



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:01 PM UTC

PDB ID : 4G7O / pdb_00004g7o
Title : Crystal structure of Thermus thermophilus transcription initiation complex containing 2 nt of RNA
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2012-07-20
Resolution : 2.99 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

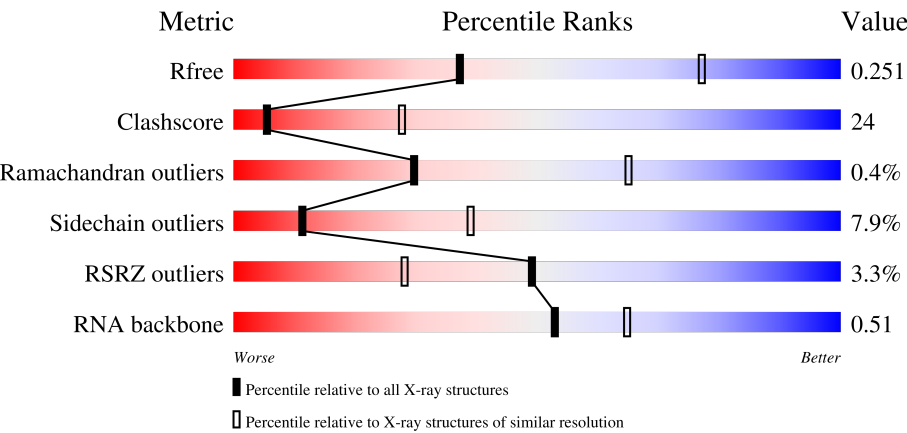
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	315	42%27%•28%
1	B	315	2% 39%26%5%30%
1	K	315	46%24%•28%
1	L	315	2% 42%25%•29%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	21	
6	Q	21	
7	H	27	
7	R	27	
8	I	2	
8	S	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1482	Total	C	N	O	S	0	0	0
			11704	7421	2059	2189	35			
3	N	1489	Total	C	N	O	S	0	0	0
			11746	7446	2066	2198	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			
6	Q	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
7	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called 5'-R(*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			
8	S	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

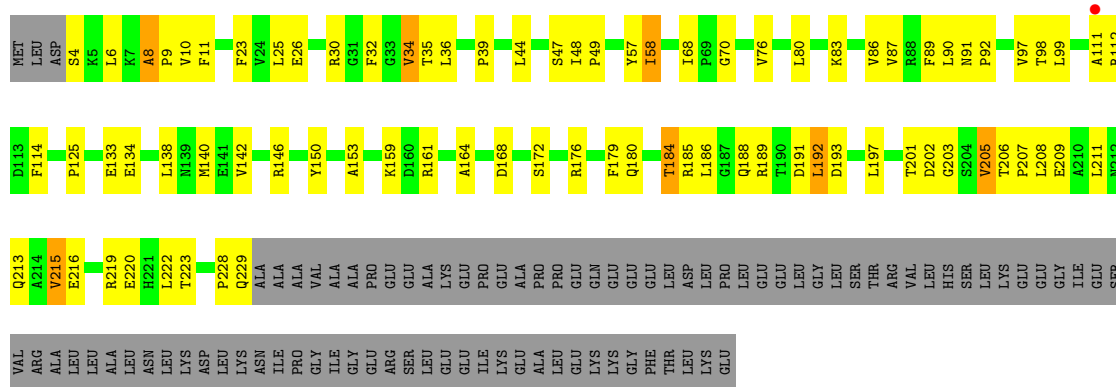
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Mg 2 2	0	0
10	K	1	Total Mg 1 1	0	0
10	N	2	Total Mg 2 2	0	0

- Molecule 11 is water.

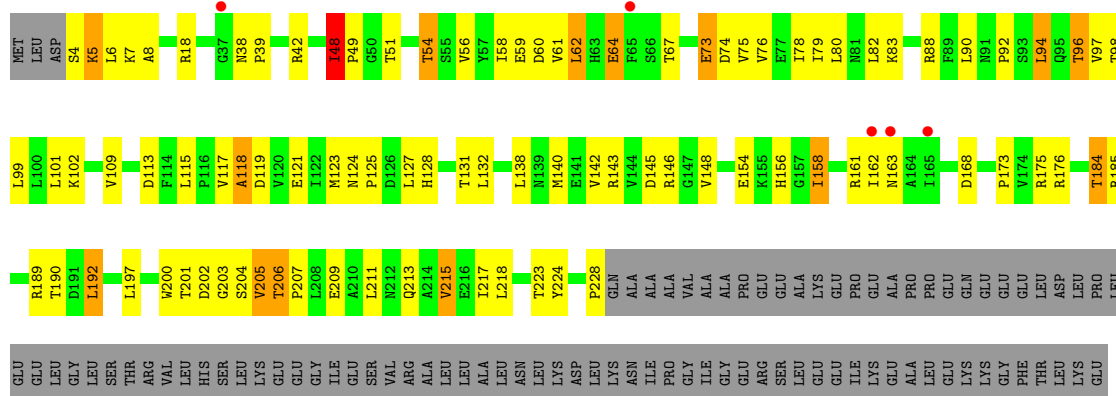
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	14	Total O 14 14	0	0
11	B	3	Total O 3 3	0	0
11	C	53	Total O 53 53	0	0
11	D	58	Total O 58 58	0	0
11	E	8	Total O 8 8	0	0
11	F	10	Total O 10 10	0	0
11	G	5	Total O 5 5	0	0
11	H	2	Total O 2 2	0	0
11	K	4	Total O 4 4	0	0
11	L	3	Total O 3 3	0	0
11	M	33	Total O 33 33	0	0
11	N	52	Total O 52 52	0	0
11	O	5	Total O 5 5	0	0
11	P	16	Total O 16 16	0	0
11	Q	2	Total O 2 2	0	0
11	R	3	Total O 3 3	0	0
11	S	1	Total O 1 1	0	0

- Molecule 1: DNA-directed RNA polymerase subunit alpha

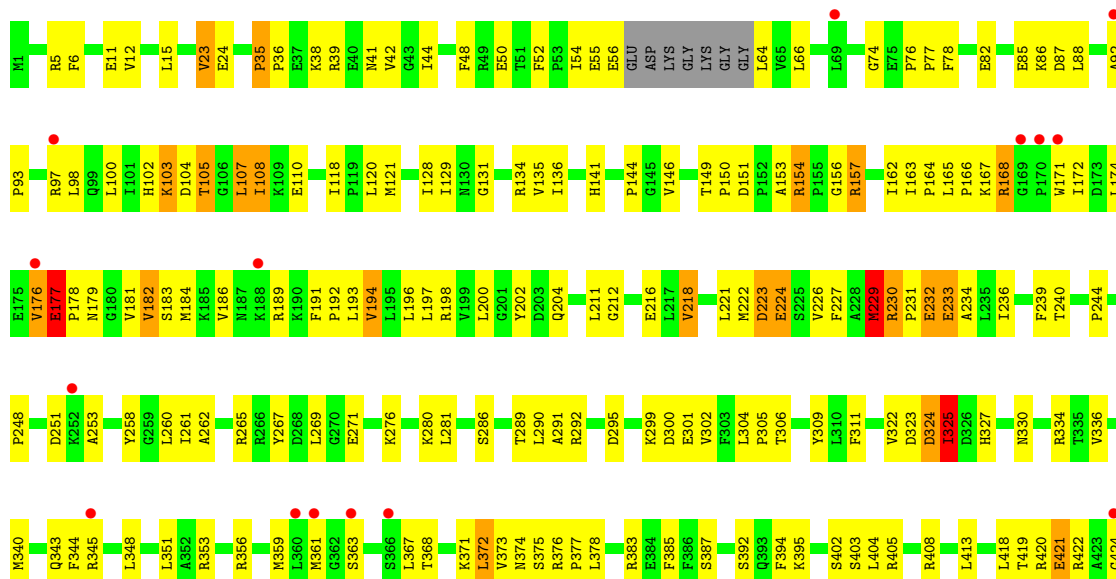


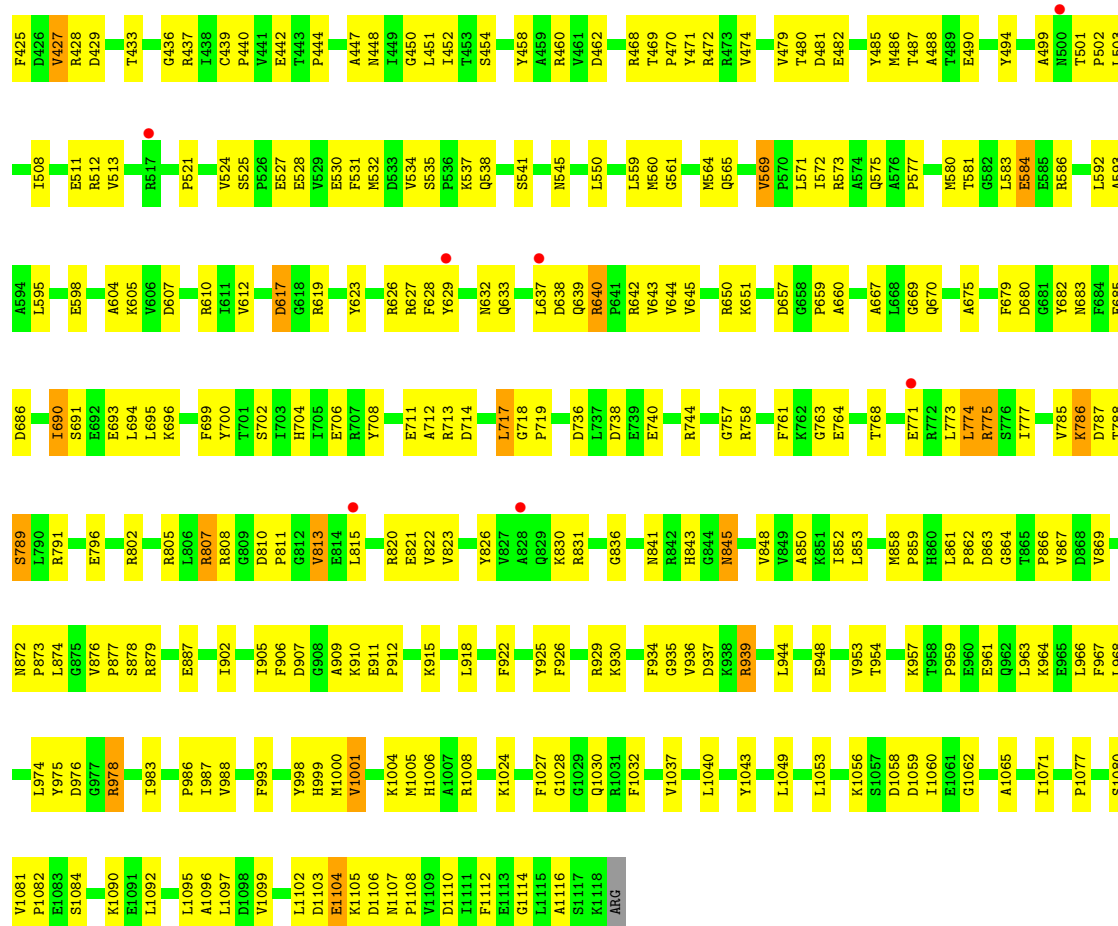


• Molecule 1: DNA-directed RNA polymerase subunit alpha

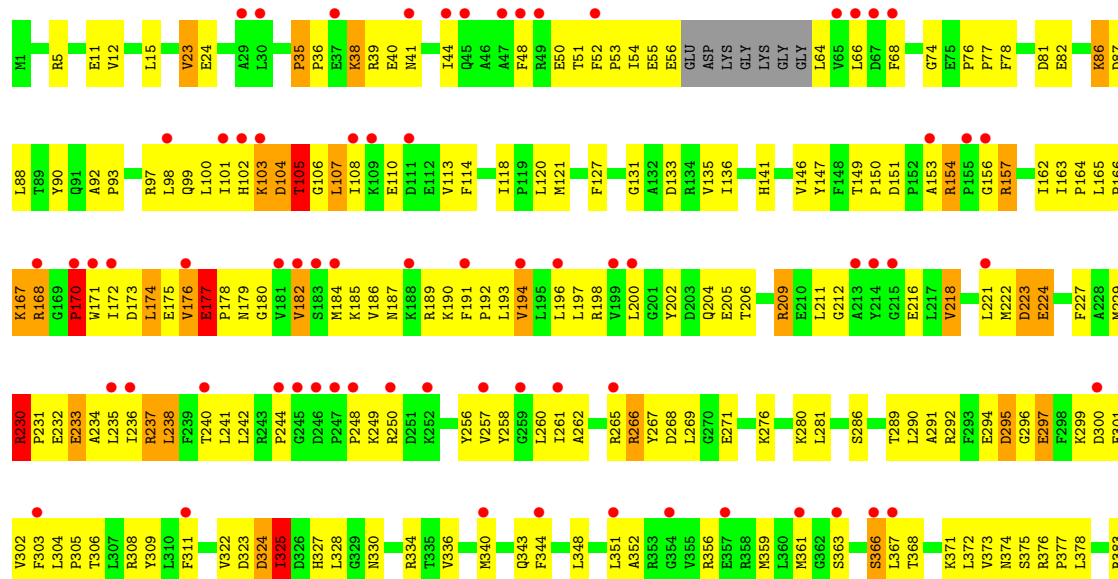


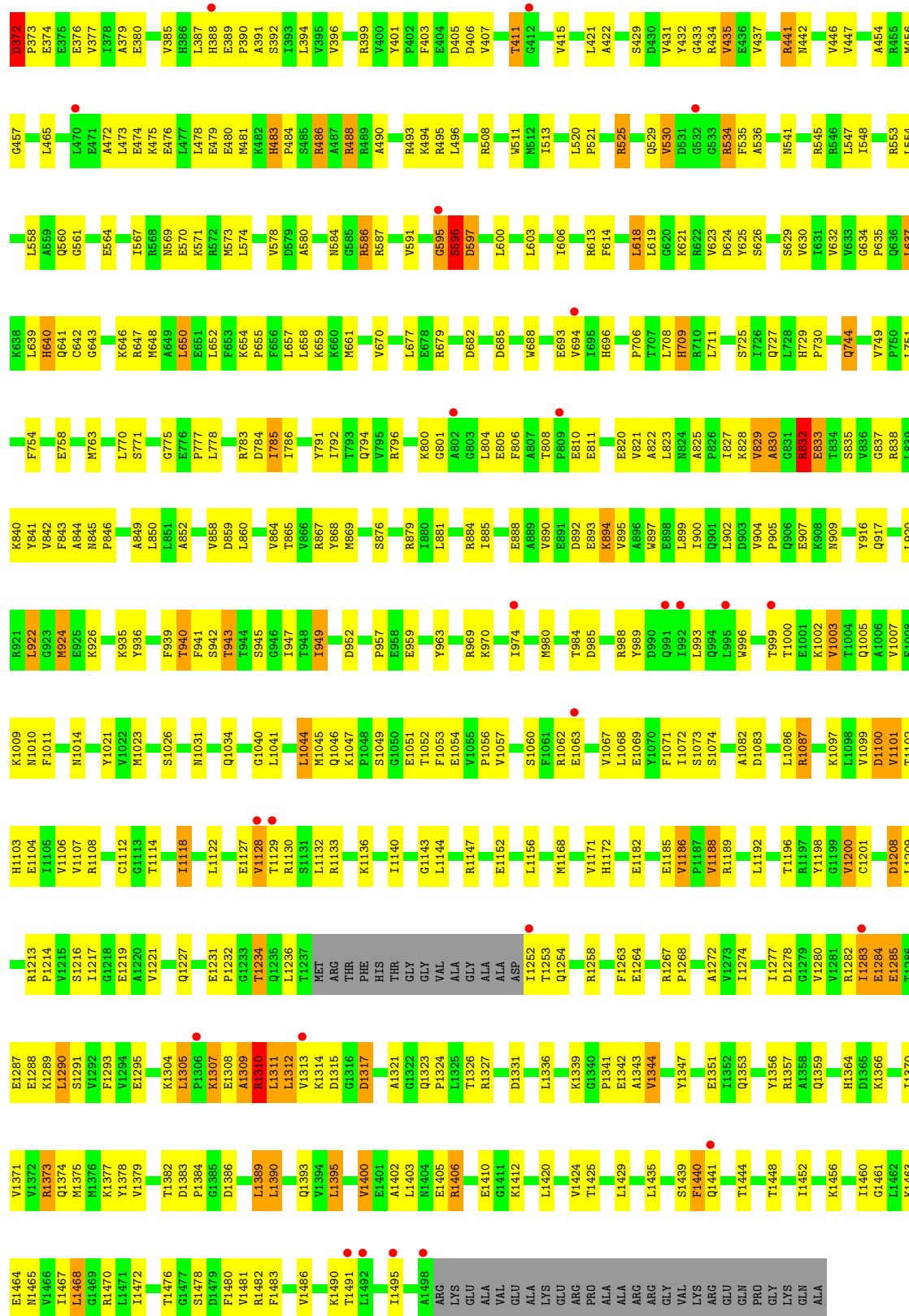
• Molecule 2: DNA-directed RNA polymerase subunit beta



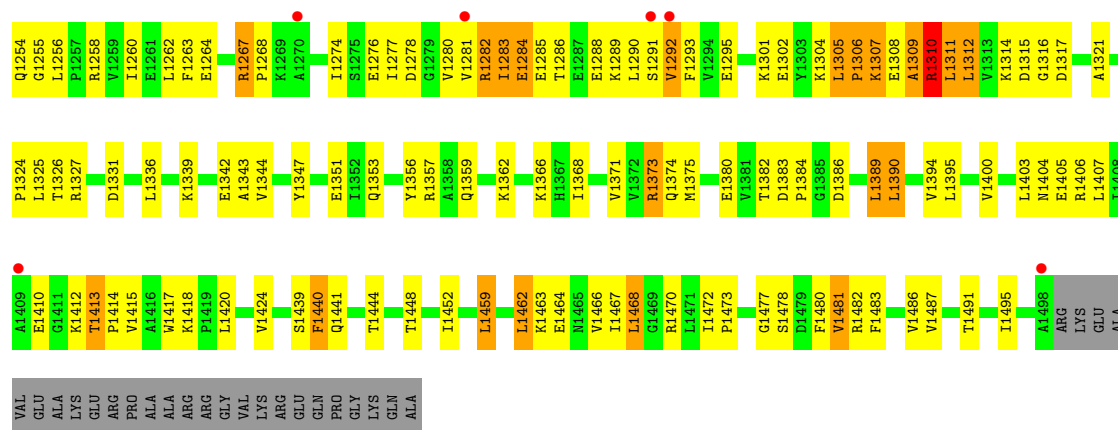


• Molecule 2: DNA-directed RNA polymerase subunit beta

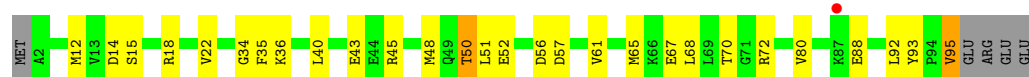




I1140	K1047	M869	L787	K671	G595	R495	A422	E338	E255	L171	R86	MET
G1143	P1048	S876	Y791	R675	S596	L496	S429	W339	E256	D181	R87	LYS
R1147	S1049	E958	I792	R676	D597	E497	D430	V347	V259	E184	R88	K3
L1156	E1051	R879	I793	L677	P599	V498	Y431	Q348	E260	K187	N90	E4
R1159	T1052	I880	Q794	R678	L600	W511	Y432	P349	L264	T97	K7	V5
V1171	F1053	L881	R795	R679	R601	M512	R433	H550	E265	P98		R6
I1175	E1054	R884	R796	Q880	S602	I513	V435	N351	E266			K7
E1182	P1056	I885	K800	R681	L603		E436	M352	E267	L191	S14	
V1188	V1057	E888	G801	D682	1606		V437	V354	F269	W103	P15	
R1189	E889	L804	D685		R613	R525	D438	P356	L270	K106	K17	
C1194	V890	E805	W688		F614	P526	V439		V271	D107	I18	
Y1198	E891	F806				M527	V440		L272	V108	R19	
G1199	D892	E693	V694		L618		R441		R273	P109	S20	
V1200	E893	V694				V530	N442		R274	S110		
C1204	K894	P706				R534	R445		D275	K111	E30	
D1208	W897	T707				R546	V446		E277	T114	I32	
R1213	E898	L708				A536	V447		V279	L115	N33	
P1214	I899	R709				F535			E282	L116	T34	
V1215	I900	H709				A541	Y450		T281	T121	R35	
E1219	L993	R710				M541	D451		F208		T36	
Q1227	L996	L711				R545	D452		R209	E124	L37	
E1231	Y997	E822				R546	D454		E283		K38	
P1232	I998	L823				F547	A454		V211	L127	P39	
T1234	L999	R824				I548	R455		R212		E40	
T1237	L999	A825					R456		V213		L44	
M1238	K1003	R827					M456		E214		F45	
ARG	Y1003	Q828					G457		Y215		D46	
THR	Q1004	R829					A460		K218		E47	
PHE	Q1005	A830					Q463		E219		R48	
HIS	Y1007	G831					L464		G222		G51	
THR	F1008	R832					L465		L223		P52	
GLY	K1009	T834					L468		R224		I53	
V1246	N1010	S835					A472		L225		K54	
G1248	F1011	G837					L473		P226		D55	
A1249	Y1021	R838					K475		L227		Y56	
A1250	L1020	L839					K476		W230		R65	
D1251	Y1022	Y841					L477		V231		Q66	
T1253	M1023	L850					L478		E232		R67	
	S1026	N845					E479		K233		F68	
	G1027	P846					M481		K237		E69	
	A1028	F941					K482		E240		G70	
	N1031	S942					P484		L241		C73	
	Q1034	T944					S485		A243		E74	
	G1040	S945					R486		D155		R75	
	L1041	L860					A487		L245		C76	
	L1044	L864					R488		Y249		G77	
	L1044	T865					K491		L250		V78	
	M1045	R867					A492		F251		F79	
	R1136	D952					R493		L337		V80	
	R1137						K494				I84	
											R85	



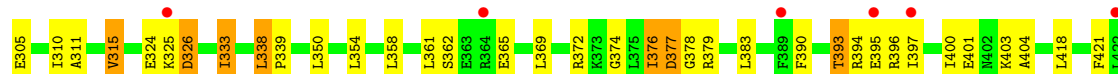
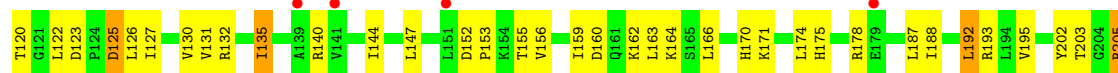
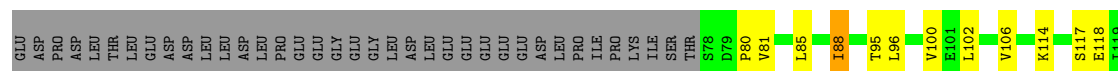
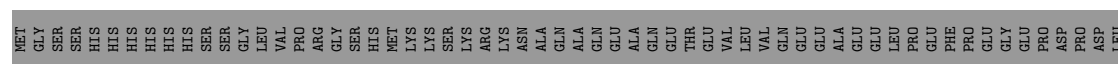
• Molecule 4: DNA-directed RNA polymerase subunit omega



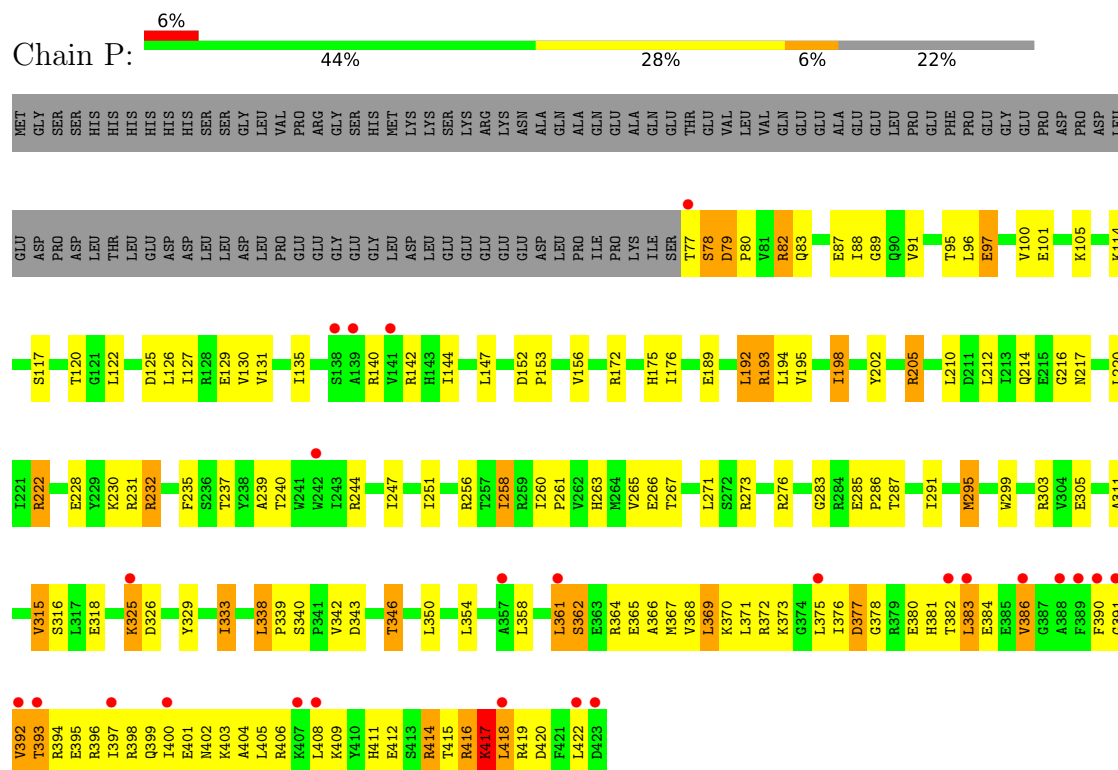
• Molecule 4: DNA-directed RNA polymerase subunit omega



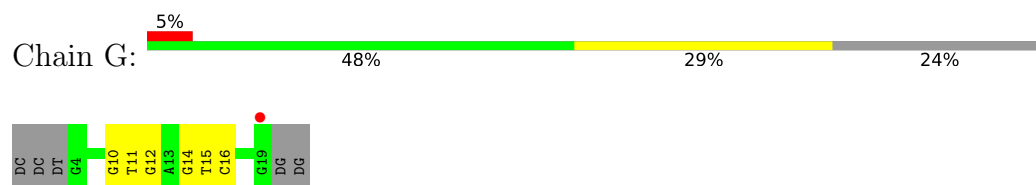
• Molecule 5: RNA polymerase sigma factor



- Molecule 5: RNA polymerase sigma factor



● Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'



● Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'



- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

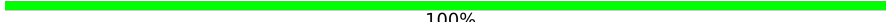


- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain R:  59% 30% 11%

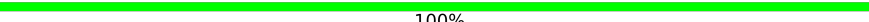


- Molecule 8: 5'-R(*GP*A)-3'

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 5'-R(*GP*A)-3'

Chain S:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.48Å 103.88Å 297.34Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	46.61 – 2.99 46.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.61-2.99) 95.5 (46.61-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.205 , 0.247 0.209 , 0.251	Depositor DCC
R_{free} test set	1946 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	57231	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	1/1814 (0.1%)	0.90	6/2466 (0.2%)
1	B	0.35	0/1782	0.88	4/2424 (0.2%)
1	K	0.34	0/1814	0.88	6/2466 (0.2%)
1	L	0.34	0/1805	0.90	7/2454 (0.3%)
2	C	0.40	0/8937	0.82	12/12087 (0.1%)
2	M	0.41	1/8937 (0.0%)	0.85	18/12087 (0.1%)
3	D	0.41	1/11910 (0.0%)	0.82	22/16105 (0.1%)
3	N	0.40	2/11952 (0.0%)	0.83	20/16162 (0.1%)
4	E	0.33	0/775	0.78	0/1045
4	O	0.31	0/775	0.77	0/1045
5	F	0.36	0/2852	0.81	7/3837 (0.2%)
5	P	0.35	0/2859	0.80	6/3847 (0.2%)
6	G	0.21	0/368	0.64	0/567
6	Q	0.17	0/368	0.59	0/567
7	H	0.18	0/556	0.71	0/858
7	R	0.18	0/556	0.68	0/858
8	I	0.16	0/47	0.29	0/72
8	S	0.16	0/47	0.25	0/72
All	All	0.39	5/58154 (0.0%)	0.83	108/79019 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
5	P	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	599	PRO	C-N	9.84	1.46	1.33
3	D	105	VAL	C-N	7.81	1.45	1.33
1	A	62	LEU	C-N	6.48	1.41	1.33
2	M	366	SER	C-N	6.20	1.41	1.33
3	N	744	GLN	C-N	5.37	1.41	1.33

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	421	GLU	N-CA-C	-8.64	101.34	112.23
2	M	421	GLU	N-CA-C	-8.64	101.35	112.23
2	M	105	THR	N-CA-C	-8.06	103.04	113.12
2	M	296	GLY	N-CA-C	7.79	122.74	112.77
5	P	326	ASP	N-CA-C	7.67	121.89	112.23
5	F	326	ASP	N-CA-C	7.52	122.21	112.89
5	P	192	LEU	N-CA-C	7.37	119.31	111.28
1	B	48	ILE	CA-C-N	7.34	128.49	119.98
1	B	48	ILE	C-N-CA	7.34	128.49	119.98
1	L	48	ILE	CA-C-N	6.92	128.00	119.98
1	L	48	ILE	C-N-CA	6.92	128.00	119.98
3	N	435	VAL	N-CA-C	6.64	118.14	109.58
3	N	1267	ARG	CA-C-N	6.60	126.62	119.89
3	N	1267	ARG	C-N-CA	6.60	126.62	119.89
3	D	595	GLY	N-CA-C	-6.44	106.35	115.43
3	N	1462	LEU	N-CA-C	6.35	118.20	111.28
2	M	493	ARG	N-CA-C	6.32	118.17	111.28
3	N	595	GLY	N-CA-C	-6.30	106.54	115.43
3	N	1440	PHE	N-CA-C	6.29	117.93	111.14
3	D	1440	PHE	N-CA-C	6.27	117.92	111.14
5	P	333	ILE	CA-C-N	6.13	126.09	120.21
5	P	333	ILE	C-N-CA	6.13	126.09	120.21
3	N	599	PRO	O-C-N	-6.08	115.81	123.10
2	C	271	GLU	N-CA-C	-6.06	104.68	111.28
3	D	483	HIS	CA-C-N	6.02	125.23	118.97
3	D	483	HIS	C-N-CA	6.02	125.23	118.97
3	N	67	ARG	N-CA-C	-6.02	104.79	111.71
2	M	271	GLU	N-CA-C	-6.01	104.73	111.28
2	M	297	GLU	N-CA-C	5.96	118.23	109.24
2	M	170	PRO	CA-C-N	-5.95	112.53	122.64
2	M	170	PRO	C-N-CA	-5.95	112.53	122.64
3	N	483	HIS	CA-C-N	5.88	125.08	118.97
3	N	483	HIS	C-N-CA	5.88	125.08	118.97
1	A	91	ASN	CA-C-N	5.86	125.56	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASN	C-N-CA	5.86	125.56	119.82
3	D	783	ARG	CB-CA-C	-5.77	109.94	116.63
3	N	597	ASP	CB-CA-C	-5.77	109.94	116.63
1	A	8	ALA	CA-C-N	5.72	125.92	120.31
1	A	8	ALA	C-N-CA	5.72	125.92	120.31
3	D	596	SER	CB-CA-C	-5.70	110.02	116.63
1	K	8	ALA	CA-C-N	5.68	125.88	120.31
1	K	8	ALA	C-N-CA	5.68	125.88	120.31
1	K	91	ASN	CA-C-N	5.67	125.38	119.82
1	K	91	ASN	C-N-CA	5.67	125.38	119.82
3	N	596	SER	CB-CA-C	-5.65	110.07	116.63
3	D	435	VAL	N-CA-C	5.63	116.84	108.23
3	D	275	GLU	CB-CA-C	-5.59	110.15	116.63
3	N	45	PHE	N-CA-C	5.58	119.39	112.59
2	C	35	PRO	CA-C-N	5.58	126.81	119.84
2	C	35	PRO	C-N-CA	5.58	126.81	119.84
2	C	229	MET	N-CA-C	5.57	117.35	111.28
2	C	1104	GLU	N-CA-C	-5.56	106.33	113.01
3	D	372	ASP	CA-C-N	5.52	124.98	119.24
3	D	372	ASP	C-N-CA	5.52	124.98	119.24
3	D	1309	ALA	CB-CA-C	-5.49	110.26	116.63
2	M	373	VAL	N-CA-C	5.48	115.84	108.17
5	F	281	GLU	N-CA-C	5.47	117.33	111.36
3	N	1309	ALA	CB-CA-C	-5.47	110.24	116.54
3	D	1186	VAL	N-CA-C	5.47	114.12	107.61
3	D	830	ALA	CB-CA-C	-5.46	110.30	116.63
3	D	597	ASP	CB-CA-C	-5.45	110.31	116.63
2	M	813	VAL	N-CA-C	5.45	115.80	108.17
2	C	813	VAL	N-CA-C	5.44	115.79	108.17
2	M	35	PRO	CA-C-N	5.44	126.64	119.84
2	M	35	PRO	C-N-CA	5.44	126.64	119.84
1	L	64	GLU	N-CA-C	5.42	117.19	111.28
2	C	295	ASP	CB-CA-C	-5.41	110.35	116.63
3	D	1087	ARG	N-CA-C	-5.39	105.40	111.28
2	M	295	ASP	CB-CA-C	-5.39	110.35	116.54
5	F	192	LEU	N-CA-C	5.36	117.88	111.71
2	M	1104	GLU	N-CA-C	-5.36	106.58	113.01
1	A	172	SER	CA-C-N	5.35	125.81	120.04
1	A	172	SER	C-N-CA	5.35	125.81	120.04
1	B	8	ALA	CA-C-N	5.33	125.33	119.89
1	B	8	ALA	C-N-CA	5.33	125.33	119.89
2	C	785	VAL	N-CA-C	5.33	115.63	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	830	ALA	CB-CA-C	-5.33	110.45	116.63
2	C	324	ASP	N-CA-C	5.30	116.74	111.07
2	M	427	VAL	N-CA-C	5.29	116.07	110.72
1	L	67	THR	CA-C-N	-5.28	117.62	123.43
1	L	67	THR	C-N-CA	-5.28	117.62	123.43
2	M	324	ASP	N-CA-C	5.28	116.72	111.07
5	P	338	LEU	CA-C-N	5.27	125.52	119.83
5	P	338	LEU	C-N-CA	5.27	125.52	119.83
2	C	373	VAL	N-CA-C	5.26	115.53	108.17
3	N	783	ARG	CB-CA-C	-5.26	110.08	117.23
3	N	1087	ARG	N-CA-C	-5.24	105.57	111.28
3	N	275	GLU	CB-CA-C	-5.21	110.58	116.63
1	K	172	SER	CA-C-N	5.19	125.64	120.04
1	K	172	SER	C-N-CA	5.19	125.64	120.04
5	F	338	LEU	CA-C-N	5.17	125.18	119.90
5	F	338	LEU	C-N-CA	5.17	125.18	119.90
2	M	303	PHE	N-CA-C	5.17	116.60	111.07
3	D	1472	ILE	CA-C-N	5.17	126.30	119.84
3	D	1472	ILE	C-N-CA	5.17	126.30	119.84
2	C	107	LEU	N-CA-C	5.15	117.69	110.23
2	M	266	ARG	N-CA-C	5.14	118.01	111.69
3	N	441	ARG	N-CA-C	5.12	119.15	113.01
3	N	832	ARG	N-CA-C	5.08	117.41	110.55
3	D	832	ARG	N-CA-C	5.05	117.37	110.55
1	L	8	ALA	CA-C-N	5.04	125.03	119.89
1	L	8	ALA	C-N-CA	5.04	125.03	119.89
3	D	28	LYS	CA-C-N	5.03	125.70	120.12
3	D	28	LYS	C-N-CA	5.03	125.70	120.12
5	F	333	ILE	CA-C-N	5.02	125.74	120.11
5	F	333	ILE	C-N-CA	5.02	125.74	120.11
3	D	924	MET	N-CA-C	5.02	116.75	111.28
3	D	441	ARG	N-CA-C	5.01	119.02	113.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	104	ASP	Peptide
5	P	82	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	86	0
1	B	1750	0	1797	97	0
1	K	1782	0	1834	61	0
1	L	1773	0	1826	79	0
2	C	8770	0	8872	451	0
2	M	8770	0	8871	531	2
3	D	11704	0	11934	563	1
3	N	11746	0	11974	697	0
4	E	761	0	778	29	0
4	O	761	0	778	27	0
5	F	2807	0	2882	112	0
5	P	2814	0	2888	177	1
6	G	328	0	181	4	0
6	Q	328	0	181	6	0
7	H	495	0	272	8	0
7	R	495	0	272	14	0
8	I	42	0	23	0	0
8	S	42	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	2	0	0	0	0
10	K	1	0	0	0	0
10	N	2	0	0	0	0
11	A	14	0	0	0	0
11	B	3	0	0	0	0
11	C	53	0	0	0	0
11	D	58	0	0	0	0
11	E	8	0	0	0	0
11	F	10	0	0	0	0
11	G	5	0	0	0	0
11	H	2	0	0	0	0
11	K	4	0	0	0	0
11	L	3	0	0	0	0
11	M	33	0	0	1	0
11	N	52	0	0	1	0
11	O	5	0	0	0	0
11	P	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Q	2	0	0	0	0
11	R	3	0	0	0	0
11	S	1	0	0	0	0
All	All	57231	0	57220	2720	2

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 24.

All (2720) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:ARG:NH1	2:M:176:VAL:HG11	1.23	1.47
2:C:64:LEU:N	2:C:103:LYS:NZ	1.61	1.47
2:M:229:MET:HE3	2:M:233:GLU:C	1.41	1.45
2:M:64:LEU:N	2:M:103:LYS:NZ	1.64	1.45
2:M:107:LEU:HD12	2:M:108:ILE:N	1.11	1.40
2:M:740:GLU:OE1	2:M:805:ARG:NH1	1.57	1.36
1:B:58:ILE:HB	1:B:61:VAL:CG1	1.56	1.35
3:D:219:GLU:CG	3:D:339:TRP:HH2	1.41	1.34
2:M:157:ARG:NH1	2:M:176:VAL:CG1	1.88	1.33
3:D:33:ASN:OD1	3:D:36:THR:HG22	1.26	1.32
3:N:1283:ILE:HG23	3:N:1315:ASP:CG	1.60	1.25
3:N:1283:ILE:CG2	3:N:1315:ASP:OD1	1.84	1.25
2:C:157:ARG:NH1	2:C:176:VAL:HG11	1.52	1.24
2:C:229:MET:O	2:C:230:ARG:CG	1.84	1.23
2:M:229:MET:HE3	2:M:233:GLU:O	1.19	1.23
2:M:157:ARG:HH11	2:M:176:VAL:CG1	1.45	1.23
3:N:219:GLU:CB	3:N:339:TRP:HH2	1.50	1.22
3:N:219:GLU:CG	3:N:339:TRP:HH2	1.51	1.22
2:C:740:GLU:OE1	2:C:805:ARG:NH1	1.73	1.21
2:C:64:LEU:N	2:C:103:LYS:HZ2	1.21	1.20
3:N:835:SER:HB3	3:N:838:ARG:NE	1.55	1.20
3:N:835:SER:CB	3:N:838:ARG:HE	1.55	1.20
2:M:229:MET:CE	2:M:233:GLU:C	2.15	1.18
2:M:231:PRO:HG2	2:M:232:GLU:OE2	1.44	1.18
2:M:229:MET:CE	2:M:233:GLU:O	1.90	1.18
3:N:1283:ILE:CG2	3:N:1315:ASP:CG	2.16	1.17
3:N:1290:LEU:CG	3:N:1307:LYS:HE2	1.73	1.17
2:C:108:ILE:HD12	2:C:108:ILE:O	1.45	1.17
3:D:256:GLU:O	3:D:274:ARG:NH1	1.77	1.17
3:N:1283:ILE:HG23	3:N:1315:ASP:OD1	1.39	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:105:THR:CG2	2:M:107:LEU:HB3	1.74	1.17
3:D:894:LYS:HD2	3:D:894:LYS:N	1.49	1.16
3:D:1305:LEU:HD23	3:D:1305:LEU:N	1.55	1.16
1:A:4:SER:O	1:A:189:ARG:NH2	1.79	1.16
3:N:1305:LEU:N	3:N:1305:LEU:HD23	1.56	1.15
2:M:107:LEU:CD1	2:M:108:ILE:N	2.08	1.15
2:C:229:MET:O	2:C:230:ARG:HG2	0.99	1.14
2:M:182:VAL:CG2	2:M:193:LEU:HB3	1.75	1.14
3:N:219:GLU:CG	3:N:339:TRP:CH2	2.31	1.14
3:D:219:GLU:HG3	3:D:339:TRP:HH2	1.11	1.13
3:N:1238:MET:C	3:N:1253:THR:OG1	1.92	1.12
2:M:105:THR:HG21	2:M:107:LEU:HB3	1.29	1.12
2:C:182:VAL:CG2	2:C:193:LEU:HB3	1.79	1.12
2:M:64:LEU:N	2:M:103:LYS:HZ2	1.25	1.12
2:M:172:ILE:HG13	2:M:186:VAL:HG22	1.21	1.11
1:B:58:ILE:HB	1:B:61:VAL:HG13	1.19	1.11
3:D:1283:ILE:H	3:D:1283:ILE:CD1	1.54	1.11
3:N:219:GLU:HB2	3:N:339:TRP:CH2	1.86	1.11
3:D:219:GLU:CG	3:D:339:TRP:CH2	2.34	1.10
5:P:416:ARG:O	5:P:417:LYS:HB3	1.44	1.10
3:N:1310:ARG:HD3	3:N:1327:ARG:NH1	1.65	1.10
2:M:198:ARG:HE	2:M:230:ARG:HA	1.13	1.10
3:N:1283:ILE:O	3:N:1283:ILE:HD13	1.49	1.10
5:F:205:ARG:HH11	5:F:205:ARG:CG	1.64	1.09
2:M:229:MET:O	2:M:230:ARG:HG2	1.51	1.09
2:M:182:VAL:HG21	2:M:193:LEU:HB3	1.32	1.09
3:D:1304:LYS:C	3:D:1305:LEU:HD23	1.77	1.08
3:N:32:ILE:CG1	5:P:258:ILE:HD13	1.82	1.08
3:N:894:LYS:H	3:N:894:LYS:HD2	1.14	1.08
2:C:157:ARG:NH1	2:C:176:VAL:CG1	2.16	1.08
3:N:1290:LEU:HG	3:N:1307:LYS:HE2	1.13	1.08
3:N:1310:ARG:CD	3:N:1327:ARG:HH11	1.67	1.08
5:F:205:ARG:HH11	5:F:205:ARG:HG2	0.96	1.07
1:B:58:ILE:CB	1:B:61:VAL:CG1	2.32	1.07
3:D:890:VAL:HB	3:D:922:LEU:CD1	1.84	1.07
3:D:1310:ARG:C	3:D:1311:LEU:HD23	1.78	1.07
2:M:105:THR:HG22	2:M:107:LEU:H	0.94	1.07
3:N:124:GLU:OE2	3:N:587:ARG:NH2	1.89	1.06
2:C:182:VAL:HG21	2:C:193:LEU:HB3	1.38	1.06
2:M:229:MET:HG2	2:M:233:GLU:HG2	1.35	1.06
3:D:1283:ILE:HD12	3:D:1283:ILE:N	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:417:LYS:HG3	5:P:418:LEU:H	1.02	1.05
5:P:231:ARG:O	5:P:232:ARG:HG3	1.53	1.05
2:M:64:LEU:HD22	2:M:100:LEU:HD11	1.33	1.05
3:D:274:ARG:HH11	3:D:274:ARG:HG3	0.92	1.05
3:D:894:LYS:H	3:D:894:LYS:CD	1.62	1.05
2:M:172:ILE:HG13	2:M:186:VAL:CG2	1.86	1.05
2:M:167:LYS:O	2:M:168:ARG:HD2	1.57	1.05
3:N:219:GLU:CB	3:N:339:TRP:CH2	2.38	1.04
3:N:32:ILE:HG13	5:P:258:ILE:HD13	1.33	1.04
3:D:219:GLU:HG3	3:D:339:TRP:CH2	1.92	1.04
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.38	1.04
5:P:417:LYS:HG3	5:P:418:LEU:N	1.71	1.04
3:D:67:ARG:NH1	3:D:67:ARG:HB2	1.71	1.03
2:C:108:ILE:HD12	2:C:108:ILE:C	1.83	1.03
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.41	1.03
3:N:46:ASP:OD1	3:N:48:ARG:N	1.91	1.03
1:A:57:TYR:CD1	1:A:161:ARG:HD2	1.94	1.03
3:D:33:ASN:OD1	3:D:36:THR:CG2	2.05	1.03
2:M:167:LYS:C	2:M:168:ARG:HD2	1.83	1.02
3:N:835:SER:HB3	3:N:838:ARG:HE	0.88	1.02
1:B:58:ILE:HB	1:B:61:VAL:HG11	1.38	1.02
3:N:260:GLU:OE1	3:N:273:ARG:NH1	1.92	1.02
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.40	1.02
2:C:230:ARG:HB2	2:C:231:PRO:HD2	1.39	1.01
2:M:179:ASN:OD1	2:M:180:GLY:N	1.93	1.01
2:C:154:ARG:HH11	2:C:154:ARG:HG2	0.84	1.00
1:K:201:THR:HG22	1:K:203:GLY:H	1.27	1.00
2:M:107:LEU:HD12	2:M:107:LEU:C	1.80	1.00
2:C:154:ARG:HG2	2:C:154:ARG:NH1	1.65	1.00
2:M:154:ARG:HG2	2:M:154:ARG:HH11	0.84	1.00
3:D:1312:LEU:CD2	3:D:1327:ARG:HG2	1.92	0.99
5:F:281:GLU:HG2	5:F:282:LEU:HD23	1.40	0.99
1:B:58:ILE:CB	1:B:61:VAL:HG11	1.91	0.99
5:F:205:ARG:HG2	5:F:205:ARG:NH1	1.70	0.99
2:M:105:THR:HG22	2:M:107:LEU:N	1.78	0.99
3:D:1311:LEU:HD23	3:D:1311:LEU:N	1.78	0.99
2:M:628:PHE:H	2:M:638:ASP:HB3	1.26	0.98
3:N:595:GLY:O	3:N:597:ASP:OD2	1.80	0.98
2:C:164:PRO:HD2	2:C:171:TRP:CD1	1.99	0.98
1:A:201:THR:HG22	1:A:203:GLY:H	1.26	0.98
1:A:184:THR:HG22	1:A:192:LEU:CB	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.46	0.98
3:D:124:GLU:OE2	3:D:587:ARG:NH2	1.96	0.97
3:N:1290:LEU:HG	3:N:1307:LYS:CE	1.94	0.97
2:C:154:ARG:HH11	2:C:154:ARG:CG	1.76	0.97
1:B:110:LYS:HZ2	1:B:128:HIS:HB2	1.27	0.97
2:M:154:ARG:HH11	2:M:154:ARG:CG	1.76	0.97
5:P:414:ARG:HG2	5:P:414:ARG:HH11	1.29	0.97
3:N:411:THR:HA	3:N:435:VAL:CG1	1.95	0.96
3:D:67:ARG:HH11	3:D:67:ARG:CG	1.76	0.96
1:B:201:THR:HG22	1:B:203:GLY:H	1.25	0.96
3:D:219:GLU:HG2	3:D:339:TRP:HH2	1.30	0.96
3:D:1283:ILE:HG13	3:D:1315:ASP:CG	1.91	0.96
3:N:1310:ARG:HD3	3:N:1327:ARG:HH11	0.81	0.96
1:L:162:ILE:O	1:L:163:ASN:HB2	1.66	0.96
2:M:154:ARG:HG2	2:M:154:ARG:NH1	1.65	0.96
5:F:231:ARG:C	5:F:232:ARG:HG3	1.89	0.96
2:M:229:MET:CB	2:M:233:GLU:HB3	1.96	0.96
5:P:91:VAL:O	5:P:193:ARG:NH2	1.97	0.96
1:L:201:THR:HG22	1:L:203:GLY:H	1.25	0.95
3:N:438:ASP:OD1	3:N:441:ARG:HD2	1.65	0.95
2:C:628:PHE:H	2:C:638:ASP:HB3	1.27	0.95
5:P:231:ARG:C	5:P:232:ARG:HG3	1.87	0.95
2:M:229:MET:O	2:M:233:GLU:HB2	1.65	0.95
2:M:198:ARG:NE	2:M:230:ARG:HA	1.81	0.95
1:K:4:SER:O	1:K:189:ARG:NH2	2.00	0.94
2:C:324:ASP:C	2:C:325:ILE:HG23	1.91	0.94
3:N:1305:LEU:N	3:N:1305:LEU:CD2	2.30	0.94
2:M:177:GLU:OE1	2:M:190:LYS:NZ	1.99	0.94
1:B:58:ILE:CB	1:B:61:VAL:HG13	1.95	0.94
2:M:324:ASP:C	2:M:325:ILE:HG23	1.91	0.94
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.48	0.94
3:D:274:ARG:NH1	3:D:274:ARG:HG3	1.72	0.93
1:L:206:THR:HG22	1:L:209:GLU:H	1.33	0.93
3:D:1309:ALA:O	3:D:1310:ARG:HB3	1.68	0.93
1:A:184:THR:HG22	1:A:192:LEU:HB3	1.50	0.93
1:B:206:THR:HG22	1:B:209:GLU:H	1.32	0.93
3:D:274:ARG:HH11	3:D:274:ARG:CG	1.80	0.93
3:D:1305:LEU:N	3:D:1305:LEU:CD2	2.30	0.93
2:C:102:HIS:HB3	2:C:105:THR:CG2	1.99	0.93
3:D:67:ARG:NH1	3:D:67:ARG:CB	2.30	0.93
3:N:209:ARG:N	3:N:389:GLU:O	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:PHE:O	3:D:86:ARG:NH2	2.01	0.93
3:N:46:ASP:OD2	3:N:48:ARG:HG3	1.69	0.93
3:N:1283:ILE:HG21	3:N:1315:ASP:OD1	1.66	0.93
3:N:890:VAL:HB	3:N:922:LEU:CD1	1.98	0.92
5:P:417:LYS:CG	5:P:418:LEU:N	2.30	0.92
2:M:198:ARG:HE	2:M:230:ARG:CA	1.82	0.92
3:N:1290:LEU:CD2	3:N:1307:LYS:HE2	1.98	0.92
3:D:894:LYS:HD2	3:D:894:LYS:H	1.01	0.92
1:B:58:ILE:CG2	1:B:61:VAL:CG1	2.48	0.92
3:D:890:VAL:HB	3:D:922:LEU:HD12	1.49	0.91
2:M:229:MET:HG2	2:M:233:GLU:CG	1.99	0.91
2:M:230:ARG:HB2	2:M:231:PRO:HD2	1.53	0.91
3:D:892:ASP:OD1	3:D:894:LYS:CD	2.18	0.91
3:N:45:PHE:O	3:N:86:ARG:NH2	2.04	0.91
2:M:172:ILE:CG1	2:M:186:VAL:CG2	2.48	0.91
2:M:107:LEU:CD1	2:M:108:ILE:H	1.77	0.91
2:C:102:HIS:HB3	2:C:105:THR:HG22	1.53	0.91
2:M:229:MET:CG	2:M:233:GLU:HB3	2.00	0.90
5:P:414:ARG:HG2	5:P:414:ARG:NH1	1.85	0.90
3:D:1284:GLU:HG2	3:D:1291:SER:HB3	1.51	0.90
2:M:229:MET:CE	2:M:234:ALA:HA	2.02	0.90
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.51	0.90
1:K:206:THR:HB	1:K:209:GLU:HG3	1.52	0.90
2:M:237:ARG:O	2:M:241:LEU:HG	1.71	0.90
1:A:206:THR:HB	1:A:209:GLU:HG3	1.52	0.90
3:N:219:GLU:HG3	3:N:339:TRP:CH2	2.06	0.90
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.53	0.90
2:C:418:LEU:HD11	2:C:427:VAL:HG11	1.54	0.90
3:N:32:ILE:CG1	5:P:258:ILE:CD1	2.50	0.89
3:N:894:LYS:HD2	3:N:894:LYS:N	1.86	0.89
3:D:821:VAL:HG11	3:D:827:ILE:HD11	1.51	0.89
2:C:168:ARG:NH2	2:C:265:ARG:O	2.05	0.89
3:N:1237:THR:HG22	3:N:1238:MET:N	1.86	0.89
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.01	0.89
3:N:227:LEU:HG	3:N:331:VAL:HG13	1.55	0.89
2:C:198:ARG:HE	2:C:230:ARG:HA	1.38	0.88
3:D:1285:GLU:OE1	3:D:1307:LYS:HE2	1.74	0.88
5:P:417:LYS:CG	5:P:418:LEU:H	1.80	0.88
3:D:67:ARG:HH11	3:D:67:ARG:HG3	1.36	0.88
3:D:892:ASP:OD1	3:D:894:LYS:HD3	1.74	0.88
3:N:894:LYS:H	3:N:894:LYS:CD	1.84	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:O	1:A:60:ASP:HB2	1.71	0.88
2:C:405:ARG:HD2	2:C:442:GLU:OE2	1.72	0.88
1:B:66:SER:O	1:B:75:VAL:HG23	1.73	0.88
3:D:209:ARG:N	3:D:389:GLU:O	2.07	0.88
2:M:105:THR:CG2	2:M:107:LEU:H	1.85	0.88
3:D:219:GLU:HG2	3:D:339:TRP:CH2	2.07	0.87
2:M:224:GLU:H	2:M:224:GLU:CD	1.78	0.87
2:M:229:MET:HE2	2:M:234:ALA:HA	1.53	0.87
2:M:487:THR:HG22	2:M:490:GLU:HB2	1.55	0.87
3:N:411:THR:HA	3:N:435:VAL:HG12	1.56	0.87
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.08	0.87
3:D:1312:LEU:CD2	3:D:1327:ARG:CG	2.53	0.87
2:M:405:ARG:HD2	2:M:442:GLU:OE2	1.73	0.87
3:N:1486:VAL:HG21	4:O:22:VAL:HG13	1.54	0.87
2:M:229:MET:HG2	2:M:233:GLU:HB3	1.57	0.86
2:C:224:GLU:H	2:C:224:GLU:CD	1.78	0.86
3:D:821:VAL:HG11	3:D:827:ILE:CD1	2.05	0.86
3:N:1311:LEU:CD2	3:N:1311:LEU:N	2.37	0.86
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.56	0.86
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.56	0.86
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.58	0.86
2:C:502:PRO:O	2:C:503:LEU:HD23	1.75	0.86
3:N:32:ILE:HD11	5:P:258:ILE:HD11	1.57	0.85
3:N:520:LEU:O	3:N:525:ARG:NH1	2.08	0.85
3:D:520:LEU:O	3:D:525:ARG:NH1	2.09	0.85
3:N:1310:ARG:HD3	3:N:1327:ARG:HD2	1.57	0.85
3:D:47:GLU:HB3	3:D:78:VAL:HG21	1.58	0.85
5:F:281:GLU:HG2	5:F:282:LEU:CD2	2.07	0.85
2:M:229:MET:HB3	2:M:233:GLU:HB3	1.58	0.85
2:M:230:ARG:CB	2:M:231:PRO:HD2	2.06	0.85
3:N:1282:ARG:HD2	3:N:1295:GLU:CD	2.01	0.85
3:N:1282:ARG:CD	3:N:1295:GLU:OE2	2.25	0.85
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.40	0.84
2:C:503:LEU:HD22	2:C:508:ILE:HA	1.60	0.84
3:D:1283:ILE:HG13	3:D:1315:ASP:CB	2.06	0.84
3:N:1283:ILE:CG2	3:N:1315:ASP:CB	2.55	0.84
3:D:274:ARG:NH2	3:D:279:VAL:HG21	1.91	0.84
1:K:201:THR:HG21	1:K:205:VAL:O	1.77	0.84
3:D:1283:ILE:HG13	3:D:1315:ASP:HB2	1.56	0.84
5:P:361:LEU:HD12	5:P:362:SER:H	1.41	0.84
2:C:177:GLU:OE2	2:C:183:SER:HB3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:864:VAL:HG12	3:D:865:THR:N	1.92	0.84
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.11	0.84
1:A:201:THR:HG21	1:A:205:VAL:O	1.77	0.84
2:C:163:ILE:HG23	2:C:171:TRP:NE1	1.93	0.84
2:M:324:ASP:O	2:M:325:ILE:HG23	1.76	0.84
2:M:182:VAL:CG2	2:M:193:LEU:CB	2.55	0.84
3:D:1304:LYS:C	3:D:1305:LEU:CD2	2.50	0.84
1:B:110:LYS:NZ	1:B:128:HIS:HB2	1.92	0.83
2:C:324:ASP:O	2:C:325:ILE:HG23	1.76	0.83
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.61	0.83
2:M:154:ARG:HH21	2:M:177:GLU:C	1.86	0.83
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.60	0.83
2:C:503:LEU:HD21	2:C:508:ILE:HD13	1.61	0.83
2:C:714:ASP:OD1	2:C:820:ARG:NH2	2.11	0.83
2:M:157:ARG:HH12	2:M:176:VAL:CG1	1.87	0.83
3:N:1237:THR:HG22	3:N:1238:MET:H	1.42	0.83
1:L:90:LEU:HB2	1:L:119:ASP:HB3	1.59	0.83
3:N:864:VAL:HG12	3:N:865:THR:N	1.93	0.83
1:A:188:GLN:HG2	1:A:189:ARG:HG3	1.60	0.82
2:C:229:MET:C	2:C:230:ARG:HG2	2.02	0.82
3:D:1283:ILE:H	3:D:1283:ILE:HD12	0.69	0.82
2:M:105:THR:CG2	2:M:107:LEU:CB	2.56	0.82
3:N:46:ASP:OD1	3:N:47:GLU:N	2.12	0.82
3:N:835:SER:HB3	3:N:838:ARG:CG	2.07	0.82
2:M:107:LEU:HD12	2:M:108:ILE:H	1.00	0.82
3:N:1305:LEU:HD23	3:N:1305:LEU:H	1.40	0.82
2:M:171:TRP:CZ3	7:R:13:DT:H2"	2.15	0.82
2:M:418:LEU:HD11	2:M:427:VAL:HG11	1.62	0.82
2:C:231:PRO:HG2	2:C:232:GLU:OE2	1.79	0.82
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.61	0.82
4:O:95:VAL:O	4:O:95:VAL:HG23	1.78	0.82
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.61	0.82
3:D:1312:LEU:HD21	3:D:1327:ARG:HG2	1.61	0.82
3:N:32:ILE:HG13	5:P:258:ILE:CD1	2.10	0.82
3:D:347:VAL:HG13	3:D:351:MET:HG3	1.61	0.82
2:M:428:ARG:NH2	2:M:447:ALA:O	2.12	0.82
3:N:1282:ARG:HD2	3:N:1295:GLU:OE2	1.80	0.82
2:C:103:LYS:O	2:C:104:ASP:HB2	1.80	0.81
2:M:229:MET:HE2	2:M:234:ALA:CA	2.10	0.81
3:N:347:VAL:HG13	3:N:351:MET:HG3	1.61	0.81
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.12	0.81
2:M:103:LYS:O	2:M:104:ASP:HB2	1.80	0.81
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.62	0.81
1:B:58:ILE:CG2	1:B:61:VAL:HG11	2.09	0.81
3:D:67:ARG:HH11	3:D:67:ARG:CB	1.89	0.81
2:M:229:MET:HG2	2:M:233:GLU:CB	2.11	0.81
3:N:1312:LEU:CD2	3:N:1327:ARG:HG2	2.10	0.81
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.11	0.81
3:N:32:ILE:HD11	5:P:258:ILE:CD1	2.10	0.81
3:D:835:SER:OG	3:D:838:ARG:HG3	1.80	0.81
3:N:411:THR:HB	3:N:437:VAL:H	1.45	0.81
2:M:78:PHE:HB3	2:M:82:GLU:HG2	1.63	0.81
2:C:164:PRO:HD2	2:C:171:TRP:HD1	1.45	0.80
3:D:411:THR:HB	3:D:437:VAL:H	1.44	0.80
3:N:219:GLU:HG3	3:N:339:TRP:CZ2	2.17	0.80
5:F:231:ARG:O	5:F:232:ARG:HG3	1.80	0.80
3:N:1304:LYS:C	3:N:1305:LEU:HD23	2.06	0.80
3:D:1439:SER:HB2	3:D:1463:LYS:NZ	1.97	0.80
3:N:1283:ILE:CG2	3:N:1315:ASP:HB2	2.09	0.80
3:N:1311:LEU:N	3:N:1311:LEU:HD22	1.96	0.80
2:M:419:THR:H	2:M:422:ARG:HG3	1.45	0.80
2:C:182:VAL:CG2	2:C:193:LEU:CB	2.60	0.79
3:N:1444:THR:O	3:N:1448:THR:HG23	1.81	0.79
2:M:172:ILE:CG1	2:M:186:VAL:HG22	2.08	0.79
2:M:229:MET:O	2:M:230:ARG:CG	2.30	0.79
3:D:821:VAL:CG1	3:D:827:ILE:HD11	2.13	0.79
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.15	0.79
2:C:419:THR:H	2:C:422:ARG:HG3	1.45	0.79
3:D:835:SER:OG	3:D:838:ARG:CG	2.31	0.79
3:D:1314:LYS:O	3:D:1317:ASP:HB2	1.81	0.79
2:M:154:ARG:NH2	2:M:177:GLU:C	2.41	0.79
2:C:78:PHE:HB3	2:C:82:GLU:HG2	1.64	0.79
2:M:717:LEU:HD23	2:M:763:GLY:HA3	1.64	0.79
3:D:693:GLU:HA	4:E:48:MET:HE1	1.65	0.79
2:M:487:THR:CG2	2:M:490:GLU:HB2	2.12	0.79
3:D:1444:THR:O	3:D:1448:THR:HG23	1.81	0.78
3:D:1384:PRO:HB3	3:D:1389:LEU:O	1.82	0.78
3:N:277:GLU:OE1	3:N:277:GLU:HA	1.83	0.78
5:P:414:ARG:HH11	5:P:414:ARG:CG	1.96	0.78
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.63	0.78
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	1.82	0.78
3:N:277:GLU:OE1	3:N:277:GLU:CA	2.31	0.78
3:N:796:ARG:HH12	3:N:859:ASP:HB2	1.48	0.78
3:N:1310:ARG:HH21	3:N:1310:ARG:HG3	1.47	0.78
3:D:1312:LEU:HD23	3:D:1327:ARG:HG3	1.64	0.78
3:N:823:LEU:HD11	3:N:837:GLY:HA2	1.64	0.78
3:N:1093:TYR:OH	3:N:1441:GLN:NE2	2.15	0.78
3:N:1283:ILE:O	3:N:1283:ILE:CD1	2.30	0.78
3:N:1284:GLU:OE1	3:N:1285:GLU:N	2.16	0.78
2:C:157:ARG:HH12	2:C:176:VAL:CG1	1.95	0.78
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.65	0.77
2:M:205:GLU:O	2:M:209:ARG:HG3	1.83	0.77
2:C:324:ASP:C	2:C:325:ILE:CG2	2.57	0.77
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.19	0.77
3:D:796:ARG:HH12	3:D:859:ASP:HB2	1.48	0.77
2:M:102:HIS:O	2:M:106:GLY:N	2.17	0.77
3:N:864:VAL:HG12	3:N:865:THR:H	1.48	0.77
2:C:151:ASP:HB3	2:C:157:ARG:O	1.84	0.77
3:N:480:GLU:OE2	3:N:488:ARG:NH2	2.17	0.77
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.20	0.77
2:M:324:ASP:C	2:M:325:ILE:CG2	2.57	0.77
3:N:821:VAL:HG11	3:N:827:ILE:HD11	1.66	0.77
3:N:1395:LEU:HD11	3:N:1400:VAL:HB	1.66	0.77
3:N:675:ARG:NH1	5:P:420:ASP:OD1	2.17	0.77
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.65	0.77
2:M:182:VAL:HG23	2:M:193:LEU:HB3	1.67	0.77
5:P:231:ARG:O	5:P:232:ARG:CG	2.30	0.77
3:N:33:ASN:HB3	3:N:36:THR:HG23	1.66	0.76
2:C:198:ARG:NE	2:C:230:ARG:HA	2.01	0.76
2:C:503:LEU:CD2	2:C:508:ILE:HA	2.15	0.76
2:C:771:GLU:OE2	2:C:775:ARG:NH2	2.18	0.76
3:D:36:THR:O	3:D:37:LEU:HB2	1.85	0.76
2:M:151:ASP:HB3	2:M:157:ARG:O	1.84	0.76
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.67	0.76
3:N:314:PRO:HG2	3:N:317:VAL:CG1	2.15	0.76
3:N:1282:ARG:HD2	3:N:1295:GLU:OE1	1.86	0.76
3:D:67:ARG:HB2	3:D:67:ARG:HH11	1.46	0.76
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.17	0.76
3:D:806:PHE:HB2	3:D:829:VAL:CG2	2.16	0.76
3:D:864:VAL:HG12	3:D:865:THR:H	1.50	0.76
2:C:108:ILE:O	2:C:108:ILE:CD1	2.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:189:ARG:HH12	2:M:244:PRO:HD3	1.50	0.76
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.65	0.76
2:M:157:ARG:HH11	2:M:157:ARG:HG3	1.50	0.76
2:M:166:PRO:O	2:M:167:LYS:HB2	1.83	0.76
5:P:383:LEU:HD23	5:P:383:LEU:H	1.50	0.76
2:M:487:THR:HG23	2:M:490:GLU:H	1.51	0.76
5:P:231:ARG:C	5:P:232:ARG:CG	2.59	0.76
2:M:157:ARG:HH11	2:M:176:VAL:HG12	1.50	0.76
2:M:229:MET:CE	2:M:234:ALA:N	2.48	0.76
2:M:238:LEU:CD1	2:M:242:LEU:HD23	2.16	0.76
3:N:835:SER:HB3	3:N:838:ARG:CD	2.14	0.76
2:C:198:ARG:HE	2:C:230:ARG:CA	1.98	0.76
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.66	0.75
3:N:1263:PHE:HD2	3:N:1375:MET:HE1	1.51	0.75
2:M:182:VAL:HG23	2:M:193:LEU:CB	2.14	0.75
3:N:1237:THR:HG21	3:N:1246:VAL:HG13	1.67	0.75
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.67	0.75
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.68	0.75
3:D:596:SER:O	3:D:597:ASP:CG	2.30	0.75
2:M:176:VAL:O	2:M:177:GLU:HB2	1.87	0.75
3:N:1237:THR:CG2	3:N:1246:VAL:HG13	2.16	0.75
3:N:1293:PHE:CZ	3:N:1302:GLU:HG3	2.21	0.75
3:D:411:THR:HA	3:D:435:VAL:HG12	1.67	0.75
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.68	0.75
3:N:1284:GLU:OE1	3:N:1284:GLU:C	2.30	0.75
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.69	0.74
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.87	0.74
1:A:59:GLU:OE1	1:A:139:ASN:ND2	2.20	0.74
2:C:157:ARG:HH11	2:C:157:ARG:HG3	1.50	0.74
2:M:229:MET:CE	2:M:234:ALA:CA	2.64	0.74
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.88	0.74
3:N:596:SER:C	3:N:597:ASP:OD2	2.30	0.74
1:A:184:THR:HG22	1:A:192:LEU:HB2	1.69	0.74
3:N:90:MET:HE3	3:N:520:LEU:HA	1.69	0.74
1:B:201:THR:HG21	1:B:205:VAL:O	1.86	0.74
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.69	0.74
3:N:219:GLU:H	3:N:339:TRP:HZ3	1.36	0.74
3:D:32:ILE:HG23	3:D:37:LEU:O	1.88	0.74
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.12	0.74
2:M:147:TYR:HA	2:M:323:ASP:OD2	1.88	0.74
5:P:416:ARG:O	5:P:417:LYS:CB	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.70	0.74
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.70	0.74
2:M:157:ARG:HH11	2:M:176:VAL:HG11	0.88	0.74
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.20	0.73
3:D:893:GLU:H	3:D:894:LYS:HE2	1.53	0.73
3:N:1283:ILE:HG21	3:N:1315:ASP:HB2	1.68	0.73
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.70	0.73
3:N:213:VAL:HG21	3:N:367:ILE:HD13	1.70	0.73
3:N:596:SER:O	3:N:597:ASP:CG	2.30	0.73
2:M:850:ALA:HA	3:N:632:VAL:CG2	2.18	0.73
3:N:274:ARG:NH1	3:N:279:VAL:HG21	2.03	0.73
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.70	0.73
5:F:202:TYR:OH	5:F:244:ARG:HG2	1.88	0.73
3:N:219:GLU:HG2	3:N:339:TRP:CH2	2.21	0.73
2:C:157:ARG:HH11	2:C:176:VAL:CG1	1.98	0.73
2:M:776:SER:OG	5:P:373:LYS:NZ	2.21	0.73
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.19	0.73
3:D:371:ILE:HD12	5:F:230:LYS:HA	1.70	0.73
3:D:373:PRO:O	3:D:376:GLU:HG2	1.89	0.73
2:C:230:ARG:HB2	2:C:231:PRO:CD	2.14	0.73
3:N:1311:LEU:CD2	3:N:1311:LEU:H	1.99	0.73
2:C:182:VAL:HG23	2:C:193:LEU:CB	2.18	0.73
3:N:1283:ILE:HG21	3:N:1315:ASP:CB	2.18	0.73
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.71	0.72
3:N:65:ARG:NH1	5:P:378:GLY:O	2.22	0.72
3:N:890:VAL:CB	3:N:922:LEU:CD1	2.67	0.72
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.04	0.72
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.90	0.72
1:K:83:LYS:HE3	1:K:168:ASP:HB2	1.71	0.72
2:M:204:GLN:HG3	2:M:222:MET:SD	2.30	0.72
3:N:255:GLU:OE1	3:N:274:ARG:NH2	2.19	0.72
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.55	0.72
3:N:892:ASP:OD1	3:N:894:LYS:CD	2.38	0.72
3:N:1263:PHE:HD2	3:N:1375:MET:CE	2.03	0.72
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.25	0.72
3:N:256:GLU:HG3	3:N:274:ARG:HE	1.54	0.72
3:N:821:VAL:HG11	3:N:827:ILE:CD1	2.19	0.72
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.71	0.72
3:D:711:LEU:HD13	3:D:778:LEU:HD12	1.70	0.72
3:D:1285:GLU:OE1	3:D:1307:LYS:CE	2.37	0.72
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.70	0.72
1:L:201:THR:HG21	1:L:205:VAL:O	1.89	0.72
2:M:238:LEU:HD12	2:M:242:LEU:HD23	1.71	0.72
2:M:48:PHE:O	2:M:52:PHE:HD2	1.72	0.72
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.04	0.72
5:P:411:HIS:O	5:P:415:THR:HB	1.89	0.72
1:B:110:LYS:HZ2	1:B:128:HIS:CB	2.03	0.72
5:F:281:GLU:CG	5:F:282:LEU:HD23	2.17	0.72
2:M:714:ASP:OD1	2:M:820:ARG:NH2	2.23	0.71
3:N:162:ARG:O	3:N:414:ARG:NH1	2.21	0.71
2:C:419:THR:H	2:C:422:ARG:CG	2.03	0.71
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.72	0.71
2:M:206:THR:HA	2:M:209:ARG:HD2	1.72	0.71
2:M:859:PRO:O	2:M:867:VAL:HG22	1.90	0.71
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.25	0.71
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.72	0.71
5:F:205:ARG:CG	5:F:205:ARG:NH1	2.37	0.71
1:K:176:ARG:NH1	2:M:863:ASP:O	2.23	0.71
3:N:1071:PHE:O	3:N:1074:SER:OG	2.09	0.71
3:D:1312:LEU:HD23	3:D:1327:ARG:CG	2.18	0.71
2:M:229:MET:HE2	2:M:234:ALA:N	2.04	0.71
3:N:1310:ARG:HG3	3:N:1310:ARG:NH2	2.05	0.71
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.73	0.71
2:M:64:LEU:CD2	2:M:100:LEU:HD11	2.16	0.71
2:M:419:THR:H	2:M:422:ARG:CG	2.03	0.71
3:N:32:ILE:CD1	5:P:258:ILE:CD1	2.68	0.71
2:M:905:ILE:HG22	2:M:906:PHE:CD2	2.26	0.71
3:N:56:TYR:HE1	3:N:69:GLU:HG3	1.54	0.71
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.55	0.70
2:C:177:GLU:HB2	2:C:181:VAL:O	1.90	0.70
2:C:204:GLN:HG3	2:C:222:MET:SD	2.31	0.70
2:M:230:ARG:HB2	2:M:231:PRO:CD	2.21	0.70
2:C:302:VAL:O	2:C:306:THR:HG23	1.91	0.70
2:M:874:LEU:HD12	3:N:784:ASP:OD2	1.90	0.70
3:N:864:VAL:CG1	3:N:865:THR:H	2.05	0.70
3:N:949:ILE:HD11	3:N:1023:MET:HE1	1.73	0.70
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.56	0.70
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.74	0.70
2:M:628:PHE:H	2:M:638:ASP:CB	2.04	0.70
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.55	0.70
2:C:418:LEU:CD1	2:C:427:VAL:HG11	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.27	0.70
3:D:864:VAL:CG1	3:D:865:THR:H	2.05	0.70
3:N:1044:LEU:H	3:N:1044:LEU:HD12	1.57	0.70
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.73	0.70
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.57	0.70
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.74	0.70
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.27	0.69
2:M:1008:ARG:O	3:N:625:TYR:HA	1.92	0.69
3:N:596:SER:C	3:N:597:ASP:CG	2.60	0.69
3:D:1071:PHE:O	3:D:1074:SER:OG	2.10	0.69
3:D:1283:ILE:CG1	3:D:1315:ASP:CG	2.65	0.69
3:N:711:LEU:HD13	3:N:778:LEU:HD12	1.73	0.69
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.27	0.69
2:M:74:GLY:HA3	2:M:93:PRO:HG2	1.74	0.69
2:M:230:ARG:CB	2:M:231:PRO:CD	2.71	0.69
3:N:266:GLU:OE2	3:N:315:ARG:NH2	2.26	0.69
5:P:415:THR:HG22	5:P:416:ARG:HG2	1.72	0.69
1:B:88:ARG:HB3	1:B:121:GLU:HB2	1.75	0.69
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.69
2:M:231:PRO:CG	2:M:232:GLU:OE2	2.33	0.69
2:C:1008:ARG:O	3:D:625:TYR:HA	1.91	0.69
3:D:47:GLU:CB	3:D:78:VAL:HG21	2.23	0.69
3:D:493:ARG:HG3	3:D:1390:LEU:HD11	1.73	0.69
3:D:1118:ILE:HD12	3:D:1192:LEU:HD12	1.73	0.69
3:D:1310:ARG:C	3:D:1311:LEU:CD2	2.63	0.69
2:M:107:LEU:HD12	2:M:108:ILE:CA	2.20	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
3:D:493:ARG:HG3	3:D:1390:LEU:CD1	2.23	0.69
3:N:71:LYS:NZ	3:N:74:GLU:OE2	2.21	0.69
3:N:1136:LYS:O	3:N:1140:ILE:HG13	1.92	0.69
3:N:1237:THR:O	3:N:1238:MET:C	2.34	0.69
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.58	0.69
3:D:1310:ARG:HD2	3:D:1327:ARG:HB2	1.75	0.69
2:C:628:PHE:H	2:C:638:ASP:CB	2.05	0.69
1:L:88:ARG:HB3	1:L:121:GLU:HB2	1.75	0.68
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.26	0.68
3:D:1314:LYS:HG3	3:D:1317:ASP:CG	2.18	0.68
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.75	0.68
2:M:238:LEU:HD12	2:M:238:LEU:O	1.92	0.68
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.75	0.68
3:N:1282:ARG:HH11	3:N:1282:ARG:CG	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1282:ARG:HD3	3:N:1295:GLU:OE2	1.92	0.68
2:M:200:LEU:HD13	2:M:300:ASP:HB2	1.75	0.68
2:M:787:ASP:OD2	2:M:791:ARG:NH2	2.27	0.68
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.57	0.68
3:N:46:ASP:OD1	3:N:46:ASP:C	2.35	0.68
5:F:231:ARG:O	5:F:232:ARG:CG	2.41	0.68
2:M:262:ALA:HA	2:M:291:ALA:O	1.93	0.68
2:M:302:VAL:O	2:M:306:THR:HG23	1.93	0.68
3:N:963:TYR:CE2	3:N:1002:LYS:HD3	2.28	0.68
2:C:262:ALA:HA	2:C:289:THR:HG21	1.76	0.68
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.75	0.68
2:M:286:SER:OG	2:M:301:GLU:OE2	2.10	0.68
3:N:675:ARG:HH12	5:P:420:ASP:HB3	1.59	0.68
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.74	0.68
3:D:864:VAL:CG1	3:D:865:THR:N	2.57	0.68
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.74	0.68
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.26	0.68
2:C:229:MET:HB3	2:C:233:GLU:HB3	1.75	0.68
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.75	0.68
2:M:230:ARG:CG	2:M:231:PRO:HD2	2.23	0.68
1:B:64:GLU:O	1:B:75:VAL:HB	1.94	0.68
3:D:1311:LEU:N	3:D:1311:LEU:CD2	2.52	0.67
2:M:165:LEU:O	2:M:168:ARG:HB2	1.94	0.67
5:P:384:GLU:HB3	5:P:394:ARG:HD2	1.74	0.67
2:C:157:ARG:NH1	2:C:176:VAL:HG12	2.07	0.67
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.75	0.67
3:N:657:LEU:HG	3:N:661:MET:HE2	1.75	0.67
1:A:27:PRO:HB3	1:A:184:THR:HG21	1.76	0.67
5:P:368:VAL:HG12	5:P:390:PHE:CE1	2.30	0.67
2:C:859:PRO:O	2:C:867:VAL:HG22	1.95	0.67
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.76	0.67
2:M:261:ILE:HG23	2:M:290:LEU:HB2	1.76	0.67
2:C:229:MET:HE2	2:C:234:ALA:HA	1.77	0.67
2:C:786:LYS:NZ	2:C:786:LYS:CB	2.57	0.67
2:M:171:TRP:CE3	7:R:13:DT:H2"	2.30	0.67
2:M:758:ARG:HH21	2:M:788:THR:HB	1.60	0.67
3:N:219:GLU:N	3:N:339:TRP:CZ3	2.63	0.67
3:N:864:VAL:CG1	3:N:865:THR:N	2.58	0.67
5:P:364:ARG:O	5:P:368:VAL:HG13	1.95	0.67
2:M:262:ALA:HA	2:M:289:THR:HG21	1.77	0.67
3:N:276:ASP:C	3:N:277:GLU:OE1	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1292:VAL:CG2	3:N:1305:LEU:HD11	2.25	0.67
3:D:46:ASP:OD1	3:D:47:GLU:N	2.28	0.66
3:N:892:ASP:OD1	3:N:894:LYS:HD3	1.95	0.66
3:D:142:LEU:HD13	3:D:161:LEU:HD11	1.77	0.66
3:D:1375:MET:HE2	3:D:1424:VAL:HG13	1.77	0.66
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.30	0.66
3:N:658:LEU:HA	3:N:661:MET:HE3	1.76	0.66
5:P:127:ILE:O	5:P:131:VAL:HG23	1.95	0.66
2:C:229:MET:CE	2:C:234:ALA:HA	2.25	0.66
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.66
3:N:1237:THR:HG21	3:N:1246:VAL:HG22	1.76	0.66
1:L:5:LYS:HA	1:L:5:LYS:HE3	1.77	0.66
3:N:1468:LEU:HB3	3:N:1470:ARG:HG3	1.77	0.66
2:M:1058:ASP:OD1	3:N:621:LYS:HE2	1.95	0.66
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.29	0.66
5:P:386:VAL:HG12	5:P:397:ILE:HG21	1.76	0.66
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.31	0.66
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.77	0.66
3:D:1482:ARG:HH21	3:D:1483:PHE:HZ	1.43	0.66
5:F:126:LEU:O	5:F:130:VAL:HG23	1.96	0.66
3:N:832:ARG:HH21	3:N:833:GLU:HG3	1.60	0.66
2:C:286:SER:OG	2:C:301:GLU:OE2	2.10	0.66
3:D:657:LEU:HG	3:D:661:MET:HE2	1.76	0.66
3:D:832:ARG:HH21	3:D:833:GLU:HG3	1.60	0.66
1:L:6:LEU:HD12	1:L:7:LYS:H	1.60	0.66
2:M:628:PHE:N	2:M:638:ASP:HB3	2.07	0.66
3:N:1375:MET:HE2	3:N:1424:VAL:HG13	1.76	0.66
2:C:108:ILE:C	2:C:108:ILE:CD1	2.57	0.66
2:M:261:ILE:CG2	2:M:291:ALA:HB3	2.26	0.66
3:N:562:ALA:O	5:P:140:ARG:NH2	2.27	0.66
3:N:1310:ARG:CD	3:N:1327:ARG:HD2	2.25	0.66
5:P:78:SER:O	5:P:80:PRO:CD	2.44	0.66
2:M:173:ASP:C	2:M:174:LEU:HD12	2.20	0.66
3:N:421:LEU:HD11	3:N:429:SER:HB2	1.77	0.66
3:N:1277:ILE:HG22	3:N:1278:ASP:H	1.61	0.66
2:C:628:PHE:N	2:C:638:ASP:HB3	2.08	0.65
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.29	0.65
3:D:213:VAL:HG21	3:D:367:ILE:HD13	1.78	0.65
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.59	0.65
2:C:166:PRO:O	2:C:167:LYS:HB2	1.95	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:348:GLN:HB3	3:D:349:PRO:HD2	1.79	0.65
3:D:1304:LYS:CA	3:D:1305:LEU:HD23	2.27	0.65
3:N:142:LEU:HD13	3:N:161:LEU:HD11	1.78	0.65
2:M:425:PHE:CE2	3:N:1086:LEU:HD12	2.31	0.65
2:M:874:LEU:CD1	3:N:784:ASP:OD2	2.45	0.65
2:C:680:ASP:OD1	3:D:943:THR:HG21	1.96	0.65
3:D:47:GLU:HB3	3:D:78:VAL:CG2	2.26	0.65
3:D:530:VAL:HG12	5:F:333:ILE:HD12	1.79	0.65
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.29	0.65
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.29	0.65
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	1.95	0.65
2:M:172:ILE:HG12	2:M:186:VAL:CG2	2.27	0.65
3:D:1100:ASP:OD1	3:D:1440:PHE:HB2	1.96	0.65
1:L:49:PRO:HA	1:L:148:VAL:HG12	1.78	0.65
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.79	0.65
1:K:228:PRO:O	1:K:229:GLN:HG3	1.96	0.65
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.77	0.65
2:M:437:ARG:NH2	2:M:491:GLU:OE2	2.29	0.65
3:N:952:ASP:HA	3:N:1062:ARG:HH21	1.62	0.65
2:C:368:THR:H	2:C:371:LYS:HD2	1.62	0.65
3:D:890:VAL:CB	3:D:922:LEU:CD1	2.70	0.65
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.79	0.65
2:M:51:THR:O	2:M:265:ARG:NH2	2.29	0.65
2:M:36:PRO:HA	2:M:39:ARG:HG3	1.79	0.64
2:M:198:ARG:CZ	2:M:230:ARG:HA	2.27	0.64
4:O:52:GLU:OE1	4:O:52:GLU:N	2.27	0.64
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.63	0.64
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.96	0.64
3:N:1143:GLY:O	3:N:1147:ARG:HD2	1.97	0.64
5:P:382:THR:HG23	5:P:384:GLU:O	1.98	0.64
2:C:176:VAL:O	2:C:177:GLU:HB2	1.97	0.64
4:E:52:GLU:OE1	4:E:52:GLU:N	2.28	0.64
2:M:1103:ASP:HB3	2:M:1105:LYS:H	1.62	0.64
3:N:348:GLN:HB3	3:N:349:PRO:HD2	1.79	0.64
3:N:661:MET:HE1	3:N:677:LEU:HD11	1.79	0.64
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.78	0.64
3:D:835:SER:OG	3:D:838:ARG:NE	2.30	0.64
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.79	0.64
2:M:368:THR:H	2:M:371:LYS:HD2	1.62	0.64
3:N:569:ASN:O	3:N:573:MET:HG3	1.98	0.64
2:C:232:GLU:OE2	2:C:232:GLU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:270:LYS:HE2	5:F:295:MET:HE1	1.78	0.64
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.78	0.64
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.79	0.64
3:N:1371:VAL:HG12	3:N:1375:MET:HE3	1.79	0.64
5:P:205:ARG:CG	5:P:205:ARG:HH11	2.11	0.64
1:A:11:PHE:O	1:B:228:PRO:HA	1.96	0.64
2:C:198:ARG:HH11	2:C:230:ARG:HA	1.63	0.64
2:C:292:ARG:HG3	2:C:299:LYS:HB2	1.78	0.64
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.79	0.64
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.28	0.64
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.78	0.64
3:N:808:THR:HG22	3:N:810:GLU:H	1.63	0.64
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.79	0.64
3:D:17:LYS:O	3:D:20:SER:HB3	1.98	0.64
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.79	0.64
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.27	0.64
1:K:11:PHE:O	1:L:228:PRO:HA	1.98	0.64
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.80	0.64
2:M:266:ARG:NH1	7:R:11:DG:O6	2.31	0.64
3:N:1315:ASP:OD2	3:N:1316:GLY:N	2.31	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:N:1309:ALA:O	3:N:1310:ARG:CB	2.46	0.64
5:P:78:SER:O	5:P:80:PRO:N	2.31	0.64
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.79	0.63
3:N:1486:VAL:CG2	4:O:22:VAL:HG13	2.26	0.63
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.78	0.63
4:O:95:VAL:O	4:O:95:VAL:CG2	2.46	0.63
1:B:58:ILE:HG21	1:B:61:VAL:HG11	1.78	0.63
2:C:911:GLU:O	2:C:915:LYS:HG2	1.99	0.63
2:C:1103:ASP:HB3	2:C:1105:LYS:H	1.63	0.63
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.80	0.63
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.62	0.63
3:D:1370:ILE:O	3:D:1373:ARG:HG2	1.99	0.63
2:C:356:ARG:HA	2:C:359:MET:HG3	1.81	0.63
3:N:639:LEU:HA	3:N:729:HIS:CD2	2.32	0.63
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	1.81	0.63
1:L:162:ILE:O	1:L:163:ASN:CB	2.43	0.63
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.79	0.63
2:M:595:LEU:HD21	2:M:623:TYR:HB3	1.80	0.63
3:N:786:ILE:HG22	3:N:1026:SER:HB2	1.81	0.63
3:N:894:LYS:N	3:N:894:LYS:CD	2.54	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.80	0.63
3:N:711:LEU:HD13	3:N:778:LEU:CD1	2.29	0.63
2:C:230:ARG:CB	2:C:231:PRO:HD2	2.20	0.63
2:C:262:ALA:HA	2:C:289:THR:CG2	2.28	0.63
2:C:786:LYS:NZ	2:C:786:LYS:HB2	2.14	0.63
3:D:808:THR:HG22	3:D:810:GLU:H	1.63	0.63
2:M:179:ASN:OD1	2:M:179:ASN:C	2.39	0.63
3:N:56:TYR:HB3	3:N:65:ARG:O	1.98	0.63
3:N:137:PRO:HB3	3:N:147:VAL:HG12	1.81	0.63
2:C:154:ARG:NH1	2:C:154:ARG:CG	2.45	0.63
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.80	0.63
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.33	0.63
2:M:168:ARG:HG3	2:M:168:ARG:NH1	2.14	0.63
2:M:911:GLU:O	2:M:915:LYS:HG2	1.99	0.63
1:A:228:PRO:O	1:A:229:GLN:HG3	1.98	0.62
2:C:503:LEU:CD2	2:C:508:ILE:HD13	2.28	0.62
2:C:773:LEU:O	2:C:777:ILE:HG13	1.99	0.62
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.99	0.62
5:P:78:SER:O	5:P:80:PRO:HD3	1.99	0.62
2:C:229:MET:HE2	2:C:234:ALA:CA	2.29	0.62
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.80	0.62
3:D:658:LEU:HA	3:D:661:MET:HE3	1.80	0.62
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.33	0.62
2:M:232:GLU:OE2	2:M:232:GLU:N	2.30	0.62
2:M:262:ALA:HA	2:M:289:THR:CG2	2.28	0.62
2:M:874:LEU:O	11:M:1229:HOH:O	2.16	0.62
3:N:493:ARG:HG3	3:N:1390:LEU:CD1	2.29	0.62
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.32	0.62
5:P:392:VAL:HG21	5:P:397:ILE:HD13	1.80	0.62
3:N:32:ILE:HG12	5:P:258:ILE:HD13	1.74	0.62
3:N:1205:TYR:CE1	3:N:1366:LYS:HD3	2.35	0.62
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.80	0.62
3:D:1236:LEU:HA	3:D:1359:GLN:HG2	1.81	0.62
3:N:493:ARG:HG3	3:N:1390:LEU:HD11	1.82	0.62
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.81	0.62
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.80	0.62
3:D:1122:LEU:HD12	3:D:1185:GLU:HA	1.80	0.62
3:D:1310:ARG:CA	3:D:1311:LEU:HD23	2.29	0.62
2:C:179:ASN:OD1	2:C:181:VAL:N	2.23	0.62
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.34	0.62
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:356:ARG:HA	2:M:359:MET:HG3	1.82	0.62
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.81	0.62
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.81	0.62
3:D:569:ASN:O	3:D:573:MET:HG3	2.00	0.62
2:M:171:TRP:CZ3	7:R:14:DG:OP1	2.53	0.62
5:P:96:LEU:O	5:P:100:VAL:HG23	2.00	0.62
1:A:176:ARG:NH1	2:C:863:ASP:O	2.32	0.62
3:D:541:ASN:O	3:D:545:ARG:HG3	2.00	0.62
3:D:786:ILE:HG22	3:D:1026:SER:HB2	1.82	0.62
3:N:675:ARG:HH12	5:P:420:ASP:CB	2.13	0.62
2:C:136:ILE:HB	2:C:336:VAL:HG12	1.81	0.62
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.14	0.62
2:C:957:LYS:HG2	2:C:961:GLU:OE1	1.99	0.62
3:D:890:VAL:CB	3:D:922:LEU:HD12	2.26	0.62
2:M:874:LEU:HD21	3:N:787:LEU:HD22	1.80	0.62
3:N:237:LYS:O	3:N:240:GLU:HB3	2.00	0.62
1:B:63:HIS:ND1	1:B:66:SER:OG	2.31	0.61
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.82	0.61
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.33	0.61
2:M:168:ARG:NH2	2:M:265:ARG:O	2.33	0.61
5:P:409:LYS:C	5:P:409:LYS:HD3	2.25	0.61
5:F:152:ASP:HB2	5:F:153:PRO:HD2	1.81	0.61
2:M:168:ARG:HG3	2:M:168:ARG:HH11	1.64	0.61
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.83	0.61
3:D:67:ARG:CB	3:D:67:ARG:CZ	2.76	0.61
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.82	0.61
1:L:213:GLN:O	1:L:217:ILE:HG13	1.99	0.61
2:M:1006:HIS:HB2	2:M:1024:LYS:HG3	1.82	0.61
3:N:592:THR:OG1	3:N:596:SER:HA	2.00	0.61
2:M:717:LEU:CD2	2:M:763:GLY:HA3	2.31	0.61
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	1.82	0.61
3:N:371:ILE:HD12	5:P:230:LYS:HA	1.81	0.61
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.81	0.61
3:N:1400:VAL:HG21	3:N:1417:TRP:CD1	2.36	0.61
1:A:184:THR:CG2	1:A:192:LEU:HB3	2.29	0.61
3:D:274:ARG:NH1	3:D:274:ARG:CG	2.48	0.61
2:M:261:ILE:HG21	2:M:291:ALA:HB3	1.83	0.61
2:M:716:LYS:HE3	3:N:35:ARG:O	2.01	0.61
3:N:1311:LEU:HB2	3:N:1325:LEU:O	2.01	0.61
2:C:1090:LYS:HE2	3:D:88:TYR:O	1.99	0.61
5:P:361:LEU:HD13	5:P:365:GLU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:198:ARG:NH1	2:M:230:ARG:HA	2.15	0.61
2:M:198:ARG:HH11	2:M:230:ARG:HA	1.64	0.61
2:M:229:MET:HE1	2:M:233:GLU:O	1.97	0.61
2:M:418:LEU:CD1	2:M:427:VAL:HG11	2.31	0.61
2:M:503:LEU:HD21	2:M:508:ILE:HD13	1.83	0.61
3:N:541:ASN:O	3:N:545:ARG:HG3	2.01	0.61
3:N:1101:VAL:HG21	3:N:1424:VAL:HB	1.82	0.61
1:A:10:VAL:HG22	1:A:26:GLU:O	2.00	0.61
2:C:15:LEU:O	2:C:586:ARG:NH2	2.28	0.61
3:D:1410:GLU:O	3:D:1410:GLU:HG2	1.99	0.61
5:F:295:MET:HA	5:F:295:MET:HE2	1.82	0.61
3:N:373:PRO:O	3:N:376:GLU:HG2	2.00	0.61
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.01	0.61
3:N:1290:LEU:HD21	3:N:1307:LYS:HE2	1.81	0.61
1:A:57:TYR:CE1	1:A:161:ARG:CD	2.84	0.61
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.36	0.61
5:F:362:SER:OG	5:F:365:GLU:HG2	2.01	0.61
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.65	0.61
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.66	0.60
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.66	0.60
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.66	0.60
3:D:1283:ILE:CD1	3:D:1283:ILE:N	2.30	0.60
2:M:136:ILE:HB	2:M:336:VAL:HG12	1.83	0.60
2:M:480:THR:HG22	2:M:482:GLU:H	1.66	0.60
2:M:957:LYS:HG2	2:M:961:GLU:OE1	2.01	0.60
5:P:205:ARG:NH1	5:P:205:ARG:HG2	2.16	0.60
3:D:33:ASN:O	3:D:37:LEU:HA	2.01	0.60
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.36	0.60
2:M:853:LEU:HB2	2:M:858:MET:CE	2.25	0.60
3:N:783:ARG:NH1	3:N:1028:ALA:O	2.34	0.60
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.81	0.60
1:B:213:GLN:O	1:B:217:ILE:HG13	2.01	0.60
2:C:383:ARG:O	2:C:387:SER:HB2	2.01	0.60
2:C:480:THR:HG22	2:C:482:GLU:H	1.66	0.60
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.82	0.60
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.84	0.60
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.83	0.60
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.82	0.60
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.82	0.60
2:C:988:VAL:HG21	3:D:949:ILE:O	2.01	0.60
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:893:GLU:N	3:D:894:LYS:HE2	2.16	0.60
3:N:15:PRO:O	3:N:19:ARG:HG3	2.02	0.60
3:N:47:GLU:CD	3:N:53:ILE:HG12	2.26	0.60
3:N:586:ARG:HH12	6:Q:10:DG:H5''	1.67	0.60
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.37	0.60
1:A:30:ARG:HD3	1:A:191:ASP:CG	2.26	0.60
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.37	0.60
3:D:1309:ALA:O	3:D:1310:ARG:CB	2.46	0.60
6:G:15:DT:H2'	6:G:16:DC:C6	2.37	0.60
2:M:626:ARG:HG3	2:M:629:TYR:CD1	2.37	0.60
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.82	0.60
1:A:184:THR:O	1:A:192:LEU:HB2	2.02	0.60
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.35	0.60
2:M:569:VAL:HG21	2:M:1000:MET:CE	2.32	0.60
2:C:177:GLU:OE2	2:C:183:SER:CB	2.48	0.60
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.37	0.60
3:D:132:TYR:HB2	3:D:153:LEU:HD12	1.83	0.60
3:D:1490:LYS:HD2	4:E:93:TYR:OH	2.01	0.60
3:N:67:ARG:HH11	3:N:67:ARG:HG3	1.67	0.60
1:A:206:THR:HG23	1:A:207:PRO:HD2	1.84	0.60
3:D:90:MET:HE3	3:D:520:LEU:HA	1.82	0.60
2:C:669:GLY:H	2:C:993:PHE:HZ	1.47	0.59
2:M:172:ILE:HG23	2:M:184:MET:HG2	1.83	0.59
2:M:773:LEU:HD22	5:P:375:LEU:HD12	1.84	0.59
3:N:1100:ASP:CG	3:N:1440:PHE:HB2	2.27	0.59
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.02	0.59
3:D:32:ILE:HD13	3:D:39:PRO:HA	1.83	0.59
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.35	0.59
3:N:127:LEU:HA	3:N:457:GLY:HA2	1.84	0.59
3:N:131:LYS:O	3:N:456:MET:HG2	2.02	0.59
3:N:412:GLY:H	3:N:435:VAL:HG12	1.66	0.59
3:N:618:LEU:HG	3:N:1467:ILE:HG23	1.84	0.59
1:K:206:THR:HG23	1:K:207:PRO:HD2	1.83	0.59
3:N:132:TYR:HB2	3:N:153:LEU:HD12	1.83	0.59
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.37	0.59
3:D:844:ALA:O	3:D:867:ARG:HB3	2.02	0.59
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.37	0.59
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.38	0.59
3:N:774:SER:HB3	3:N:1362:LYS:O	2.03	0.59
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.36	0.59
1:A:70:GLY:N	2:C:607:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.67	0.59
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.85	0.59
3:D:1285:GLU:OE1	3:D:1307:LYS:NZ	2.36	0.59
2:M:154:ARG:CG	2:M:154:ARG:NH1	2.45	0.59
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.84	0.59
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.84	0.59
2:C:151:ASP:CB	2:C:157:ARG:O	2.50	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.85	0.59
3:D:603:LEU:HA	3:D:606:ILE:HD12	1.84	0.59
2:M:15:LEU:O	2:M:586:ARG:NH2	2.29	0.59
5:P:194:LEU:O	5:P:198:ILE:HG13	2.02	0.59
3:D:1435:LEU:O	3:D:1439:SER:OG	2.13	0.59
1:K:206:THR:HG22	1:K:208:LEU:H	1.67	0.59
3:N:845:ASN:HB2	3:N:846:PRO:HD2	1.85	0.59
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.84	0.59
3:N:1205:TYR:CZ	3:N:1366:LYS:HD3	2.38	0.59
2:C:157:ARG:HD3	2:C:157:ARG:N	2.18	0.59
3:D:67:ARG:NH1	5:F:379:ARG:HB2	2.18	0.59
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.85	0.59
3:D:388:HIS:O	3:D:390:PRO:HD3	2.02	0.59
3:D:580:ALA:O	3:D:584:ASN:HB2	2.03	0.59
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.03	0.59
5:F:230:LYS:O	5:F:232:ARG:HG3	2.02	0.59
1:L:115:LEU:O	1:L:117:VAL:HG23	2.02	0.59
1:A:219:ARG:HG3	1:A:220:GLU:N	2.17	0.59
3:N:844:ALA:O	3:N:867:ARG:HB3	2.03	0.59
3:N:963:TYR:HE2	3:N:1002:LYS:HD3	1.68	0.59
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.38	0.59
1:B:115:LEU:O	1:B:117:VAL:HG23	2.02	0.59
2:C:134:ARG:NH1	2:C:392:SER:O	2.35	0.59
2:C:482:GLU:HG3	2:C:482:GLU:O	2.01	0.59
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.85	0.59
3:D:1439:SER:HB2	3:D:1463:LYS:HZ3	1.67	0.59
1:K:219:ARG:HG3	1:K:220:GLU:N	2.17	0.59
2:M:184:MET:HE3	2:M:186:VAL:CG2	2.33	0.59
2:M:383:ARG:O	2:M:387:SER:HB2	2.03	0.59
2:M:482:GLU:HG3	2:M:482:GLU:O	2.03	0.59
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.01	0.59
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.85	0.59
3:N:202:VAL:HG21	3:N:400:VAL:HG13	1.83	0.59
6:Q:15:DT:H2'	6:Q:16:DC:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:HIS:CB	2:C:105:THR:CG2	2.78	0.58
2:C:420:ARG:NH2	2:C:448:ASN:OD1	2.33	0.58
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.36	0.58
3:D:876:SER:OG	3:D:879:ARG:HG3	2.02	0.58
1:K:10:VAL:HG22	1:K:26:GLU:O	2.03	0.58
2:M:858:MET:HG3	2:M:867:VAL:HG23	1.85	0.58
3:N:260:GLU:OE1	3:N:273:ARG:CZ	2.51	0.58
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.38	0.58
1:B:123:MET:HE2	1:B:204:SER:HA	1.85	0.58
2:C:105:THR:O	2:C:105:THR:HG23	2.03	0.58
2:C:157:ARG:HH11	2:C:157:ARG:CG	2.15	0.58
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.85	0.58
3:N:1286:THR:HG22	3:N:1288:GLU:H	1.68	0.58
4:O:50:THR:HG22	4:O:51:LEU:H	1.67	0.58
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.86	0.58
3:D:56:TYR:HB3	3:D:65:ARG:O	2.01	0.58
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.84	0.58
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.38	0.58
2:C:487:THR:HG23	2:C:490:GLU:H	1.68	0.58
3:D:33:ASN:HB3	3:D:36:THR:HG23	1.84	0.58
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.44	0.58
2:M:302:VAL:O	2:M:305:PRO:HD2	2.03	0.58
3:N:1384:PRO:HB3	3:N:1389:LEU:O	2.04	0.58
5:P:382:THR:CG2	5:P:384:GLU:HG2	2.33	0.58
2:C:198:ARG:NH1	2:C:230:ARG:HA	2.17	0.58
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.36	0.58
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.39	0.58
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.84	0.58
1:L:123:MET:HE2	1:L:204:SER:HA	1.85	0.58
2:M:167:LYS:O	2:M:168:ARG:CD	2.44	0.58
2:M:772:ARG:HH22	5:P:380:GLU:HB3	1.69	0.58
3:N:658:LEU:HD23	3:N:661:MET:CE	2.33	0.58
5:P:228:GLU:OE2	5:P:231:ARG:NE	2.37	0.58
5:P:394:ARG:HG2	5:P:395:GLU:HG2	1.85	0.58
1:A:211:LEU:O	1:A:215:VAL:HG23	2.03	0.58
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.02	0.58
1:K:30:ARG:CD	1:K:191:ASP:OD1	2.51	0.58
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.86	0.58
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.18	0.58
2:M:229:MET:HE1	2:M:234:ALA:HA	1.85	0.58
3:N:37:LEU:HD13	3:N:535:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.69	0.58
1:L:94:LEU:HD11	1:L:96:THR:O	2.03	0.58
3:N:149:LYS:O	3:N:150:ARG:HB2	2.03	0.58
3:N:233:LYS:HD2	3:N:240:GLU:OE2	2.03	0.58
3:N:437:VAL:HG11	5:P:175:HIS:CD2	2.39	0.58
2:M:235:LEU:CD1	2:M:257:VAL:HG21	2.34	0.58
2:M:1090:LYS:HE2	3:N:88:TYR:O	2.04	0.58
3:N:317:VAL:HG23	3:N:339:TRP:HB3	1.86	0.58
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.31	0.58
3:D:1331:ASP:C	3:D:1331:ASP:OD1	2.45	0.58
3:N:876:SER:OG	3:N:879:ARG:HG3	2.02	0.58
3:N:1263:PHE:CD2	3:N:1375:MET:HE1	2.38	0.58
2:C:786:LYS:HB2	2:C:786:LYS:HZ2	1.69	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.38	0.58
3:D:264:LEU:HD12	3:D:264:LEU:O	2.04	0.57
3:D:490:ALA:O	3:D:494:LYS:HG3	2.04	0.57
2:M:420:ARG:NH2	2:M:448:ASN:OD1	2.36	0.57
3:D:433:GLY:HA3	3:D:446:VAL:CG1	2.33	0.57
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.87	0.57
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.17	0.57
5:F:202:TYR:HE2	5:F:248:ASN:OD1	1.87	0.57
3:N:36:THR:O	3:N:37:LEU:HB2	2.03	0.57
3:N:835:SER:HB3	3:N:838:ARG:HG2	1.85	0.57
3:N:1194:CYS:O	3:N:1373:ARG:NH2	2.37	0.57
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.17	0.57
1:B:76:VAL:O	1:B:79:ILE:HG12	2.04	0.57
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.39	0.57
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.86	0.57
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.85	0.57
2:M:114:PHE:CD2	5:P:283:GLY:HA2	2.39	0.57
2:M:157:ARG:HD3	2:M:157:ARG:N	2.17	0.57
3:N:259:VAL:HG13	3:N:270:LEU:HD11	1.85	0.57
3:N:276:ASP:O	3:N:277:GLU:OE1	2.22	0.57
5:P:376:ILE:HD12	5:P:377:ASP:HB3	1.86	0.57
2:C:580:MET:HB3	2:C:584:GLU:CD	2.29	0.57
3:D:405:ASP:CG	3:D:406:ASP:H	2.11	0.57
3:D:890:VAL:HB	3:D:922:LEU:HD11	1.82	0.57
2:M:127:PHE:O	2:M:133:ASP:HA	2.03	0.57
2:M:146:VAL:HG22	2:M:162:ILE:HG12	1.86	0.57
2:M:156:GLY:C	2:M:157:ARG:HD3	2.29	0.57
3:N:405:ASP:CG	3:N:406:ASP:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:O	1:A:114:PHE:HD1	1.87	0.57
1:A:206:THR:HG22	1:A:208:LEU:H	1.70	0.57
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.85	0.57
5:F:202:TYR:O	5:F:205:ARG:HD3	2.04	0.57
1:L:138:LEU:HD21	1:L:140:MET:HE3	1.86	0.57
2:M:151:ASP:CB	2:M:157:ARG:O	2.50	0.57
3:N:558:LEU:HD13	5:P:142:ARG:HD2	1.86	0.57
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.19	0.57
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.86	0.57
2:C:327:HIS:NE2	2:C:433:THR:HG21	2.19	0.57
3:D:808:THR:HB	3:D:811:GLU:HG3	1.87	0.57
4:E:50:THR:HG22	4:E:51:LEU:H	1.68	0.57
2:M:157:ARG:HG3	2:M:176:VAL:CG1	2.35	0.57
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.86	0.57
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.86	0.57
5:P:256:ARG:NH2	5:P:311:ALA:O	2.37	0.57
1:A:57:TYR:CD1	1:A:161:ARG:CD	2.80	0.57
2:C:617:ASP:N	2:C:617:ASP:OD1	2.37	0.57
2:M:182:VAL:HG23	2:M:193:LEU:HB2	1.86	0.57
3:N:388:HIS:O	3:N:390:PRO:HD3	2.04	0.57
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.40	0.57
2:M:238:LEU:HD11	2:M:242:LEU:HD23	1.86	0.57
5:P:397:ILE:O	5:P:400:ILE:HG22	2.05	0.57
1:B:138:LEU:HD21	1:B:140:MET:HE3	1.87	0.57
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.04	0.57
1:K:211:LEU:O	1:K:215:VAL:HG23	2.05	0.57
1:L:76:VAL:O	1:L:79:ILE:HG12	2.05	0.57
2:M:150:PRO:HD3	2:M:322:VAL:CG1	2.35	0.57
3:N:103:TRP:CE2	3:N:1444:THR:HG22	2.40	0.57
3:N:1282:ARG:HH11	3:N:1282:ARG:HG3	1.67	0.57
2:C:171:TRP:CZ3	7:H:13:DT:H2"	2.40	0.57
2:C:174:LEU:HD11	2:C:184:MET:HG3	1.86	0.57
3:D:1010:ASN:OD1	3:D:1014:ASN:ND2	2.37	0.57
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.70	0.57
5:F:287:THR:O	5:F:291:ILE:HG13	2.05	0.57
3:N:563:PRO:HB3	5:P:189:GLU:HG3	1.86	0.57
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.40	0.56
3:D:1264:GLU:OE1	3:D:1264:GLU:HA	2.05	0.56
3:N:808:THR:HB	3:N:811:GLU:HG3	1.87	0.56
5:P:222:ARG:HD2	5:P:222:ARG:N	2.18	0.56
2:C:157:ARG:HH11	2:C:176:VAL:HG11	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:15:PRO:O	3:D:19:ARG:HG3	2.05	0.56
1:L:58:ILE:HB	1:L:61:VAL:HB	1.87	0.56
2:M:150:PRO:HD3	2:M:322:VAL:HG13	1.87	0.56
2:M:248:PRO:C	2:M:250:ARG:H	2.12	0.56
2:M:617:ASP:N	2:M:617:ASP:OD1	2.37	0.56
1:A:30:ARG:HD3	1:A:191:ASP:OD2	2.06	0.56
2:C:156:GLY:C	2:C:157:ARG:HD3	2.29	0.56
2:C:184:MET:HE3	2:C:186:VAL:CG2	2.34	0.56
2:C:302:VAL:O	2:C:305:PRO:HD2	2.06	0.56
2:C:363:SER:O	2:C:367:LEU:HD21	2.04	0.56
3:D:1231:GLU:N	3:D:1232:PRO:HD2	2.21	0.56
1:K:111:ALA:O	1:K:114:PHE:HD1	1.89	0.56
2:M:294:GLU:O	2:M:295:ASP:C	2.48	0.56
3:N:1276:GLU:OE2	3:N:1301:LYS:HE3	2.04	0.56
5:P:383:LEU:HD12	5:P:398:ARG:HD2	1.87	0.56
2:C:861:LEU:HD23	2:C:974:LEU:CD1	2.35	0.56
3:N:273:ARG:HG3	3:N:278:PRO:HA	1.87	0.56
3:N:1237:THR:CG2	3:N:1238:MET:H	2.09	0.56
3:N:1290:LEU:HG	3:N:1307:LYS:CD	2.35	0.56
3:N:1439:SER:HB2	3:N:1463:LYS:NZ	2.20	0.56
3:D:693:GLU:HA	4:E:48:MET:CE	2.32	0.56
2:M:105:THR:HG22	2:M:107:LEU:HB3	1.79	0.56
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.39	0.56
5:F:377:ASP:OD1	5:F:379:ARG:N	2.38	0.56
3:N:207:PHE:CZ	5:P:101:GLU:OE2	2.59	0.56
2:C:690:ILE:CD1	2:C:869:VAL:HG22	2.36	0.56
2:C:758:ARG:HH21	2:C:788:THR:HB	1.70	0.56
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.87	0.56
3:D:128:TYR:CZ	3:D:587:ARG:CD	2.88	0.56
2:M:176:VAL:HG12	2:M:177:GLU:N	2.21	0.56
3:N:16:GLU:OE2	3:N:16:GLU:N	2.26	0.56
3:N:835:SER:O	3:N:838:ARG:HG3	2.06	0.56
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.38	0.56
2:M:524:VAL:CG1	2:M:528:GLU:HB2	2.35	0.56
3:N:1311:LEU:CB	3:N:1325:LEU:O	2.54	0.56
5:P:358:LEU:O	5:P:366:ALA:HB2	2.05	0.56
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.06	0.56
2:M:118:ILE:HD11	2:M:344:PHE:CE2	2.40	0.56
2:M:230:ARG:HG3	2:M:231:PRO:HD2	1.88	0.56
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.34	0.56
1:A:220:GLU:O	1:A:223:THR:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.40	0.55
2:C:717:LEU:CD2	2:C:763:GLY:HA2	2.35	0.55
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.42	0.55
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.55
2:M:154:ARG:NH2	2:M:178:PRO:N	2.53	0.55
2:M:157:ARG:HH11	2:M:157:ARG:CG	2.15	0.55
5:P:153:PRO:HA	5:P:156:VAL:HG22	1.88	0.55
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.19	0.55
5:F:354:LEU:O	5:F:358:LEU:HG	2.06	0.55
1:K:25:LEU:HD11	1:L:224:TYR:O	2.07	0.55
3:N:478:LEU:O	3:N:481:MET:HB2	2.06	0.55
3:N:1263:PHE:HA	3:N:1375:MET:HE1	1.88	0.55
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.88	0.55
2:C:858:MET:HG3	2:C:867:VAL:HG23	1.88	0.55
5:F:377:ASP:OD1	5:F:377:ASP:C	2.50	0.55
1:K:138:LEU:HD21	1:K:140:MET:HE2	1.88	0.55
1:L:4:SER:O	1:L:189:ARG:NH1	2.39	0.55
2:M:637:LEU:HD23	2:M:659:PRO:HG2	1.88	0.55
3:N:835:SER:CB	3:N:838:ARG:CG	2.82	0.55
5:P:144:ILE:HB	5:P:147:LEU:HB2	1.88	0.55
1:B:102:LYS:HA	1:B:138:LEU:O	2.06	0.55
5:F:259:ARG:HG2	5:F:259:ARG:HH11	1.72	0.55
1:L:102:LYS:HA	1:L:138:LEU:O	2.07	0.55
2:M:157:ARG:HG3	2:M:176:VAL:HG12	1.88	0.55
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.06	0.55
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.88	0.55
5:P:380:GLU:H	5:P:380:GLU:CD	2.14	0.55
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.36	0.55
2:C:858:MET:HG2	2:C:867:VAL:O	2.06	0.55
3:D:16:GLU:OE2	3:D:16:GLU:N	2.34	0.55
2:M:224:GLU:OE2	2:M:224:GLU:N	2.30	0.55
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.47	0.55
3:D:274:ARG:HH22	3:D:279:VAL:HG21	1.70	0.55
3:D:372:ASP:OD1	3:D:372:ASP:N	2.40	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
2:C:151:ASP:OD1	2:C:153:ALA:N	2.39	0.55
3:D:149:LYS:O	3:D:150:ARG:HB2	2.05	0.55
1:K:39:PRO:CG	1:L:39:PRO:HG3	2.36	0.55
2:M:141:HIS:CE1	2:M:334:ARG:HD2	2.42	0.55
2:M:1097:LEU:HD11	3:N:103:TRP:HZ3	1.72	0.55
5:P:364:ARG:NH1	5:P:392:VAL:HG11	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:32:ILE:O	5:P:258:ILE:HG23	2.07	0.55
3:N:56:TYR:CE1	3:N:69:GLU:HG3	2.38	0.55
3:N:1237:THR:CG2	3:N:1238:MET:N	2.57	0.55
5:P:364:ARG:HH12	5:P:392:VAL:HG11	1.72	0.55
2:C:325:ILE:H	2:C:330:ASN:HD22	1.55	0.55
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.89	0.55
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.36	0.55
3:D:696:HIS:CD2	4:E:57:ASP:OD1	2.60	0.55
3:D:1312:LEU:CD2	3:D:1327:ARG:HG3	2.30	0.55
1:L:211:LEU:O	1:L:215:VAL:HG13	2.07	0.55
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.55
2:M:680:ASP:OD2	2:M:978:ARG:NH2	2.39	0.55
2:M:922:PHE:CE2	2:M:964:LYS:HB2	2.42	0.55
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.72	0.55
3:N:1156:LEU:HD23	3:N:1182:GLU:OE2	2.07	0.55
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.40	0.55
5:P:125:ASP:OD1	5:P:125:ASP:N	2.40	0.55
1:B:18:ARG:O	1:B:207:PRO:HD3	2.07	0.54
1:B:211:LEU:O	1:B:215:VAL:HG13	2.06	0.54
2:C:35:PRO:CG	2:C:38:LYS:HD2	2.36	0.54
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.71	0.54
3:N:227:LEU:O	3:N:227:LEU:HD23	2.07	0.54
3:N:1410:GLU:HG2	3:N:1410:GLU:O	2.06	0.54
5:P:299:TRP:CE3	5:P:303:ARG:HD3	2.41	0.54
5:P:358:LEU:HD23	5:P:370:LYS:HE2	1.88	0.54
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.89	0.54
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.07	0.54
3:N:671:LYS:NZ	5:P:420:ASP:O	2.40	0.54
3:N:771:SER:O	3:N:775:GLY:HA2	2.07	0.54
2:C:164:PRO:CD	2:C:171:TRP:HD1	2.16	0.54
2:M:151:ASP:OD1	2:M:153:ALA:N	2.39	0.54
2:M:236:ILE:HD12	2:M:248:PRO:HB3	1.90	0.54
3:N:1292:VAL:HG21	3:N:1305:LEU:HD11	1.88	0.54
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.42	0.54
3:D:478:LEU:O	3:D:481:MET:HB2	2.07	0.54
3:D:658:LEU:HD23	3:D:661:MET:CE	2.37	0.54
1:K:133:GLU:HG2	1:K:134:GLU:N	2.22	0.54
1:L:92:PRO:O	1:L:146:ARG:NH1	2.35	0.54
2:M:174:LEU:CD1	2:M:174:LEU:N	2.70	0.54
3:N:274:ARG:O	3:N:275:GLU:HB2	2.06	0.54
2:C:176:VAL:O	2:C:177:GLU:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:478:LEU:O	3:D:481:MET:N	2.41	0.54
3:D:536:ALA:HA	5:F:315:VAL:O	2.08	0.54
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.90	0.54
3:N:1482:ARG:HH21	3:N:1483:PHE:HZ	1.55	0.54
5:P:382:THR:HG23	5:P:384:GLU:HG2	1.89	0.54
5:P:383:LEU:H	5:P:383:LEU:CD2	2.17	0.54
1:K:220:GLU:O	1:K:223:THR:HB	2.08	0.54
2:M:988:VAL:HG21	3:N:949:ILE:O	2.08	0.54
3:N:143:ASN:OD1	3:N:144:GLY:N	2.40	0.54
3:N:800:LYS:HB3	3:N:822:ALA:HB2	1.90	0.54
3:D:596:SER:C	3:D:597:ASP:CG	2.76	0.54
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.89	0.54
1:K:184:THR:O	1:K:192:LEU:HB2	2.08	0.54
2:M:437:ARG:CZ	2:M:491:GLU:OE2	2.55	0.54
2:M:545:ASN:HB3	2:M:583:LEU:HD22	1.90	0.54
2:M:704:HIS:CD2	2:M:831:ARG:HD2	2.42	0.54
3:N:1282:ARG:CG	3:N:1282:ARG:NH1	2.66	0.54
3:N:1400:VAL:HG21	3:N:1417:TRP:HD1	1.70	0.54
5:P:125:ASP:O	5:P:129:GLU:HG2	2.08	0.54
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.90	0.54
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.89	0.54
3:D:433:GLY:HA3	3:D:446:VAL:HG13	1.89	0.54
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.89	0.54
2:M:206:THR:CA	2:M:209:ARG:HD2	2.38	0.54
3:N:372:ASP:N	3:N:372:ASP:OD1	2.36	0.54
3:N:475:LYS:O	3:N:479:GLU:HG2	2.08	0.54
3:N:1264:GLU:OE1	3:N:1264:GLU:HA	2.07	0.54
5:P:383:LEU:HD23	5:P:383:LEU:N	2.18	0.54
2:C:758:ARG:H	2:C:789:SER:HB3	1.72	0.54
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.89	0.54
3:N:573:MET:CE	5:P:214:GLN:HG3	2.38	0.54
3:N:1213:ARG:HB2	3:N:1214:PRO:HD2	1.89	0.54
2:C:198:ARG:CZ	2:C:230:ARG:HA	2.38	0.54
5:F:155:THR:O	5:F:159:ILE:HG12	2.07	0.54
5:F:231:ARG:O	5:F:232:ARG:CB	2.56	0.54
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.90	0.54
3:N:595:GLY:C	3:N:597:ASP:OD2	2.48	0.54
3:N:1292:VAL:HG23	3:N:1305:LEU:HD11	1.89	0.54
3:N:1314:LYS:O	3:N:1317:ASP:HB2	2.07	0.54
1:B:92:PRO:O	1:B:146:ARG:NH1	2.33	0.53
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:598:GLU:O	2:C:651:LYS:HG3	2.08	0.53
2:C:999:HIS:HB3	2:C:1004:LYS:HE3	1.90	0.53
3:D:1283:ILE:CG1	3:D:1315:ASP:HB2	2.35	0.53
2:M:242:LEU:HD12	2:M:256:TYR:OH	2.08	0.53
2:M:581:THR:N	2:M:584:GLU:OE2	2.40	0.53
2:M:966:LEU:HD13	2:M:986:PRO:HB3	1.90	0.53
3:N:259:VAL:HG13	3:N:270:LEU:CD1	2.37	0.53
3:N:1304:LYS:C	3:N:1305:LEU:CD2	2.78	0.53
3:N:1312:LEU:HD22	3:N:1327:ARG:HG2	1.90	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.91	0.53
3:D:1310:ARG:CD	3:D:1327:ARG:HB2	2.37	0.53
3:N:187:LYS:N	3:N:200:ASP:HB3	2.23	0.53
3:N:433:GLY:HA3	3:N:446:VAL:CG1	2.39	0.53
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.89	0.53
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.89	0.53
5:P:140:ARG:HH11	5:P:140:ARG:HG2	1.73	0.53
1:A:201:THR:HG22	1:A:202:ASP:N	2.23	0.53
2:C:581:THR:N	2:C:584:GLU:OE2	2.41	0.53
3:D:187:LYS:N	3:D:200:ASP:HB3	2.23	0.53
1:L:18:ARG:O	1:L:207:PRO:HD3	2.09	0.53
2:M:419:THR:HB	2:M:422:ARG:HG2	1.91	0.53
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.89	0.53
2:C:177:GLU:CG	2:C:178:PRO:HD2	2.30	0.53
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.90	0.53
3:D:580:ALA:HA	3:D:584:ASN:HA	1.88	0.53
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.74	0.53
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.23	0.53
2:C:640:ARG:HH11	2:C:642:ARG:NH2	2.07	0.53
3:D:143:ASN:OD1	3:D:144:GLY:N	2.40	0.53
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.89	0.53
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.91	0.53
3:N:840:LYS:HE3	3:N:841:TYR:OH	2.09	0.53
2:C:229:MET:O	2:C:230:ARG:CB	2.55	0.53
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.90	0.53
3:D:1386:ASP:CB	3:D:1412:LYS:HD2	2.39	0.53
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.09	0.53
2:M:184:MET:HE3	2:M:186:VAL:HG23	1.89	0.53
3:N:1232:PRO:HG2	3:N:1356:TYR:HE2	1.73	0.53
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.92	0.53
2:C:55:GLU:HG3	2:C:56:GLU:H	1.73	0.53
2:C:191:PHE:HB2	2:C:192:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:GLU:OE2	2:C:224:GLU:N	2.30	0.53
2:C:229:MET:HE3	2:C:233:GLU:HB3	1.90	0.53
2:M:157:ARG:HH12	2:M:176:VAL:HG13	1.71	0.53
1:A:58:ILE:HB	1:A:61:VAL:HB	1.90	0.53
2:C:419:THR:HB	2:C:422:ARG:HG2	1.91	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.90	0.53
5:F:394:ARG:O	5:F:397:ILE:HG22	2.08	0.53
2:M:419:THR:N	2:M:422:ARG:HG3	2.21	0.53
5:P:152:ASP:OD1	5:P:152:ASP:N	2.42	0.53
5:P:343:ASP:O	5:P:346:THR:HB	2.09	0.53
1:A:30:ARG:CD	1:A:191:ASP:OD2	2.57	0.53
2:C:560:MET:O	2:C:564:MET:HG3	2.09	0.53
2:M:535:SER:O	2:M:538:GLN:HG2	2.08	0.53
2:M:759:THR:HB	2:M:785:VAL:HB	1.90	0.53
3:N:478:LEU:O	3:N:481:MET:N	2.42	0.53
3:N:1462:LEU:O	3:N:1466:VAL:HG23	2.08	0.53
5:P:295:MET:HE2	5:P:295:MET:HA	1.90	0.53
5:P:368:VAL:HG11	5:P:397:ILE:HD11	1.91	0.53
3:D:693:GLU:CA	4:E:48:MET:HE1	2.38	0.53
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.44	0.53
3:D:1280:VAL:HG12	3:D:1295:GLU:O	2.10	0.53
4:E:95:VAL:HG23	4:E:95:VAL:O	2.08	0.53
2:M:121:MET:HE1	2:M:336:VAL:HG21	1.89	0.53
2:M:164:PRO:HA	2:M:269:LEU:HD12	1.91	0.53
3:N:288:MET:HE2	3:N:307:ALA:HB2	1.91	0.53
4:O:14:ASP:OD1	4:O:18:ARG:NH1	2.42	0.53
1:A:112:ARG:HB3	1:A:125:PRO:HB2	1.91	0.52
2:C:845:ASN:C	2:C:845:ASN:HD22	2.17	0.52
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.90	0.52
3:D:74:GLU:CD	3:D:74:GLU:H	2.17	0.52
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.09	0.52
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.52
3:D:1044:LEU:HD12	3:D:1044:LEU:N	2.23	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.91	0.52
2:M:363:SER:O	2:M:367:LEU:HD21	2.09	0.52
3:N:32:ILE:CD1	5:P:258:ILE:HD11	2.33	0.52
4:O:43:GLU:OE1	4:O:43:GLU:N	2.36	0.52
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.90	0.52
3:D:801:GLY:HA3	3:D:825:ALA:CB	2.40	0.52
3:D:945:SER:OG	3:D:947:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:15:LEU:HD12	2:M:458:TYR:CZ	2.44	0.52
2:M:55:GLU:HG3	2:M:56:GLU:H	1.72	0.52
3:N:255:GLU:HB3	3:N:279:VAL:HG11	1.91	0.52
5:P:366:ALA:O	5:P:370:LYS:HG3	2.09	0.52
5:P:395:GLU:HA	5:P:398:ARG:HG2	1.90	0.52
1:A:138:LEU:HD21	1:A:140:MET:HE2	1.91	0.52
1:B:110:LYS:NZ	1:B:128:HIS:CB	2.67	0.52
2:C:182:VAL:HG23	2:C:193:LEU:HB2	1.90	0.52
2:C:184:MET:HE3	2:C:186:VAL:HG23	1.90	0.52
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.91	0.52
3:D:786:ILE:CG2	3:D:1026:SER:HB2	2.39	0.52
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	1.90	0.52
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.74	0.52
5:F:390:PHE:HD1	5:F:397:ILE:HD11	1.74	0.52
2:M:229:MET:C	2:M:233:GLU:HB2	2.33	0.52
2:M:858:MET:HG2	2:M:867:VAL:O	2.09	0.52
3:N:945:SER:OG	3:N:947:ILE:HG12	2.09	0.52
3:N:1044:LEU:HD12	3:N:1044:LEU:N	2.22	0.52
1:B:67:THR:O	1:B:69:PRO:HD3	2.10	0.52
2:M:191:PHE:HB2	2:M:192:PRO:HD2	1.90	0.52
2:M:999:HIS:HB3	2:M:1004:LYS:HE3	1.92	0.52
3:N:260:GLU:OE1	3:N:273:ARG:NH2	2.42	0.52
3:N:407:VAL:HG23	3:N:422:ALA:HB2	1.91	0.52
3:N:601:ARG:HD3	5:P:318:GLU:HG2	1.92	0.52
3:N:669:ASN:HD22	5:P:417:LYS:HD3	1.73	0.52
3:N:1311:LEU:N	3:N:1311:LEU:HD23	2.18	0.52
5:P:361:LEU:CD1	5:P:362:SER:H	2.16	0.52
2:C:292:ARG:HG3	2:C:299:LYS:CB	2.39	0.52
2:C:807:ARG:NH2	2:C:810:ASP:OD2	2.43	0.52
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.92	0.52
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.52
1:K:201:THR:HG22	1:K:202:ASP:N	2.25	0.52
3:N:192:ALA:HB1	3:N:193:PRO:HD2	1.91	0.52
3:N:860:LEU:O	3:N:876:SER:HB2	2.09	0.52
5:P:97:GLU:H	5:P:97:GLU:CD	2.18	0.52
1:A:133:GLU:HG2	1:A:134:GLU:N	2.24	0.52
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.92	0.52
1:K:112:ARG:HB3	1:K:125:PRO:HB2	1.92	0.52
2:M:954:THR:OG1	2:M:957:LYS:HE3	2.10	0.52
2:M:1090:LYS:HD3	2:M:1112:PHE:CZ	2.44	0.52
3:N:277:GLU:OE1	3:N:277:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1310:ARG:HD3	3:N:1327:ARG:CD	2.35	0.52
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.92	0.52
3:D:371:ILE:CD1	5:F:230:LYS:HA	2.40	0.52
3:D:399:ARG:HB2	3:D:401:TYR:CE1	2.45	0.52
3:D:475:LYS:O	3:D:479:GLU:HG2	2.09	0.52
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.25	0.52
2:M:757:GLY:HA2	2:M:789:SER:CB	2.36	0.52
2:M:787:ASP:OD1	2:M:789:SER:OG	2.26	0.52
3:N:801:GLY:HA3	3:N:825:ALA:CB	2.40	0.52
3:N:1267:ARG:HG2	3:N:1331:ASP:OD2	2.09	0.52
5:P:372:ARG:HD2	5:P:381:HIS:O	2.09	0.52
1:A:209:GLU:O	1:A:213:GLN:HG3	2.10	0.52
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.91	0.52
3:D:1282:ARG:NE	3:D:1295:GLU:OE2	2.41	0.52
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.90	0.52
2:M:1097:LEU:HD11	3:N:103:TRP:CZ3	2.45	0.52
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.91	0.52
3:N:399:ARG:HB2	3:N:401:TYR:CE1	2.45	0.52
2:C:424:GLY:O	2:C:428:ARG:HG3	2.09	0.52
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.45	0.52
1:K:4:SER:HA	1:K:189:ARG:HH21	1.74	0.52
2:M:550:LEU:HB3	2:M:905:ILE:HG23	1.92	0.52
2:M:768:THR:HB	2:M:771:GLU:HB2	1.91	0.52
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.43	0.52
2:M:876:VAL:N	2:M:877:PRO:HD2	2.25	0.52
2:M:1053:LEU:HA	3:N:621:LYS:HD2	1.91	0.52
3:N:786:ILE:CG2	3:N:1026:SER:HB2	2.39	0.52
2:C:954:THR:OG1	2:C:957:LYS:HE3	2.10	0.52
2:C:966:LEU:HD13	2:C:986:PRO:HB3	1.92	0.52
2:M:229:MET:O	2:M:230:ARG:CB	2.58	0.52
2:M:580:MET:HB3	2:M:584:GLU:OE2	2.10	0.52
3:N:693:GLU:HA	4:O:48:MET:CE	2.40	0.52
3:N:835:SER:H	3:N:838:ARG:NE	2.07	0.52
3:N:881:LEU:O	3:N:885:ILE:HG13	2.09	0.52
5:P:402:ASN:O	5:P:406:ARG:HG3	2.09	0.52
2:C:229:MET:C	2:C:230:ARG:CG	2.74	0.51
3:D:860:LEU:O	3:D:876:SER:HB2	2.09	0.51
2:M:212:GLY:HA2	2:M:218:VAL:HG21	1.91	0.51
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.44	0.51
3:N:1336:LEU:HB2	3:N:1344:VAL:HG21	1.92	0.51
2:C:1090:LYS:HD3	2:C:1112:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.91	0.51
2:M:983:ILE:HG21	2:M:987:ILE:CD1	2.40	0.51
3:N:890:VAL:CG1	3:N:922:LEU:CD1	2.88	0.51
3:N:1283:ILE:CD1	3:N:1283:ILE:H	2.23	0.51
3:N:1290:LEU:CG	3:N:1307:LYS:CE	2.64	0.51
5:P:404:ALA:O	5:P:408:LEU:HB2	2.11	0.51
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.41	0.51
3:D:596:SER:C	3:D:597:ASP:OD2	2.54	0.51
3:D:804:LEU:O	3:D:827:ILE:HG23	2.11	0.51
3:D:895:VAL:HG11	3:D:922:LEU:CD2	2.40	0.51
5:F:95:THR:HG22	5:F:96:LEU:N	2.25	0.51
2:M:66:LEU:HD11	2:M:98:LEU:HB3	1.92	0.51
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.92	0.51
2:M:323:ASP:O	2:M:325:ILE:CG2	2.59	0.51
2:M:807:ARG:NH2	2:M:810:ASP:OD2	2.43	0.51
2:M:948:GLU:HB3	2:M:953:VAL:HG23	1.92	0.51
3:N:46:ASP:OD2	3:N:48:ARG:CG	2.53	0.51
3:N:147:VAL:HG21	3:N:161:LEU:HD21	1.93	0.51
5:P:83:GLN:O	5:P:87:GLU:HG3	2.09	0.51
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.26	0.51
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.91	0.51
2:M:170:PRO:HA	7:R:13:DT:H3	1.74	0.51
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.91	0.51
2:M:669:GLY:H	2:M:993:PHE:HZ	1.56	0.51
5:P:419:ARG:HD2	5:P:422:LEU:HD11	1.92	0.51
1:A:180:GLN:NE2	2:C:935:GLY:O	2.43	0.51
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.91	0.51
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.52	0.51
1:K:209:GLU:O	1:K:213:GLN:HG3	2.09	0.51
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.93	0.51
2:M:861:LEU:HD23	2:M:974:LEU:CD1	2.40	0.51
3:N:675:ARG:HH12	5:P:420:ASP:CG	2.18	0.51
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.73	0.51
5:P:231:ARG:O	5:P:232:ARG:CB	2.56	0.51
5:P:399:GLN:O	5:P:402:ASN:HB2	2.11	0.51
1:A:47:SER:O	1:A:49:PRO:HD3	2.11	0.51
2:C:97:ARG:HD3	2:C:110:GLU:OE1	2.11	0.51
3:D:614:PHE:HA	3:D:618:LEU:HD23	1.93	0.51
6:G:11:DT:H2''	6:G:12:DG:H5''	1.92	0.51
2:M:154:ARG:NH2	2:M:178:PRO:HA	2.26	0.51
2:M:1065:ALA:HB1	2:M:1077:PRO:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:823:LEU:HD11	3:N:837:GLY:CA	2.37	0.51
3:N:823:LEU:CD1	3:N:837:GLY:HA2	2.37	0.51
3:N:834:THR:HG23	3:N:835:SER:O	2.11	0.51
3:N:959:GLU:HB3	3:N:963:TYR:CE1	2.45	0.51
3:N:1248:GLY:C	3:N:1250:ALA:H	2.18	0.51
5:P:386:VAL:CG1	5:P:397:ILE:HG21	2.41	0.51
2:C:48:PHE:HA	2:C:348:LEU:HD21	1.93	0.51
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.46	0.51
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.46	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.44	0.51
3:D:1312:LEU:HD21	3:D:1327:ARG:CG	2.29	0.51
2:M:267:TYR:CE2	2:M:290:LEU:HG	2.46	0.51
3:N:709:HIS:HA	3:N:1227:GLN:HB3	1.92	0.51
3:N:1481:VAL:HG23	4:O:21:VAL:HG21	1.93	0.51
3:D:619:LEU:HD11	3:D:1439:SER:HB3	1.93	0.51
2:M:845:ASN:HD22	2:M:845:ASN:C	2.18	0.51
3:N:71:LYS:HG3	3:N:72:VAL:N	2.25	0.51
3:N:218:LYS:HA	3:N:337:LEU:O	2.11	0.51
3:N:566:ILE:HD13	5:P:217:ASN:HB3	1.91	0.51
3:N:1283:ILE:HG21	3:N:1315:ASP:CG	2.08	0.51
2:C:223:ASP:O	2:C:227:PHE:HD2	1.94	0.51
2:C:1103:ASP:OD2	2:C:1107:ASN:HB2	2.10	0.51
2:M:97:ARG:HD3	2:M:110:GLU:OE1	2.11	0.51
2:M:171:TRP:HZ3	7:R:14:DG:OP1	1.94	0.51
2:M:250:ARG:HG3	2:M:250:ARG:HH11	1.76	0.51
2:M:325:ILE:H	2:M:330:ASN:HD22	1.57	0.51
2:M:503:LEU:CD2	2:M:508:ILE:HD13	2.41	0.51
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.76	0.51
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.92	0.51
3:N:573:MET:SD	5:P:210:LEU:HB3	2.51	0.51
3:N:1231:GLU:N	3:N:1232:PRO:HD2	2.26	0.51
3:N:1386:ASP:OD2	3:N:1413:THR:OG1	2.17	0.51
2:C:637:LEU:HD23	2:C:659:PRO:HG3	1.91	0.51
5:F:418:LEU:HD12	5:F:418:LEU:N	2.25	0.51
1:K:90:LEU:O	1:K:92:PRO:HD3	2.11	0.51
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.93	0.51
3:N:47:GLU:C	3:N:78:VAL:HG22	2.36	0.51
3:N:1099:VAL:O	3:N:1103:HIS:HB3	2.11	0.51
1:B:156:HIS:ND1	1:B:158:ILE:HG23	2.26	0.50
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.93	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1103:ASP:OD2	2:M:1107:ASN:HB2	2.11	0.50
3:N:111:LYS:HG3	3:N:1452:ILE:HD11	1.93	0.50
3:N:646:LYS:HB3	3:N:688:TRP:CZ3	2.46	0.50
1:B:123:MET:C	1:B:125:PRO:HD3	2.36	0.50
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.11	0.50
3:D:258:VAL:HG12	3:D:297:ILE:HD13	1.92	0.50
3:D:376:GLU:HG3	3:D:376:GLU:O	2.11	0.50
1:K:206:THR:O	1:K:207:PRO:C	2.54	0.50
1:L:154:GLU:H	1:L:154:GLU:CD	2.19	0.50
2:M:223:ASP:O	2:M:227:PHE:HD2	1.94	0.50
2:M:758:ARG:H	2:M:789:SER:HB3	1.76	0.50
2:M:1065:ALA:CB	2:M:1077:PRO:HG3	2.41	0.50
3:N:1305:LEU:O	3:N:1306:PRO:C	2.55	0.50
5:P:261:PRO:O	5:P:265:VAL:HG23	2.11	0.50
1:A:27:PRO:HB2	1:A:192:LEU:HD13	1.93	0.50
2:C:105:THR:CG2	2:C:105:THR:O	2.58	0.50
2:C:418:LEU:HD21	7:H:14:DG:C8	2.46	0.50
3:D:47:GLU:CB	3:D:78:VAL:CG2	2.87	0.50
3:D:1232:PRO:HG2	3:D:1356:TYR:HE2	1.75	0.50
2:M:189:ARG:HH12	2:M:244:PRO:CD	2.20	0.50
3:N:114:THR:HG21	3:N:498:VAL:HG21	1.94	0.50
3:N:693:GLU:CB	4:O:48:MET:HE1	2.41	0.50
1:B:94:LEU:HD22	1:B:96:THR:H	1.76	0.50
2:C:15:LEU:HD12	2:C:458:TYR:CZ	2.46	0.50
3:D:1339:LYS:HG2	3:D:1343:ALA:HB2	1.91	0.50
3:D:1465:ASN:HB3	3:D:1470:ARG:HB2	1.92	0.50
4:E:67:GLU:O	4:E:70:THR:OG1	2.29	0.50
1:L:156:HIS:ND1	1:L:158:ILE:HG23	2.26	0.50
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.93	0.50
3:N:279:VAL:HG13	3:N:279:VAL:O	2.10	0.50
3:N:323:GLU:HB2	3:N:334:THR:HB	1.93	0.50
3:N:1282:ARG:CD	3:N:1295:GLU:CD	2.75	0.50
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.93	0.50
2:M:171:TRP:CH2	7:R:13:DT:H2"	2.45	0.50
2:M:173:ASP:C	2:M:174:LEU:CD1	2.85	0.50
3:N:558:LEU:HD23	3:N:567:ILE:HD12	1.93	0.50
1:A:184:THR:N	1:A:192:LEU:O	2.38	0.50
2:C:198:ARG:HH11	2:C:230:ARG:CA	2.24	0.50
3:D:147:VAL:HG21	3:D:161:LEU:HD21	1.94	0.50
3:D:291:LEU:HD12	3:D:303:PRO:HB2	1.94	0.50
3:D:596:SER:O	3:D:597:ASP:OD2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:829:VAL:O	3:D:830:ALA:HB3	2.11	0.50
2:M:1005:MET:HE1	3:N:647:ARG:HB2	1.94	0.50
3:D:69:GLU:HA	3:D:80:VAL:HG23	1.92	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.46	0.50
2:M:327:HIS:CE1	2:M:488:ALA:HB1	2.46	0.50
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.45	0.50
2:C:48:PHE:O	2:C:52:PHE:HD2	1.94	0.50
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.46	0.50
2:C:550:LEU:HB3	2:C:905:ILE:HG23	1.94	0.50
2:C:787:ASP:OD1	2:C:789:SER:OG	2.30	0.50
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.94	0.50
3:D:483:HIS:ND1	3:D:484:PRO:HD2	2.27	0.50
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.12	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.50
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.45	0.50
3:N:44:LEU:O	3:N:525:ARG:NH2	2.40	0.50
3:N:412:GLY:N	3:N:435:VAL:HG12	2.26	0.50
3:N:483:HIS:ND1	3:N:484:PRO:HD2	2.27	0.50
1:B:154:GLU:H	1:B:154:GLU:CD	2.20	0.50
1:B:176:ARG:HG2	1:B:200:TRP:CE3	2.47	0.50
2:C:524:VAL:HG12	2:C:525:SER:N	2.27	0.50
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.75	0.50
3:D:23:TYR:CD2	3:D:89:ARG:HD3	2.47	0.50
3:D:970:LYS:O	3:D:974:ILE:HG13	2.11	0.50
1:K:47:SER:O	1:K:49:PRO:HD3	2.11	0.50
1:K:153:ALA:N	1:K:168:ASP:OD1	2.33	0.50
2:M:690:ILE:CD1	2:M:869:VAL:HG22	2.42	0.50
2:M:926:PHE:HE1	2:M:929:ARG:HH11	1.59	0.50
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.94	0.50
3:N:1440:PHE:O	3:N:1441:GLN:HG3	2.12	0.50
2:C:82:GLU:O	2:C:86:LYS:HG3	2.12	0.49
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.94	0.49
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.94	0.49
2:M:460:ARG:HD2	2:M:485:TYR:CZ	2.46	0.49
3:N:368:VAL:HB	3:N:377:VAL:HB	1.94	0.49
3:N:661:MET:CE	3:N:677:LEU:HD11	2.42	0.49
5:P:152:ASP:HB2	5:P:153:PRO:HD2	1.92	0.49
5:P:398:ARG:O	5:P:401:GLU:HG2	2.10	0.49
1:A:90:LEU:O	1:A:92:PRO:HD3	2.11	0.49
2:C:535:SER:OG	2:C:537:LYS:HG3	2.12	0.49
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:33:ASN:HB2	3:D:40:GLU:OE1	2.11	0.49
3:D:217:LYS:HB2	3:D:339:TRP:CE2	2.47	0.49
3:D:595:GLY:O	3:D:597:ASP:OD2	2.30	0.49
3:D:1347:TYR:O	3:D:1351:GLU:HB2	2.11	0.49
2:M:211:LEU:HD23	2:M:311:PHE:HD2	1.76	0.49
2:M:229:MET:HE1	2:M:237:ARG:HB3	1.94	0.49
2:M:302:VAL:C	2:M:305:PRO:HD2	2.37	0.49
3:N:274:ARG:CZ	3:N:279:VAL:HG21	2.42	0.49
5:P:403:LYS:NZ	5:P:406:ARG:HH12	2.10	0.49
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.49
2:C:289:THR:HG22	2:C:291:ALA:H	1.76	0.49
2:C:660:ALA:O	2:C:667:ALA:N	2.39	0.49
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.93	0.49
3:D:567:ILE:HG22	3:D:571:LYS:HE3	1.94	0.49
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.46	0.49
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.94	0.49
5:F:372:ARG:HE	5:F:383:LEU:HG	1.77	0.49
1:L:123:MET:C	1:L:125:PRO:HD3	2.37	0.49
2:M:425:PHE:CZ	3:N:1086:LEU:HD12	2.47	0.49
2:M:1056:LYS:NZ	3:N:749:VAL:O	2.40	0.49
2:M:1090:LYS:HD3	2:M:1112:PHE:CE2	2.47	0.49
3:N:315:ARG:O	3:N:316:GLN:HB3	2.12	0.49
5:P:140:ARG:HG2	5:P:140:ARG:NH1	2.27	0.49
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.42	0.49
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.47	0.49
2:C:436:GLY:HA2	2:C:538:GLN:O	2.12	0.49
3:D:230:TRP:CZ2	3:D:232:GLU:HA	2.47	0.49
3:N:619:LEU:HD11	3:N:1439:SER:HB3	1.92	0.49
3:N:806:PHE:HB2	3:N:829:VAL:HG22	1.94	0.49
2:C:231:PRO:HG2	2:C:232:GLU:CD	2.37	0.49
2:C:711:GLU:HB2	2:C:713:ARG:NH1	2.28	0.49
3:D:32:ILE:HG23	3:D:37:LEU:C	2.36	0.49
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.47	0.49
3:D:1031:ASN:C	3:D:1031:ASN:OD1	2.56	0.49
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.92	0.49
4:E:43:GLU:OE1	4:E:43:GLU:N	2.37	0.49
1:K:34:VAL:CG2	1:L:42:ARG:CZ	2.90	0.49
1:L:176:ARG:HG2	1:L:200:TRP:CE3	2.47	0.49
2:M:56:GLU:CD	2:M:359:MET:HE3	2.37	0.49
2:M:157:ARG:NH1	2:M:157:ARG:CG	2.74	0.49
3:N:473:LEU:HD21	3:N:495:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:708:TYR:OH	2:C:796:GLU:OE1	2.25	0.49
3:D:1305:LEU:HD23	3:D:1305:LEU:H	1.66	0.49
1:L:80:LEU:HD11	3:N:842:VAL:HG12	1.95	0.49
2:M:86:LYS:HB2	2:M:88:LEU:HG	1.94	0.49
2:M:289:THR:CG2	2:M:291:ALA:O	2.61	0.49
2:M:327:HIS:CE1	2:M:433:THR:HG21	2.47	0.49
2:M:708:TYR:OH	2:M:796:GLU:OE1	2.21	0.49
3:N:614:PHE:HA	3:N:618:LEU:HD23	1.94	0.49
5:P:391:GLY:O	5:P:392:VAL:O	2.31	0.49
2:M:23:VAL:HG12	2:M:24:GLU:N	2.26	0.49
2:M:136:ILE:HB	2:M:336:VAL:CG1	2.43	0.49
2:M:261:ILE:HG22	2:M:291:ALA:HB3	1.94	0.49
2:M:424:GLY:O	2:M:428:ARG:HG3	2.12	0.49
3:N:1238:MET:CG	3:N:1359:GLN:OE1	2.61	0.49
2:C:23:VAL:HG12	2:C:24:GLU:N	2.27	0.49
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.27	0.49
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.31	0.49
5:F:123:ASP:HB3	5:F:125:ASP:OD1	2.12	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.95	0.49
2:M:685:GLU:OE1	2:M:685:GLU:HA	2.12	0.49
3:N:729:HIS:ND1	3:N:730:PRO:HD2	2.28	0.49
3:N:832:ARG:HD2	3:N:833:GLU:H	1.77	0.49
1:A:9:PRO:HD3	1:B:224:TYR:CE2	2.47	0.49
1:A:25:LEU:HD22	1:B:225:PHE:CZ	2.47	0.49
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.95	0.49
3:D:272:LEU:O	3:D:279:VAL:N	2.43	0.49
3:D:431:VAL:HG12	3:D:432:TYR:N	2.27	0.49
5:F:156:VAL:O	5:F:160:ASP:HB2	2.13	0.49
2:M:238:LEU:HD11	2:M:242:LEU:CD2	2.43	0.49
2:M:878:SER:HA	3:N:1034:GLN:OE1	2.13	0.49
3:N:433:GLY:HA3	3:N:446:VAL:HG13	1.95	0.49
3:N:1237:THR:O	3:N:1238:MET:O	2.30	0.49
2:C:50:GLU:OE1	2:C:345:ARG:NE	2.46	0.49
2:C:290:LEU:HD23	2:C:302:VAL:HG21	1.95	0.49
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.42	0.49
5:F:376:ILE:C	5:F:378:GLY:H	2.21	0.49
1:L:48:ILE:HG22	1:L:173:PRO:HD2	1.95	0.49
1:L:58:ILE:HD12	1:L:140:MET:HE2	1.94	0.49
2:M:560:MET:O	2:M:564:MET:HG3	2.13	0.49
2:M:660:ALA:O	2:M:667:ALA:N	2.41	0.49
3:N:80:VAL:O	3:N:80:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:313:MET:HG3	3:N:314:PRO:HD2	1.95	0.49
3:N:437:VAL:HG11	5:P:175:HIS:HD2	1.78	0.49
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.77	0.48
3:N:219:GLU:N	3:N:339:TRP:CH2	2.81	0.48
3:N:286:VAL:HG13	3:N:312:ARG:O	2.13	0.48
3:N:770:LEU:HD23	3:N:777:PRO:HA	1.95	0.48
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.28	0.48
3:N:890:VAL:HG21	3:N:922:LEU:HD11	1.95	0.48
3:N:1283:ILE:H	3:N:1283:ILE:HD12	1.78	0.48
2:M:858:MET:HG3	2:M:867:VAL:CG2	2.43	0.48
2:M:1043:TYR:CG	3:N:763:MET:HG2	2.49	0.48
3:N:890:VAL:CB	3:N:922:LEU:HD11	2.41	0.48
5:P:89:GLY:HA3	7:R:7:DG:C6	2.48	0.48
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.95	0.48
1:B:58:ILE:C	1:B:61:VAL:HG13	2.39	0.48
2:C:836:GLY:C	2:C:1001:VAL:HG22	2.39	0.48
2:C:876:VAL:N	2:C:877:PRO:HD2	2.28	0.48
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.95	0.48
5:F:226:LYS:HD2	7:H:1:DT:H72	1.95	0.48
2:M:99:GLN:NE2	2:M:101:ILE:HD11	2.28	0.48
2:M:154:ARG:HH22	2:M:178:PRO:HA	1.77	0.48
2:M:810:ASP:HB2	2:M:811:PRO:HD2	1.95	0.48
2:M:850:ALA:HA	3:N:632:VAL:HG21	1.93	0.48
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.53	0.48
1:A:206:THR:O	1:A:207:PRO:C	2.54	0.48
1:L:60:ASP:O	1:L:62:LEU:HD12	2.13	0.48
2:M:553:ASP:OD1	2:M:843:HIS:ND1	2.38	0.48
2:M:1053:LEU:HD11	3:N:1466:VAL:HG13	1.94	0.48
3:N:574:LEU:O	3:N:578:VAL:HG23	2.13	0.48
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.28	0.48
2:C:511:GLU:HG3	2:C:512:ARG:HG2	1.96	0.48
2:C:810:ASP:HB2	2:C:811:PRO:HD2	1.94	0.48
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.96	0.48
1:K:180:GLN:NE2	2:M:935:GLY:O	2.47	0.48
2:M:805:ARG:HG3	2:M:823:VAL:HG22	1.96	0.48
3:N:255:GLU:HA	3:N:300:LYS:HE2	1.95	0.48
3:N:1284:GLU:O	3:N:1285:GLU:CD	2.57	0.48
3:N:1400:VAL:CG2	3:N:1417:TRP:CD1	2.96	0.48
1:B:117:VAL:O	1:B:118:ALA:C	2.57	0.48
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.13	0.48
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.94	0.48
2:M:76:PRO:HG3	2:M:120:LEU:CD1	2.44	0.48
2:M:511:GLU:HG3	2:M:512:ARG:HG2	1.96	0.48
3:N:314:PRO:HG2	3:N:317:VAL:HG12	1.95	0.48
3:N:315:ARG:H	3:N:315:ARG:HD3	1.78	0.48
3:N:658:LEU:HD23	3:N:661:MET:HE3	1.94	0.48
3:N:835:SER:CB	3:N:838:ARG:NE	2.37	0.48
3:N:936:TYR:O	3:N:940:THR:OG1	2.28	0.48
2:C:174:LEU:CD1	2:C:184:MET:HG3	2.43	0.48
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.44	0.48
2:C:1030:GLN:H	3:D:626:SER:HG	1.62	0.48
3:D:629:SER:C	3:D:744:GLN:HG2	2.39	0.48
3:D:999:THR:O	3:D:1003:VAL:HG13	2.13	0.48
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.94	0.48
3:N:394:LEU:HG	3:N:396:VAL:HG23	1.95	0.48
5:P:361:LEU:HD21	5:P:408:LEU:HD12	1.96	0.48
1:B:58:ILE:HG22	1:B:61:VAL:CG1	2.40	0.48
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.44	0.48
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.79	0.48
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.96	0.48
2:M:524:VAL:HG12	2:M:525:SER:N	2.27	0.48
2:M:925:TYR:CD1	2:M:967:PHE:CE1	3.02	0.48
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.96	0.48
3:N:567:ILE:HG22	3:N:571:LYS:HE3	1.96	0.48
3:N:1049:SER:OG	3:N:1051:GLU:HG2	2.12	0.48
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.29	0.48
1:A:185:ARG:HE	1:A:187:GLY:HA2	1.79	0.48
1:B:58:ILE:HD12	1:B:140:MET:HE2	1.96	0.48
2:C:141:HIS:CE1	2:C:334:ARG:HD2	2.49	0.48
2:C:157:ARG:NH1	2:C:157:ARG:CG	2.74	0.48
2:C:1056:LYS:O	3:D:624:ASP:N	2.43	0.48
3:D:208:PRO:HA	3:D:390:PRO:HA	1.95	0.48
3:D:832:ARG:HD2	3:D:833:GLU:H	1.77	0.48
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.94	0.48
2:M:172:ILE:HA	2:M:185:LYS:O	2.14	0.48
2:M:177:GLU:CB	2:M:178:PRO:HD2	2.44	0.48
2:M:351:LEU:HD12	2:M:374:ASN:O	2.14	0.48
2:M:404:LEU:O	2:M:408:ARG:HG3	2.14	0.48
3:N:250:LEU:H	3:N:250:LEU:HD12	1.78	0.48
3:N:255:GLU:HB3	3:N:279:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.92	0.48
2:C:136:ILE:HB	2:C:336:VAL:CG1	2.44	0.48
2:C:425:PHE:CZ	3:D:1086:LEU:HD12	2.49	0.48
2:C:580:MET:SD	2:C:584:GLU:HG3	2.54	0.48
2:C:925:TYR:CD1	2:C:967:PHE:CE1	3.01	0.48
3:D:71:LYS:HG3	3:D:72:VAL:N	2.28	0.48
3:D:529:GLN:HG2	3:D:535:PHE:CE1	2.49	0.48
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.78	0.48
3:D:1403:LEU:HD12	3:D:1406:ARG:HH11	1.78	0.48
5:F:365:GLU:O	5:F:369:LEU:HD13	2.14	0.48
1:K:219:ARG:HG3	1:K:220:GLU:H	1.78	0.48
2:M:182:VAL:HG21	2:M:193:LEU:CB	2.22	0.48
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.94	0.48
3:N:465:LEU:HD12	3:N:513:ILE:HD13	1.96	0.48
3:N:493:ARG:NH1	11:N:2121:HOH:O	2.47	0.48
3:N:706:PRO:HB2	3:N:708:LEU:HD21	1.96	0.48
1:A:188:GLN:HG2	1:A:189:ARG:N	2.29	0.47
2:C:302:VAL:C	2:C:305:PRO:HD2	2.38	0.47
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.44	0.47
2:C:757:GLY:HA2	2:C:789:SER:CB	2.42	0.47
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.29	0.47
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.13	0.47
2:M:168:ARG:HH11	2:M:168:ARG:CG	2.27	0.47
3:N:1413:THR:HG22	3:N:1414:PRO:HD2	1.94	0.47
1:L:117:VAL:O	1:L:118:ALA:C	2.57	0.47
2:M:685:GLU:O	2:M:686:ASP:HB2	2.15	0.47
3:N:134:VAL:HG23	3:N:150:ARG:N	2.29	0.47
3:N:1208:ASP:C	3:N:1208:ASP:OD1	2.57	0.47
5:P:78:SER:O	5:P:79:ASP:C	2.58	0.47
5:P:205:ARG:HH11	5:P:205:ARG:HG2	1.72	0.47
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.95	0.47
1:B:223:THR:O	1:B:226:SER:OG	2.30	0.47
2:C:404:LEU:O	2:C:408:ARG:HG3	2.14	0.47
2:C:419:THR:N	2:C:422:ARG:HG3	2.21	0.47
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.93	0.47
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.96	0.47
3:D:574:LEU:O	3:D:578:VAL:HG23	2.13	0.47
3:D:868:TYR:CE2	3:D:869:MET:HG3	2.49	0.47
1:L:175:ARG:N	1:L:200:TRP:O	2.44	0.47
2:M:260:LEU:C	2:M:261:ILE:HD12	2.39	0.47
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HE3	2:C:643:VAL:O	2.14	0.47
3:D:219:GLU:CB	3:D:339:TRP:CH2	2.97	0.47
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.96	0.47
5:F:279:GLN:HA	5:F:284:ARG:O	2.15	0.47
1:K:32:PHE:HA	1:K:35:THR:HB	1.95	0.47
3:N:431:VAL:HG12	3:N:432:TYR:N	2.29	0.47
3:N:536:ALA:HA	5:P:315:VAL:O	2.13	0.47
3:N:868:TYR:CE2	3:N:869:MET:HG3	2.50	0.47
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.47
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.50	0.47
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.14	0.47
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.14	0.47
1:K:57:TYR:CG	1:K:161:ARG:HD2	2.49	0.47
2:M:418:LEU:HD21	7:R:14:DG:C8	2.48	0.47
2:M:680:ASP:OD1	3:N:943:THR:HG21	2.15	0.47
2:M:841:ASN:C	2:M:841:ASN:OD1	2.57	0.47
2:M:905:ILE:C	2:M:907:ASP:H	2.22	0.47
3:N:650:LEU:HD12	3:N:657:LEU:CD2	2.45	0.47
1:A:9:PRO:CD	1:B:224:TYR:CE2	2.98	0.47
1:A:159:LYS:HE3	1:A:164:ALA:O	2.14	0.47
1:A:219:ARG:HG3	1:A:220:GLU:H	1.79	0.47
2:C:128:ILE:O	2:C:129:ILE:HD13	2.15	0.47
3:D:214:GLU:HG2	3:D:342:PRO:HB3	1.97	0.47
5:F:234:LYS:HD3	7:H:5:DA:OP2	2.15	0.47
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.65	0.47
1:K:39:PRO:HG3	1:L:39:PRO:CG	2.44	0.47
2:M:173:ASP:O	2:M:174:LEU:HD12	2.14	0.47
3:N:204:LEU:HD23	3:N:441:ARG:NH2	2.29	0.47
3:N:273:ARG:CG	3:N:278:PRO:HA	2.44	0.47
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.97	0.47
1:B:206:THR:H	1:B:209:GLU:HB2	1.80	0.47
2:C:35:PRO:HG2	2:C:38:LYS:CD	2.44	0.47
2:C:56:GLU:HA	2:C:56:GLU:OE2	2.14	0.47
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.95	0.47
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.47
2:C:559:LEU:C	2:C:559:LEU:HD23	2.39	0.47
2:C:1090:LYS:HD3	2:C:1112:PHE:CE2	2.49	0.47
3:D:47:GLU:HA	3:D:51:GLY:O	2.15	0.47
3:D:134:VAL:HG23	3:D:150:ARG:N	2.29	0.47
3:D:661:MET:CE	3:D:677:LEU:HD11	2.43	0.47
3:D:1100:ASP:OD2	3:D:1440:PHE:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:295:MET:HA	5:F:295:MET:CE	2.44	0.47
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.96	0.47
2:M:580:MET:SD	2:M:584:GLU:HG3	2.54	0.47
2:M:711:GLU:HB2	2:M:713:ARG:NH1	2.30	0.47
2:M:836:GLY:C	2:M:1001:VAL:HG22	2.39	0.47
2:M:850:ALA:HA	3:N:632:VAL:HG22	1.92	0.47
3:N:134:VAL:HG23	3:N:150:ARG:H	1.80	0.47
3:N:208:PRO:HA	3:N:390:PRO:HA	1.95	0.47
3:N:271:VAL:HG22	3:N:281:THR:HG23	1.96	0.47
3:N:1031:ASN:C	3:N:1031:ASN:OD1	2.58	0.47
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.15	0.47
3:N:1347:TYR:O	3:N:1351:GLU:HB2	2.15	0.47
5:P:247:ILE:O	5:P:251:ILE:HG13	2.14	0.47
5:P:365:GLU:O	5:P:368:VAL:HG22	2.15	0.47
2:C:56:GLU:CD	2:C:359:MET:HE3	2.39	0.47
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.42	0.47
2:C:535:SER:O	2:C:538:GLN:HG2	2.14	0.47
3:D:131:LYS:O	3:D:456:MET:HG2	2.15	0.47
3:D:265:GLU:HB3	3:D:266:GLU:H	1.51	0.47
3:D:936:TYR:O	3:D:940:THR:OG1	2.30	0.47
3:N:310:LEU:HD23	3:N:310:LEU:H	1.80	0.47
3:N:1407:LEU:O	3:N:1410:GLU:N	2.44	0.47
2:C:841:ASN:C	2:C:841:ASN:OD1	2.56	0.47
3:D:47:GLU:C	3:D:78:VAL:CG2	2.88	0.47
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.97	0.47
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.30	0.47
3:D:1128:VAL:HG22	3:D:1129:THR:HG23	1.96	0.47
3:D:1216:SER:HB3	4:E:15:SER:HA	1.97	0.47
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.47
1:K:159:LYS:HE3	1:K:164:ALA:O	2.15	0.47
2:M:327:HIS:HE1	2:M:488:ALA:C	2.23	0.47
2:M:436:GLY:HA2	2:M:538:GLN:O	2.15	0.47
2:M:550:LEU:HD23	2:M:905:ILE:HG21	1.97	0.47
2:M:571:LEU:HD23	2:M:702:SER:HB3	1.97	0.47
2:M:936:VAL:HG11	2:M:959:PRO:CB	2.44	0.47
3:N:1005:GLN:O	3:N:1009:LYS:HG2	2.14	0.47
3:N:1101:VAL:HG12	3:N:1374:GLN:HB3	1.96	0.47
3:N:1284:GLU:OE1	3:N:1285:GLU:CA	2.63	0.47
6:Q:14:DG:H5'	6:Q:14:DG:H8	1.80	0.47
2:C:164:PRO:CD	2:C:171:TRP:CD1	2.85	0.47
2:C:261:ILE:O	2:C:289:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.50	0.47
2:C:988:VAL:HG21	3:D:949:ILE:C	2.40	0.47
2:M:816:LYS:HA	2:M:816:LYS:HD2	1.61	0.47
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.79	0.47
3:N:434:ARG:O	3:N:447:VAL:HG23	2.15	0.47
3:N:970:LYS:O	3:N:974:ILE:HG13	2.14	0.47
5:P:153:PRO:O	5:P:156:VAL:HG22	2.14	0.47
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.50	0.46
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.95	0.46
2:M:168:ARG:HG3	2:M:268:ASP:HB3	1.97	0.46
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.50	0.46
3:N:17:LYS:O	3:N:20:SER:HB3	2.15	0.46
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.97	0.46
3:N:693:GLU:HA	4:O:48:MET:HE1	1.96	0.46
3:N:1283:ILE:HG22	3:N:1315:ASP:HB2	1.92	0.46
3:N:1290:LEU:HD21	3:N:1307:LYS:CE	2.43	0.46
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.96	0.46
3:D:368:VAL:HB	3:D:377:VAL:HB	1.97	0.46
3:D:1252:ILE:HG23	3:D:1253:THR:HG23	1.96	0.46
4:E:12:MET:HE1	4:E:68:LEU:O	2.15	0.46
2:M:154:ARG:NH2	2:M:177:GLU:O	2.47	0.46
3:N:1276:GLU:O	3:N:1277:ILE:HD13	2.15	0.46
3:N:1404:ASN:OD1	3:N:1415:VAL:HB	2.14	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.97	0.46
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.49	0.46
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.96	0.46
3:D:843:PHE:CD1	3:D:864:VAL:HG11	2.50	0.46
1:K:34:VAL:HG22	1:L:42:ARG:NH2	2.31	0.46
1:L:54:THR:OG1	1:L:145:ASP:OD1	2.28	0.46
2:M:503:LEU:HD23	2:M:508:ILE:HA	1.97	0.46
2:M:541:SER:O	2:M:545:ASN:ND2	2.41	0.46
3:N:84:ILE:CD1	3:N:87:ARG:HD3	2.45	0.46
3:N:136:ASP:H	3:N:453:ASP:HB3	1.78	0.46
3:N:1284:GLU:O	3:N:1285:GLU:OE2	2.33	0.46
3:N:1486:VAL:HG22	4:O:75:PHE:HB3	1.97	0.46
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.96	0.46
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.74	0.46
2:C:1071:ILE:O	3:D:659:LYS:HD3	2.14	0.46
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.15	0.46
3:D:58:CYS:HA	3:D:78:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:939:PHE:O	3:D:942:SER:OG	2.20	0.46
2:M:52:PHE:HB3	2:M:53:PRO:HA	1.97	0.46
2:M:135:VAL:HG23	2:M:395:LYS:HG3	1.96	0.46
2:M:289:THR:HG22	2:M:291:ALA:H	1.80	0.46
2:M:366:SER:O	2:M:367:LEU:HD23	2.15	0.46
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.98	0.46
2:M:690:ILE:HD13	2:M:690:ILE:HA	1.74	0.46
3:N:892:ASP:OD1	3:N:894:LYS:HD2	2.12	0.46
3:N:1310:ARG:CD	3:N:1327:ARG:NH1	2.47	0.46
1:A:32:PHE:HA	1:A:35:THR:HB	1.97	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.97	0.46
2:C:102:HIS:CB	2:C:105:THR:HG21	2.45	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.30	0.46
3:D:373:PRO:HA	3:D:376:GLU:OE2	2.16	0.46
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.79	0.46
3:N:134:VAL:CG2	3:N:151:GLN:H	2.28	0.46
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.46
3:N:1353:GLN:O	3:N:1357:ARG:HG3	2.15	0.46
7:R:2:DA:H5'	7:R:2:DA:C8	2.50	0.46
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.46
3:D:56:TYR:CE1	3:D:69:GLU:HG3	2.49	0.46
3:D:243:ALA:HB3	3:D:311:LEU:HD21	1.97	0.46
3:D:1283:ILE:CD1	3:D:1315:ASP:OD2	2.64	0.46
2:M:1001:VAL:HG11	3:N:725:SER:HB3	1.97	0.46
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.31	0.46
3:N:273:ARG:HG2	3:N:277:GLU:C	2.41	0.46
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.28	0.46
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.16	0.46
5:P:95:THR:OG1	5:P:97:GLU:OE1	2.29	0.46
1:A:30:ARG:CD	1:A:191:ASP:CG	2.89	0.46
2:C:102:HIS:CG	2:C:105:THR:HB	2.50	0.46
2:C:236:ILE:O	2:C:240:THR:HG23	2.16	0.46
2:C:340:MET:SD	2:C:340:MET:C	2.98	0.46
2:C:502:PRO:C	2:C:503:LEU:HD23	2.41	0.46
2:C:550:LEU:HD23	2:C:905:ILE:HG21	1.97	0.46
3:D:274:ARG:CZ	3:D:279:VAL:HG21	2.46	0.46
7:H:18:DC:H2'	7:H:19:DG:C8	2.51	0.46
2:M:1056:LYS:O	3:N:624:ASP:N	2.44	0.46
3:N:829:VAL:O	3:N:830:ALA:HB3	2.15	0.46
4:O:68:LEU:HD12	4:O:68:LEU:HA	1.79	0.46
5:P:220:LEU:HD11	5:P:235:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:18:DA:H2''	6:Q:19:DG:H5'	1.98	0.46
3:D:134:VAL:HG23	3:D:150:ARG:H	1.81	0.46
3:D:907:GLU:OE1	3:D:909:ASN:N	2.48	0.46
5:F:393:THR:O	5:F:396:ARG:HB3	2.16	0.46
1:L:94:LEU:HD12	1:L:96:THR:H	1.81	0.46
2:M:444:PRO:CG	2:M:452:ILE:HB	2.45	0.46
2:M:559:LEU:HD23	2:M:559:LEU:C	2.40	0.46
3:N:36:THR:HG1	3:N:38:LYS:HB2	1.81	0.46
3:N:135:LEU:HD23	3:N:463:GLN:HG2	1.98	0.46
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.97	0.46
3:N:613:ARG:HG3	3:N:618:LEU:CD2	2.46	0.46
3:N:661:MET:HE1	3:N:677:LEU:CD1	2.46	0.46
3:N:1339:LYS:HG2	3:N:1343:ALA:HB2	1.97	0.46
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.98	0.46
2:C:764:GLU:OE1	2:C:764:GLU:N	2.42	0.46
3:D:36:THR:O	3:D:37:LEU:CB	2.58	0.46
3:D:46:ASP:OD2	3:D:48:ARG:NE	2.46	0.46
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.27	0.46
1:L:97:VAL:HG12	1:L:98:THR:N	2.31	0.46
2:M:77:PRO:HB2	2:M:78:PHE:CD1	2.51	0.46
3:N:222:GLY:HA2	3:N:333:LEU:O	2.16	0.46
3:N:1280:VAL:HG22	3:N:1281:VAL:N	2.31	0.46
5:P:114:LYS:O	5:P:117:SER:OG	2.24	0.46
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.98	0.46
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.85	0.46
3:D:134:VAL:CG2	3:D:151:GLN:H	2.29	0.46
3:D:331:VAL:O	3:D:331:VAL:HG13	2.16	0.46
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.97	0.46
3:D:1314:LYS:HG3	3:D:1317:ASP:OD2	2.16	0.46
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.97	0.46
5:F:281:GLU:OE2	5:F:282:LEU:HD21	2.15	0.46
1:L:38:ASN:HB2	1:L:39:PRO:HD3	1.97	0.46
1:L:88:ARG:HH11	1:L:123:MET:HE1	1.80	0.46
2:M:198:ARG:HH11	2:M:230:ARG:CA	2.28	0.46
2:M:238:LEU:HD12	2:M:238:LEU:C	2.40	0.46
2:M:404:LEU:O	2:M:404:LEU:HG	2.15	0.46
3:N:472:ALA:O	3:N:476:GLU:HG3	2.16	0.46
3:N:778:LEU:HD23	3:N:778:LEU:HA	1.63	0.46
3:N:890:VAL:HG11	3:N:922:LEU:CD1	2.46	0.46
3:N:916:TYR:CE1	3:N:920:LEU:HD11	2.51	0.46
3:N:1400:VAL:CG2	3:N:1417:TRP:HD1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:PRO:HD3	2:C:322:VAL:HG13	1.96	0.45
2:C:685:GLU:O	2:C:686:ASP:HB2	2.15	0.45
2:C:691:SER:HA	2:C:858:MET:HE3	1.98	0.45
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.29	0.45
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.49	0.45
3:D:650:LEU:HD12	3:D:657:LEU:CD2	2.46	0.45
3:D:808:THR:HG22	3:D:810:GLU:N	2.31	0.45
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.50	0.45
1:L:206:THR:H	1:L:209:GLU:HB2	1.81	0.45
2:M:604:ALA:O	2:M:645:VAL:HG13	2.16	0.45
2:M:644:VAL:HG22	2:M:645:VAL:N	2.32	0.45
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.98	0.45
1:A:201:THR:CG2	1:A:202:ASP:N	2.79	0.45
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.51	0.45
3:D:33:ASN:CG	3:D:36:THR:CG2	2.87	0.45
3:D:38:LYS:HD2	3:D:38:LYS:HA	1.68	0.45
3:D:145:VAL:HB	3:D:146:PRO:HD2	1.98	0.45
3:D:1136:LYS:O	3:D:1140:ILE:HG13	2.16	0.45
5:F:374:GLY:HA2	5:F:379:ARG:O	2.15	0.45
1:K:193:ASP:HB3	2:M:938:LYS:CE	2.45	0.45
1:L:73:GLU:CD	1:L:73:GLU:H	2.24	0.45
3:N:1100:ASP:OD1	3:N:1440:PHE:HB2	2.16	0.45
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.16	0.45
3:N:1459:LEU:HD12	3:N:1464:GLU:HB3	1.99	0.45
5:P:260:ILE:HG22	5:P:265:VAL:HG23	1.99	0.45
5:P:273:ARG:HA	5:P:276:ARG:NH1	2.31	0.45
1:B:88:ARG:HH11	1:B:123:MET:HE1	1.81	0.45
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.82	0.45
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.97	0.45
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.97	0.45
3:D:355:VAL:HG13	3:D:359:ALA:HB3	1.98	0.45
3:D:890:VAL:O	3:D:926:LYS:NZ	2.47	0.45
3:D:922:LEU:N	3:D:922:LEU:HD23	2.32	0.45
3:D:1102:THR:CG2	3:D:1371:VAL:HG22	2.47	0.45
2:M:56:GLU:OE2	2:M:56:GLU:HA	2.16	0.45
2:M:419:THR:HB	2:M:422:ARG:CG	2.47	0.45
2:M:469:THR:HG23	2:M:471:TYR:CE1	2.51	0.45
3:N:904:VAL:HG23	3:N:905:PRO:HD2	1.98	0.45
3:N:1248:GLY:O	3:N:1249:ALA:HB3	2.16	0.45
3:N:1276:GLU:OE2	3:N:1301:LYS:CE	2.64	0.45
3:N:1283:ILE:CD1	3:N:1283:ILE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1304:LYS:CA	3:N:1305:LEU:HD23	2.45	0.45
3:N:1342:GLU:H	3:N:1342:GLU:CD	2.25	0.45
2:C:121:MET:HE1	2:C:336:VAL:HG21	1.96	0.45
2:C:229:MET:O	2:C:230:ARG:CD	2.58	0.45
2:C:1005:MET:HE1	3:D:647:ARG:HB2	1.99	0.45
3:D:47:GLU:C	3:D:78:VAL:HG23	2.42	0.45
3:D:573:MET:SD	5:F:210:LEU:HB3	2.56	0.45
3:D:778:LEU:HA	3:D:778:LEU:HD23	1.63	0.45
2:M:86:LYS:O	2:M:87:ASP:HB2	2.17	0.45
2:M:157:ARG:NH1	2:M:176:VAL:HG12	2.09	0.45
3:N:890:VAL:O	3:N:926:LYS:NZ	2.48	0.45
2:C:230:ARG:HD3	2:C:233:GLU:OE1	2.16	0.45
2:C:323:ASP:O	2:C:325:ILE:CG2	2.65	0.45
2:C:444:PRO:CG	2:C:452:ILE:HB	2.47	0.45
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.60	0.45
3:D:1267:ARG:HG2	3:D:1331:ASP:OD2	2.16	0.45
3:D:1439:SER:HB2	3:D:1463:LYS:HZ1	1.77	0.45
3:D:1440:PHE:O	3:D:1441:GLN:CG	2.65	0.45
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.53	0.45
5:F:278:LEU:O	5:F:282:LEU:HG	2.17	0.45
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.17	0.45
5:F:418:LEU:HD12	5:F:418:LEU:H	1.81	0.45
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.52	0.45
2:M:230:ARG:HG3	2:M:231:PRO:CD	2.46	0.45
3:N:843:PHE:CD1	3:N:864:VAL:HG11	2.50	0.45
1:B:201:THR:HG22	1:B:202:ASP:N	2.32	0.45
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.99	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.98	0.45
3:D:661:MET:HE1	3:D:677:LEU:CD1	2.46	0.45
3:D:1440:PHE:O	3:D:1441:GLN:HG3	2.17	0.45
2:M:582:GLY:N	2:M:584:GLU:OE2	2.44	0.45
3:N:30:GLU:OE1	3:N:40:GLU:HG2	2.16	0.45
3:N:573:MET:HE1	5:P:214:GLN:HG3	1.99	0.45
3:N:1237:THR:HG21	3:N:1246:VAL:CG1	2.42	0.45
3:N:1309:ALA:O	3:N:1310:ARG:HB3	2.16	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.64	0.45
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.98	0.45
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.78	0.45
5:F:394:ARG:HG3	5:F:395:GLU:N	2.32	0.45
2:M:87:ASP:HA	2:M:131:GLY:HA3	1.98	0.45
5:P:401:GLU:HG3	5:P:402:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:717:LEU:HD12	2:C:717:LEU:N	2.32	0.45
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.98	0.45
3:D:1460:ILE:N	3:D:1460:ILE:HD13	2.30	0.45
5:F:390:PHE:CD1	5:F:397:ILE:HD11	2.51	0.45
1:L:64:GLU:O	1:L:75:VAL:HB	2.16	0.45
1:L:201:THR:HG22	1:L:202:ASP:N	2.31	0.45
2:M:680:ASP:H	3:N:943:THR:CG2	2.30	0.45
3:N:355:VAL:HG13	3:N:359:ALA:HB3	1.99	0.45
3:N:640:HIS:ND1	3:N:641:GLN:HG3	2.32	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.98	0.45
5:P:222:ARG:HA	5:P:222:ARG:HE	1.82	0.45
5:P:391:GLY:O	5:P:392:VAL:C	2.58	0.45
2:C:419:THR:HB	2:C:422:ARG:CG	2.47	0.45
2:C:858:MET:HG3	2:C:867:VAL:CG2	2.46	0.45
3:D:534:ARG:HH21	3:D:534:ARG:HG3	1.82	0.45
3:D:805:GLU:HA	3:D:828:LYS:O	2.17	0.45
1:L:190:THR:O	1:L:190:THR:HG22	2.17	0.45
2:M:261:ILE:O	2:M:289:THR:HG23	2.16	0.45
2:M:281:LEU:HD11	2:M:306:THR:HG22	1.98	0.45
5:P:237:THR:OG1	7:R:4:DA:H8	2.00	0.45
5:P:358:LEU:HD23	5:P:370:LYS:CE	2.47	0.45
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.88	0.45
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.98	0.45
1:B:143:ARG:HD3	1:B:158:ILE:HD13	1.99	0.45
1:B:190:THR:O	1:B:190:THR:HG22	2.17	0.45
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.52	0.45
2:C:1104:GLU:HB3	3:D:6:ARG:HG3	1.98	0.45
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.98	0.45
5:F:96:LEU:O	5:F:100:VAL:HG23	2.17	0.45
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.99	0.45
2:M:154:ARG:NH2	2:M:178:PRO:CA	2.80	0.45
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.99	0.45
3:N:806:PHE:O	3:N:830:ALA:N	2.48	0.45
3:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.51	0.45
3:N:1478:SER:O	3:N:1482:ARG:HB2	2.17	0.45
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.84	0.45
1:A:153:ALA:N	1:A:168:ASP:OD1	2.33	0.44
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.99	0.44
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.47	0.44
3:D:203:ALA:C	3:D:204:LEU:HD12	2.42	0.44
3:D:791:TYR:CD1	3:D:945:SER:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1310:ARG:O	3:D:1310:ARG:HG2	2.17	0.44
5:F:221:ILE:O	5:F:222:ARG:C	2.61	0.44
2:M:280:LYS:HE3	2:M:309:TYR:CZ	2.52	0.44
2:M:480:THR:HG22	2:M:481:ASP:N	2.32	0.44
2:M:684:PHE:HE1	3:N:783:ARG:HB2	1.81	0.44
3:N:47:GLU:HG2	3:N:51:GLY:O	2.17	0.44
3:N:241:ILE:HD13	3:N:312:ARG:HB3	1.99	0.44
3:N:634:GLY:O	3:N:637:LEU:CD1	2.65	0.44
2:C:604:ALA:O	2:C:645:VAL:HG13	2.17	0.44
3:D:1200:VAL:CG1	3:D:1201:CYS:N	2.80	0.44
3:N:97:THR:HG22	3:N:98:PRO:O	2.17	0.44
1:A:34:VAL:HG22	1:B:42:ARG:NH2	2.33	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.98	0.44
2:C:738:ASP:C	2:C:738:ASP:OD1	2.61	0.44
2:C:1060:ILE:HD13	5:F:338:LEU:HD13	1.98	0.44
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.98	0.44
3:D:1406:ARG:O	3:D:1410:GLU:HB3	2.17	0.44
1:L:56:VAL:HG21	1:L:82:LEU:CD1	2.47	0.44
2:M:340:MET:C	2:M:340:MET:SD	3.01	0.44
2:M:486:MET:HE1	2:M:531:PHE:CD1	2.52	0.44
2:M:639:GLN:HA	2:M:657:ASP:O	2.18	0.44
2:M:767:PRO:HB2	2:M:772:ARG:HD2	1.99	0.44
3:N:14:SER:HB3	3:N:511:TRP:CZ2	2.53	0.44
3:N:46:ASP:OD1	3:N:48:ARG:HG2	2.18	0.44
3:N:213:VAL:HG21	3:N:367:ILE:CD1	2.44	0.44
3:N:1126:ASP:OD2	3:N:1126:ASP:N	2.49	0.44
3:N:1255:GLY:O	3:N:1258:ARG:HB3	2.16	0.44
3:N:1439:SER:OG	3:N:1467:ILE:HD11	2.17	0.44
5:P:202:TYR:HB2	5:P:212:LEU:HD13	1.98	0.44
5:P:286:PRO:HB2	5:P:291:ILE:HG13	1.99	0.44
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.98	0.44
2:C:639:GLN:HA	2:C:657:ASP:O	2.18	0.44
2:C:873:PRO:HB2	3:D:949:ILE:CD1	2.48	0.44
3:D:133:ILE:HD12	3:D:152:LEU:HD23	2.00	0.44
3:D:237:LYS:N	3:D:240:GLU:OE1	2.49	0.44
1:K:30:ARG:HD3	1:K:191:ASP:OD1	2.17	0.44
2:M:323:ASP:O	2:M:325:ILE:HG22	2.17	0.44
3:N:71:LYS:O	3:N:80:VAL:HG22	2.17	0.44
3:N:215:TYR:CE1	3:N:380:GLU:O	2.70	0.44
3:N:252:ARG:NH2	3:N:303:PRO:HD3	2.32	0.44
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:808:THR:HG22	3:N:810:GLU:N	2.30	0.44
3:N:1315:ASP:OD2	3:N:1315:ASP:C	2.60	0.44
3:N:1477:GLY:O	3:N:1482:ARG:HD3	2.17	0.44
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.53	0.44
2:C:644:VAL:HG22	2:C:645:VAL:N	2.33	0.44
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.52	0.44
2:C:1059:ASP:OD2	2:C:1062:GLY:HA3	2.18	0.44
2:M:237:ARG:HD2	2:M:241:LEU:HD21	1.99	0.44
2:M:439:CYS:HA	2:M:440:PRO:HD3	1.82	0.44
3:N:142:LEU:HG	3:N:143:ASN:H	1.82	0.44
3:N:170:PRO:HA	3:N:392:SER:HB3	2.00	0.44
3:N:203:ALA:C	3:N:204:LEU:HD12	2.42	0.44
3:N:1282:ARG:HB3	3:N:1293:PHE:HB2	1.98	0.44
3:N:1321:ALA:O	3:N:1339:LYS:HD3	2.17	0.44
5:P:412:GLU:O	5:P:416:ARG:HG3	2.18	0.44
1:B:58:ILE:HD13	1:B:140:MET:HB2	2.00	0.44
2:C:86:LYS:O	2:C:87:ASP:HB2	2.18	0.44
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.82	0.44
3:D:775:GLY:HA2	3:D:1209:LEU:O	2.17	0.44
5:F:259:ARG:HH11	5:F:259:ARG:CG	2.31	0.44
1:L:97:VAL:HG12	1:L:99:LEU:HD12	1.99	0.44
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.53	0.44
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.29	0.44
3:N:264:LEU:O	3:N:264:LEU:HD12	2.17	0.44
3:N:679:ARG:HD3	3:N:682:ASP:OD2	2.18	0.44
3:N:693:GLU:HB3	4:O:48:MET:HE1	1.99	0.44
2:C:224:GLU:CD	2:C:224:GLU:N	2.60	0.44
3:D:170:PRO:HA	3:D:392:SER:HB3	1.98	0.44
3:D:230:TRP:CD1	3:D:331:VAL:HG11	2.52	0.44
3:D:629:SER:O	3:D:744:GLN:HG2	2.17	0.44
3:D:679:ARG:HD3	3:D:682:ASP:OD2	2.18	0.44
1:K:201:THR:CG2	1:K:202:ASP:N	2.81	0.44
2:M:167:LYS:HD3	2:M:167:LYS:HA	1.72	0.44
2:M:422:ARG:HH22	7:R:13:DT:H5''	1.82	0.44
2:M:437:ARG:HH22	2:M:491:GLU:HB2	1.83	0.44
2:M:535:SER:OG	2:M:537:LYS:HG3	2.18	0.44
2:M:604:ALA:HB3	2:M:612:VAL:HG12	1.99	0.44
2:M:815:LEU:O	2:M:816:LYS:C	2.59	0.44
3:N:145:VAL:HB	3:N:146:PRO:HD2	1.99	0.44
3:N:411:THR:CA	3:N:435:VAL:HG12	2.40	0.44
1:A:9:PRO:HB3	1:A:26:GLU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:351:LEU:HD12	2:C:374:ASN:O	2.18	0.44
3:D:890:VAL:CG2	3:D:922:LEU:HD11	2.48	0.44
1:L:123:MET:O	1:L:125:PRO:HD3	2.17	0.44
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.53	0.44
5:P:393:THR:HG23	5:P:396:ARG:HB3	1.99	0.44
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.47	0.44
2:C:853:LEU:HB2	2:C:858:MET:CE	2.28	0.44
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.99	0.44
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.18	0.44
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.53	0.44
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.44	0.44
3:D:904:VAL:HG23	3:D:905:PRO:HD2	1.99	0.44
3:D:1353:GLN:OE1	3:D:1353:GLN:HA	2.17	0.44
1:K:206:THR:HG22	1:K:208:LEU:N	2.32	0.44
1:L:74:ASP:O	1:L:78:ILE:HG13	2.18	0.44
2:M:206:THR:O	2:M:209:ARG:HD2	2.18	0.44
2:M:717:LEU:N	2:M:717:LEU:HD12	2.32	0.44
2:M:1095:LEU:O	2:M:1096:ALA:HB3	2.18	0.44
3:N:669:ASN:HD22	5:P:417:LYS:CD	2.30	0.44
3:N:1311:LEU:HD22	3:N:1311:LEU:H	1.71	0.44
3:N:1331:ASP:C	3:N:1331:ASP:OD1	2.61	0.44
3:N:1386:ASP:HB2	3:N:1412:LYS:HD2	2.00	0.44
3:N:1487:VAL:CG2	3:N:1491:THR:HB	2.47	0.44
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.85	0.44
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.33	0.43
2:C:281:LEU:HD11	2:C:306:THR:HG22	2.00	0.43
2:C:572:ILE:HG13	2:C:573:ARG:HG3	2.00	0.43
2:C:680:ASP:H	3:D:943:THR:CG2	2.32	0.43
3:D:314:PRO:HD2	3:D:317:VAL:CG1	2.48	0.43
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.99	0.43
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.99	0.43
5:F:278:LEU:HD11	5:F:294:ALA:CB	2.47	0.43
1:L:161:ARG:HE	1:L:161:ARG:HB2	1.63	0.43
1:L:185:ARG:CG	1:L:190:THR:HG23	2.48	0.43
2:M:223:ASP:HA	2:M:224:GLU:OE2	2.18	0.43
2:M:376:ARG:HB2	2:M:377:PRO:HD3	2.00	0.43
2:M:684:PHE:HB3	3:N:633:VAL:HG21	2.00	0.43
3:N:314:PRO:HG2	3:N:317:VAL:HG11	1.99	0.43
3:N:598:ARG:NH2	5:P:316:SER:OG	2.51	0.43
3:N:835:SER:HB2	3:N:838:ARG:HE	1.66	0.43
3:N:907:GLU:OE1	3:N:909:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:HG12	2:C:177:GLU:O	2.19	0.43
2:C:541:SER:O	2:C:545:ASN:ND2	2.40	0.43
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.43	0.43
5:F:81:VAL:O	5:F:85:LEU:HG	2.18	0.43
1:K:83:LYS:CE	1:K:168:ASP:HB2	2.46	0.43
1:L:58:ILE:HD13	1:L:140:MET:HB2	2.00	0.43
2:M:572:ILE:HG13	2:M:573:ARG:HG3	2.00	0.43
2:M:637:LEU:HA	2:M:659:PRO:HG3	2.00	0.43
3:N:597:ASP:HB2	3:N:598:ARG:H	1.56	0.43
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	1.98	0.43
4:O:12:MET:HE1	4:O:68:LEU:O	2.18	0.43
5:P:350:LEU:O	5:P:354:LEU:HG	2.18	0.43
1:A:57:TYR:CZ	1:A:161:ARG:HD2	2.52	0.43
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.54	0.43
2:C:706:GLU:OE1	2:C:706:GLU:HA	2.18	0.43
2:C:911:GLU:N	2:C:912:PRO:CD	2.81	0.43
2:C:937:ASP:OD1	2:C:939:ARG:CG	2.66	0.43
3:D:142:LEU:HG	3:D:143:ASN:H	1.84	0.43
3:D:1373:ARG:HE	3:D:1373:ARG:HB2	1.55	0.43
2:M:1058:ASP:OD2	2:M:1084:SER:HB2	2.19	0.43
3:N:204:LEU:HD23	3:N:441:ARG:CZ	2.49	0.43
3:N:648:MET:O	3:N:652:LEU:HG	2.18	0.43
3:N:1171:VAL:O	3:N:1175:ILE:HG13	2.18	0.43
5:P:371:LEU:HA	5:P:381:HIS:HD2	1.83	0.43
5:P:372:ARG:O	5:P:380:GLU:HB2	2.17	0.43
1:B:131:THR:C	1:B:132:LEU:HD12	2.43	0.43
1:B:185:ARG:CG	1:B:190:THR:HG23	2.49	0.43
2:C:223:ASP:HA	2:C:224:GLU:OE2	2.19	0.43
2:C:480:THR:HG22	2:C:481:ASP:N	2.32	0.43
2:C:699:PHE:O	2:C:700:TYR:HB2	2.18	0.43
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.82	0.43
2:C:937:ASP:OD1	2:C:939:ARG:HG3	2.17	0.43
4:E:43:GLU:H	4:E:43:GLU:CD	2.26	0.43
7:H:2:DA:H5'	7:H:2:DA:C8	2.53	0.43
2:M:375:SER:O	2:M:378:LEU:N	2.51	0.43
2:M:499:ALA:HA	2:M:532:MET:HE3	1.99	0.43
3:N:65:ARG:NH1	5:P:378:GLY:C	2.76	0.43
3:N:827:ILE:CG2	3:N:828:LYS:N	2.80	0.43
1:B:56:VAL:HG21	1:B:82:LEU:CD1	2.48	0.43
1:B:58:ILE:HG21	1:B:61:VAL:CG1	2.37	0.43
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:529:GLN:HA	3:D:534:ARG:O	2.18	0.43
3:D:1313:VAL:HG23	3:D:1313:VAL:O	2.19	0.43
5:F:95:THR:HG22	5:F:96:LEU:H	1.82	0.43
5:F:144:ILE:HB	5:F:147:LEU:HB2	2.01	0.43
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.49	0.43
1:K:9:PRO:HB3	1:K:26:GLU:C	2.43	0.43
2:M:90:TYR:CD2	2:M:120:LEU:HB2	2.54	0.43
2:M:308:ARG:HE	2:M:308:ARG:HB3	1.70	0.43
2:M:524:VAL:HG11	2:M:528:GLU:HB2	1.99	0.43
2:M:706:GLU:OE1	2:M:706:GLU:HA	2.18	0.43
2:M:738:ASP:C	2:M:738:ASP:OD1	2.61	0.43
3:N:315:ARG:O	3:N:316:GLN:CB	2.65	0.43
3:N:1403:LEU:O	3:N:1406:ARG:HB2	2.18	0.43
5:P:172:ARG:O	5:P:176:ILE:HG12	2.18	0.43
1:B:123:MET:O	1:B:125:PRO:HD3	2.18	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HB2	2.00	0.43
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.43
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.43
2:C:910:LYS:HB3	2:C:912:PRO:HD2	2.00	0.43
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.27	0.43
3:D:1429:LEU:HD21	3:D:1441:GLN:HB2	2.01	0.43
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.81	0.43
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.85	0.43
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.99	0.43
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	2.00	0.43
3:N:68:PHE:O	3:N:80:VAL:HG21	2.17	0.43
3:N:570:GLU:OE2	5:P:214:GLN:NE2	2.48	0.43
3:N:900:ILE:H	3:N:900:ILE:HG13	1.63	0.43
3:N:959:GLU:HB3	3:N:963:TYR:HE1	1.84	0.43
1:B:73:GLU:H	1:B:73:GLU:CD	2.22	0.43
2:C:486:MET:HE1	2:C:531:PHE:CD1	2.54	0.43
2:C:499:ALA:HA	2:C:532:MET:HE3	2.00	0.43
2:C:561:GLY:O	2:C:565:GLN:HG3	2.19	0.43
3:D:45:PHE:C	3:D:86:ARG:HH22	2.25	0.43
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.48	0.43
3:D:696:HIS:HD2	4:E:57:ASP:OD1	2.00	0.43
5:F:383:LEU:O	5:F:397:ILE:HG21	2.19	0.43
1:K:89:PHE:HB2	1:K:146:ARG:NH2	2.33	0.43
1:L:143:ARG:HD3	1:L:158:ILE:HD13	1.99	0.43
2:M:136:ILE:HD13	2:M:392:SER:HA	2.01	0.43
2:M:176:VAL:CG1	2:M:177:GLU:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:911:GLU:N	2:M:912:PRO:CD	2.81	0.43
3:N:367:ILE:HB	3:N:377:VAL:HG12	2.01	0.43
3:N:1462:LEU:HD23	3:N:1473:PRO:HG2	2.00	0.43
2:C:524:VAL:HG11	2:C:528:GLU:HB2	1.99	0.43
3:D:145:VAL:HB	3:D:146:PRO:CD	2.48	0.43
3:D:207:PHE:HB2	3:D:391:ALA:HB2	2.01	0.43
3:D:356:PRO:HB3	3:D:441:ARG:HA	2.01	0.43
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.91	0.43
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.86	0.43
3:D:1403:LEU:O	3:D:1406:ARG:HB2	2.18	0.43
1:L:131:THR:C	1:L:132:LEU:HD12	2.44	0.43
2:M:12:VAL:HG11	2:M:472:ARG:NH1	2.34	0.43
2:M:48:PHE:O	2:M:52:PHE:CD2	2.61	0.43
2:M:164:PRO:HB2	2:M:168:ARG:O	2.19	0.43
2:M:171:TRP:CE3	7:R:14:DG:OP1	2.72	0.43
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.43
2:M:428:ARG:HB3	2:M:450:GLY:HA3	2.00	0.43
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.00	0.43
2:M:937:ASP:OD1	2:M:939:ARG:CG	2.66	0.43
2:M:1104:GLU:H	2:M:1104:GLU:CD	2.27	0.43
3:N:245:LEU:HD22	3:N:249:TYR:HB3	2.01	0.43
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.99	0.43
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.18	0.43
2:C:807:ARG:HE	2:C:807:ARG:HB2	1.56	0.43
3:D:403:PHE:CE2	3:D:442:ASN:C	2.97	0.43
3:D:1005:GLN:O	3:D:1009:LYS:HG2	2.19	0.43
3:D:1188:VAL:HG13	3:D:1189:ARG:O	2.19	0.43
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.71	0.43
2:M:1032:PHE:HZ	2:M:1040:LEU:HG	1.84	0.43
2:M:1059:ASP:OD2	2:M:1062:GLY:HA3	2.19	0.43
3:N:133:ILE:CG2	3:N:460:ALA:HB1	2.48	0.43
3:N:801:GLY:HA2	3:N:821:VAL:HG13	2.01	0.43
3:N:1309:ALA:O	3:N:1310:ARG:HB2	2.18	0.43
5:P:362:SER:HB3	5:P:365:GLU:CG	2.49	0.43
2:C:36:PRO:HA	2:C:39:ARG:HG3	2.01	0.43
3:D:634:GLY:O	3:D:637:LEU:CD1	2.66	0.43
3:D:984:THR:HG22	3:D:985:ASP:N	2.34	0.43
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.27	0.43
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.51	0.43
1:L:124:ASN:OD1	1:L:124:ASN:N	2.52	0.43
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG12	1:B:98:THR:N	2.33	0.42
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.53	0.42
3:D:155:ASP:O	3:D:159:ARG:HG3	2.18	0.42
2:M:248:PRO:C	2:M:250:ARG:N	2.77	0.42
3:N:269:PHE:CE2	3:N:283:PHE:HD1	2.37	0.42
3:N:959:GLU:OE1	3:N:959:GLU:N	2.45	0.42
3:N:1495:ILE:HG21	4:O:80:VAL:HG21	2.00	0.42
5:P:101:GLU:CG	5:P:105:LYS:HE2	2.49	0.42
1:A:154:GLU:H	1:A:154:GLU:CD	2.27	0.42
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.01	0.42
2:C:184:MET:HE2	2:C:191:PHE:CZ	2.54	0.42
2:C:292:ARG:NE	2:C:299:LYS:HD3	2.34	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.42
2:C:683:ASN:CG	2:C:872:ASN:HB2	2.45	0.42
3:D:434:ARG:NH1	5:F:135:ILE:O	2.52	0.42
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.01	0.42
5:F:114:LYS:O	5:F:118:GLU:HG3	2.19	0.42
1:K:133:GLU:HG2	1:K:134:GLU:H	1.83	0.42
2:M:51:THR:HG21	2:M:352:ALA:HB2	2.01	0.42
2:M:552:HIS:CD2	2:M:886:LEU:HD12	2.54	0.42
2:M:879:ARG:N	2:M:879:ARG:HD2	2.34	0.42
2:M:1056:LYS:HE2	3:N:751:LEU:HG	2.01	0.42
3:N:108:VAL:HB	3:N:109:PRO:CD	2.46	0.42
3:N:367:ILE:HD11	3:N:379:ALA:HB2	2.01	0.42
3:N:593:ASN:OD1	3:N:594:PRO:HD3	2.20	0.42
3:N:719:VAL:O	3:N:721:VAL:HG13	2.20	0.42
3:N:890:VAL:HG11	3:N:922:LEU:HD12	2.01	0.42
3:N:1101:VAL:HG21	3:N:1424:VAL:CB	2.49	0.42
3:N:1283:ILE:HD13	3:N:1283:ILE:C	2.21	0.42
5:P:239:ALA:O	5:P:240:THR:C	2.63	0.42
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.33	0.42
2:C:231:PRO:CG	2:C:232:GLU:OE2	2.59	0.42
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.34	0.42
2:C:1001:VAL:HG13	3:D:630:VAL:HB	2.00	0.42
3:D:65:ARG:HG3	5:F:378:GLY:O	2.19	0.42
3:D:142:LEU:HD13	3:D:161:LEU:CD1	2.48	0.42
3:D:894:LYS:N	3:D:894:LYS:CD	2.30	0.42
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.01	0.42
1:L:5:LYS:HE3	1:L:6:LEU:H	1.84	0.42
3:N:791:TYR:CD1	3:N:945:SER:HB2	2.53	0.42
3:N:957:PRO:HG3	3:N:1007:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1238:MET:HE3	3:N:1238:MET:HB3	1.88	0.42
5:P:375:LEU:HD23	5:P:375:LEU:C	2.43	0.42
3:D:275:GLU:HB3	3:D:276:ASP:H	1.57	0.42
3:D:405:ASP:CG	3:D:406:ASP:N	2.77	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
3:D:890:VAL:CB	3:D:922:LEU:HD11	2.45	0.42
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.85	0.42
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.42
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.55	0.42
5:F:418:LEU:H	5:F:418:LEU:CD1	2.32	0.42
1:K:34:VAL:HG22	1:L:42:ARG:CZ	2.49	0.42
1:L:124:ASN:HD22	1:L:127:LEU:HB2	1.84	0.42
2:M:54:ILE:HG23	2:M:356:ARG:HG3	2.01	0.42
2:M:105:THR:CG2	2:M:107:LEU:N	2.60	0.42
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.55	0.42
2:M:937:ASP:OD1	2:M:939:ARG:HG3	2.18	0.42
2:M:998:TYR:CG	2:M:998:TYR:O	2.73	0.42
3:N:138:LYS:HB2	3:N:451:ASP:O	2.17	0.42
3:N:598:ARG:NH2	5:P:316:SER:CB	2.83	0.42
3:N:693:GLU:CA	4:O:48:MET:HE1	2.49	0.42
3:N:827:ILE:O	3:N:834:THR:N	2.45	0.42
3:N:1286:THR:HG22	3:N:1288:GLU:N	2.32	0.42
3:N:1404:ASN:O	3:N:1405:GLU:C	2.63	0.42
5:P:340:SER:C	5:P:342:VAL:N	2.77	0.42
1:A:44:LEU:HA	1:A:48:ILE:HG12	2.01	0.42
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.50	0.42
2:C:236:ILE:HG23	2:C:248:PRO:CB	2.50	0.42
2:C:462:ASP:OD1	2:C:462:ASP:C	2.62	0.42
3:D:128:TYR:CZ	3:D:587:ARG:HD2	2.55	0.42
3:D:367:ILE:HD11	3:D:379:ALA:HB2	2.01	0.42
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.42
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.20	0.42
3:D:1373:ARG:HG3	3:D:1374:GLN:N	2.35	0.42
1:L:201:THR:CG2	1:L:202:ASP:N	2.82	0.42
2:M:151:ASP:OD2	2:M:175:GLU:OE2	2.38	0.42
2:M:1071:ILE:HG23	3:N:670:VAL:HG21	2.02	0.42
2:M:1081:VAL:HA	2:M:1082:PRO:HD3	1.85	0.42
3:N:1312:LEU:CD2	3:N:1327:ARG:CG	2.90	0.42
1:B:201:THR:CG2	1:B:202:ASP:N	2.83	0.42
2:C:774:LEU:HD21	5:F:418:LEU:HB3	2.02	0.42
3:D:187:LYS:HG3	3:D:198:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:259:VAL:O	3:D:295:GLY:N	2.44	0.42
3:D:640:HIS:ND1	3:D:641:GLN:HG3	2.34	0.42
4:E:34:GLY:O	4:E:35:PHE:HB2	2.19	0.42
2:M:187:ASN:HD22	2:M:187:ASN:HA	1.63	0.42
2:M:918:LEU:HD23	2:M:918:LEU:HA	1.95	0.42
3:N:48:ARG:CZ	3:N:76:CYS:O	2.68	0.42
3:N:266:GLU:HG2	3:N:286:VAL:HB	2.01	0.42
3:N:553:ARG:HD3	5:P:214:GLN:HB3	2.01	0.42
3:N:801:GLY:HA3	3:N:825:ALA:HB1	2.01	0.42
3:N:1003:VAL:O	3:N:1007:VAL:HG23	2.20	0.42
5:P:222:ARG:HA	5:P:222:ARG:NE	2.34	0.42
2:C:690:ILE:HG23	2:C:694:LEU:HD12	2.01	0.42
2:C:1001:VAL:HG11	3:D:725:SER:HB3	2.01	0.42
3:D:67:ARG:CZ	5:F:379:ARG:HB2	2.50	0.42
3:D:231:VAL:O	3:D:231:VAL:HG22	2.20	0.42
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.19	0.42
5:F:230:LYS:O	5:F:232:ARG:CG	2.67	0.42
2:M:289:THR:HG21	2:M:291:ALA:O	2.19	0.42
2:M:717:LEU:HD23	2:M:763:GLY:CA	2.43	0.42
2:M:1001:VAL:HG13	3:N:630:VAL:HB	2.02	0.42
3:N:33:ASN:CB	3:N:36:THR:HG23	2.43	0.42
3:N:35:ARG:CB	3:N:35:ARG:HH11	2.32	0.42
3:N:111:LYS:HG3	3:N:1452:ILE:CD1	2.49	0.42
3:N:134:VAL:HG22	3:N:151:GLN:O	2.20	0.42
3:N:568:ARG:HD2	5:P:87:GLU:OE1	2.20	0.42
3:N:784:ASP:HB2	3:N:939:PHE:HE2	1.84	0.42
3:N:827:ILE:HG23	3:N:828:LYS:N	2.34	0.42
3:N:1057:VAL:HG13	3:N:1069:GLU:CD	2.45	0.42
3:N:1256:LEU:O	3:N:1260:ILE:HG13	2.19	0.42
3:N:1283:ILE:O	3:N:1283:ILE:CG1	2.67	0.42
1:B:74:ASP:O	1:B:78:ILE:HG13	2.20	0.42
1:B:179:PHE:CB	1:B:197:LEU:HD13	2.49	0.42
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.02	0.42
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.80	0.42
2:C:604:ALA:HB3	2:C:612:VAL:HG12	2.01	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH11	1.68	0.42
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.55	0.42
2:M:48:PHE:HA	2:M:348:LEU:HD21	2.02	0.42
2:M:289:THR:HG22	2:M:291:ALA:O	2.20	0.42
2:M:695:LEU:HD23	2:M:695:LEU:N	2.34	0.42
3:N:33:ASN:OD1	3:N:36:THR:CG2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:140:ALA:HA	3:N:450:TYR:CG	2.55	0.42
3:N:187:LYS:HG3	3:N:198:ARG:O	2.20	0.42
3:N:230:TRP:HA	3:N:243:ALA:HB2	2.01	0.42
3:N:530:VAL:HG22	3:N:534:ARG:O	2.20	0.42
3:N:1232:PRO:O	3:N:1233:GLY:C	2.63	0.42
4:O:61:VAL:O	4:O:65:MET:HG3	2.20	0.42
5:P:368:VAL:HG23	5:P:369:LEU:N	2.35	0.42
1:A:4:SER:C	1:A:189:ARG:HH21	2.26	0.42
1:B:58:ILE:O	1:B:61:VAL:HG13	2.20	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
2:C:1104:GLU:H	2:C:1104:GLU:CD	2.27	0.42
3:D:530:VAL:HG22	3:D:534:ARG:HB3	2.01	0.42
3:D:637:LEU:HD22	3:D:642:CYS:HA	2.02	0.42
3:D:1168:MET:HE3	3:D:1171:VAL:HB	2.02	0.42
3:D:1168:MET:HE2	3:D:1172:HIS:CE1	2.54	0.42
3:D:1285:GLU:HA	3:D:1290:LEU:HD22	2.02	0.42
5:F:102:LEU:O	5:F:106:VAL:HG23	2.20	0.42
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.01	0.42
2:M:118:ILE:HD11	2:M:344:PHE:HE2	1.81	0.42
2:M:693:GLU:HA	2:M:696:LYS:HD2	2.02	0.42
2:M:751:PRO:HB2	3:N:680:GLN:HB2	2.02	0.42
3:N:36:THR:OG1	3:N:38:LYS:HB2	2.20	0.42
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.35	0.42
3:N:580:ALA:HA	3:N:584:ASN:HA	2.02	0.42
3:N:829:VAL:O	3:N:830:ALA:C	2.61	0.42
3:N:1284:GLU:C	3:N:1284:GLU:CD	2.88	0.42
5:P:391:GLY:C	5:P:392:VAL:O	2.63	0.42
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.01	0.42
2:C:786:LYS:HB3	2:C:786:LYS:HZ3	1.84	0.42
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.55	0.42
3:D:553:ARG:HD2	3:D:570:GLU:CD	2.45	0.42
3:D:801:GLY:HA3	3:D:825:ALA:HB1	2.01	0.42
4:E:70:THR:HB	4:E:72:ARG:HG3	2.02	0.42
2:M:41:ASN:OD1	2:M:41:ASN:C	2.63	0.42
2:M:98:LEU:HD12	2:M:113:VAL:HG21	2.02	0.42
2:M:248:PRO:O	2:M:250:ARG:N	2.53	0.42
2:M:690:ILE:HG23	2:M:694:LEU:HD12	2.02	0.42
2:M:691:SER:HA	2:M:858:MET:HE3	2.01	0.42
2:M:736:ASP:O	2:M:744:ARG:HG2	2.20	0.42
3:N:145:VAL:HB	3:N:146:PRO:CD	2.49	0.42
3:N:317:VAL:CG2	3:N:339:TRP:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:602:SER:O	3:N:606:ILE:HG13	2.19	0.42
3:N:1394:VAL:HG12	3:N:1395:LEU:N	2.34	0.42
1:A:216:GLU:CD	1:A:219:ARG:HH21	2.28	0.41
2:C:54:ILE:HG23	2:C:356:ARG:HG3	2.02	0.41
2:C:64:LEU:HD11	2:C:367:LEU:HD12	2.02	0.41
2:C:592:LEU:N	2:C:592:LEU:HD23	2.35	0.41
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.90	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD2	1.88	0.41
3:D:45:PHE:C	3:D:86:ARG:NH2	2.77	0.41
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.89	0.41
1:L:101:LEU:HD21	1:L:109:VAL:HG11	2.02	0.41
1:L:128:HIS:HE1	1:L:131:THR:CG2	2.33	0.41
2:M:102:HIS:O	2:M:106:GLY:CA	2.68	0.41
2:M:820:ARG:HE	2:M:820:ARG:HB2	1.59	0.41
2:M:999:HIS:HB3	2:M:1004:LYS:CE	2.49	0.41
3:N:133:ILE:HD12	3:N:152:LEU:HD23	2.02	0.41
3:N:326:GLU:HG2	3:N:331:VAL:HG12	2.02	0.41
3:N:403:PHE:CE2	3:N:442:ASN:C	2.98	0.41
3:N:405:ASP:CG	3:N:406:ASP:N	2.77	0.41
3:N:1374:GLN:OE1	3:N:1374:GLN:HA	2.19	0.41
5:P:228:GLU:OE2	5:P:231:ARG:NH2	2.53	0.41
1:A:23:PHE:HE1	1:A:208:LEU:HD12	1.85	0.41
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.56	0.41
2:C:404:LEU:O	2:C:404:LEU:HG	2.20	0.41
3:D:80:VAL:HG23	3:D:80:VAL:O	2.20	0.41
3:D:261:LEU:HD12	3:D:269:PHE:O	2.20	0.41
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.19	0.41
3:D:801:GLY:O	3:D:804:LEU:HG	2.21	0.41
5:F:228:GLU:OE2	5:F:231:ARG:NH2	2.48	0.41
6:G:14:DG:H5'	6:G:14:DG:H8	1.85	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.55	0.41
2:M:100:LEU:HD23	2:M:367:LEU:O	2.20	0.41
2:M:487:THR:HG23	2:M:490:GLU:HB2	1.96	0.41
2:M:571:LEU:HD22	2:M:700:TYR:HA	2.01	0.41
2:M:776:SER:O	5:P:405:LEU:HD21	2.21	0.41
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.85	0.41
3:N:564:GLU:O	3:N:565:ILE:C	2.63	0.41
3:N:794:GLN:HA	3:N:794:GLN:OE1	2.19	0.41
3:N:1439:SER:HB2	3:N:1463:LYS:HZ1	1.84	0.41
5:P:263:HIS:HA	5:P:266:GLU:HG2	2.01	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:289:THR:HG22	2:C:290:LEU:N	2.34	0.41
2:C:736:ASP:O	2:C:744:ARG:HG2	2.19	0.41
2:C:999:HIS:HB3	2:C:1004:LYS:CE	2.49	0.41
3:D:264:LEU:O	3:D:265:GLU:C	2.63	0.41
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.20	0.41
2:M:163:ILE:HA	2:M:164:PRO:HD2	1.93	0.41
3:N:468:LEU:HD23	3:N:468:LEU:HA	1.86	0.41
3:N:890:VAL:CG2	3:N:922:LEU:HD11	2.49	0.41
1:B:185:ARG:HA	1:B:189:ARG:O	2.21	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.89	0.41
2:C:1032:PHE:HZ	2:C:1040:LEU:HG	1.85	0.41
3:D:243:ALA:O	3:D:311:LEU:HD23	2.20	0.41
3:D:288:MET:CE	3:D:305:ALA:HB3	2.50	0.41
4:E:36:LYS:HE3	4:E:36:LYS:HB3	1.76	0.41
2:M:394:PHE:CE2	2:M:632:ASN:HB3	2.55	0.41
3:N:37:LEU:HD13	3:N:535:PHE:CE1	2.54	0.41
3:N:103:TRP:CZ2	3:N:1444:THR:HG22	2.55	0.41
3:N:116:LEU:HD21	3:N:465:LEU:HD23	2.02	0.41
3:N:785:ILE:HD13	3:N:935:LYS:HA	2.02	0.41
5:P:135:ILE:HD13	5:P:135:ILE:HA	1.96	0.41
5:P:408:LEU:O	5:P:408:LEU:HD23	2.20	0.41
6:Q:11:DT:H2"	6:Q:12:DG:C8	2.55	0.41
1:A:184:THR:CG2	1:A:192:LEU:CB	2.81	0.41
1:A:184:THR:CG2	1:A:192:LEU:HB2	2.45	0.41
2:C:918:LEU:HD23	2:C:918:LEU:HA	1.94	0.41
3:D:207:PHE:HB2	3:D:391:ALA:CB	2.51	0.41
3:D:472:ALA:O	3:D:476:GLU:HG3	2.19	0.41
3:D:849:ALA:O	3:D:852:ALA:HB3	2.21	0.41
3:D:959:GLU:OE1	3:D:959:GLU:N	2.44	0.41
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.20	0.41
5:F:256:ARG:NH2	5:F:311:ALA:O	2.53	0.41
1:K:44:LEU:HA	1:K:48:ILE:HG12	2.02	0.41
3:N:356:PRO:HB3	3:N:441:ARG:HA	2.02	0.41
3:N:410:SER:O	3:N:435:VAL:HG11	2.19	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.19	0.41
3:N:632:VAL:O	3:N:727:GLN:HA	2.20	0.41
3:N:792:ILE:HD13	3:N:941:PHE:CE1	2.56	0.41
3:N:823:LEU:CD1	3:N:837:GLY:CA	2.98	0.41
3:N:1045:MET:HE2	3:N:1073:SER:HA	2.03	0.41
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.90	0.41
5:P:384:GLU:HB3	5:P:394:ARG:CD	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:VAL:HG21	2:C:193:LEU:CB	2.27	0.41
2:C:864:GLY:O	2:C:866:PRO:HD3	2.20	0.41
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.36	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG13	2.02	0.41
3:D:1464:GLU:OE1	3:D:1464:GLU:N	2.36	0.41
5:F:264:MET:O	5:F:268:ILE:HG13	2.20	0.41
1:L:224:TYR:N	1:L:224:TYR:CD1	2.86	0.41
3:N:648:MET:HE2	3:N:648:MET:HB3	1.88	0.41
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	2.02	0.41
3:N:1238:MET:HG2	3:N:1359:GLN:OE1	2.21	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.41
1:A:206:THR:HG22	1:A:208:LEU:N	2.34	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.71	0.41
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.34	0.41
2:C:786:LYS:CB	2:C:786:LYS:HZ3	2.32	0.41
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.54	0.41
2:M:206:THR:C	2:M:209:ARG:HD2	2.45	0.41
2:M:223:ASP:O	2:M:227:PHE:CD2	2.73	0.41
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	2.03	0.41
3:N:275:GLU:HB3	3:N:276:ASP:H	1.60	0.41
3:N:984:THR:HG22	3:N:985:ASP:N	2.36	0.41
3:N:1353:GLN:HG2	3:N:1368:ILE:CD1	2.51	0.41
3:N:1495:ILE:HG21	4:O:80:VAL:CG2	2.51	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.92	0.41
1:B:124:ASN:HD22	1:B:127:LEU:HB2	1.86	0.41
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.55	0.41
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.54	0.41
3:D:567:ILE:CG2	3:D:571:LYS:HE3	2.50	0.41
3:D:586:ARG:HH12	6:G:10:DG:H5"	1.86	0.41
3:D:648:MET:O	3:D:652:LEU:HG	2.21	0.41
3:D:806:PHE:HB2	3:D:829:VAL:HG23	1.98	0.41
3:D:1011:PHE:HB3	3:D:1021:TYR:CG	2.55	0.41
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.20	0.41
5:F:195:VAL:HG13	5:F:216:GLY:HA3	2.01	0.41
2:M:569:VAL:HG21	2:M:1000:MET:HE1	2.03	0.41
2:M:976:ASP:OD2	2:M:978:ARG:NH1	2.54	0.41
3:N:107:ASP:O	3:N:108:VAL:C	2.63	0.41
3:N:132:TYR:HB2	3:N:153:LEU:CD1	2.50	0.41
3:N:232:GLU:O	3:N:232:GLU:HG2	2.21	0.41
3:N:553:ARG:HD2	3:N:570:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:939:PHE:O	3:N:942:SER:OG	2.23	0.41
3:N:1011:PHE:HB3	3:N:1021:TYR:CG	2.56	0.41
5:P:126:LEU:O	5:P:130:VAL:HG23	2.21	0.41
5:P:394:ARG:C	5:P:395:GLU:HG2	2.45	0.41
1:B:80:LEU:O	1:B:83:LYS:HB2	2.21	0.41
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.90	0.41
2:C:41:ASN:C	2:C:42:VAL:HG13	2.46	0.41
2:C:163:ILE:HG23	2:C:171:TRP:CD1	2.55	0.41
2:C:204:GLN:HB2	2:C:227:PHE:CD1	2.56	0.41
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.88	0.41
2:C:494:TYR:HD1	2:C:530:GLU:OE2	2.04	0.41
2:C:679:PHE:HA	3:D:943:THR:HB	2.03	0.41
2:C:786:LYS:NZ	2:C:786:LYS:HB3	2.33	0.41
2:C:998:TYR:O	2:C:998:TYR:CG	2.74	0.41
2:C:1105:LYS:O	2:C:1106:ASP:HB2	2.20	0.41
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.56	0.41
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.21	0.41
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.51	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
3:D:1468:LEU:HD22	3:D:1468:LEU:HA	1.79	0.41
5:F:259:ARG:CG	5:F:259:ARG:NH1	2.83	0.41
5:F:278:LEU:HD11	5:F:294:ALA:HB3	2.02	0.41
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.03	0.41
7:H:13:DT:H6	7:H:13:DT:H2'	1.70	0.41
1:K:57:TYR:CE1	1:K:161:ARG:HD2	2.55	0.41
2:M:230:ARG:HG3	2:M:232:GLU:H	1.86	0.41
2:M:561:GLY:O	2:M:565:GLN:HG3	2.21	0.41
2:M:763:GLY:O	2:M:764:GLU:C	2.64	0.41
2:M:944:LEU:HD22	2:M:962:GLN:HB3	2.03	0.41
2:M:1071:ILE:O	3:N:659:LYS:HD3	2.21	0.41
3:N:132:TYR:HE2	3:N:155:ASP:HB3	1.86	0.41
3:N:155:ASP:O	3:N:159:ARG:HG3	2.21	0.41
3:N:230:TRP:HA	3:N:243:ALA:CB	2.50	0.41
3:N:567:ILE:CG2	3:N:571:LYS:HE3	2.51	0.41
3:N:597:ASP:OD2	3:N:597:ASP:N	2.54	0.41
3:N:731:LEU:CD1	3:N:931:LEU:HB3	2.51	0.41
3:N:784:ASP:HB2	3:N:939:PHE:CE2	2.56	0.41
3:N:1290:LEU:CD2	3:N:1307:LYS:CE	2.85	0.41
5:P:101:GLU:O	5:P:105:LYS:HG3	2.21	0.41
5:P:120:THR:HG22	5:P:122:LEU:HD13	2.02	0.41
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:VAL:HA	2:C:229:MET:HG3	2.03	0.41
2:C:229:MET:HB3	2:C:233:GLU:CB	2.47	0.41
2:C:375:SER:O	2:C:378:LEU:N	2.53	0.41
2:C:682:TYR:CD1	3:D:635:PRO:HG2	2.56	0.41
2:C:879:ARG:N	2:C:879:ARG:HD2	2.35	0.41
3:D:215:TYR:CE1	3:D:380:GLU:O	2.74	0.41
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.03	0.41
3:D:1060:SER:OG	3:D:1063:GLU:HG3	2.21	0.41
2:M:258:TYR:CD2	2:M:262:ALA:HB3	2.56	0.41
2:M:767:PRO:O	2:M:768:THR:C	2.64	0.41
2:M:1105:LYS:O	2:M:1106:ASP:HB2	2.20	0.41
5:P:195:VAL:HG13	5:P:216:GLY:HA3	2.02	0.41
5:P:369:LEU:HD12	5:P:401:GLU:HB2	2.03	0.41
1:B:184:THR:O	1:B:192:LEU:HB2	2.21	0.40
2:C:229:MET:O	2:C:233:GLU:HB2	2.21	0.40
2:C:1027:PHE:CD2	2:C:1027:PHE:O	2.74	0.40
3:D:134:VAL:HG22	3:D:151:GLN:O	2.21	0.40
3:D:632:VAL:O	3:D:727:GLN:HA	2.21	0.40
3:D:1045:MET:HE2	3:D:1073:SER:HA	2.04	0.40
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.35	0.40
5:F:324:GLU:HB2	5:F:326:ASP:OD1	2.21	0.40
1:L:80:LEU:O	1:L:83:LYS:HB2	2.22	0.40
3:N:659:LYS:HZ1	3:N:663:GLU:HG2	1.87	0.40
3:N:1100:ASP:OD2	3:N:1440:PHE:HB2	2.21	0.40
3:N:1310:ARG:CG	3:N:1327:ARG:NH1	2.84	0.40
2:C:229:MET:HE1	2:C:234:ALA:HA	2.00	0.40
2:C:501:THR:HG21	2:C:513:VAL:HB	2.03	0.40
3:D:106:LYS:HE3	3:D:587:ARG:HG3	2.03	0.40
3:D:486:ARG:H	3:D:486:ARG:HG3	1.58	0.40
3:D:634:GLY:O	3:D:637:LEU:HG	2.21	0.40
3:D:771:SER:O	3:D:775:GLY:HA2	2.21	0.40
4:E:61:VAL:O	4:E:65:MET:HG3	2.21	0.40
4:E:70:THR:CB	4:E:72:ARG:HG3	2.52	0.40
5:F:281:GLU:CG	5:F:282:LEU:CD2	2.86	0.40
1:L:94:LEU:HD21	1:L:97:VAL:CG2	2.51	0.40
2:M:395:LYS:HE2	2:M:403:SER:CB	2.51	0.40
2:M:474:VAL:HG22	2:M:479:VAL:HG22	2.03	0.40
2:M:707:ARG:NE	2:M:824:ARG:HD3	2.37	0.40
2:M:729:LEU:HD23	2:M:729:LEU:HA	1.91	0.40
2:M:1053:LEU:CD1	3:N:1466:VAL:HG13	2.51	0.40
3:N:138:LYS:CB	3:N:451:ASP:O	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.57	0.40
3:N:547:LEU:O	3:N:548:ILE:C	2.63	0.40
3:N:637:LEU:HD22	3:N:642:CYS:HA	2.03	0.40
3:N:1289:LYS:O	3:N:1290:LEU:HD23	2.20	0.40
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.78	0.40
5:P:325:LYS:HE2	5:P:325:LYS:HB2	1.80	0.40
5:P:396:ARG:C	5:P:396:ARG:HD3	2.46	0.40
1:A:39:PRO:O	1:A:43:ILE:HG13	2.22	0.40
2:C:626:ARG:HG3	2:C:629:TYR:CG	2.56	0.40
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.56	0.40
2:C:830:LYS:HB3	2:C:830:LYS:HE2	1.89	0.40
3:D:47:GLU:CD	3:D:53:ILE:HG12	2.46	0.40
3:D:132:TYR:HB2	3:D:153:LEU:CD1	2.51	0.40
3:D:293:VAL:O	3:D:294:HIS:C	2.65	0.40
3:D:547:LEU:O	3:D:548:ILE:C	2.64	0.40
3:D:900:ILE:H	3:D:900:ILE:HG13	1.62	0.40
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	2.03	0.40
3:D:1341:PRO:O	3:D:1342:GLU:C	2.63	0.40
1:K:23:PHE:HE1	1:K:208:LEU:HD12	1.85	0.40
2:M:557:ARG:HG3	2:M:844:GLY:HA3	2.02	0.40
2:M:864:GLY:O	2:M:866:PRO:HD3	2.20	0.40
2:M:899:GLN:HE21	2:M:901:TYR:HE2	1.67	0.40
2:M:1012:PRO:HB2	2:M:1021:LEU:HD12	2.03	0.40
3:N:121:THR:O	3:N:124:GLU:HB3	2.21	0.40
3:N:527:MET:HE2	3:N:527:MET:HB2	1.98	0.40
3:N:622:ARG:NH1	6:Q:17:DG:OP1	2.43	0.40
3:N:801:GLY:O	3:N:804:LEU:HG	2.21	0.40
3:N:1130:ARG:C	3:N:1130:ARG:HD3	2.46	0.40
3:N:1258:ARG:NH2	3:N:1262:LEU:HD21	2.36	0.40
1:A:97:VAL:HG12	1:A:98:THR:N	2.36	0.40
2:C:223:ASP:O	2:C:227:PHE:CD2	2.73	0.40
2:C:717:LEU:N	2:C:717:LEU:CD1	2.84	0.40
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.57	0.40
3:D:208:PRO:HA	3:D:389:GLU:O	2.22	0.40
4:E:14:ASP:CG	4:E:18:ARG:HH11	2.29	0.40
5:F:260:ILE:HG23	5:F:261:PRO:HD2	2.03	0.40
1:L:184:THR:O	1:L:192:LEU:HB2	2.22	0.40
1:L:185:ARG:HA	1:L:189:ARG:O	2.21	0.40
1:L:205:VAL:HG12	1:L:206:THR:H	1.86	0.40
2:M:385:PHE:O	2:M:389:SER:HB3	2.21	0.40
2:M:988:VAL:HG21	3:N:949:ILE:C	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:252:ARG:HD3	3:N:301:GLY:O	2.21	0.40
3:N:832:ARG:HD2	3:N:833:GLU:N	2.37	0.40
3:N:899:LEU:HD22	3:N:917:GLN:HB3	2.02	0.40
3:N:1102:THR:CG2	3:N:1371:VAL:HG22	2.52	0.40
3:N:1293:PHE:CE2	3:N:1302:GLU:HG3	2.54	0.40
5:P:101:GLU:HG3	5:P:105:LYS:HE2	2.02	0.40
5:P:398:ARG:C	5:P:401:GLU:HG2	2.46	0.40
7:R:18:DC:H2'	7:R:19:DG:C8	2.57	0.40
1:A:73:GLU:OE1	1:A:73:GLU:N	2.54	0.40
2:C:103:LYS:H	2:C:103:LYS:HG3	1.55	0.40
2:C:176:VAL:O	2:C:181:VAL:O	2.39	0.40
2:C:758:ARG:N	2:C:789:SER:HB3	2.36	0.40
2:C:1071:ILE:CG2	3:D:670:VAL:HG21	2.52	0.40
3:D:285:PRO:HG2	3:D:311:LEU:HD12	2.04	0.40
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.03	0.40
1:K:97:VAL:HG12	1:K:98:THR:N	2.35	0.40
2:M:328:LEU:HD12	2:M:433:THR:O	2.22	0.40
2:M:719:PRO:HD2	2:M:761:PHE:CE1	2.57	0.40
3:N:39:PRO:HB3	3:N:45:PHE:O	2.22	0.40
3:N:223:LEU:HD21	3:N:225:LEU:HD21	2.03	0.40
3:N:245:LEU:HD12	3:N:245:LEU:N	2.35	0.40
3:N:512:MET:C	3:N:513:ILE:HD12	2.47	0.40
3:N:1258:ARG:HH21	3:N:1351:GLU:HG3	1.86	0.40
3:N:1406:ARG:HB3	3:N:1406:ARG:NH2	2.36	0.40
4:O:67:GLU:O	4:O:70:THR:OG1	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1314:LYS:NZ	2:M:784:ASP:OD2[1_445]	1.83	0.37
2:M:40:GLU:OE1	5:P:364:ARG:NH1[1_545]	2.03	0.17

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	218 (97%)	5 (2%)	1 (0%)	30	65
1	B	220/315 (70%)	212 (96%)	6 (3%)	2 (1%)	14	48
1	K	224/315 (71%)	218 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	213 (96%)	8 (4%)	2 (1%)	14	48
2	C	1107/1119 (99%)	1066 (96%)	37 (3%)	4 (0%)	30	65
2	M	1107/1119 (99%)	1063 (96%)	39 (4%)	5 (0%)	24	60
3	D	1478/1524 (97%)	1423 (96%)	53 (4%)	2 (0%)	48	80
3	N	1485/1524 (97%)	1423 (96%)	57 (4%)	5 (0%)	36	70
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	335 (97%)	9 (3%)	0	100	100
5	P	345/443 (78%)	329 (95%)	12 (4%)	4 (1%)	10	40
All	All	6941/7630 (91%)	6677 (96%)	239 (3%)	25 (0%)	30	65

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	325	ILE
5	P	78	SER
5	P	417	LYS
3	D	1310	ARG
3	N	1310	ARG
5	P	392	VAL
3	N	1237	THR
5	P	79	ASP
1	A	60	ASP
1	B	59	GLU
1	B	118	ALA
2	C	429	ASP
1	L	118	ALA
2	M	230	ARG
2	C	230	ARG
2	M	249	LYS
3	N	1137	ARG
3	N	1306	PRO

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Mol	Chain	Res	Type
1	L	59	GLU
2	C	177	GLU
2	M	170	PRO
3	D	530	VAL
3	N	530	VAL
2	M	177	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	185 (93%)	14 (7%)	14	44
1	B	195/273 (71%)	178 (91%)	17 (9%)	9	35
1	K	199/273 (73%)	184 (92%)	15 (8%)	12	41
1	L	198/273 (72%)	182 (92%)	16 (8%)	11	38
2	C	936/941 (100%)	873 (93%)	63 (7%)	15	46
2	M	936/941 (100%)	864 (92%)	72 (8%)	12	40
3	D	1250/1279 (98%)	1137 (91%)	113 (9%)	9	34
3	N	1253/1279 (98%)	1150 (92%)	103 (8%)	10	37
4	E	83/88 (94%)	80 (96%)	3 (4%)	31	65
4	O	83/88 (94%)	80 (96%)	3 (4%)	31	65
5	F	301/388 (78%)	281 (93%)	20 (7%)	15	46
5	P	302/388 (78%)	273 (90%)	29 (10%)	8	31
All	All	5935/6484 (92%)	5467 (92%)	468 (8%)	11	39

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	58	ILE
1	A	76	VAL

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Mol	Chain	Res	Type
1	A	80	LEU
1	A	86	VAL
1	A	87	VAL
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	192	LEU
1	A	198	ARG
1	A	205	VAL
1	A	215	VAL
1	B	48	ILE
1	B	51	THR
1	B	54	THR
1	B	61	VAL
1	B	63	HIS
1	B	66	SER
1	B	73	GLU
1	B	94	LEU
1	B	96	THR
1	B	158	ILE
1	B	165	ILE
1	B	184	THR
1	B	192	LEU
1	B	197	LEU
1	B	205	VAL
1	B	206	THR
1	B	215	VAL
2	C	11	GLU
2	C	23	VAL
2	C	44	ILE
2	C	85	GLU
2	C	103	LYS
2	C	105	THR
2	C	107	LEU
2	C	108	ILE
2	C	149	THR
2	C	154	ARG
2	C	157	ARG
2	C	168	ARG
2	C	176	VAL
2	C	177	GLU
2	C	182	VAL

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Mol	Chain	Res	Type
2	C	194	VAL
2	C	196	LEU
2	C	216	GLU
2	C	218	VAL
2	C	221	LEU
2	C	223	ASP
2	C	224	GLU
2	C	229	MET
2	C	232	GLU
2	C	233	GLU
2	C	251	ASP
2	C	276	LYS
2	C	325	ILE
2	C	353	ARG
2	C	361	MET
2	C	372	LEU
2	C	402	SER
2	C	421	GLU
2	C	427	VAL
2	C	454	SER
2	C	527	GLU
2	C	569	VAL
2	C	575	GLN
2	C	584	GLU
2	C	617	ASP
2	C	633	GLN
2	C	640	ARG
2	C	650	ARG
2	C	670	GLN
2	C	690	ILE
2	C	695	LEU
2	C	717	LEU
2	C	768	THR
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	789	SER
2	C	807	ARG
2	C	813	VAL
2	C	815	LEU
2	C	845	ASN
2	C	848	VAL

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Mol	Chain	Res	Type
2	C	930	LYS
2	C	939	ARG
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1080	SER
3	D	10	ILE
3	D	36	THR
3	D	38	LYS
3	D	40	GLU
3	D	54	LYS
3	D	67	ARG
3	D	68	PHE
3	D	69	GLU
3	D	78	VAL
3	D	81	THR
3	D	106	LYS
3	D	141	ILE
3	D	153	LEU
3	D	154	THR
3	D	184	GLU
3	D	191	LEU
3	D	199	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	265	GLU
3	D	270	LEU
3	D	273	ARG
3	D	274	ARG
3	D	275	GLU
3	D	299	GLU
3	D	335	LEU
3	D	354	VAL
3	D	372	ASP
3	D	374	GLU
3	D	387	LEU
3	D	411	THR
3	D	415	VAL
3	D	447	VAL
3	D	486	ARG
3	D	488	ARG

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Mol	Chain	Res	Type
3	D	508	ARG
3	D	525	ARG
3	D	534	ARG
3	D	586	ARG
3	D	591	VAL
3	D	596	SER
3	D	600	LEU
3	D	618	LEU
3	D	623	VAL
3	D	637	LEU
3	D	640	HIS
3	D	650	LEU
3	D	694	VAL
3	D	709	HIS
3	D	744	GLN
3	D	754	PHE
3	D	785	ILE
3	D	820	GLU
3	D	829	VAL
3	D	832	ARG
3	D	833	GLU
3	D	858	VAL
3	D	894	LYS
3	D	922	LEU
3	D	924	MET
3	D	940	THR
3	D	943	THR
3	D	949	ILE
3	D	969	ARG
3	D	980	MET
3	D	1003	VAL
3	D	1041	LEU
3	D	1044	LEU
3	D	1067	VAL
3	D	1083	ASP
3	D	1100	ASP
3	D	1101	VAL
3	D	1118	ILE
3	D	1127	GLU
3	D	1128	VAL
3	D	1130	ARG
3	D	1132	LEU

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Mol	Chain	Res	Type
3	D	1133	ARG
3	D	1152	GLU
3	D	1188	VAL
3	D	1200	VAL
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1234	THR
3	D	1283	ILE
3	D	1284	GLU
3	D	1285	GLU
3	D	1287	GLU
3	D	1288	GLU
3	D	1289	LYS
3	D	1290	LEU
3	D	1305	LEU
3	D	1307	LYS
3	D	1308	GLU
3	D	1310	ARG
3	D	1311	LEU
3	D	1312	LEU
3	D	1317	ASP
3	D	1344	VAL
3	D	1373	ARG
3	D	1382	THR
3	D	1383	ASP
3	D	1389	LEU
3	D	1390	LEU
3	D	1393	GLN
3	D	1395	LEU
3	D	1400	VAL
3	D	1406	ARG
3	D	1456	LYS
3	D	1468	LEU
3	D	1481	VAL
4	E	50	THR
4	E	92	LEU
4	E	95	VAL
5	F	88	ILE
5	F	117	SER
5	F	125	ASP
5	F	135	ILE

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Mol	Chain	Res	Type
5	F	203	THR
5	F	205	ARG
5	F	218	GLN
5	F	226	LYS
5	F	230	LYS
5	F	259	ARG
5	F	262	VAL
5	F	281	GLU
5	F	287	THR
5	F	295	MET
5	F	310	ILE
5	F	315	VAL
5	F	325	LYS
5	F	376	ILE
5	F	377	ASP
5	F	393	THR
1	K	6	LEU
1	K	34	VAL
1	K	58	ILE
1	K	76	VAL
1	K	80	LEU
1	K	86	VAL
1	K	87	VAL
1	K	142	VAL
1	K	184	THR
1	K	185	ARG
1	K	186	LEU
1	K	188	GLN
1	K	192	LEU
1	K	205	VAL
1	K	215	VAL
1	L	5	LYS
1	L	48	ILE
1	L	51	THR
1	L	54	THR
1	L	62	LEU
1	L	73	GLU
1	L	94	LEU
1	L	96	THR
1	L	158	ILE
1	L	184	THR
1	L	192	LEU

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Mol	Chain	Res	Type
1	L	197	LEU
1	L	205	VAL
1	L	206	THR
1	L	215	VAL
1	L	223	THR
2	M	11	GLU
2	M	23	VAL
2	M	38	LYS
2	M	44	ILE
2	M	50	GLU
2	M	81	ASP
2	M	86	LYS
2	M	103	LYS
2	M	105	THR
2	M	107	LEU
2	M	149	THR
2	M	154	ARG
2	M	157	ARG
2	M	167	LYS
2	M	168	ARG
2	M	174	LEU
2	M	176	VAL
2	M	177	GLU
2	M	182	VAL
2	M	194	VAL
2	M	196	LEU
2	M	209	ARG
2	M	216	GLU
2	M	218	VAL
2	M	221	LEU
2	M	223	ASP
2	M	224	GLU
2	M	230	ARG
2	M	233	GLU
2	M	237	ARG
2	M	238	LEU
2	M	240	THR
2	M	276	LYS
2	M	292	ARG
2	M	297	GLU
2	M	299	LYS
2	M	325	ILE

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Mol	Chain	Res	Type
2	M	361	MET
2	M	372	LEU
2	M	421	GLU
2	M	427	VAL
2	M	454	SER
2	M	490	GLU
2	M	493	ARG
2	M	527	GLU
2	M	569	VAL
2	M	575	GLN
2	M	584	GLU
2	M	585	GLU
2	M	617	ASP
2	M	633	GLN
2	M	640	ARG
2	M	650	ARG
2	M	670	GLN
2	M	690	ILE
2	M	695	LEU
2	M	717	LEU
2	M	781	LYS
2	M	789	SER
2	M	807	ARG
2	M	813	VAL
2	M	815	LEU
2	M	816	LYS
2	M	845	ASN
2	M	848	VAL
2	M	905	ILE
2	M	930	LYS
2	M	939	ARG
2	M	968	LEU
2	M	978	ARG
2	M	1001	VAL
2	M	1080	SER
3	N	35	ARG
3	N	36	THR
3	N	37	LEU
3	N	48	ARG
3	N	54	LYS
3	N	106	LYS
3	N	107	ASP

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Mol	Chain	Res	Type
3	N	141	ILE
3	N	153	LEU
3	N	154	THR
3	N	184	GLU
3	N	191	LEU
3	N	199	LEU
3	N	211	VAL
3	N	225	LEU
3	N	264	LEU
3	N	266	GLU
3	N	270	LEU
3	N	275	GLU
3	N	277	GLU
3	N	279	VAL
3	N	286	VAL
3	N	298	VAL
3	N	306	GLU
3	N	311	LEU
3	N	354	VAL
3	N	387	LEU
3	N	411	THR
3	N	415	VAL
3	N	435	VAL
3	N	442	ASN
3	N	447	VAL
3	N	486	ARG
3	N	488	ARG
3	N	525	ARG
3	N	586	ARG
3	N	587	ARG
3	N	591	VAL
3	N	597	ASP
3	N	598	ARG
3	N	600	LEU
3	N	618	LEU
3	N	623	VAL
3	N	637	LEU
3	N	640	HIS
3	N	650	LEU
3	N	694	VAL
3	N	709	HIS
3	N	744	GLN

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Mol	Chain	Res	Type
3	N	754	PHE
3	N	820	GLU
3	N	827	ILE
3	N	832	ARG
3	N	833	GLU
3	N	834	THR
3	N	838	ARG
3	N	858	VAL
3	N	894	LYS
3	N	940	THR
3	N	943	THR
3	N	949	ILE
3	N	969	ARG
3	N	980	MET
3	N	1003	VAL
3	N	1020	LEU
3	N	1041	LEU
3	N	1044	LEU
3	N	1067	VAL
3	N	1083	ASP
3	N	1100	ASP
3	N	1124	GLN
3	N	1128	VAL
3	N	1129	THR
3	N	1130	ARG
3	N	1131	SER
3	N	1132	LEU
3	N	1159	ARG
3	N	1188	VAL
3	N	1200	VAL
3	N	1219	GLU
3	N	1234	THR
3	N	1238	MET
3	N	1282	ARG
3	N	1283	ILE
3	N	1284	GLU
3	N	1291	SER
3	N	1292	VAL
3	N	1305	LEU
3	N	1307	LYS
3	N	1308	GLU
3	N	1310	ARG

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Mol	Chain	Res	Type
3	N	1311	LEU
3	N	1312	LEU
3	N	1373	ARG
3	N	1382	THR
3	N	1383	ASP
3	N	1389	LEU
3	N	1390	LEU
3	N	1413	THR
3	N	1418	LYS
3	N	1459	LEU
3	N	1468	LEU
3	N	1481	VAL
4	O	50	THR
4	O	92	LEU
4	O	95	VAL
5	P	77	THR
5	P	82	ARG
5	P	88	ILE
5	P	97	GLU
5	P	193	ARG
5	P	198	ILE
5	P	205	ARG
5	P	222	ARG
5	P	232	ARG
5	P	244	ARG
5	P	258	ILE
5	P	267	THR
5	P	271	LEU
5	P	287	THR
5	P	295	MET
5	P	315	VAL
5	P	325	LYS
5	P	346	THR
5	P	361	LEU
5	P	362	SER
5	P	369	LEU
5	P	377	ASP
5	P	383	LEU
5	P	386	VAL
5	P	393	THR
5	P	414	ARG
5	P	416	ARG

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Mol	Chain	Res	Type
5	P	417	LYS
5	P	418	LEU

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

Mol	Chain	Res	Type
2	C	99	GLN
2	C	117	HIS
2	C	130	ASN
2	C	187	ASN
2	C	330	ASN
2	C	845	ASN
2	C	884	GLN
3	D	442	ASN
3	D	483	HIS
3	D	703	ASN
3	D	1172	HIS
5	F	170	HIS
5	F	263	HIS
5	F	280	GLN
1	L	128	HIS
1	L	221	HIS
2	M	99	GLN
2	M	117	HIS
2	M	130	ASN
2	M	187	ASN
2	M	330	ASN
2	M	845	ASN
2	M	860	HIS
2	M	884	GLN
3	N	316	GLN
3	N	483	HIS
3	N	611	GLN
3	N	703	ASN
3	N	744	GLN
3	N	1103	HIS
3	N	1195	GLN
3	N	1202	GLN
3	N	1227	GLN
3	N	1441	GLN
3	N	1442	ASN
5	P	263	HIS

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Mol	Chain	Res	Type
5	P	381	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	S	1/2 (50%)	0	0
All	All	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/315 (71%)	0.02	0 100 100	47, 67, 98, 118	0
1	B	222/315 (70%)	0.25	7 (3%) 50 29	50, 79, 119, 142	0
1	K	226/315 (71%)	0.14	1 (0%) 88 76	49, 73, 103, 122	0
1	L	225/315 (71%)	0.36	5 (2%) 62 39	51, 81, 126, 148	0
2	C	1111/1119 (99%)	0.07	22 (1%) 65 41	34, 62, 122, 168	0
2	M	1111/1119 (99%)	0.46	91 (8%) 17 9	38, 76, 142, 179	0
3	D	1482/1524 (97%)	0.11	40 (2%) 56 33	32, 66, 130, 178	1 (0%)
3	N	1489/1524 (97%)	0.15	30 (2%) 65 41	34, 69, 129, 201	1 (0%)
4	E	94/99 (94%)	0.21	1 (1%) 78 57	44, 66, 113, 121	0
4	O	94/99 (94%)	0.04	2 (2%) 63 40	49, 72, 116, 130	0
5	F	346/443 (78%)	0.20	10 (2%) 53 31	42, 70, 124, 147	0
5	P	347/443 (78%)	0.55	25 (7%) 21 11	46, 83, 156, 214	0
6	G	16/21 (76%)	-0.05	1 (6%) 26 13	42, 78, 172, 179	0
6	Q	16/21 (76%)	-0.02	1 (6%) 26 13	53, 80, 182, 183	0
7	H	24/27 (88%)	0.22	0 100 100	67, 95, 146, 201	0
7	R	24/27 (88%)	0.24	0 100 100	65, 106, 160, 210	0
8	I	2/2 (100%)	-0.82	0 100 100	50, 50, 50, 55	0
8	S	2/2 (100%)	-0.43	0 100 100	62, 62, 62, 63	0
All	All	7057/7730 (91%)	0.20	236 (3%) 49 28	32, 71, 132, 214	2 (0%)

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	391	GLY	5.1
2	M	191	PHE	5.0
3	N	1249	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	M	196	LEU	4.7
5	P	375	LEU	4.5
5	P	392	VAL	4.5
2	M	200	LEU	4.5
5	P	418	LEU	4.5
2	M	68	PHE	4.3
3	N	355	VAL	4.3
2	M	184	MET	4.2
5	P	388	ALA	4.2
2	M	477	GLY	4.2
2	C	361	MET	4.2
5	F	141	VAL	4.1
4	O	95	VAL	4.0
2	M	48	PHE	3.9
5	P	389	PHE	3.9
3	N	1498	ALA	3.9
3	N	1246	VAL	3.9
2	M	248	PRO	3.9
2	M	247	PRO	3.8
3	D	1498	ALA	3.8
2	M	188	LYS	3.8
3	N	1252	ILE	3.7
2	M	245	GLY	3.7
1	B	157	GLY	3.7
2	M	172	ILE	3.7
5	P	77	THR	3.7
3	N	1270	ALA	3.7
3	N	394	LEU	3.6
3	D	184	GLU	3.6
2	C	366	SER	3.6
5	P	141	VAL	3.6
2	M	236	ILE	3.6
3	D	1252	ILE	3.5
3	N	184	GLU	3.5
3	D	203	ALA	3.4
5	P	139	ALA	3.4
2	M	182	VAL	3.4
2	M	812	GLY	3.3
5	F	139	ALA	3.3
1	B	63	HIS	3.3
5	P	393	THR	3.2
2	M	29	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	M	199	VAL	3.2
2	M	47	ALA	3.2
2	M	102	HIS	3.2
2	M	44	ILE	3.2
2	M	41	ASN	3.2
2	M	367	LEU	3.1
2	M	52	PHE	3.1
3	D	412	GLY	3.1
2	M	155	PRO	3.1
2	M	778	PHE	3.1
2	M	476	GLY	3.1
2	C	828	ALA	3.1
2	M	488	ALA	3.1
2	M	594	ALA	3.1
2	M	257	VAL	3.1
2	M	170	PRO	3.1
2	M	194	VAL	3.0
3	D	175	VAL	3.0
5	P	138	SER	3.0
2	M	357	GLU	3.0
2	M	171	TRP	2.9
3	N	978	TYR	2.9
2	M	363	SER	2.9
2	M	65	VAL	2.9
2	M	101	ILE	2.9
5	P	383	LEU	2.9
3	N	1247	ALA	2.9
2	C	176	VAL	2.9
5	P	357	ALA	2.9
5	P	390	PHE	2.9
3	D	1491	THR	2.9
5	P	422	LEU	2.9
5	P	325	LYS	2.8
3	N	352	ASN	2.8
2	C	69	LEU	2.8
5	P	408	LEU	2.8
3	D	343	LYS	2.8
1	L	165	ILE	2.8
3	N	1250	ALA	2.8
2	M	311	PHE	2.8
2	M	153	ALA	2.7
2	M	66	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	361	MET	2.7
2	C	363	SER	2.7
2	M	593	ALA	2.7
2	C	171	TRP	2.7
5	P	423	ASP	2.7
2	M	45	GLN	2.7
3	N	108	VAL	2.7
2	M	767	PRO	2.6
6	Q	4	DG	2.6
3	D	335	LEU	2.6
5	P	400	ILE	2.6
1	B	190	THR	2.6
3	N	1409	ALA	2.6
2	M	49	ARG	2.6
2	C	170	PRO	2.6
2	C	637	LEU	2.6
3	D	207	PHE	2.6
2	C	517	ARG	2.6
2	M	103	LYS	2.6
3	N	279	VAL	2.6
3	D	991	GLN	2.6
5	F	325	LYS	2.5
2	M	354	GLY	2.5
2	M	261	ILE	2.5
2	M	244	PRO	2.5
5	F	151	LEU	2.5
2	M	30	LEU	2.5
5	P	361	LEU	2.5
2	M	156	GLY	2.5
3	D	595	GLY	2.5
3	D	213	VAL	2.5
2	M	240	THR	2.5
2	M	98	LEU	2.5
2	M	221	LEU	2.5
2	M	769	PRO	2.5
2	M	215	GLY	2.5
2	M	804	VAL	2.5
3	N	107	ASP	2.4
2	M	176	VAL	2.4
2	C	345	ARG	2.4
2	M	998	TYR	2.4
3	D	218	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	339	TRP	2.4
5	P	382	THR	2.4
2	M	475	VAL	2.4
3	D	532	GLY	2.4
2	C	97	ARG	2.4
6	G	19	DG	2.4
3	N	1291	SER	2.4
2	C	629	TYR	2.4
2	M	629	TYR	2.4
2	M	300	ASP	2.4
5	P	242	TRP	2.4
3	D	388	HIS	2.4
1	L	163	ASN	2.3
2	C	500	ASN	2.3
2	M	340	MET	2.3
2	M	265	ARG	2.3
3	N	586	ARG	2.3
2	M	741	GLY	2.3
1	L	162	ILE	2.3
2	M	168	ARG	2.3
2	M	250	ARG	2.3
3	N	434	ARG	2.3
1	L	37	GLY	2.3
2	M	252	LYS	2.3
2	M	181	VAL	2.3
5	F	389	PHE	2.3
2	M	764	GLU	2.3
1	B	160	ASP	2.3
2	M	351	LEU	2.3
1	B	162	ILE	2.3
3	D	1495	ILE	2.3
2	M	461	VAL	2.3
3	N	1281	VAL	2.3
1	K	111	ALA	2.2
3	N	232	GLU	2.2
2	M	717	LEU	2.2
3	D	1313	VAL	2.2
5	P	386	VAL	2.2
2	C	360	LEU	2.2
2	C	771	GLU	2.2
2	M	774	LEU	2.2
3	D	1492	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
5	F	422	LEU	2.2
3	D	974	ILE	2.2
5	P	397	ILE	2.2
3	D	212	ARG	2.2
3	D	999	THR	2.2
1	L	65	PHE	2.2
2	C	188	LYS	2.2
2	M	109	LYS	2.2
2	M	806	LEU	2.2
3	N	256	GLU	2.2
3	N	388	HIS	2.2
2	M	656	ALA	2.2
3	D	1063	GLU	2.2
5	F	395	GLU	2.2
3	N	809	PRO	2.2
1	B	66	SER	2.2
3	D	470	LEU	2.2
2	M	213	ALA	2.2
3	D	694	VAL	2.1
3	D	1306	PRO	2.1
3	N	1292	VAL	2.1
2	M	344	PHE	2.1
2	M	214	TYR	2.1
2	C	92	ALA	2.1
5	F	179	GLU	2.1
2	M	108	ILE	2.1
3	D	992	ILE	2.1
3	D	298	VAL	2.1
2	M	259	GLY	2.1
2	M	235	LEU	2.1
1	B	185	ARG	2.1
3	D	802	ALA	2.1
2	M	183	SER	2.1
3	D	1283	ILE	2.1
3	N	626	SER	2.1
3	D	1441	GLN	2.1
2	M	303	PHE	2.1
3	D	1129	THR	2.1
3	N	1052	THR	2.1
3	N	567	ILE	2.1
2	M	514	VAL	2.1
5	P	407	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	815	LEU	2.1
2	M	592	LEU	2.1
4	O	51	LEU	2.1
2	M	67	ASP	2.1
2	M	111	ASP	2.1
2	M	246	ASP	2.1
2	M	37	GLU	2.1
2	C	252	LYS	2.0
3	D	193	PRO	2.0
3	D	809	PRO	2.0
2	C	169	GLY	2.0
5	F	364	ARG	2.0
3	D	53	ILE	2.0
3	N	307	ALA	2.0
4	E	87	LYS	2.0
2	M	366	SER	2.0
3	D	350	HIS	2.0
3	N	440	VAL	2.0
3	D	995	LEU	2.0
2	C	424	GLY	2.0
5	F	397	ILE	2.0
3	D	322	VAL	2.0
3	D	1128	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	K	1001	1/1	0.76	0.35	69,69,69,69	0
10	MG	N	2004	1/1	0.79	0.31	65,65,65,65	0
10	MG	D	2004	1/1	0.84	0.29	63,63,63,63	0
10	MG	N	2003	1/1	0.93	0.08	46,46,46,46	0
10	MG	D	2003	1/1	0.93	0.08	40,40,40,40	0
9	ZN	N	2002	1/1	0.99	0.03	107,107,107,107	0
9	ZN	D	2001	1/1	0.99	0.01	62,62,62,62	0
9	ZN	D	2002	1/1	0.99	0.02	83,83,83,83	0
9	ZN	N	2001	1/1	1.00	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.