25	0.54
3:I:107:VAL:O	3:I:109:PRO:HD3	2.07	0.54
3:I:364:ASP:HB3	3:I:368:HIS:CE1	2.43	0.54
3:I:699:VAL:HG22	3:I:741:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:120:HIS:CD2	3:A:239:ILE:HD12	2.43	0.54
3:E:640:ASN:ND2	3:E:760:VAL:O	2.35	0.54
3:F:175:GLY:O	3:F:179:HIS:ND1	2.40	0.54
3:G:375:LYS:HA	3:G:378:ILE:HD13	1.89	0.54
3:K:647:ARG:HG2	3:K:651:MET:HE3	1.90	0.54
3:K:717:ARG:NH2	3:J:719:LEU:HD13	2.22	0.54
3:J:30:LEU:HA	3:J:34:GLU:OE1	2.08	0.54
3:H:289:SER:O	3:H:293:LEU:HG	2.08	0.54
3:A:376:ARG:NH2	3:A:537:GLN:OE1	2.35	0.54
3:A:804:LYS:HD2	3:A:807:LYS:HE3	1.90	0.54
3:C:95:MET:HA	3:C:95:MET:HE3	1.89	0.54
3:D:140:HIS:ND1	3:D:228:GLU:OE1	2.41	0.54
3:D:565:ALA:N	3:D:803:GLU:OE2	2.41	0.54
3:E:416:TYR:O	3:E:420:LYS:HG2	2.08	0.54
3:E:789:ASP:OD1	3:E:790:CYS:N	2.40	0.54
3:F:94:LEU:HD13	3:F:170:LYS:HE3	1.90	0.54
3:I:254:SER:O	3:I:260:ASN:ND2	2.38	0.54
3:A:752:ARG:NH2	4:B:1001:ANP:O2G	2.41	0.54
3:A:862:TYR:O	3:A:866:TYR:HB2	2.08	0.54
3:B:866:TYR:HA	3:B:870:ILE:CD1	2.38	0.54
3:C:347:PRO:HA	3:C:350:TRP:HB3	1.90	0.54
3:C:821:ILE:O	3:C:822:GLU:HG3	2.08	0.54
3:D:867:ASN:CG	3:D:872:VAL:HA	2.33	0.54
3:E:97:ASP:OD1	3:E:203:SER:OG	2.26	0.54
3:K:116:SER:O	3:K:120:HIS:ND1	2.31	0.54
3:K:309:LEU:HD22	3:K:389:GLN:HE22	1.73	0.54
3:J:681:MET:HG3	3:J:718:GLU:HB3	1.89	0.54
3:I:147:PRO:HA	3:I:222:GLN:HE22	1.73	0.54
3:H:53:ILE:HG22	3:H:54:THR:HG23	1.89	0.54
3:B:766:PRO:HG3	3:B:775:LYS:HB2	1.91	0.53
3:C:305:LYS:HB3	3:C:393:ILE:HD11	1.90	0.53
3:D:332:SER:OG	3:D:333:ALA:N	2.38	0.53
3:E:31:LEU:HD23	3:E:35:LEU:HD12	1.89	0.53
3:E:634:TRP:O	3:E:642:LYS:NZ	2.29	0.53
3:G:536:ARG:NH1	3:L:467:ASP:OD2	2.38	0.53
3:L:30:LEU:HD21	3:L:68:LEU:HD22	1.90	0.53
3:L:53:ILE:HG13	3:L:83:TYR:HB2	1.89	0.53
3:L:499:ASN:OD1	3:L:500:ILE:N	2.41	0.53
3:K:344:GLN:HA	3:K:350:TRP:CZ3	2.42	0.53
3:K:872:VAL:HG12	3:K:874:ARG:HH12	1.72	0.53
3:J:626:LEU:HD22	3:J:711:PRO:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:LEU:HD22	3:H:60:LEU:HD22	1.90	0.53
3:A:321:TRP:HZ2	3:A:358:LEU:HB2	1.73	0.53
3:B:720:ASN:O	3:B:721:GLN:NE2	2.41	0.53
3:C:242:HIS:HB2	3:I:240:PRO:O	2.08	0.53
3:F:115:LEU:HA	3:F:118:LEU:HD12	1.89	0.53
3:F:156:PHE:O	3:F:157:HIS:ND1	2.41	0.53
3:F:631:MET:HB3	3:F:753:LEU:HA	1.90	0.53
3:G:647:ARG:NH2	3:H:713:ASP:OD1	2.34	0.53
3:L:30:LEU:HD22	3:L:71:HIS:ND1	2.22	0.53
3:J:783:GLU:O	3:J:784:TYR:HB2	2.08	0.53
3:I:315:TYR:CE2	3:I:346:CYS:HB2	2.43	0.53
3:I:499:ASN:OD1	3:I:500:ILE:N	2.42	0.53
3:H:62:SER:OG	3:H:262:GLN:NE2	2.41	0.53
3:A:140:HIS:NE2	3:A:266:VAL:HA	2.23	0.53
3:G:292:ILE:O	3:G:296:HIS:ND1	2.40	0.53
3:G:414:GLU:OE2	3:L:520:ASN:HB2	2.07	0.53
3:L:153:LYS:HG3	3:L:154:TYR:N	2.20	0.53
3:L:605:ILE:O	3:L:611:ARG:NH1	2.42	0.53
3:K:145:LEU:HD22	3:K:224:LYS:HB2	1.89	0.53
3:I:536:ARG:NH1	3:H:467:ASP:OD2	2.41	0.53
3:C:630:LEU:HD11	3:C:754:ARG:HG2	1.90	0.53
3:D:85:LEU:HD23	3:D:209:LEU:HB3	1.90	0.53
3:D:120:HIS:CE1	3:D:241:ILE:HD11	2.44	0.53
3:E:87:ARG:HG3	3:E:207:PRO:HG3	1.89	0.53
3:E:563:ILE:HG12	3:E:803:GLU:HG2	1.90	0.53
3:F:60:LEU:HB3	3:F:64:GLU:HB2	1.90	0.53
3:J:651:MET:HG3	3:J:785:ILE:HG22	1.90	0.53
3:A:521:ASP:OD1	3:F:530:GLN:NE2	2.33	0.53
3:A:674:GLU:HG2	3:B:677:ASN:HA	1.90	0.53
3:B:64:GLU:OE1	3:B:67:ARG:NH2	2.35	0.53
3:C:750:TRP:HB3	3:C:829:ARG:HD3	1.91	0.53
3:D:600:ALA:O	3:D:604:ILE:HG12	2.09	0.53
3:G:521:ASP:OD1	3:H:530:GLN:NE2	2.40	0.53
3:I:52:ARG:HH22	3:I:215:LYS:HA	1.74	0.53
3:C:866:TYR:CD1	3:C:870:ILE:HD13	2.44	0.53
3:F:497:GLU:OE1	3:F:497:GLU:N	2.42	0.53
3:F:636:GLY:HA2	3:F:757:ARG:NH1	2.24	0.53
3:G:626:LEU:HD22	3:G:711:PRO:HB2	1.91	0.53
3:J:701:ASN:HB2	3:J:704:ARG:HH12	1.74	0.53
3:I:162:GLY:O	3:I:269:VAL:N	2.42	0.53
3:I:337:PRO:O	3:I:341:TRP:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:294:MET:SD	3:B:301:ARG:HA	2.49	0.53
3:B:892:TYR:O	3:B:904:LYS:N	2.38	0.53
3:D:238:TYR:HA	3:J:239:ILE:HD11	1.91	0.53
3:D:388:GLN:HG2	3:D:391:LYS:HE3	1.91	0.53
3:E:140:HIS:ND1	3:E:228:GLU:OE1	2.42	0.53
3:F:107:VAL:O	3:F:109:PRO:HD3	2.08	0.53
3:I:111:GLU:HB3	3:I:113:PRO:HD2	1.90	0.53
3:A:103:ASN:HB3	3:A:193:THR:HB	1.91	0.53
3:D:665:LEU:O	3:D:704:ARG:HG3	2.08	0.53
3:E:315:TYR:OH	3:E:343:SER:HA	2.09	0.53
3:E:807:LYS:NZ	3:E:808:GLU:OE2	2.36	0.53
3:G:107:VAL:O	3:G:109:PRO:HD3	2.09	0.53
3:L:414:GLU:OE2	3:K:520:ASN:HB2	2.07	0.53
3:K:634:TRP:HA	3:K:755:HIS:HD1	1.73	0.53
3:K:672:THR:HG22	3:K:674:GLU:H	1.73	0.53
3:J:642:LYS:O	4:J:1001:ANP:O2A	2.27	0.53
3:E:375:LYS:HA	3:E:378:ILE:HD13	1.91	0.53
3:F:98:TYR:HB3	3:F:100:LEU:HG	1.91	0.53
3:G:752:ARG:NH2	4:L:1001:ANP:O3G	2.37	0.53
3:L:35:LEU:HA	3:L:38:PHE:HD2	1.74	0.53
3:K:30:LEU:HD22	3:K:71:HIS:ND1	2.23	0.53
3:K:405:TYR:OH	3:K:420:LYS:NZ	2.41	0.53
3:J:821:ILE:O	3:J:822:GLU:HG3	2.09	0.53
3:H:153:LYS:HG3	3:H:154:TYR:H	1.74	0.53
3:A:892:TYR:HB3	3:A:904:LYS:H	1.74	0.53
3:C:837:ARG:O	3:C:841:GLU:HB2	2.08	0.53
3:D:240:PRO:HB3	3:J:120:HIS:NE2	2.24	0.53
3:F:314:TYR:HB3	3:F:320:LEU:HD22	1.91	0.53
3:G:866:TYR:HE2	3:G:873:LYS:HB3	1.73	0.53
3:I:692:GLU:OE2	3:I:735:ALA:N	2.42	0.53
3:D:945:TRP:O	3:D:950:SER:OG	2.27	0.52
3:E:29:THR:O	3:E:33:ARG:HG2	2.09	0.52
3:L:626:LEU:HD12	3:L:711:PRO:HB2	1.89	0.52
3:K:406:VAL:HG23	3:K:411:GLY:HA2	1.91	0.52
3:J:781:ILE:HG12	4:J:1001:ANP:H3'	1.90	0.52
3:H:30:LEU:HD21	3:H:68:LEU:HD22	1.90	0.52
3:H:154:TYR:CE2	3:H:156:PHE:HB2	2.43	0.52
3:H:642:LYS:HG3	3:H:643:THR:HG23	1.89	0.52
3:D:767:ASP:N	3:D:767:ASP:OD1	2.41	0.52
3:E:751:ARG:NH2	4:F:1001:ANP:O3G	2.41	0.52
3:F:375:LYS:HA	3:F:378:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:643:THR:OG1	4:L:1001:ANP:O2B	2.24	0.52
3:I:23:GLU:HG3	3:I:75:CYS:HA	1.90	0.52
3:A:132:LEU:HB3	3:A:231:PHE:HE2	1.73	0.52
3:K:363:ASN:O	3:K:367:HIS:ND1	2.42	0.52
3:J:753:LEU:O	3:J:754:ARG:NH1	2.34	0.52
3:I:342:PHE:HA	3:I:345:LYS:HE2	1.91	0.52
3:I:804:LYS:HD2	3:I:807:LYS:HE3	1.91	0.52
3:H:340:GLU:OE2	3:H:344:GLN:NE2	2.42	0.52
3:A:842:ARG:HD3	3:A:909:LEU:HD23	1.92	0.52
3:B:946:SER:HB3	3:B:947:PRO:HD2	1.90	0.52
3:C:168:SER:HA	3:C:171:LYS:HE2	1.91	0.52
3:D:766:PRO:HG3	3:D:775:LYS:HB2	1.90	0.52
3:E:356:GLU:O	3:E:359:GLU:HG2	2.09	0.52
3:E:742:ILE:H	3:E:832:GLN:CD	2.17	0.52
3:K:751:ARG:NH2	3:J:639:CYS:SG	2.83	0.52
3:J:162:GLY:O	3:J:269:VAL:N	2.42	0.52
3:I:607:GLU:HB2	3:I:610:ALA:HB3	1.90	0.52
3:A:64:GLU:OE1	3:A:67:ARG:NH2	2.40	0.52
3:C:139:ILE:HG12	3:C:231:PHE:H	1.74	0.52
3:C:876:ILE:HD12	3:D:871:ASN:HD22	1.75	0.52
3:G:290:LEU:HD13	3:G:341:TRP:CG	2.45	0.52
3:K:91:TYR:HB3	3:K:164:LYS:HB2	1.92	0.52
3:K:350:TRP:O	3:K:355:LYS:N	2.39	0.52
3:J:332:SER:HB3	3:J:335:TYR:HE1	1.75	0.52
3:H:607:GLU:HB2	3:H:610:ALA:HB3	1.92	0.52
3:H:786:MET:O	3:H:787:ASP:C	2.52	0.52
3:H:821:ILE:O	3:H:822:GLU:HG3	2.10	0.52
1:O:4:DT:H1'	1:O:5:DT:H5'	1.92	0.52
3:C:142:PHE:HA	3:C:226:GLY:HA2	1.91	0.52
3:G:866:TYR:CE2	3:G:873:LYS:HB3	2.45	0.52
3:K:121:ARG:HH11	3:K:121:ARG:HA	1.75	0.52
3:K:229:LEU:HD12	3:K:241:ILE:HG13	1.91	0.52
3:K:652:VAL:HG21	3:K:794:PHE:HD2	1.73	0.52
3:H:107:VAL:O	3:H:109:PRO:HD3	2.09	0.52
3:H:211:TYR:HB3	3:H:253:VAL:HG22	1.92	0.52
3:H:615:MET:HE1	3:H:798:LEU:HD22	1.91	0.52
3:B:47:THR:HG23	3:B:87:ARG:HH22	1.74	0.52
3:B:163:LEU:HD23	3:B:163:LEU:H	1.75	0.52
3:B:375:LYS:HA	3:B:378:ILE:HD13	1.91	0.52
3:L:110:LEU:HB3	3:L:115:LEU:HD11	1.90	0.52
3:J:103:ASN:OD1	3:J:104:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:347:PRO:HA	3:J:350:TRP:HB3	1.92	0.52
3:H:892:TYR:HB3	3:H:904:LYS:H	1.75	0.52
3:C:902:ILE:HG13	3:C:903:LEU:H	1.74	0.52
3:E:93:GLY:HA3	3:E:161:PRO:HA	1.92	0.52
3:F:855:LEU:HG	3:F:902:ILE:HG22	1.90	0.52
3:L:293:LEU:HD13	3:L:338:LEU:HD12	1.91	0.52
3:L:766:PRO:HG3	3:L:775:LYS:HB2	1.92	0.52
3:K:629:ALA:HB1	3:K:709:VAL:HG22	1.91	0.52
3:H:337:PRO:O	3:H:341:TRP:N	2.31	0.52
3:C:154:TYR:CE2	3:C:192:VAL:HG22	2.44	0.52
3:D:20:TYR:CE1	3:D:500:ILE:HD12	2.45	0.52
3:D:103:ASN:OD1	3:D:104:THR:N	2.43	0.52
3:D:662:ASN:HB3	3:D:665:LEU:HD23	1.92	0.52
3:F:634:TRP:HB3	3:F:756:TYR:HB3	1.92	0.52
3:G:682:ARG:HH21	3:G:686:ARG:HH22	1.56	0.52
3:K:767:ASP:OD1	3:K:767:ASP:N	2.43	0.52
3:J:216:LEU:O	3:J:218:HIS:ND1	2.43	0.52
3:I:938:PRO:HG3	3:I:942:TRP:HB3	1.90	0.52
3:A:107:VAL:O	3:A:109:PRO:HD3	2.09	0.52
3:A:309:LEU:HB3	3:A:389:GLN:HE22	1.74	0.52
3:A:615:MET:HE2	3:A:615:MET:HA	1.91	0.52
3:C:98:TYR:HB3	3:C:100:LEU:HG	1.92	0.52
3:C:675:LYS:HG3	3:C:717:ARG:NH1	2.25	0.52
3:C:946:SER:HB3	3:C:947:PRO:HD2	1.92	0.52
3:D:946:SER:HB3	3:D:947:PRO:HD2	1.91	0.52
3:E:615:MET:HA	3:E:615:MET:HE2	1.92	0.52
3:G:605:ILE:HD12	3:G:611:ARG:HA	1.90	0.52
3:G:740:PHE:O	3:G:828:TYR:OH	2.27	0.52
3:L:652:VAL:HG21	3:L:794:PHE:HD2	1.73	0.52
3:K:757:ARG:NH1	3:K:758:SER:OG	2.43	0.52
3:J:107:VAL:O	3:J:109:PRO:HD3	2.09	0.52
3:J:746:ASP:N	3:J:746:ASP:OD1	2.41	0.52
3:H:945:TRP:CG	3:H:946:SER:H	2.26	0.52
1:M:3:DT:H4'	1:M:4:DT:OP1	2.09	0.51
3:B:153:LYS:HG3	3:B:154:TYR:CD1	2.43	0.51
3:D:883:GLU:HA	3:D:886:ASN:HB2	1.91	0.51
3:D:909:LEU:HG	3:D:913:GLU:HG2	1.92	0.51
3:E:893:LEU:HA	3:E:903:LEU:HA	1.92	0.51
3:F:732:MET:HE2	3:F:732:MET:HA	1.92	0.51
3:G:148:GLU:HG3	3:G:154:TYR:HB3	1.92	0.51
3:G:677:ASN:O	3:G:718:GLU:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:818:CYS:SG	3:K:821:ILE:HG12	2.51	0.51
3:J:122:ILE:HD11	3:J:141:PHE:HE2	1.74	0.51
3:I:315:TYR:HE2	3:I:346:CYS:HB2	1.74	0.51
1:O:2:DT:H2"	1:O:3:DT:C5	2.45	0.51
3:A:340:GLU:OE2	3:A:344:GLN:NE2	2.43	0.51
3:B:666:LEU:HD13	3:B:700:LEU:HD11	1.90	0.51
3:B:672:THR:O	3:B:675:LYS:HG2	2.10	0.51
3:C:670:ARG:NH1	3:C:671:GLU:O	2.44	0.51
3:D:605:ILE:O	3:D:611:ARG:NH1	2.43	0.51
3:F:147:PRO:HA	3:F:222:GLN:HE22	1.75	0.51
3:G:478:SER:HA	3:G:481:MET:HB2	1.92	0.51
3:L:103:ASN:OD1	3:L:104:THR:N	2.44	0.51
3:K:159:LEU:HD11	3:K:258:LEU:HD21	1.92	0.51
3:H:290:LEU:HD13	3:H:341:TRP:CD2	2.46	0.51
3:H:615:MET:HE2	3:H:797:ILE:HG22	1.91	0.51
4:H:1001:ANP:O2A	4:H:1001:ANP:O2B	2.29	0.51
3:C:187:LEU:HD13	3:C:192:VAL:HG11	1.92	0.51
3:D:705:LEU:HG	3:D:706:LYS:N	2.25	0.51
3:D:854:ASN:HA	3:D:902:ILE:HG22	1.92	0.51
3:F:140:HIS:NE2	3:F:266:VAL:HA	2.26	0.51
3:G:467:ASP:OD2	3:H:536:ARG:NH1	2.44	0.51
3:L:676:PRO:HB2	3:L:718:GLU:O	2.10	0.51
3:L:746:ASP:OD1	3:L:749:THR:OG1	2.25	0.51
3:K:332:SER:OG	3:K:333:ALA:N	2.44	0.51
3:K:593:TRP:NE1	3:K:789:ASP:OD2	2.43	0.51
3:J:395:GLU:HA	3:J:398:TYR:CE1	2.44	0.51
3:I:145:LEU:HD22	3:I:224:LYS:HB2	1.92	0.51
3:I:877:ALA:HB3	3:H:870:ILE:HA	1.93	0.51
3:H:604:ILE:HG22	3:H:605:ILE:HG23	1.92	0.51
3:A:29:THR:O	3:A:33:ARG:HG2	2.10	0.51
3:C:62:SER:HA	3:C:65:LEU:HD12	1.92	0.51
3:C:102:LEU:HD21	3:C:192:VAL:HA	1.92	0.51
3:D:410:ASN:HB2	3:D:507:LEU:HD13	1.92	0.51
3:E:695:ASN:O	3:E:696:LYS:HG2	2.10	0.51
3:F:91:TYR:HB3	3:F:164:LYS:HB2	1.91	0.51
3:F:395:GLU:HA	3:F:398:TYR:CE1	2.46	0.51
3:L:664:SER:HA	3:L:667:THR:HG22	1.92	0.51
3:K:354:GLY:HA2	3:K:357:LYS:CD	2.40	0.51
3:H:779:ARG:HB3	3:H:783:GLU:HG2	1.93	0.51
3:B:187:LEU:HB3	3:B:192:VAL:HB	1.91	0.51
3:B:821:ILE:C	3:B:823:SER:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ASN:ND2	3:C:60:LEU:O	2.43	0.51
3:C:111:GLU:HG3	3:C:113:PRO:HG2	1.92	0.51
3:D:107:VAL:O	3:D:109:PRO:HD3	2.10	0.51
3:D:336:ARG:HH12	3:D:359:GLU:HG3	1.74	0.51
3:L:69:TYR:OH	3:L:259:THR:OG1	2.28	0.51
3:K:457:ILE:HG22	3:K:458:TRP:CD1	2.46	0.51
3:K:476:ASN:HA	3:K:479:ARG:HH21	1.74	0.51
3:B:391:LYS:O	3:B:394:VAL:N	2.44	0.51
3:D:50:ILE:HG12	3:D:57:THR:HG22	1.93	0.51
3:D:616:PHE:HB3	3:D:805:LEU:HD12	1.91	0.51
3:E:293:LEU:HA	3:E:296:HIS:HB2	1.93	0.51
3:F:140:HIS:ND1	3:F:228:GLU:OE1	2.44	0.51
3:F:744:THR:OG1	3:F:746:ASP:OD1	2.26	0.51
3:G:330:ASN:ND2	3:G:373:ILE:O	2.39	0.51
3:G:639:CYS:HA	4:G:1001:ANP:HNB1	1.76	0.51
3:G:718:GLU:HG2	3:G:719:LEU:N	2.25	0.51
3:G:750:TRP:HB3	3:G:829:ARG:HD3	1.93	0.51
3:L:640:ASN:ND2	3:L:760:VAL:O	2.43	0.51
3:K:368:HIS:HB3	3:K:370:GLU:OE1	2.10	0.51
3:I:192:VAL:HG12	3:I:194:ASN:H	1.76	0.51
1:M:6:DT:OP1	3:F:717:ARG:NH2	2.44	0.51
3:B:629:ALA:HB2	3:B:711:PRO:HD3	1.93	0.51
3:C:204:ALA:C	3:C:206:VAL:N	2.69	0.51
3:C:406:VAL:HG23	3:C:411:GLY:HA2	1.93	0.51
3:C:583:CYS:O	3:C:792:ASN:ND2	2.41	0.51
3:D:294:MET:HE2	3:D:294:MET:N	2.25	0.51
3:E:457:ILE:HG22	3:E:458:TRP:CD1	2.46	0.51
3:F:140:HIS:CE1	3:F:265:LEU:HG	2.46	0.51
3:G:290:LEU:HD12	3:G:338:LEU:HG	1.92	0.51
3:G:708:MET:SD	3:G:728:MET:HE1	2.51	0.51
3:G:718:GLU:OE2	3:G:718:GLU:N	2.33	0.51
3:J:356:GLU:O	3:J:359:GLU:HG2	2.11	0.51
3:J:939:LYS:HG3	3:J:940:ASN:H	1.76	0.51
3:B:311:PRO:HB2	3:B:313:GLU:HG2	1.90	0.51
3:B:347:PRO:HA	3:B:350:TRP:HB3	1.93	0.51
3:C:132:LEU:H	3:C:231:PHE:HE2	1.59	0.51
3:C:403:ALA:HA	3:C:406:VAL:HG12	1.92	0.51
3:E:415:HIS:HD2	3:E:527:VAL:HG23	1.75	0.51
3:E:652:VAL:HG21	3:E:794:PHE:HD2	1.75	0.51
3:E:752:ARG:NH2	4:F:1001:ANP:O3G	2.43	0.51
3:E:821:ILE:O	3:E:822:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:415:HIS:O	3:L:519:PHE:HB3	2.11	0.51
3:L:615:MET:HE1	3:L:798:LEU:HD22	1.92	0.51
3:K:50:ILE:HG12	3:K:57:THR:HG22	1.92	0.51
3:J:111:GLU:HB3	3:J:113:PRO:HD2	1.92	0.51
3:A:47:THR:HG23	3:A:87:ARG:HH12	1.75	0.51
3:A:50:ILE:HG12	3:A:57:THR:HG22	1.92	0.51
3:A:869:ASN:OD1	3:A:870:ILE:HG12	2.09	0.51
3:C:294:MET:O	3:C:301:ARG:NH1	2.44	0.51
3:C:883:GLU:O	3:C:887:SER:N	2.43	0.51
3:D:785:ILE:O	3:D:791:GLN:NE2	2.43	0.51
3:K:15:THR:O	3:K:19:LYS:HG2	2.11	0.51
3:K:58:TYR:HB3	3:K:60:LEU:HG	1.92	0.51
3:K:621:ALA:HB1	3:K:688:TYR:HB2	1.93	0.51
3:J:170:LYS:HE3	3:J:204:ALA:HB1	1.92	0.51
3:J:403:ALA:HA	3:J:406:VAL:HG12	1.93	0.51
3:I:605:ILE:HD12	3:I:611:ARG:HA	1.93	0.51
3:I:709:VAL:HG21	3:I:752:ARG:HB3	1.92	0.51
3:I:761:LYS:NZ	3:I:762:PHE:O	2.44	0.51
3:I:838:PHE:HB2	3:I:865:TRP:CH2	2.46	0.51
3:I:854:ASN:CG	3:I:855:LEU:H	2.17	0.51
3:H:339:ALA:O	3:H:343:SER:OG	2.25	0.51
3:A:192:VAL:HG12	3:A:194:ASN:H	1.75	0.51
3:B:497:GLU:O	3:B:501:LEU:HD23	2.11	0.51
3:C:238:TYR:CB	3:C:240:PRO:HD3	2.41	0.51
3:G:103:ASN:OD1	3:G:104:THR:N	2.44	0.51
3:G:639:CYS:SG	3:H:751:ARG:NH2	2.84	0.51
3:G:878:LEU:HD13	3:L:870:ILE:HG23	1.92	0.51
3:K:326:PHE:HE1	3:K:361:LEU:HB3	1.75	0.51
3:K:364:ASP:C	3:K:368:HIS:HD1	2.19	0.51
3:J:96:LEU:HD21	3:J:98:TYR:CE1	2.46	0.51
3:H:121:ARG:HE	3:H:125:HIS:HD2	1.58	0.51
3:H:146:LYS:H	3:H:154:TYR:HB2	1.76	0.51
3:A:294:MET:HE1	3:A:301:ARG:HA	1.93	0.50
3:B:605:ILE:HD11	3:B:611:ARG:HA	1.94	0.50
3:B:939:LYS:HG3	3:B:940:ASN:H	1.76	0.50
3:E:341:TRP:O	3:E:345:LYS:NZ	2.45	0.50
3:F:406:VAL:HG23	3:F:411:GLY:HA2	1.91	0.50
3:F:709:VAL:HG11	3:F:752:ARG:HD3	1.92	0.50
3:J:56:LYS:HD3	3:J:58:TYR:CE2	2.46	0.50
3:I:544:LEU:HD23	3:I:575:PRO:HB2	1.93	0.50
3:I:670:ARG:HH22	3:H:663:ILE:HG23	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:713:ASP:H	3:H:647:ARG:NH1	2.02	0.50
3:H:140:HIS:ND1	3:H:228:GLU:OE1	2.44	0.50
3:H:635:LEU:HD22	3:H:739:ASN:HA	1.93	0.50
3:H:695:ASN:O	3:H:696:LYS:HG2	2.11	0.50
3:A:103:ASN:OD1	3:A:104:THR:N	2.45	0.50
3:B:642:LYS:HG2	4:B:1001:ANP:O1B	2.11	0.50
3:D:681:MET:HG3	3:D:717:ARG:HH11	1.76	0.50
3:E:120:HIS:CE1	3:E:241:ILE:HD11	2.46	0.50
3:E:370:GLU:O	3:E:372:LYS:NZ	2.39	0.50
3:E:395:GLU:HA	3:E:398:TYR:CE1	2.46	0.50
3:E:851:THR:O	3:E:853:TYR:N	2.44	0.50
3:F:635:LEU:HD22	3:F:739:ASN:HA	1.94	0.50
3:G:777:ASP:O	4:G:1001:ANP:O2'	2.29	0.50
3:L:336:ARG:HH22	3:L:359:GLU:HB3	1.76	0.50
3:L:415:HIS:O	3:K:519:PHE:HB3	2.11	0.50
3:K:337:PRO:O	3:K:341:TRP:N	2.34	0.50
3:K:344:GLN:HA	3:K:350:TRP:CE3	2.47	0.50
3:I:171:LYS:NZ	3:I:201:PRO:O	2.43	0.50
3:I:779:ARG:O	3:I:783:GLU:HG3	2.10	0.50
3:H:703:SER:O	3:H:704:ARG:HG2	2.10	0.50
3:A:744:THR:OG1	3:A:746:ASP:OD1	2.28	0.50
3:C:96:LEU:HD11	3:C:199:LEU:CG	2.40	0.50
3:E:66:LEU:HG	3:E:67:ARG:N	2.27	0.50
3:E:237:ASP:CG	3:K:117:ARG:HH12	2.20	0.50
3:F:857:GLU:OE1	3:F:857:GLU:N	2.44	0.50
3:G:585:VAL:O	3:G:796:SER:OG	2.27	0.50
3:G:695:ASN:ND2	3:H:702:THR:O	2.44	0.50
3:I:330:ASN:HB3	3:I:372:LYS:NZ	2.26	0.50
3:I:753:LEU:O	3:I:754:ARG:NH1	2.36	0.50
3:H:435:ASP:OD1	3:H:439:LYS:N	2.39	0.50
3:H:602:GLN:HB2	3:H:942:TRP:HE1	1.76	0.50
3:C:143:PHE:HA	3:C:158:VAL:HG13	1.93	0.50
3:D:711:PRO:HA	3:D:728:MET:SD	2.51	0.50
3:E:676:PRO:HG2	3:E:719:LEU:HD23	1.93	0.50
3:E:872:VAL:O	3:E:873:LYS:HD2	2.10	0.50
3:F:30:LEU:HA	3:F:34:GLU:OE1	2.11	0.50
3:F:368:HIS:CE1	3:F:370:GLU:HB3	2.47	0.50
3:J:98:TYR:HB3	3:J:100:LEU:HG	1.92	0.50
3:J:120:HIS:CD2	3:J:239:ILE:HD12	2.46	0.50
3:J:303:LEU:HA	3:J:306:ILE:HG12	1.94	0.50
4:J:1001:ANP:O2B	4:J:1001:ANP:O1A	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:364:ASP:HA	3:I:367:HIS:CE1	2.46	0.50
3:I:751:ARG:NH2	3:H:639:CYS:SG	2.84	0.50
3:I:851:THR:OG1	3:I:852:VAL:N	2.44	0.50
3:H:826:GLU:HA	3:H:829:ARG:HB2	1.92	0.50
3:A:870:ILE:HA	3:F:878:LEU:HD21	1.93	0.50
3:C:190:GLN:HB3	3:C:192:VAL:HG23	1.93	0.50
3:E:706:LYS:HD3	3:E:749:THR:HG22	1.94	0.50
3:L:363:ASN:O	3:L:367:HIS:ND1	2.44	0.50
3:I:121:ARG:HG2	3:I:183:VAL:HG13	1.93	0.50
3:I:176:SER:HA	3:I:179:HIS:CD2	2.47	0.50
3:H:395:GLU:HA	3:H:398:TYR:CE1	2.47	0.50
3:B:945:TRP:O	3:B:950:SER:OG	2.29	0.50
3:C:314:TYR:CG	3:C:320:LEU:HD22	2.47	0.50
3:D:51:ASN:HB3	3:D:56:LYS:HG2	1.93	0.50
3:D:250:TYR:HE2	3:D:265:LEU:HD13	1.76	0.50
3:D:893:LEU:HA	3:D:903:LEU:HA	1.94	0.50
3:E:115:LEU:HB3	3:E:143:PHE:CE2	2.46	0.50
3:E:237:ASP:OD1	3:K:117:ARG:NH2	2.44	0.50
3:L:140:HIS:NE2	3:L:265:LEU:O	2.45	0.50
3:L:311:PRO:HB2	3:L:313:GLU:HG2	1.94	0.50
3:K:633:LEU:O	3:K:755:HIS:ND1	2.44	0.50
3:I:676:PRO:HB2	3:I:718:GLU:C	2.37	0.50
3:H:61:PRO:HD2	3:H:64:GLU:HG3	1.92	0.50
3:A:380:TYR:CZ	3:A:384:LYS:HD3	2.47	0.50
3:B:30:LEU:HD21	3:B:68:LEU:HD22	1.94	0.50
3:C:88:GLN:HA	3:C:207:PRO:HG3	1.94	0.50
3:D:290:LEU:HG	3:D:294:MET:HE3	1.93	0.50
3:D:681:MET:HG2	3:D:717:ARG:HD3	1.94	0.50
3:A:232:ASP:OD2	3:A:234:SER:OG	2.27	0.50
3:B:302:TYR:OH	3:B:379:MET:HE1	2.12	0.50
3:C:496:HIS:HB3	3:C:500:ILE:HG21	1.92	0.50
3:E:415:HIS:CD2	3:E:527:VAL:HG23	2.47	0.50
3:F:63:THR:O	3:F:66:LEU:HG	2.10	0.50
3:L:107:VAL:O	3:L:109:PRO:HD3	2.12	0.50
3:K:176:SER:HA	3:K:179:HIS:CE1	2.46	0.50
3:J:786:MET:N	3:J:786:MET:SD	2.84	0.50
3:I:103:ASN:OD1	3:I:104:THR:N	2.45	0.50
3:H:746:ASP:OD1	3:H:746:ASP:N	2.44	0.50
3:A:52:ARG:HH22	3:A:215:LYS:HA	1.77	0.50
3:B:364:ASP:O	3:B:368:HIS:ND1	2.23	0.50
3:D:335:TYR:HD2	3:D:338:LEU:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:644:PHE:HB2	3:E:781:ILE:HD11	1.93	0.50
3:G:105:ASN:HA	3:G:153:LYS:HD3	1.93	0.50
3:G:444:GLU:OE2	3:G:461:ARG:NH2	2.39	0.50
1:M:2:DT:H2'	1:M:3:DT:H5"	1.94	0.49
3:A:395:GLU:HA	3:A:398:TYR:CE1	2.47	0.49
3:C:229:LEU:HD12	3:C:240:PRO:HD2	1.94	0.49
3:C:452:MET:HG3	3:C:453:ASN:O	2.12	0.49
3:C:821:ILE:C	3:C:823:SER:H	2.20	0.49
3:D:298:PRO:O	3:D:301:ARG:HG2	2.11	0.49
3:E:237:ASP:OD1	3:E:237:ASP:N	2.44	0.49
3:E:243:GLN:HB2	3:K:242:HIS:CE1	2.47	0.49
3:E:821:ILE:C	3:E:823:SER:H	2.20	0.49
3:E:945:TRP:CH2	3:E:948:ASN:HA	2.48	0.49
3:L:226:GLY:H	3:L:247:LEU:HD11	1.76	0.49
3:L:563:ILE:HG12	3:L:803:GLU:HG2	1.93	0.49
3:L:761:LYS:NZ	3:L:762:PHE:O	2.44	0.49
3:I:347:PRO:HA	3:I:350:TRP:HB3	1.94	0.49
3:I:350:TRP:HA	3:I:354:GLY:HA3	1.94	0.49
1:M:18:DT:H2'	1:M:19:DT:O4'	2.11	0.49
3:A:62:SER:OG	3:A:262:GLN:NE2	2.45	0.49
3:A:302:TYR:O	3:A:306:ILE:HG12	2.12	0.49
3:A:771:PRO:O	3:A:774:LYS:NZ	2.44	0.49
3:D:499:ASN:OD1	3:D:500:ILE:N	2.44	0.49
3:D:666:LEU:O	3:D:704:ARG:NH2	2.42	0.49
3:F:804:LYS:HD2	3:F:807:LYS:HE3	1.93	0.49
3:K:356:GLU:O	3:K:359:GLU:HG2	2.12	0.49
3:K:746:ASP:OD1	3:K:746:ASP:N	2.44	0.49
3:K:883:GLU:O	3:K:887:SER:N	2.43	0.49
3:J:646:MET:SD	3:J:647:ARG:N	2.85	0.49
3:H:370:GLU:CD	3:H:371:LYS:H	2.20	0.49
3:H:415:HIS:CE1	3:H:526:GLY:HA3	2.47	0.49
3:H:709:VAL:HG21	3:H:752:ARG:HB3	1.93	0.49
3:A:161:PRO:HB3	3:A:258:LEU:HD23	1.94	0.49
3:A:563:ILE:HG12	3:A:803:GLU:HG2	1.95	0.49
3:D:661:LEU:HD12	3:D:732:MET:HE1	1.94	0.49
3:F:337:PRO:O	3:F:341:TRP:N	2.37	0.49
3:F:676:PRO:HB2	3:F:718:GLU:O	2.11	0.49
3:G:740:PHE:O	3:G:832:GLN:NE2	2.44	0.49
3:K:677:ASN:N	3:K:717:ARG:O	2.46	0.49
3:I:646:MET:SD	3:I:647:ARG:N	2.85	0.49
3:H:87:ARG:HG3	3:H:207:PRO:HG3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:146:LYS:HE2	3:H:154:TYR:HA	1.94	0.49
3:A:229:LEU:HD21	3:A:239:ILE:HA	1.92	0.49
3:A:332:SER:OG	3:A:333:ALA:N	2.46	0.49
3:C:98:TYR:CE1	3:C:199:LEU:HD12	2.47	0.49
3:C:731:THR:O	3:C:732:MET:HE2	2.12	0.49
3:F:496:HIS:HB3	3:F:500:ILE:HG21	1.94	0.49
3:F:867:ASN:HA	3:F:871:ASN:O	2.11	0.49
3:J:298:PRO:O	3:J:301:ARG:HG2	2.12	0.49
3:J:587:PHE:HA	3:J:796:SER:HB3	1.93	0.49
3:I:344:GLN:HA	3:I:350:TRP:CZ3	2.47	0.49
3:H:51:ASN:HD21	3:H:53:ILE:HD12	1.77	0.49
3:A:96:LEU:HD21	3:A:98:TYR:CE1	2.47	0.49
3:A:311:PRO:CD	3:A:385:HIS:HB3	2.43	0.49
3:A:370:GLU:O	3:A:372:LYS:NZ	2.34	0.49
3:A:864:GLU:O	3:A:868:THR:HG23	2.12	0.49
3:B:294:MET:O	3:B:301:ARG:NE	2.42	0.49
3:C:391:LYS:O	3:C:394:VAL:HG22	2.12	0.49
3:D:364:ASP:HA	3:D:367:HIS:CE1	2.47	0.49
3:D:395:GLU:HA	3:D:398:TYR:CZ	2.48	0.49
3:F:31:LEU:HD23	3:F:35:LEU:HD12	1.94	0.49
3:L:102:LEU:HD21	3:L:108:PRO:HG3	1.95	0.49
3:L:703:SER:O	3:L:704:ARG:HG2	2.12	0.49
3:K:118:LEU:HD23	3:K:183:VAL:HG12	1.95	0.49
3:K:513:ARG:NH1	3:K:513:ARG:HB2	2.28	0.49
3:J:50:ILE:O	3:J:85:LEU:N	2.39	0.49
3:I:744:THR:O	3:I:750:TRP:NE1	2.43	0.49
3:I:818:CYS:SG	3:I:820:THR:OG1	2.70	0.49
3:H:15:THR:O	3:H:19:LYS:HG2	2.12	0.49
3:H:481:MET:HA	3:H:481:MET:HE3	1.94	0.49
3:H:744:THR:OG1	3:H:746:ASP:OD1	2.29	0.49
3:C:197:SER:O	3:C:198:CYS:C	2.56	0.49
3:D:339:ALA:HB1	3:D:358:LEU:HD11	1.95	0.49
3:F:718:GLU:HG2	3:F:719:LEU:N	2.28	0.49
3:G:613:TRP:HZ3	3:G:632:LEU:HD11	1.77	0.49
3:L:91:TYR:HB2	3:L:164:LYS:HB2	1.94	0.49
3:K:250:TYR:CZ	3:K:265:LEU:HB2	2.48	0.49
3:K:403:ALA:HA	3:K:406:VAL:HG12	1.95	0.49
3:K:695:ASN:O	3:K:696:LYS:HG2	2.12	0.49
3:J:174:ILE:HD12	3:J:199:LEU:HD21	1.94	0.49
3:J:703:SER:HB2	3:I:695:ASN:ND2	2.27	0.49
3:I:375:LYS:O	3:I:379:MET:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:939:LYS:HG3	3:I:940:ASN:H	1.78	0.49
3:H:388:GLN:HG2	3:H:391:LYS:HE3	1.95	0.49
1:M:7:DT:H2"	1:M:8:DT:O5'	2.12	0.49
3:A:87:ARG:HG3	3:A:207:PRO:HG3	1.95	0.49
3:B:804:LYS:HD2	3:B:807:LYS:HE3	1.95	0.49
3:D:866:TYR:CE2	3:D:873:LYS:HB2	2.48	0.49
3:E:35:LEU:HD21	3:E:67:ARG:HH21	1.78	0.49
3:G:751:ARG:HH22	3:L:639:CYS:HG	1.60	0.49
3:K:74:GLN:HA	3:K:77:LYS:HE2	1.93	0.49
3:J:105:ASN:HA	3:J:153:LYS:HD3	1.93	0.49
3:J:767:ASP:OD1	3:J:767:ASP:N	2.44	0.49
3:I:343:SER:HB3	3:I:350:TRP:NE1	2.27	0.49
1:M:17:DT:H2'	1:M:18:DT:O4'	2.12	0.49
3:D:116:SER:HB3	3:D:241:ILE:HG12	1.95	0.49
3:D:643:THR:O	3:D:647:ARG:NE	2.45	0.49
3:D:666:LEU:C	3:D:704:ARG:HH21	2.20	0.49
3:F:704:ARG:O	3:F:708:MET:HG2	2.12	0.49
3:K:298:PRO:O	3:K:301:ARG:HG2	2.13	0.49
3:K:626:LEU:HD22	3:K:711:PRO:HB2	1.94	0.49
3:J:13:GLN:OE1	3:J:491:HIS:NE2	2.42	0.49
3:J:665:LEU:HD11	3:J:680:PHE:HB2	1.94	0.49
3:J:713:ASP:OD1	3:I:647:ARG:NH1	2.44	0.49
3:I:851:THR:HG23	3:I:853:TYR:H	1.76	0.49
3:H:187:LEU:HB3	3:H:192:VAL:HB	1.94	0.49
3:H:652:VAL:HG21	3:H:794:PHE:HD2	1.78	0.49
3:B:95:MET:SD	3:B:96:LEU:N	2.86	0.49
3:C:140:HIS:ND1	3:C:228:GLU:HB2	2.27	0.49
3:F:674:GLU:OE1	3:F:674:GLU:N	2.44	0.49
3:L:946:SER:HB3	3:L:947:PRO:HD2	1.94	0.49
3:J:192:VAL:HG12	3:J:194:ASN:H	1.78	0.49
3:H:426:MET:CE	3:H:429:LYS:HB2	2.42	0.49
3:B:403:ALA:HA	3:B:406:VAL:HG12	1.95	0.49
3:B:696:LYS:HA	3:B:738:TYR:CD2	2.47	0.49
3:C:64:GLU:HG3	3:C:67:ARG:NH2	2.25	0.49
3:C:752:ARG:NH1	4:D:1001:ANP:O1G	2.26	0.49
3:E:52:ARG:HH22	3:E:215:LYS:HA	1.77	0.49
3:E:368:HIS:HB3	3:E:370:GLU:OE1	2.13	0.49
3:F:159:LEU:HG	3:F:256:LEU:HD23	1.94	0.49
3:K:73:GLU:HB3	3:K:77:LYS:HZ3	1.78	0.49
3:K:303:LEU:HA	3:K:306:ILE:HG12	1.94	0.49
3:K:350:TRP:NE1	3:K:355:LYS:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:780:PHE:HB2	4:J:1001:ANP:O2'	2.12	0.49
3:I:412:MET:N	3:I:412:MET:SD	2.86	0.49
3:H:332:SER:OG	3:H:333:ALA:N	2.46	0.49
3:H:356:GLU:O	3:H:359:GLU:HG2	2.13	0.49
3:H:676:PRO:HB2	3:H:718:GLU:O	2.13	0.49
3:H:818:CYS:SG	3:H:821:ILE:HG12	2.53	0.49
3:A:170:LYS:O	3:A:174:ILE:HG12	2.14	0.48
3:B:425:MET:HE1	3:B:477:PHE:HD1	1.78	0.48
3:C:115:LEU:HB2	3:C:143:PHE:CZ	2.47	0.48
3:C:144:THR:HA	3:C:223:LEU:HD23	1.95	0.48
3:C:198:CYS:O	3:C:199:LEU:C	2.55	0.48
3:C:332:SER:OG	3:C:333:ALA:N	2.46	0.48
3:C:718:GLU:HG3	3:C:719:LEU:H	1.77	0.48
3:C:777:ASP:H	4:C:1001:ANP:H8	1.78	0.48
3:C:809:TYR:CZ	3:C:816:VAL:HG23	2.48	0.48
3:D:53:ILE:HG13	3:D:83:TYR:HB2	1.95	0.48
3:D:605:ILE:HD11	3:D:611:ARG:HA	1.94	0.48
3:D:652:VAL:HG21	3:D:794:PHE:HD2	1.78	0.48
3:D:703:SER:O	3:D:704:ARG:HD3	2.14	0.48
3:D:706:LYS:O	3:D:709:VAL:HG12	2.13	0.48
3:E:232:ASP:OD2	3:E:235:ASP:N	2.44	0.48
3:E:703:SER:O	3:E:704:ARG:HG2	2.13	0.48
3:L:166:ALA:HA	3:L:170:LYS:HG3	1.95	0.48
3:L:700:LEU:HD23	3:L:700:LEU:H	1.77	0.48
3:L:818:CYS:SG	3:L:821:ILE:HG12	2.53	0.48
3:K:227:PHE:HA	3:K:243:GLN:HA	1.95	0.48
3:J:607:GLU:HB2	3:J:610:ALA:HB3	1.93	0.48
3:H:289:SER:O	3:H:292:ILE:HG22	2.13	0.48
3:D:353:GLY:O	3:D:356:GLU:HG2	2.13	0.48
3:E:302:TYR:OH	3:E:394:VAL:HG12	2.13	0.48
3:F:701:ASN:C	3:F:703:SER:H	2.20	0.48
3:G:521:ASP:HB2	3:H:530:GLN:HG2	1.95	0.48
3:L:303:LEU:HD23	3:L:306:ILE:HD11	1.95	0.48
3:I:347:PRO:O	3:I:351:ASN:N	2.46	0.48
3:I:380:TYR:CE2	3:I:571:PHE:HB3	2.48	0.48
3:I:807:LYS:NZ	3:I:808:GLU:OE2	2.44	0.48
3:I:894:GLN:N	3:I:902:ILE:O	2.41	0.48
3:H:56:LYS:HD3	3:H:58:TYR:HE2	1.77	0.48
1:M:19:DT:H2'	1:M:20:DT:O4'	2.14	0.48
3:A:852:VAL:HB	3:A:902:ILE:HB	1.95	0.48
3:C:779:ARG:HG2	3:C:783:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:LEU:HD13	3:D:153:LYS:HG2	1.95	0.48
3:D:416:TYR:HA	3:D:419:ALA:HB3	1.94	0.48
3:D:457:ILE:H	3:D:457:ILE:HD12	1.77	0.48
3:D:621:ALA:HB1	3:D:688:TYR:HB2	1.94	0.48
3:E:102:LEU:HG	3:E:192:VAL:HA	1.94	0.48
3:E:794:PHE:HA	3:E:797:ILE:HD12	1.95	0.48
3:G:615:MET:HE2	3:G:615:MET:HA	1.96	0.48
3:L:497:GLU:O	3:L:501:LEU:HD23	2.13	0.48
3:L:607:GLU:HB2	3:L:610:ALA:HB3	1.95	0.48
3:K:416:TYR:HA	3:K:419:ALA:HB3	1.96	0.48
3:K:777:ASP:OD2	3:K:780:PHE:N	2.45	0.48
3:J:140:HIS:ND1	3:J:228:GLU:OE1	2.46	0.48
3:J:294:MET:HE2	3:J:294:MET:N	2.29	0.48
3:J:761:LYS:NZ	3:J:762:PHE:O	2.46	0.48
3:I:16:ALA:HB1	3:I:20:TYR:CE2	2.47	0.48
3:I:616:PHE:HB3	3:I:805:LEU:HD12	1.95	0.48
3:H:701:ASN:OD1	3:H:704:ARG:NH2	2.40	0.48
3:H:780:PHE:HB2	4:H:1001:ANP:O2'	2.13	0.48
3:C:99:ASP:H	3:C:198:CYS:HB3	1.79	0.48
3:D:120:HIS:NE2	3:D:241:ILE:HD11	2.28	0.48
3:D:680:PHE:HB2	3:D:717:ARG:CZ	2.44	0.48
3:F:821:ILE:C	3:F:823:SER:H	2.22	0.48
3:G:607:GLU:HB2	3:G:610:ALA:HB3	1.96	0.48
3:L:587:PHE:HA	3:L:796:SER:HB3	1.95	0.48
3:J:766:PRO:HA	3:J:773:GLU:OE2	2.13	0.48
3:J:786:MET:O	3:J:787:ASP:C	2.56	0.48
3:A:97:ASP:HA	3:A:157:HIS:ND1	2.29	0.48
3:C:110:LEU:HD21	3:C:115:LEU:HD23	1.95	0.48
3:C:896:SER:HB2	3:C:900:THR:HB	1.95	0.48
3:D:722:LYS:HD2	3:D:722:LYS:HA	1.45	0.48
3:E:174:ILE:HD12	3:E:199:LEU:HD21	1.94	0.48
3:F:671:GLU:CD	3:F:675:LYS:HB2	2.39	0.48
3:L:94:LEU:HB2	3:L:160:ILE:HB	1.95	0.48
3:K:51:ASN:HB3	3:K:56:LYS:HG2	1.94	0.48
3:J:171:LYS:HD3	3:J:171:LYS:HA	1.63	0.48
3:J:383:HIS:ND1	3:J:390:TYR:OH	2.41	0.48
3:J:631:MET:HB3	3:J:753:LEU:HD23	1.95	0.48
3:J:946:SER:HB3	3:J:947:PRO:HD2	1.96	0.48
3:I:50:ILE:O	3:I:85:LEU:N	2.39	0.48
3:I:609:ASP:OD1	3:I:610:ALA:N	2.46	0.48
3:H:69:TYR:HB3	3:H:254:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:99:ASP:N	3:H:198:CYS:O	2.42	0.48
3:H:363:ASN:O	3:H:367:HIS:ND1	2.47	0.48
3:A:102:LEU:HD22	3:A:153:LYS:HG2	1.96	0.48
3:C:851:THR:HG23	3:C:853:TYR:H	1.78	0.48
3:D:290:LEU:HD22	3:D:341:TRP:CD1	2.49	0.48
3:E:101:LYS:HA	3:E:152:GLY:O	2.13	0.48
3:F:746:ASP:OD1	3:F:746:ASP:N	2.46	0.48
3:G:54:THR:HG1	3:G:56:LYS:HZ2	1.55	0.48
3:G:707:GLU:OE1	3:G:707:GLU:N	2.39	0.48
3:K:607:GLU:HB2	3:K:610:ALA:HB3	1.94	0.48
3:K:644:PHE:CE1	3:K:780:PHE:HB3	2.48	0.48
3:K:867:ASN:HA	3:K:871:ASN:O	2.13	0.48
3:J:339:ALA:HB1	3:J:358:LEU:HD11	1.95	0.48
3:I:345:LYS:O	3:I:346:CYS:C	2.54	0.48
3:H:161:PRO:HB3	3:H:258:LEU:HD23	1.96	0.48
3:D:368:HIS:HB3	3:D:370:GLU:HB2	1.96	0.48
3:E:67:ARG:O	3:E:70:GLU:HG3	2.14	0.48
3:E:232:ASP:HB2	3:E:238:TYR:CD2	2.48	0.48
3:F:401:ILE:O	3:F:404:GLU:HG3	2.13	0.48
3:G:332:SER:OG	3:G:333:ALA:N	2.45	0.48
3:K:102:LEU:HB2	3:K:153:LYS:HG2	1.96	0.48
3:K:565:ALA:N	3:K:803:GLU:OE2	2.46	0.48
3:J:145:LEU:HD22	3:J:224:LYS:HB2	1.95	0.48
3:J:379:MET:HE1	3:J:390:TYR:CD2	2.48	0.48
3:J:780:PHE:HA	3:J:784:TYR:CD2	2.46	0.48
3:I:40:THR:O	3:I:57:THR:OG1	2.32	0.48
3:I:708:MET:HE1	3:I:714:VAL:HG21	1.94	0.48
3:H:879:GLU:O	3:H:883:GLU:HG3	2.14	0.48
3:A:668:SER:OG	3:A:669:CYS:N	2.46	0.48
3:A:818:CYS:SG	3:A:820:THR:OG1	2.72	0.48
3:A:945:TRP:O	3:A:950:SER:OG	2.31	0.48
3:B:121:ARG:NH1	3:B:121:ARG:O	2.47	0.48
3:B:292:ILE:HB	3:B:296:HIS:NE2	2.28	0.48
3:E:412:MET:HE3	3:E:412:MET:H	1.79	0.48
3:E:604:ILE:HG22	3:E:605:ILE:HG23	1.95	0.48
3:E:841:GLU:OE1	3:E:865:TRP:NE1	2.45	0.48
3:G:767:ASP:N	3:G:767:ASP:OD1	2.45	0.48
3:L:162:GLY:O	3:L:269:VAL:N	2.45	0.48
3:L:939:LYS:HG3	3:L:940:ASN:H	1.79	0.48
3:J:228:GLU:N	3:J:242:HIS:O	2.30	0.48
3:J:330:ASN:ND2	3:J:373:ILE:O	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:457:ILE:HG22	3:J:458:TRP:CD1	2.49	0.48
3:J:818:CYS:SG	3:J:821:ILE:HG12	2.54	0.48
3:I:614:ILE:HG13	3:I:632:LEU:HD11	1.95	0.48
3:I:699:VAL:HG12	3:I:701:ASN:H	1.79	0.48
3:I:779:ARG:HB3	3:I:783:GLU:OE2	2.14	0.48
3:H:762:PHE:HB3	3:H:776:GLU:HA	1.94	0.48
3:C:60:LEU:HB2	3:C:64:GLU:HB3	1.96	0.48
3:C:101:LYS:HD2	3:C:152:GLY:HA2	1.96	0.48
3:C:416:TYR:HA	3:C:419:ALA:HB3	1.96	0.48
3:C:719:LEU:O	3:C:721:GLN:HG2	2.13	0.48
3:D:52:ARG:HE	3:D:83:TYR:HB3	1.79	0.48
3:D:807:LYS:NZ	3:D:808:GLU:OE2	2.32	0.48
3:G:646:MET:SD	3:G:647:ARG:N	2.87	0.48
3:G:766:PRO:HG3	3:G:775:LYS:HD2	1.95	0.48
3:L:182:THR:O	3:L:185:LYS:HG3	2.14	0.48
3:L:403:ALA:HA	3:L:406:VAL:HG12	1.96	0.48
3:H:297:ASP:OD2	3:H:299:GLU:HB3	2.14	0.48
3:A:52:ARG:HD3	3:A:85:LEU:HD11	1.95	0.48
3:C:115:LEU:HD13	3:C:143:PHE:CE1	2.49	0.48
3:D:164:LYS:NZ	3:D:268:PRO:O	2.47	0.48
3:E:111:GLU:HB3	3:E:113:PRO:HD2	1.96	0.48
3:E:224:LYS:HG3	3:E:225:THR:HG23	1.95	0.48
3:E:876:ILE:HB	3:E:879:GLU:OE2	2.14	0.48
3:F:105:ASN:HA	3:F:153:LYS:HD3	1.96	0.48
3:L:305:LYS:O	3:L:309:LEU:HG	2.14	0.48
3:L:852:VAL:HG23	3:L:854:ASN:H	1.78	0.48
3:K:452:MET:HG3	3:K:453:ASN:O	2.13	0.48
3:I:342:PHE:HA	3:I:345:LYS:CE	2.43	0.48
3:H:294:MET:CE	3:H:300:ALA:HB1	2.41	0.48
3:H:774:LYS:HE2	3:H:774:LYS:HB2	1.56	0.48
3:A:674:GLU:HG2	3:B:676:PRO:O	2.14	0.47
3:C:821:ILE:HG22	3:C:822:GLU:H	1.79	0.47
3:D:162:GLY:O	3:D:269:VAL:N	2.45	0.47
3:D:376:ARG:HH11	3:D:573:GLU:HG3	1.79	0.47
3:D:714:VAL:HG13	3:D:726:PHE:CE1	2.49	0.47
3:F:708:MET:HA	3:F:728:MET:HE2	1.96	0.47
3:G:301:ARG:HA	3:G:304:HIS:HB3	1.95	0.47
3:L:380:TYR:CE2	3:L:571:PHE:HB3	2.49	0.47
3:L:717:ARG:N	3:L:723:GLN:OE1	2.47	0.47
3:K:122:ILE:HD11	3:K:141:PHE:HE2	1.79	0.47
3:K:444:GLU:OE2	3:K:461:ARG:NH2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:854:ASN:HA	3:K:902:ILE:HG22	1.96	0.47
3:J:433:ASP:OD1	3:J:434:VAL:N	2.41	0.47
3:H:140:HIS:NE2	3:H:266:VAL:HA	2.28	0.47
3:H:708:MET:HE1	3:H:714:VAL:HG21	1.96	0.47
1:M:8:DT:H2'	1:M:9:DT:C6	2.49	0.47
3:B:375:LYS:O	3:B:379:MET:HG2	2.14	0.47
3:C:156:PHE:CE1	3:C:158:VAL:HB	2.49	0.47
3:C:746:ASP:OD1	3:C:749:THR:OG1	2.27	0.47
3:C:837:ARG:O	3:C:841:GLU:CB	2.63	0.47
3:F:47:THR:O	3:F:87:ARG:NH1	2.46	0.47
3:G:101:LYS:HA	3:G:152:GLY:O	2.14	0.47
3:G:153:LYS:HG3	3:G:154:TYR:H	1.79	0.47
3:G:604:ILE:HG22	3:G:605:ILE:HG23	1.96	0.47
3:G:838:PHE:HB2	3:G:865:TRP:CZ3	2.49	0.47
3:K:82:MET:SD	3:K:84:PHE:HB2	2.54	0.47
3:I:680:PHE:CZ	3:I:714:VAL:HG21	2.49	0.47
3:H:764:HIS:HA	3:H:775:LYS:HZ3	1.79	0.47
3:A:709:VAL:CG1	3:A:752:ARG:HD3	2.44	0.47
3:A:870:ILE:HA	3:F:878:LEU:CD2	2.45	0.47
3:B:306:ILE:HG21	3:B:378:ILE:HG22	1.96	0.47
3:C:73:GLU:CD	3:C:251:ASN:HB2	2.39	0.47
3:C:616:PHE:HB3	3:C:805:LEU:HD12	1.95	0.47
3:E:153:LYS:HG3	3:E:154:TYR:HD1	1.78	0.47
3:E:908:ILE:O	3:E:908:ILE:HG13	2.13	0.47
3:F:228:GLU:HB3	3:F:242:HIS:HB2	1.96	0.47
3:F:874:ARG:HA	3:F:874:ARG:NE	2.28	0.47
3:G:290:LEU:O	3:G:294:MET:N	2.46	0.47
3:G:870:ILE:HG23	3:H:878:LEU:HD23	1.96	0.47
3:L:125:HIS:HE2	3:L:180:ASP:CG	2.23	0.47
3:I:634:TRP:HB3	3:I:756:TYR:HB3	1.95	0.47
3:H:634:TRP:CZ3	3:H:758:SER:HB3	2.49	0.47
3:H:718:GLU:OE1	3:H:718:GLU:N	2.47	0.47
3:B:29:THR:O	3:B:33:ARG:HG2	2.14	0.47
3:B:718:GLU:HG2	3:B:719:LEU:N	2.27	0.47
3:B:880:LEU:HA	3:B:883:GLU:OE2	2.15	0.47
3:C:148:GLU:O	3:C:149:VAL:C	2.58	0.47
3:D:634:TRP:HA	3:D:756:TYR:O	2.14	0.47
3:D:674:GLU:HB3	3:E:719:LEU:HD11	1.97	0.47
3:E:50:ILE:O	3:E:85:LEU:N	2.41	0.47
3:E:483:ARG:O	3:E:486:GLU:HG3	2.14	0.47
3:E:565:ALA:N	3:E:803:GLU:OE2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:224:LYS:HG3	3:F:225:THR:HG23	1.97	0.47
3:F:638:GLY:O	3:F:640:ASN:ND2	2.48	0.47
3:G:337:PRO:O	3:G:341:TRP:N	2.40	0.47
3:G:388:GLN:HG2	3:G:391:LYS:HE3	1.96	0.47
3:G:909:LEU:HG	3:G:913:GLU:OE1	2.15	0.47
3:K:107:VAL:O	3:K:109:PRO:HD3	2.14	0.47
3:K:639:CYS:HA	4:K:1001:ANP:O3A	2.13	0.47
3:J:722:LYS:HZ3	3:I:718:GLU:HB2	1.79	0.47
3:H:159:LEU:HD11	3:H:258:LEU:HD21	1.96	0.47
3:H:605:ILE:HD11	3:H:611:ARG:HA	1.96	0.47
3:B:412:MET:HA	3:B:412:MET:HE2	1.96	0.47
3:E:107:VAL:O	3:E:109:PRO:HD3	2.14	0.47
3:E:289:SER:O	3:E:292:ILE:HG22	2.14	0.47
3:F:188:HIS:CE1	3:F:195:PRO:HB3	2.49	0.47
3:L:627:LYS:HZ2	3:L:731:THR:N	2.12	0.47
3:K:634:TRP:HZ3	3:K:758:SER:HB3	1.79	0.47
3:J:544:LEU:HD23	3:J:575:PRO:HB2	1.95	0.47
3:J:743:ASP:OD1	3:J:743:ASP:N	2.46	0.47
3:I:228:GLU:N	3:I:242:HIS:O	2.35	0.47
3:I:604:ILE:HG13	4:I:1001:ANP:HN61	1.79	0.47
3:I:882:GLN:O	3:I:885:GLU:HG2	2.15	0.47
3:A:153:LYS:HG3	3:A:154:TYR:CD1	2.50	0.47
3:B:144:THR:HA	3:B:224:LYS:H	1.79	0.47
3:B:894:GLN:O	3:B:902:ILE:N	2.44	0.47
3:C:375:LYS:HA	3:C:378:ILE:HD13	1.96	0.47
3:D:715:THR:HG23	3:D:725:SER:N	2.30	0.47
3:E:96:LEU:HD21	3:E:98:TYR:CE1	2.50	0.47
3:E:332:SER:OG	3:E:333:ALA:N	2.47	0.47
3:E:732:MET:N	3:E:732:MET:SD	2.88	0.47
3:L:398:TYR:CE1	3:L:425:MET:HE2	2.48	0.47
3:J:760:VAL:HB	3:J:774:LYS:HZ3	1.79	0.47
3:I:403:ALA:HA	3:I:406:VAL:HG12	1.97	0.47
3:H:647:ARG:O	3:H:651:MET:HE3	2.14	0.47
3:A:378:ILE:HA	3:A:381:TRP:CE3	2.49	0.47
3:A:837:ARG:O	3:A:841:GLU:HB2	2.15	0.47
3:A:867:ASN:HA	3:A:871:ASN:O	2.15	0.47
3:B:101:LYS:HG2	3:B:194:ASN:ND2	2.30	0.47
3:B:125:HIS:CE1	3:B:180:ASP:HB2	2.50	0.47
3:B:619:SER:HA	3:B:798:LEU:HD22	1.96	0.47
3:C:40:THR:OG1	3:C:59:ALA:N	2.48	0.47
3:C:92:SER:HB2	3:C:258:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:OG1	3:C:145:LEU:N	2.47	0.47
3:D:344:GLN:HA	3:D:350:TRP:CZ3	2.49	0.47
3:D:350:TRP:HA	3:D:354:GLY:CA	2.42	0.47
3:D:350:TRP:O	3:D:354:GLY:N	2.48	0.47
3:D:609:ASP:N	3:D:609:ASP:OD1	2.47	0.47
3:E:61:PRO:HD2	3:E:64:GLU:HG3	1.97	0.47
3:E:122:ILE:HD11	3:E:141:PHE:HE2	1.79	0.47
3:E:145:LEU:HD22	3:E:224:LYS:HB2	1.95	0.47
3:F:416:TYR:HA	3:F:419:ALA:HB3	1.95	0.47
3:F:709:VAL:CG1	3:F:752:ARG:HD3	2.45	0.47
3:F:947:PRO:O	3:F:950:SER:OG	2.28	0.47
3:G:108:PRO:HD3	3:G:153:LYS:HE2	1.96	0.47
3:G:821:ILE:C	3:G:823:SER:H	2.22	0.47
3:G:844:VAL:HG13	3:G:907:ARG:NH2	2.30	0.47
3:K:321:TRP:HZ3	3:K:357:LYS:HD3	1.79	0.47
3:K:475:GLU:O	3:K:478:SER:OG	2.33	0.47
3:J:318:TYR:HE1	3:J:361:LEU:HD11	1.79	0.47
3:J:321:TRP:O	3:J:325:VAL:HG23	2.15	0.47
3:J:380:TYR:CE2	3:J:571:PHE:HB3	2.48	0.47
3:J:700:LEU:HD23	3:J:705:LEU:HD13	1.96	0.47
3:J:762:PHE:HB3	3:J:776:GLU:HG3	1.95	0.47
3:I:56:LYS:HD3	3:I:58:TYR:CE2	2.50	0.47
3:I:148:GLU:HG2	3:I:153:LYS:HE3	1.97	0.47
3:I:433:ASP:OD1	3:I:434:VAL:N	2.44	0.47
3:I:622:ILE:HG13	3:I:623:PHE:N	2.29	0.47
3:H:321:TRP:HZ3	3:H:357:LYS:HD3	1.79	0.47
3:H:753:LEU:O	3:H:754:ARG:NH1	2.41	0.47
1:M:8:DT:O3'	3:C:720:ASN:ND2	2.47	0.47
3:A:694:THR:HG21	3:A:736:SER:HB2	1.97	0.47
3:C:238:TYR:O	3:C:239:ILE:C	2.58	0.47
3:C:743:ASP:OD1	3:C:743:ASP:N	2.45	0.47
3:D:544:LEU:HD23	3:D:575:PRO:HB2	1.96	0.47
3:F:192:VAL:HG12	3:F:194:ASN:H	1.80	0.47
3:F:305:LYS:O	3:F:309:LEU:HG	2.14	0.47
3:F:699:VAL:HG12	3:F:741:ILE:HB	1.97	0.47
3:K:490:TYR:O	3:K:493:SER:OG	2.25	0.47
3:J:364:ASP:HA	3:J:367:HIS:CE1	2.50	0.47
3:H:318:TYR:HE1	3:H:361:LEU:HD11	1.80	0.47
3:A:499:ASN:OD1	3:A:500:ILE:N	2.48	0.47
3:A:533:PHE:HB3	3:B:471:ILE:HD11	1.97	0.47
3:C:938:PRO:HG3	3:C:942:TRP:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:ASP:OD1	3:D:97:ASP:N	2.46	0.47
3:E:867:ASN:HA	3:E:871:ASN:O	2.14	0.47
3:F:235:ASP:HB2	3:L:117:ARG:NH2	2.30	0.47
3:G:53:ILE:HG12	3:G:83:TYR:HD2	1.80	0.47
3:G:123:PHE:O	3:G:127:LYS:HG2	2.14	0.47
3:G:364:ASP:C	3:G:368:HIS:HD1	2.20	0.47
3:L:452:MET:HE3	3:L:457:ILE:HG13	1.97	0.47
3:K:117:ARG:HG3	3:K:186:ILE:HD11	1.95	0.47
3:K:889:LEU:O	3:K:893:LEU:N	2.47	0.47
3:J:228:GLU:O	3:J:242:HIS:HB2	2.15	0.47
3:I:332:SER:OG	3:I:333:ALA:N	2.48	0.47
3:H:56:LYS:HD3	3:H:58:TYR:CE2	2.50	0.47
3:H:297:ASP:O	3:H:300:ALA:HB3	2.14	0.47
3:A:121:ARG:HE	3:A:180:ASP:CG	2.23	0.47
3:C:139:ILE:HG12	3:C:230:VAL:HA	1.95	0.47
3:C:841:GLU:HG2	3:C:842:ARG:HE	1.79	0.47
3:D:92:SER:HB2	3:D:258:LEU:HB3	1.97	0.47
3:D:674:GLU:C	3:D:676:PRO:HD3	2.40	0.47
3:D:675:LYS:HG3	3:D:717:ARG:NH2	2.30	0.47
3:D:709:VAL:HG11	3:D:752:ARG:HD2	1.96	0.47
3:E:718:GLU:HB3	3:E:721:GLN:OE1	2.15	0.47
3:E:780:PHE:HA	3:E:784:TYR:HD2	1.80	0.47
3:F:240:PRO:HB3	3:L:116:SER:OG	2.15	0.47
3:F:600:ALA:O	3:F:604:ILE:HG12	2.15	0.47
3:G:336:ARG:HB2	3:G:362:TRP:CE2	2.50	0.47
3:L:163:LEU:HA	3:L:269:VAL:HB	1.96	0.47
3:L:821:ILE:C	3:L:823:SER:H	2.22	0.47
3:K:634:TRP:O	3:K:735:ALA:HA	2.15	0.47
3:J:672:THR:HG22	3:J:674:GLU:H	1.80	0.47
3:I:250:TYR:CZ	3:I:265:LEU:HB2	2.50	0.47
3:A:746:ASP:OD1	3:A:746:ASP:N	2.47	0.46
3:B:144:THR:HG1	3:B:222:GLN:C	2.23	0.46
3:B:744:THR:OG1	3:C:738:TYR:OH	2.27	0.46
3:C:851:THR:OG1	3:C:852:VAL:N	2.37	0.46
3:D:13:GLN:OE1	3:D:491:HIS:NE2	2.47	0.46
3:D:171:LYS:HD3	3:D:171:LYS:HA	1.71	0.46
3:E:86:GLU:O	3:E:208:SER:N	2.42	0.46
3:F:121:ARG:HH11	3:F:121:ARG:HA	1.79	0.46
3:L:565:ALA:N	3:L:803:GLU:OE2	2.46	0.46
3:L:894:GLN:HB2	3:L:904:LYS:HZ2	1.80	0.46
3:I:174:ILE:HG23	3:I:199:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:783:GLU:C	3:I:785:ILE:H	2.23	0.46
3:H:153:LYS:HG3	3:H:154:TYR:HD1	1.80	0.46
3:H:670:ARG:NH1	3:H:707:GLU:OE2	2.48	0.46
3:H:779:ARG:O	3:H:783:GLU:N	2.48	0.46
3:A:723:GLN:HG3	3:B:679:ALA:HA	1.97	0.46
3:B:100:LEU:O	3:B:153:LYS:HB3	2.16	0.46
3:C:64:GLU:HG3	3:C:67:ARG:HE	1.80	0.46
3:F:97:ASP:OD1	3:F:97:ASP:N	2.49	0.46
3:F:655:ASP:N	3:F:655:ASP:OD1	2.48	0.46
3:G:170:LYS:HE3	3:G:204:ALA:HB1	1.97	0.46
3:L:174:ILE:HD12	3:L:199:LEU:HD21	1.97	0.46
3:L:237:ASP:OD1	3:L:237:ASP:N	2.47	0.46
3:K:636:GLY:O	3:K:737:ASN:HA	2.16	0.46
3:I:354:GLY:HA2	3:I:357:LYS:CD	2.45	0.46
3:H:16:ALA:HB1	3:H:20:TYR:CE2	2.50	0.46
3:A:73:GLU:OE2	3:A:252:LEU:N	2.43	0.46
3:B:947:PRO:O	3:B:950:SER:OG	2.29	0.46
3:C:692:GLU:N	3:C:692:GLU:OE1	2.49	0.46
3:D:247:LEU:O	3:D:252:LEU:HD21	2.15	0.46
3:E:162:GLY:O	3:E:269:VAL:N	2.44	0.46
3:E:232:ASP:HB2	3:E:238:TYR:CE2	2.50	0.46
3:E:306:ILE:HA	3:E:309:LEU:HG	1.97	0.46
3:F:61:PRO:HD2	3:F:64:GLU:HG3	1.97	0.46
3:F:228:GLU:O	3:F:242:HIS:ND1	2.48	0.46
3:F:375:LYS:O	3:F:379:MET:HG2	2.15	0.46
3:L:326:PHE:CD1	3:L:365:ALA:HB2	2.49	0.46
3:K:355:LYS:C	3:K:355:LYS:HZ3	2.24	0.46
3:I:341:TRP:HA	3:I:344:GLN:CD	2.41	0.46
3:I:632:LEU:HD21	3:I:634:TRP:HD1	1.81	0.46
3:H:295:LEU:HG	3:H:296:HIS:N	2.29	0.46
3:H:457:ILE:HD12	3:H:457:ILE:H	1.80	0.46
3:B:141:PHE:HE2	3:B:229:LEU:HG	1.79	0.46
3:B:663:ILE:HG21	3:B:693:GLU:O	2.16	0.46
3:C:147:PRO:O	3:C:148:GLU:HB2	2.15	0.46
3:C:290:LEU:HD22	3:C:341:TRP:CD1	2.51	0.46
3:C:376:ARG:NH1	3:C:428:ASN:O	2.48	0.46
3:E:629:ALA:HB1	3:E:709:VAL:HG22	1.96	0.46
3:L:159:LEU:HD21	3:L:256:LEU:O	2.16	0.46
3:L:297:ASP:HB3	3:L:300:ALA:HB2	1.97	0.46
3:K:380:TYR:CE2	3:K:571:PHE:HB3	2.51	0.46
3:K:701:ASN:O	3:K:701:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:140:HIS:NE2	3:I:266:VAL:HA	2.31	0.46
3:I:457:ILE:H	3:I:457:ILE:HD12	1.79	0.46
3:I:607:GLU:OE2	3:I:756:TYR:OH	2.29	0.46
3:I:682:ARG:HH21	3:I:686:ARG:HH22	1.64	0.46
3:A:290:LEU:HD11	3:A:341:TRP:HB2	1.96	0.46
3:B:105:ASN:O	3:B:153:LYS:NZ	2.48	0.46
3:B:297:ASP:OD2	3:B:299:GLU:HG3	2.15	0.46
3:B:644:PHE:HE2	4:B:1001:ANP:H2'	1.81	0.46
3:C:749:THR:C	3:C:751:ARG:H	2.24	0.46
3:D:200:ASP:O	3:D:203:SER:OG	2.30	0.46
3:D:336:ARG:HB2	3:D:362:TRP:CE2	2.51	0.46
3:D:354:GLY:O	3:D:358:LEU:N	2.44	0.46
3:D:808:GLU:HG3	3:D:945:TRP:CE2	2.51	0.46
3:E:153:LYS:HA	3:E:153:LYS:HD2	1.61	0.46
3:E:337:PRO:O	3:E:341:TRP:N	2.34	0.46
3:E:852:VAL:HG13	3:E:853:TYR:N	2.29	0.46
3:F:544:LEU:HD23	3:F:575:PRO:HB2	1.98	0.46
3:G:64:GLU:OE1	3:G:67:ARG:NH2	2.37	0.46
3:G:171:LYS:HA	3:G:171:LYS:HD3	1.71	0.46
3:G:294:MET:O	3:G:301:ARG:NH2	2.49	0.46
3:G:813:ILE:O	3:G:816:VAL:HG12	2.16	0.46
3:K:86:GLU:OE1	3:K:210:LEU:HD12	2.15	0.46
3:K:95:MET:HE2	3:K:208:SER:HB2	1.97	0.46
3:K:699:VAL:HG12	3:K:741:ILE:HB	1.97	0.46
3:K:838:PHE:HB2	3:K:865:TRP:CZ3	2.50	0.46
3:I:328:LEU:HD11	3:I:339:ALA:HB2	1.97	0.46
1:M:10:DT:H2'	1:M:11:DT:C6	2.51	0.46
3:D:56:LYS:HD3	3:D:58:TYR:CZ	2.51	0.46
3:E:116:SER:HB3	3:E:241:ILE:HD13	1.98	0.46
3:E:140:HIS:NE2	3:E:266:VAL:HA	2.30	0.46
3:E:497:GLU:O	3:E:501:LEU:HD23	2.15	0.46
3:E:626:LEU:HD23	3:E:729:THR:HG22	1.98	0.46
3:E:643:THR:C	3:E:645:LEU:H	2.24	0.46
3:F:101:LYS:HA	3:F:152:GLY:O	2.16	0.46
3:F:208:SER:OG	3:F:209:LEU:N	2.48	0.46
3:F:457:ILE:H	3:F:457:ILE:HD12	1.80	0.46
3:L:86:GLU:OE1	3:L:210:LEU:HD12	2.15	0.46
3:K:98:TYR:HD2	3:K:100:LEU:HD21	1.81	0.46
3:K:783:GLU:HA	3:K:786:MET:HE1	1.98	0.46
3:I:305:LYS:O	3:I:309:LEU:HG	2.16	0.46
3:I:318:TYR:HE1	3:I:361:LEU:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:LEU:HD11	3:H:68:LEU:HD21	1.96	0.46
3:H:626:LEU:HD22	3:H:711:PRO:HB2	1.96	0.46
3:H:938:PRO:HG3	3:H:942:TRP:HB3	1.97	0.46
2:N:3:DA:H2"	2:N:4:DA:C8	2.51	0.46
3:A:457:ILE:H	3:A:457:ILE:HD12	1.80	0.46
3:A:670:ARG:HH21	3:A:703:SER:HB2	1.81	0.46
3:A:813:ILE:O	3:A:816:VAL:HG12	2.16	0.46
3:B:309:LEU:HD13	3:B:390:TYR:HB2	1.98	0.46
3:C:131:VAL:HB	3:C:231:PHE:CZ	2.51	0.46
3:C:867:ASN:HA	3:C:871:ASN:O	2.15	0.46
3:D:335:TYR:HA	3:D:338:LEU:HD13	1.97	0.46
3:D:717:ARG:HB2	3:D:723:GLN:CB	2.46	0.46
3:E:169:THR:O	3:E:173:ILE:HG12	2.15	0.46
3:E:499:ASN:OD1	3:E:500:ILE:N	2.48	0.46
3:E:851:THR:HA	3:E:906:CYS:H	1.81	0.46
3:G:309:LEU:HB3	3:G:389:GLN:HE22	1.80	0.46
3:K:30:LEU:HD21	3:K:68:LEU:HD22	1.98	0.46
3:K:789:ASP:OD1	3:K:790:CYS:N	2.49	0.46
3:J:894:GLN:HB2	3:J:904:LYS:NZ	2.31	0.46
3:A:888:VAL:O	3:A:888:VAL:HG13	2.16	0.46
3:B:159:LEU:HD12	3:B:256:LEU:HD23	1.97	0.46
3:B:717:ARG:HH21	3:C:719:LEU:CD1	2.26	0.46
3:C:35:LEU:HD21	3:C:68:LEU:HD21	1.98	0.46
3:C:121:ARG:CZ	3:C:181:ALA:H	2.28	0.46
3:C:122:ILE:HA	3:C:125:HIS:CD2	2.51	0.46
3:C:467:ASP:OD1	3:C:468:GLU:N	2.48	0.46
3:D:88:GLN:HE22	3:D:204:ALA:HA	1.79	0.46
3:D:403:ALA:HA	3:D:406:VAL:HG12	1.97	0.46
3:D:496:HIS:HB3	3:D:500:ILE:HG21	1.98	0.46
3:E:852:VAL:HG23	3:E:902:ILE:HB	1.97	0.46
3:G:519:PHE:HB3	3:H:415:HIS:O	2.15	0.46
3:G:700:LEU:O	3:G:704:ARG:NH2	2.46	0.46
3:G:804:LYS:HD2	3:G:807:LYS:HE3	1.98	0.46
3:L:332:SER:OG	3:L:333:ALA:N	2.49	0.46
3:B:457:ILE:H	3:B:457:ILE:HD12	1.81	0.46
3:C:145:LEU:HB3	3:C:222:GLN:CG	2.42	0.46
3:C:236:PRO:HD2	3:C:238:TYR:CZ	2.51	0.46
3:C:356:GLU:O	3:C:359:GLU:HG2	2.16	0.46
3:C:631:MET:HB3	3:C:753:LEU:HD23	1.97	0.46
3:D:347:PRO:HA	3:D:350:TRP:HE3	1.81	0.46
3:D:867:ASN:HA	3:D:871:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:146:LYS:HE2	3:E:155:GLY:N	2.30	0.46
3:F:631:MET:O	3:F:754:ARG:N	2.48	0.46
3:G:120:HIS:HE1	3:G:241:ILE:HD13	1.81	0.46
3:G:782:HIS:NE2	3:H:628:GLU:HA	2.31	0.46
3:G:883:GLU:HA	3:G:886:ASN:HB2	1.97	0.46
3:K:73:GLU:O	3:K:76:ARG:HG2	2.15	0.46
3:K:364:ASP:HA	3:K:367:HIS:CE1	2.51	0.46
3:J:452:MET:HE1	3:J:457:ILE:HG13	1.98	0.46
3:I:350:TRP:NE1	3:I:355:LYS:HA	2.30	0.46
3:I:388:GLN:HA	3:I:391:LYS:HD3	1.96	0.46
3:H:143:PHE:HB3	3:H:156:PHE:HE1	1.80	0.46
3:H:598:LEU:HD13	3:H:943:TRP:CE2	2.50	0.46
3:A:63:THR:O	3:A:66:LEU:HG	2.15	0.46
3:A:309:LEU:HD22	3:A:389:GLN:HE22	1.81	0.46
3:A:391:LYS:O	3:A:394:VAL:N	2.49	0.46
3:A:457:ILE:O	3:A:459:LYS:NZ	2.46	0.46
3:A:682:ARG:HE	3:A:686:ARG:HH12	1.64	0.46
3:B:74:GLN:HA	3:B:77:LYS:HG2	1.97	0.46
3:B:851:THR:OG1	3:B:852:VAL:N	2.39	0.46
3:D:188:HIS:CE1	3:D:195:PRO:HB3	2.51	0.46
3:D:332:SER:HB3	3:D:335:TYR:CE1	2.51	0.46
3:D:376:ARG:HG2	3:D:428:ASN:OD1	2.16	0.46
3:D:715:THR:HG22	3:D:723:GLN:O	2.15	0.46
3:L:328:LEU:HD11	3:L:339:ALA:HB2	1.96	0.46
3:K:838:PHE:HB2	3:K:865:TRP:CH2	2.50	0.46
3:J:746:ASP:OD1	3:J:749:THR:OG1	2.32	0.46
3:J:813:ILE:O	3:J:816:VAL:HG12	2.16	0.46
3:I:170:LYS:O	3:I:174:ILE:HG12	2.16	0.46
3:I:350:TRP:CD1	3:I:355:LYS:HA	2.51	0.46
3:I:783:GLU:C	3:I:785:ILE:N	2.73	0.46
3:H:305:LYS:O	3:H:309:LEU:HG	2.15	0.46
1:M:4:DT:H2"	1:M:5:DT:C6	2.51	0.45
3:A:85:LEU:HD23	3:A:209:LEU:HB3	1.97	0.45
3:A:497:GLU:O	3:A:501:LEU:HD23	2.17	0.45
3:B:332:SER:OG	3:B:333:ALA:N	2.48	0.45
3:C:139:ILE:N	3:C:230:VAL:HA	2.31	0.45
3:C:201:PRO:C	3:C:203:SER:H	2.24	0.45
3:E:303:LEU:HA	3:E:306:ILE:HG12	1.98	0.45
3:E:699:VAL:HG12	3:E:741:ILE:HB	1.99	0.45
3:E:888:VAL:HG13	3:E:888:VAL:O	2.16	0.45
3:G:53:ILE:HG13	3:G:83:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:LEU:HD23	3:G:209:LEU:HB3	1.97	0.45
3:L:298:PRO:O	3:L:301:ARG:HG2	2.17	0.45
3:L:566:LYS:HZ3	3:L:568:ILE:HG12	1.80	0.45
3:L:867:ASN:HA	3:L:871:ASN:O	2.16	0.45
3:K:140:HIS:CE1	3:K:266:VAL:HA	2.51	0.45
3:J:140:HIS:CE1	3:J:265:LEU:HG	2.51	0.45
3:I:97:ASP:HA	3:I:157:HIS:ND1	2.31	0.45
3:I:946:SER:HB3	3:I:947:PRO:HD2	1.98	0.45
3:A:403:ALA:HA	3:A:406:VAL:HG12	1.98	0.45
3:A:651:MET:HE2	3:A:651:MET:HB2	1.82	0.45
3:D:675:LYS:HG3	3:D:717:ARG:HH21	1.81	0.45
3:D:696:LYS:NZ	3:D:698:GLU:OE2	2.34	0.45
3:E:804:LYS:HD2	3:E:807:LYS:HE3	1.98	0.45
3:G:305:LYS:O	3:G:309:LEU:HG	2.16	0.45
3:G:563:ILE:HG12	3:G:803:GLU:HG2	1.97	0.45
3:G:616:PHE:HB3	3:G:805:LEU:HD12	1.99	0.45
3:G:700:LEU:C	3:G:704:ARG:HH22	2.23	0.45
3:L:773:GLU:C	3:L:774:LYS:HD3	2.41	0.45
3:K:867:ASN:CG	3:K:872:VAL:HA	2.41	0.45
3:J:115:LEU:HB3	3:J:143:PHE:CE2	2.51	0.45
3:J:639:CYS:HA	4:J:1001:ANP:N3B	2.31	0.45
3:J:700:LEU:HD21	3:J:705:LEU:HB3	1.98	0.45
3:I:307:LEU:HD23	3:I:341:TRP:HZ3	1.80	0.45
3:H:298:PRO:HA	3:H:301:ARG:CZ	2.46	0.45
3:A:171:LYS:NZ	3:A:205:SER:HB3	2.32	0.45
3:A:381:TRP:HA	3:A:384:LYS:NZ	2.32	0.45
3:B:101:LYS:HG2	3:B:194:ASN:HD22	1.82	0.45
3:B:336:ARG:HH12	3:B:359:GLU:HA	1.80	0.45
3:B:736:SER:OG	3:B:737:ASN:N	2.48	0.45
3:B:838:PHE:HD1	3:B:865:TRP:CG	2.34	0.45
3:C:433:ASP:OD1	3:C:434:VAL:N	2.49	0.45
3:D:103:ASN:HB3	3:D:193:THR:HG21	1.98	0.45
3:D:332:SER:HB3	3:D:335:TYR:HE1	1.81	0.45
3:D:497:GLU:O	3:D:501:LEU:HD23	2.16	0.45
3:E:777:ASP:O	4:E:1001:ANP:O2'	2.33	0.45
3:F:876:ILE:HB	3:F:879:GLU:HG3	1.98	0.45
3:G:328:LEU:HD11	3:G:339:ALA:HB2	1.97	0.45
3:G:391:LYS:HA	3:G:394:VAL:HG22	1.99	0.45
3:L:224:LYS:HG3	3:L:225:THR:HG23	1.98	0.45
3:K:294:MET:O	3:K:301:ARG:NH2	2.49	0.45
3:J:30:LEU:HD21	3:J:68:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:153:LYS:HG3	3:I:154:TYR:CD1	2.52	0.45
3:I:707:GLU:OE1	3:I:707:GLU:N	2.42	0.45
3:H:433:ASP:OD1	3:H:434:VAL:N	2.49	0.45
3:H:894:GLN:HB3	3:H:902:ILE:HG13	1.98	0.45
3:A:105:ASN:HA	3:A:153:LYS:HD3	1.98	0.45
3:A:709:VAL:HG11	3:A:752:ARG:HD3	1.98	0.45
3:B:52:ARG:HD3	3:B:85:LEU:HD11	1.98	0.45
3:B:305:LYS:O	3:B:309:LEU:HG	2.16	0.45
3:B:336:ARG:HH22	3:B:359:GLU:HB3	1.81	0.45
3:C:52:ARG:NH1	3:C:216:LEU:HD21	2.32	0.45
3:C:844:VAL:HG23	3:C:907:ARG:HE	1.81	0.45
3:D:442:TRP:HZ2	3:D:532:GLU:HG2	1.81	0.45
3:D:706:LYS:HA	3:D:706:LYS:HD2	1.43	0.45
3:L:437:ASN:HB3	3:L:439:LYS:NZ	2.32	0.45
3:K:328:LEU:HD11	3:K:339:ALA:HB2	1.98	0.45
3:J:416:TYR:HA	3:J:419:ALA:HB3	1.97	0.45
3:H:97:ASP:N	3:H:97:ASP:OD1	2.50	0.45
3:H:294:MET:O	3:H:301:ARG:NH2	2.49	0.45
3:H:767:ASP:OD1	3:H:767:ASP:N	2.49	0.45
3:A:153:LYS:HG3	3:A:154:TYR:H	1.81	0.45
3:C:47:THR:O	3:C:87:ARG:HG3	2.16	0.45
3:C:297:ASP:HB2	3:C:299:GLU:CD	2.42	0.45
3:C:696:LYS:HD2	3:C:697:SER:N	2.31	0.45
3:D:74:GLN:HA	3:D:77:LYS:HG3	1.97	0.45
3:D:98:TYR:HE1	3:D:199:LEU:HD12	1.81	0.45
3:D:821:ILE:O	3:D:822:GLU:HG3	2.17	0.45
3:D:942:TRP:CD1	3:D:942:TRP:H	2.34	0.45
3:E:23:GLU:HG3	3:E:75:CYS:HA	1.99	0.45
3:E:164:LYS:NZ	3:E:269:VAL:O	2.49	0.45
3:F:171:LYS:HD3	3:F:171:LYS:HA	1.72	0.45
3:G:94:LEU:HD13	3:G:170:LYS:HD2	1.99	0.45
3:G:229:LEU:HG	3:G:240:PRO:HD2	1.97	0.45
3:G:670:ARG:HH22	3:G:704:ARG:HG2	1.81	0.45
3:G:717:ARG:HH22	1:O:4:DT:P	2.39	0.45
3:L:894:GLN:HB2	3:L:904:LYS:NZ	2.31	0.45
3:J:315:TYR:CE2	3:J:345:LYS:HB2	2.51	0.45
3:I:97:ASP:HA	3:I:157:HIS:HD1	1.82	0.45
3:I:355:LYS:C	3:I:355:LYS:HZ3	2.25	0.45
3:I:861:ALA:O	3:I:864:GLU:HG3	2.16	0.45
3:H:648:LEU:O	3:H:651:MET:HG2	2.17	0.45
3:H:786:MET:SD	3:H:786:MET:N	2.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:93:GLY:HA3	3:A:161:PRO:HA	1.98	0.45
3:A:383:HIS:CD2	3:A:384:LYS:HG3	2.52	0.45
3:A:752:ARG:C	3:A:753:LEU:HD12	2.41	0.45
3:C:390:TYR:O	3:C:393:ILE:HG22	2.16	0.45
3:D:100:LEU:O	3:D:153:LYS:HB3	2.16	0.45
3:D:255:GLU:OE1	3:D:265:LEU:N	2.49	0.45
3:D:635:LEU:HD23	3:D:740:PHE:CE2	2.51	0.45
3:D:867:ASN:HA	3:D:871:ASN:C	2.41	0.45
3:F:895:TRP:HA	3:F:901:ARG:HA	1.99	0.45
3:L:248:GLU:CD	3:L:248:GLU:H	2.25	0.45
3:L:777:ASP:OD2	3:L:780:PHE:N	2.49	0.45
3:K:780:PHE:HB2	4:K:1001:ANP:O2'	2.17	0.45
3:J:306:ILE:HA	3:J:309:LEU:HG	1.99	0.45
3:I:719:LEU:O	3:I:721:GLN:NE2	2.49	0.45
3:H:31:LEU:HD23	3:H:35:LEU:HD12	1.98	0.45
3:A:390:TYR:O	3:A:393:ILE:HB	2.16	0.45
3:B:708:MET:HA	3:B:728:MET:SD	2.57	0.45
3:B:898:ASN:O	3:B:900:THR:HG23	2.17	0.45
3:C:123:PHE:O	3:C:127:LYS:HG2	2.17	0.45
3:C:604:ILE:HD12	3:C:641:GLY:HA3	1.99	0.45
3:D:557:VAL:HG13	3:D:568:ILE:HB	1.98	0.45
3:E:73:GLU:O	3:E:77:LYS:HG2	2.17	0.45
3:F:183:VAL:HA	3:F:186:ILE:HD12	1.98	0.45
3:G:744:THR:HG23	3:G:750:TRP:CD1	2.52	0.45
3:G:946:SER:HB3	3:G:947:PRO:HD2	1.99	0.45
3:L:72:LEU:HD13	3:L:82:MET:HE1	1.98	0.45
3:L:180:ASP:O	3:L:184:GLN:NE2	2.36	0.45
3:K:293:LEU:HD13	3:K:338:LEU:HD12	1.97	0.45
3:J:186:ILE:HA	3:J:189:GLU:CD	2.42	0.45
3:I:429:LYS:NZ	3:I:445:PHE:O	2.50	0.45
3:I:652:VAL:HG12	3:I:791:GLN:HB3	1.99	0.45
3:A:235:ASP:HB2	3:A:238:TYR:CE2	2.51	0.45
3:A:295:LEU:O	3:A:301:ARG:NH2	2.50	0.45
3:B:416:TYR:HA	3:B:419:ALA:HB3	1.99	0.45
3:B:682:ARG:O	3:B:683:LEU:HG	2.17	0.45
3:C:96:LEU:HB3	3:C:156:PHE:CD2	2.52	0.45
3:E:140:HIS:CE1	3:E:265:LEU:HG	2.52	0.45
3:E:215:LYS:HB2	3:E:218:HIS:HB2	1.99	0.45
3:F:390:TYR:O	3:F:393:ILE:HB	2.16	0.45
3:G:371:LYS:HE3	3:G:574:HIS:CD2	2.51	0.45
3:L:364:ASP:C	3:L:368:HIS:HD1	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:750:TRP:HB3	3:L:829:ARG:NH1	2.32	0.45
3:K:343:SER:HB3	3:K:350:TRP:CD1	2.52	0.45
3:K:383:HIS:HA	3:K:390:TYR:CE1	2.51	0.45
3:K:894:GLN:HB3	3:K:902:ILE:HG13	1.99	0.45
3:J:63:THR:O	3:J:66:LEU:HG	2.15	0.45
3:J:626:LEU:HD21	3:J:727:GLN:HE21	1.82	0.45
3:H:670:ARG:HH12	3:H:704:ARG:H	1.65	0.45
3:H:677:ASN:CG	3:H:680:PHE:HB2	2.42	0.45
3:A:132:LEU:HB3	3:A:231:PHE:CE2	2.51	0.45
3:A:215:LYS:HB2	3:A:218:HIS:HB2	1.99	0.45
3:A:710:ASN:OD1	3:A:711:PRO:HD2	2.17	0.45
3:B:119:CYS:HA	3:B:122:ILE:HG12	1.98	0.45
3:C:215:LYS:HE3	3:C:221:TYR:HE1	1.82	0.45
3:C:894:GLN:HB2	3:C:904:LYS:HG3	1.99	0.45
3:D:16:ALA:HB1	3:D:20:TYR:HE2	1.81	0.45
3:E:867:ASN:CB	3:E:872:VAL:HA	2.47	0.45
3:G:292:ILE:HG13	3:G:296:HIS:CE1	2.52	0.45
3:L:116:SER:O	3:L:120:HIS:ND1	2.50	0.45
3:L:374:THR:O	3:L:377:SER:OG	2.33	0.45
3:L:746:ASP:OD1	3:L:746:ASP:N	2.50	0.45
3:K:115:LEU:HD22	3:K:143:PHE:CG	2.52	0.45
3:K:364:ASP:O	3:K:368:HIS:ND1	2.47	0.45
3:K:380:TYR:CE2	3:K:384:LYS:HD2	2.52	0.45
3:I:336:ARG:HB2	3:I:362:TRP:CE2	2.52	0.45
3:I:710:ASN:OD1	3:I:752:ARG:NH1	2.50	0.45
3:B:16:ALA:HB1	3:B:20:TYR:CE2	2.52	0.45
3:C:469:LEU:HD12	3:C:469:LEU:HA	1.82	0.45
3:C:530:GLN:NE2	3:D:521:ASP:OD1	2.46	0.45
3:E:61:PRO:HD2	3:E:64:GLU:CG	2.46	0.45
3:F:239:ILE:O	3:F:239:ILE:HG13	2.17	0.45
3:G:97:ASP:HA	3:G:157:HIS:ND1	2.31	0.45
3:G:315:TYR:CE2	3:G:345:LYS:HB2	2.52	0.45
3:G:695:ASN:O	3:G:696:LYS:HG2	2.17	0.45
3:L:73:GLU:O	3:L:77:LYS:HG3	2.17	0.45
3:K:748:GLY:O	3:K:752:ARG:NH2	2.46	0.45
3:J:224:LYS:HA	3:J:224:LYS:HD2	1.77	0.45
4:J:1001:ANP:O2B	4:J:1001:ANP:O3G	2.35	0.45
3:I:661:LEU:HD11	3:I:689:GLY:HA3	1.99	0.45
3:I:894:GLN:HB3	3:I:902:ILE:HG13	1.99	0.45
3:H:598:LEU:HD13	3:H:943:TRP:CD2	2.52	0.45
3:H:794:PHE:O	3:H:798:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:838:PHE:HB2	3:H:865:TRP:CE3	2.52	0.45
3:A:238:TYR:O	3:A:240:PRO:HD3	2.17	0.44
3:E:651:MET:HE2	3:E:651:MET:HB2	1.85	0.44
3:E:889:LEU:O	3:E:893:LEU:N	2.35	0.44
3:G:13:GLN:C	3:G:17:GLN:HE21	2.25	0.44
3:G:228:GLU:N	3:G:242:HIS:O	2.50	0.44
3:G:457:ILE:H	3:G:457:ILE:HD12	1.82	0.44
3:G:846:SER:HB3	3:G:905:GLY:CA	2.36	0.44
3:L:69:TYR:O	3:L:73:GLU:HG3	2.17	0.44
3:J:153:LYS:HA	3:J:153:LYS:HD2	1.67	0.44
3:I:121:ARG:HE	3:I:125:HIS:CD2	2.35	0.44
3:I:176:SER:HA	3:I:179:HIS:NE2	2.32	0.44
3:H:617:TYR:O	3:H:620:THR:OG1	2.30	0.44
1:M:25:DT:O4	2:N:1:DA:N6	2.50	0.44
3:A:163:LEU:HA	3:A:269:VAL:HB	1.98	0.44
3:A:713:ASP:O	3:B:660:LYS:NZ	2.45	0.44
3:A:821:ILE:C	3:A:823:SER:H	2.25	0.44
3:B:56:LYS:HD3	3:B:58:TYR:CE2	2.52	0.44
3:C:66:LEU:HA	3:C:69:TYR:CD2	2.52	0.44
3:C:117:ARG:HG3	3:I:238:TYR:HE1	1.82	0.44
3:C:192:VAL:HG12	3:C:194:ASN:H	1.83	0.44
3:C:866:TYR:HD1	3:C:870:ILE:HD13	1.82	0.44
3:E:309:LEU:HD22	3:E:389:GLN:HE22	1.82	0.44
3:E:391:LYS:O	3:E:394:VAL:HG22	2.17	0.44
3:F:73:GLU:O	3:F:77:LYS:HG2	2.18	0.44
3:F:681:MET:CG	3:F:718:GLU:HB3	2.44	0.44
3:G:834:THR:OG1	3:G:862:TYR:OH	2.25	0.44
3:L:139:ILE:N	3:L:267:ARG:HH12	2.15	0.44
3:K:13:GLN:OE1	3:K:491:HIS:NE2	2.50	0.44
3:J:674:GLU:OE1	3:I:678:SER:N	2.47	0.44
3:J:683:LEU:HD13	3:J:728:MET:SD	2.57	0.44
3:I:171:LYS:HD3	3:I:171:LYS:HA	1.73	0.44
3:I:364:ASP:HA	3:I:367:HIS:NE2	2.32	0.44
3:I:425:MET:HE3	3:I:425:MET:HB2	1.78	0.44
3:A:947:PRO:O	3:A:950:SER:OG	2.33	0.44
3:B:203:SER:OG	3:B:204:ALA:N	2.49	0.44
3:C:146:LYS:HB3	3:C:221:TYR:CE2	2.52	0.44
3:C:292:ILE:O	3:C:296:HIS:ND1	2.27	0.44
3:D:303:LEU:HA	3:D:306:ILE:HG12	1.98	0.44
3:E:12:ILE:H	3:E:12:ILE:HD12	1.82	0.44
3:E:444:GLU:OE2	3:E:461:ARG:NH2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:639:CYS:N	4:F:1001:ANP:O2B	2.50	0.44
3:G:254:SER:O	3:G:260:ASN:ND2	2.44	0.44
3:G:473:ILE:O	3:G:477:PHE:HB3	2.17	0.44
3:K:483:ARG:O	3:K:486:GLU:HG3	2.16	0.44
3:K:601:LEU:HD23	3:K:942:TRP:CH2	2.52	0.44
3:I:30:LEU:HD12	3:I:34:GLU:HB2	2.00	0.44
3:I:336:ARG:HB2	3:I:362:TRP:CZ2	2.52	0.44
3:I:381:TRP:HD1	3:I:384:LYS:HE2	1.82	0.44
3:I:671:GLU:HB2	3:I:675:LYS:HE3	2.00	0.44
3:I:701:ASN:HB2	3:I:704:ARG:NH1	2.24	0.44
3:H:40:THR:O	3:H:57:THR:OG1	2.36	0.44
3:H:380:TYR:CE2	3:H:571:PHE:HB3	2.52	0.44
3:H:642:LYS:O	4:H:1001:ANP:O2B	2.35	0.44
3:A:52:ARG:HH21	3:A:83:TYR:HD1	1.65	0.44
3:C:601:LEU:HD23	3:C:611:ARG:HD2	1.99	0.44
3:C:761:LYS:NZ	3:C:763:CYS:HB3	2.32	0.44
3:F:412:MET:HA	3:F:412:MET:HE3	2.00	0.44
3:G:102:LEU:HB2	3:G:153:LYS:HB2	2.00	0.44
3:G:866:TYR:OH	3:G:873:LYS:HE3	2.18	0.44
3:J:671:GLU:HB2	3:J:675:LYS:HE3	1.99	0.44
3:J:872:VAL:O	3:J:872:VAL:HG13	2.16	0.44
3:J:883:GLU:HA	3:J:886:ASN:HB2	2.00	0.44
3:J:888:VAL:HG13	3:J:888:VAL:O	2.17	0.44
3:I:294:MET:SD	3:I:295:LEU:N	2.91	0.44
3:I:471:ILE:O	3:I:475:GLU:HG2	2.17	0.44
3:A:353:GLY:N	3:A:356:GLU:OE2	2.46	0.44
3:C:30:LEU:HD11	3:C:67:ARG:NH1	2.32	0.44
3:C:414:GLU:HG3	3:C:415:HIS:H	1.83	0.44
3:C:643:THR:OG1	4:C:1001:ANP:O1B	2.34	0.44
3:C:878:LEU:O	3:C:881:SER:OG	2.24	0.44
3:C:945:TRP:O	3:C:950:SER:OG	2.35	0.44
3:D:645:LEU:HA	3:D:648:LEU:HB3	1.99	0.44
3:F:696:LYS:HD3	3:F:697:SER:N	2.32	0.44
3:G:761:LYS:NZ	3:G:762:PHE:O	2.50	0.44
3:L:51:ASN:HB3	3:L:56:LYS:HG2	1.99	0.44
3:L:292:ILE:HG13	3:L:296:HIS:CE1	2.52	0.44
3:L:481:MET:HE3	3:L:481:MET:HB3	1.85	0.44
3:L:851:THR:OG1	3:L:852:VAL:N	2.49	0.44
3:J:140:HIS:NE2	3:J:266:VAL:HA	2.32	0.44
3:J:530:GLN:NE2	3:I:521:ASP:OD1	2.41	0.44
3:I:101:LYS:HA	3:I:152:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:416:TYR:HA	3:I:419:ALA:HB3	1.99	0.44
3:I:563:ILE:HG12	3:I:803:GLU:HG2	1.98	0.44
3:H:294:MET:SD	3:H:304:HIS:HB2	2.57	0.44
3:H:837:ARG:O	3:H:841:GLU:HB2	2.17	0.44
3:A:566:LYS:NZ	3:A:567:LEU:O	2.47	0.44
3:B:260:ASN:HD21	3:B:262:GLN:HG2	1.83	0.44
3:B:303:LEU:O	3:B:307:LEU:HG	2.18	0.44
3:B:813:ILE:O	3:B:816:VAL:HG12	2.18	0.44
3:C:112:PRO:O	3:C:115:LEU:HG	2.18	0.44
3:D:250:TYR:CE2	3:D:265:LEU:HD13	2.52	0.44
3:D:676:PRO:C	3:D:717:ARG:HH12	2.25	0.44
3:D:703:SER:O	3:D:705:LEU:N	2.50	0.44
3:E:16:ALA:HB1	3:E:20:TYR:HE2	1.82	0.44
3:F:23:GLU:H	3:F:23:GLU:CD	2.25	0.44
3:G:132:LEU:HB3	3:G:231:PHE:CE2	2.53	0.44
3:G:141:PHE:CE1	3:G:229:LEU:HB3	2.53	0.44
3:G:846:SER:CB	3:G:905:GLY:HA2	2.36	0.44
3:L:255:GLU:OE1	3:L:265:LEU:N	2.50	0.44
3:L:457:ILE:HG22	3:L:458:TRP:CD1	2.53	0.44
3:K:184:GLN:OE1	3:K:195:PRO:HB2	2.18	0.44
3:K:818:CYS:SG	3:K:820:THR:OG1	2.75	0.44
3:J:321:TRP:HZ3	3:J:357:LYS:HD3	1.82	0.44
3:J:326:PHE:CZ	3:J:361:LEU:HD22	2.53	0.44
3:J:375:LYS:HA	3:J:378:ILE:HD13	2.00	0.44
3:J:640:ASN:ND2	3:J:760:VAL:O	2.51	0.44
3:H:47:THR:HG21	3:H:50:ILE:HD11	2.00	0.44
3:H:414:GLU:H	3:H:417:MET:CE	2.31	0.44
3:A:311:PRO:HD3	3:A:385:HIS:CB	2.47	0.44
3:B:40:THR:HG21	3:B:47:THR:HB	2.00	0.44
3:B:785:ILE:O	3:B:791:GLN:NE2	2.51	0.44
3:C:182:THR:O	3:C:186:ILE:HG12	2.18	0.44
3:C:312:PRO:O	3:C:316:VAL:HG23	2.17	0.44
3:E:379:MET:HE1	3:E:390:TYR:CD2	2.53	0.44
3:L:108:PRO:HD2	3:L:154:TYR:HE1	1.82	0.44
3:L:290:LEU:HA	3:L:293:LEU:HD12	1.98	0.44
3:K:336:ARG:HH22	3:K:359:GLU:HB3	1.83	0.44
3:J:790:CYS:SG	3:J:791:GLN:N	2.91	0.44
3:I:631:MET:HE3	3:I:753:LEU:HD22	1.99	0.44
3:B:123:PHE:CE1	3:B:127:LYS:HE3	2.52	0.44
3:C:497:GLU:O	3:C:501:LEU:HD23	2.18	0.44
3:C:601:LEU:HD11	3:C:615:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:159:LEU:HD21	3:D:256:LEU:O	2.18	0.44
3:D:381:TRP:HA	3:D:384:LYS:HD3	1.99	0.44
3:F:583:CYS:O	3:F:792:ASN:ND2	2.51	0.44
3:L:700:LEU:HG	3:L:702:THR:H	1.82	0.44
3:K:98:TYR:HE1	3:K:199:LEU:HD12	1.83	0.44
3:K:631:MET:HE3	3:K:709:VAL:HA	2.00	0.44
3:J:755:HIS:HD2	3:J:828:TYR:HB2	1.82	0.44
3:H:103:ASN:OD1	3:H:104:THR:N	2.51	0.44
3:H:118:LEU:HD23	3:H:183:VAL:HG12	2.00	0.44
3:H:347:PRO:HA	3:H:350:TRP:HB3	2.00	0.44
3:H:383:HIS:HA	3:H:390:TYR:CE1	2.53	0.44
3:H:587:PHE:HA	3:H:796:SER:HB3	2.00	0.44
3:H:861:ALA:O	3:H:864:GLU:HG3	2.18	0.44
3:B:162:GLY:O	3:B:269:VAL:N	2.45	0.44
3:B:457:ILE:O	3:B:459:LYS:NZ	2.48	0.44
3:B:467:ASP:O	3:B:471:ILE:HD12	2.18	0.44
3:C:627:LYS:NZ	3:C:731:THR:HG23	2.32	0.44
3:C:946:SER:HB2	3:C:950:SER:HA	1.99	0.44
3:D:76:ARG:HH22	3:D:252:LEU:HD12	1.82	0.44
3:D:240:PRO:HA	3:J:240:PRO:HA	2.00	0.44
3:D:716:ALA:C	3:D:717:ARG:HG2	2.42	0.44
3:F:123:PHE:HZ	3:F:231:PHE:HB2	1.81	0.44
3:F:146:LYS:HD2	3:F:154:TYR:HA	2.00	0.44
3:G:298:PRO:O	3:G:301:ARG:HG2	2.17	0.44
3:G:312:PRO:O	3:G:316:VAL:HG23	2.18	0.44
3:G:475:GLU:O	3:G:478:SER:OG	2.20	0.44
3:L:97:ASP:OD1	3:L:97:ASP:N	2.48	0.44
3:L:661:LEU:HD12	3:L:732:MET:HE1	1.99	0.44
3:K:946:SER:HB3	3:K:947:PRO:HD2	1.99	0.44
3:J:293:LEU:HD13	3:J:338:LEU:HD12	1.99	0.44
3:J:648:LEU:HG	3:J:794:PHE:CD2	2.53	0.44
3:J:713:ASP:OD1	3:J:713:ASP:N	2.42	0.44
3:I:351:ASN:O	3:I:352:THR:C	2.61	0.44
3:I:676:PRO:HB3	3:I:717:ARG:NE	2.33	0.44
3:H:743:ASP:OD1	3:H:743:ASP:N	2.51	0.44
3:A:58:TYR:HB3	3:A:60:LEU:HG	2.00	0.43
3:A:891:LYS:HE2	3:A:892:TYR:CZ	2.53	0.43
3:B:148:GLU:HG2	3:B:154:TYR:HB3	2.00	0.43
3:B:600:ALA:O	3:B:604:ILE:HG12	2.18	0.43
3:C:660:LYS:HG2	3:C:661:LEU:N	2.32	0.43
3:C:690:TYR:HA	3:C:733:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:715:THR:HA	3:C:725:SER:HA	2.00	0.43
3:D:749:THR:C	3:D:751:ARG:H	2.26	0.43
3:G:86:GLU:O	3:G:208:SER:N	2.44	0.43
3:G:499:ASN:OD1	3:G:500:ILE:N	2.51	0.43
3:G:613:TRP:CZ3	3:G:632:LEU:HD11	2.53	0.43
3:L:364:ASP:HA	3:L:367:HIS:CE1	2.53	0.43
3:L:700:LEU:HD22	3:L:742:ILE:HD13	1.99	0.43
3:J:744:THR:HG23	3:J:750:TRP:CD1	2.53	0.43
3:I:289:SER:O	3:I:293:LEU:HG	2.17	0.43
3:I:410:ASN:N	3:I:410:ASN:OD1	2.51	0.43
3:I:676:PRO:HB2	3:I:718:GLU:O	2.18	0.43
3:I:706:LYS:HD3	3:I:749:THR:HG22	1.98	0.43
3:H:303:LEU:HA	3:H:306:ILE:HG12	2.00	0.43
3:H:315:TYR:CE2	3:H:345:LYS:HB2	2.53	0.43
3:C:242:HIS:CE1	3:I:243:GLN:H	2.36	0.43
3:C:444:GLU:OE2	3:C:461:ARG:NH2	2.46	0.43
3:E:364:ASP:HB3	3:E:368:HIS:HE1	1.80	0.43
3:E:364:ASP:HA	3:E:367:HIS:CE1	2.53	0.43
3:F:139:ILE:N	3:F:229:LEU:O	2.51	0.43
3:F:391:LYS:O	3:F:394:VAL:N	2.50	0.43
3:G:27:LEU:HD12	3:G:30:LEU:HD23	2.00	0.43
3:G:343:SER:HB3	3:G:350:TRP:CD1	2.53	0.43
3:K:391:LYS:O	3:K:394:VAL:HG22	2.18	0.43
3:J:121:ARG:HG2	3:J:183:VAL:HG13	1.99	0.43
3:I:755:HIS:HD2	3:I:828:TYR:HB2	1.83	0.43
3:I:757:ARG:NH1	3:I:758:SER:O	2.51	0.43
3:A:766:PRO:HG3	3:A:775:LYS:HD2	2.00	0.43
3:B:146:LYS:O	3:B:148:GLU:HG3	2.17	0.43
3:C:604:ILE:HG22	3:C:605:ILE:HG23	2.01	0.43
3:D:707:GLU:H	3:D:707:GLU:CD	2.26	0.43
3:E:98:TYR:CE1	3:E:199:LEU:HD12	2.53	0.43
3:G:312:PRO:HA	3:G:315:TYR:HB3	1.99	0.43
3:G:715:THR:HG23	3:G:723:GLN:HE21	1.83	0.43
3:G:746:ASP:OD1	3:G:749:THR:OG1	2.28	0.43
3:G:751:ARG:NH2	3:L:639:CYS:SG	2.84	0.43
3:G:891:LYS:HE2	3:G:892:TYR:CZ	2.53	0.43
3:L:115:LEU:HD22	3:L:143:PHE:CG	2.53	0.43
3:L:388:GLN:HA	3:L:391:LYS:HD3	1.99	0.43
3:L:416:TYR:HA	3:L:419:ALA:HB3	2.00	0.43
3:J:309:LEU:HD13	3:J:389:GLN:HE22	1.83	0.43
3:I:355:LYS:HZ2	3:I:355:LYS:HG3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:718:GLU:HG2	3:I:719:LEU:N	2.32	0.43
3:H:222:GLN:OE1	3:H:222:GLN:N	2.48	0.43
3:H:565:ALA:N	3:H:803:GLU:OE2	2.46	0.43
3:H:682:ARG:HH21	3:H:686:ARG:HH22	1.65	0.43
3:H:751:ARG:HH21	3:H:752:ARG:NH2	2.16	0.43
3:A:700:LEU:HD13	3:A:742:ILE:HD13	2.01	0.43
3:B:742:ILE:HB	3:B:832:GLN:HG2	2.01	0.43
3:C:321:TRP:HZ3	3:C:357:LYS:HD3	1.83	0.43
3:C:755:HIS:H	3:C:825:THR:HG22	1.83	0.43
3:D:48:ASN:OD1	3:D:49:ILE:N	2.51	0.43
3:D:121:ARG:HE	3:D:180:ASP:CG	2.26	0.43
3:D:607:GLU:HB2	3:D:610:ALA:HB3	1.99	0.43
3:F:364:ASP:HA	3:F:367:HIS:HE1	1.81	0.43
3:L:520:ASN:OD1	3:L:522:SER:N	2.51	0.43
3:K:96:LEU:HA	3:K:203:SER:HB3	2.00	0.43
3:K:209:LEU:HD13	3:K:213:SER:HB2	2.00	0.43
3:K:718:GLU:HG2	3:K:721:GLN:HE21	1.83	0.43
3:J:64:GLU:OE1	3:J:67:ARG:NH2	2.50	0.43
3:J:113:PRO:O	3:J:117:ARG:HG2	2.17	0.43
3:J:475:GLU:O	3:J:478:SER:OG	2.26	0.43
3:H:52:ARG:HD3	3:H:85:LEU:HD11	2.00	0.43
3:H:414:GLU:H	3:H:417:MET:HE3	1.82	0.43
3:H:473:ILE:O	3:H:477:PHE:HB3	2.18	0.43
3:A:15:THR:O	3:A:19:LYS:HG2	2.18	0.43
3:A:245:LYS:HE2	3:G:245:LYS:HE2	2.01	0.43
3:A:376:ARG:HA	3:A:379:MET:HE2	2.00	0.43
3:A:696:LYS:HD2	3:A:697:SER:O	2.18	0.43
3:B:110:LEU:HD21	3:B:115:LEU:HD21	2.01	0.43
3:B:145:LEU:HD22	3:B:224:LYS:HB2	1.99	0.43
3:B:248:GLU:OE1	3:B:248:GLU:N	2.51	0.43
3:D:357:LYS:HB3	3:D:357:LYS:HE2	1.59	0.43
3:D:593:TRP:NE1	3:D:789:ASP:OD2	2.52	0.43
3:E:96:LEU:HD22	3:E:158:VAL:HG12	2.01	0.43
3:E:391:LYS:O	3:E:392:GLU:C	2.61	0.43
3:F:12:ILE:H	3:F:12:ILE:HD12	1.83	0.43
3:F:682:ARG:NE	3:F:686:ARG:HH12	2.16	0.43
3:F:755:HIS:H	3:F:825:THR:HG22	1.83	0.43
3:F:883:GLU:O	3:F:887:SER:N	2.52	0.43
3:G:30:LEU:HD22	3:G:71:HIS:ND1	2.33	0.43
3:G:364:ASP:HA	3:G:367:HIS:CE1	2.53	0.43
3:G:939:LYS:HG3	3:G:940:ASN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:187:LEU:HB3	3:K:192:VAL:HB	2.00	0.43
3:K:318:TYR:N	3:K:319:PRO:HD2	2.34	0.43
3:K:821:ILE:C	3:K:823:SER:H	2.26	0.43
3:J:364:ASP:HA	3:J:367:HIS:NE2	2.33	0.43
3:I:52:ARG:NH2	3:I:215:LYS:HA	2.33	0.43
3:I:63:THR:O	3:I:66:LEU:HG	2.18	0.43
3:H:416:TYR:HA	3:H:419:ALA:HB3	1.98	0.43
3:A:97:ASP:OD1	3:A:97:ASP:N	2.50	0.43
3:B:227:PHE:HA	3:B:242:HIS:O	2.19	0.43
3:B:696:LYS:HG3	3:B:697:SER:N	2.27	0.43
3:C:794:PHE:HA	3:C:797:ILE:HD12	1.99	0.43
3:C:834:THR:HG21	3:C:870:ILE:HG12	1.99	0.43
3:D:433:ASP:OD1	3:D:434:VAL:N	2.47	0.43
3:D:821:ILE:C	3:D:823:SER:H	2.26	0.43
3:E:866:TYR:CE2	3:E:873:LYS:HB2	2.39	0.43
3:F:497:GLU:O	3:F:501:LEU:HD23	2.19	0.43
3:F:604:ILE:HG23	3:F:641:GLY:HA3	2.00	0.43
3:G:355:LYS:NZ	3:G:359:GLU:OE1	2.51	0.43
3:L:681:MET:HB3	3:L:718:GLU:HB2	1.99	0.43
3:L:743:ASP:OD1	3:L:743:ASP:N	2.51	0.43
3:K:13:GLN:O	3:K:17:GLN:NE2	2.51	0.43
3:J:208:SER:OG	3:J:209:LEU:N	2.49	0.43
3:J:728:MET:HE3	3:J:729:THR:H	1.82	0.43
3:I:662:ASN:HB3	3:I:665:LEU:HD23	2.00	0.43
3:I:821:ILE:C	3:I:823:SER:H	2.25	0.43
3:H:251:ASN:CG	3:H:254:SER:HB3	2.43	0.43
3:B:371:LYS:NZ	3:B:373:ILE:HB	2.34	0.43
3:C:51:ASN:O	3:C:55:GLY:N	2.52	0.43
3:C:118:LEU:O	3:C:122:ILE:HG23	2.19	0.43
3:C:159:LEU:HG	3:C:161:PRO:HG3	2.00	0.43
3:D:318:TYR:N	3:D:319:PRO:HD2	2.33	0.43
3:E:30:LEU:HD12	3:E:34:GLU:OE1	2.18	0.43
3:E:353:GLY:H	3:E:356:GLU:CD	2.26	0.43
3:E:746:ASP:N	3:E:746:ASP:OD1	2.52	0.43
3:E:947:PRO:O	3:E:950:SER:OG	2.36	0.43
3:G:156:PHE:CZ	3:G:158:VAL:HB	2.54	0.43
3:L:85:LEU:HD23	3:L:209:LEU:HB3	2.01	0.43
3:L:107:VAL:HG12	3:L:148:GLU:HG2	2.01	0.43
3:L:642:LYS:O	3:L:643:THR:OG1	2.36	0.43
3:K:52:ARG:HH21	3:K:83:TYR:HD1	1.66	0.43
3:K:770:ASN:ND2	3:K:773:GLU:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:23:GLU:CD	3:J:23:GLU:H	2.26	0.43
3:J:320:LEU:O	3:J:324:VAL:HG13	2.18	0.43
3:J:751:ARG:NH2	3:I:639:CYS:SG	2.92	0.43
3:J:866:TYR:HA	3:J:870:ILE:HD13	2.00	0.43
3:I:671:GLU:OE2	3:I:677:ASN:HB2	2.18	0.43
3:H:364:ASP:C	3:H:368:HIS:HD1	2.26	0.43
3:H:609:ASP:OD1	3:H:609:ASP:N	2.51	0.43
3:A:187:LEU:HB3	3:A:192:VAL:HB	2.01	0.43
3:A:469:LEU:HD12	3:A:469:LEU:HA	1.78	0.43
3:A:783:GLU:OE1	3:A:784:TYR:N	2.51	0.43
3:B:102:LEU:HG	3:B:192:VAL:HA	2.00	0.43
3:B:184:GLN:CD	3:B:196:GLU:HG2	2.43	0.43
3:B:483:ARG:O	3:B:486:GLU:HG3	2.17	0.43
3:C:146:LYS:HE3	3:C:146:LYS:HB2	1.41	0.43
3:C:149:VAL:N	3:C:153:LYS:HZ2	2.16	0.43
3:C:318:TYR:N	3:C:319:PRO:HD2	2.33	0.43
3:C:336:ARG:HH22	3:C:359:GLU:HB3	1.84	0.43
3:D:63:THR:O	3:D:66:LEU:HG	2.19	0.43
3:D:681:MET:CG	3:D:717:ARG:HD3	2.49	0.43
3:D:757:ARG:HD3	3:D:758:SER:O	2.18	0.43
3:D:947:PRO:O	3:D:950:SER:OG	2.31	0.43
3:E:146:LYS:HE2	3:E:155:GLY:H	1.82	0.43
3:E:374:THR:O	3:E:377:SER:OG	2.35	0.43
3:E:380:TYR:CZ	3:E:384:LYS:HD2	2.54	0.43
3:E:391:LYS:HG3	3:E:392:GLU:N	2.34	0.43
3:G:97:ASP:OD1	3:G:97:ASP:N	2.50	0.43
3:G:118:LEU:HD23	3:G:183:VAL:HG12	2.00	0.43
3:G:763:CYS:N	3:G:776:GLU:HB3	2.33	0.43
3:G:777:ASP:OD2	3:G:780:PHE:N	2.51	0.43
3:G:857:GLU:HG2	3:G:858:VAL:N	2.32	0.43
3:K:164:LYS:HG3	3:K:164:LYS:O	2.19	0.43
3:J:563:ILE:HG12	3:J:803:GLU:HG2	2.00	0.43
3:H:694:THR:HG21	3:H:736:SER:HB2	2.01	0.43
3:A:821:ILE:HG22	3:A:822:GLU:H	1.84	0.43
3:B:183:VAL:O	3:B:187:LEU:HG	2.19	0.43
3:B:307:LEU:HA	3:B:310:LEU:CD2	2.48	0.43
3:B:751:ARG:NH2	4:C:1001:ANP:HNB1	2.11	0.43
3:C:813:ILE:O	3:C:816:VAL:HG12	2.19	0.43
3:C:869:ASN:HB2	3:C:870:ILE:HD12	2.00	0.43
3:E:457:ILE:HD12	3:E:457:ILE:H	1.83	0.43
3:G:353:GLY:N	3:G:356:GLU:OE2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:594:THR:HG23	3:L:797:ILE:HD11	2.01	0.43
3:K:87:ARG:HA	3:K:207:PRO:HA	2.01	0.43
3:K:289:SER:O	3:K:292:ILE:HG22	2.18	0.43
3:K:757:ARG:HD3	3:K:758:SER:O	2.19	0.43
3:K:795:PHE:HA	3:K:798:LEU:HD12	2.01	0.43
3:J:326:PHE:HZ	3:J:361:LEU:HD22	1.84	0.43
3:J:328:LEU:HD11	3:J:339:ALA:HB2	1.99	0.43
3:J:369:THR:HA	3:J:372:LYS:HZ1	1.84	0.43
3:J:604:ILE:HG22	3:J:605:ILE:HG23	2.00	0.43
3:I:70:GLU:OE2	3:I:74:GLN:NE2	2.52	0.43
3:H:229:LEU:HG	3:H:240:PRO:HD2	2.00	0.43
1:M:6:DT:OP1	3:F:676:PRO:HG3	2.19	0.43
3:A:228:GLU:C	3:A:242:HIS:HB2	2.44	0.43
3:A:254:SER:OG	3:A:260:ASN:ND2	2.52	0.43
3:B:56:LYS:HD3	3:B:58:TYR:CZ	2.54	0.43
3:B:148:GLU:HG2	3:B:154:TYR:CG	2.53	0.43
3:B:353:GLY:N	3:B:356:GLU:OE2	2.45	0.43
3:C:736:SER:OG	3:C:737:ASN:N	2.52	0.43
3:D:444:GLU:OE2	3:D:461:ARG:NH2	2.40	0.43
3:D:502:ASN:HA	3:D:505:LYS:HE2	2.00	0.43
3:E:883:GLU:O	3:E:887:SER:N	2.51	0.43
3:F:444:GLU:OE2	3:F:461:ARG:NH2	2.43	0.43
3:F:708:MET:SD	3:F:708:MET:N	2.92	0.43
3:G:147:PRO:HA	3:G:222:GLN:HE22	1.84	0.43
3:G:378:ILE:H	3:G:378:ILE:HD12	1.84	0.43
3:G:715:THR:HA	3:G:725:SER:HA	2.01	0.43
3:K:209:LEU:HB2	3:K:213:SER:HB2	2.00	0.43
3:K:244:ILE:HG21	3:K:247:LEU:HD13	1.99	0.43
3:K:587:PHE:HA	3:K:796:SER:HB3	2.01	0.43
3:K:719:LEU:HD11	1:O:2:DT:H3'	2.01	0.43
3:K:941:LYS:HD2	3:K:943:TRP:NE1	2.33	0.43
3:J:47:THR:HG21	3:J:50:ILE:HD11	2.01	0.43
3:J:86:GLU:OE1	3:J:210:LEU:HD12	2.19	0.43
3:J:452:MET:HG3	3:J:453:ASN:O	2.19	0.43
3:I:121:ARG:HE	3:I:125:HIS:HD2	1.66	0.43
3:H:336:ARG:HB2	3:H:362:TRP:CE2	2.54	0.43
2:N:1:DA:H2"	2:N:2:DA:C8	2.54	0.42
3:A:32:THR:O	3:A:36:SER:HB3	2.19	0.42
3:A:315:TYR:CE1	3:A:321:TRP:CD1	3.06	0.42
3:A:467:ASP:O	3:A:471:ILE:HD12	2.19	0.42
3:A:775:LYS:NZ	3:A:776:GLU:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:302:TYR:HA	3:B:305:LYS:HD2	2.01	0.42
3:B:616:PHE:CD1	3:B:805:LEU:HB2	2.54	0.42
3:C:105:ASN:HB3	3:C:149:VAL:HA	2.00	0.42
3:C:442:TRP:CG	3:C:466:PRO:HG3	2.54	0.42
3:C:663:ILE:HG21	3:C:693:GLU:O	2.19	0.42
3:C:854:ASN:C	3:C:902:ILE:HD11	2.44	0.42
3:C:876:ILE:HG23	3:D:871:ASN:HB3	2.01	0.42
3:D:350:TRP:CG	3:D:351:ASN:N	2.87	0.42
3:D:617:TYR:OH	3:D:732:MET:O	2.32	0.42
3:E:110:LEU:HD21	3:E:154:TYR:OH	2.19	0.42
3:E:336:ARG:HH22	3:E:359:GLU:HB3	1.84	0.42
3:L:49:ILE:HD12	3:L:210:LEU:HD11	2.00	0.42
3:L:177:LEU:HA	3:L:180:ASP:HB2	1.99	0.42
3:L:356:GLU:O	3:L:359:GLU:HG2	2.19	0.42
3:J:153:LYS:HG3	3:J:154:TYR:H	1.84	0.42
3:J:653:LEU:HD23	3:J:653:LEU:HA	1.86	0.42
3:I:254:SER:OG	3:I:260:ASN:ND2	2.51	0.42
3:I:356:GLU:O	3:I:359:GLU:HG2	2.19	0.42
3:I:602:GLN:HB2	3:I:942:TRP:NE1	2.34	0.42
3:I:744:THR:HG23	3:I:750:TRP:CD1	2.54	0.42
3:H:838:PHE:HB2	3:H:865:TRP:CZ3	2.54	0.42
3:A:183:VAL:HA	3:A:186:ILE:HD12	2.00	0.42
3:A:708:MET:C	3:A:728:MET:HE1	2.44	0.42
3:C:74:GLN:HA	3:C:77:LYS:HG2	2.00	0.42
3:D:95:MET:HE1	3:D:157:HIS:CD2	2.54	0.42
3:D:305:LYS:O	3:D:309:LEU:HG	2.19	0.42
3:D:700:LEU:C	3:D:702:THR:H	2.27	0.42
3:E:132:LEU:HB3	3:E:231:PHE:CE2	2.54	0.42
3:E:139:ILE:N	3:E:267:ARG:HH22	2.17	0.42
3:E:880:LEU:HD23	3:E:880:LEU:HA	1.91	0.42
3:F:706:LYS:NZ	3:F:752:ARG:HD2	2.35	0.42
3:F:838:PHE:HB2	3:F:865:TRP:CZ3	2.54	0.42
3:G:180:ASP:O	3:G:184:GLN:NE2	2.31	0.42
3:L:103:ASN:OD1	3:L:104:THR:HG22	2.20	0.42
3:K:121:ARG:HE	3:K:182:THR:HB	1.83	0.42
3:J:16:ALA:HB1	3:J:20:TYR:CE2	2.54	0.42
3:J:164:LYS:NZ	3:J:269:VAL:O	2.52	0.42
3:J:761:LYS:HZ2	3:J:763:CYS:HB3	1.83	0.42
3:J:945:TRP:O	3:J:950:SER:OG	2.33	0.42
3:I:95:MET:HG3	3:I:208:SER:HB2	1.99	0.42
3:I:237:ASP:OD1	3:I:237:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:390:TYR:HE1	3:I:391:LYS:HZ2	1.67	0.42
3:H:113:PRO:O	3:H:117:ARG:HG2	2.19	0.42
3:H:633:LEU:O	3:H:755:HIS:HA	2.19	0.42
3:A:140:HIS:CE1	3:A:265:LEU:HG	2.53	0.42
3:A:162:GLY:O	3:A:269:VAL:N	2.50	0.42
3:C:395:GLU:O	3:C:399:PHE:HB3	2.20	0.42
3:D:418:ILE:HD12	3:D:523:PHE:HE1	1.84	0.42
3:E:749:THR:C	3:E:751:ARG:H	2.28	0.42
3:F:93:GLY:HA3	3:F:161:PRO:HA	2.01	0.42
3:G:232:ASP:OD2	3:G:235:ASP:N	2.52	0.42
3:G:291:SER:O	3:G:294:MET:HB2	2.20	0.42
3:G:683:LEU:H	3:G:686:ARG:HH11	1.67	0.42
3:L:777:ASP:C	3:L:779:ARG:H	2.27	0.42
3:K:23:GLU:CD	3:K:23:GLU:H	2.28	0.42
3:K:681:MET:HA	3:K:684:LYS:NZ	2.34	0.42
3:K:773:GLU:C	3:K:774:LYS:HD3	2.44	0.42
3:I:303:LEU:HA	3:I:306:ILE:HG12	2.01	0.42
3:I:775:LYS:NZ	3:I:776:GLU:HG2	2.34	0.42
3:H:315:TYR:OH	3:H:345:LYS:O	2.23	0.42
3:H:403:ALA:HA	3:H:406:VAL:HG12	2.01	0.42
3:A:239:ILE:HG13	3:A:239:ILE:O	2.20	0.42
3:C:364:ASP:HA	3:C:367:HIS:CE1	2.54	0.42
3:C:780:PHE:HD1	3:C:784:TYR:CD2	2.38	0.42
3:D:316:VAL:HG22	3:D:346:CYS:SG	2.59	0.42
3:E:239:ILE:N	3:E:240:PRO:HD3	2.35	0.42
3:E:804:LYS:HE3	3:E:804:LYS:HB3	1.81	0.42
3:F:332:SER:OG	3:F:333:ALA:N	2.52	0.42
3:G:153:LYS:HA	3:G:153:LYS:HD2	1.66	0.42
3:L:86:GLU:OE1	3:L:86:GLU:N	2.52	0.42
3:L:695:ASN:O	3:L:696:LYS:HG2	2.19	0.42
3:K:530:GLN:HG2	3:J:521:ASP:HB2	2.01	0.42
3:K:672:THR:HB	3:K:675:LYS:HG3	2.01	0.42
3:J:50:ILE:HG12	3:J:57:THR:HA	2.01	0.42
3:J:250:TYR:CZ	3:J:265:LEU:HB2	2.54	0.42
3:J:775:LYS:HE2	3:J:775:LYS:HB2	1.23	0.42
3:J:866:TYR:O	3:J:870:ILE:HB	2.19	0.42
3:I:52:ARG:HD3	3:I:85:LEU:HD11	2.02	0.42
3:I:159:LEU:HD11	3:I:258:LEU:HD21	2.01	0.42
3:H:750:TRP:HA	3:H:753:LEU:HD12	2.02	0.42
3:H:777:ASP:HB3	4:H:1001:ANP:C8	2.49	0.42
3:A:356:GLU:OE1	3:A:356:GLU:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:893:LEU:O	3:C:904:LYS:NZ	2.51	0.42
3:D:378:ILE:H	3:D:378:ILE:HD12	1.84	0.42
3:D:879:GLU:OE1	3:D:879:GLU:N	2.40	0.42
3:E:342:PHE:HD1	3:E:345:LYS:HE2	1.84	0.42
3:E:601:LEU:HD11	3:E:615:MET:SD	2.60	0.42
3:F:295:LEU:O	3:F:301:ARG:NH2	2.52	0.42
3:F:403:ALA:HA	3:F:406:VAL:HG12	2.01	0.42
3:G:497:GLU:O	3:G:501:LEU:HD23	2.18	0.42
3:L:215:LYS:HB2	3:L:218:HIS:HB2	2.00	0.42
3:K:115:LEU:HD13	3:K:143:PHE:CD2	2.55	0.42
3:K:292:ILE:HG13	3:K:296:HIS:CE1	2.55	0.42
3:K:513:ARG:HB2	3:K:513:ARG:HH11	1.85	0.42
3:K:683:LEU:H	3:K:686:ARG:NH1	2.15	0.42
3:H:52:ARG:HH21	3:H:83:TYR:HD1	1.67	0.42
3:H:290:LEU:HD13	3:H:341:TRP:CE3	2.55	0.42
3:H:339:ALA:HB1	3:H:358:LEU:HD11	2.01	0.42
3:H:681:MET:HB3	3:H:718:GLU:HB3	2.01	0.42
3:A:118:LEU:HD13	3:A:183:VAL:HG12	2.02	0.42
3:B:128:ASN:OD1	3:B:129:SER:N	2.52	0.42
3:B:340:GLU:CD	3:B:344:GLN:HE22	2.26	0.42
3:D:447:LEU:N	3:D:450:GLN:OE1	2.37	0.42
3:D:636:GLY:H	3:D:642:LYS:HZ3	1.66	0.42
3:E:433:ASP:OD1	3:E:434:VAL:N	2.46	0.42
3:F:379:MET:HE3	3:F:379:MET:HB3	1.88	0.42
3:L:414:GLU:HG2	3:L:415:HIS:H	1.84	0.42
3:L:767:ASP:N	3:L:767:ASP:OD1	2.51	0.42
3:H:63:THR:O	3:H:66:LEU:HG	2.19	0.42
3:H:216:LEU:O	3:H:218:HIS:ND1	2.52	0.42
3:H:633:LEU:HD13	3:H:734:ALA:HB3	2.02	0.42
1:M:6:DT:H2"	1:M:7:DT:H5"	2.02	0.42
3:A:98:TYR:HB3	3:A:100:LEU:HG	2.02	0.42
3:A:186:ILE:HA	3:A:189:GLU:CD	2.44	0.42
3:B:391:LYS:HG3	3:B:392:GLU:N	2.33	0.42
3:C:97:ASP:OD1	3:C:97:ASP:N	2.53	0.42
3:D:833:ASP:OD1	3:D:833:ASP:N	2.53	0.42
3:E:115:LEU:HD22	3:E:143:PHE:CG	2.55	0.42
3:E:171:LYS:HD3	3:E:171:LYS:HA	1.76	0.42
3:E:673:ALA:HB1	3:F:679:ALA:HB3	2.00	0.42
3:E:717:ARG:HD2	3:E:721:GLN:O	2.20	0.42
3:E:841:GLU:HG2	3:E:842:ARG:HE	1.84	0.42
3:E:879:GLU:O	3:E:880:LEU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:111:GLU:HB3	3:F:113:PRO:HD2	2.01	0.42
3:G:681:MET:HE3	3:G:681:MET:HB3	1.82	0.42
3:G:692:GLU:OE2	3:G:735:ALA:N	2.36	0.42
3:L:96:LEU:HD11	3:L:174:ILE:HD11	2.01	0.42
3:L:219:LYS:HE2	3:L:219:LYS:HB2	1.90	0.42
3:L:317:GLU:HB2	3:L:319:PRO:HD2	2.01	0.42
3:K:171:LYS:HD3	3:K:171:LYS:HA	1.74	0.42
3:J:414:GLU:H	3:J:417:MET:HE3	1.84	0.42
3:J:852:VAL:HG21	3:J:902:ILE:HD12	2.02	0.42
3:H:192:VAL:HG12	3:H:194:ASN:H	1.84	0.42
3:H:666:LEU:O	3:H:704:ARG:NH2	2.48	0.42
3:A:757:ARG:NH1	3:A:758:SER:O	2.53	0.42
3:B:31:LEU:HD23	3:B:35:LEU:HD12	2.00	0.42
3:B:496:HIS:HB3	3:B:500:ILE:HG21	2.01	0.42
3:B:751:ARG:HD3	3:C:639:CYS:SG	2.60	0.42
3:D:889:LEU:O	3:D:893:LEU:N	2.32	0.42
3:E:222:GLN:OE1	3:E:222:GLN:N	2.51	0.42
3:F:187:LEU:HB3	3:F:192:VAL:HB	2.02	0.42
3:F:340:GLU:CD	3:F:344:GLN:HE22	2.27	0.42
3:G:153:LYS:HG3	3:G:154:TYR:HD1	1.84	0.42
3:L:609:ASP:OD2	3:L:819:PRO:HG2	2.19	0.42
3:L:744:THR:HG23	3:L:750:TRP:CD1	2.55	0.42
3:L:867:ASN:HA	3:L:871:ASN:C	2.45	0.42
3:K:148:GLU:HG2	3:K:153:LYS:NZ	2.34	0.42
3:K:167:ALA:H	3:K:170:LYS:HG3	1.84	0.42
3:J:39:LEU:HD23	3:J:58:TYR:HE1	1.85	0.42
3:J:731:THR:O	3:J:732:MET:HE2	2.20	0.42
3:J:941:LYS:HB2	3:J:944:GLU:HB2	2.02	0.42
3:I:64:GLU:OE1	3:I:67:ARG:NH2	2.53	0.42
3:I:670:ARG:HH12	3:H:663:ILE:HG22	1.83	0.42
3:H:147:PRO:HG2	3:H:219:LYS:HB3	2.01	0.42
3:H:613:TRP:HH2	3:H:630:LEU:HD21	1.84	0.42
3:H:676:PRO:HG3	1:O:5:DT:OP1	2.20	0.42
3:A:140:HIS:ND1	3:A:228:GLU:OE1	2.53	0.42
3:A:420:LYS:HE2	3:A:420:LYS:HB3	1.90	0.42
3:B:719:LEU:O	3:B:721:GLN:HG2	2.19	0.42
3:C:664:SER:O	3:C:668:SER:OG	2.30	0.42
3:D:11:THR:HA	3:D:14:LEU:HD13	2.01	0.42
3:D:429:LYS:NZ	3:D:445:PHE:O	2.53	0.42
3:E:187:LEU:HB3	3:E:192:VAL:HB	2.02	0.42
3:E:356:GLU:OE1	3:E:356:GLU:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:499:ASN:OD1	3:F:500:ILE:N	2.52	0.42
3:F:833:ASP:N	3:F:833:ASP:OD1	2.53	0.42
3:G:153:LYS:HG3	3:G:154:TYR:CD1	2.54	0.42
3:G:641:GLY:HA2	4:G:1001:ANP:N7	2.35	0.42
3:G:660:LYS:HE3	3:H:713:ASP:O	2.20	0.42
3:L:16:ALA:HB1	3:L:20:TYR:HE2	1.85	0.42
3:K:52:ARG:HE	3:K:83:TYR:HB3	1.85	0.42
3:K:305:LYS:O	3:K:309:LEU:HG	2.19	0.42
3:K:669:CYS:HA	3:K:704:ARG:NH1	2.35	0.42
3:J:593:TRP:HZ3	3:J:784:TYR:HE1	1.68	0.42
3:I:290:LEU:HA	3:I:293:LEU:HD12	2.01	0.42
3:I:653:LEU:HD23	3:I:653:LEU:HA	1.89	0.42
3:A:66:LEU:HA	3:A:69:TYR:CD2	2.55	0.42
3:A:159:LEU:HD21	3:A:256:LEU:O	2.20	0.42
3:A:452:MET:CE	3:A:457:ILE:HG13	2.50	0.42
3:B:356:GLU:OE1	3:B:356:GLU:N	2.49	0.42
3:B:807:LYS:NZ	3:B:808:GLU:OE2	2.43	0.42
3:B:893:LEU:O	3:B:904:LYS:NZ	2.53	0.42
3:C:121:ARG:HG2	3:C:180:ASP:OD2	2.19	0.42
3:C:146:LYS:HB3	3:C:221:TYR:CD2	2.55	0.42
3:E:60:LEU:H	3:E:60:LEU:HG	1.48	0.42
3:E:92:SER:H	3:E:166:ALA:HB2	1.85	0.42
3:E:452:MET:HE3	3:E:456:GLU:HG3	2.01	0.42
3:F:780:PHE:HD1	3:F:784:TYR:CD2	2.38	0.42
3:G:87:ARG:HA	3:G:207:PRO:HA	2.02	0.42
3:G:97:ASP:HA	3:G:157:HIS:HD1	1.85	0.42
3:G:847:PRO:HA	3:G:917:PRO:C	2.45	0.42
3:L:171:LYS:HA	3:L:171:LYS:HD3	1.75	0.42
3:L:422:ILE:HD13	3:L:422:ILE:HA	1.94	0.42
3:L:446:VAL:HG21	3:L:456:GLU:O	2.19	0.42
3:K:145:LEU:HD22	3:K:224:LYS:HE2	2.00	0.42
3:I:53:ILE:HG13	3:I:83:TYR:HB2	2.02	0.42
3:I:349:LYS:HB2	3:I:349:LYS:HE2	1.21	0.42
3:I:476:ASN:HA	3:I:479:ARG:HH11	1.85	0.42
3:H:23:GLU:CD	3:H:23:GLU:H	2.28	0.42
3:H:718:GLU:HG2	3:H:719:LEU:N	2.27	0.42
3:A:17:GLN:OE1	3:A:81:LEU:N	2.51	0.41
3:A:114:ALA:O	3:A:118:LEU:HD23	2.20	0.41
3:A:164:LYS:HG3	3:A:164:LYS:O	2.20	0.41
3:A:178:GLN:NE2	3:A:196:GLU:OE1	2.53	0.41
3:A:627:LYS:HZ2	3:A:731:THR:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:442:TRP:CZ2	3:B:532:GLU:HG2	2.55	0.41
3:B:605:ILE:HA	3:B:606:PRO:HD3	1.92	0.41
3:B:713:ASP:C	3:C:660:LYS:HZ1	2.21	0.41
3:D:707:GLU:CG	3:D:708:MET:HE2	2.49	0.41
3:E:553:VAL:HG23	3:E:555:ASN:H	1.84	0.41
3:E:846:SER:OG	3:E:905:GLY:HA2	2.21	0.41
3:F:180:ASP:O	3:F:184:GLN:NE2	2.37	0.41
3:F:251:ASN:CG	3:F:254:SER:HB3	2.44	0.41
3:F:853:TYR:CD2	3:F:906:CYS:HB2	2.55	0.41
3:G:751:ARG:HH21	3:G:752:ARG:NH2	2.17	0.41
3:L:132:LEU:HD23	3:L:231:PHE:HZ	1.85	0.41
3:K:751:ARG:HD2	3:K:752:ARG:HG3	2.02	0.41
3:J:245:LYS:HA	3:J:245:LYS:HD2	1.92	0.41
3:J:605:ILE:HD12	3:J:611:ARG:HA	2.02	0.41
3:J:613:TRP:CD2	3:J:821:ILE:HG13	2.55	0.41
3:I:414:GLU:HG3	3:I:415:HIS:H	1.85	0.41
3:I:867:ASN:CG	3:I:872:VAL:HA	2.45	0.41
3:H:336:ARG:HH12	3:H:359:GLU:HA	1.84	0.41
3:H:475:GLU:O	3:H:478:SER:OG	2.23	0.41
3:A:780:PHE:HB2	4:A:1001:ANP:O2'	2.20	0.41
3:B:91:TYR:HB3	3:B:164:LYS:HB2	2.02	0.41
3:B:165:LEU:HG	3:B:169:THR:OG1	2.20	0.41
3:C:30:LEU:HD11	3:C:67:ARG:HH11	1.85	0.41
3:C:110:LEU:HD13	3:C:224:LYS:HD3	2.02	0.41
3:C:165:LEU:HD23	3:C:165:LEU:HA	1.95	0.41
3:D:244:ILE:HD11	3:D:265:LEU:HD11	2.02	0.41
3:D:508:LEU:O	3:D:512:GLU:HG2	2.19	0.41
3:D:653:LEU:HD23	3:D:653:LEU:HA	1.85	0.41
3:E:703:SER:C	3:E:705:LEU:H	2.27	0.41
3:F:909:LEU:HG	3:F:913:GLU:OE1	2.19	0.41
3:G:164:LYS:O	3:G:164:LYS:HG3	2.20	0.41
3:L:703:SER:OG	3:L:704:ARG:N	2.53	0.41
3:K:146:LYS:HD2	3:K:154:TYR:HA	2.02	0.41
3:K:499:ASN:OD1	3:K:500:ILE:N	2.53	0.41
3:J:101:LYS:HA	3:J:152:GLY:O	2.20	0.41
3:J:289:SER:O	3:J:292:ILE:HG22	2.19	0.41
3:I:232:ASP:OD1	3:I:233:SER:N	2.53	0.41
3:I:615:MET:HE1	3:I:801:PHE:CG	2.55	0.41
3:H:755:HIS:H	3:H:825:THR:HG22	1.84	0.41
3:H:842:ARG:CZ	3:H:865:TRP:HD1	2.32	0.41
3:A:69:TYR:HB3	3:A:254:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:97:ASP:OD1	3:A:203:SER:OG	2.28	0.41
3:A:364:ASP:O	3:A:368:HIS:HB2	2.20	0.41
3:A:852:VAL:HG11	3:A:902:ILE:HD12	2.01	0.41
3:B:414:GLU:HG3	3:B:415:HIS:H	1.85	0.41
3:C:145:LEU:HD22	3:C:224:LYS:HD2	2.02	0.41
3:C:326:PHE:CD1	3:C:365:ALA:HB2	2.55	0.41
3:D:47:THR:HG21	3:D:50:ILE:HD11	2.01	0.41
3:D:153:LYS:HG3	3:D:154:TYR:H	1.84	0.41
3:D:426:MET:HE3	3:D:426:MET:HB2	1.57	0.41
3:E:488:ILE:HD13	3:E:488:ILE:HA	1.94	0.41
3:E:633:LEU:O	3:E:755:HIS:HA	2.20	0.41
3:F:883:GLU:HA	3:F:886:ASN:HB2	2.02	0.41
3:G:61:PRO:HD2	3:G:64:GLU:HG3	2.02	0.41
3:G:145:LEU:HD12	3:G:148:GLU:OE2	2.20	0.41
3:G:661:LEU:HD11	3:G:689:GLY:HA3	2.02	0.41
3:G:879:GLU:OE2	3:L:697:SER:HB2	2.20	0.41
3:L:61:PRO:HD2	3:L:64:GLU:HG3	2.01	0.41
3:K:98:TYR:CE1	3:K:199:LEU:HD12	2.55	0.41
3:K:127:LYS:HA	3:K:127:LYS:HE2	2.01	0.41
3:K:161:PRO:HB3	3:K:258:LEU:HD23	2.01	0.41
3:K:174:ILE:O	3:K:178:GLN:HG2	2.19	0.41
3:K:355:LYS:O	3:K:358:LEU:HB3	2.20	0.41
3:J:101:LYS:HA	3:J:101:LYS:HD2	1.92	0.41
3:J:335:TYR:HA	3:J:338:LEU:HD13	2.01	0.41
3:J:722:LYS:HD2	3:J:722:LYS:HA	1.67	0.41
3:I:349:LYS:H	3:I:349:LYS:HG3	1.57	0.41
3:I:350:TRP:O	3:I:350:TRP:CG	2.73	0.41
3:I:555:ASN:ND2	3:I:584:TYR:O	2.47	0.41
3:I:681:MET:HG3	3:I:718:GLU:OE1	2.21	0.41
3:I:683:LEU:H	3:I:686:ARG:HH11	1.67	0.41
3:A:94:LEU:HB2	3:A:160:ILE:HB	2.01	0.41
3:A:732:MET:HE3	3:A:732:MET:HB3	1.91	0.41
3:A:749:THR:C	3:A:751:ARG:H	2.29	0.41
3:B:183:VAL:HA	3:B:186:ILE:HD12	2.03	0.41
3:B:356:GLU:O	3:B:359:GLU:HG2	2.20	0.41
3:C:236:PRO:HD2	3:C:238:TYR:OH	2.21	0.41
3:C:335:TYR:HA	3:C:338:LEU:HD13	2.02	0.41
3:C:879:GLU:OE2	3:D:697:SER:HB2	2.21	0.41
3:D:866:TYR:HE2	3:D:873:LYS:HB2	1.84	0.41
3:E:33:ARG:HG3	3:E:34:GLU:N	2.35	0.41
3:E:938:PRO:HG3	3:E:942:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:290:LEU:HD11	3:F:341:TRP:HB2	2.02	0.41
3:F:945:TRP:CH2	3:F:948:ASN:HA	2.56	0.41
3:G:16:ALA:HB1	3:G:20:TYR:HE2	1.85	0.41
3:G:23:GLU:H	3:G:23:GLU:CD	2.29	0.41
3:G:139:ILE:N	3:G:267:ARG:HH22	2.19	0.41
3:G:682:ARG:O	3:G:683:LEU:HG	2.21	0.41
3:G:766:PRO:HG3	3:G:775:LYS:HB2	2.03	0.41
3:G:780:PHE:HD1	3:G:784:TYR:HD2	1.68	0.41
3:L:169:THR:O	3:L:173:ILE:HG12	2.20	0.41
3:K:229:LEU:HA	3:K:241:ILE:HA	2.02	0.41
3:J:506:LYS:HE2	3:J:506:LYS:HB2	1.93	0.41
3:J:664:SER:HA	3:J:667:THR:HG22	2.01	0.41
3:J:777:ASP:HB3	4:J:1001:ANP:C8	2.50	0.41
3:J:821:ILE:HG22	3:J:822:GLU:H	1.86	0.41
3:I:87:ARG:HA	3:I:207:PRO:HA	2.02	0.41
3:I:141:PHE:HB2	3:I:227:PHE:HB2	2.02	0.41
3:I:238:TYR:C	3:I:240:PRO:HD3	2.45	0.41
3:I:326:PHE:CZ	3:I:361:LEU:HD22	2.55	0.41
3:I:347:PRO:HB2	3:I:351:ASN:OD1	2.20	0.41
3:I:852:VAL:HG11	3:I:902:ILE:HD12	2.02	0.41
3:A:16:ALA:HB1	3:A:20:TYR:CE2	2.56	0.41
3:A:328:LEU:HD11	3:A:339:ALA:HB2	2.02	0.41
3:A:761:LYS:NZ	3:A:763:CYS:HB3	2.35	0.41
3:A:780:PHE:HD1	3:A:784:TYR:CD2	2.38	0.41
3:A:938:PRO:HG3	3:A:942:TRP:HB3	2.02	0.41
3:B:144:THR:OG1	3:B:145:LEU:N	2.53	0.41
3:B:298:PRO:HA	3:B:301:ARG:CD	2.50	0.41
3:B:728:MET:HE3	3:B:728:MET:HB2	1.80	0.41
3:C:499:ASN:OD1	3:C:500:ILE:N	2.53	0.41
3:C:701:ASN:C	3:C:703:SER:N	2.78	0.41
3:D:777:ASP:O	4:D:1001:ANP:O2'	2.34	0.41
3:E:77:LYS:HD3	3:E:77:LYS:HA	1.79	0.41
3:E:674:GLU:O	3:E:717:ARG:NH2	2.54	0.41
3:F:457:ILE:HG22	3:F:458:TRP:CD1	2.55	0.41
3:G:30:LEU:HA	3:G:34:GLU:OE1	2.20	0.41
3:G:130:SER:HB2	3:G:165:LEU:HD21	2.01	0.41
3:G:310:LEU:HB2	3:G:385:HIS:ND1	2.35	0.41
3:L:66:LEU:O	3:L:70:GLU:HG2	2.20	0.41
3:L:392:GLU:O	3:L:395:GLU:HG3	2.21	0.41
3:L:606:PRO:HA	3:L:611:ARG:HH12	1.84	0.41
3:J:570:HIS:ND1	3:J:571:PHE:O	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:585:VAL:O	3:J:796:SER:OG	2.30	0.41
3:J:796:SER:HA	3:J:799:VAL:HG12	2.02	0.41
3:J:945:TRP:CH2	3:J:948:ASN:HA	2.55	0.41
3:I:821:ILE:HG22	3:I:822:GLU:H	1.84	0.41
3:I:883:GLU:O	3:I:887:SER:N	2.53	0.41
3:H:335:TYR:HA	3:H:338:LEU:HD13	2.03	0.41
3:H:589:PRO:HA	3:H:594:THR:HG21	2.02	0.41
3:H:821:ILE:HG22	3:H:822:GLU:H	1.85	0.41
3:H:879:GLU:HG2	3:H:880:LEU:N	2.34	0.41
3:A:23:GLU:H	3:A:23:GLU:CD	2.28	0.41
3:A:818:CYS:SG	3:A:821:ILE:HG12	2.61	0.41
3:A:862:TYR:CE1	3:A:865:TRP:CZ3	3.09	0.41
3:B:140:HIS:HD2	3:B:142:PHE:HE2	1.67	0.41
3:B:216:LEU:O	3:B:218:HIS:ND1	2.54	0.41
3:B:895:TRP:HA	3:B:901:ARG:HA	2.03	0.41
3:C:63:THR:O	3:C:66:LEU:HG	2.20	0.41
3:C:173:ILE:O	3:C:177:LEU:HG	2.21	0.41
3:C:655:ASP:N	3:C:655:ASP:OD1	2.52	0.41
3:E:97:ASP:OD1	3:E:97:ASP:N	2.54	0.41
3:E:353:GLY:N	3:E:356:GLU:OE2	2.41	0.41
3:E:403:ALA:HA	3:E:406:VAL:HG12	2.03	0.41
3:G:328:LEU:HD12	3:G:362:TRP:HZ3	1.86	0.41
3:G:907:ARG:HH11	3:G:916:GLN:HG3	1.85	0.41
3:L:833:ASP:OD1	3:L:833:ASP:N	2.51	0.41
3:K:616:PHE:HB3	3:K:805:LEU:HD12	2.03	0.41
3:J:826:GLU:HA	3:J:829:ARG:HB3	2.03	0.41
3:I:74:GLN:HA	3:I:77:LYS:HE2	2.01	0.41
3:I:97:ASP:OD1	3:I:97:ASP:N	2.53	0.41
3:I:315:TYR:CZ	3:I:349:LYS:HD3	2.55	0.41
3:I:616:PHE:HZ	3:I:945:TRP:HD1	1.68	0.41
3:H:651:MET:HE2	3:H:651:MET:HB3	1.89	0.41
3:H:665:LEU:O	3:H:704:ARG:HD2	2.20	0.41
3:A:416:TYR:HB3	3:B:519:PHE:HD1	1.86	0.41
3:B:99:ASP:OD1	3:B:99:ASP:N	2.52	0.41
3:B:105:ASN:HA	3:B:153:LYS:HD3	2.02	0.41
3:B:123:PHE:O	3:B:127:LYS:HG2	2.20	0.41
3:B:728:MET:O	3:B:728:MET:HG3	2.21	0.41
3:B:752:ARG:NH1	4:C:1001:ANP:O3G	2.51	0.41
3:C:211:TYR:CE1	3:C:223:LEU:HG	2.55	0.41
3:C:237:ASP:O	3:I:117:ARG:NH2	2.54	0.41
3:C:293:LEU:HD11	3:C:337:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:370:GLU:H	3:C:372:LYS:NZ	2.19	0.41
3:C:633:LEU:O	3:C:755:HIS:HA	2.21	0.41
3:C:783:GLU:OE1	3:C:784:TYR:N	2.52	0.41
3:C:903:LEU:HD12	3:C:903:LEU:HA	1.83	0.41
3:E:681:MET:HG3	3:E:718:GLU:CG	2.50	0.41
3:E:857:GLU:OE1	3:E:857:GLU:N	2.54	0.41
3:F:362:TRP:O	3:F:366:SER:OG	2.28	0.41
3:K:842:ARG:NH1	3:K:865:TRP:HD1	2.19	0.41
3:J:229:LEU:HB3	3:J:241:ILE:HD13	2.02	0.41
3:J:779:ARG:O	3:J:783:GLU:N	2.46	0.41
3:I:302:TYR:OH	3:I:394:VAL:HG12	2.20	0.41
3:I:435:ASP:OD1	3:I:439:LYS:N	2.47	0.41
3:I:633:LEU:HD13	3:I:734:ALA:HB3	2.02	0.41
3:H:362:TRP:O	3:H:366:SER:OG	2.33	0.41
3:H:469:LEU:HD12	3:H:469:LEU:HA	1.89	0.41
3:A:242:HIS:CE1	3:G:113:PRO:HG3	2.56	0.41
3:A:332:SER:OG	3:A:334:ASN:OD1	2.26	0.41
3:A:752:ARG:H	3:A:752:ARG:HG2	1.60	0.41
3:B:140:HIS:CD2	3:B:161:PRO:HD2	2.56	0.41
3:B:326:PHE:CD1	3:B:365:ALA:HB2	2.56	0.41
3:B:442:TRP:CG	3:B:466:PRO:HG3	2.55	0.41
3:B:866:TYR:O	3:B:871:ASN:N	2.54	0.41
3:C:73:GLU:HG3	3:C:253:VAL:HB	2.02	0.41
3:C:894:GLN:O	3:C:902:ILE:N	2.49	0.41
3:D:406:VAL:O	3:D:410:ASN:HA	2.21	0.41
3:D:717:ARG:O	3:D:718:GLU:C	2.61	0.41
3:D:808:GLU:HG3	3:D:945:TRP:NE1	2.35	0.41
3:F:132:LEU:HB3	3:F:231:PHE:HE2	1.85	0.41
3:G:229:LEU:HD12	3:G:241:ILE:HG23	2.03	0.41
3:L:867:ASN:CG	3:L:872:VAL:HA	2.45	0.41
3:K:96:LEU:HD11	3:K:158:VAL:HG12	2.02	0.41
3:K:226:GLY:HA3	3:K:247:LEU:HD22	2.01	0.41
3:K:627:LYS:NZ	3:K:731:THR:HG23	2.36	0.41
3:K:757:ARG:NH1	3:K:758:SER:O	2.54	0.41
3:J:32:THR:O	3:J:36:SER:HB3	2.20	0.41
3:J:96:LEU:HA	3:J:203:SER:HB3	2.02	0.41
3:J:255:GLU:OE2	3:J:264:SER:OG	2.33	0.41
3:J:509:LYS:O	3:J:512:GLU:HG3	2.20	0.41
3:J:627:LYS:NZ	3:J:731:THR:HG23	2.35	0.41
3:J:674:GLU:CD	3:I:677:ASN:HA	2.46	0.41
3:I:318:TYR:N	3:I:319:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:484:ILE:O	3:I:488:ILE:HG12	2.21	0.41
3:H:240:PRO:HB2	3:H:242:HIS:CE1	2.55	0.41
3:H:312:PRO:O	3:H:316:VAL:HG23	2.21	0.41
3:H:462:LYS:H	3:H:577:HIS:CE1	2.38	0.41
3:H:618:LEU:HD23	3:H:618:LEU:HA	1.90	0.41
3:A:117:ARG:HA	3:A:117:ARG:HD3	1.87	0.41
3:A:140:HIS:CG	3:A:266:VAL:HG12	2.56	0.41
3:A:321:TRP:CZ2	3:A:358:LEU:HB2	2.53	0.41
3:A:878:LEU:O	3:A:881:SER:OG	2.35	0.41
3:C:99:ASP:N	3:C:198:CYS:HB3	2.35	0.41
3:C:119:CYS:HA	3:C:122:ILE:HG12	2.02	0.41
3:C:163:LEU:O	3:C:164:LYS:HE2	2.20	0.41
3:C:290:LEU:O	3:C:294:MET:HG2	2.21	0.41
3:D:347:PRO:O	3:D:351:ASN:N	2.54	0.41
3:D:402:LEU:HD23	3:D:480:VAL:HG12	2.03	0.41
3:D:636:GLY:H	3:D:642:LYS:NZ	2.19	0.41
3:D:750:TRP:HB3	3:D:829:ARG:HD3	2.03	0.41
3:E:73:GLU:CD	3:E:251:ASN:HA	2.45	0.41
3:E:298:PRO:HA	3:E:301:ARG:HG2	2.03	0.41
3:E:452:MET:HG3	3:E:453:ASN:O	2.20	0.41
3:E:653:LEU:HD23	3:E:653:LEU:HA	1.82	0.41
3:E:701:ASN:C	3:E:703:SER:H	2.28	0.41
3:E:751:ARG:HH21	3:E:752:ARG:NH2	2.19	0.41
3:F:16:ALA:HB1	3:F:20:TYR:CE2	2.56	0.41
3:F:44:SER:HB2	3:F:46:LYS:HE2	2.02	0.41
3:F:415:HIS:CE1	3:F:526:GLY:HA3	2.56	0.41
3:F:670:ARG:HD3	3:F:704:ARG:HB3	2.02	0.41
3:G:76:ARG:HH12	3:G:253:VAL:HG22	1.86	0.41
3:G:112:PRO:HB3	3:G:227:PHE:HZ	1.86	0.41
3:G:162:GLY:O	3:G:269:VAL:N	2.50	0.41
3:G:184:GLN:HG2	3:G:195:PRO:O	2.20	0.41
3:G:309:LEU:HD13	3:G:389:GLN:HE22	1.85	0.41
3:G:340:GLU:CD	3:G:344:GLN:HE22	2.29	0.41
3:G:416:TYR:HA	3:G:419:ALA:HB3	2.02	0.41
3:G:670:ARG:NH2	3:G:704:ARG:HG2	2.35	0.41
3:L:380:TYR:CE2	3:L:384:LYS:HD2	2.55	0.41
3:L:627:LYS:NZ	3:L:731:THR:HG23	2.36	0.41
3:L:632:LEU:HA	3:L:754:ARG:HB2	2.02	0.41
3:K:452:MET:HE1	3:K:457:ILE:HG13	2.01	0.41
3:K:605:ILE:HA	3:K:606:PRO:HD3	1.94	0.41
3:K:666:LEU:HD11	3:K:691:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:766:PRO:HG3	3:K:775:LYS:HB2	2.02	0.41
3:K:804:LYS:HE3	3:K:804:LYS:HB3	1.86	0.41
3:J:372:LYS:HD3	3:J:372:LYS:HA	1.81	0.41
3:J:780:PHE:HB2	4:J:1001:ANP:H2'	2.03	0.41
3:J:839:ILE:HD13	3:J:839:ILE:HA	1.97	0.41
3:I:80:ALA:C	3:I:81:LEU:HD12	2.46	0.41
3:I:139:ILE:N	3:I:229:LEU:O	2.54	0.41
3:I:222:GLN:OE1	3:I:222:GLN:N	2.53	0.41
3:H:52:ARG:NH2	3:H:215:LYS:HA	2.26	0.41
3:H:110:LEU:HD23	3:H:115:LEU:HD21	2.02	0.41
3:H:471:ILE:H	3:H:471:ILE:HD12	1.86	0.41
3:H:490:TYR:O	3:H:493:SER:OG	2.32	0.41
3:A:174:ILE:HG23	3:A:199:LEU:HD21	2.03	0.41
3:B:97:ASP:HA	3:B:157:HIS:ND1	2.36	0.41
3:B:121:ARG:NH1	3:B:125:HIS:HB2	2.36	0.41
3:B:153:LYS:HD2	3:B:153:LYS:HA	1.68	0.41
3:B:337:PRO:HA	3:B:340:GLU:HB3	2.01	0.41
3:B:651:MET:HE3	3:B:651:MET:HB3	1.87	0.41
3:B:821:ILE:HG22	3:B:822:GLU:H	1.85	0.41
3:C:60:LEU:HB2	3:C:64:GLU:CB	2.51	0.41
3:C:184:GLN:NE2	3:C:196:GLU:HG2	2.36	0.41
3:C:911:LYS:HA	3:C:911:LYS:HD2	1.77	0.41
3:D:120:HIS:CD2	3:D:239:ILE:HD12	2.55	0.41
3:D:351:ASN:HD22	3:D:351:ASN:HA	1.52	0.41
3:D:642:LYS:O	3:D:643:THR:OG1	2.37	0.41
3:E:417:MET:HE3	3:E:417:MET:HB2	1.65	0.41
3:F:763:CYS:N	3:F:776:GLU:HB3	2.35	0.41
3:G:216:LEU:O	3:G:218:HIS:ND1	2.54	0.41
3:L:336:ARG:HB2	3:L:362:TRP:CZ2	2.55	0.41
3:L:882:GLN:HA	3:L:885:GLU:HG2	2.03	0.41
3:K:100:LEU:O	3:K:153:LYS:HB3	2.21	0.41
3:K:744:THR:HG23	3:K:750:TRP:CD1	2.56	0.41
3:J:321:TRP:O	3:J:324:VAL:HG22	2.21	0.41
3:J:356:GLU:OE1	3:J:356:GLU:N	2.53	0.41
3:J:371:LYS:HE3	3:J:574:HIS:CD2	2.56	0.41
3:I:320:LEU:O	3:I:324:VAL:HG13	2.21	0.41
3:I:335:TYR:HA	3:I:338:LEU:HD13	2.03	0.41
3:H:17:GLN:OE1	3:H:81:LEU:N	2.53	0.41
3:A:821:ILE:HG22	3:A:822:GLU:N	2.35	0.40
3:B:222:GLN:OE1	3:B:222:GLN:N	2.54	0.40
3:B:675:LYS:HA	3:B:675:LYS:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:715:THR:HA	3:B:725:SER:HA	2.03	0.40
3:D:251:ASN:OD1	3:D:251:ASN:N	2.54	0.40
3:D:551:LEU:HD23	3:D:551:LEU:HA	1.88	0.40
3:E:30:LEU:HD22	3:E:71:HIS:ND1	2.36	0.40
3:E:350:TRP:CZ2	3:E:355:LYS:HD3	2.56	0.40
3:E:470:HIS:NE2	3:E:528:ILE:HG13	2.36	0.40
3:F:33:ARG:HG3	3:F:34:GLU:OE1	2.21	0.40
3:F:433:ASP:OD1	3:F:434:VAL:N	2.51	0.40
3:F:766:PRO:HG3	3:F:775:LYS:HB2	2.03	0.40
3:G:140:HIS:CD2	3:G:266:VAL:HA	2.56	0.40
3:G:174:ILE:HD13	3:G:174:ILE:HA	1.92	0.40
3:G:652:VAL:HG21	3:G:794:PHE:HD2	1.87	0.40
3:L:471:ILE:H	3:L:471:ILE:HD12	1.86	0.40
3:L:653:LEU:HD23	3:L:653:LEU:HA	1.90	0.40
3:K:102:LEU:HD11	3:K:192:VAL:HG22	2.03	0.40
3:K:602:GLN:HB2	3:K:942:TRP:NE1	2.36	0.40
3:J:15:THR:O	3:J:19:LYS:HG2	2.21	0.40
3:J:602:GLN:HB2	3:J:942:TRP:NE1	2.35	0.40
3:I:248:GLU:H	3:I:248:GLU:CD	2.28	0.40
3:I:593:TRP:NE1	3:I:789:ASP:OD2	2.54	0.40
3:B:318:TYR:N	3:B:319:PRO:HD2	2.36	0.40
3:C:187:LEU:HD12	3:C:195:PRO:O	2.21	0.40
3:C:237:ASP:OD2	3:C:239:ILE:HG12	2.21	0.40
3:C:629:ALA:O	3:C:752:ARG:HG2	2.21	0.40
3:D:821:ILE:HG22	3:D:822:GLU:H	1.86	0.40
3:E:942:TRP:CD1	3:E:942:TRP:H	2.38	0.40
3:F:247:LEU:HD23	3:F:247:LEU:H	1.86	0.40
3:F:250:TYR:CZ	3:F:265:LEU:HD13	2.56	0.40
3:F:651:MET:HE2	3:F:651:MET:HB2	1.92	0.40
3:F:804:LYS:HE3	3:F:804:LYS:HB3	1.85	0.40
3:L:318:TYR:N	3:L:319:PRO:HD2	2.36	0.40
3:L:941:LYS:HE3	3:L:944:GLU:HB2	2.02	0.40
3:J:16:ALA:HB1	3:J:20:TYR:HE2	1.85	0.40
3:J:17:GLN:OE1	3:J:81:LEU:N	2.54	0.40
3:J:140:HIS:CG	3:J:266:VAL:HG12	2.56	0.40
3:J:692:GLU:OE1	3:J:692:GLU:N	2.54	0.40
3:I:413:LEU:HB2	3:I:514:SER:OG	2.22	0.40
3:I:585:VAL:O	3:I:796:SER:OG	2.26	0.40
3:H:64:GLU:OE1	3:H:67:ARG:NH2	2.39	0.40
3:H:426:MET:HE3	3:H:427:GLY:N	2.37	0.40
3:H:706:LYS:NZ	3:H:748:GLY:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:742:ILE:HG12	3:H:832:GLN:HG2	2.02	0.40
3:A:309:LEU:HB3	3:A:389:GLN:NE2	2.36	0.40
3:B:907:ARG:NH1	3:B:915:LEU:HA	2.36	0.40
3:C:776:GLU:CA	4:C:1001:ANP:H8	2.43	0.40
3:D:616:PHE:CB	3:D:805:LEU:HD12	2.51	0.40
3:D:804:LYS:HD2	3:D:807:LYS:HE3	2.02	0.40
3:F:73:GLU:CD	3:F:251:ASN:HA	2.46	0.40
3:F:121:ARG:HA	3:F:121:ARG:HD2	1.72	0.40
3:F:121:ARG:HE	3:F:182:THR:HB	1.85	0.40
3:G:208:SER:OG	3:G:209:LEU:N	2.54	0.40
3:G:321:TRP:HZ3	3:G:357:LYS:HD3	1.86	0.40
3:G:818:CYS:SG	3:G:821:ILE:HG12	2.61	0.40
3:G:844:VAL:HG22	3:G:907:ARG:CZ	2.51	0.40
3:L:52:ARG:HE	3:L:83:TYR:HB3	1.86	0.40
3:L:95:MET:SD	3:L:159:LEU:HD13	2.61	0.40
3:L:102:LEU:HD22	3:L:153:LYS:HG2	2.03	0.40
3:L:312:PRO:O	3:L:316:VAL:HG23	2.22	0.40
3:L:425:MET:HE3	3:L:425:MET:HB2	1.86	0.40
3:L:473:ILE:O	3:L:477:PHE:HB3	2.21	0.40
3:L:529:ARG:O	3:L:532:GLU:HG2	2.21	0.40
3:L:892:TYR:O	3:L:903:LEU:HA	2.21	0.40
3:K:630:LEU:O	3:K:631:MET:HE2	2.21	0.40
3:J:148:GLU:HB3	3:J:149:VAL:H	1.68	0.40
3:J:292:ILE:HG13	3:J:296:HIS:CE1	2.56	0.40
3:J:804:LYS:HE3	3:J:804:LYS:HB3	1.88	0.40
3:I:183:VAL:O	3:I:187:LEU:HG	2.22	0.40
3:I:415:HIS:O	3:H:519:PHE:HB3	2.22	0.40
3:I:432:VAL:O	3:I:536:ARG:HA	2.22	0.40
3:I:804:LYS:HE3	3:I:804:LYS:HB3	1.83	0.40
3:H:120:HIS:NE2	3:H:239:ILE:HB	2.36	0.40
3:H:293:LEU:HD11	3:H:337:PRO:HG2	2.04	0.40
3:H:636:GLY:O	3:H:737:ASN:HA	2.20	0.40
3:A:598:LEU:HD13	3:A:943:TRP:CE3	2.56	0.40
3:B:196:GLU:O	3:B:197:SER:OG	2.35	0.40
3:B:783:GLU:OE1	3:B:784:TYR:N	2.54	0.40
3:C:238:TYR:C	3:C:239:ILE:HG13	2.46	0.40
3:C:718:GLU:CG	3:C:719:LEU:H	2.34	0.40
3:C:777:ASP:N	4:C:1001:ANP:H8	2.35	0.40
3:D:692:GLU:OE1	3:D:692:GLU:N	2.53	0.40
3:D:781:ILE:HD13	3:D:781:ILE:HA	1.94	0.40
3:E:66:LEU:HA	3:E:69:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:426:MET:HE2	3:E:472:TYR:CD2	2.56	0.40
3:F:86:GLU:O	3:F:208:SER:N	2.51	0.40
3:G:97:ASP:O	3:G:199:LEU:HA	2.21	0.40
3:G:237:ASP:OD1	3:G:237:ASP:N	2.54	0.40
3:G:833:ASP:OD1	3:G:833:ASP:N	2.55	0.40
3:L:108:PRO:HB3	3:L:190:GLN:O	2.22	0.40
3:L:563:ILE:HD11	3:L:806:GLN:HB2	2.03	0.40
3:K:590:GLU:O	3:K:595:LYS:NZ	2.37	0.40
3:J:471:ILE:H	3:J:471:ILE:HD12	1.87	0.40
3:J:759:LYS:HB3	3:J:772:TYR:CZ	2.56	0.40
3:I:120:HIS:NE2	3:I:239:ILE:HB	2.37	0.40
3:I:627:LYS:NZ	3:I:731:THR:HG23	2.36	0.40
3:I:644:PHE:CE1	3:I:780:PHE:HB3	2.56	0.40
3:H:336:ARG:HB2	3:H:362:TRP:CZ2	2.56	0.40
3:H:672:THR:HB	3:H:675:LYS:HG3	2.04	0.40
3:H:762:PHE:CE1	3:H:774:LYS:HE2	2.57	0.40
1:O:1:DT:H4'	1:O:2:DT:OP1	2.20	0.40
3:A:405:TYR:CD2	3:A:417:MET:HB3	2.57	0.40
3:A:617:TYR:OH	3:A:732:MET:O	2.32	0.40
3:A:877:ALA:HB3	3:B:869:ASN:O	2.22	0.40
3:B:97:ASP:HA	3:B:157:HIS:CE1	2.55	0.40
3:B:470:HIS:NE2	3:B:528:ILE:HG13	2.36	0.40
3:C:437:ASN:OD1	3:C:721:GLN:NE2	2.46	0.40
3:C:544:LEU:HD12	3:C:575:PRO:HB2	2.02	0.40
3:D:483:ARG:O	3:D:486:GLU:HG3	2.21	0.40
3:E:185:LYS:HE2	3:E:185:LYS:HB3	1.96	0.40
3:E:185:LYS:HE3	3:E:186:ILE:HG13	2.04	0.40
3:F:473:ILE:O	3:F:477:PHE:HB3	2.21	0.40
3:G:96:LEU:HD21	3:G:98:TYR:CE1	2.57	0.40
3:L:63:THR:O	3:L:66:LEU:HG	2.22	0.40
3:K:156:PHE:CZ	3:K:158:VAL:HB	2.56	0.40
3:K:378:ILE:HD12	3:K:378:ILE:H	1.86	0.40
3:K:762:PHE:HB3	3:K:776:GLU:HA	2.04	0.40
3:J:141:PHE:N	3:J:227:PHE:O	2.52	0.40
3:J:174:ILE:HD13	3:J:174:ILE:HA	1.95	0.40
3:J:336:ARG:HH22	3:J:359:GLU:HB3	1.87	0.40
3:J:718:GLU:CD	3:J:719:LEU:H	2.29	0.40
3:J:894:GLN:HB2	3:J:904:LYS:HZ2	1.86	0.40
3:I:756:TYR:CG	3:I:757:ARG:N	2.90	0.40
3:H:328:LEU:HD11	3:H:339:ALA:HB2	2.04	0.40
3:H:457:ILE:HG22	3:H:458:TRP:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:634:TRP:HA	3:H:755:HIS:HD1	1.87	0.40
3:H:666:LEU:HA	3:H:704:ARG:HE	1.86	0.40
3:H:781:ILE:HD12	3:H:781:ILE:HA	1.86	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	
3	A	877/972 (90%)	798 (91%)	77 (9%)	2 (0%)	43	71
3	B	879/972 (90%)	795 (90%)	82 (9%)	2 (0%)	43	71
3	C	882/972 (91%)	781 (88%)	98 (11%)	3 (0%)	36	66
3	D	879/972 (90%)	803 (91%)	72 (8%)	4 (0%)	24	55
3	E	890/972 (92%)	817 (92%)	70 (8%)	3 (0%)	36	66
3	F	878/972 (90%)	796 (91%)	80 (9%)	2 (0%)	43	71
3	G	890/972 (92%)	811 (91%)	77 (9%)	2 (0%)	43	71
3	H	873/972 (90%)	801 (92%)	71 (8%)	1 (0%)	48	76
3	I	872/972 (90%)	806 (92%)	64 (7%)	2 (0%)	43	71
3	J	874/972 (90%)	814 (93%)	58 (7%)	2 (0%)	43	71
3	K	871/972 (90%)	796 (91%)	72 (8%)	3 (0%)	36	66
3	L	868/972 (89%)	794 (92%)	73 (8%)	1 (0%)	48	76
All	All	10533/11664 (90%)	9612 (91%)	894 (8%)	27 (0%)	37	66

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	852	VAL

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Mol	Chain	Res	Type
3	C	675	LYS
3	F	946	SER
3	C	148	GLU
3	D	946	SER
3	E	946	SER
3	L	946	SER
3	J	946	SER
3	A	946	SER
3	B	946	SER
3	C	946	SER
3	D	704	ARG
3	G	946	SER
3	K	355	LYS
3	K	946	SER
3	I	719	LEU
3	I	946	SER
3	H	870	ILE
3	D	696	LYS
3	G	241	ILE
3	F	241	ILE
3	A	241	ILE
3	B	241	ILE
3	E	241	ILE
3	K	297	ASP
3	J	297	ASP
3	D	297	ASP

5.3.2 Protein sidechains (i)

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
3	A	800/879 (91%)	798 (100%)	2 (0%)	86 86
3	B	802/879 (91%)	793 (99%)	9 (1%)	65 76
3	C	805/879 (92%)	793 (98%)	12 (2%)	57 73
3	D	802/879 (91%)	781 (97%)	21 (3%)	40 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	810/879 (92%)	805 (99%)	5 (1%)	78 82
3	F	801/879 (91%)	801 (100%)	0	100 100
3	G	810/879 (92%)	809 (100%)	1 (0%)	88 91
3	H	797/879 (91%)	787 (99%)	10 (1%)	61 75
3	I	796/879 (91%)	790 (99%)	6 (1%)	73 79
3	J	798/879 (91%)	790 (99%)	8 (1%)	68 77
3	K	795/879 (90%)	790 (99%)	5 (1%)	78 82
3	L	794/879 (90%)	794 (100%)	0	100 100
All	All	9610/10548 (91%)	9531 (99%)	79 (1%)	70 79

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	383	HIS
3	A	870	ILE
3	B	299	GLU
3	B	303	LEU
3	B	304	HIS
3	B	389	GLN
3	B	642	LYS
3	B	646	MET
3	B	647	ARG
3	B	866	TYR
3	B	872	VAL
3	C	144	THR
3	C	146	LYS
3	C	194	ASN
3	C	196	GLU
3	C	199	LEU
3	C	200	ASP
3	C	202	HIS
3	C	229	LEU
3	C	230	VAL
3	C	235	ASP
3	C	239	ILE
3	C	871	ASN
3	D	345	LYS
3	D	349	LYS
3	D	351	ASN

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Mol	Chain	Res	Type
3	D	356	GLU
3	D	357	LYS
3	D	359	GLU
3	D	360	LYS
3	D	361	LEU
3	D	705	LEU
3	D	706	LYS
3	D	707	GLU
3	D	709	VAL
3	D	714	VAL
3	D	715	THR
3	D	717	ARG
3	D	718	GLU
3	D	719	LEU
3	D	720	ASN
3	D	722	LYS
3	D	725	SER
3	D	739	ASN
3	E	60	LEU
3	E	66	LEU
3	E	414	GLU
3	E	417	MET
3	E	421	VAL
3	G	843	VAL
3	K	348	GLU
3	K	349	LYS
3	K	355	LYS
3	K	642	LYS
3	K	645	LEU
3	J	774	LYS
3	J	775	LYS
3	J	777	ASP
3	J	779	ARG
3	J	781	ILE
3	J	782	HIS
3	J	783	GLU
3	J	785	ILE
3	I	343	SER
3	I	345	LYS
3	I	349	LYS
3	I	355	LYS
3	I	714	VAL

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Mol	Chain	Res	Type
3	I	781	ILE
3	H	290	LEU
3	H	295	LEU
3	H	299	GLU
3	H	738	TYR
3	H	740	PHE
3	H	742	ILE
3	H	774	LYS
3	H	777	ASP
3	H	779	ARG
3	H	781	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	78	GLN
3	A	120	HIS
3	A	178	GLN
3	A	202	HIS
3	A	308	ASN
3	A	323	ASN
3	A	330	ASN
3	A	351	ASN
3	A	491	HIS
3	A	530	GLN
3	A	695	ASN
3	A	701	ASN
3	A	747	HIS
3	B	51	ASN
3	B	260	ASN
3	B	262	GLN
3	B	351	ASN
3	B	836	HIS
3	B	854	ASN
3	B	886	ASN
3	B	910	HIS
3	C	17	GLN
3	C	105	ASN
3	C	179	HIS
3	C	202	HIS
3	C	308	ASN
3	C	330	ASN

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Mol	Chain	Res	Type
3	C	428	ASN
3	C	578	GLN
3	C	720	ASN
3	C	871	ASN
3	C	886	ASN
3	D	51	ASN
3	D	105	ASN
3	D	351	ASN
3	D	389	GLN
3	D	502	ASN
3	D	677	ASN
3	D	770	ASN
3	D	854	ASN
3	D	886	ASN
3	E	78	GLN
3	E	105	ASN
3	E	260	ASN
3	E	323	ASN
3	E	330	ASN
3	E	415	HIS
3	E	755	HIS
3	E	770	ASN
3	E	869	ASN
3	E	886	ASN
3	F	304	HIS
3	F	389	GLN
3	F	502	ASN
3	F	898	ASN
3	F	910	HIS
3	G	51	ASN
3	G	179	HIS
3	G	190	GLN
3	G	260	ASN
3	G	262	GLN
3	G	308	ASN
3	G	351	ASN
3	G	494	GLN
3	G	701	ASN
3	G	721	GLN
3	G	723	GLN
3	G	832	GLN
3	G	854	ASN

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Mol	Chain	Res	Type
3	G	867	ASN
3	G	875	HIS
3	G	916	GLN
3	L	17	GLN
3	L	51	ASN
3	L	105	ASN
3	L	202	HIS
3	L	262	GLN
3	L	296	HIS
3	L	330	ASN
3	L	502	ASN
3	L	530	GLN
3	L	701	ASN
3	L	869	ASN
3	L	875	HIS
3	K	17	GLN
3	K	74	GLN
3	K	105	ASN
3	K	242	HIS
3	K	262	GLN
3	K	502	ASN
3	K	530	GLN
3	K	695	ASN
3	K	721	GLN
3	K	770	ASN
3	K	832	GLN
3	K	854	ASN
3	K	898	ASN
3	J	78	GLN
3	J	190	GLN
3	J	202	HIS
3	J	396	GLN
3	J	494	GLN
3	J	574	HIS
3	J	701	ASN
3	J	770	ASN
3	J	832	GLN
3	J	869	ASN
3	J	886	ASN
3	I	51	ASN
3	I	105	ASN
3	I	190	GLN

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Mol	Chain	Res	Type
3	I	262	GLN
3	I	323	ASN
3	I	351	ASN
3	I	367	HIS
3	I	415	HIS
3	I	542	GLN
3	I	721	GLN
3	I	792	ASN
3	I	886	ASN
3	I	948	ASN
3	H	51	ASN
3	H	190	GLN
3	H	260	ASN
3	H	262	GLN
3	H	323	ASN
3	H	330	ASN
3	H	396	GLN
3	H	502	ASN
3	H	721	GLN
3	H	832	GLN

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

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ANP	A	1001	5	33,33,33	0.94	4 (12%)	45,52,52	0.59	0
4	ANP	B	1001	5	33,33,33	0.89	4 (12%)	45,52,52	0.53	0
4	ANP	F	1001	5	33,33,33	0.93	4 (12%)	45,52,52	0.60	0
4	ANP	G	1001	-	33,33,33	0.92	4 (12%)	45,52,52	0.61	0
4	ANP	L	1001	-	33,33,33	0.95	4 (12%)	45,52,52	0.64	0
4	ANP	J	1001	-	33,33,33	0.88	4 (12%)	45,52,52	0.67	2 (4%)
4	ANP	E	1001	5	33,33,33	0.96	4 (12%)	45,52,52	0.56	0
4	ANP	C	1001	5	33,33,33	0.93	4 (12%)	45,52,52	0.62	0
4	ANP	I	1001	-	33,33,33	0.93	4 (12%)	45,52,52	0.60	0
4	ANP	H	1001	-	33,33,33	0.92	4 (12%)	45,52,52	0.59	0
4	ANP	K	1001	-	33,33,33	0.93	4 (12%)	45,52,52	0.60	0
4	ANP	D	1001	5	33,33,33	0.92	4 (12%)	45,52,52	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	A	1001	5	-	5/18/38/38	0/3/3/3
4	ANP	B	1001	5	-	7/18/38/38	0/3/3/3
4	ANP	F	1001	5	-	8/18/38/38	0/3/3/3
4	ANP	G	1001	-	-	7/18/38/38	0/3/3/3
4	ANP	L	1001	-	-	9/18/38/38	0/3/3/3
4	ANP	J	1001	-	-	7/18/38/38	0/3/3/3
4	ANP	E	1001	5	-	10/18/38/38	0/3/3/3
4	ANP	C	1001	5	-	8/18/38/38	0/3/3/3
4	ANP	I	1001	-	-	7/18/38/38	0/3/3/3
4	ANP	H	1001	-	-	7/18/38/38	0/3/3/3
4	ANP	K	1001	-	-	3/18/38/38	0/3/3/3
4	ANP	D	1001	5	-	7/18/38/38	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1001	ANP	PB-O3A	-2.71	1.55	1.59
4	E	1001	ANP	PB-O3A	-2.68	1.55	1.59
4	A	1001	ANP	PB-O3A	-2.66	1.55	1.59
4	B	1001	ANP	PB-O3A	-2.65	1.55	1.59
4	F	1001	ANP	PB-O3A	-2.60	1.55	1.59
4	I	1001	ANP	PG-O1G	2.56	1.50	1.46
4	D	1001	ANP	PB-O3A	-2.56	1.55	1.59
4	E	1001	ANP	PG-O1G	2.54	1.50	1.46
4	G	1001	ANP	PG-O1G	2.54	1.50	1.46
4	F	1001	ANP	PG-O1G	2.51	1.50	1.46
4	L	1001	ANP	PG-O1G	2.49	1.50	1.46
4	K	1001	ANP	PG-O1G	2.48	1.49	1.46
4	L	1001	ANP	PG-N3B	2.48	1.69	1.63
4	H	1001	ANP	PG-O1G	2.48	1.49	1.46
4	C	1001	ANP	PG-O1G	2.47	1.49	1.46
4	K	1001	ANP	PB-O3A	-2.46	1.56	1.59
4	A	1001	ANP	PG-O1G	2.45	1.49	1.46
4	K	1001	ANP	PB-O1B	2.44	1.49	1.46
4	J	1001	ANP	PG-O1G	2.43	1.49	1.46
4	L	1001	ANP	PB-O3A	-2.43	1.56	1.59
4	D	1001	ANP	PG-O1G	2.43	1.49	1.46
4	I	1001	ANP	PB-O3A	-2.43	1.56	1.59
4	B	1001	ANP	PG-O1G	2.43	1.49	1.46
4	L	1001	ANP	PB-O1B	2.40	1.49	1.46
4	G	1001	ANP	PG-N3B	2.39	1.69	1.63
4	I	1001	ANP	PB-O1B	2.37	1.49	1.46
4	H	1001	ANP	PG-N3B	2.36	1.69	1.63
4	H	1001	ANP	PB-O3A	-2.36	1.56	1.59
4	K	1001	ANP	PG-N3B	2.35	1.69	1.63
4	H	1001	ANP	PB-O1B	2.35	1.49	1.46
4	G	1001	ANP	PB-O3A	-2.34	1.56	1.59
4	E	1001	ANP	PB-O1B	2.34	1.49	1.46
4	D	1001	ANP	PB-O1B	2.33	1.49	1.46
4	D	1001	ANP	PG-N3B	2.33	1.69	1.63
4	G	1001	ANP	PB-O1B	2.32	1.49	1.46
4	I	1001	ANP	PG-N3B	2.32	1.69	1.63
4	E	1001	ANP	PG-N3B	2.31	1.69	1.63
4	J	1001	ANP	PG-N3B	2.30	1.69	1.63
4	F	1001	ANP	PG-N3B	2.29	1.69	1.63
4	C	1001	ANP	PB-O1B	2.28	1.49	1.46
4	A	1001	ANP	PB-O1B	2.28	1.49	1.46
4	A	1001	ANP	PG-N3B	2.27	1.69	1.63
4	J	1001	ANP	PB-O3A	-2.25	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1001	ANP	PB-O1B	2.17	1.49	1.46
4	F	1001	ANP	PB-O1B	2.16	1.49	1.46
4	C	1001	ANP	PG-N3B	2.13	1.68	1.63
4	B	1001	ANP	PB-O1B	2.11	1.49	1.46
4	B	1001	ANP	PG-N3B	2.10	1.68	1.63

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1001	ANP	O1G-PG-N3B	-2.03	108.79	111.77
4	J	1001	ANP	O1B-PB-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	ANP	PB-N3B-PG-O1G
4	A	1001	ANP	PG-N3B-PB-O1B
4	A	1001	ANP	C5'-O5'-PA-O3A
4	B	1001	ANP	PB-N3B-PG-O1G
4	B	1001	ANP	C5'-O5'-PA-O1A
4	B	1001	ANP	C5'-O5'-PA-O2A
4	B	1001	ANP	C5'-O5'-PA-O3A
4	C	1001	ANP	PB-N3B-PG-O1G
4	C	1001	ANP	PG-N3B-PB-O1B
4	C	1001	ANP	PA-O3A-PB-O2B
4	D	1001	ANP	PG-N3B-PB-O1B
4	D	1001	ANP	PG-N3B-PB-O3A
4	D	1001	ANP	PA-O3A-PB-O2B
4	D	1001	ANP	C5'-O5'-PA-O2A
4	D	1001	ANP	C5'-O5'-PA-O3A
4	E	1001	ANP	PG-N3B-PB-O1B
4	E	1001	ANP	PG-N3B-PB-O3A
4	E	1001	ANP	C5'-O5'-PA-O2A
4	E	1001	ANP	C5'-O5'-PA-O3A
4	F	1001	ANP	PB-N3B-PG-O1G
4	F	1001	ANP	PG-N3B-PB-O1B
4	F	1001	ANP	C5'-O5'-PA-O1A
4	F	1001	ANP	C5'-O5'-PA-O2A
4	F	1001	ANP	C5'-O5'-PA-O3A
4	G	1001	ANP	C5'-O5'-PA-O1A
4	G	1001	ANP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	G	1001	ANP	C5'-O5'-PA-O3A
4	G	1001	ANP	O4'-C4'-C5'-O5'
4	L	1001	ANP	PB-N3B-PG-O1G
4	L	1001	ANP	PG-N3B-PB-O1B
4	L	1001	ANP	PG-N3B-PB-O3A
4	K	1001	ANP	PB-N3B-PG-O1G
4	K	1001	ANP	C5'-O5'-PA-O1A
4	K	1001	ANP	C5'-O5'-PA-O3A
4	J	1001	ANP	PG-N3B-PB-O1B
4	J	1001	ANP	PA-O3A-PB-O2B
4	J	1001	ANP	C5'-O5'-PA-O1A
4	J	1001	ANP	C5'-O5'-PA-O2A
4	J	1001	ANP	C5'-O5'-PA-O3A
4	I	1001	ANP	PB-N3B-PG-O1G
4	I	1001	ANP	PG-N3B-PB-O1B
4	I	1001	ANP	C5'-O5'-PA-O1A
4	H	1001	ANP	PG-N3B-PB-O1B
4	H	1001	ANP	C5'-O5'-PA-O1A
4	A	1001	ANP	C3'-C4'-C5'-O5'
4	D	1001	ANP	O4'-C4'-C5'-O5'
4	D	1001	ANP	C3'-C4'-C5'-O5'
4	G	1001	ANP	C3'-C4'-C5'-O5'
4	L	1001	ANP	C3'-C4'-C5'-O5'
4	C	1001	ANP	O4'-C1'-N9-C8
4	A	1001	ANP	O4'-C4'-C5'-O5'
4	L	1001	ANP	O4'-C4'-C5'-O5'
4	I	1001	ANP	O4'-C4'-C5'-O5'
4	H	1001	ANP	O4'-C4'-C5'-O5'
4	C	1001	ANP	O4'-C1'-N9-C4
4	B	1001	ANP	C3'-C4'-C5'-O5'
4	B	1001	ANP	O4'-C4'-C5'-O5'
4	E	1001	ANP	O4'-C4'-C5'-O5'
4	F	1001	ANP	O4'-C4'-C5'-O5'
4	F	1001	ANP	C3'-C4'-C5'-O5'
4	I	1001	ANP	C3'-C4'-C5'-O5'
4	H	1001	ANP	C3'-C4'-C5'-O5'
4	E	1001	ANP	PB-O3A-PA-O1A
4	E	1001	ANP	C3'-C4'-C5'-O5'
4	J	1001	ANP	O4'-C4'-C5'-O5'
4	L	1001	ANP	C4'-C5'-O5'-PA
4	J	1001	ANP	C3'-C4'-C5'-O5'
4	G	1001	ANP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
4	L	1001	ANP	O4'-C1'-N9-C4
4	C	1001	ANP	C4'-C5'-O5'-PA
4	L	1001	ANP	O4'-C1'-N9-C8
4	B	1001	ANP	PG-N3B-PB-O3A
4	L	1001	ANP	C5'-O5'-PA-O1A
4	E	1001	ANP	C4'-C5'-O5'-PA
4	H	1001	ANP	C4'-C5'-O5'-PA
4	H	1001	ANP	PB-O3A-PA-O2A
4	E	1001	ANP	C2'-C1'-N9-C8
4	I	1001	ANP	C4'-C5'-O5'-PA
4	F	1001	ANP	PB-O3A-PA-O1A
4	I	1001	ANP	PB-O3A-PA-O2A
4	G	1001	ANP	C4'-C5'-O5'-PA
4	C	1001	ANP	PA-O3A-PB-O1B
4	C	1001	ANP	C3'-C4'-C5'-O5'
4	H	1001	ANP	PB-O3A-PA-O1A
4	E	1001	ANP	O4'-C1'-N9-C8

There are no ring outliers.

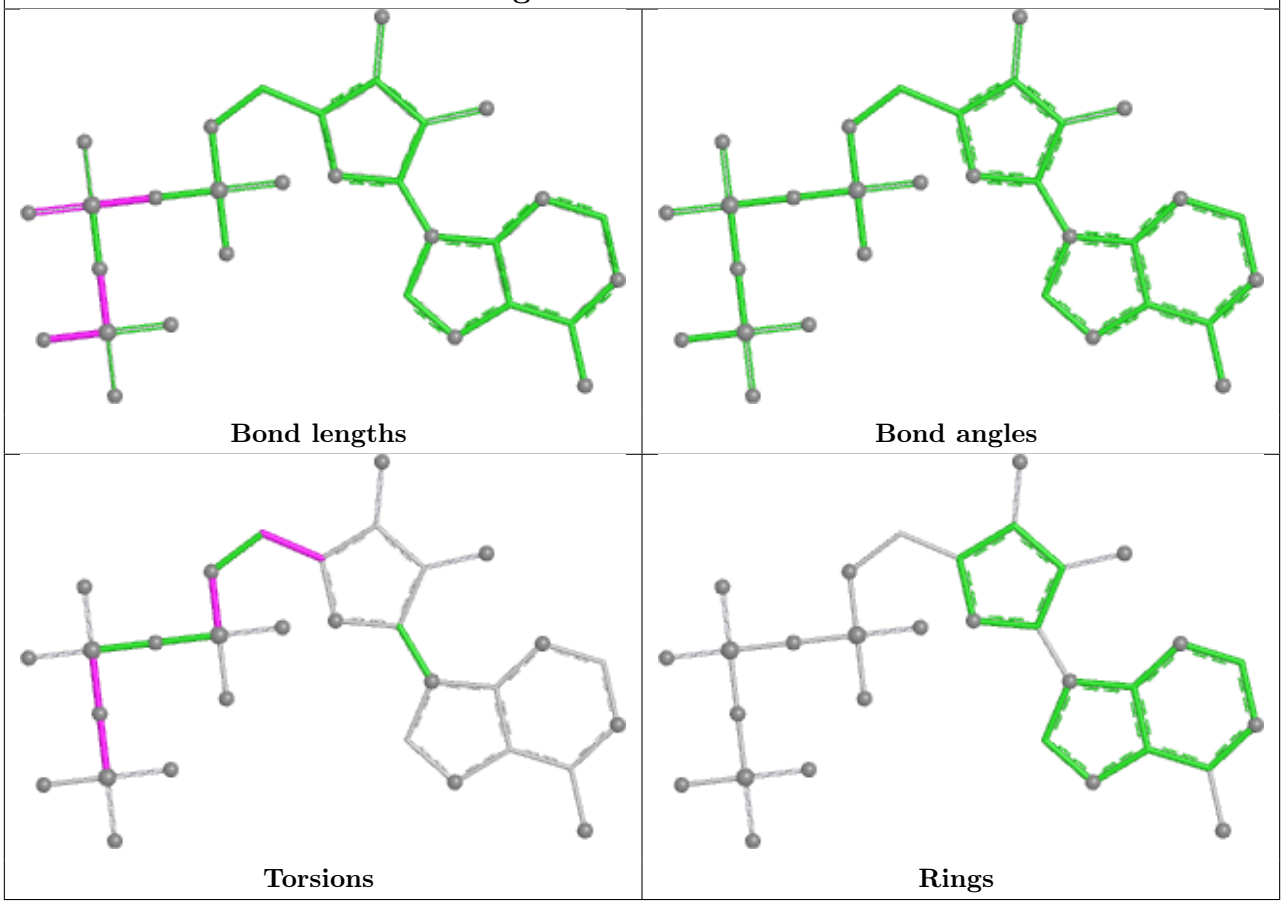
12 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	ANP	1	0
4	B	1001	ANP	5	0
4	F	1001	ANP	3	0
4	G	1001	ANP	3	0
4	L	1001	ANP	4	0
4	J	1001	ANP	11	0
4	E	1001	ANP	2	0
4	C	1001	ANP	8	0
4	I	1001	ANP	4	0
4	H	1001	ANP	5	0
4	K	1001	ANP	3	0
4	D	1001	ANP	2	0

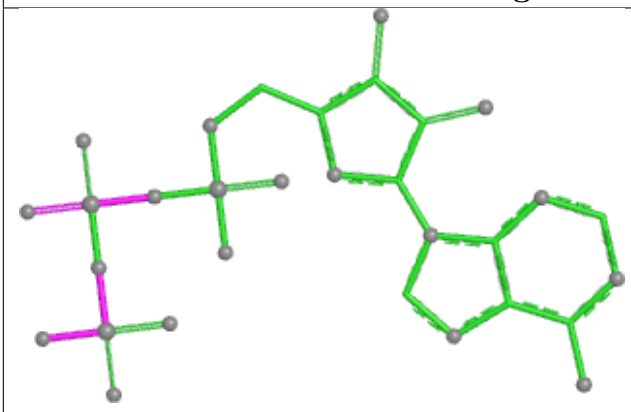
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

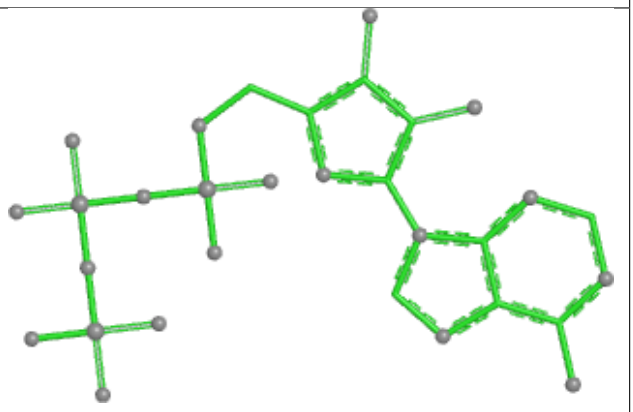
Ligand ANP A 1001



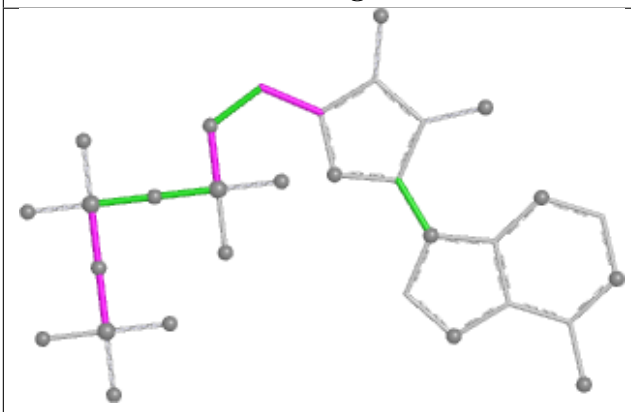
Ligand ANP B 1001



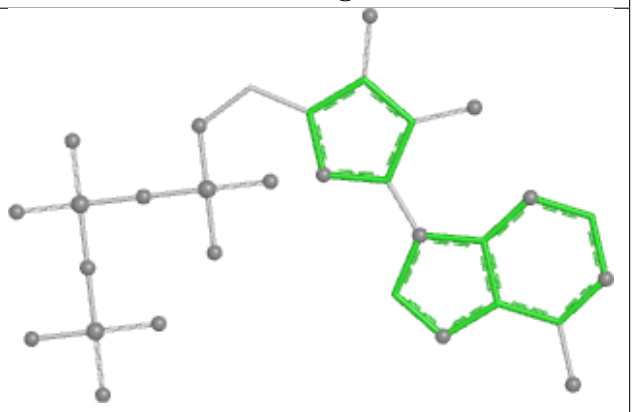
Bond lengths



Bond angles

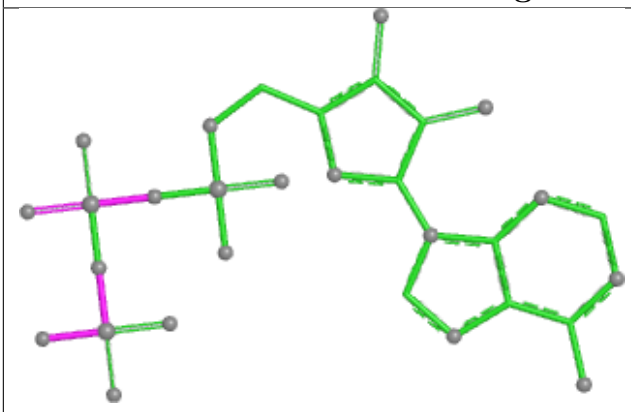


Torsions

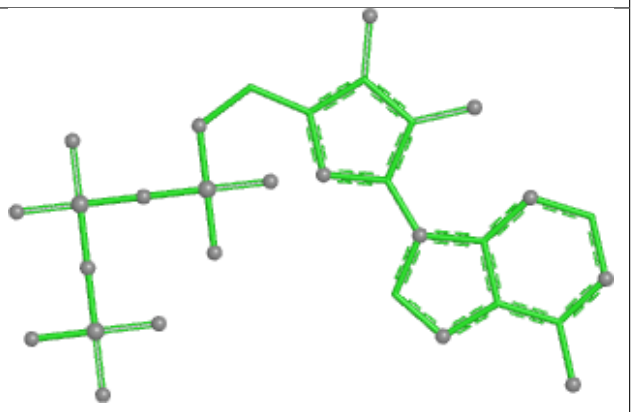


Rings

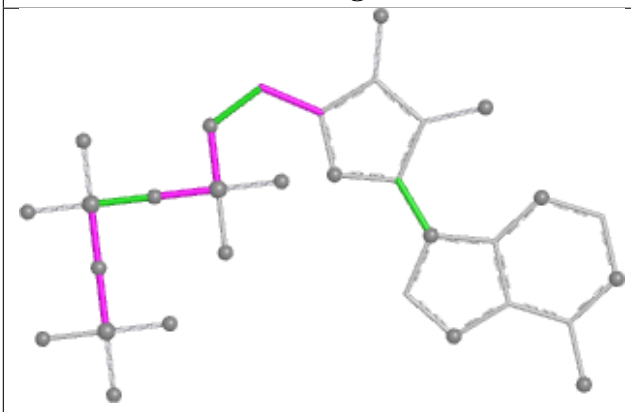
Ligand ANP F 1001



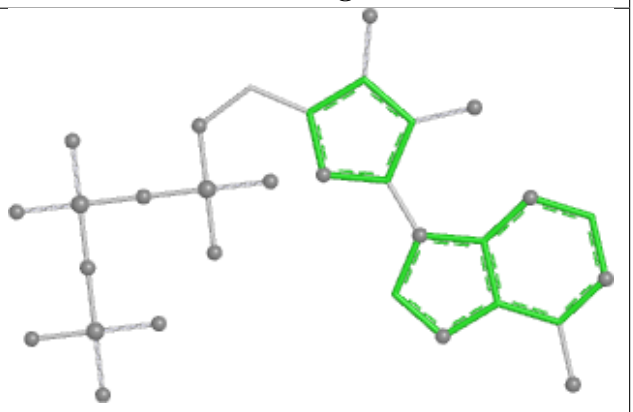
Bond lengths



Bond angles

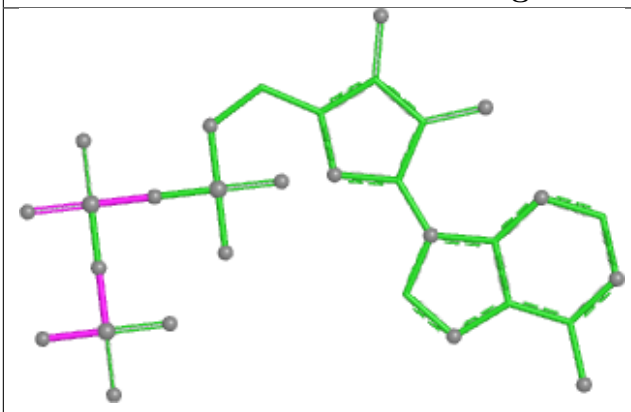


Torsions

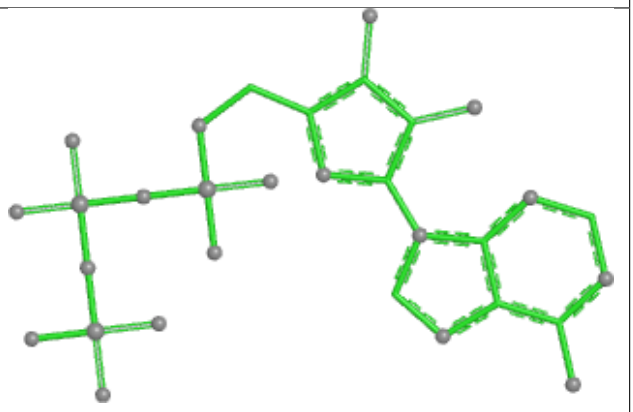


Rings

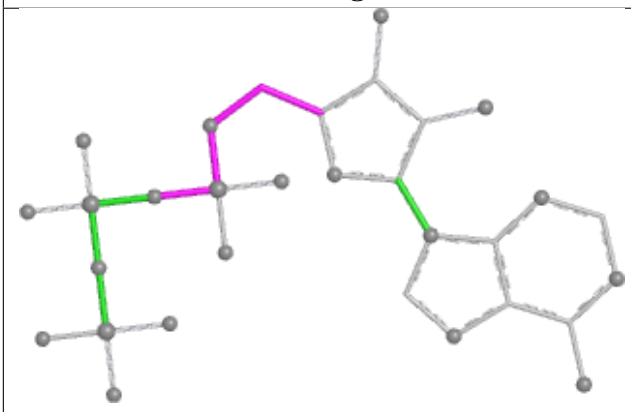
Ligand ANP G 1001



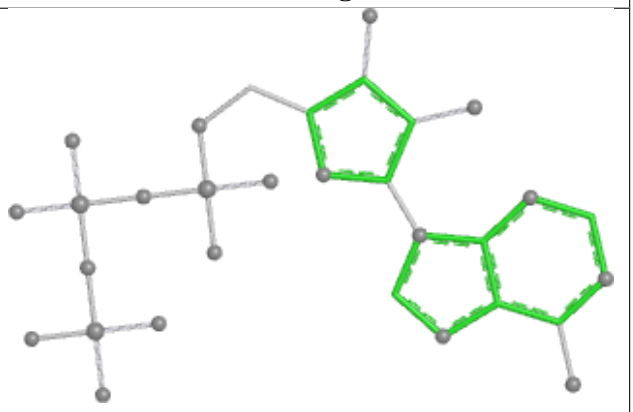
Bond lengths



Bond angles

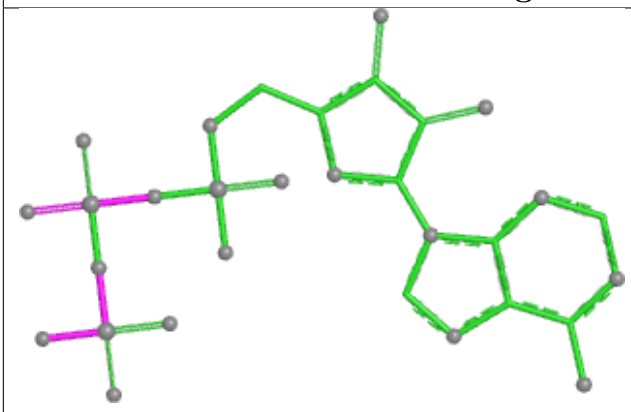


Torsions



Rings

Ligand ANP L 1001



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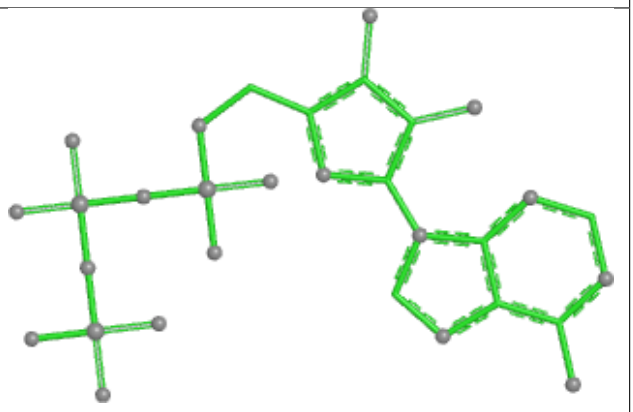
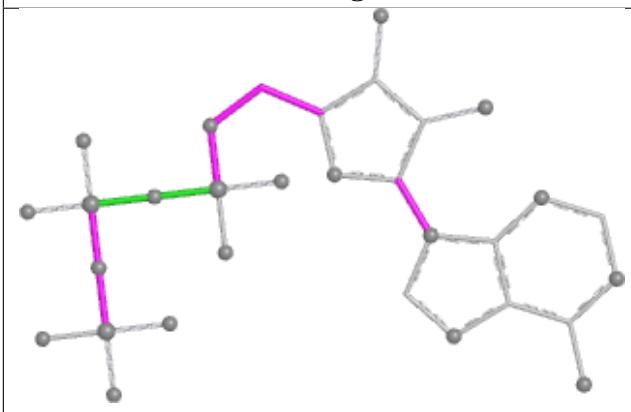
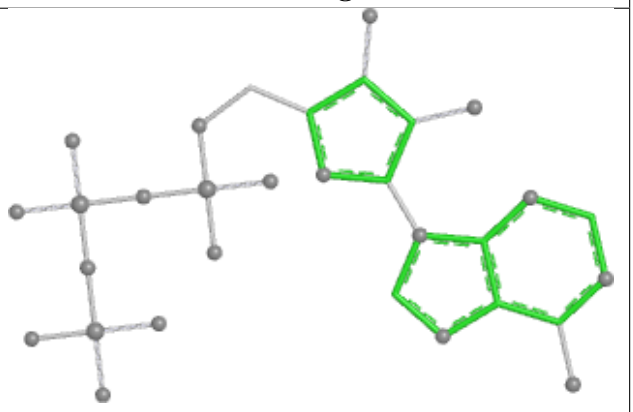


Bond angles

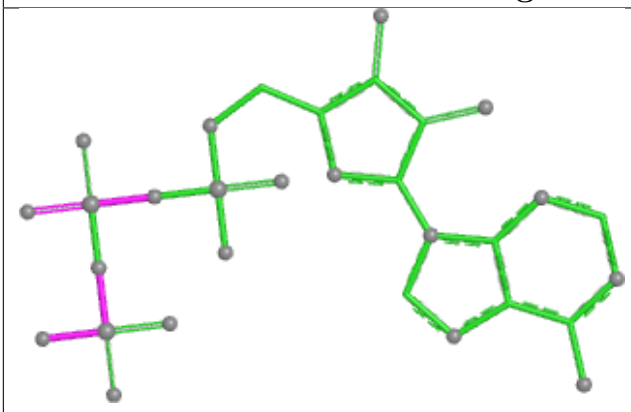


Torsions

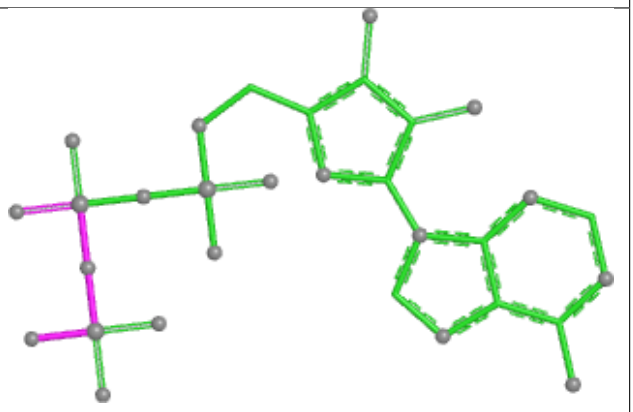


Rings

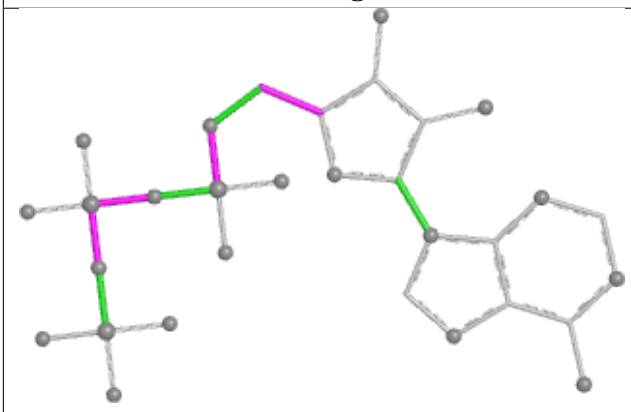
Ligand ANP J 1001



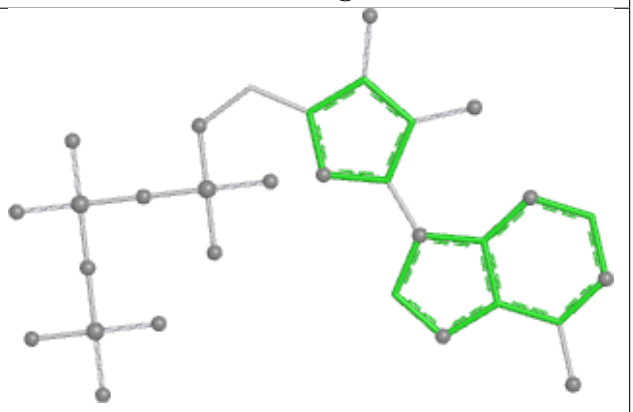
Bond lengths



Bond angles

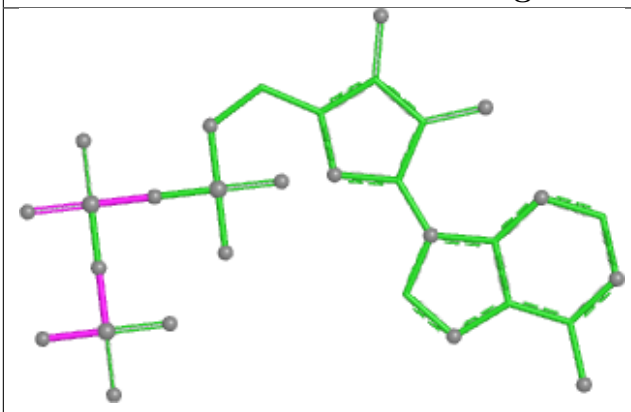


Torsions

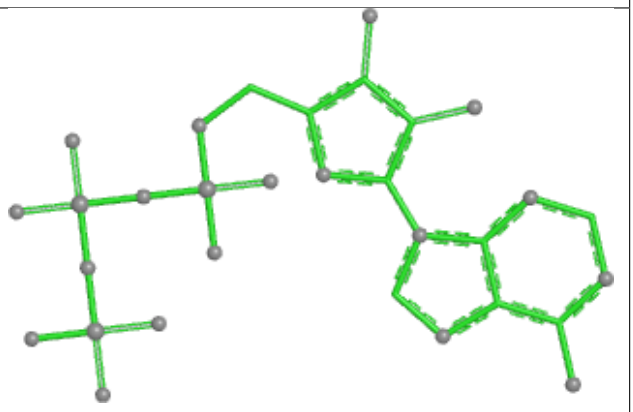


Rings

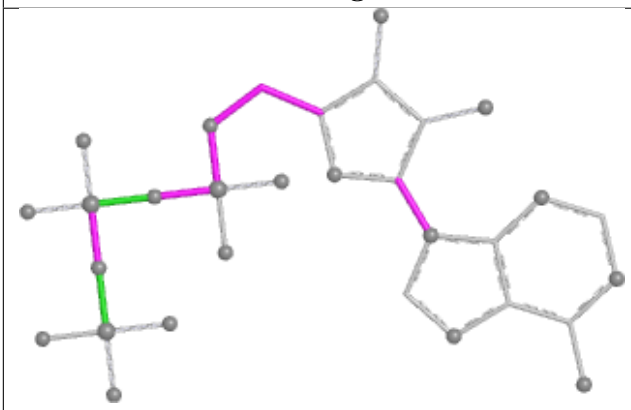
Ligand ANP E 1001



Bond lengths



Bond angles



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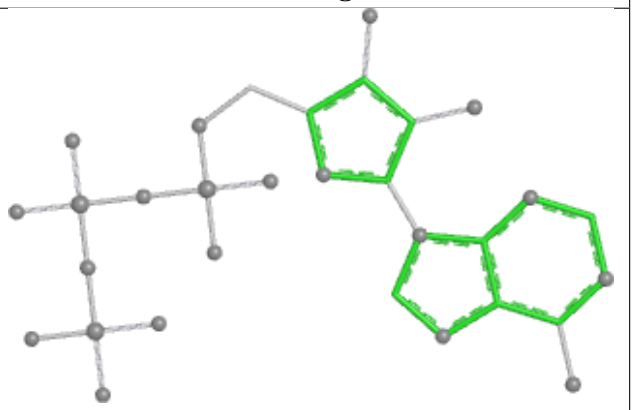
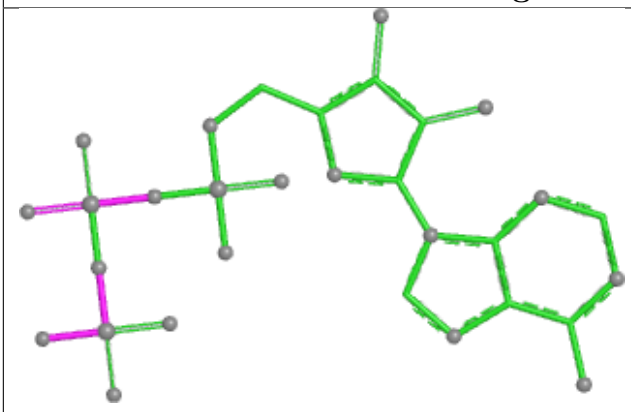
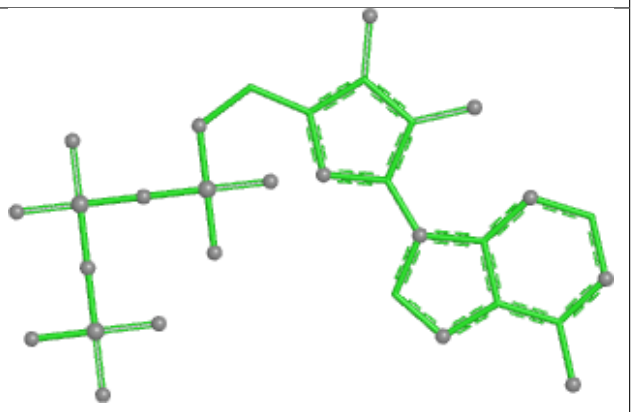


Rings

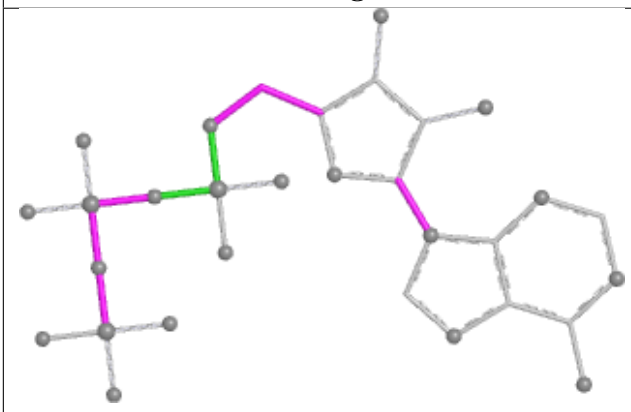
Ligand ANP C 1001



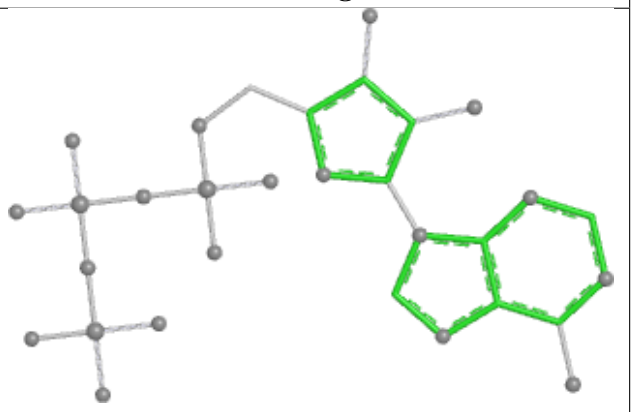
Bond lengths



Bond angles

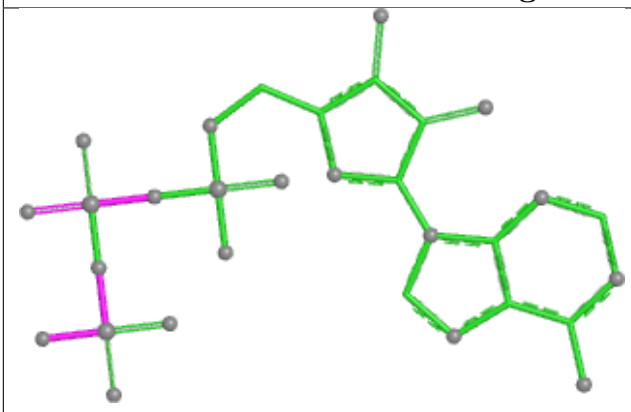


Torsions



Rings

Ligand ANP I 1001



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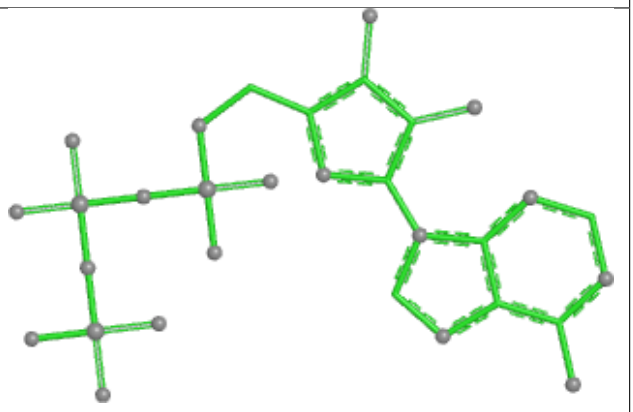
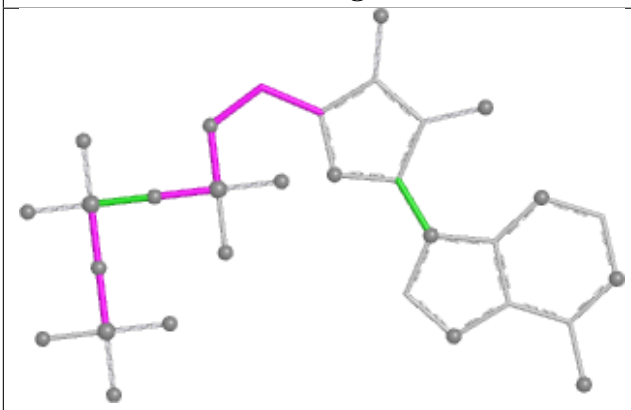
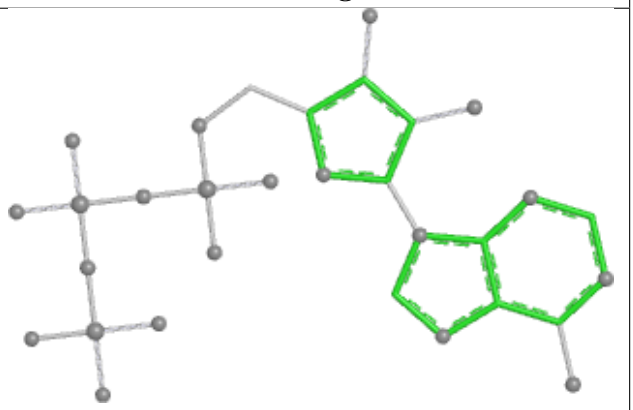


Bond angles

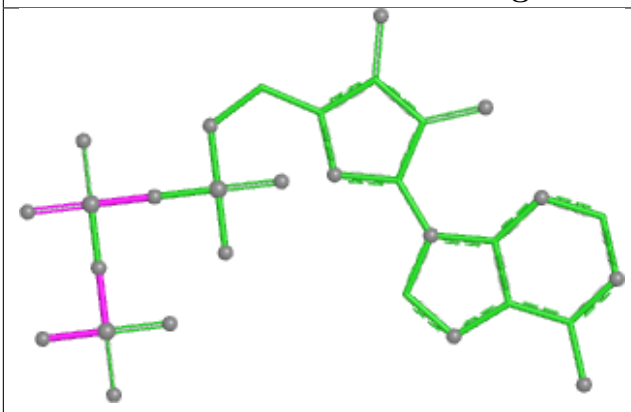


Torsions

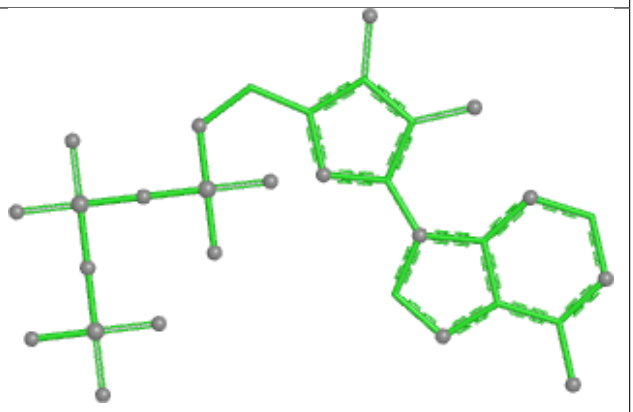


Rings

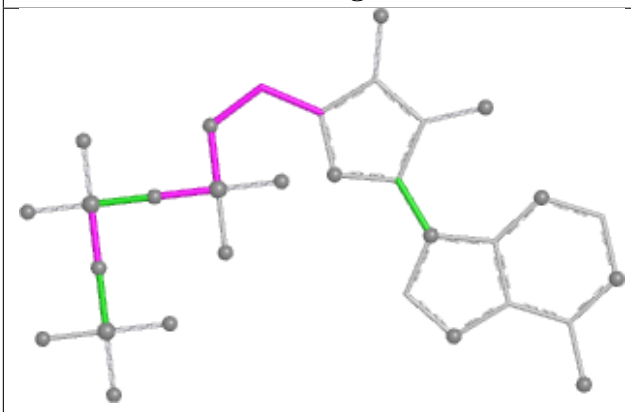
Ligand ANP H 1001



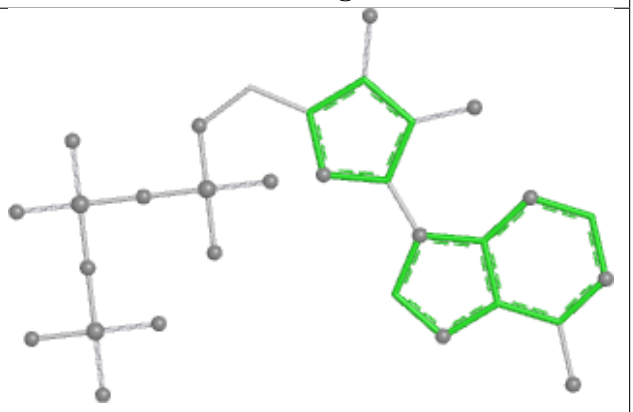
Bond lengths



Bond angles

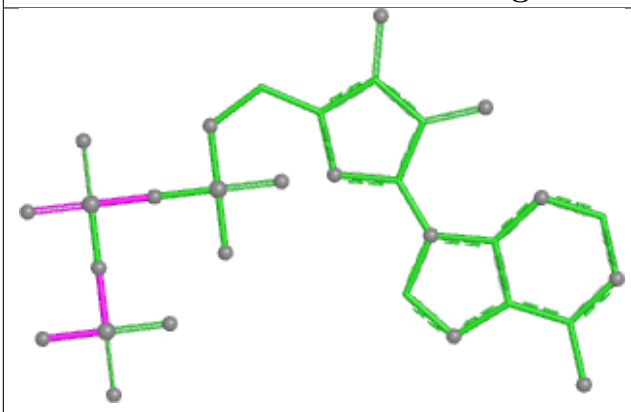


Torsions

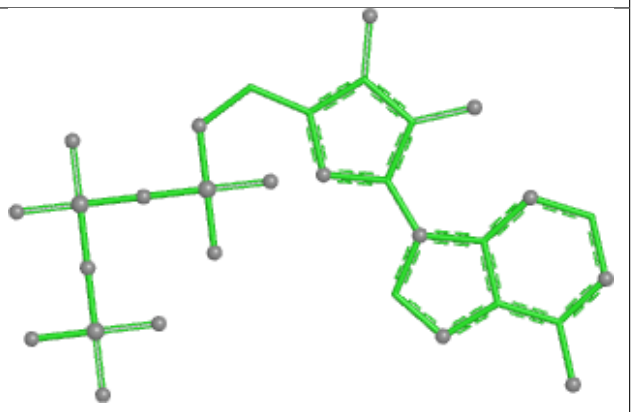


Rings

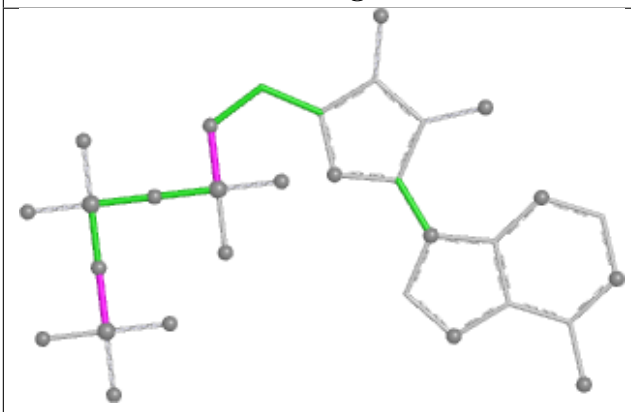
Ligand ANP K 1001



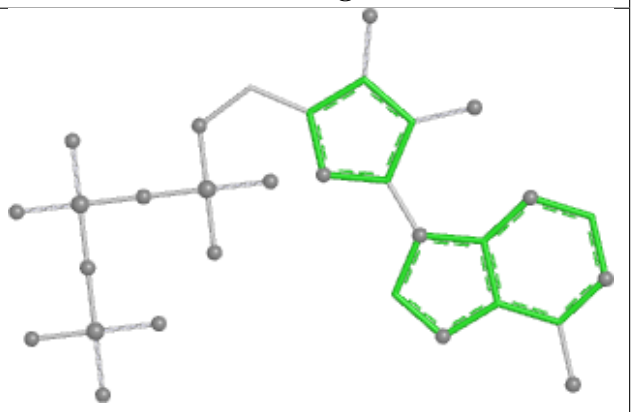
Bond lengths



Bond angles

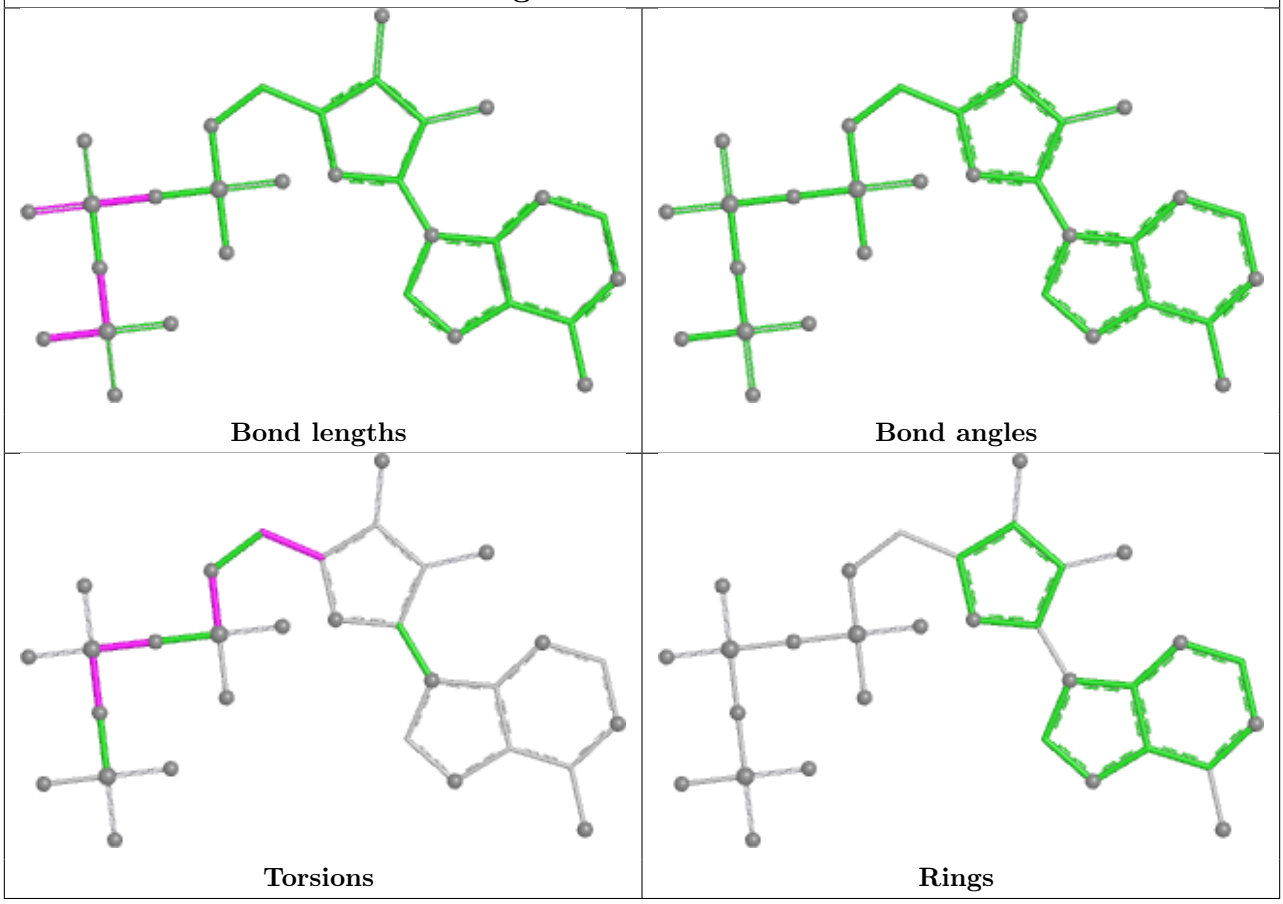


Torsions



Rings

Ligand ANP D 1001



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.

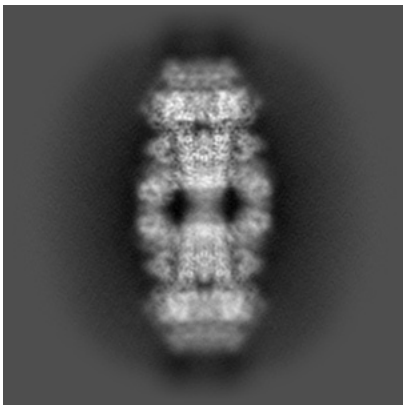
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37883. These allow visual inspection of the internal detail of the map and identification of artifacts.

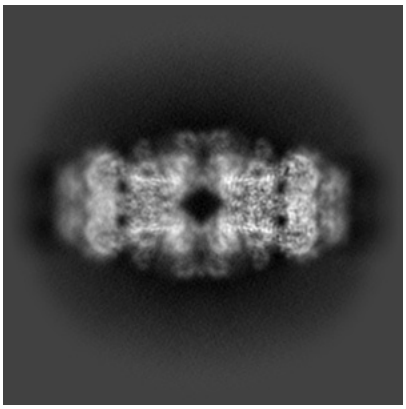
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

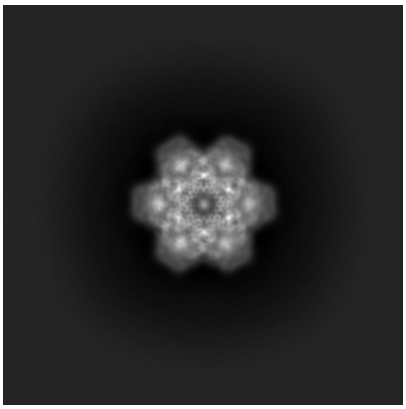
6.1.1 Primary map



X

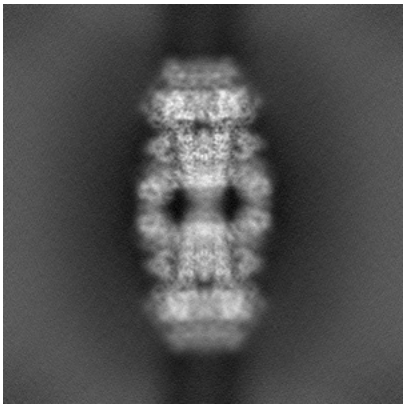


Y

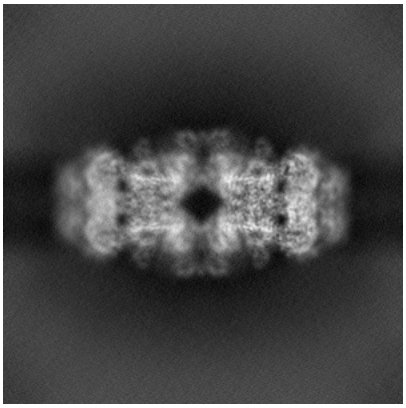


Z

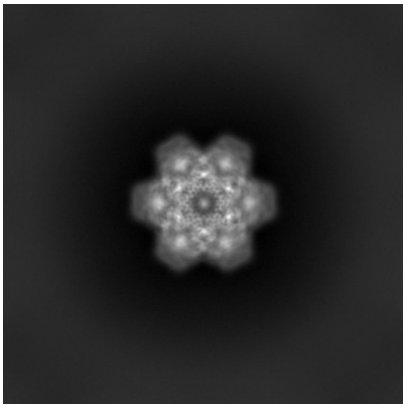
6.1.2 Raw map



X



Y

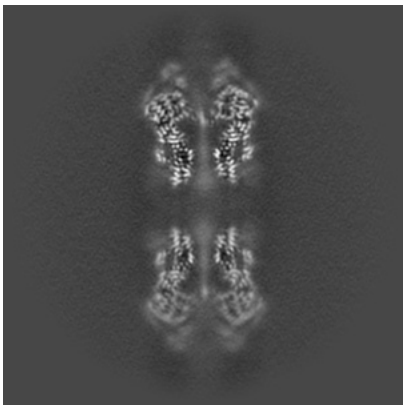


Z

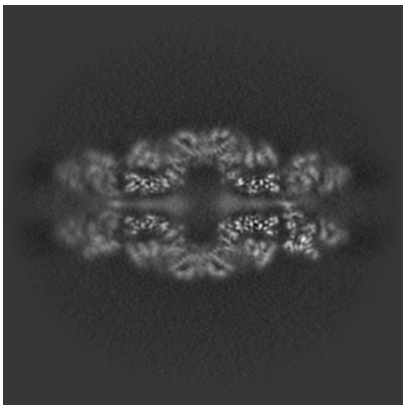
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

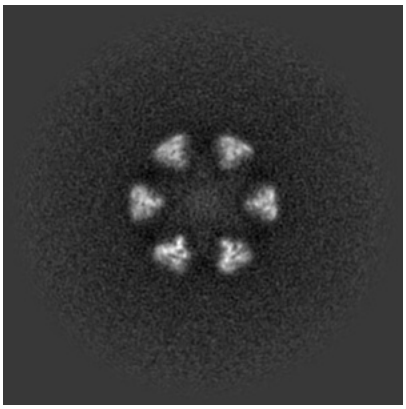
6.2.1 Primary map



X Index: 192

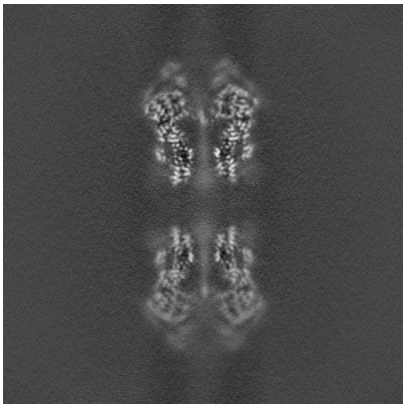


Y Index: 192

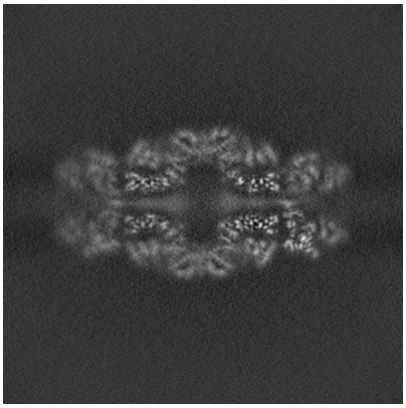


Z Index: 192

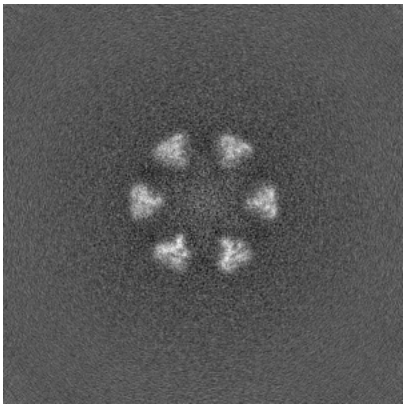
6.2.2 Raw map



X Index: 192



Y Index: 192

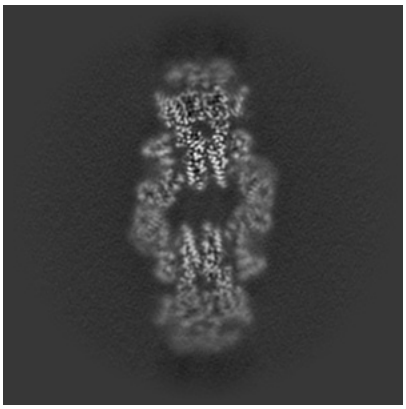


Z Index: 192

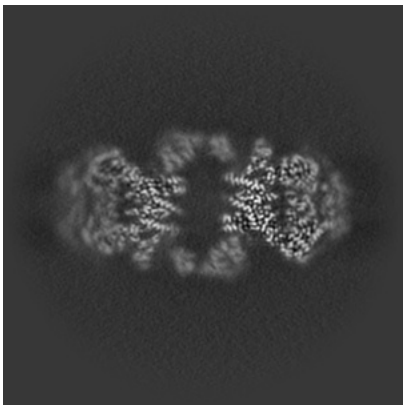
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

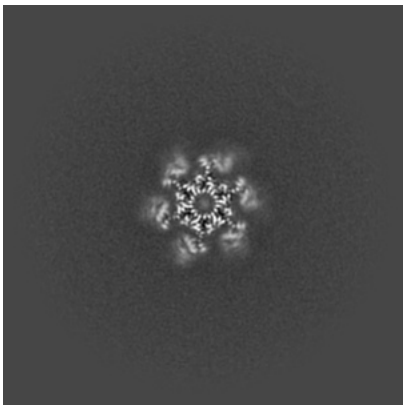
6.3.1 Primary map



X Index: 169

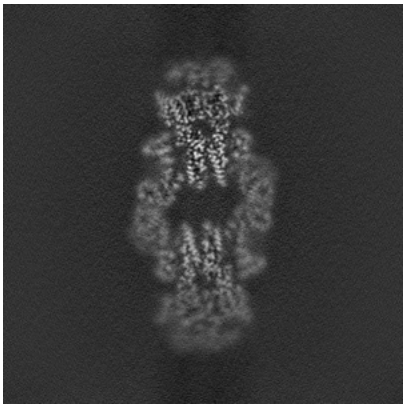


Y Index: 208

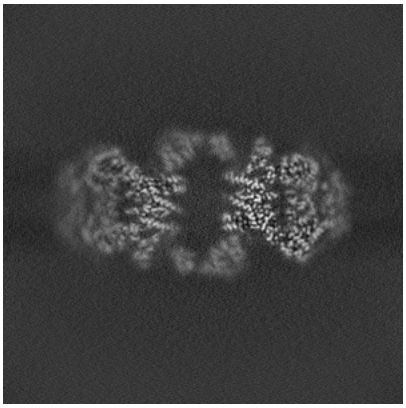


Z Index: 238

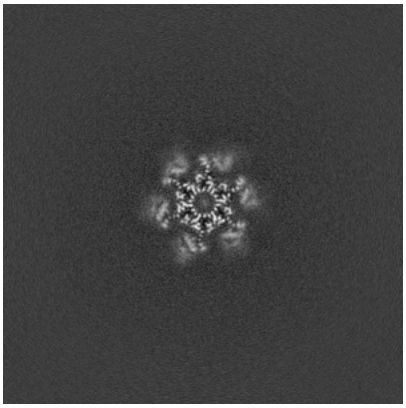
6.3.2 Raw map



X Index: 169



Y Index: 208

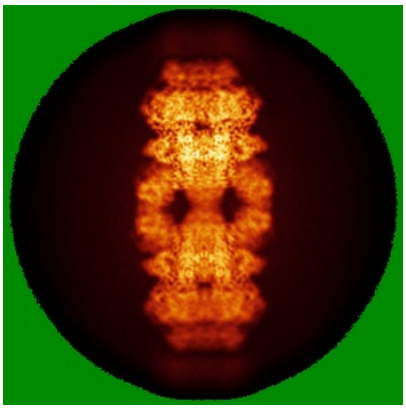


Z Index: 238

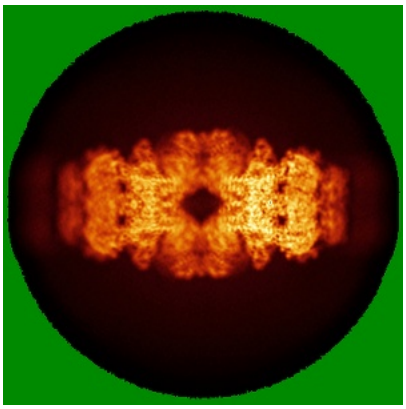
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

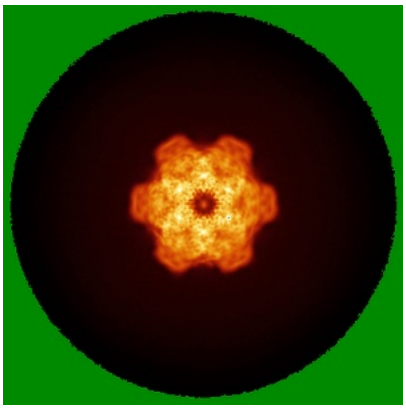
6.4.1 Primary map



X

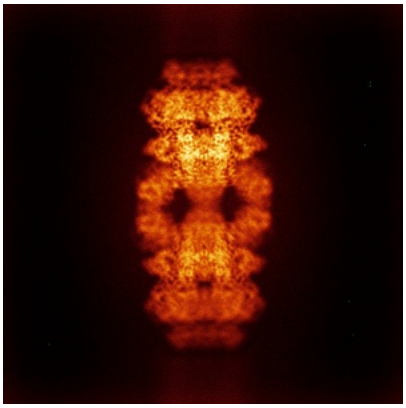


Y

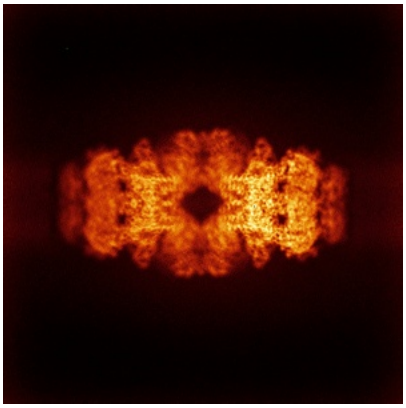


Z

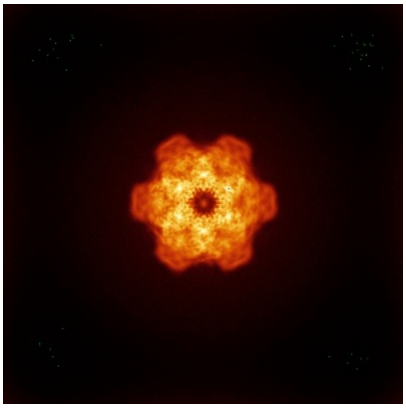
6.4.2 Raw map



X



Y

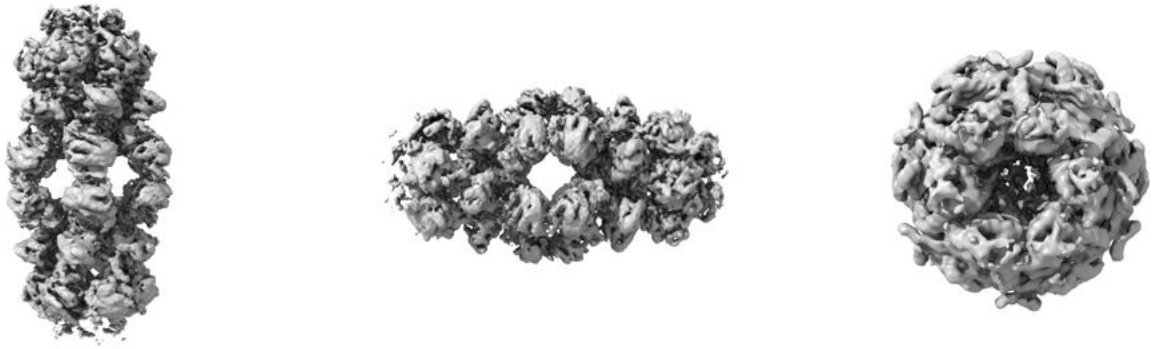


Z

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

6.5 Orthogonal surface views (i)

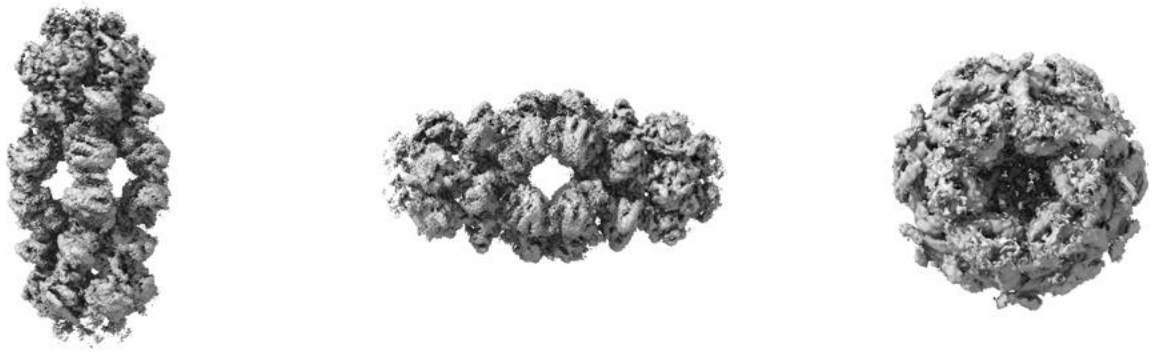
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.258. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

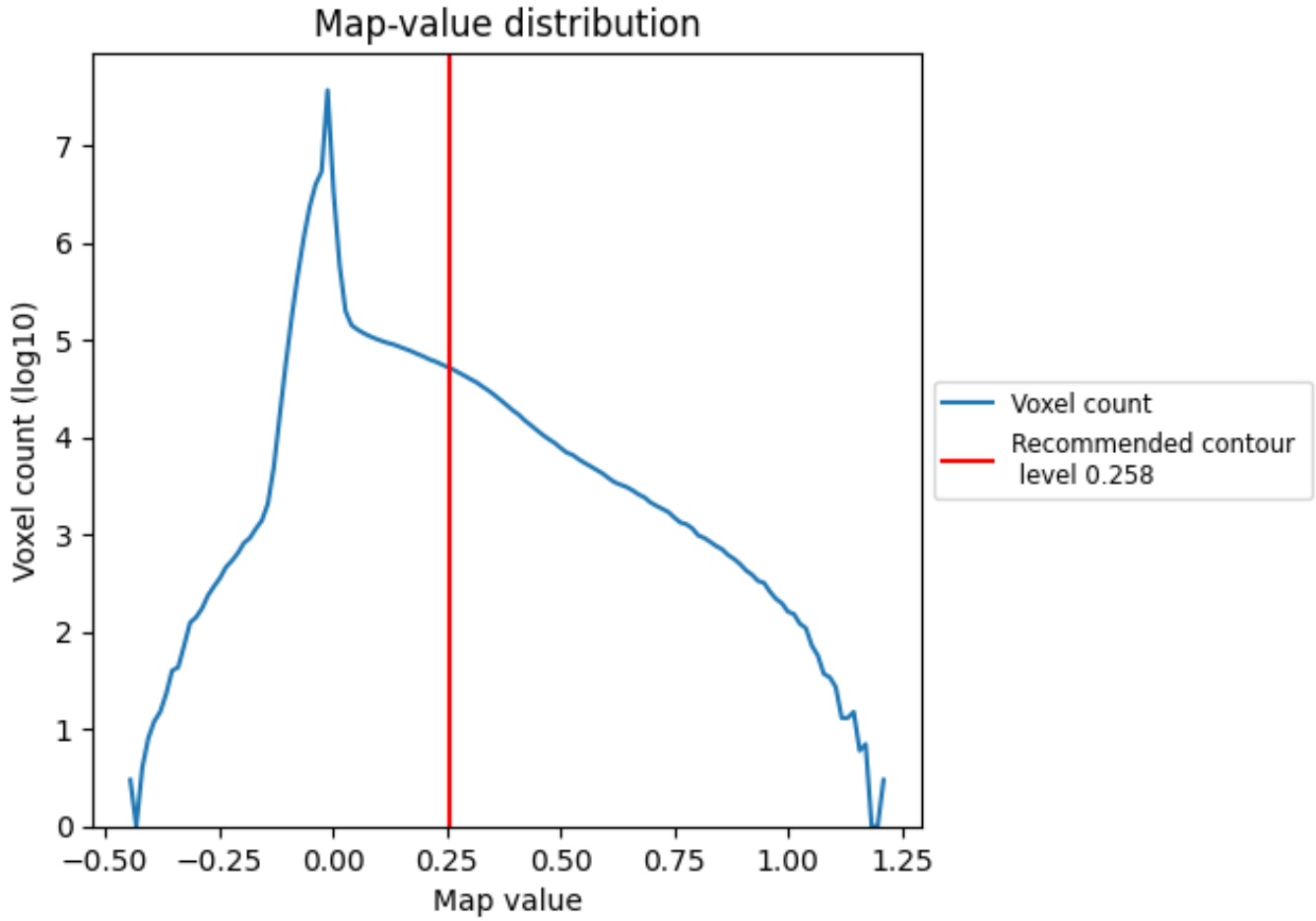
6.6 Mask visualisation (i)

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

7 Map analysis

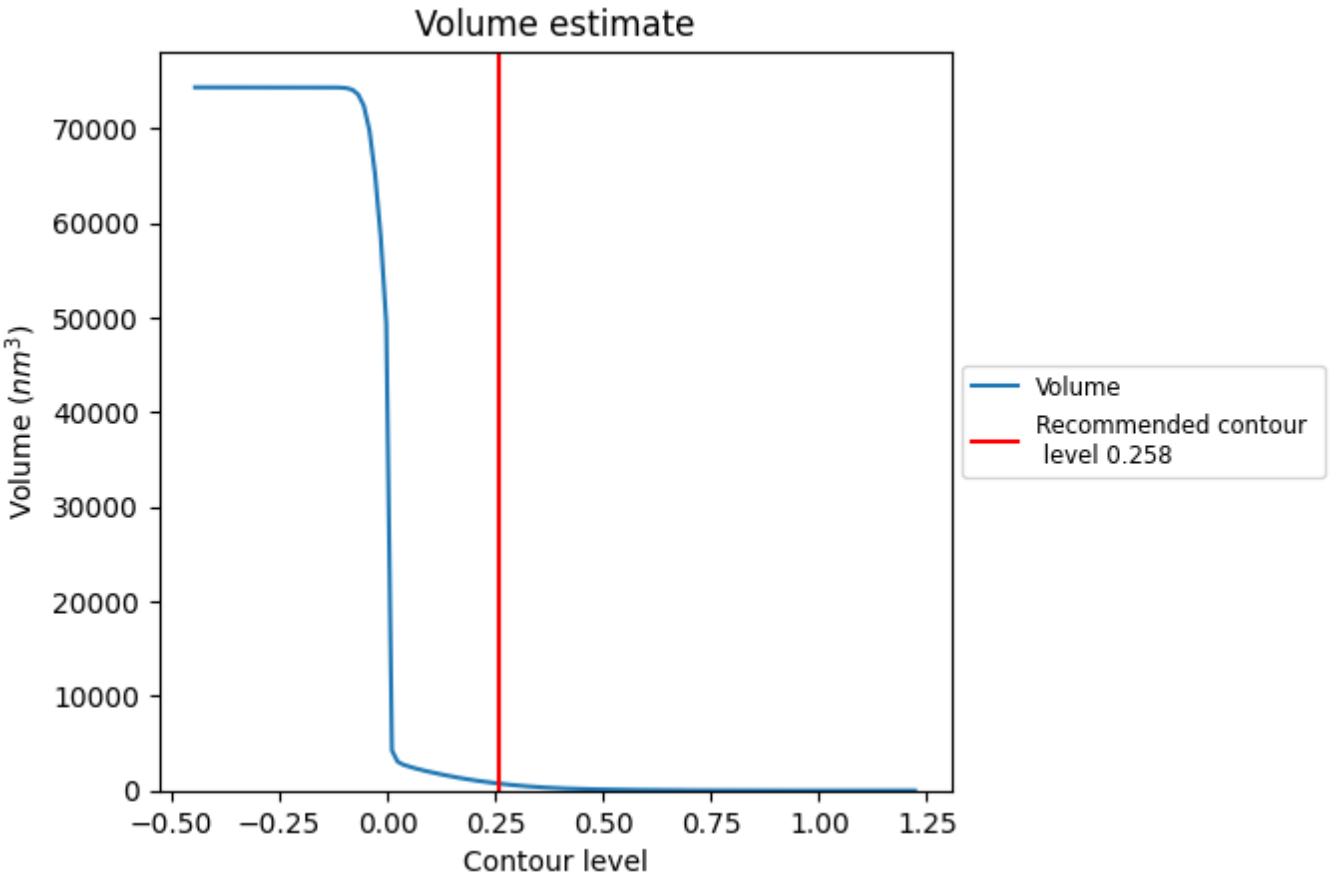
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

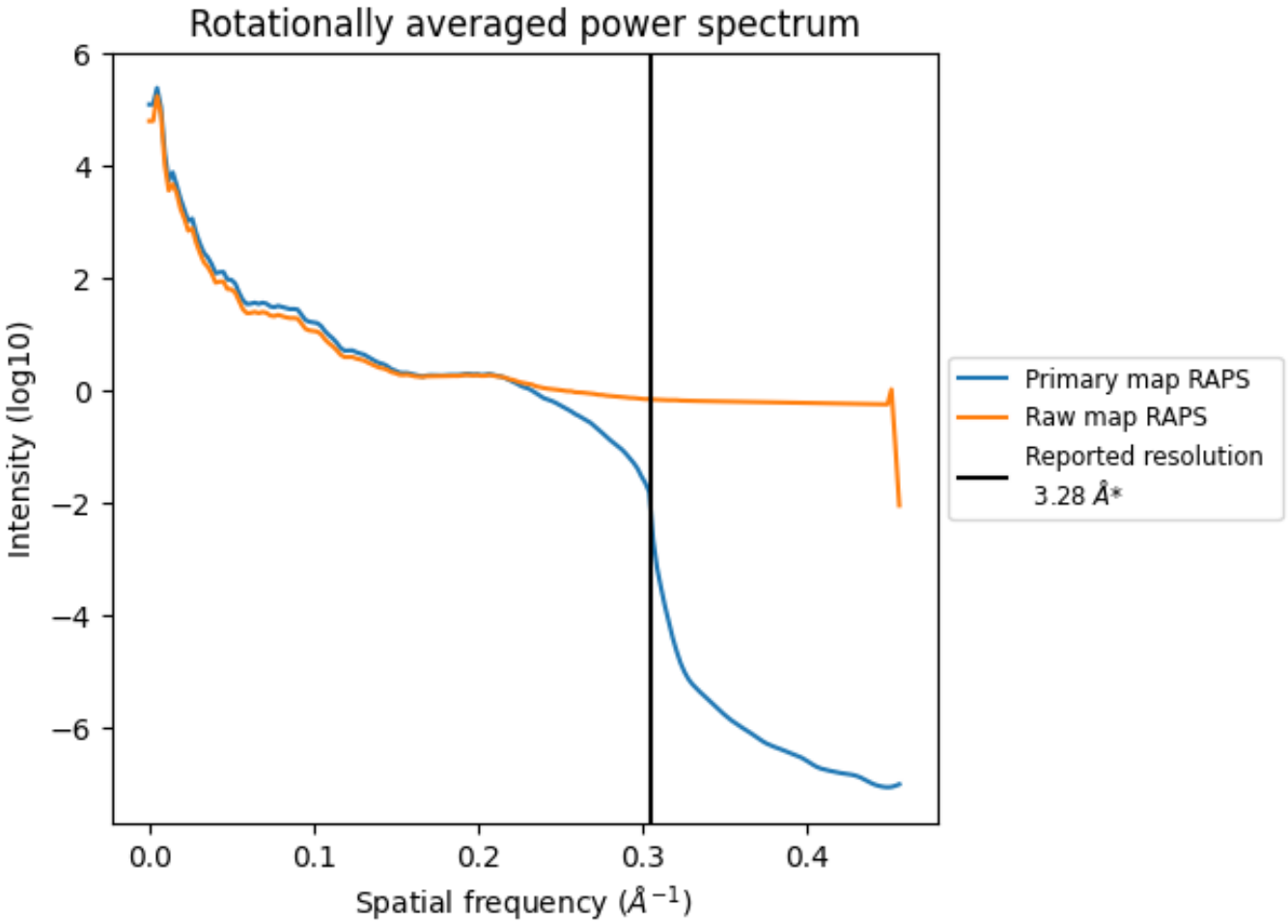
7.2 Volume estimate



The volume at the recommended contour level is 746 nm^3; this corresponds to an approximate mass of 674 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 (i)

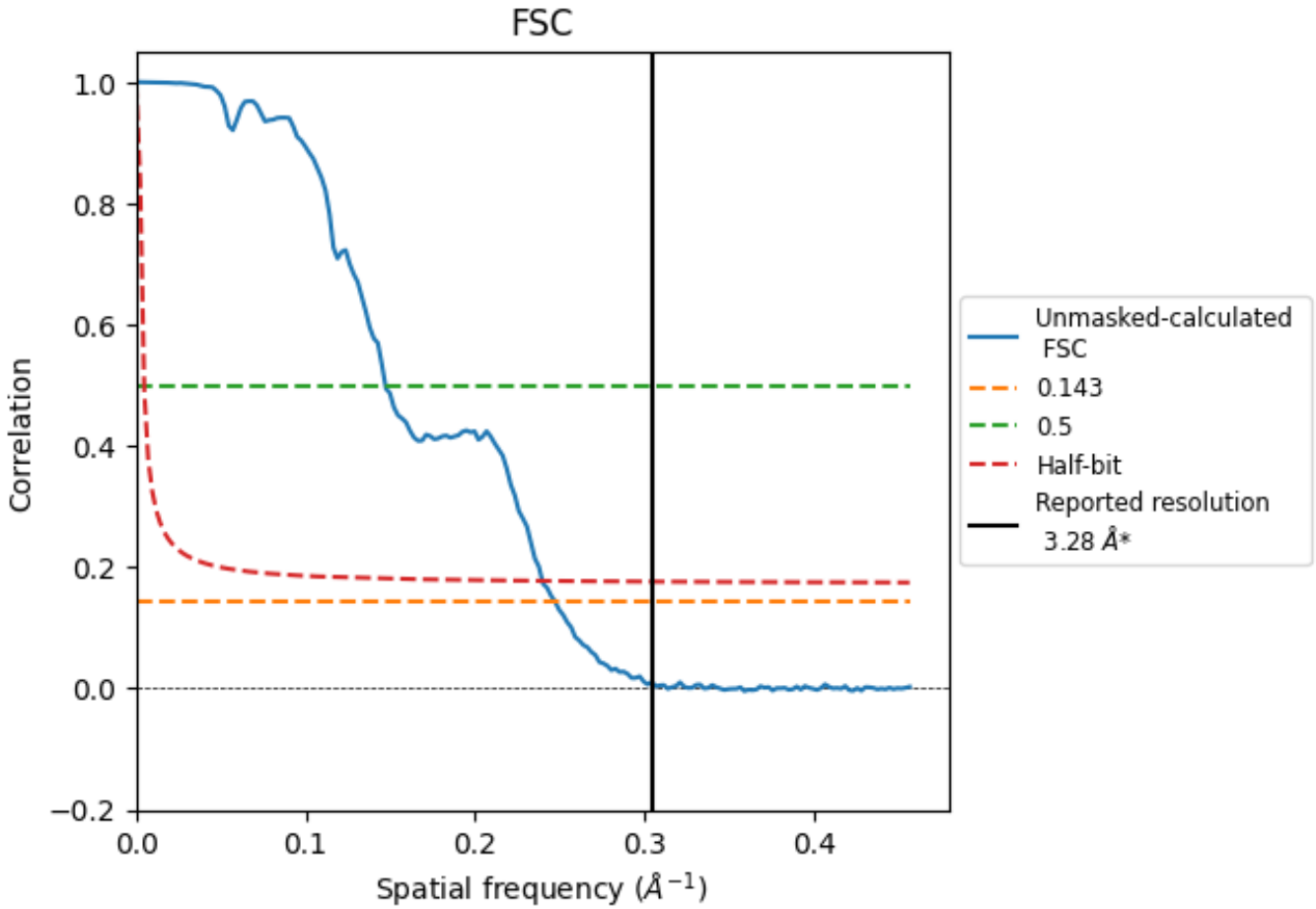


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

8.2 Resolution estimates (i)

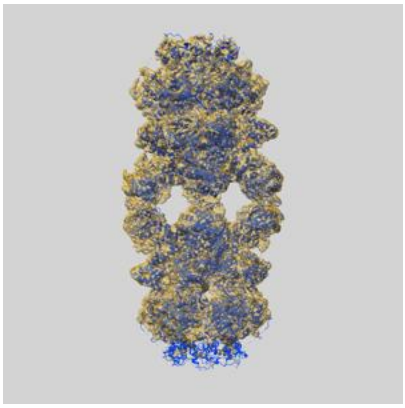
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	6.80	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.28 by more than 10 %

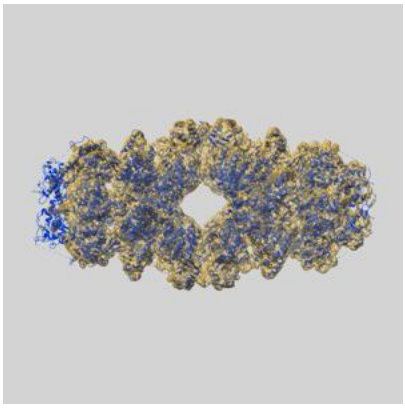
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37883 and PDB model 8WW7. Per-residue inclusion information can be found in section 3 on page 10.

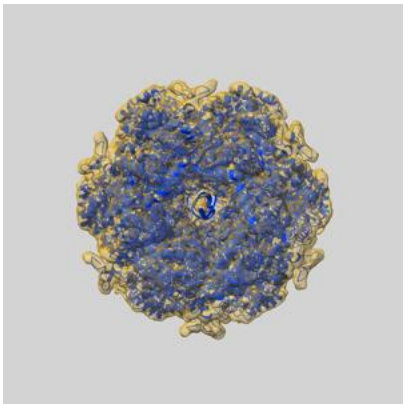
9.1 Map-model overlay



X



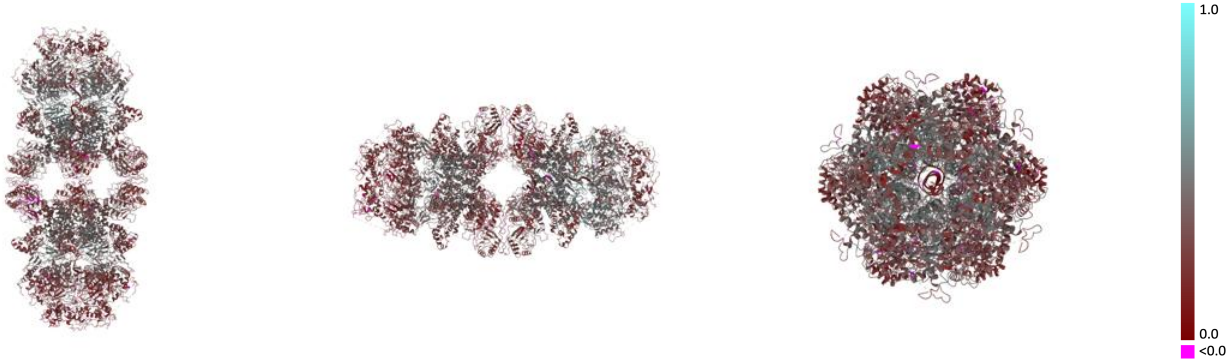
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.258 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.

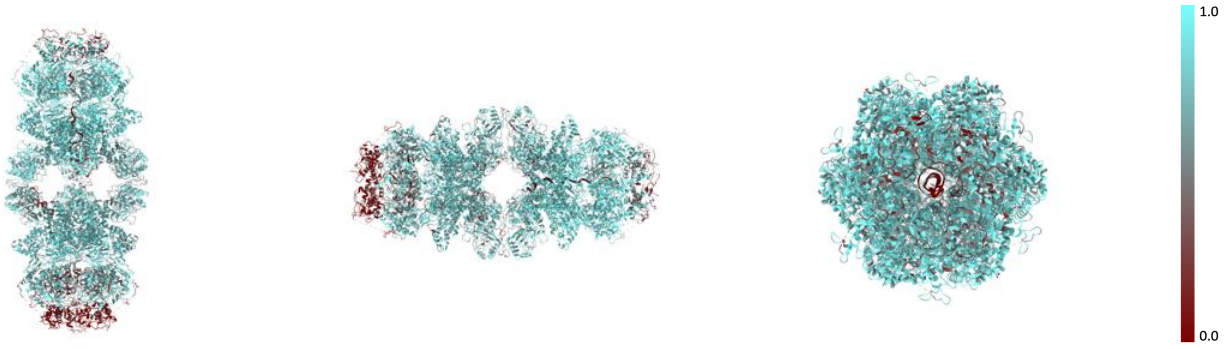
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

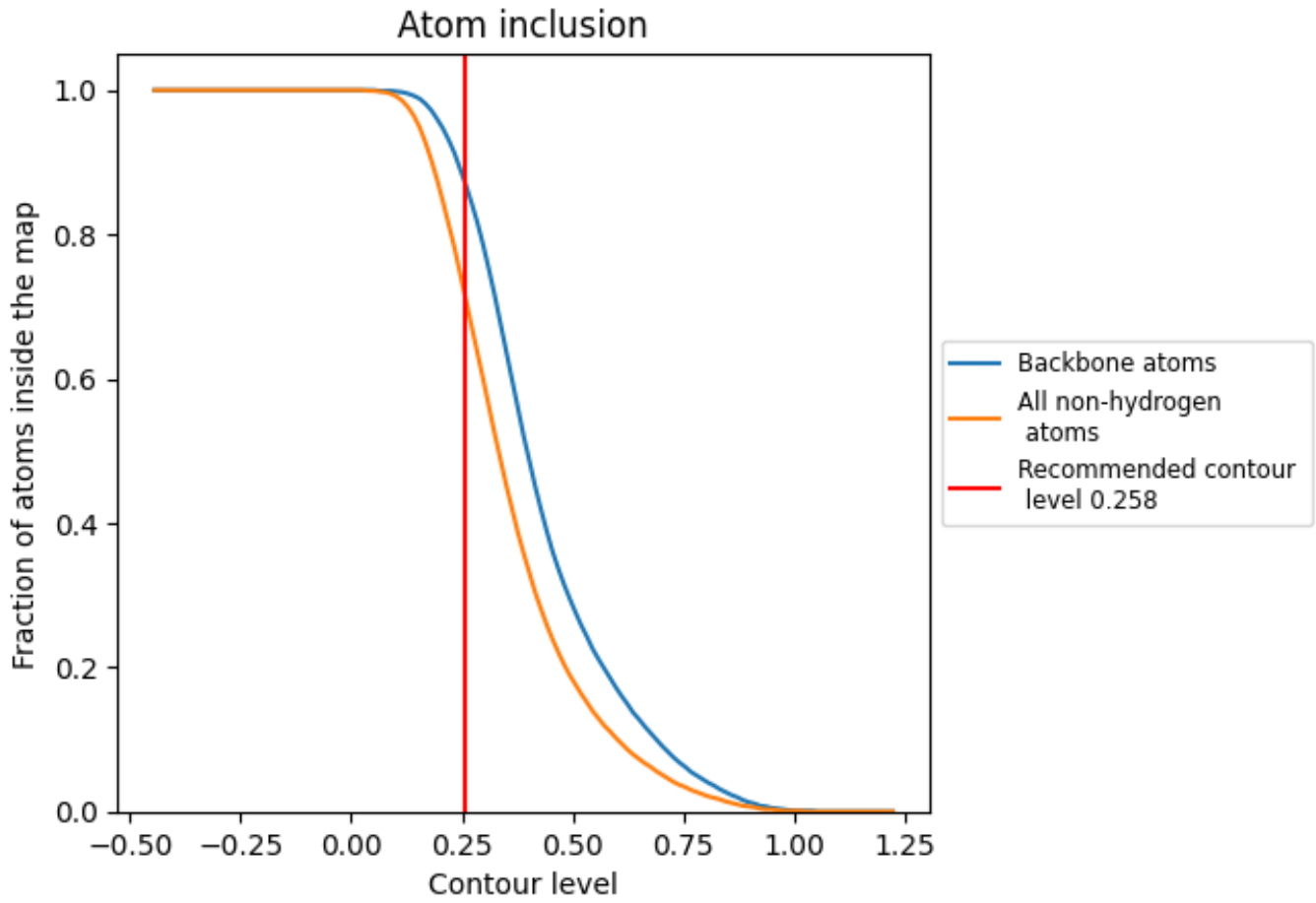
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.258).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.3280
A	0.8110	0.3840
B	0.7880	0.3790
C	0.7700	0.3570
D	0.7530	0.3390
E	0.7920	0.3670
F	0.8270	0.3850
G	0.6360	0.2890
H	0.6490	0.2910
I	0.6570	0.2980
J	0.6550	0.3030
K	0.6340	0.2870
L	0.6200	0.2750
M	0.1370	0.1510
N	0.1790	0.1410
O	0.2900	0.1630