Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 PM GMT

PDB ID	:	4G7O
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

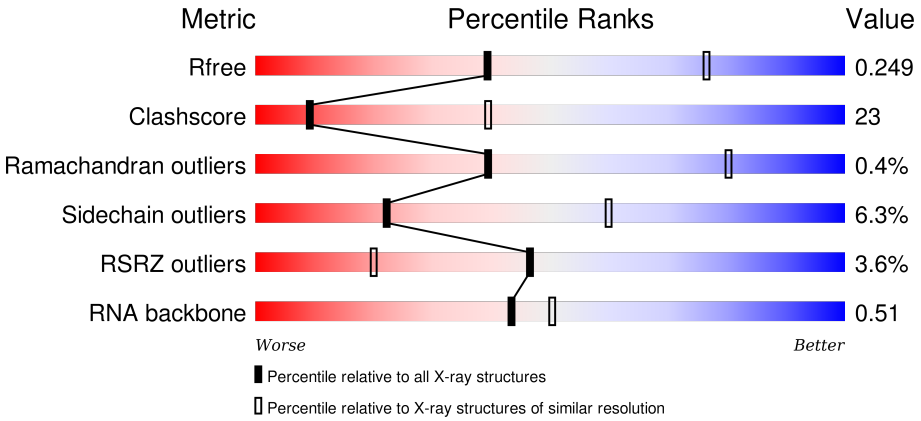
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	44% 26% • 28%
1	B	315	% 41% 26% • 30%
1	K	315	48% 23% • 28%
1	L	315	% 43% 26% • 29%

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Mol	Chain	Length	Quality of chain
2	C	1119	3% 59% 38%
2	M	1119	8% 56% 40%
3	D	1524	3% 59% 34%
3	N	1524	4% 56% 38%
4	E	99	3% 68% 25% 5%
4	O	99	3% 71% 23% 5%
5	F	443	% 51% 25% 22%
5	P	443	4% 46% 28% 22%
6	G	21	48% 19% 10% 24%
6	Q	21	33% 43% 24%
7	H	27	52% 33% 11%
7	R	27	52% 37% 11%
8	I	2	100%
8	S	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MG	D	2004	-	-	-	X
10	MG	K	1001	-	-	-	X
10	MG	N	2004	-	-	-	X

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*CP*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 (three-letter code: 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 (three-letter code: 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.

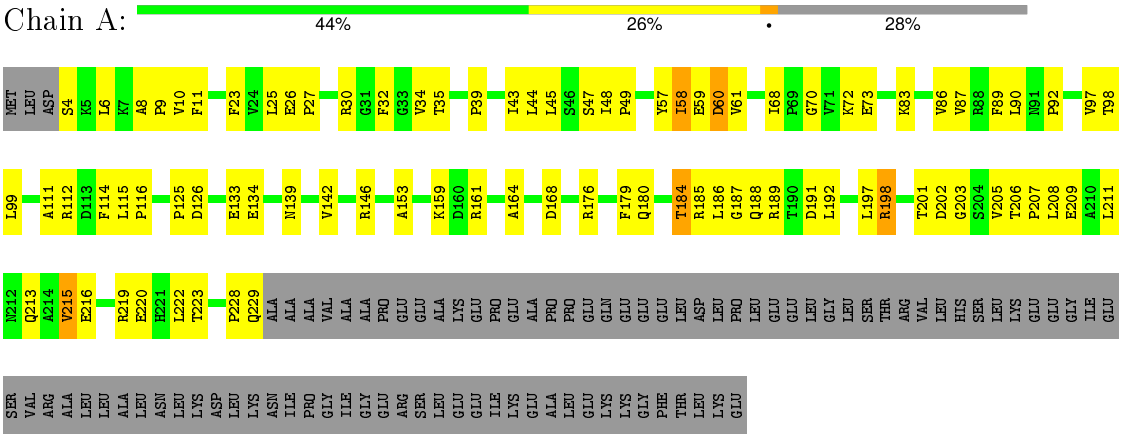
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	14	Total O 14 14	0	0
11	B	3	Total O 3 3	0	0
11	C	53	Total O 53 53	0	0
11	D	58	Total O 58 58	0	0
11	E	8	Total O 8 8	0	0
11	F	10	Total O 10 10	0	0
11	G	5	Total O 5 5	0	0
11	H	2	Total O 2 2	0	0
11	K	4	Total O 4 4	0	0
11	L	3	Total O 3 3	0	0
11	M	33	Total O 33 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

3 Residue-property plots (i)

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

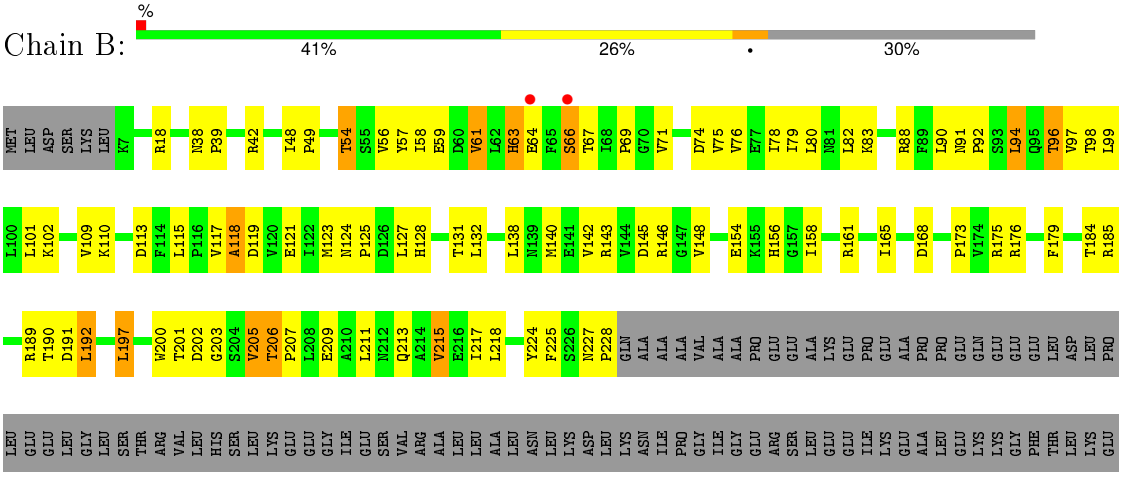
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



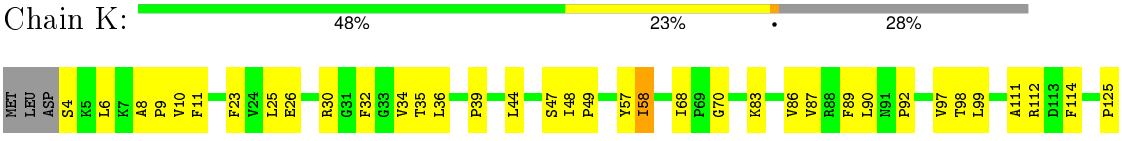
- Molecule 1: DNA-directed RNA polymerase subunit alpha

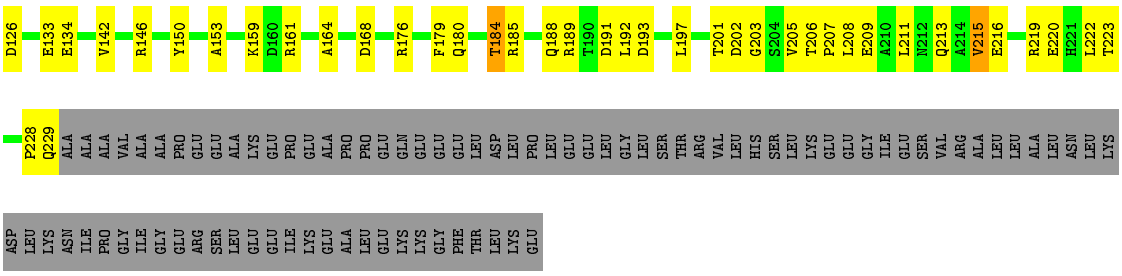
Chain B:



- Molecule 1: DNA-directed RNA polymerase subunit alpha

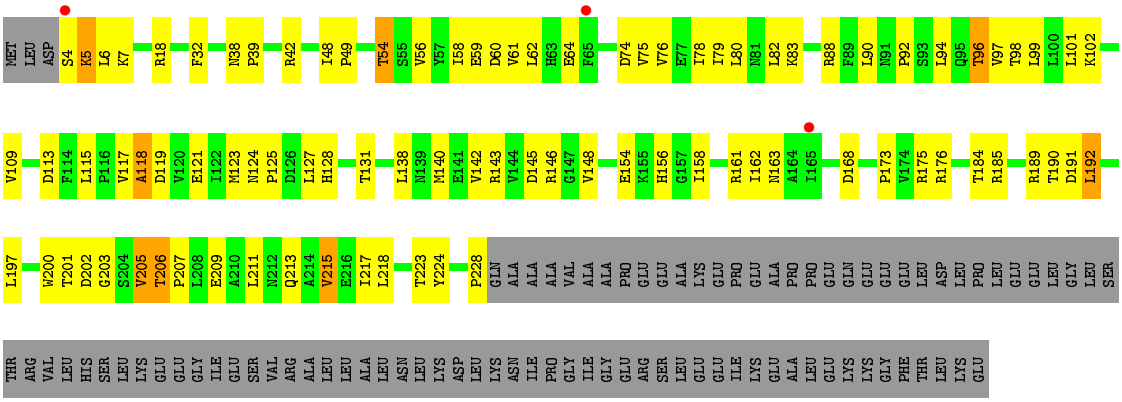
Chain K:





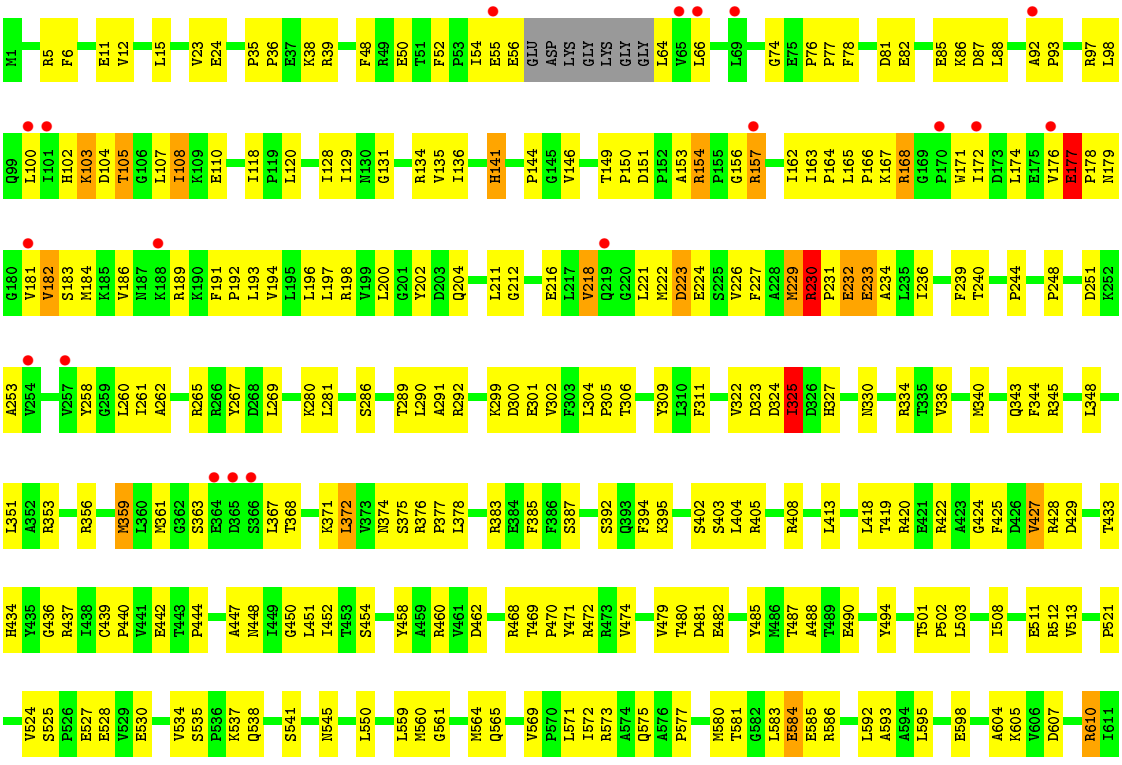
• Molecule 1: DNA-directed RNA polymerase subunit alpha

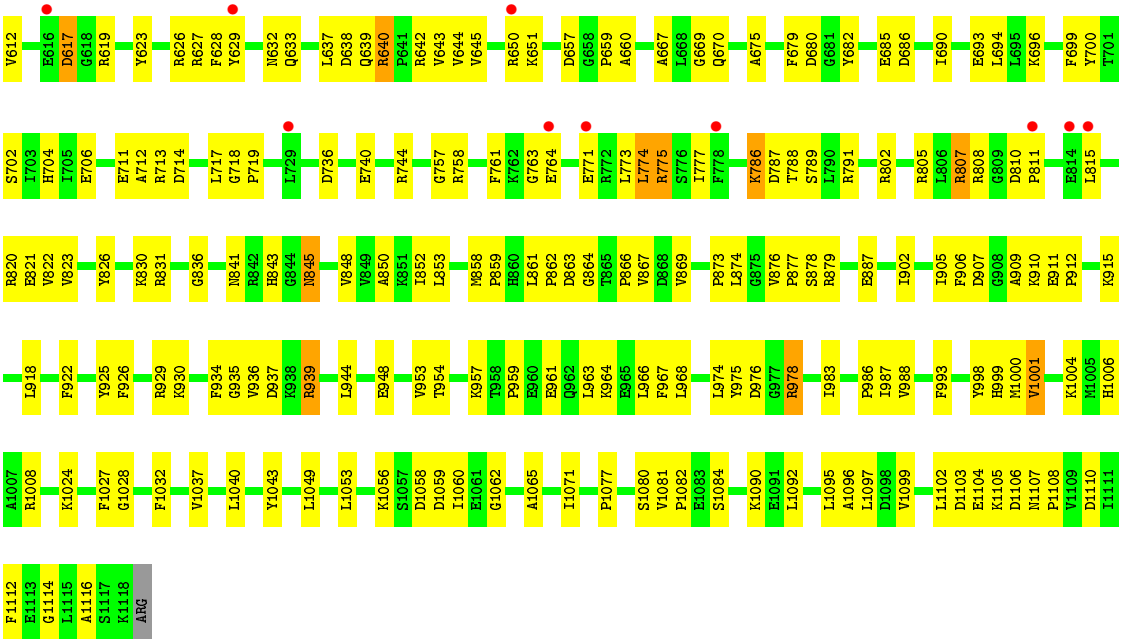
Chain L:



• Molecule 2: DNA-directed RNA polymerase subunit beta

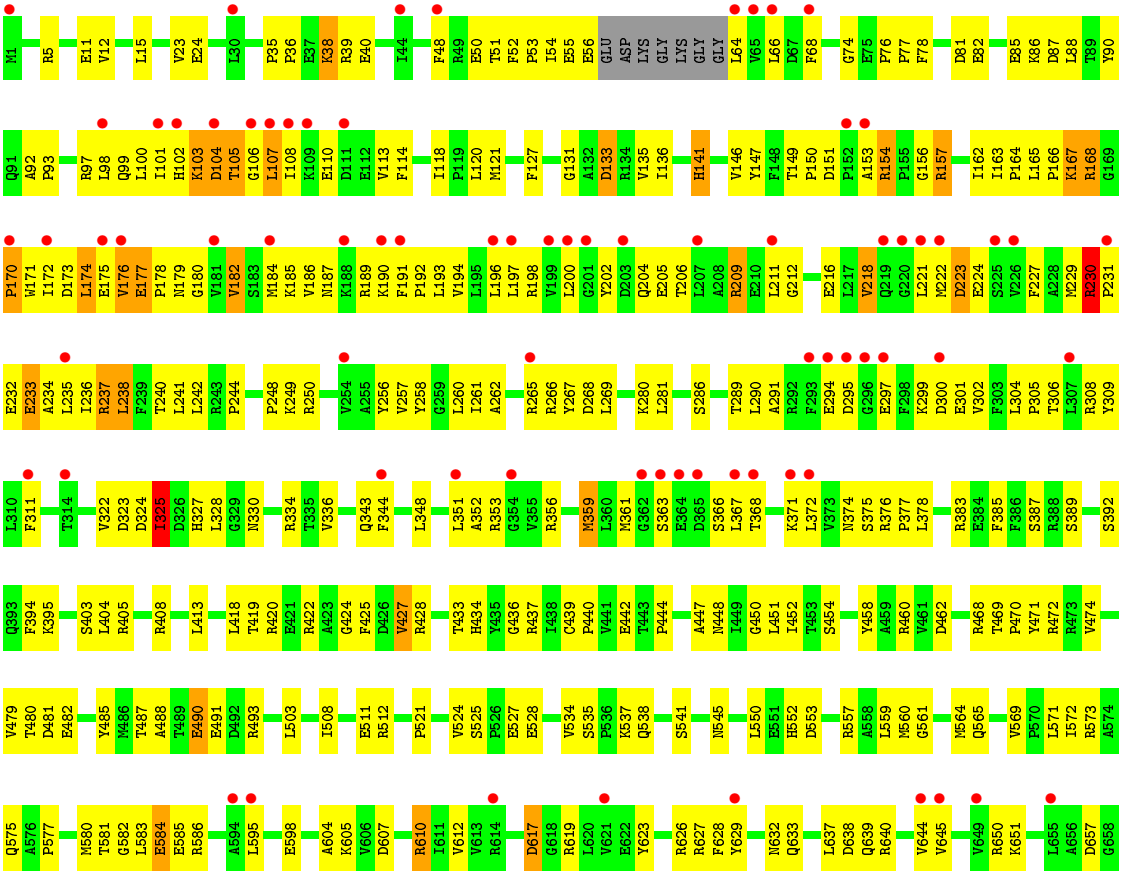
Chain C:

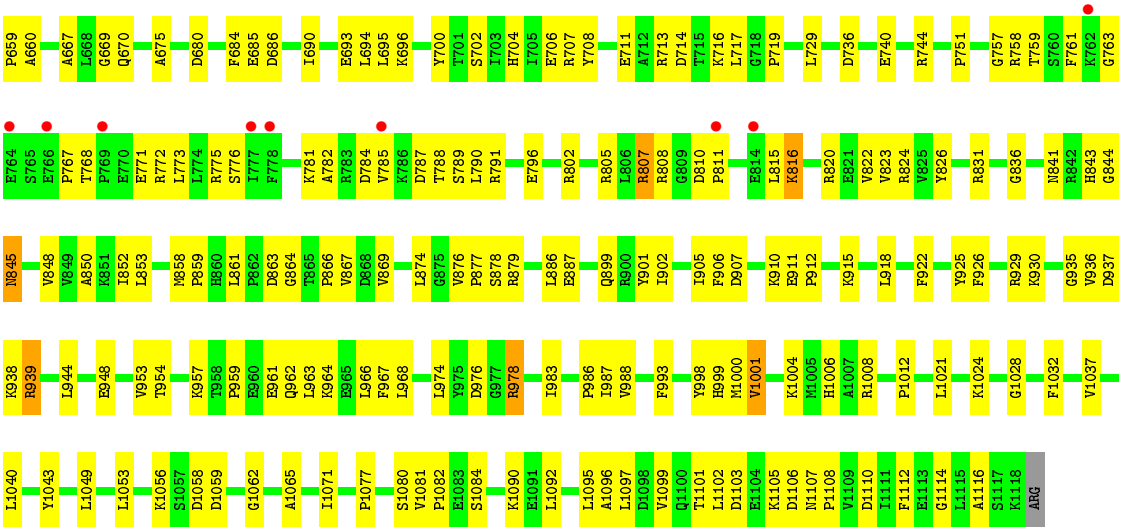




• Molecule 2: DNA-directed RNA polymerase subunit beta

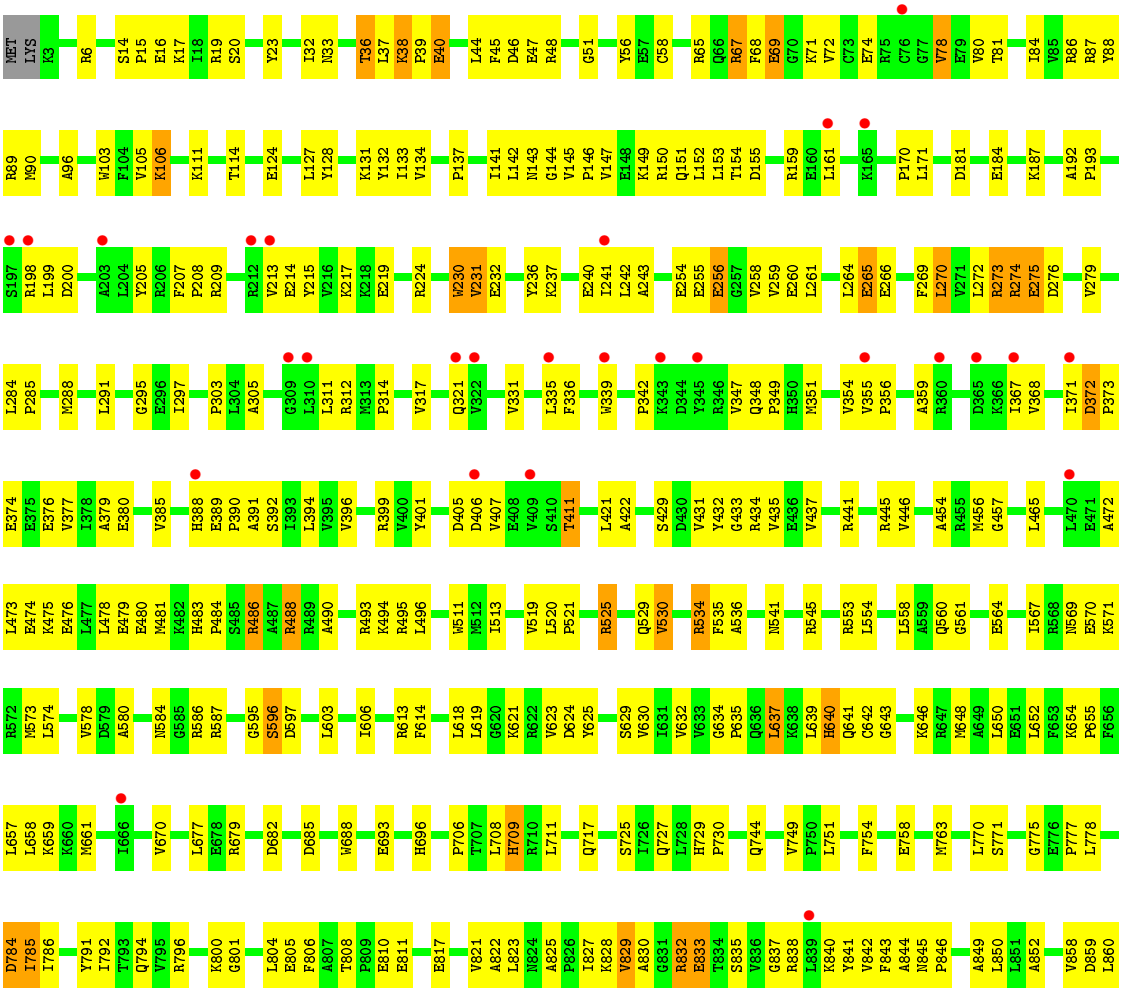
Chain M:

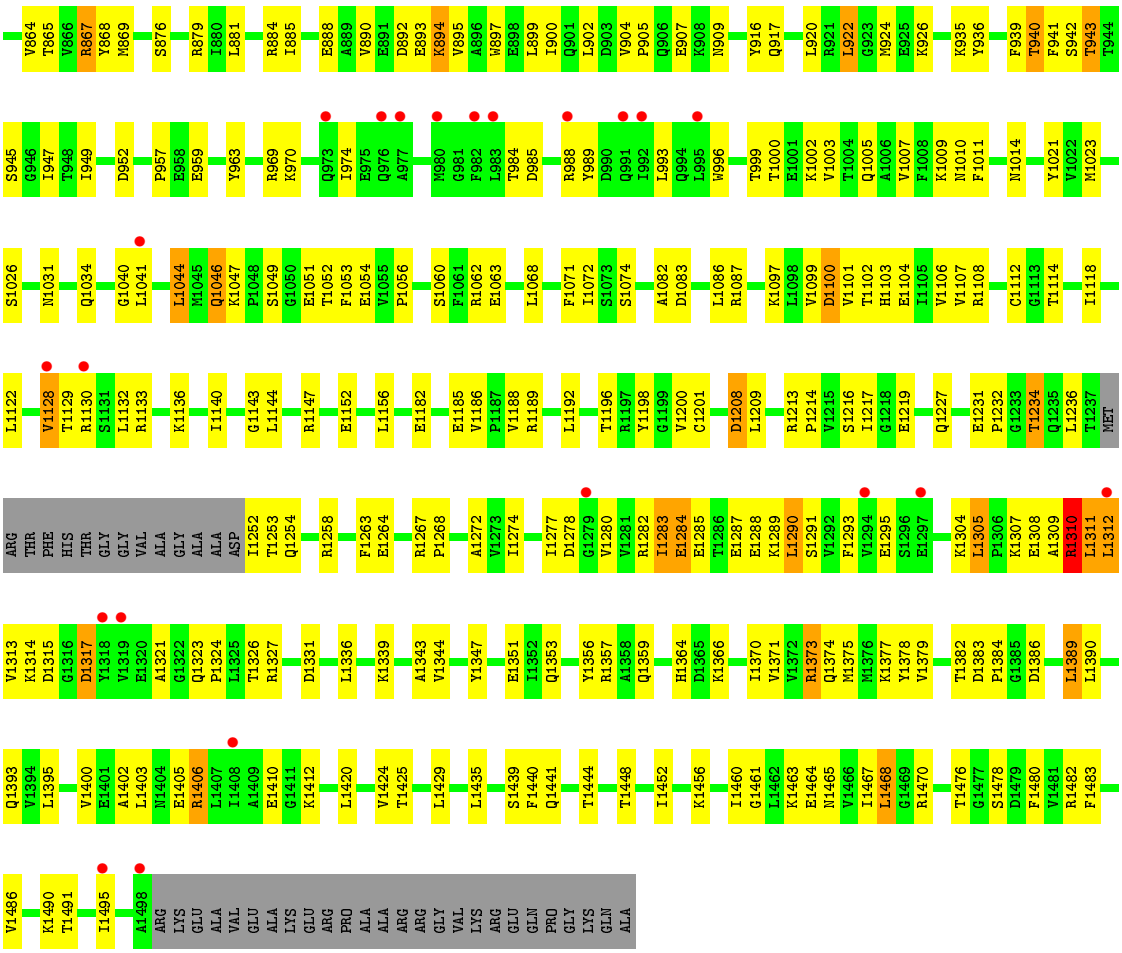




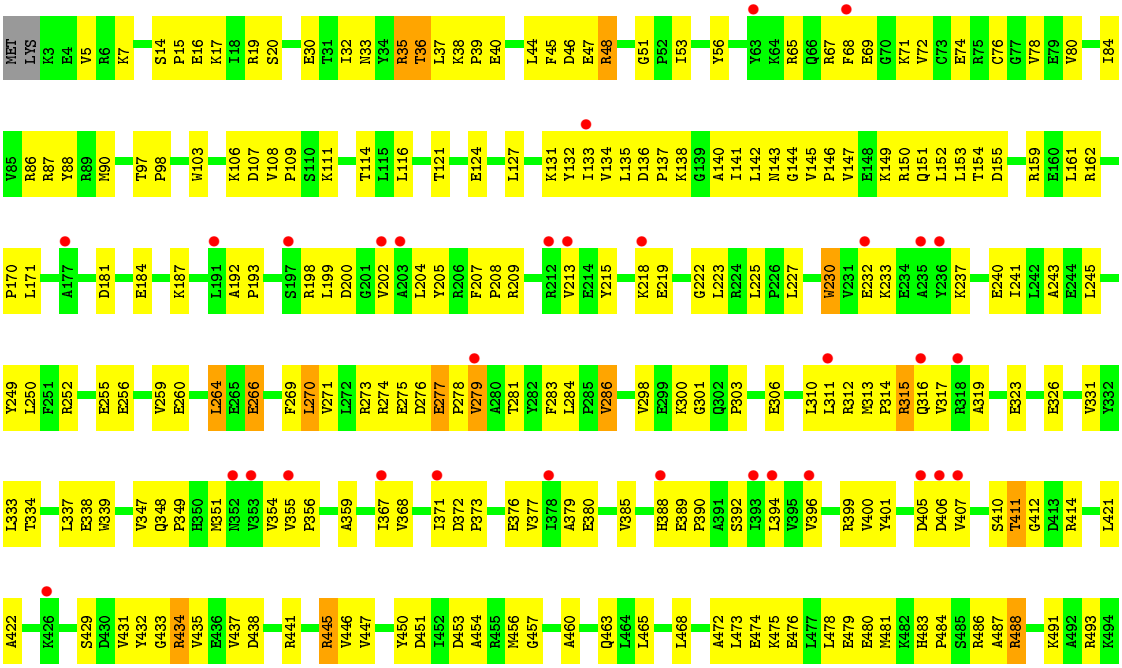
- Molecule 3: DNA-directed RNA polymerase subunit beta'

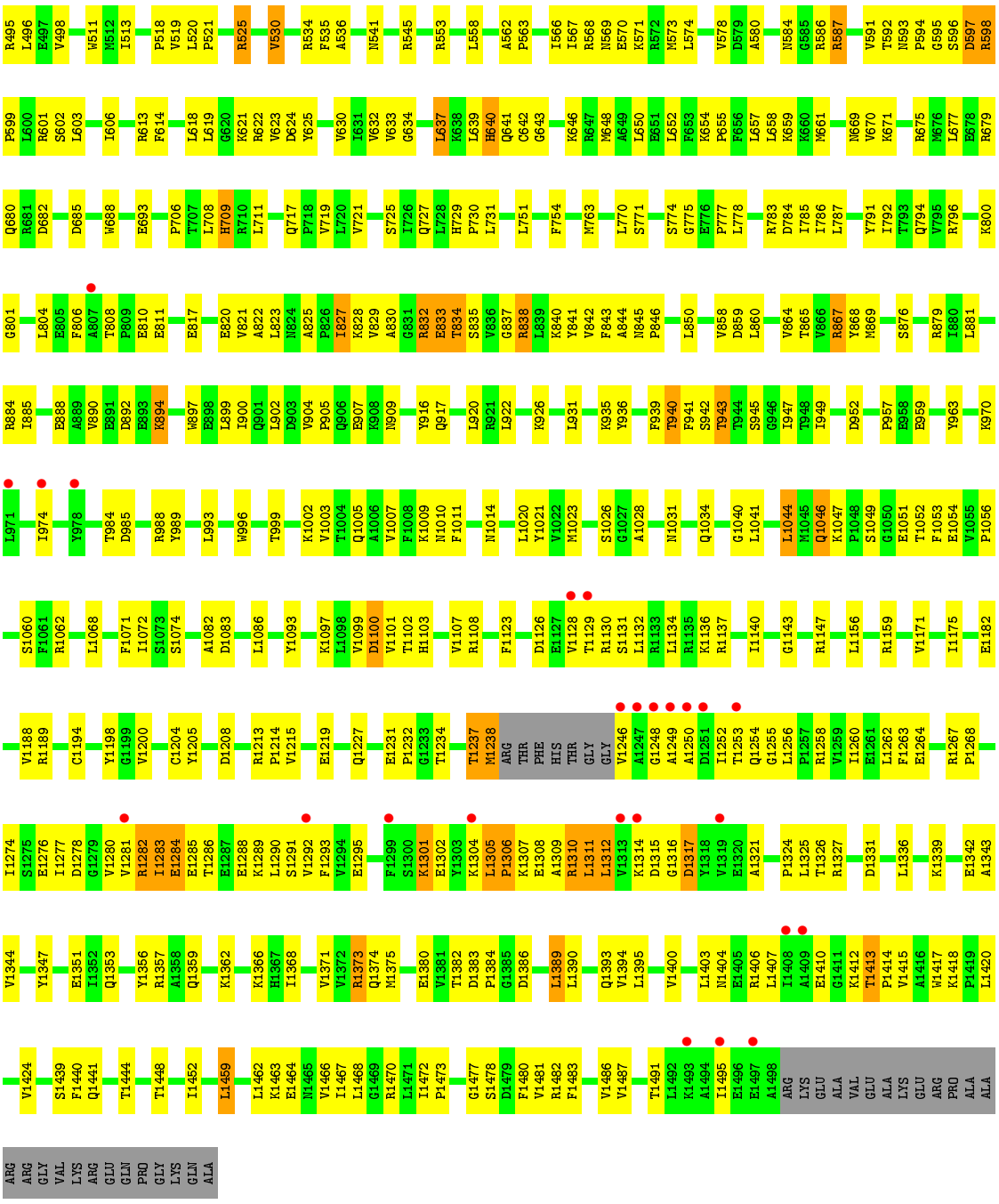
Chain D:



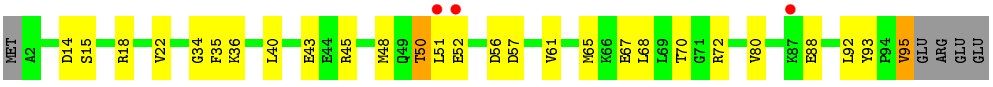


• Molecule 3: DNA-directed RNA polymerase subunit beta'

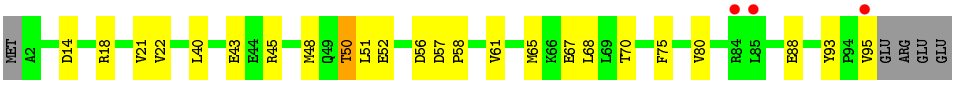




• Molecule 4: DNA-directed RNA polymerase subunit omega

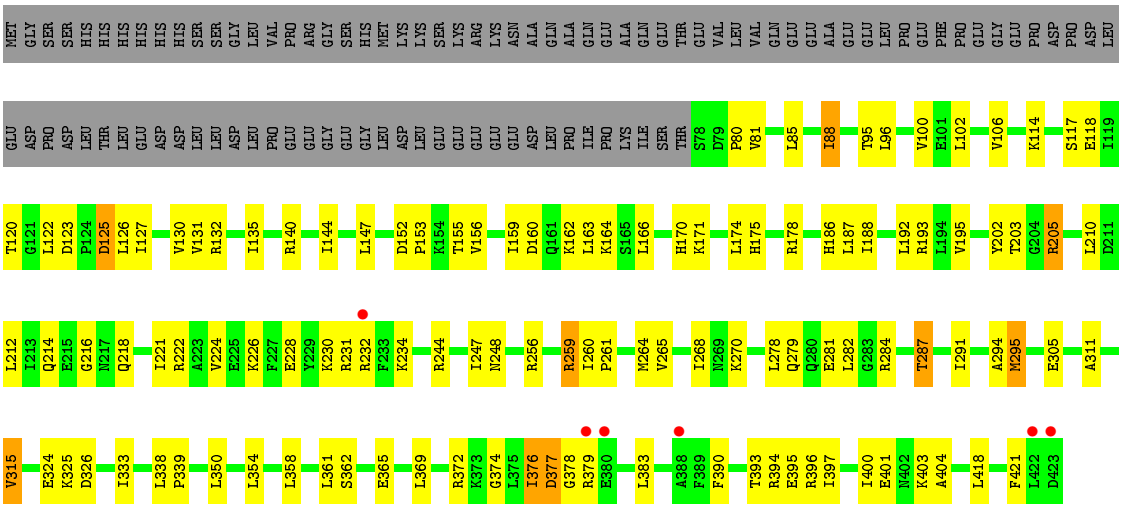


• Molecule 4: DNA-directed RNA polymerase subunit omega



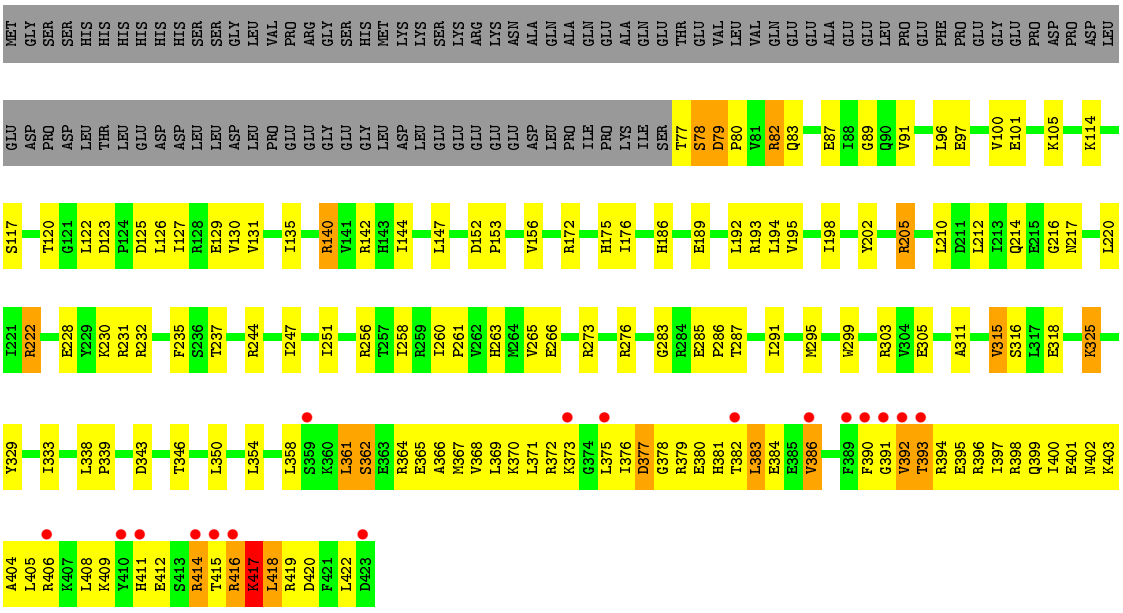
• Molecule 5: RNA polymerase sigma factor

Chain F:



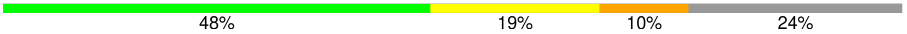
• Molecule 5: RNA polymerase sigma factor

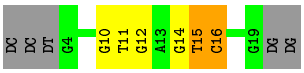
Chain P:



• 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'

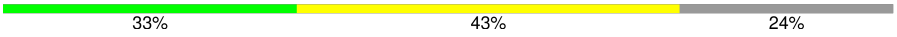
Chain G:





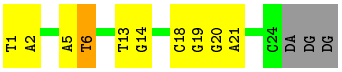
• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

Chain Q:



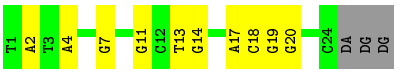
• Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H:



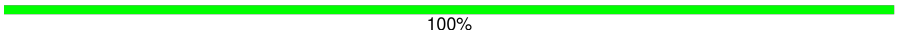
• Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain R:



• Molecule 8: 5'-R(*GP*A)-3'

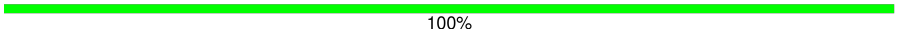
Chain I:



There are no outlier residues recorded for this chain.

• Molecule 8: 5'-R(*GP*A)-3'

Chain S:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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 49.59 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.61-2.99) 95.5 (49.59-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.205 , 0.247 0.205 , 0.249	Depositor DCC
R_{free} test set	1903 reflections (0.88%)	DCC
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 , 42.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	6 of 221179 reflections (0.003%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.29	0/1814	0.50	0/2466
1	B	0.27	0/1782	0.49	0/2424
1	K	0.27	0/1814	0.49	0/2466
1	L	0.28	0/1805	0.51	0/2454
2	C	0.30	0/8937	0.49	0/12087
2	M	0.31	0/8937	0.50	0/12087
3	D	0.31	1/11910 (0.0%)	0.49	0/16105
3	N	0.31	1/11952 (0.0%)	0.50	0/16162
4	E	0.28	0/775	0.44	0/1045
4	O	0.26	0/775	0.44	0/1045
5	F	0.28	0/2852	0.46	0/3837
5	P	0.28	0/2859	0.45	0/3847
6	G	0.55	0/368	1.09	2/567 (0.4%)
6	Q	0.47	0/368	1.05	0/567
7	H	0.51	0/556	1.26	3/858 (0.3%)
7	R	0.52	0/556	1.23	2/858 (0.2%)
8	I	0.35	0/47	0.68	0/72
8	S	0.25	0/47	0.55	0/72
All	All	0.31	2/58154 (0.0%)	0.53	7/79019 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	599	PRO	C-N	5.34	1.46	1.34
3	D	105	VAL	C-N	5.13	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	17	DA	O4'-C1'-N9	6.77	112.74	108.00
7	H	6	DT	O4'-C1'-N1	-6.45	103.49	108.00
7	H	20	DG	C1'-O4'-C4'	-6.17	103.93	110.10
6	G	16	DC	O4'-C4'-C3'	-5.77	102.19	104.50
7	R	20	DG	C1'-O4'-C4'	-5.40	104.70	110.10
6	G	15	DT	O4'-C4'-C3'	-5.27	102.39	104.50
7	H	21	DA	O4'-C1'-N9	5.21	111.65	108.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	81	0
1	B	1750	0	1797	92	0
1	K	1782	0	1834	60	0
1	L	1773	0	1826	76	0
2	C	8770	0	8872	436	0
2	M	8770	0	8871	518	2
3	D	11704	0	11934	544	1
3	N	11746	0	11974	664	0
4	E	761	0	778	26	0
4	O	761	0	778	25	0
5	F	2807	0	2882	111	0
5	P	2814	0	2888	168	1
6	G	328	0	181	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	2617	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 23.

All (2617) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:M:229:MET:HE3	2:M:233:GLU:O	1.07	1.21
2:C:64:LEU:N	2:C:103:LYS:HZ2	1.21	1.20
3:N:1283:ILE:HG23	3:N:1315:ASP:CG	1.60	1.20
3:N:835:SER:CB	3:N:838:ARG:HE	1.55	1.20
3:N:835:SER:HB3	3:N:838:ARG:NE	1.55	1.20
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: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:N:1283:ILE:HG23	3:N:1315:ASP:OD1	1.39	1.17
3:D:256:GLU:O	3:D:274:ARG:NH1	1.77	1.17
2:M:105:THR:CG2	2:M:107:LEU:HB3	1.74	1.17
3:D:894:LYS:N	3:D:894:LYS:HD2	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:229:MET:CE	2:M:233:GLU:C	2.15	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:1283:ILE:CG2	3:N:1315:ASP:CG	2.16	1.13
2:M:105:THR:HG21	2:M:107:LEU:HB3	1.29	1.12
2:M:64:LEU:N	2:M:103:LYS:HZ2	1.25	1.12
2:C:182:VAL:CG2	2:C:193:LEU:HB3	1.79	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:CD1	3:D:1283:ILE:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:1283:ILE:O	3:N:1283:ILE:HD13	1.49	1.10
2:M:198:ARG:HE	2:M:230:ARG:HA	1.13	1.10
2:M:229:MET:O	2:M:230:ARG:HG2	1.51	1.09
5:F:205:ARG:CG	5:F:205:ARG:HH11	1.64	1.09
2:M:182:VAL:HG21	2:M:193:LEU:HB3	1.32	1.09
2:M:229:MET:HE3	2:M:233:GLU:C	1.72	1.08
3:N:32:ILE:CG1	5:P:258:ILE:HD13	1.82	1.08
3:N:894:LYS:HD2	3:N:894:LYS:H	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:HG2	5:F:205:ARG:HH11	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
2:M:105:THR:HG22	2:M:107:LEU:H	0.94	1.07
3:N:1238:MET:C	3:N:1253:THR:OG1	1.92	1.07
3:N:124:GLU:OE2	3:N:587:ARG:NH2	1.89	1.06
2:M:229:MET:HG2	2:M:233:GLU:HG2	1.35	1.06
2:C:182:VAL:HG21	2:C:193:LEU:HB3	1.38	1.06
3:D:1283:ILE:HD12	3:D:1283:ILE:N	1.55	1.06
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:CD	3:D:894:LYS:H	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
3:D:1304:LYS:C	3:D:1305:LEU:HD23	1.77	1.04
5:P:417:LYS:HG3	5:P:418:LEU:N	1.71	1.04
3:D:1310:ARG:C	3:D:1311:LEU:HD23	1.78	1.03
3:D:67:ARG:HB2	3:D:67:ARG:NH1	1.71	1.03
3:N:46:ASP:OD1	3:N:48:ARG:N	1.91	1.03
3:D:33:ASN:OD1	3:D:36:THR:CG2	2.05	1.03
1:A:57:TYR:CD1	1:A:161:ARG:HD2	1.94	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	2:C:154:ARG:HH11	0.84	1.00
1:K:201:THR:HG22	1:K:203:GLY:H	1.27	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:N	3:D:1311:LEU:HD23	1.78	0.99
2:M:628:PHE:H	2:M:638:ASP:HB3	1.26	0.98
2:C:108:ILE:C	2:C:108:ILE:HD12	1.83	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
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.46	0.98
2:M:167:LYS:C	2:M:168:ARG:HD2	1.83	0.97
3:N:1290:LEU:HG	3:N:1307:LYS:CE	1.94	0.97
3:D:124:GLU:OE2	3:D:587:ARG:NH2	1.96	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:CG	2:M:154:ARG:HH11	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:CG	3:D:67:ARG:HH11	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:N:1310:ARG:HD3	3:N:1327:ARG:HH11	0.81	0.96
2:M:154:ARG:HG2	2:M:154:ARG:NH1	1.65	0.96
1:L:162:ILE:O	1:L:163:ASN:HB2	1.66	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
3:N:438:ASP:OD1	3:N:441:ARG:HD2	1.65	0.95
1:L:201:THR:HG22	1:L:203:GLY:H	1.25	0.95
2:M:107:LEU:HD12	2:M:107:LEU:C	1.80	0.95
2:C:628:PHE:H	2:C:638:ASP:HB3	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:229:MET:HE2	2:M:233:GLU:C	1.86	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:521:PRO:HB3	3:N:1068:LEU:HD21	1.48	0.94
3:D:274:ARG:HG3	3:D:274:ARG:NH1	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
2:M:229:MET:HE2	2:M:234:ALA:N	1.84	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:CD2	3:D:1305:LEU:N	2.30	0.93
3:D:67:ARG:CB	3:D:67:ARG:NH1	2.30	0.93
2:C:102:HIS:HB3	2:C:105:THR:CG2	1.99	0.93
2:M:229:MET:HE1	2:M:234:ALA:HA	1.51	0.93
3:N:209:ARG:N	3:N:389:GLU:O	2.01	0.93
3:D:45:PHE:O	3:D:86:ARG:NH2	2.01	0.93
3:N:1283:ILE:HG21	3:N:1315:ASP:OD1	1.66	0.93
3:N:46:ASP:OD2	3:N:48:ARG:HG3	1.69	0.93
5:P:417:LYS:CG	5:P:418:LEU:N	2.30	0.92
3:N:890:VAL:HB	3:N:922:LEU:CD1	1.98	0.92
2:M:198:ARG:HE	2:M:230:ARG:CA	1.82	0.92
5:F:231:ARG:C	5:F:232:ARG:HG3	1.89	0.92
3:N:1290:LEU:CD2	3:N:1307:LYS:HE2	1.98	0.92
3:D:894:LYS:H	3:D:894:LYS:HD2	1.01	0.92
1:B:58:ILE:CG2	1:B:61:VAL:CG1	2.48	0.92
2:M:229:MET:HG2	2:M:233:GLU:CG	1.99	0.91
3:D:890:VAL:HB	3:D:922:LEU:HD12	1.49	0.91
2:M:230:ARG:HB2	2:M:231:PRO:HD2	1.53	0.91
3:D:1283:ILE:HG13	3:D:1315:ASP:CG	1.91	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
5:P:231:ARG:C	5:P:232:ARG:HG3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:M:237:ARG:O	2:M:241:LEU:HG	1.71	0.90
1:K:206:THR:HB	1:K:209:GLU:HG3	1.52	0.90
3:N:219:GLU:HG3	3:N:339:TRP:CH2	2.06	0.90
1:A:206:THR:HB	1:A:209:GLU:HG3	1.52	0.90
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.53	0.90
2:C:324:ASP:C	2:C:325:ILE:HG23	1.91	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:M:324:ASP:C	2:M:325:ILE:HG23	1.91	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
3:N:227:LEU:HG	3:N:331:VAL:HG13	1.55	0.89
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.01	0.89
2:C:198:ARG:HE	2:C:230:ARG:HA	1.38	0.88
5:P:417:LYS:CG	5:P:418:LEU:H	1.80	0.88
3:D:1285:GLU:OE1	3:D:1307:LYS:HE2	1.74	0.88
3:D:892:ASP:OD1	3:D:894:LYS:HD3	1.74	0.88
3:N:894:LYS:CD	3:N:894:LYS:H	1.84	0.88
3:D:67:ARG:HG3	3:D:67:ARG:HH11	1.36	0.88
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
2:M:105:THR:CG2	2:M:107:LEU:H	1.85	0.88
3:D:209:ARG:N	3:D:389:GLU:O	2.07	0.88
1:B:66:SER:O	1:B:75:VAL:HG23	1.73	0.88
3:D:219:GLU:HG2	3:D:339:TRP:CH2	2.07	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
3:D:821:VAL:HG11	3:D:827:ILE:CD1	2.05	0.86
3:N:1311:LEU:N	3:N:1311:LEU:CD2	2.37	0.86
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:1310:ARG:HD3	3:N:1327:ARG:HD2	1.57	0.85
3:D:520:LEU:O	3:D:525:ARG:NH1	2.09	0.85
5:F:281:GLU:HG2	5:F:282:LEU:CD2	2.07	0.85
3:D:47:GLU:HB3	3:D:78:VAL:HG21	1.58	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: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:N:1283:ILE:CG2	3:N:1315:ASP:CB	2.55	0.84
3:D:1283:ILE:HG13	3:D:1315:ASP:CB	2.06	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
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
2:C:163:ILE:HG23	2:C:171:TRP:NE1	1.93	0.84
1:A:201:THR:HG21	1:A:205:VAL:O	1.77	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
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:N:218:LYS:HG2	3:N:338:GLU:HG2	1.60	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
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
3:N:864:VAL:HG12	3:N:865:THR:N	1.93	0.83
1:L:90:LEU:HB2	1:L:119:ASP:HB3	1.59	0.83
2:M:224:GLU:CD	2:M:224:GLU:H	1.78	0.83
1:A:188:GLN:HG2	1:A:189:ARG:HG3	1.60	0.82
2:M:105:THR:CG2	2:M:107:LEU:CB	2.56	0.82
3:N:835:SER:HB3	3:N:838:ARG:CG	2.07	0.82
3:D:1283:ILE:HD12	3:D:1283:ILE:H	0.69	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:46:ASP:OD1	3:N:47:GLU:N	2.12	0.82
2:M:107:LEU:HD12	2:M:108:ILE:H	1.00	0.82
3:N:1305:LEU:H	3:N:1305:LEU:HD23	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:224:GLU:CD	2:C:224:GLU:H	1.78	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:N:32:ILE:HG13	5:P:258:ILE:CD1	2.10	0.82
3:D:1312:LEU:HD21	3:D:1327:ARG:HG2	1.61	0.82
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.61	0.82
3:D:347:VAL:HG13	3:D:351:MET:HG3	1.61	0.82
3:N:1282:ARG:HD2	3:N:1295:GLU:OE2	1.80	0.82
2:M:428:ARG:NH2	2:M:447:ALA:O	2.12	0.82
2:C:103:LYS:O	2:C:104:ASP:HB2	1.80	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
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
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
3:D:67:ARG:CB	3:D:67:ARG:HH11	1.89	0.81
3:N:1282:ARG:HD2	3:N:1295:GLU:CD	2.01	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:N:411:THR:HB	3:N:437:VAL:H	1.45	0.81
3:D:835:SER:OG	3:D:838:ARG:HG3	1.80	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:1283:ILE:CG2	3:N:1315:ASP:HB2	2.09	0.80
3:D:1439:SER:HB2	3:D:1463:LYS:NZ	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:229:MET:O	2:M:230:ARG:CG	2.30	0.79
2:M:172:ILE:CG1	2:M:186:VAL:HG22	2.08	0.79
3:D:821:VAL:CG1	3:D:827:ILE:HD11	2.13	0.79
3:D:835:SER:OG	3:D:838:ARG:CG	2.31	0.79
2:C:419:THR:H	2:C:422:ARG:HG3	1.45	0.79
3:D:1304:LYS:C	3:D:1305:LEU:CD2	2.50	0.79
3:D:1314:LYS:O	3:D:1317:ASP:HB2	1.81	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
2:M:487:THR:CG2	2:M:490:GLU:HB2	2.12	0.79
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.64	0.79
2:M:154:ARG:HH21	2:M:177:GLU:C	1.86	0.79
3:D:1444:THR:O	3:D:1448:THR:HG23	1.81	0.78
3:N:277:GLU:HA	3:N:277:GLU:OE1	1.83	0.78
5:P:414:ARG:CG	5:P:414:ARG:HH11	1.96	0.78
3:D:1384:PRO:HB3	3:D:1389:LEU:O	1.82	0.78
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.63	0.78
3:N:1310:ARG:HG3	3:N:1310:ARG:HH21	1.47	0.78
3:N:277:GLU:CA	3:N:277:GLU:OE1	2.31	0.78
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	1.82	0.78
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.64	0.78
3:N:796:ARG:HH12	3:N:859:ASP:HB2	1.48	0.78
3:D:1312:LEU:HD23	3:D:1327:ARG:HG3	1.64	0.78
3:N:1093:TYR:OH	3:N:1441:GLN:NE2	2.15	0.78
3:N:823:LEU:HD11	3:N:837:GLY:HA2	1.64	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
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
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.15	0.77
3:N:821:VAL:HG11	3:N:827:ILE:HD11	1.66	0.77
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.65	0.77
3:N:33:ASN:HB3	3:N:36:THR:HG23	1.66	0.76
3:D:36:THR:O	3:D:37:LEU:HB2	1.85	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
2:M:151:ASP:HB3	2:M:157:ARG:O	1.84	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
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.67	0.76
3:D:67:ARG:HB2	3:D:67:ARG:HH11	1.46	0.76
3:D:864:VAL:HG12	3:D:865:THR:H	1.50	0.76
3:D:806:PHE:HB2	3:D:829:VAL:CG2	2.16	0.76
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.17	0.76
2:C:108:ILE:CD1	2:C:108:ILE:O	2.30	0.76
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:HG3	2:M:157:ARG:HH11	1.50	0.76
2:M:166:PRO:O	2:M:167:LYS:HB2	1.83	0.76
5:P:383:LEU:H	5:P:383:LEU:HD23	1.50	0.76
2:M:487:THR:HG23	2:M:490:GLU:H	1.51	0.76
2:M:157:ARG:HH11	2:M:176:VAL:HG12	1.50	0.76
3:N:835:SER:HB3	3:N:838:ARG:CD	2.14	0.76
2:M:238:LEU:CD1	2:M:242:LEU:HD23	2.16	0.76
2:C:198:ARG:HE	2:C:230:ARG:CA	1.98	0.76
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.67	0.76
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.66	0.75
3:N:1304:LYS:C	3:N:1305:LEU:HD23	2.06	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
2:M:176:VAL:O	2:M:177:GLU:HB2	1.87	0.75
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.68	0.75
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.67	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:ARG:HG3	2:C:157:ARG:HH11	1.50	0.74
1:A:59:GLU:OE1	1:A:139:ASN:ND2	2.20	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
2:M:154:ARG:NH2	2:M:177:GLU:C	2.41	0.74
1:A:184:THR:HG22	1:A:192:LEU:HB2	1.69	0.74
3:N:219:GLU:H	3:N:339:TRP:HZ3	1.36	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:D:32:ILE:HG23	3:D:37:LEU:O	1.88	0.74
3:D:693:GLU:HA	4:E:48:MET:HE1	1.69	0.74
5:P:416:ARG:O	5:P:417:LYS:CB	2.30	0.74
2:M:147:TYR:HA	2:M:323:ASP:OD2	1.88	0.74
2:M:157:ARG:HH11	2:M:176:VAL:HG11	0.88	0.74
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
3:N:1283:ILE:HG21	3:N:1315:ASP:HB2	1.68	0.73
3:D:893:GLU:H	3:D:894:LYS:HE2	1.53	0.73
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.20	0.73
3:N:213:VAL:HG21	3:N:367:ILE:HD13	1.70	0.73
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.70	0.73
3:N:274:ARG:NH1	3:N:279:VAL:HG21	2.03	0.73
2:M:850:ALA:HA	3:N:632:VAL:CG2	2.18	0.73
3:N:219:GLU:HG2	3:N:339:TRP:CH2	2.21	0.73
5:F:202:TYR:OH	5:F:244:ARG:HG2	1.88	0.73
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.70	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
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:850:ALA:HA	3:D:632:VAL:CG2	2.19	0.73
2:C:230:ARG:HB2	2:C:231:PRO:CD	2.14	0.73
3:N:1311:LEU:H	3:N:1311:LEU:CD2	1.99	0.73
3:N:1283:ILE:HG21	3:N:1315:ASP:CB	2.18	0.73
2:C:182:VAL:HG23	2:C:193:LEU:CB	2.18	0.73
2:C:324:ASP:C	2:C:325:ILE:CG2	2.57	0.73
3:N:890:VAL:CB	3:N:922:LEU:CD1	2.67	0.72
3:N:65:ARG:NH1	5:P:378:GLY:O	2.22	0.72
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:892:ASP:OD1	3:N:894:LYS:CD	2.38	0.72
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.55	0.72
3:N:1263:PHE:HD2	3:N:1375:MET:CE	2.03	0.72
3:N:821:VAL:HG11	3:N:827:ILE:CD1	2.19	0.72
3:N:256:GLU:HG3	3:N:274:ARG:HE	1.54	0.72
2:M:324:ASP:C	2:M:325:ILE:CG2	2.57	0.72
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.25	0.72
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.71	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
3:D:711:LEU:HD13	3:D:778:LEU:HD12	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:C:229:MET:C	2:C:230:ARG:HG2	2.02	0.72
5:P:411:HIS:O	5:P:415:THR:HB	1.89	0.72
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.04	0.72
2:M:48:PHE:O	2:M:52:PHE:HD2	1.72	0.72
5:F:281:GLU:CG	5:F:282:LEU:HD23	2.17	0.72
1:B:110:LYS:HZ2	1:B:128:HIS:CB	2.03	0.72
3:N:162:ARG:O	3:N:414:ARG:NH1	2.21	0.71
2:M:714:ASP:OD1	2:M:820:ARG:NH2	2.23	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
3:N:658:LEU:HA	3:N:661:MET:HE3	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
5:F:205:ARG:CG	5:F:205:ARG:NH1	2.37	0.71
5:P:231:ARG:C	5:P:232:ARG:CG	2.59	0.71
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.25	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
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.72	0.71
3:D:1312:LEU:HD23	3:D:1327:ARG:CG	2.18	0.71
3:N:1310:ARG:HG3	3:N:1310:ARG:NH2	2.05	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:D:284:LEU:HD22	3:D:288:MET:HE2	1.72	0.71
3:N:32:ILE:CD1	5:P:258:ILE:CD1	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:56:TYR:HE1	3:N:69:GLU:HG3	1.54	0.71
2:M:905:ILE:HG22	2:M:906:PHE:CD2	2.26	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
3:D:596:SER:O	3:D:597:ASP:CG	2.30	0.70
3:N:864:VAL:CG1	3:N:865:THR:H	2.05	0.70
2:M:874:LEU:HD12	3:N:784:ASP:OD2	1.90	0.70
2:C:302:VAL:O	2:C:306:THR:HG23	1.91	0.70
2:M:628:PHE:H	2:M:638:ASP:CB	2.04	0.70
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.74	0.70
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.56	0.70
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.55	0.70
3:N:1284:GLU:C	3:N:1284:GLU:OE1	2.30	0.70
2:C:418:LEU:CD1	2:C:427:VAL:HG11	2.21	0.70
3:D:864:VAL:CG1	3:D:865:THR:H	2.05	0.70
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.27	0.70
3:N:1044:LEU:HD12	3:N:1044:LEU:H	1.57	0.70
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.73	0.70
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.74	0.70
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.57	0.70
3:N:596:SER:C	3:N:597:ASP:OD2	2.30	0.69
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:711:LEU:HD13	3:N:778:LEU:HD12	1.73	0.69
3:D:1071:PHE:O	3:D:1074:SER:OG	2.10	0.69
2:M:230:ARG:CB	2:M:231:PRO:CD	2.71	0.69
5:P:415:THR:HG22	5:P:416:ARG:HG2	1.72	0.69
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.27	0.69
3:N:266:GLU:OE2	3:N:315:ARG:NH2	2.26	0.69
2:M:74:GLY:HA3	2:M:93:PRO:HG2	1.74	0.69
2:M:231:PRO:CG	2:M:232:GLU:OE2	2.33	0.69
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.69
1:B:88:ARG:HB3	1:B:121:GLU:HB2	1.75	0.69
3:D:47:GLU:CB	3:D:78:VAL:HG21	2.23	0.69
2:C:1008:ARG:O	3:D:625:TYR:HA	1.91	0.69
3:D:493:ARG:HG3	3:D:1390:LEU:HD11	1.73	0.69
2:M:107:LEU:HD12	2:M:108:ILE:CA	2.20	0.69
3:N:596:SER:O	3:N:597:ASP:CG	2.30	0.69
3:D:1118:ILE:HD12	3:D:1192:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.12	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
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
3:D:1310:ARG:HD2	3:D:1327:ARG:HB2	1.75	0.69
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.58	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
3:N:1282:ARG:HH11	3:N:1282:ARG:CG	2.05	0.68
3:N:1282:ARG:HD3	3:N:1295:GLU:OE2	1.92	0.68
2:M:238:LEU:O	2:M:238:LEU:HD12	1.92	0.68
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.26	0.68
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.75	0.68
3:N:108:VAL:HB	3:N:109:PRO:HD3	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
2:M:200:LEU:HD13	2:M:300:ASP:HB2	1.75	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:229:MET:HE1	2:C:234:ALA:HA	1.75	0.68
3:N:675:ARG:HH12	5:P:420:ASP:HB3	1.59	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:D:864:VAL:CG1	3:D:865:THR:N	2.57	0.68
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.74	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
2:M:230:ARG:CG	2:M:231:PRO:HD2	2.23	0.68
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.75	0.68
1:B:64:GLU:O	1:B:75:VAL:HB	1.94	0.68
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.59	0.68
2:M:165:LEU:O	2:M:168:ARG:HB2	1.94	0.67
3:D:1311:LEU:N	3:D:1311:LEU:CD2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:658:LEU:HA	3:D:661:MET:HE3	1.76	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
2:M:261:ILE:HG23	2:M:290:LEU:HB2	1.76	0.67
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.76	0.67
3:N:219:GLU:N	3:N:339:TRP:CZ3	2.63	0.67
2:M:758:ARG:HH21	2:M:788:THR:HB	1.60	0.67
5:P:364:ARG:O	5:P:368:VAL:HG13	1.95	0.67
3:N:864:VAL:CG1	3:N:865:THR:N	2.58	0.67
2:M:171:TRP:CE3	7:R:13:DT:H2"	2.30	0.67
2:C:786:LYS:NZ	2:C:786:LYS:CB	2.57	0.67
3:N:1292:VAL:CG2	3:N:1305:LEU:HD11	2.25	0.67
2:M:853:LEU:HB2	2:M:858:MET:CE	2.25	0.67
2:M:262:ALA:HA	2:M:289:THR:HG21	1.77	0.67
3:N:892:ASP:OD1	3:N:894:LYS:HD3	1.95	0.66
3:D:46:ASP:OD1	3:D:47:GLU:N	2.28	0.66
5:P:127:ILE:O	5:P:131:VAL:HG23	1.95	0.66
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.30	0.66
3:D:142:LEU:HD13	3:D:161:LEU:HD11	1.77	0.66
2:C:229:MET:CE	2:C:234:ALA:HA	2.25	0.66
3:N:1237:THR:HG21	3:N:1246:VAL:HG22	1.76	0.66
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.66
1:L:5:LYS:HE3	1:L:5:LYS:HA	1.77	0.66
3:N:1468:LEU:HB3	3:N:1470:ARG:HG3	1.77	0.66
5:P:386:VAL:HG12	5:P:397:ILE:HG21	1.76	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
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.31	0.66
3:D:1482:ARG:HH21	3:D:1483:PHE:HZ	1.43	0.66
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.77	0.66
3:N:832:ARG:HH21	3:N:833:GLU:HG3	1.60	0.66
5:F:126:LEU:O	5:F:130:VAL:HG23	1.96	0.66
2:M:628:PHE:N	2:M:638:ASP:HB3	2.07	0.66
1:L:6:LEU:HD12	1:L:7:LYS:H	1.60	0.66
3:D:832:ARG:HH21	3:D:833:GLU:HG3	1.60	0.66
2:C:286:SER:OG	2:C:301:GLU:OE2	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:1311:LEU:H	3:N:1311:LEU:HD23	1.59	0.65
3:D:213:VAL:HG21	3:D:367:ILE:HD13	1.78	0.65
2:M:229:MET:HE2	2:M:234:ALA:CA	2.26	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:C:166:PRO:O	2:C:167:LYS:HB2	1.95	0.65
3:D:348:GLN:HB3	3:D:349:PRO:HD2	1.79	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.28	0.65
2:M:874:LEU:CD1	3:N:784:ASP:OD2	2.45	0.65
2:M:425:PHE:CE2	3:N:1086:LEU:HD12	2.31	0.65
2:M:229:MET:CE	2:M:234:ALA:N	2.48	0.65
3:D:47:GLU:HB3	3:D:78:VAL:CG2	2.26	0.65
2:C:680:ASP:OD1	3:D:943:THR:HG21	1.96	0.65
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.29	0.65
3:D:530:VAL:HG12	5:F:333:ILE:HD12	1.79	0.65
2:M:172:ILE:HG12	2:M:186:VAL:CG2	2.27	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
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:1283:ILE:CG1	3:D:1315:ASP:CG	2.65	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:M:12:VAL:HG21	2:M:472:ARG:HD3	1.77	0.65
1:K:228:PRO:O	1:K:229:GLN:HG3	1.96	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:C:368:THR:H	2:C:371:LYS:HD2	1.62	0.65
2:M:51:THR:O	2:M:265:ARG:NH2	2.29	0.65
2:M:198:ARG:CZ	2:M:230:ARG:HA	2.27	0.64
3:D:1310:ARG:C	3:D:1311:LEU:CD2	2.63	0.64
2:M:36:PRO:HA	2:M:39:ARG:HG3	1.79	0.64
4:O:52:GLU:OE1	4:O:52:GLU:N	2.27	0.64
5:P:382:THR:HG23	5:P:384:GLU:O	1.98	0.64
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.96	0.64
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.63	0.64
3:N:1143:GLY:O	3:N:1147:ARG:HD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:O	2:C:177:GLU:HB2	1.97	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
4:E:52:GLU:N	4:E:52:GLU:OE1	2.28	0.64
3:N:1237:THR:O	3:N:1238:MET:C	2.34	0.64
3:D:835:SER:OG	3:D:838:ARG:NE	2.30	0.64
3:N:569:ASN:O	3:N:573:MET:HG3	1.98	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
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.78	0.64
2:C:232:GLU:OE2	2:C:232:GLU:N	2.30	0.64
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.79	0.64
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.78	0.64
5:P:205:ARG:CG	5:P:205:ARG:HH11	2.11	0.64
2:C:198:ARG:HH11	2:C:230:ARG:HA	1.63	0.64
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.79	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
2:C:292:ARG:HG3	2:C:299:LYS:HB2	1.78	0.64
1:A:11:PHE:O	1:B:228:PRO:HA	1.96	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:D:711:LEU:HD13	3:D:778:LEU:CD1	2.27	0.64
3:D:17:LYS:O	3:D:20:SER:HB3	1.98	0.64
1:K:11:PHE:O	1:L:228:PRO:HA	1.98	0.64
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.79	0.64
3:N:1315:ASP:OD2	3:N:1316:GLY:N	2.31	0.64
2:M:266:ARG:NH1	7:R:11:DG:O6	2.31	0.64
1:K:222:LEU:HD21	1:L: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
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:N:46:ASP:C	3:N:46:ASP:OD1	2.35	0.63
3:N:1486:VAL:CG2	4:O:22:VAL:HG13	2.26	0.63
4:O:95:VAL:O	4:O:95:VAL:CG2	2.46	0.63
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.78	0.63
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.79	0.63
1:B:58:ILE:HG21	1:B:61:VAL:HG11	1.78	0.63
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.62	0.63
2:C:853:LEU:HB2	2:C:858:MET:CE	2.28	0.63
2:C:911:GLU:O	2:C:915:LYS:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:894:LYS:CD	3:N:894:LYS:N	2.54	0.63
1:L:162:ILE:O	1:L:163:ASN:CB	2.43	0.63
3:N:786:ILE:HG22	3:N:1026:SER:HB2	1.81	0.63
2:M:595:LEU:HD21	2:M:623:TYR:HB3	1.80	0.63
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.79	0.63
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	1.81	0.63
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.80	0.63
3:D:1314:LYS:HG3	3:D:1317:ASP:CG	2.18	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
3:N:56:TYR:HB3	3:N:65:ARG:O	1.98	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:N:137:PRO:HB3	3:N:147:VAL:HG12	1.81	0.63
3:D:808:THR:HG22	3:D:810:GLU:H	1.63	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:NH1	2:M:168:ARG:HG3	2.14	0.63
2:M:911:GLU:O	2:M:915:LYS:HG2	1.99	0.63
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.99	0.62
2:C:503:LEU:CD2	2:C:508:ILE:HD13	2.28	0.62
5:P:78:SER:O	5:P:80:PRO:HD3	1.99	0.62
1:A:228:PRO:O	1:A:229:GLN:HG3	1.98	0.62
2:C:773:LEU:O	2:C:777:ILE:HG13	1.99	0.62
2:M:232:GLU:OE2	2:M:232:GLU:N	2.30	0.62
5:P:392:VAL:HG21	5:P:397:ILE:HD13	1.80	0.62
2:M:874:LEU:O	11:M:1229:HOH:O	2.16	0.62
2:M:262:ALA:HA	2:M:289:THR:CG2	2.28	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
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.33	0.62
2:C:462:ASP:HB3	2:C:468:ARG:HD2	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
3:N:493:ARG:HG3	3:N:1390:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1236:LEU:HA	3:D:1359:GLN:HG2	1.81	0.62
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.80	0.62
3:D:1310:ARG:CA	3:D:1311:LEU:HD23	2.29	0.62
3:D:1122:LEU:HD12	3:D:1185:GLU:HA	1.80	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
2:C:179:ASN:OD1	2:C:181:VAL:N	2.23	0.62
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.32	0.62
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.34	0.62
2:M:356:ARG:HA	2:M:359:MET:HG3	1.82	0.62
2:C:108:ILE:C	2:C:108:ILE:CD1	2.57	0.62
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.81	0.62
2:M:171:TRP:CZ3	7:R:14:DG:OP1	2.53	0.62
3:D:657:LEU:HG	3:D:661:MET:HE2	1.81	0.62
3:D:569:ASN:O	3:D:573:MET:HG3	2.00	0.62
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.81	0.62
5:P:96:LEU:O	5:P:100:VAL:HG23	2.00	0.62
3:N:276:ASP:C	3:N:277:GLU:OE1	2.38	0.62
3:N:675:ARG:HH12	5:P:420:ASP:CB	2.13	0.62
1:A:176:ARG:NH1	2:C:863:ASP:O	2.32	0.62
3:D:786:ILE:HG22	3:D:1026:SER:HB2	1.82	0.62
3:D:541:ASN:O	3:D:545:ARG:HG3	2.00	0.62
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.14	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
2:C:957:LYS:HG2	2:C:961:GLU:OE1	1.99	0.62
2:C:136:ILE:HB	2:C:336:VAL:HG12	1.81	0.62
2:M:168:ARG:NH2	2:M:265:ARG:O	2.33	0.61
1:B:63:HIS:ND1	1:B:66:SER:OG	2.31	0.61
3:N:657:LEU:HG	3:N:661:MET:HE2	1.80	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:HH11	2:M:168:ARG:HG3	1.64	0.61
5:F:152:ASP:HB2	5:F:153:PRO:HD2	1.81	0.61
3:D:67:ARG:CB	3:D:67:ARG:CZ	2.76	0.61
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.83	0.61
1:L:213:GLN:O	1:L:217:ILE:HG13	1.99	0.61
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.82	0.61
3:N:592:THR:OG1	3:N:596:SER:HA	2.00	0.61
2:M:1006:HIS:HB2	2:M:1024:LYS:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1400:VAL:HG21	3:N:1417:TRP:CD1	2.36	0.61
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.81	0.61
3:N:371:ILE:HD12	5:P:230:LYS:HA	1.81	0.61
3:D:274:ARG:NH1	3:D:274:ARG:CG	2.48	0.61
1:A:184:THR:CG2	1:A:192:LEU:HB3	2.29	0.61
3:N:1311:LEU:HB2	3:N:1325:LEU:O	2.01	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
5:P:361:LEU:HD13	5:P:365:GLU:HB2	1.81	0.61
2:C:1090:LYS:HE2	3:D:88:TYR:O	1.99	0.61
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.81	0.61
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: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
3:N:1290:LEU:HD21	3:N:1307:LYS:HE2	1.81	0.61
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.01	0.61
1:A:10:VAL:HG22	1:A:26:GLU:O	2.00	0.61
2:M:173:ASP:C	2:M:174:LEU:HD12	2.20	0.61
3:D:1410:GLU:O	3:D:1410:GLU:HG2	1.99	0.61
3:N:373:PRO:O	3:N:376:GLU:HG2	2.00	0.61
2:C:15:LEU:O	2:C:586:ARG:NH2	2.28	0.61
1:A:57:TYR:CE1	1:A:161:ARG:CD	2.84	0.61
5:F:362:SER:OG	5:F:365:GLU:HG2	2.01	0.61
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.36	0.61
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.65	0.61
3:D:1283:ILE:CD1	3:D:1283:ILE:N	2.30	0.60
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.66	0.60
5:P:205:ARG:NH1	5:P:205:ARG:HG2	2.16	0.60
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.66	0.60
2:M:136:ILE:HB	2:M:336:VAL:HG12	1.83	0.60
2:M:957:LYS:HG2	2:M:961:GLU:OE1	2.01	0.60
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.66	0.60
2:M:480:THR:HG22	2:M:482:GLU:H	1.66	0.60
3:D:33:ASN:O	3:D:37:LEU:HA	2.01	0.60
3:N:783:ARG:NH1	3:N:1028:ALA:O	2.34	0.60
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.84	0.60
2:C:383:ARG:O	2:C:387:SER:HB2	2.01	0.60
1:B:213:GLN:O	1:B:217:ILE:HG13	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
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.81	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
3:N:596:SER:C	3:N:597:ASP:CG	2.60	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
3:D:893:GLU:N	3:D:894:LYS:HE2	2.16	0.60
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.81	0.60
3:N:586:ARG:HH12	6:Q:10:DG:H5”	1.67	0.60
3:N:15:PRO:O	3:N:19:ARG:HG3	2.02	0.60
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.37	0.60
3:D:1309:ALA:O	3:D:1310:ARG:CB	2.46	0.60
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.82	0.60
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.37	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
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
3:D:1490:LYS:HD2	4:E:93:TYR:OH	2.01	0.60
3:D:132:TYR:HB2	3:D:153:LEU:HD12	1.83	0.60
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.37	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
1:A:219:ARG:HG3	1:A:220:GLU:N	2.17	0.60
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:D:1263:PHE:O	3:D:1375:MET:HE2	2.03	0.59
2:C:669:GLY:H	2:C:993:PHE:HZ	1.47	0.59
3:D:32:ILE:HD13	3:D:39:PRO:HA	1.83	0.59
3:N:412:GLY:H	3:N:435:VAL:HG12	1.66	0.59
3:D:693:GLU:HA	4:E:48:MET:CE	2.32	0.59
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.02	0.59
3:N:127:LEU:HA	3:N:457:GLY:HA2	1.84	0.59
3:N:618:LEU:HG	3:N:1467:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.35	0.59
3:N:131:LYS:O	3:N:456:MET:HG2	2.02	0.59
1:K:206:THR:HG23	1:K:207:PRO:HD2	1.83	0.59
1:K:219:ARG:HG3	1:K:220:GLU:N	2.17	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: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:D:844:ALA:O	3:D:867:ARG:HB3	2.02	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
2:M:154:ARG:NH1	2:M:154:ARG:CG	2.45	0.59
3:D:1285:GLU:OE1	3:D:1307:LYS:NZ	2.36	0.59
1:A:70:GLY:N	2:C:607:ASP:OD1	2.36	0.59
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.85	0.59
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.84	0.59
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.67	0.59
2:C:151:ASP:CB	2:C:157:ARG:O	2.50	0.59
5:P:194:LEU:O	5:P:198:ILE:HG13	2.02	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.85	0.59
2:M:15:LEU:O	2:M:586:ARG:NH2	2.29	0.59
3:D:603:LEU:HA	3:D:606:ILE:HD12	1.84	0.59
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.84	0.59
1:K:206:THR:HG22	1:K:208:LEU:H	1.67	0.59
3:D:1435:LEU:O	3:D:1439:SER:OG	2.13	0.59
3:N:1205:TYR:CZ	3:N:1366:LYS:HD3	2.38	0.59
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.84	0.59
3:N:845:ASN:HB2	3:N:846:PRO:HD2	1.85	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
5:F:230:LYS:O	5:F:232:ARG:HG3	2.02	0.59
3:D:388:HIS:O	3:D:390:PRO:HD3	2.02	0.59
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.03	0.59
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.85	0.59
3:D:580:ALA:O	3:D:584:ASN:HB2	2.03	0.59
1:L:115:LEU:O	1:L:117:VAL:HG23	2.02	0.59
3:N:963:TYR:HE2	3:N:1002:LYS:HD3	1.68	0.59
3:N:844:ALA:O	3:N:867:ARG:HB3	2.03	0.59
3:D:1439:SER:HB2	3:D:1463:LYS:HZ3	1.67	0.59
2:M:482:GLU:O	2:M:482:GLU:HG3	2.03	0.59
2:C:482:GLU:O	2:C:482:GLU:HG3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:15:DT:H2'	6:Q:16:DC:C6	2.38	0.59
1:B:115:LEU:O	1:B:117:VAL:HG23	2.02	0.59
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.01	0.59
2:C:134:ARG:NH1	2:C:392:SER:O	2.35	0.59
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.85	0.59
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.38	0.59
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.85	0.59
2:M:383:ARG:O	2:M:387:SER:HB2	2.03	0.59
3:N:202:VAL:HG21	3:N:400:VAL:HG13	1.83	0.59
3:N:260:GLU:OE1	3:N:273:ARG:CZ	2.51	0.58
2:C:102:HIS:CB	2:C:105:THR:CG2	2.78	0.58
2:M:858:MET:HG3	2:M:867:VAL:HG23	1.85	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:C:420:ARG:NH2	2:C:448:ASN:OD1	2.33	0.58
2:C:157:ARG:HH11	2:C:157:ARG:CG	2.15	0.58
2:C:105:THR:O	2:C:105:THR:HG23	2.03	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:B:57:TYR:CG	1:B:161:ARG:HD2	2.38	0.58
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.86	0.58
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.38	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:D:33:ASN:HB3	3:D:36:THR:HG23	1.84	0.58
5:P:382:THR:CG2	5:P:384:GLU:HG2	2.33	0.58
2:M:302:VAL:O	2:M:305:PRO:HD2	2.03	0.58
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.44	0.58
2:C:487:THR:HG23	2:C:490:GLU:H	1.68	0.58
3:N:1384:PRO:HB3	3:N:1389:LEU:O	2.04	0.58
2:C:198:ARG:NH1	2:C:230:ARG:HA	2.17	0.58
5:P:228:GLU:OE2	5:P:231:ARG:NE	2.37	0.58
2:M:167:LYS:O	2:M:168:ARG:CD	2.44	0.58
5:P:394:ARG:HG2	5:P:395:GLU:HG2	1.85	0.58
3:N:658:LEU:HD23	3:N:661:MET:CE	2.33	0.58
2:M:772:ARG:HH22	5:P:380:GLU:HB3	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.02	0.58
3:N:37:LEU:HD13	3:N:535:PHE:CZ	2.39	0.58
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.18	0.58
1:K:30:ARG:CD	1:K:191:ASP:OD1	2.51	0.58
1:A:211:LEU:O	1:A:215:VAL:HG23	2.03	0.58
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.86	0.58
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.69	0.58
3:N:437:VAL:HG11	5:P:175:HIS:CD2	2.39	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
1:L:94:LEU:HD11	1:L:96:THR:O	2.03	0.58
3:N:317:VAL:HG23	3:N:339:TRP:HB3	1.86	0.58
2:M:1090:LYS:HE2	3:N:88:TYR:O	2.04	0.58
2:M:235:LEU:CD1	2:M:257:VAL:HG21	2.34	0.58
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.31	0.58
3:N:876:SER:OG	3:N:879:ARG:HG3	2.02	0.58
2:C:786:LYS:HZ2	2:C:786:LYS:HB2	1.69	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.38	0.58
2:M:420:ARG:NH2	2:M:448:ASN:OD1	2.36	0.57
3:D:490:ALA:O	3:D:494:LYS:HG3	2.04	0.57
3:D:264:LEU:O	3:D:264:LEU:HD12	2.04	0.57
3:N:835:SER:HB3	3:N:838:ARG:HG2	1.85	0.57
5:F:202:TYR:HE2	5:F:248:ASN:OD1	1.87	0.57
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.17	0.57
3:N:36:THR:O	3:N:37:LEU:HB2	2.03	0.57
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.87	0.57
3:N:1194:CYS:O	3:N:1373:ARG:NH2	2.37	0.57
3:D:433:GLY:HA3	3:D:446:VAL:CG1	2.33	0.57
2:M:157:ARG:HD3	2:M:157:ARG:N	2.17	0.57
3:N:276:ASP:O	3:N:277:GLU:OE1	2.22	0.57
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.39	0.57
5:P:376:ILE:HD12	5:P:377:ASP:HB3	1.86	0.57
2:M:114:PHE:CD2	5:P:283:GLY:HA2	2.39	0.57
1:B:76:VAL:O	1:B:79:ILE:HG12	2.04	0.57
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.85	0.57
3:N:259:VAL:HG13	3:N:270:LEU:HD11	1.85	0.57
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.86	0.57
3:D:890:VAL:HB	3:D:922:LEU:HD11	1.82	0.57
2:M:179:ASN:C	2:M:179:ASN:OD1	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:151:ASP:CB	2:M:157:ARG:O	2.50	0.57
5:F:202:TYR:O	5:F:205:ARG:HD3	2.04	0.57
1:A:206:THR:HG22	1:A:208:LEU:H	1.70	0.57
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.19	0.57
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.85	0.57
3:N:558:LEU:HD13	5:P:142:ARG:HD2	1.86	0.57
1:A:111:ALA:O	1:A:114:PHE:HD1	1.87	0.57
2:M:157:ARG:HG3	2:M:176:VAL:CG1	2.35	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
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
4:E:50:THR:HG22	4:E:51:LEU:H	1.68	0.57
5:P:256:ARG:NH2	5:P:311:ALA:O	2.37	0.57
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.86	0.57
2:M:182:VAL:HG23	2:M:193:LEU:HB2	1.86	0.57
1:A:57:TYR:CD1	1:A:161:ARG:CD	2.80	0.57
2:C:617:ASP:OD1	2:C:617:ASP:N	2.37	0.57
3:N:388:HIS:O	3:N:390:PRO:HD3	2.04	0.57
5:P:397:ILE:O	5:P:400:ILE:HG22	2.05	0.57
2:M:238:LEU:HD11	2:M:242:LEU:HD23	1.86	0.57
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.85	0.57
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.40	0.57
3:N:1282:ARG:HG3	3:N:1282:ARG:HH11	1.67	0.57
3:N:103:TRP:CE2	3:N:1444:THR:HG22	2.40	0.57
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.04	0.57
2:M:150:PRO:HD3	2:M:322:VAL:CG1	2.35	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
3:N:47:GLU:CD	3:N:53:ILE:HG12	2.26	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
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:N:808:THR:HB	3:N:811:GLU:HG3	1.87	0.56
5:P:222:ARG:N	5:P:222:ARG:HD2	2.18	0.56
3:D:1264:GLU:HA	3:D:1264:GLU:OE1	2.05	0.56
2:C:157:ARG:HH11	2:C:176:VAL:HG11	1.52	0.56
2:M:617:ASP:OD1	2:M:617:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:150:PRO:HD3	2:M:322:VAL:HG13	1.87	0.56
1:L:58:ILE:HB	1:L:61:VAL:HB	1.87	0.56
3:D:15:PRO:O	3:D:19:ARG:HG3	2.05	0.56
2:C:363:SER:O	2:C:367:LEU:HD21	2.04	0.56
5:P:383:LEU:HD12	5:P:398:ARG:HD2	1.87	0.56
2:C:302:VAL:O	2:C:305:PRO:HD2	2.06	0.56
3:N:1276:GLU:OE2	3:N:1301:LYS:HE3	2.04	0.56
1:K:111:ALA:O	1:K:114:PHE:HD1	1.89	0.56
1:A:30:ARG:HD3	1:A:191:ASP:OD2	2.06	0.56
3:D:1231:GLU:N	3:D:1232:PRO:HD2	2.21	0.56
3:N:1290:LEU:HG	3:N:1307:LYS:CD	2.35	0.56
3:N:1237:THR:CG2	3:N:1238:MET:H	2.09	0.56
3:N:273:ARG:HG3	3:N:278:PRO:HA	1.87	0.56
3:N:1439:SER:HB2	3:N:1463:LYS:NZ	2.20	0.56
5:P:409:LYS:HD3	5:P:409:LYS:C	2.25	0.56
2:C:861:LEU:HD23	2:C:974:LEU:CD1	2.35	0.56
2:M:105:THR:HG22	2:M:107:LEU:HB3	1.79	0.56
5:F:377:ASP:OD1	5:F:379:ARG:N	2.38	0.56
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.39	0.56
3:N:207:PHE:CZ	5:P:101:GLU:OE2	2.59	0.56
2:M:176:VAL:HG12	2:M:177:GLU:N	2.21	0.56
3:N:835:SER:O	3:N:838:ARG:HG3	2.06	0.56
3:D:128:TYR:CZ	3:D:587:ARG:CD	2.88	0.56
2:C:758:ARG:HH21	2:C:788:THR:HB	1.70	0.56
3:N:16:GLU:N	3:N:16:GLU:OE2	2.26	0.56
2:C:690:ILE:CD1	2:C:869:VAL:HG22	2.36	0.56
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.87	0.56
3:N:1311:LEU:CB	3:N:1325:LEU:O	2.54	0.56
3:N:573:MET:HE1	5:P:214:GLN:HG3	1.88	0.56
2:M:524:VAL:CG1	2:M:528:GLU:HB2	2.35	0.56
5:P:358:LEU:O	5:P:366:ALA:HB2	2.05	0.56
2:M:230:ARG:HG3	2:M:231:PRO:HD2	1.88	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:56:GLU:HG2	2:M:359:MET:HE3	1.88	0.56
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.34	0.56
2:M:157:ARG:CG	2:M:157:ARG:HH11	2.15	0.55
2:M:154:ARG:NH2	2:M:178:PRO:N	2.53	0.55
2:C:717:LEU:CD2	2:C:763:GLY:HA2	2.35	0.55
3:N:1263:PHE:HD2	3:N:1375:MET:HE1	1.71	0.55
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.55

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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	0.55
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.17	0.55
1:A:220:GLU:O	1:A:223:THR:HB	2.07	0.55
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.40	0.55
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.42	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
3:N:478:LEU:O	3:N:481:MET:HB2	2.06	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:835:SER:CB	3:N:838:ARG:CG	2.82	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
1:A:30:ARG:HD3	1:A:191:ASP:CG	2.26	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
5:P:144:ILE:HB	5:P:147:LEU:HB2	1.88	0.55
2:M:157:ARG:HG3	2:M:176:VAL:HG12	1.88	0.55
1:B:102:LYS:HA	1:B:138:LEU:O	2.06	0.55
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.06	0.55
1:L:102:LYS:HA	1:L:138:LEU:O	2.07	0.55
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.88	0.55
5:F:259:ARG:HG2	5:F:259:ARG:HH11	1.72	0.55
2:M:224:GLU:OE2	2:M:224:GLU:N	2.30	0.55
2:C:858:MET:HG2	2:C:867:VAL:O	2.06	0.55
3:D:16:GLU:N	3:D:16:GLU:OE2	2.34	0.55
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.36	0.55
3:D:274:ARG:HH22	3:D:279:VAL:HG21	1.70	0.55
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.47	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
3:D:372:ASP:N	3:D:372:ASP:OD1	2.40	0.55
2:C:151:ASP:OD1	2:C:153:ALA:N	2.39	0.55
5:P:364:ARG:NH1	5:P:392:VAL:HG11	2.22	0.55
2:M:1097:LEU:HD11	3:N:103:TRP:HZ3	1.72	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
3:D:1331:ASP:C	3:D:1331:ASP:OD1	2.45	0.55
3:D:149:LYS:O	3:D:150:ARG:HB2	2.05	0.55
3:N:32:ILE:O	5:P:258:ILE:HG23	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1100:ASP:CG	3:N:1440:PHE:HB2	2.27	0.55
3:N:56:TYR:CE1	3:N:69:GLU:HG3	2.38	0.55
3:N:1264:GLU:HA	3:N:1264:GLU:OE1	2.07	0.55
3:D:1312:LEU:CD2	3:D:1327:ARG:HG3	2.30	0.55
2:C:325:ILE:H	2:C:330:ASN:HD22	1.55	0.55
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.36	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:D:696:HIS:CD2	4:E:57:ASP:OD1	2.60	0.55
3:N:1156:LEU:HD23	3:N:1182:GLU:OE2	2.07	0.55
1:L:211:LEU:O	1:L:215:VAL:HG13	2.07	0.55
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.89	0.55
5:P:125:ASP:N	5:P:125:ASP:OD1	2.40	0.55
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.40	0.55
3:N:227:LEU:HD23	3:N:227:LEU:O	2.07	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
5:P:358:LEU:HD23	5:P:370:LYS:HE2	1.88	0.54
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
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
3:N:771:SER:O	3:N:775:GLY:HA2	2.07	0.54
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.07	0.54
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.89	0.54
2:M:151:ASP:OD1	2:M:153:ALA:N	2.39	0.54
3:N:1292:VAL:HG21	3:N:1305:LEU:HD11	1.88	0.54
2:C:164:PRO:CD	2:C:171:TRP:HD1	2.16	0.54
2:M:236:ILE:HD12	2:M:248:PRO:HB3	1.90	0.54
3:N:274:ARG:O	3:N:275:GLU:HB2	2.06	0.54
3:D:658:LEU:HD23	3:D:661:MET:CE	2.37	0.54
2:M:174:LEU:CD1	2:M:174:LEU:N	2.70	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
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:C:176:VAL:O	2:C:177:GLU:CB	2.56	0.54
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.90	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

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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
3:N:1482:ARG:HH21	3:N:1483:PHE:HZ	1.55	0.54
3:N:143:ASN:OD1	3:N:144:GLY:N	2.40	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:800:LYS:HB3	3:N:822:ALA:HB2	1.90	0.54
3:N:1282:ARG:CG	3:N:1282:ARG:NH1	2.66	0.54
2:M:437:ARG:CZ	2:M:491:GLU:OE2	2.55	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
1:K:184:THR:O	1:K:192:LEU:HB2	2.08	0.54
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.89	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
5:P:383:LEU:N	5:P:383:LEU:HD23	2.18	0.54
2:M:206:THR:CA	2:M:209:ARG:HD2	2.38	0.54
3:D:433:GLY:HA3	3:D:446:VAL:HG13	1.89	0.54
3:N:372:ASP:N	3:N:372:ASP:OD1	2.36	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:1046:GLN:HA	3:D:1052:THR:HA	1.89	0.54
3:N:475:LYS:O	3:N:479:GLU:HG2	2.08	0.54
2:C:758:ARG:H	2:C:789:SER:HB3	1.72	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
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.90	0.54
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.89	0.54
2:C:198:ARG:CZ	2:C:230:ARG:HA	2.38	0.54
3:N:1292:VAL:HG23	3:N:1305:LEU:HD11	1.89	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
5:F:155:THR:O	5:F:159:ILE:HG12	2.07	0.54
3:N:1314:LYS:O	3:N:1317:ASP:HB2	2.07	0.54
3:D:1283:ILE:CG1	3:D:1315:ASP:HB2	2.35	0.53
3:N:1312:LEU:HD22	3:N:1327:ARG:HG2	1.90	0.53
2:C:184:MET:HE3	2:C:186:VAL:CG2	2.37	0.53
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.90	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
3:N:259:VAL:HG13	3:N:270:LEU:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:966:LEU:HD13	2:M:986:PRO:HB3	1.90	0.53
1:B:92:PRO:O	1:B:146:ARG:NH1	2.33	0.53
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:1310:ARG:CD	3:D:1327:ARG:HB2	2.37	0.53
2:C:184:MET:HE3	2:C:186:VAL:HG21	1.90	0.53
5:P:140:ARG:HH11	5:P:140:ARG:HG2	1.73	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.91	0.53
3:N:433:GLY:HA3	3:N:446:VAL:CG1	2.39	0.53
3:N:187:LYS:N	3:N:200:ASP:HB3	2.23	0.53
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.89	0.53
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.89	0.53
1:A:201:THR:HG22	1:A:202:ASP:N	2.23	0.53
2:M:419:THR:HB	2:M:422:ARG:HG2	1.91	0.53
2:C:581:THR:N	2:C:584:GLU:OE2	2.41	0.53
1:L:18:ARG:O	1:L:207:PRO:HD3	2.09	0.53
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.89	0.53
3:D:187:LYS:N	3:D:200:ASP:HB3	2.23	0.53
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.23	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:184:MET:HE3	2:M:186:VAL:HG21	1.90	0.53
3:N:1263:PHE:HA	3:N:1375:MET:HE1	1.89	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:D:143:ASN:OD1	3:D:144:GLY:N	2.40	0.53
2:C:640:ARG:HH11	2:C:642:ARG:NH2	2.07	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:N:1232:PRO:HG2	3:N:1356:TYR:HE2	1.73	0.53
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.09	0.53
3:D:1386:ASP:CB	3:D:1412:LYS:HD2	2.39	0.53
2:M:157:ARG:HH12	2:M:176:VAL:HG13	1.71	0.53
2:C:224:GLU:N	2:C:224:GLU:OE2	2.30	0.53
2:C:55:GLU:HG3	2:C:56:GLU:H	1.73	0.53
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.92	0.53
2:C:191:PHE:HB2	2:C:192:PRO:HD2	1.90	0.53
2:M:419:THR:N	2:M:422:ARG:HG3	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:419:THR:HB	2:C:422:ARG:HG2	1.91	0.53
5:F:394:ARG:O	5:F:397:ILE:HG22	2.08	0.53
5:P:152:ASP:N	5:P:152:ASP:OD1	2.42	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.90	0.53
5:P:343:ASP:O	5:P:346:THR:HB	2.09	0.53
1:A:58:ILE:HB	1:A:61:VAL:HB	1.90	0.53
2:M:156:GLY:C	2:M:157:ARG:HD3	2.29	0.53
5:P:368:VAL:HG11	5:P:397:ILE:HD11	1.91	0.53
2:C:580:MET:HB3	2:C:584:GLU:CD	2.29	0.53
3:N:1462:LEU:O	3:N:1466:VAL:HG23	2.08	0.53
1:A:30:ARG:CD	1:A:191:ASP:OD2	2.57	0.53
3:N:478:LEU:O	3:N:481:MET:N	2.42	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
2:M:164:PRO:HA	2:M:269:LEU:HD12	1.91	0.53
4:E:95:VAL:HG23	4:E:95:VAL:O	2.08	0.53
3:N:405:ASP:CG	3:N:406:ASP:H	2.11	0.53
3:D:1280:VAL:HG12	3:D:1295:GLU:O	2.10	0.53
3:D:405:ASP:CG	3:D:406:ASP:H	2.11	0.53
4:O:14:ASP:OD1	4:O:18:ARG:NH1	2.42	0.53
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.44	0.53
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
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
3:D:1044:LEU:HD12	3:D:1044:LEU:N	2.23	0.52
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.91	0.52
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.09	0.52
1:A:112:ARG:HB3	1:A:125:PRO:HB2	1.91	0.52
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.52
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.90	0.52
4:O:43:GLU:OE1	4:O:43:GLU:N	2.36	0.52
3:N:255:GLU:HB3	3:N:279:VAL:HG11	1.91	0.52
3:D:801:GLY:HA3	3:D:825:ALA:CB	2.40	0.52
5:P:395:GLU:HA	5:P:398:ARG:HG2	1.90	0.52
2:M:55:GLU:HG3	2:M:56:GLU:H	1.72	0.52
2:M:15:LEU:HD12	2:M:458:TYR:CZ	2.44	0.52
5:P:366:ALA:O	5:P:370:LYS:HG3	2.09	0.52
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.90	0.52
3:D:945:SER:OG	3:D:947:ILE:HG12	2.09	0.52
2:C:182:VAL:HG23	2:C:193:LEU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.74	0.52
1:B:110:LYS:NZ	1:B:128:HIS:CB	2.67	0.52
2:M:858:MET:HG2	2:M:867:VAL:O	2.09	0.52
5:F:390:PHE:HD1	5:F:397:ILE:HD11	1.74	0.52
3:N:1044:LEU:N	3:N:1044:LEU:HD12	2.22	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
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.91	0.52
3:N:945:SER:OG	3:N:947:ILE:HG12	2.09	0.52
2:M:191:PHE:HB2	2:M:192:PRO:HD2	1.90	0.52
3:N:669:ASN:HD22	5:P:417:LYS:HD3	1.73	0.52
3:N:260:GLU:OE1	3:N:273:ARG:NH2	2.42	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
3:N:407:VAL:HG23	3:N:422:ALA:HB2	1.91	0.52
2:M:999:HIS:HB3	2:M:1004:LYS:HE3	1.92	0.52
3:N:601:ARG:HD3	5:P:318:GLU:HG2	1.92	0.52
1:B:67:THR:O	1:B:69:PRO:HD3	2.10	0.52
1:K:201:THR:HG22	1:K:202:ASP:N	2.25	0.52
2:C:292:ARG:HG3	2:C:299:LYS:CB	2.39	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
3:N:860:LEU:O	3:N:876:SER:HB2	2.09	0.52
2:C:807:ARG:NH2	2:C:810:ASP:OD2	2.43	0.52
3:N:192:ALA:HB1	3:N:193:PRO:HD2	1.91	0.52
3:N:1310:ARG:HD3	3:N:1327:ARG:CD	2.35	0.52
3:N:277:GLU:N	3:N:277:GLU:OE1	2.42	0.52
2:M:1090:LYS:HD3	2:M:1112:PHE:CZ	2.44	0.52
2:M:954:THR:OG1	2:M:957:LYS:HE3	2.10	0.52
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.92	0.52
1:A:133:GLU:HG2	1:A:134:GLU:N	2.24	0.52
1:K:112:ARG:HB3	1:K:125:PRO:HB2	1.92	0.52
3:N:801:GLY:HA3	3:N:825:ALA:CB	2.40	0.52
3:D:371:ILE:CD1	5:F:230:LYS:HA	2.40	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
5:P:372:ARG:HD2	5:P:381:HIS:O	2.09	0.52
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.25	0.52
3:D:475:LYS:O	3:D:479:GLU:HG2	2.09	0.52
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.92	0.52
3:D:399:ARG:HB2	3:D:401:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1267:ARG:HG2	3:N:1331:ASP:OD2	2.09	0.52
1:A:209:GLU:O	1:A:213:GLN:HG3	2.10	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
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
3:N:399:ARG:HB2	3:N:401:TYR:CE1	2.45	0.52
2:C:156:GLY:C	2:C:157:ARG:HD3	2.29	0.52
5:P:231:ARG:O	5:P:232:ARG:CB	2.56	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:1053:LEU:HA	3:N:621:LYS:HD2	1.91	0.52
2:C:424:GLY:O	2:C:428:ARG:HG3	2.09	0.52
3:N:786:ILE:CG2	3:N:1026:SER:HB2	2.39	0.52
2:M:248:PRO:C	2:M:250:ARG:H	2.12	0.52
2:M:876:VAL:N	2:M:877:PRO:HD2	2.25	0.52
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.45	0.52
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.43	0.52
2:M:768:THR:HB	2:M:771:GLU:HB2	1.91	0.52
2:M:229:MET:O	2:M:230:ARG:CB	2.58	0.52
3:N:835:SER:H	3:N:838:ARG:NE	2.07	0.52
5:P:402:ASN:O	5:P:406:ARG:HG3	2.09	0.52
2:M:580:MET:HB3	2:M:584:GLU:OE2	2.10	0.52
2:C:954:THR:OG1	2:C:957:LYS:HE3	2.10	0.52
3:N:693:GLU:HA	4:O:48:MET:CE	2.40	0.52
3:N:881:LEU:O	3:N:885:ILE:HG13	2.09	0.52
2:C:966:LEU:HD13	2:C:986:PRO:HB3	1.92	0.52
2:M:294:GLU:O	2:M:295:ASP:C	2.48	0.52
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
3:N:1283:ILE:H	3:N:1283:ILE:CD1	2.23	0.51
3:N:1290:LEU:CG	3:N:1307:LYS:CE	2.64	0.51
3:N:890:VAL:CG1	3:N:922:LEU:CD1	2.88	0.51
5:P:404:ALA:O	5:P:408:LEU:HB2	2.11	0.51
2:C:1090:LYS:HD3	2:C:1112:PHE:CZ	2.45	0.51
2:M:983:ILE:HG21	2:M:987:ILE:CD1	2.40	0.51
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.91	0.51
3:D:895:VAL:HG11	3:D:922:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:46:ASP:OD2	3:N:48:ARG:CG	2.53	0.51
3:D:804:LEU:O	3:D:827:ILE:HG23	2.11	0.51
2:M:323:ASP:O	2:M:325:ILE:CG2	2.59	0.51
3:N:147:VAL:HG21	3:N:161:LEU:HD21	1.93	0.51
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.41	0.51
2:M:66:LEU:HD11	2:M:98:LEU:HB3	1.92	0.51
2:M:807:ARG:NH2	2:M:810:ASP:OD2	2.43	0.51
5:P:83:GLN:O	5:P:87:GLU:HG3	2.09	0.51
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.92	0.51
5:F:95:THR:HG22	5:F:96:LEU:N	2.25	0.51
2:M:948:GLU:HB3	2:M:953:VAL:HG23	1.92	0.51
2:M:170:PRO:HA	7:R:13:DT:H3	1.74	0.51
2:M:669:GLY:H	2:M:993:PHE:HZ	1.56	0.51
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.91	0.51
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.91	0.51
5:P:419:ARG:HD2	5:P:422:LEU:HD11	1.92	0.51
2:M:184:MET:HE3	2:M:186:VAL:CG2	2.40	0.51
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.73	0.51
1:K:209:GLU:O	1:K:213:GLN:HG3	2.09	0.51
5:P:399:GLN:O	5:P:402:ASN:HB2	2.11	0.51
3:N:693:GLU:HA	4:O:48:MET:HE1	1.92	0.51
1:A:180:GLN:NE2	2:C:935:GLY:O	2.43	0.51
2:M:861:LEU:HD23	2:M:974:LEU:CD1	2.40	0.51
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.91	0.51
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.93	0.51
2:M:154:ARG:NH2	2:M:178:PRO:HA	2.26	0.51
3:N:834:THR:HG23	3:N:835:SER:O	2.11	0.51
5:P:386:VAL:CG1	5:P:397:ILE:HG21	2.41	0.51
3:N:823:LEU:CD1	3:N:837:GLY:HA2	2.37	0.51
3:N:823:LEU:HD11	3:N:837:GLY:CA	2.37	0.51
3:N:959:GLU:HB3	3:N:963:TYR:CE1	2.45	0.51
3:D:614:PHE:HA	3:D:618:LEU:HD23	1.93	0.51
2:C:97:ARG:HD3	2:C:110:GLU:OE1	2.11	0.51
2:M:1065:ALA:HB1	2:M:1077:PRO:HG3	1.91	0.51
6:G:11:DT:H2"	6:G:12:DG:H5"	1.92	0.51
1:A:47:SER:O	1:A:49:PRO:HD3	2.11	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:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.46	0.51
2:C:48:PHE:HA	2:C:348:LEU:HD21	1.93	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1481:VAL:HG23	4:O:21:VAL:HG21	1.93	0.51
3:N:709:HIS:HA	3:N:1227:GLN:HB3	1.92	0.51
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.46	0.51
3:N:218:LYS:HA	3:N:337:LEU:O	2.11	0.51
3:D:619:LEU:HD11	3:D:1439:SER:HB3	1.93	0.51
3:N:71:LYS:HG3	3:N:72:VAL:N	2.25	0.51
3:N:566:ILE:HD13	5:P:217:ASN:HB3	1.91	0.51
2:M:325:ILE:H	2:M:330:ASN:HD22	1.57	0.51
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.76	0.51
2:M:171:TRP:HZ3	7:R:14:DG:OP1	1.94	0.51
2:C:223:ASP:O	2:C:227:PHE:HD2	1.94	0.51
3:N:573:MET:SD	5:P:210:LEU:HB3	2.51	0.51
2:C:1103:ASP:OD2	2:C:1107:ASN:HB2	2.10	0.51
2:M:503:LEU:CD2	2:M:508:ILE:HD13	2.41	0.51
2:M:250:ARG:HH11	2:M:250:ARG:HG3	1.76	0.51
3:N:1231:GLU:N	3:N:1232:PRO:HD2	2.26	0.51
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.92	0.51
2:M:97:ARG:HD3	2:M:110:GLU:OE1	2.11	0.51
3:N:1386:ASP:OD2	3:N:1413:THR:OG1	2.17	0.51
5:F:377:ASP:OD1	5:F:377:ASP:C	2.50	0.51
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.93	0.51
2:C:637:LEU:HD23	2:C:659:PRO:HG3	1.91	0.51
5:F:418:LEU:N	5:F:418:LEU:HD12	2.25	0.51
1:K:90:LEU:O	1:K:92:PRO:HD3	2.11	0.51
3:N:1099:VAL:O	3:N:1103:HIS:HB3	2.11	0.51
2:M:1103:ASP:OD2	2:M:1107:ASN:HB2	2.11	0.50
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.93	0.50
2:C:56:GLU:HG2	2:C:359:MET:HE3	1.92	0.50
5:P:380:GLU:H	5:P:380:GLU:CD	2.14	0.50
3:N:646:LYS:HB3	3:N:688:TRP:CZ3	2.46	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.93	0.50
1:B:156:HIS:ND1	1:B:158:ILE:HG23	2.26	0.50
3:N:111:LYS:HG3	3:N:1452:ILE:HD11	1.93	0.50
2:M:758:ARG:H	2:M:789:SER:HB3	1.76	0.50
2:M:223:ASP:O	2:M:227:PHE:HD2	1.94	0.50
3:D:376:GLU:O	3:D:376:GLU:HG3	2.11	0.50
2:M:1065:ALA:CB	2:M:1077:PRO:HG3	2.41	0.50
3:D:258:VAL:HG12	3:D:297:ILE:HD13	1.92	0.50
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:THR:O	2:C:105:THR:CG2	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
2:M:189:ARG:HH12	2:M:244:PRO:CD	2.20	0.50
3:D:1263:PHE:HA	3:D:1375:MET:HE2	1.94	0.50
3:N:114:THR:HG21	3:N:498:VAL:HG21	1.94	0.50
3:D:1232:PRO:HG2	3:D:1356:TYR:HE2	1.75	0.50
3:N:279:VAL:HG13	3:N:279:VAL:O	2.10	0.50
3:D:1465:ASN:HB3	3:D:1470:ARG:HB2	1.92	0.50
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.93	0.50
2:C:15:LEU:HD12	2:C:458:TYR:CZ	2.46	0.50
1:B:94:LEU:HD22	1:B:96:THR:H	1.76	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
3:N:323:GLU:HB2	3:N:334:THR:HB	1.93	0.50
3:D:1339:LYS:HG2	3:D:1343:ALA:HB2	1.91	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
3:N:558:LEU:HD23	3:N:567:ILE:HD12	1.93	0.50
2:C:198:ARG:HH11	2:C:230:ARG:CA	2.24	0.50
1:A:184:THR:N	1:A:192:LEU:O	2.38	0.50
3:D:829:VAL:O	3:D:830:ALA:HB3	2.11	0.50
3:D:693:GLU:CA	4:E:48:MET:HE1	2.41	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.50
3:D:596:SER:O	3:D:597:ASP:OD2	2.30	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
2:M:327:HIS:CE1	2:M:488:ALA:HB1	2.46	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.46	0.50
3:D:69:GLU:HA	3:D:80:VAL:HG23	1.92	0.50
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.45	0.50
3:N:412:GLY:N	3:N:435:VAL:HG12	2.26	0.50
3:N:44:LEU:O	3:N:525:ARG:NH2	2.40	0.50
2:C:787:ASP:OD1	2:C:789:SER:OG	2.30	0.50
2:C:550:LEU:HB3	2:C:905:ILE:HG23	1.94	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.50
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.12	0.50
2:C:48:PHE:O	2:C:52:PHE:HD2	1.94	0.50
3:N:483:HIS:ND1	3:N:484:PRO:HD2	2.27	0.50
3:D:483:HIS:ND1	3:D:484:PRO:HD2	2.27	0.50
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.46	0.50
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.45	0.50
3:N:1440:PHE:O	3:N:1441:GLN:HG3	2.12	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:C:524:VAL:HG12	2:C:525:SER:N	2.27	0.50
1:B:176:ARG:HG2	1:B:200:TRP:CE3	2.47	0.50
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.94	0.50
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.75	0.50
1:K:47:SER:O	1:K:49:PRO:HD3	2.11	0.50
3:D:23:TYR:CD2	3:D:89:ARG:HD3	2.47	0.50
2:M:926:PHE:HE1	2:M:929:ARG:HH11	1.59	0.50
3:D:970:LYS:O	3:D:974:ILE:HG13	2.11	0.50
5:P:398:ARG:O	5:P:401:GLU:HG2	2.10	0.49
2:C:82:GLU:O	2:C:86:LYS:HG3	2.12	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
2:M:460:ARG:HD2	2:M:485:TYR:CZ	2.46	0.49
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.94	0.49
3:D:217:LYS:HB2	3:D:339:TRP:CE2	2.47	0.49
3:D:33:ASN:HB2	3:D:40:GLU:OE1	2.11	0.49
3:N:274:ARG:CZ	3:N:279:VAL:HG21	2.42	0.49
3:D:1347:TYR:O	3:D:1351:GLU:HB2	2.11	0.49
5:P:403:LYS:NZ	5:P:406:ARG:HH12	2.10	0.49
3:D:595:GLY:O	3:D:597:ASP:OD2	2.30	0.49
2:M:524:VAL:HG12	2:M:525:SER:N	2.27	0.49
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.60	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:M:211:LEU:HD23	2:M:311:PHE:HD2	1.76	0.49
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.94	0.49
2:M:1090:LYS:HD3	2:M:1112:PHE:CE2	2.47	0.49
5:F:372:ARG:HE	5:F:383:LEU:HG	1.77	0.49
2:C:289:THR:HG22	2:C:291:ALA:H	1.76	0.49
3:N:315:ARG:O	3:N:316:GLN:HB3	2.12	0.49
5:P:140:ARG:NH1	5:P:140:ARG:HG2	2.27	0.49
2:M:425:PHE:CZ	3:N:1086:LEU:HD12	2.47	0.49
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.49
1:K:47:SER:HG	1:L:32:PHE:HE1	1.60	0.49
2:C:660:ALA:O	2:C:667:ALA:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.46	0.49
3:D:567:ILE:HG22	3:D:571:LYS:HE3	1.94	0.49
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.93	0.49
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.47	0.49
3:N:619:LEU:HD11	3:N:1439:SER:HB3	1.92	0.49
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.42	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:806:PHE:HB2	3:N:829:VAL:HG22	1.94	0.49
2:M:157:ARG:CG	2:M:157:ARG:NH1	2.74	0.49
2:M:229:MET:HE2	2:M:234:ALA:HA	1.87	0.49
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.47	0.49
2:C:711:GLU:HB2	2:C:713:ARG:NH1	2.28	0.49
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.92	0.49
1:L:176:ARG:HG2	1:L:200:TRP:CE3	2.47	0.49
3:N:473:LEU:HD21	3:N:495:ARG:NH2	2.27	0.49
1:K:34:VAL:CG2	1:L:42:ARG:CZ	2.90	0.49
4:E:43:GLU:N	4:E:43:GLU:OE1	2.37	0.49
3:D:1305:LEU:HD23	3:D:1305:LEU:H	1.66	0.49
2:M:327:HIS:CE1	2:M:433:THR:HG21	2.47	0.49
5:P:391:GLY:O	5:P:392:VAL:O	2.31	0.49
2:M:289:THR:CG2	2:M:291:ALA:O	2.61	0.49
3:D:661:MET:CE	3:D:677:LEU:HD11	2.43	0.49
3:N:614:PHE:HA	3:N:618:LEU:HD23	1.94	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
3:N:1238:MET:CG	3:N:1359:GLN:OE1	2.61	0.49
2:M:424:GLY:O	2:M:428:ARG:HG3	2.12	0.49
3:N:671:LYS:NZ	5:P:420:ASP:O	2.40	0.49
2:M:261:ILE:HG22	2:M:291:ALA:HB3	1.94	0.49
2:M:136:ILE:HB	2:M:336:VAL:CG1	2.43	0.49
2:M:23:VAL:HG12	2:M:24:GLU:N	2.26	0.49
3:N:595:GLY:C	3:N:597:ASP:OD2	2.48	0.49
3:N:832:ARG:HD2	3:N:833:GLU:H	1.77	0.49
3:N:729:HIS:ND1	3:N:730:PRO:HD2	2.28	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
2:M:685:GLU:HA	2:M:685:GLU:OE1	2.12	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.95	0.49
2:C:23:VAL:HG12	2:C:24:GLU:N	2.27	0.49
5:F:123:ASP:HB3	5:F:125:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:272:LEU:O	3:D:279:VAL:N	2.43	0.49
3:N:1237:THR:O	3:N:1238:MET:O	2.30	0.49
2:M:238:LEU:HD11	2:M:242:LEU:CD2	2.43	0.49
5:F:156:VAL:O	5:F:160:ASP:HB2	2.13	0.49
1:A:9:PRO:HD3	1:B:224:TYR:CE2	2.47	0.49
3:N:433:GLY:HA3	3:N:446:VAL:HG13	1.95	0.49
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.95	0.49
2:M:878:SER:HA	3:N:1034:GLN:OE1	2.13	0.49
1:A:25:LEU:HD22	1:B:225:PHE:CZ	2.47	0.49
3:D:431:VAL:HG12	3:D:432:TYR:N	2.27	0.49
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
2:C:290:LEU:HD23	2:C:302:VAL:HG21	1.95	0.49
3:N:80:VAL:O	3:N:80:VAL:HG23	2.13	0.49
1:L:48:ILE:HG22	1:L:173:PRO:HD2	1.95	0.49
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.42	0.49
2:C:50:GLU:OE1	2:C:345:ARG:NE	2.46	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:D:74:GLU:CD	3:D:74:GLU:H	2.17	0.49
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.77	0.48
3:N:1283:ILE:HD12	3:N:1283:ILE:H	1.78	0.48
3:N:219:GLU:N	3:N:339:TRP:CH2	2.81	0.48
3:N:890:VAL:HG21	3:N:922:LEU:HD11	1.95	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	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:CB	3:N:922:LEU:HD11	2.41	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
5:P:89:GLY:HA3	7:R:7:DG:C6	2.48	0.48
2:M:154:ARG:HH22	2:M:178:PRO:HA	1.77	0.48
3:D:371:ILE:HG23	5:F:230:LYS: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:B:48:ILE:HG22	1:B:173:PRO:HD2	1.95	0.48
2:M:810:ASP:HB2	2:M:811:PRO:HD2	1.95	0.48
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.12	0.48
2:C:876:VAL:N	2:C:877:PRO:HD2	2.28	0.48
2:M:99:GLN:NE2	2:M:101:ILE:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:226:LYS:HD2	7:H:1:DT:H72	1.95	0.48
2:M:1053:LEU:HD11	3:N:1466:VAL:HG13	1.94	0.48
2:M:553:ASP:OD1	2:M:843:HIS:ND1	2.38	0.48
3:N:574:LEU:O	3:N:578:VAL:HG23	2.13	0.48
1:L:60:ASP:O	1:L:62:LEU:HD12	2.13	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:1400:VAL:CG2	3:N:1417:TRP:CD1	2.96	0.48
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.43	0.48
2:C:810:ASP:HB2	2:C:811:PRO:HD2	1.94	0.48
1:K:180:GLN:NE2	2:M:935:GLY:O	2.47	0.48
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.28	0.48
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.96	0.48
2:C:511:GLU:HG3	2:C:512:ARG:HG2	1.96	0.48
3:N:314:PRO:HG2	3:N:317:VAL:HG12	1.95	0.48
3:N:835:SER:CB	3:N:838:ARG:NE	2.37	0.48
3:N:315:ARG:HD3	3:N:315:ARG:H	1.78	0.48
2:M:511:GLU:HG3	2:M:512:ARG:HG2	1.96	0.48
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
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
5:P:361:LEU:HD21	5:P:408:LEU:HD12	1.96	0.48
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.44	0.48
5:F:295:MET:CE	5:F:295:MET:HA	2.44	0.48
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.94	0.48
3:D:999:THR:O	3:D:1003:VAL:HG13	2.13	0.48
3:N:394:LEU:HG	3:N:396:VAL:HG23	1.95	0.48
1:B:58:ILE:HG22	1:B:61:VAL:CG1	2.40	0.48
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.29	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
2:M:925:TYR:CD1	2:M:967:PHE:CE1	3.02	0.48
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.96	0.48
3:N:1049:SER:OG	3:N:1051:GLU:HG2	2.12	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
2:M:177:GLU:CB	2:M:178:PRO:HD2	2.44	0.48
2:C:157:ARG:NH1	2:C:157:ARG:CG	2.74	0.48
2:M:172:ILE:HA	2:M:185:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:255:GLU:HB3	3:N:279:VAL:CG1	2.44	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:C:141:HIS:CE1	2:C:334:ARG:HD2	2.49	0.48
2:C:1056:LYS:O	3:D:624:ASP:N	2.43	0.48
1:A:185:ARG:HE	1:A:187:GLY:HA2	1.79	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
2:C:845:ASN:HD22	2:C:845:ASN:C	2.17	0.48
3:N:250:LEU:H	3:N:250:LEU:HD12	1.78	0.48
2:M:182:VAL:HG21	2:M:193:LEU:CB	2.22	0.48
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.78	0.48
3:N:1282:ARG:CD	3:N:1295:GLU:CD	2.75	0.48
2:C:580:MET:SD	2:C:584:GLU:HG3	2.54	0.48
5:F:365:GLU:O	5:F:369:LEU:HD13	2.14	0.48
3:D:529:GLN:HG2	3:D:535:PHE:CE1	2.49	0.48
3:N:493:ARG:NH1	11:N:2121:HOH:O	2.47	0.48
1:K:219:ARG:HG3	1:K:220:GLU:H	1.78	0.48
2:C:136:ILE:HB	2:C:336:VAL:CG1	2.44	0.48
3:D:1403:LEU:HD12	3:D:1406:ARG:HH11	1.78	0.48
2:M:121:MET:HE1	2:M:336:VAL:HG21	1.96	0.48
2:C:425:PHE:CZ	3:D:1086:LEU:HD12	2.49	0.48
5:P:97:GLU:CD	5:P:97:GLU:H	2.18	0.48
3:D:71:LYS:HG3	3:D:72:VAL:N	2.28	0.48
3:N:706:PRO:HB2	3:N:708:LEU:HD21	1.96	0.48
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.92	0.48
3:N:465:LEU:HD12	3:N:513:ILE:HD13	1.96	0.48
2:C:925:TYR:CD1	2:C:967:PHE:CE1	3.01	0.48
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.94	0.48
1:A:188:GLN:HG2	1:A:189:ARG:N	2.29	0.47
2:M:168:ARG:HH11	2:M:168:ARG:CG	2.27	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
3:N:1413:THR:HG22	3:N:1414:PRO:HD2	1.94	0.47
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.44	0.47
5:P:205:ARG:HH11	5:P:205:ARG:HG2	1.72	0.47
3:N:134:VAL:HG23	3:N:150:ARG:N	2.29	0.47
2:M:685:GLU:O	2:M:686:ASP:HB2	2.15	0.47
2:C:419:THR:N	2:C:422:ARG:HG3	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.93	0.47
1:L:175:ARG:N	1:L:200:TRP:O	2.44	0.47
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.95	0.47
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.49	0.47
3:D:574:LEU:O	3:D:578:VAL:HG23	2.13	0.47
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.96	0.47
2:C:404:LEU:O	2:C:408:ARG:HG3	2.14	0.47
3:D:868:TYR:CE2	3:D:869:MET:HG3	2.49	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
3:N:868:TYR:CE2	3:N:869:MET:HG3	2.50	0.47
1:K:32:PHE:HA	1:K:35:THR:HB	1.95	0.47
1:A:72:LYS:HE3	2:C:643:VAL:O	2.14	0.47
3:N:431:VAL:HG12	3:N:432:TYR:N	2.29	0.47
5:F:279:GLN:HA	5:F:284:ARG:O	2.15	0.47
3:N:536:ALA:HA	5:P:315:VAL:O	2.13	0.47
2:M:418:LEU:HD21	7:R:14:DG:C8	2.48	0.47
3:N:650:LEU:HD12	3:N:657:LEU:CD2	2.45	0.47
1:K:57:TYR:CG	1:K:161:ARG:HD2	2.49	0.47
2:M:680:ASP:OD1	3:N:943:THR:HG21	2.15	0.47
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.14	0.47
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.14	0.47
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.50	0.47
3:D:890:VAL:O	3:D:926:LYS:NZ	2.47	0.47
3:N:273:ARG:CG	3:N:278:PRO:HA	2.44	0.47
3:N:204:LEU:HD23	3:N:441:ARG:NH2	2.29	0.47
1:K:39:PRO:HG3	1:L:39:PRO:CG	2.44	0.47
1:A:219:ARG:HG3	1:A:220:GLU:H	1.79	0.47
2:M:173:ASP:O	2:M:174:LEU:HD12	2.14	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
2:C:128:ILE:O	2:C:129:ILE:HD13	2.15	0.47
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.65	0.47
5:F:234:LYS:HD3	7:H:5:DA:OP2	2.15	0.47
3:D:214:GLU:HG2	3:D:342:PRO:HB3	1.97	0.47
3:N:1347:TYR:O	3:N:1351:GLU:HB2	2.15	0.47
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.15	0.47
1:B:206:THR:H	1:B:209:GLU:HB2	1.80	0.47
3:D:47:GLU:HA	3:D:51:GLY:O	2.15	0.47
5:P:365:GLU:O	5:P:368:VAL:HG22	2.15	0.47
2:M:711:GLU:HB2	2:M:713:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:850:ALA:HA	3:N:632:VAL:HG22	1.92	0.47
2:C:1090:LYS:HD3	2:C:1112:PHE:CE2	2.49	0.47
2:M:580:MET:SD	2:M:584:GLU:HG3	2.54	0.47
3:D:1100:ASP:OD2	3:D:1440:PHE:HB2	2.13	0.47
3:N:134:VAL:HG23	3:N:150:ARG:H	1.80	0.47
2:C:56:GLU:OE2	2:C:56:GLU:HA	2.14	0.47
2:C:35:PRO:HG2	2:C:38:LYS:CD	2.44	0.47
3:N:208:PRO:HA	3:N:390:PRO:HA	1.95	0.47
3:D:134:VAL:HG23	3:D:150:ARG:N	2.29	0.47
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.97	0.47
3:N:693:GLU:CB	4:O:48:MET:HE1	2.45	0.47
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.95	0.47
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.96	0.47
3:N:271:VAL:HG22	3:N:281:THR:HG23	1.96	0.47
5:P:247:ILE:O	5:P:251:ILE:HG13	2.14	0.47
2:C:229:MET:C	2:C:230:ARG:CG	2.74	0.47
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.42	0.47
3:D:265:GLU:HB3	3:D:266:GLU:H	1.51	0.47
3:N:1407:LEU:O	3:N:1410:GLU:N	2.44	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: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:1284:GLU:OE1	3:N:1285:GLU:CA	2.63	0.47
2:M:550:LEU:HD23	2:M:905:ILE:HG21	1.97	0.47
3:N:1101:VAL:HG12	3:N:1374:GLN:HB3	1.96	0.47
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.97	0.47
2:M:936:VAL:HG11	2:M:959:PRO:CB	2.44	0.47
2:M:436:GLY:HA2	2:M:538:GLN:O	2.15	0.47
2:M:571:LEU:HD23	2:M:702:SER:HB3	1.97	0.47
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.47
3:D:1216:SER:HB3	4:E:15:SER:HA	1.97	0.47
3:D:1128:VAL:HG22	3:D:1129:THR:HG23	1.96	0.47
1:K:159:LYS:HE3	1:K:164:ALA:O	2.15	0.47
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.30	0.47
3:N:1005:GLN:O	3:N:1009:LYS:HG2	2.14	0.47
6:Q:14:DG:H8	6:Q:14:DG:H5'	1.80	0.47
2:C:164:PRO:CD	2:C:171:TRP:CD1	2.85	0.47
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.79	0.47
3:D:596:SER:C	3:D:597:ASP:OD2	2.54	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)
5:P:153:PRO:O	5:P:156:VAL:HG22	2.14	0.47
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.50	0.47
3:N:970:LYS:O	3:N:974:ILE:HG13	2.14	0.47
3:N:434:ARG:O	3:N:447:VAL:HG23	2.15	0.47
2:M:816:LYS:HA	2:M:816:LYS:HD2	1.61	0.47
3:N:1283:ILE:HG22	3:N:1315:ASP:HB2	1.92	0.46
2:M:229:MET:C	2:M:233:GLU:HB2	2.33	0.46
3:N:1290:LEU:HD21	3:N:1307:LYS:CE	2.43	0.46
2:M:168:ARG:HG3	2:M:268:ASP:HB3	1.97	0.46
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.97	0.46
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:577:PRO:HB3	2:M:993:PHE:CG	2.50	0.46
2:C:685:GLU:O	2:C:686:ASP:HB2	2.15	0.46
3:N:17:LYS:O	3:N:20:SER:HB3	2.15	0.46
2:M:154:ARG:NH2	2:M:177:GLU:O	2.47	0.46
3:N:675:ARG:HH12	5:P:420:ASP:CG	2.18	0.46
3:N:1276:GLU:O	3:N:1277:ILE:HD13	2.15	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:N:1404:ASN:OD1	3:N:1415:VAL:HB	2.14	0.46
3:N:1248:GLY:C	3:N:1250:ALA:H	2.18	0.46
3:D:1252:ILE:HG23	3:D:1253:THR:HG23	1.96	0.46
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.52	0.46
3:N:1486:VAL:HG22	4:O:75:PHE:HB3	1.97	0.46
3:D:843:PHE:CD1	3:D:864:VAL:HG11	2.50	0.46
3:N:1284:GLU:O	3:N:1285:GLU:OE2	2.33	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
2:M:503:LEU:HD23	2:M:508:ILE:HA	1.97	0.46
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.97	0.46
2:M:541:SER:O	2:M:545:ASN:ND2	2.41	0.46
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.96	0.46
1:K:34:VAL:HG22	1:L:42:ARG:NH2	2.31	0.46
3:N:84:ILE:CD1	3:N:87:ARG:HD3	2.45	0.46
1:L:54:THR:OG1	1:L:145:ASP:OD1	2.28	0.46
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.49	0.46
3:N:136:ASP:H	3:N:453:ASP:HB3	1.78	0.46
2:M:366:SER:O	2:M:367:LEU:HD23	2.15	0.46
3:N:1310:ARG:CD	3:N:1327:ARG:NH1	2.47	0.46
3:N:892:ASP:OD1	3:N:894:LYS:HD2	2.12	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)
2:M:52:PHE:HB3	2:M:53:PRO:HA	1.97	0.46
2:M:289:THR:HG22	2:M:291:ALA:H	1.80	0.46
2:M:690:ILE:HD13	2:M:690:ILE:HA	1.74	0.46
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.74	0.46
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.96	0.46
2:M:135:VAL:HG23	2:M:395:LYS:HG3	1.96	0.46
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.98	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
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:N:134:VAL:CG2	3:N:151:GLN:H	2.28	0.46
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.79	0.46
7:R:2:DA:H5'	7:R:2:DA:C8	2.50	0.46
2:M:845:ASN:C	2:M:845:ASN:HD22	2.18	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.97	0.46
3:N:1353:GLN:O	3:N:1357:ARG:HG3	2.15	0.46
1:A:32:PHE:HA	1:A:35:THR:HB	1.97	0.46
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.46
3:D:1283:ILE:CD1	3:D:1315:ASP:OD2	2.64	0.46
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.28	0.46
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.31	0.46
3:N:90:MET:HE3	3:N:519:VAL:O	2.16	0.46
3:D:56:TYR:CE1	3:D:69:GLU:HG3	2.49	0.46
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.46
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.16	0.46
3:D:243:ALA:HB3	3:D:311:LEU:HD21	1.97	0.46
2:M:1001:VAL:HG11	3:N:725:SER:HB3	1.97	0.46
3:D:274:ARG:CZ	3:D:279:VAL:HG21	2.46	0.46
3:N:47:GLU:C	3:N:78:VAL:HG22	2.36	0.46
2:C:102:HIS:CG	2:C:105:THR:HB	2.50	0.46
2:C:550:LEU:HD23	2:C:905:ILE:HG21	1.97	0.46
3:N:829:VAL:O	3:N:830:ALA:HB3	2.15	0.46
2:M:1056:LYS:O	3:N:624:ASP:N	2.44	0.46
2:C:236:ILE:O	2:C:240:THR:HG23	2.16	0.46
5:P:220:LEU:HD11	5:P:235:PHE:HE2	1.81	0.46
7:H:18:DC:H2'	7:H:19:DG:C8	2.51	0.46
6:Q:18:DA:H2"	6:Q:19:DG:H5'	1.98	0.46
4:O:68:LEU:HD12	4:O:68:LEU:HA	1.79	0.46
3:N:613:ARG:HG3	3:N:618:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:LEU:HD12	1:L:96:THR:H	1.81	0.46
3:D:134:VAL:HG23	3:D:150:ARG:H	1.81	0.46
3:N:135:LEU:HD23	3:N:463:GLN:HG2	1.98	0.46
3:N:1339:LYS:HG2	3:N:1343:ALA:HB2	1.97	0.46
2:M:444:PRO:CG	2:M:452:ILE:HB	2.45	0.46
5:F:393:THR:O	5:F:396:ARG:HB3	2.16	0.46
3:D:907:GLU:OE1	3:D:909:ASN:N	2.48	0.46
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.97	0.46
3:D:36:THR:O	3:D:37:LEU:CB	2.58	0.46
3:N:1305:LEU:O	3:N:1306:PRO:C	2.55	0.46
1:K:206:THR:O	1:K:207:PRO:C	2.54	0.46
3:D:46:ASP:OD2	3:D:48:ARG:NE	2.46	0.46
2:M:77:PRO:HB2	2:M:78:PHE:CD1	2.51	0.46
2:M:173:ASP:C	2:M:174:LEU:CD1	2.85	0.46
1:L:97:VAL:HG12	1:L:98:THR:N	2.31	0.46
3:N:222:GLY:HA2	3:N:333:LEU:O	2.16	0.46
5:P:114:LYS:O	5:P:117:SER:OG	2.24	0.46
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.98	0.46
3:N:1280:VAL:HG22	3:N:1281:VAL:N	2.31	0.46
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.27	0.46
2:C:764:GLU:N	2:C:764:GLU:OE1	2.42	0.46
2:M:198:ARG:HH11	2:M:230:ARG:CA	2.28	0.46
3:N:890:VAL:HG11	3:N:922:LEU:CD1	2.46	0.46
5:F:281:GLU:OE2	5:F:282:LEU:HD21	2.15	0.46
3:D:1314:LYS:HG3	3:D:1317:ASP:OD2	2.16	0.46
3:N:1400:VAL:CG2	3:N:1417:TRP:HD1	2.29	0.46
1:L:38:ASN:HB2	1:L:39:PRO:HD3	1.97	0.46
3:N:778:LEU:HA	3:N:778:LEU:HD23	1.63	0.46
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.97	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
2:M:404:LEU:HG	2:M:404:LEU:O	2.15	0.46
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.98	0.46
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.97	0.46
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.85	0.46
3:N:916:TYR:CE1	3:N:920:LEU:HD11	2.51	0.46
3:N:472:ALA:O	3:N:476:GLU:HG3	2.16	0.46
1:L:154:GLU:H	1:L:154:GLU:CD	2.19	0.46
1:L:206:THR:H	1:L:209:GLU:HB2	1.81	0.45
2:C:150:PRO:HD3	2:C:322:VAL:HG13	1.96	0.45
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.29	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
1:L:138:LEU:HD11	1:L:140:MET:HE2	1.98	0.45
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.50	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
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.49	0.45
5:F:374:GLY:HA2	5:F:379:ARG:O	2.15	0.45
1:A:201:THR:CG2	1:A:202:ASP:N	2.79	0.45
5:P:273:ARG:HA	5:P:276:ARG:NH1	2.31	0.45
3:N:1100:ASP:OD1	3:N:1440:PHE:HB2	2.16	0.45
3:D:1136:LYS:O	3:D:1140:ILE:HG13	2.16	0.45
5:P:260:ILE:HG22	5:P:265:VAL:HG23	1.99	0.45
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.51	0.45
1:K:193:ASP:HB3	2:M:938:LYS:CE	2.45	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
3:D:145:VAL:HB	3:D:146:PRO:HD2	1.98	0.45
3:D:38:LYS:HD2	3:D:38:LYS:HA	1.68	0.45
3:N:1283:ILE:CD1	3:N:1283:ILE:N	2.79	0.45
3:N:1304:LYS:CA	3:N:1305:LEU:HD23	2.45	0.45
3:D:922:LEU:N	3:D:922:LEU:HD23	2.32	0.45
2:M:419:THR:HB	2:M:422:ARG:CG	2.47	0.45
3:N:1276:GLU:OE2	3:N:1301:LYS:CE	2.64	0.45
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.97	0.45
2:M:56:GLU:OE2	2:M:56:GLU:HA	2.16	0.45
3:D:355:VAL:HG13	3:D:359:ALA:HB3	1.98	0.45
3:N:1248:GLY:O	3:N:1249:ALA:HB3	2.16	0.45
3:D:1102:THR:CG2	3:D:1371:VAL:HG22	2.47	0.45
3:N:904:VAL:HG23	3:N:905:PRO:HD2	1.98	0.45
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.97	0.45
2:M:469:THR:HG23	2:M:471:TYR:CE1	2.51	0.45
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.82	0.45
2:M:157:ARG:NH1	2:M:176:VAL:HG12	2.09	0.45
2:C:229:MET:O	2:C:230:ARG:CD	2.58	0.45
3:N:890:VAL:O	3:N:926:LYS:NZ	2.48	0.45
3:D:778:LEU:HA	3:D:778:LEU:HD23	1.63	0.45
3:D:573:MET:SD	5:F:210:LEU:HB3	2.56	0.45
2:M:86:LYS:O	2:M:87:ASP:HB2	2.17	0.45
2:C:229:MET:HE2	2:C:234:ALA:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:HD3	2:C:233:GLU:OE1	2.16	0.45
2:M:230:ARG:HG3	2:M:231:PRO:CD	2.46	0.45
5:F:278:LEU:O	5:F:282:LEU:HG	2.17	0.45
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.60	0.45
2:C:323:ASP:O	2:C:325:ILE:CG2	2.65	0.45
3:N:843:PHE:CD1	3:N:864:VAL:HG11	2.50	0.45
3:D:1439:SER:HB2	3:D:1463:LYS:HZ1	1.77	0.45
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.17	0.45
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.52	0.45
3:D:1440:PHE:O	3:D:1441:GLN:CG	2.65	0.45
1:L:123:MET:C	1:L:125:PRO:HD3	2.37	0.45
3:D:1267:ARG:HG2	3:D:1331:ASP:OD2	2.16	0.45
5:F:418:LEU:H	5:F:418:LEU:HD12	1.81	0.45
2:C:444:PRO:CG	2:C:452:ILE:HB	2.47	0.45
5:F:162:LYS:HB2	5:F:162:LYS:HE3	1.53	0.45
3:N:1309:ALA:O	3:N:1310:ARG:HB3	2.16	0.45
3:N:1237:THR:HG21	3:N:1246:VAL:CG1	2.42	0.45
1:B:201:THR:HG22	1:B:202:ASP:N	2.32	0.45
2:M:582:GLY:N	2:M:584:GLU:OE2	2.44	0.45
3:D:1440:PHE:O	3:D:1441:GLN:HG3	2.17	0.45
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.99	0.45
3:N:693:GLU:CA	4:O:48:MET:HE1	2.46	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.98	0.45
3:N:30:GLU:OE1	3:N:40:GLU:HG2	2.16	0.45
5:P:401:GLU:HG3	5:P:402:ASN:N	2.32	0.45
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.98	0.45
5:F:394:ARG:HG3	5:F:395:GLU:N	2.32	0.45
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.78	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.64	0.45
2:M:87:ASP:HA	2:M:131:GLY:HA3	1.98	0.45
3:N:355:VAL:HG13	3:N:359:ALA:HB3	1.99	0.45
1:L:201:THR:HG22	1:L:202:ASP:N	2.31	0.45
2:C:717:LEU:HD12	2:C:717:LEU:N	2.32	0.45
5:F:390:PHE:CD1	5:F:397:ILE:HD11	2.51	0.45
2:M:302:VAL:C	2:M:305:PRO:HD2	2.37	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.98	0.45
2:M:680:ASP:H	3:N:943:THR:CG2	2.30	0.45
5:P:222:ARG:HA	5:P:222:ARG:HE	1.82	0.45
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.98	0.45
3:N:640:HIS:ND1	3:N:641:GLN:HG3	2.32	0.45
1:L:64:GLU:O	1:L:75:VAL:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1460:ILE:N	3:D:1460:ILE:HD13	2.30	0.45
3:D:805:GLU:HA	3:D:828:LYS:O	2.17	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
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
3:D:534:ARG:HG3	3:D:534:ARG:HH21	1.82	0.45
5:P:358:LEU:HD23	5:P:370:LYS:CE	2.47	0.45
1:L:190:THR:O	1:L:190:THR:HG22	2.17	0.45
5:P:237:THR:OG1	7:R:4:DA:H8	2.00	0.45
2:M:154:ARG:NH2	2:M:178:PRO:CA	2.80	0.45
1:B:123:MET:C	1:B:125:PRO:HD3	2.36	0.45
3:N:1478:SER:O	3:N:1482:ARG:HB2	2.17	0.45
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.88	0.45
5:F:96:LEU:O	5:F:100:VAL:HG23	2.17	0.45
1:B:143:ARG:HD3	1:B:158:ILE:HD13	1.99	0.45
3:N:806:PHE:O	3:N:830:ALA:N	2.48	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:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.51	0.45
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.98	0.45
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.99	0.45
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.84	0.45
1:B:190:THR:O	1:B:190:THR:HG22	2.17	0.45
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.99	0.45
3:D:32:ILE:HG23	3:D:37:LEU:C	2.36	0.44
2:C:231:PRO:HG2	2:C:232:GLU:CD	2.37	0.44
3:D:1310:ARG:O	3:D:1310:ARG:HG2	2.17	0.44
3:N:47:GLU:HG2	3:N:51:GLY:O	2.17	0.44
1:A:153:ALA:N	1:A:168:ASP:OD1	2.33	0.44
3:D:596:SER:C	3:D:597:ASP:CG	2.76	0.44
3:N:241:ILE:HD13	3:N:312:ARG:HB3	1.99	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:D:791:TYR:CD1	3:D:945:SER:HB2	2.52	0.44
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.99	0.44
2:M:280:LYS:HE3	2:M:309:TYR:CZ	2.52	0.44
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.47	0.44
3:N:634:GLY:O	3:N:637:LEU:CD1	2.65	0.44
3:D:1031:ASN:OD1	3:D:1031:ASN:C	2.56	0.44
3:N:313:MET:HE1	3:N:319:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.98	0.44
2:C:604:ALA:O	2:C:645:VAL:HG13	2.17	0.44
3:N:97:THR:HG22	3:N:98:PRO:O	2.17	0.44
3:D:1200:VAL:CG1	3:D:1201:CYS:N	2.80	0.44
3:N:46:ASP:OD1	3:N:48:ARG:HG2	2.18	0.44
3:N:1255:GLY:O	3:N:1258:ARG:HB3	2.16	0.44
3:N:213:VAL:HG21	3:N:367:ILE:CD1	2.44	0.44
1:L:56:VAL:HG21	1:L:82:LEU:CD1	2.47	0.44
3:D:1406:ARG:O	3:D:1410:GLU:HB3	2.17	0.44
3:N:1439:SER:OG	3:N:1467:ILE:HD11	2.17	0.44
3:N:14:SER:HB3	3:N:511:TRP:CZ2	2.53	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.98	0.44
2:M:767:PRO:HB2	2:M:772:ARG:HD2	1.99	0.44
1:A:34:VAL:HG22	1:B:42:ARG:NH2	2.33	0.44
2:C:1060:ILE:HD13	5:F:338:LEU:HD13	1.98	0.44
5:P:286:PRO:HB2	5:P:291:ILE:HG13	1.99	0.44
5:P:202:TYR:HB2	5:P:212:LEU:HD13	1.98	0.44
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.98	0.44
2:M:639:GLN:HA	2:M:657:ASP:O	2.18	0.44
3:N:1126:ASP:OD2	3:N:1126:ASP:N	2.49	0.44
2:M:229:MET:HB3	2:M:229:MET:HE2	1.86	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:808:THR:HG22	3:N:810:GLU:N	2.30	0.44
2:C:873:PRO:HB2	3:D:949:ILE:CD1	2.48	0.44
1:K:30:ARG:HD3	1:K:191:ASP:OD1	2.17	0.44
3:N:1477:GLY:O	3:N:1482:ARG:HD3	2.17	0.44
2:C:639:GLN:HA	2:C:657:ASP:O	2.18	0.44
3:N:252:ARG:NH2	3:N:303:PRO:HD3	2.32	0.44
3:N:215:TYR:CE1	3:N:380:GLU:O	2.70	0.44
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.98	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
3:N:1304:LYS:C	3:N:1305:LEU:CD2	2.78	0.44
5:P:412:GLU:O	5:P:416:ARG:HG3	2.18	0.44
2:M:237:ARG:HD2	2:M:241:LEU:HD21	1.99	0.44
3:N:1282:ARG:HB3	3:N:1293:PHE:HB2	1.98	0.44
3:N:142:LEU:HG	3:N:143:ASN:H	1.82	0.44
3:N:1321:ALA:O	3:N:1339:LYS:HD3	2.17	0.44
2:C:644:VAL:HG22	2:C:645:VAL:N	2.33	0.44
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:439:CYS:HA	2:M:440:PRO:HD3	1.82	0.44
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.52	0.44
3:N:170:PRO:HA	3:N:392:SER:HB3	2.00	0.44
2:C:1059:ASP:OD2	2:C:1062:GLY:HA3	2.18	0.44
1:B:58:ILE:HD13	1:B:140:MET:HB2	2.00	0.44
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.82	0.44
2:C:86:LYS:O	2:C:87:ASP:HB2	2.18	0.44
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.29	0.44
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.53	0.44
1:L:97:VAL:HG12	1:L:99:LEU:HD12	1.99	0.44
5:F:259:ARG:HH11	5:F:259:ARG:CG	2.31	0.44
3:N:264:LEU:HD12	3:N:264:LEU:O	2.17	0.44
3:N:679:ARG:HD3	3:N:682:ASP:OD2	2.18	0.44
3:D:775:GLY:HA2	3:D:1209:LEU:O	2.17	0.44
2:M:167:LYS:HD3	2:M:167:LYS:HA	1.72	0.44
1:K:201:THR:CG2	1:K:202:ASP:N	2.81	0.44
3:N:411:THR:CA	3:N:435:VAL:HG12	2.40	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
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.99	0.44
2:M:535:SER:OG	2:M:537:LYS:HG3	2.18	0.44
3:D:230:TRP:CD1	3:D:331:VAL:HG11	2.52	0.44
2:M:604:ALA:HB3	2:M:612:VAL:HG12	1.99	0.44
3:D:629:SER:O	3:D:744:GLN:HG2	2.17	0.44
3:N:145:VAL:HB	3:N:146:PRO:HD2	1.99	0.44
3:D:170:PRO:HA	3:D:392:SER:HB3	1.98	0.44
3:D:679:ARG:HD3	3:D:682:ASP:OD2	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
5:P:393:THR:HG23	5:P:396:ARG:HB3	1.99	0.44
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.53	0.44
2:C:351:LEU:HD12	2:C:374:ASN:O	2.18	0.44
1:B:58:ILE:C	1:B:61:VAL:HG13	2.39	0.44
3:N:669:ASN:HD22	5:P:417:LYS:CD	2.30	0.44
1:K:206:THR:HG22	1:K:208:LEU:N	2.32	0.44
3:N:1311:LEU:H	3:N:1311:LEU:HD22	1.71	0.44
2:M:717:LEU:HD12	2:M:717:LEU:N	2.32	0.44
2:M:206:THR:O	2:M:209:ARG:HD2	2.18	0.44
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.44	0.44
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.18	0.44
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1386:ASP:HB2	3:N:1412:LYS:HD2	2.00	0.44
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.99	0.44
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.85	0.44
3:N:1487:VAL:CG2	3:N:1491:THR:HB	2.47	0.44
3:D:1353:GLN:OE1	3:D:1353:GLN:HA	2.17	0.44
2:M:1095:LEU:O	2:M:1096:ALA:HB3	2.18	0.44
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.53	0.44
1:L:74:ASP:O	1:L:78:ILE:HG13	2.18	0.44
3:D:904:VAL:HG23	3:D:905:PRO:HD2	1.99	0.44
3:N:314:PRO:HG2	3:N:317:VAL:HG11	1.99	0.43
3:N:835:SER:HB2	3:N:838:ARG:HE	1.66	0.43
5:F:278:LEU:HD11	5:F:294:ALA:CB	2.47	0.43
3:N:598:ARG:NH2	5:P:316:SER:OG	2.51	0.43
1:A:206:THR:O	1:A:207:PRO:C	2.54	0.43
2:M:223:ASP:HA	2:M:224:GLU:OE2	2.18	0.43
2:C:281:LEU:HD11	2:C:306:THR:HG22	2.00	0.43
3:D:314:PRO:HD2	3:D:317:VAL:CG1	2.48	0.43
2:C:680:ASP:H	3:D:943:THR:CG2	2.32	0.43
2:M:684:PHE:HB3	3:N:633:VAL:HG21	2.00	0.43
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.33	0.43
1:L:185:ARG:CG	1:L:190:THR:HG23	2.48	0.43
2:C:572:ILE:HG13	2:C:573:ARG:HG3	2.00	0.43
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.99	0.43
2:M:376:ARG:HB2	2:M:377:PRO:HD3	2.00	0.43
3:N:907:GLU:OE1	3:N:909:ASN:N	2.51	0.43
2:C:836:GLY:C	2:C:1001:VAL:HG22	2.39	0.43
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.99	0.43
1:L:161:ARG:HB2	1:L:161:ARG:HE	1.63	0.43
2:C:176:VAL:HG12	2:C:177:GLU:O	2.19	0.43
3:N:597:ASP:HB2	3:N:598:ARG:H	1.56	0.43
3:N:1284:GLU:O	3:N:1285:GLU:CD	2.57	0.43
5:P:350:LEU:O	5:P:354:LEU:HG	2.18	0.43
1:K:83:LYS:CE	1:K:168:ASP:HB2	2.46	0.43
1:L:88:ARG:HD2	1:L:123:MET:HE2	2.00	0.43
5:F:376:ILE:C	5:F:378:GLY:H	2.21	0.43
2:C:541:SER:O	2:C:545:ASN:ND2	2.40	0.43
1:L:58:ILE:HD13	1:L:140:MET:HB2	2.00	0.43
2:M:637:LEU:HA	2:M:659:PRO:HG3	2.00	0.43
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	1.98	0.43
2:M:572:ILE:HG13	2:M:573:ARG:HG3	2.00	0.43
5:F:81:VAL:O	5:F:85:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:841:ASN:C	2:C:841:ASN:OD1	2.56	0.43
1:A:57:TYR:CZ	1:A:161:ARG:HD2	2.52	0.43
3:N:204:LEU:HD23	3:N:441:ARG:CZ	2.49	0.43
3:D:142:LEU:HG	3:D:143:ASN:H	1.84	0.43
2:M:1058:ASP:OD2	2:M:1084:SER:HB2	2.19	0.43
2:C:911:GLU:N	2:C:912:PRO:CD	2.81	0.43
3:D:1373:ARG:HE	3:D:1373:ARG:HB2	1.55	0.43
1:B:117:VAL:O	1:B:118:ALA:C	2.57	0.43
5:P:372:ARG:O	5:P:380:GLU:HB2	2.17	0.43
5:P:371:LEU:HA	5:P:381:HIS:HD2	1.83	0.43
2:C:706:GLU:OE1	2:C:706:GLU:HA	2.18	0.43
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.54	0.43
2:C:937:ASP:OD1	2:C:939:ARG:CG	2.66	0.43
3:N:1171:VAL:O	3:N:1175:ILE:HG13	2.18	0.43
3:N:648:MET:O	3:N:652:LEU:HG	2.18	0.43
1:B:138:LEU:HD11	1:B:140:MET:HE2	2.00	0.43
3:N:827:ILE:CG2	3:N:828:LYS:N	2.80	0.43
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.82	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
1:B:185:ARG:CG	1:B:190:THR:HG23	2.49	0.43
2:C:937:ASP:OD1	2:C:939:ARG:HG3	2.17	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:C:699:PHE:O	2:C:700:TYR:HB2	2.18	0.43
1:B:58:ILE:HG21	1:B:61:VAL:CG1	2.37	0.43
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.49	0.43
3:N:315:ARG:O	3:N:316:GLN:CB	2.65	0.43
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.99	0.43
3:D:529:GLN:HA	3:D:534:ARG:O	2.18	0.43
1:B:56:VAL:HG21	1:B:82:LEU:CD1	2.48	0.43
2:M:524:VAL:HG11	2:M:528:GLU:HB2	1.99	0.43
5:F:295:MET:HA	5:F:295:MET:HE3	2.00	0.43
5:F:95:THR:HG22	5:F:96:LEU:H	1.82	0.43
2:M:90:TYR:CD2	2:M:120:LEU:HB2	2.54	0.43
3:D:629:SER:C	3:D:744:GLN:HG2	2.39	0.43
3:D:1313:VAL:O	3:D:1313:VAL:HG23	2.19	0.43
3:N:1403:LEU:O	3:N:1406:ARG:HB2	2.18	0.43
5:F:144:ILE:HB	5:F:147:LEU:HB2	2.01	0.43
5:P:172:ARG:O	5:P:176:ILE:HG12	2.18	0.43
2:M:308:ARG:HE	2:M:308:ARG:HB3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:706:GLU:OE1	2:M:706:GLU:HA	2.18	0.43
2:M:905:ILE:C	2:M:907:ASP:H	2.22	0.43
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.27	0.43
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.43
1:B:123:MET:O	1:B:125:PRO:HD3	2.18	0.43
3:D:1429:LEU:HD21	3:D:1441:GLN:HB2	2.01	0.43
3:N:68:PHE:O	3:N:80:VAL:HG21	2.17	0.43
3:N:959:GLU:HB3	3:N:963:TYR:HE1	1.84	0.43
3:N:570:GLU:OE2	5:P:214:GLN:NE2	2.48	0.43
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.99	0.43
2:C:910:LYS:HB3	2:C:912:PRO:HD2	2.00	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HB2	2.00	0.43
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.81	0.43
3:N:900:ILE:HG13	3:N:900:ILE:H	1.63	0.43
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.43
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	2.00	0.43
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.85	0.43
2:M:176:VAL:CG1	2:M:177:GLU:O	2.67	0.43
5:F:383:LEU:O	5:F:397:ILE:HG21	2.19	0.43
3:N:367:ILE:HB	3:N:377:VAL:HG12	2.01	0.43
1:B:88:ARG:HD2	1:B:123:MET:HE2	2.00	0.43
3:N:1462:LEU:HD23	3:N:1473:PRO:HG2	2.00	0.43
2:M:911:GLU:N	2:M:912:PRO:CD	2.81	0.43
2:M:136:ILE:HD13	2:M:392:SER:HA	2.01	0.43
3:D:696:HIS:HD2	4:E:57:ASP:OD1	2.00	0.43
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.48	0.43
1:L:143:ARG:HD3	1:L:158:ILE:HD13	1.99	0.43
2:C:561:GLY:O	2:C:565:GLN:HG3	2.19	0.43
1:K:89:PHE:HB2	1:K:146:ARG:NH2	2.33	0.43
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.43
2:M:164:PRO:HB2	2:M:168:ARG:O	2.19	0.43
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.99	0.43
2:M:171:TRP:CE3	7:R:14:DG:OP1	2.72	0.43
2:M:428:ARG:HB3	2:M:450:GLY:HA3	2.00	0.43
2:M:48:PHE:O	2:M:52:PHE:CD2	2.61	0.43
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.43
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.18	0.43
2:M:12:VAL:HG11	2:M:472:ARG:NH1	2.34	0.43
3:D:1403:LEU:O	3:D:1406:ARG:HB2	2.18	0.43
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.91	0.43
3:D:356:PRO:HB3	3:D:441:ARG:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:524:VAL:HG11	2:C:528:GLU:HB2	1.99	0.43
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.86	0.43
3:D:145:VAL:HB	3:D:146:PRO:CD	2.48	0.43
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.00	0.43
3:D:207:PHE:HB2	3:D:391:ALA:HB2	2.01	0.43
3:N:245:LEU:HD22	3:N:249:TYR:HB3	2.01	0.43
2:M:937:ASP:OD1	2:M:939:ARG:CG	2.66	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
3:D:1188:VAL:HG13	3:D:1189:ARG:O	2.19	0.43
2:C:302:VAL:C	2:C:305:PRO:HD2	2.38	0.43
5:P:78:SER:O	5:P:79:ASP:C	2.58	0.43
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.71	0.43
1:L:117:VAL:O	1:L:118:ALA:C	2.57	0.43
2:C:807:ARG:HE	2:C:807:ARG:HB2	1.56	0.43
3:N:1208:ASP:OD1	3:N:1208:ASP:C	2.57	0.43
2:M:1032:PHE:HZ	2:M:1040:LEU:HG	1.84	0.43
3:D:1005:GLN:O	3:D:1009:LYS:HG2	2.19	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
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.01	0.43
2:C:36:PRO:HA	2:C:39:ARG:HG3	2.01	0.43
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.51	0.43
2:M:841:ASN:C	2:M:841:ASN:OD1	2.57	0.43
3:D:984:THR:HG22	3:D:985:ASP:N	2.34	0.43
1:L:124:ASN:N	1:L:124:ASN:OD1	2.52	0.43
3:D:634:GLY:O	3:D:637:LEU:CD1	2.66	0.43
3:N:1495:ILE:HG21	4:O:80:VAL:HG21	2.00	0.42
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.53	0.42
3:N:959:GLU:N	3:N:959:GLU:OE1	2.45	0.42
5:P:101:GLU:CG	5:P:105:LYS:HE2	2.49	0.42
1:B:97:VAL:HG12	1:B:98:THR:N	2.33	0.42
3:N:269:PHE:CE2	3:N:283:PHE:HD1	2.37	0.42
3:D:155:ASP:O	3:D:159:ARG:HG3	2.18	0.42
2:M:51:THR:HG21	2:M:352:ALA:HB2	2.01	0.42
3:N:890:VAL:HG11	3:N:922:LEU:HD12	2.01	0.42
3:N:367:ILE:HD11	3:N:379:ALA:HB2	2.01	0.42
3:N:108:VAL:HB	3:N:109:PRO:CD	2.46	0.42
2:C:292:ARG:NE	2:C:299:LYS:HD3	2.34	0.42
3:N:1101:VAL:HG21	3:N:1424:VAL:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:GLU:HG2	1:K:134:GLU:H	1.83	0.42
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.01	0.42
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.01	0.42
2:M:1056:LYS:HE2	3:N:751:LEU:HG	2.01	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.42
3:N:593:ASN:OD1	3:N:594:PRO:HD3	2.20	0.42
2:M:552:HIS:CD2	2:M:886:LEU:HD12	2.54	0.42
3:N:719:VAL:O	3:N:721:VAL:HG13	2.20	0.42
5:F:114:LYS:O	5:F:118:GLU:HG3	2.19	0.42
3:D:434:ARG:NH1	5:F:135:ILE:O	2.52	0.42
2:M:879:ARG:HD2	2:M:879:ARG:N	2.34	0.42
2:C:231:PRO:CG	2:C:232:GLU:OE2	2.59	0.42
3:D:894:LYS:N	3:D:894:LYS:CD	2.30	0.42
3:D:827:ILE:CG2	3:D:828:LYS:N	2.82	0.42
3:D:142:LEU:HD13	3:D:161:LEU:CD1	2.48	0.42
1:L:5:LYS:HE3	1:L:6:LEU:H	1.84	0.42
3:D:65:ARG:HG3	5:F:378:GLY:O	2.19	0.42
3:N:791:TYR:CD1	3:N:945:SER:HB2	2.53	0.42
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.01	0.42
3:N:957:PRO:HG3	3:N:1007:VAL:HA	2.02	0.42
2:C:1001:VAL:HG13	3:D:630:VAL:HB	2.00	0.42
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.33	0.42
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.34	0.42
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.26	0.42
2:M:105:THR:CG2	2:M:107:LEU:N	2.60	0.42
3:N:827:ILE:O	3:N:834:THR:N	2.45	0.42
3:D:890:VAL:CB	3:D:922:LEU:HD11	2.45	0.42
3:N:598:ARG:NH2	5:P:316:SER:CB	2.83	0.42
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.85	0.42
2:M:54:ILE:HG23	2:M:356:ARG:HG3	2.01	0.42
3:N:1286:THR:HG22	3:N:1288:GLU:N	2.32	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
2:M:470:PRO:HD3	2:M:485:TYR:CE2	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
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.42
2:M:836:GLY:C	2:M:1001:VAL:HG22	2.39	0.42
2:M:937:ASP:OD1	2:M:939:ARG:HG3	2.18	0.42
1:L:124:ASN:HD22	1:L:127:LEU:HB2	1.84	0.42
3:D:275:GLU:HB3	3:D:276:ASP:H	1.57	0.42
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:138:LYS:HB2	3:N:451:ASP:O	2.17	0.42
2:M:998:TYR:O	2:M:998:TYR:CG	2.73	0.42
2:M:151:ASP:OD2	2:M:175:GLU:OE2	2.38	0.42
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.50	0.42
3:N:1312:LEU:CD2	3:N:1327:ARG:CG	2.90	0.42
3:D:128:TYR:CZ	3:D:587:ARG:HD2	2.55	0.42
1:L:201:THR:CG2	1:L:202:ASP:N	2.82	0.42
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.42
3:D:367:ILE:HD11	3:D:379:ALA:HB2	2.01	0.42
3:D:1373:ARG:HG3	3:D:1374:GLN:N	2.35	0.42
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.20	0.42
2:C:236:ILE:HG23	2:C:248:PRO:CB	2.50	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
1:A:44:LEU:HA	1:A:48:ILE:HG12	2.01	0.42
2:C:559:LEU:C	2:C:559:LEU:HD23	2.39	0.42
3:N:1031:ASN:OD1	3:N:1031:ASN:C	2.58	0.42
2:C:229:MET:CE	2:C:234:ALA:CA	2.96	0.42
3:N:801:GLY:HA3	3:N:825:ALA:HB1	2.01	0.42
3:N:48:ARG:CZ	3:N:76:CYS:O	2.68	0.42
1:B:201:THR:CG2	1:B:202:ASP:N	2.83	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
5:P:222:ARG:NE	5:P:222:ARG:HA	2.34	0.42
3:D:187:LYS:HG3	3:D:198:ARG:O	2.20	0.42
2:C:774:LEU:HD21	5:F:418:LEU:HB3	2.02	0.42
3:N:1003:VAL:O	3:N:1007:VAL:HG23	2.20	0.42
2:M:187:ASN:HD22	2:M:187:ASN:HA	1.63	0.42
2:M:918:LEU:HA	2:M:918:LEU:HD23	1.95	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
3:D:259:VAL:O	3:D:295:GLY:N	2.44	0.42
3:N:1283:ILE:O	3:N:1283:ILE:CG1	2.67	0.42
3:N:827:ILE:HG23	3:N:828:LYS:N	2.34	0.42
3:D:67:ARG:CZ	5:F:379:ARG:HB2	2.50	0.42
5:F:230:LYS:O	5:F:232:ARG:CG	2.67	0.42
2:M:327:HIS:HE1	2:M:488:ALA:C	2.23	0.42
3:D:47:GLU:C	3:D:78:VAL:CG2	2.88	0.42
2:M:717:LEU:HD23	2:M:763:GLY:CA	2.43	0.42
3:N:33:ASN:CB	3:N:36:THR:HG23	2.43	0.42
3:N:784:ASP:HB2	3:N:939:PHE:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:289:THR:HG21	2:M:291:ALA:O	2.19	0.42
3:N:134:VAL:HG22	3:N:151:GLN:O	2.20	0.42
3:N:35:ARG:HH11	3:N:35:ARG:CB	2.32	0.42
2:C:690:ILE:HG23	2:C:694:LEU:HD12	2.01	0.42
3:N:568:ARG:HD2	5:P:87:GLU:OE1	2.20	0.42
3:N:111:LYS:HG3	3:N:1452:ILE:CD1	2.49	0.42
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.19	0.42
2:M:1001:VAL:HG13	3:N:630:VAL:HB	2.02	0.42
2:C:1001:VAL:HG11	3:D:725:SER:HB3	2.01	0.42
3:D:231:VAL:O	3:D:231:VAL:HG22	2.20	0.42
3:N:1256:LEU:O	3:N:1260:ILE:HG13	2.19	0.42
5:P:368:VAL:HG23	5:P:369:LEU:N	2.35	0.42
3:N:33:ASN:OD1	3:N:36:THR:CG2	2.67	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
1:B:179:PHE:CB	1:B:197:LEU:HD13	2.49	0.42
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.80	0.42
5:F:270:LYS:HE2	5:F:295:MET:CE	2.50	0.42
3:N:187:LYS:HG3	3:N:198:ARG:O	2.20	0.42
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.02	0.42
2:C:604:ALA:HB3	2:C:612:VAL:HG12	2.01	0.42
1:B:74:ASP:O	1:B:78:ILE:HG13	2.20	0.42
4:O:61:VAL:O	4:O:65:MET:HG3	2.20	0.42
3:N:230:TRP:HA	3:N:243:ALA:HB2	2.01	0.42
3:N:140:ALA:HA	3:N:450:TYR:CG	2.55	0.42
3:N:530:VAL:HG22	3:N:534:ARG:O	2.20	0.42
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.55	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH11	1.68	0.42
2:M:695:LEU:N	2:M:695:LEU:HD23	2.34	0.42
1:B:58:ILE:O	1:B:61:VAL:HG13	2.20	0.42
3:D:1285:GLU:HA	3:D:1290:LEU:HD22	2.02	0.42
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.35	0.42
3:N:36:THR:OG1	3:N:38:LYS:HB2	2.20	0.42
2:M:260:LEU:C	2:M:261:ILE:HD12	2.39	0.42
3:D:530:VAL:HG22	3:D:534:ARG:HB3	2.01	0.42
2:C:988:VAL:HG21	3:D:949:ILE:C	2.40	0.42
2:M:118:ILE:HD11	2:M:344:PHE:HE2	1.81	0.42
3:D:637:LEU:HD22	3:D:642:CYS:HA	2.02	0.42
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.19	0.42
2:M:693:GLU:HA	2:M:696:LYS:HD2	2.02	0.42
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:102:LEU:O	5:F:106:VAL:HG23	2.20	0.42
2:M:751:PRO:HB2	3:N:680:GLN:HB2	2.02	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
3:N:580:ALA:HA	3:N:584:ASN:HA	2.02	0.42
3:N:317:VAL:CG2	3:N:339:TRP:HB3	2.49	0.42
3:D:801:GLY:HA3	3:D:825:ALA:HB1	2.01	0.42
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.55	0.42
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.01	0.42
3:N:1394:VAL:HG12	3:N:1395:LEU:N	2.34	0.42
2:C:786:LYS:HZ3	2:C:786:LYS:HB3	1.84	0.42
3:N:602:SER:O	3:N:606:ILE:HG13	2.19	0.42
2:M:690:ILE:HG23	2:M:694:LEU:HD12	2.02	0.42
2:M:248:PRO:O	2:M:250:ARG:N	2.53	0.42
2:M:98:LEU:HD12	2:M:113:VAL:HG21	2.02	0.42
4:E:70:THR:HB	4:E:72:ARG:HG3	2.02	0.42
3:N:145:VAL:HB	3:N:146:PRO:CD	2.49	0.42
2:M:736:ASP:O	2:M:744:ARG:HG2	2.20	0.42
2:C:64:LEU:HD11	2:C:367:LEU:HD12	2.02	0.41
5:P:228:GLU:OE2	5:P:231:ARG:NH2	2.53	0.41
3:N:326:GLU:HG2	3:N:331:VAL:HG12	2.02	0.41
2:M:102:HIS:O	2:M:106:GLY:CA	2.68	0.41
3:N:36:THR:HG1	3:N:38:LYS:HB2	1.84	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD2	1.88	0.41
2:M:820:ARG:HB2	2:M:820:ARG:HE	1.59	0.41
2:C:289:THR:HG22	2:C:290:LEU:N	2.34	0.41
2:C:54:ILE:HG23	2:C:356:ARG:HG3	2.02	0.41
3:N:1374:GLN:OE1	3:N:1374:GLN:HA	2.19	0.41
2:C:642:ARG:HA	2:C:642:ARG:HD3	1.90	0.41
2:M:999:HIS:HB3	2:M:1004:LYS:CE	2.49	0.41
1:L:101:LEU:HD21	1:L:109:VAL:HG11	2.02	0.41
3:N:133:ILE:HD12	3:N:152:LEU:HD23	2.02	0.41
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.89	0.41
1:L:128:HIS:HE1	1:L:131:THR:CG2	2.33	0.41
2:C:592:LEU:HD23	2:C:592:LEU:N	2.35	0.41
2:M:100:LEU:HD23	2:M:367:LEU:O	2.20	0.41
5:F:228:GLU:OE2	5:F:231:ARG:NH2	2.48	0.41
1:A:23:PHE:HE1	1:A:208:LEU:HD12	1.85	0.41
3:D:801:GLY:O	3:D:804:LEU:HG	2.21	0.41
2:M:487:THR:HG23	2:M:490:GLU:HB2	1.96	0.41
2:M:776:SER:O	5:P:405:LEU:HD21	2.21	0.41
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:VAL:O	3:D:80:VAL:HG23	2.20	0.41
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.85	0.41
2:C:404:LEU:HG	2:C:404:LEU:O	2.20	0.41
2:M:571:LEU:HD22	2:M:700:TYR:HA	2.01	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.55	0.41
3:D:261:LEU:HD12	3:D:269:PHE:O	2.20	0.41
5:P:263:HIS:HA	5:P:266:GLU:HG2	2.01	0.41
3:N:794:GLN:HA	3:N:794:GLN:OE1	2.19	0.41
6:G:14:DG:H8	6:G:14:DG:H5'	1.85	0.41
2:M:163:ILE:HA	2:M:164:PRO:HD2	1.93	0.41
3:N:890:VAL:CG2	3:N:922:LEU:HD11	2.49	0.41
2:C:999:HIS:HB3	2:C:1004:LYS:CE	2.49	0.41
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.20	0.41
3:N:468:LEU:HA	3:N:468:LEU:HD23	1.86	0.41
2:C:736:ASP:O	2:C:744:ARG:HG2	2.19	0.41
1:B:124:ASN:N	1:B:124:ASN:OD1	2.54	0.41
2:M:184:MET:HE1	2:M:191:PHE:CZ	2.56	0.41
3:N:273:ARG:HG2	3:N:277:GLU:C	2.41	0.41
2:M:325:ILE:HG13	2:M:325:ILE:O	2.13	0.41
5:P:408:LEU:O	5:P:408:LEU:HD23	2.20	0.41
3:N:103:TRP:CZ2	3:N:1444:THR:HG22	2.55	0.41
3:N:37:LEU:HD13	3:N:535:PHE:CE1	2.54	0.41
3:D:288:MET:CE	3:D:305:ALA:HB3	2.50	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.89	0.41
3:N:116:LEU:HD21	3:N:465:LEU:HD23	2.02	0.41
3:D:243:ALA:O	3:D:311:LEU:HD23	2.20	0.41
1:B:185:ARG:HA	1:B:189:ARG:O	2.21	0.41
5:P:135:ILE:HD13	5:P:135:ILE:HA	1.96	0.41
2:C:340:MET:SD	2:C:340:MET:C	2.98	0.41
3:N:785:ILE:HD13	3:N:935:LYS:HA	2.02	0.41
2:C:1032:PHE:HZ	2:C:1040:LEU:HG	1.85	0.41
6:Q:11:DT:H2"	6:Q:12:DG:C8	2.55	0.41
2:M:394:PHE:CE2	2:M:632:ASN:HB3	2.55	0.41
4:E:36:LYS:HB3	4:E:36:LYS:HE3	1.76	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
3:N:410:SER:O	3:N:435:VAL:HG11	2.19	0.41
3:N:356:PRO:HB3	3:N:441:ARG:HA	2.02	0.41
5:P:384:GLU:HB3	5:P:394:ARG:CD	2.47	0.41
3:N:823:LEU:CD1	3:N:837:GLY:CA	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:632:VAL:O	3:N:727:GLN:HA	2.20	0.41
3:D:959:GLU:N	3:D:959:GLU:OE1	2.44	0.41
2:M:569:VAL:HG21	2:M:1000:MET:HE1	2.02	0.41
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.90	0.41
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.20	0.41
3:D:207:PHE:HB2	3:D:391:ALA:CB	2.51	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.19	0.41
3:D:472:ALA:O	3:D:476:GLU:HG3	2.19	0.41
1:K:44:LEU:HA	1:K:48:ILE:HG12	2.02	0.41
3:D:849:ALA:O	3:D:852:ALA:HB3	2.21	0.41
3:N:792:ILE:HD13	3:N:941:PHE:CE1	2.56	0.41
5:F:256:ARG:NH2	5:F:311:ALA:O	2.53	0.41
2:C:918:LEU:HA	2:C:918:LEU:HD23	1.94	0.41
2:C:182:VAL:HG21	2:C:193:LEU:CB	2.27	0.41
3:N:1238:MET:HG2	3:N:1359:GLN:OE1	2.21	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG13	2.02	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.36	0.41
1:L:224:TYR:CD1	1:L:224:TYR:N	2.86	0.41
2:M:559:LEU:C	2:M:559:LEU:HD23	2.40	0.41
5:F:264:MET:O	5:F:268:ILE:HG13	2.20	0.41
2:C:864:GLY:O	2:C:866:PRO:HD3	2.20	0.41
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	2.02	0.41
3:D:1464:GLU:OE1	3:D:1464:GLU:N	2.36	0.41
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.54	0.41
3:N:275:GLU:HB3	3:N:276:ASP:H	1.60	0.41
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.34	0.41
1:A:206:THR:HG22	1:A:208:LEU:N	2.34	0.41
2:M:223:ASP:O	2:M:227:PHE:CD2	2.73	0.41
3:N:1495:ILE:HG21	4:O:80:VAL:CG2	2.51	0.41
3:N:1100:ASP:OD2	3:N:1440:PHE:HB2	2.21	0.41
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	2.03	0.41
3:N:1263:PHE:HD2	3:N:1375:MET:HE3	1.80	0.41
2:C:786:LYS:HZ3	2:C:786:LYS:CB	2.32	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.71	0.41
3:N:1353:GLN:HG2	3:N:1368:ILE:CD1	2.51	0.41
3:N:984:THR:HG22	3:N:985:ASP:N	2.36	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.41
1:B:154:GLU:H	1:B:154:GLU:CD	2.20	0.41
3:D:806:PHE:HB2	3:D:829:VAL:HG23	1.98	0.41
2:M:238:LEU:C	2:M:238:LEU:HD12	2.40	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
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.54	0.41
3:N:132:TYR:HB2	3:N:153:LEU:CD1	2.50	0.41
2:M:976:ASP:OD2	2:M:978:ARG:NH1	2.54	0.41
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.20	0.41
3:D:567:ILE:CG2	3:D:571:LYS:HE3	2.50	0.41
1:B:124:ASN:HD22	1:B:127:LEU:HB2	1.86	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.92	0.41
3:D:648:MET:O	3:D:652:LEU:HG	2.21	0.41
3:D:586:ARG:HH12	6:G:10:DG:H5"	1.86	0.41
3:D:1011:PHE:HB3	3:D:1021:TYR:CG	2.55	0.41
5:P:126:LEU:O	5:P:130:VAL:HG23	2.21	0.41
5:F:195:VAL:HG13	5:F:216:GLY:HA3	2.01	0.41
3:N:1011:PHE:HB3	3:N:1021:TYR:CG	2.56	0.41
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.55	0.41
3:N:232:GLU:HG2	3:N:232:GLU:O	2.21	0.41
2:M:230:ARG:HG3	2:M:232:GLU:H	1.86	0.41
3:N:1290:LEU:CD2	3:N:1307:LYS:CE	2.85	0.41
5:F:278:LEU:HD11	5:F:294:ALA:HB3	2.02	0.41
3:N:597:ASP:OD2	3:N:597:ASP:N	2.54	0.41
7:H:13:DT:H6	7:H:13:DT:H2'	1.70	0.41
2:C:163:ILE:HG23	2:C:171:TRP:CD1	2.55	0.41
5:P:391:GLY:O	5:P:392:VAL:C	2.58	0.41
2:C:204:GLN:HB2	2:C:227:PHE:CD1	2.56	0.41
3:N:784:ASP:HB2	3:N:939:PHE:CE2	2.56	0.41
3:D:1468:LEU:HA	3:D:1468:LEU:HD22	1.79	0.41
2:C:786:LYS:HB3	2:C:786:LYS:NZ	2.33	0.41
1:K:57:TYR:CE1	1:K:161:ARG:HD2	2.55	0.41
2:C:679:PHE:HA	3:D:943:THR:HB	2.03	0.41
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.90	0.41
2:C:1105:LYS:O	2:C:1106:ASP:HB2	2.20	0.41
3:N:155:ASP:O	3:N:159:ARG:HG3	2.21	0.41
3:N:132:TYR:HE2	3:N:155:ASP:HB3	1.86	0.41
1:B:80:LEU:O	1:B:83:LYS:HB2	2.21	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
3:N:567:ILE:CG2	3:N:571:LYS:HE3	2.51	0.41
5:P:101:GLU:O	5:P:105:LYS:HG3	2.21	0.41
5:F:259:ARG:NH1	5:F:259:ARG:CG	2.83	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
2:M:944:LEU:HD22	2:M:962:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.03	0.41
2:M:1071:ILE:O	3:N:659:LYS:HD3	2.21	0.41
3:N:230:TRP:HA	3:N:243:ALA:CB	2.50	0.41
3:D:90:MET:HE3	3:D:519:VAL:O	2.21	0.41
2:C:998:TYR:CG	2:C:998:TYR:O	2.74	0.41
2:C:494:TYR:HD1	2:C:530:GLU:OE2	2.04	0.41
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.51	0.41
5:P:120:THR:HG22	5:P:122:LEU:HD13	2.02	0.41
2:M:561:GLY:O	2:M:565:GLN:HG3	2.21	0.41
3:N:731:LEU:CD1	3:N:931:LEU:HB3	2.51	0.41
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.88	0.41
2:C:229:MET:HB3	2:C:233:GLU:CB	2.47	0.41
2:C:226:VAL:HA	2:C:229:MET:HG3	2.03	0.41
5:P:369:LEU:HD12	5:P:401:GLU:HB2	2.03	0.41
2:M:1105:LYS:O	2:M:1106:ASP:HB2	2.20	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:C:6:PHE:CD2	2:C:909:ALA:HB2	2.56	0.41
5:P:195:VAL:HG13	5:P:216:GLY:HA3	2.02	0.41
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.03	0.41
2:C:682:TYR:CD1	3:D:635:PRO:HG2	2.56	0.41
2:C:375:SER:O	2:C:378:LEU:N	2.53	0.41
3:D:215:TYR:CE1	3:D:380:GLU:O	2.74	0.41
2:C:879:ARG:HD2	2:C:879:ARG:N	2.35	0.41
3:N:1342:GLU:H	3:N:1342:GLU:CD	2.25	0.41
2:C:229:MET:O	2:C:233:GLU:HB2	2.21	0.40
3:N:1310:ARG:CG	3:N:1327:ARG:NH1	2.84	0.40
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.35	0.40
3:D:47:GLU:C	3:D:78:VAL:HG23	2.42	0.40
3:D:632:VAL:O	3:D:727:GLN:HA	2.21	0.40
1:L:80:LEU:O	1:L:83:LYS:HB2	2.22	0.40
3:D:134:VAL:HG22	3:D:151:GLN:O	2.21	0.40
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.38	0.40
5:F:324:GLU:HB2	5:F:326:ASP:OD1	2.21	0.40
1:B:184:THR:O	1:B:192:LEU:HB2	2.21	0.40
2:C:1027:PHE:CD2	2:C:1027:PHE:O	2.74	0.40
3:N:1289:LYS:O	3:N:1290:LEU:HD23	2.20	0.40
5:F:281:GLU:CG	5:F:282:LEU:CD2	2.86	0.40
3:D:106:LYS:HE3	3:D:587:ARG:HG3	2.03	0.40
3:N:90:MET:HE3	3:N:520:LEU:HA	2.02	0.40
2:M:1053:LEU:CD1	3:N:1466:VAL:HG13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:LEU:HD21	1:L:97:VAL:CG2	2.51	0.40
1:A:30:ARG:CD	1:A:191:ASP:CG	2.89	0.40
2:M:395:LYS:HE2	2:M:403:SER:CB	2.51	0.40
4:E:70:THR:CB	4:E:72:ARG:HG3	2.52	0.40
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.57	0.40
3:N:637:LEU:HD22	3:N:642:CYS:HA	2.03	0.40
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.78	0.40
3:D:771:SER:O	3:D:775:GLY:HA2	2.21	0.40
2:M:708:TYR:OH	2:M:796:GLU:OE1	2.21	0.40
3:D:634:GLY:O	3:D:637:LEU:HG	2.21	0.40
3:N:138:LYS:CB	3:N:451:ASP:O	2.69	0.40
5:P:325:LYS:HB2	5:P:325:LYS:HE2	1.80	0.40
2:M:707:ARG:NE	2:M:824:ARG:HD3	2.37	0.40
4:E:61:VAL:O	4:E:65:MET:HG3	2.21	0.40
2:C:501:THR:HG21	2:C:513:VAL:HB	2.03	0.40
2:M:474:VAL:HG22	2:M:479:VAL:HG22	2.03	0.40
3:D:486:ARG:HG3	3:D:486:ARG:H	1.58	0.40
2:M:729:LEU:HD23	2:M:729:LEU:HA	1.91	0.40
2:C:229:MET:HE2	2:C:229:MET:HB2	1.91	0.40
3:N:801:GLY:O	3:N:804:LEU:HG	2.21	0.40
3:N:121:THR:O	3:N:124:GLU:HB3	2.21	0.40
3:N:1258:ARG:NH2	3:N:1262:LEU:HD21	2.36	0.40
1:K:23:PHE:HE1	1:K:208:LEU:HD12	1.85	0.40
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.56	0.40
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	2.03	0.40
3:D:132:TYR:HB2	3:D:153:LEU:CD1	2.51	0.40
2:C:626:ARG:HG3	2:C:629:TYR:CG	2.56	0.40
1:A:39:PRO:O	1:A:43:ILE:HG13	2.22	0.40
2:M:899:GLN:HE21	2:M:901:TYR:HE2	1.67	0.40
2:M:864:GLY:O	2:M:866:PRO:HD3	2.20	0.40
3:N:622:ARG:NH1	6:Q:17:DG:OP1	2.43	0.40
2:M:557:ARG:HG3	2:M:844:GLY:HA3	2.02	0.40
2:M:1012:PRO:HB2	2:M:1021:LEU:HD12	2.03	0.40
3:D:900:ILE:H	3:D:900:ILE:HG13	1.62	0.40
2:C:830:LYS:HE2	2:C:830:LYS:HB3	1.89	0.40
5:P:295:MET:HE2	5:P:295:MET:HA	2.02	0.40
1:L:205:VAL:HG12	1:L:206:THR:H	1.86	0.40
3:D:208:PRO:HA	3:D:389:GLU:O	2.22	0.40
3:N:1293:PHE:CE2	3:N:1302:GLU:HG3	2.54	0.40
2:C:223:ASP:O	2:C:227:PHE:CD2	2.73	0.40
2:M:385:PHE:O	2:M:389:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:717:LEU:CD1	2:C:717:LEU:N	2.84	0.40
3:N:832:ARG:HD2	3:N:833:GLU:N	2.37	0.40
1:A:97:VAL:HG12	1:A:98:THR:N	2.36	0.40
5:P:101:GLU:HG3	5:P:105:LYS:HE2	2.02	0.40
1:L:185:ARG:HA	1:L:189:ARG:O	2.21	0.40
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.57	0.40
3:N:252:ARG:HD3	3:N:301:GLY:O	2.21	0.40
5:F:260:ILE:HG23	5:F:261:PRO:HD2	2.03	0.40
3:N:1102:THR:CG2	3:N:1371:VAL:HG22	2.52	0.40
7:R:18:DC:H2'	7:R:19:DG:C8	2.57	0.40
1:L:184:THR:O	1:L:192:LEU:HB2	2.22	0.40
3:N:899:LEU:HD22	3:N:917:GLN:HB3	2.02	0.40
2:C:103:LYS:HG3	2:C:103:LYS:H	1.55	0.40
2:C:176:VAL:O	2:C:181:VAL:O	2.39	0.40
3:N:1258:ARG:HH21	3:N:1351:GLU:HG3	1.86	0.40
3:N:39:PRO:HB3	3:N:45:PHE:O	2.22	0.40
2:M:328:LEU:HD12	2:M:433:THR:O	2.22	0.40
2:C:758:ARG:N	2:C:789:SER:HB3	2.36	0.40
1:K:97:VAL:HG12	1:K:98:THR:N	2.35	0.40
4:O:67:GLU:O	4:O:70:THR:OG1	2.36	0.40
3:D:285:PRO:HG2	3:D:311:LEU:HD12	2.04	0.40
2:C:1071:ILE:CG2	3:D:670:VAL:HG21	2.52	0.40
3:N:1406:ARG:HB3	3:N:1406:ARG:NH2	2.36	0.40
3:N:245:LEU:N	3:N:245:LEU:HD12	2.35	0.40
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.03	0.40
3:N:223:LEU:HD21	3:N:225:LEU:HD21	2.03	0.40
2:M:719:PRO:HD2	2:M:761:PHE:CE1	2.57	0.40
1:A:73:GLU:OE1	1:A:73:GLU:N	2.54	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%)	39	80
1	B	220/315 (70%)	212 (96%)	6 (3%)	2 (1%)	21	64
1	K	224/315 (71%)	218 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	213 (96%)	8 (4%)	2 (1%)	21	64
2	C	1107/1119 (99%)	1066 (96%)	37 (3%)	4 (0%)	39	80
2	M	1107/1119 (99%)	1063 (96%)	39 (4%)	5 (0%)	34	76
3	D	1478/1524 (97%)	1423 (96%)	53 (4%)	2 (0%)	56	90
3	N	1485/1524 (97%)	1423 (96%)	57 (4%)	5 (0%)	46	84
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%)	16	56
All	All	6941/7630 (91%)	6677 (96%)	239 (3%)	25 (0%)	39	80

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

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Mol	Chain	Res	Type
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
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 (i)

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%)	189 (95%)	10 (5%)	30	70
1	B	195/273 (71%)	182 (93%)	13 (7%)	20	57
1	K	199/273 (73%)	189 (95%)	10 (5%)	30	70
1	L	198/273 (72%)	188 (95%)	10 (5%)	29	69
2	C	936/941 (100%)	880 (94%)	56 (6%)	24	62
2	M	936/941 (100%)	873 (93%)	63 (7%)	20	57
3	D	1250/1279 (98%)	1165 (93%)	85 (7%)	20	56
3	N	1253/1279 (98%)	1169 (93%)	84 (7%)	20	57
4	E	83/88 (94%)	80 (96%)	3 (4%)	42	79
4	O	83/88 (94%)	81 (98%)	2 (2%)	57	87
5	F	301/388 (78%)	287 (95%)	14 (5%)	32	72
5	P	302/388 (78%)	280 (93%)	22 (7%)	17	52
All	All	5935/6484 (92%)	5563 (94%)	372 (6%)	22	60

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	58	ILE
1	A	86	VAL
1	A	87	VAL
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	198	ARG
1	A	215	VAL
1	B	54	THR
1	B	61	VAL
1	B	63	HIS
1	B	66	SER
1	B	94	LEU
1	B	96	THR
1	B	165	ILE
1	B	191	ASP
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	81	ASP
2	C	85	GLU
2	C	103	LYS
2	C	105	THR
2	C	107	LEU
2	C	108	ILE
2	C	141	HIS
2	C	149	THR
2	C	154	ARG
2	C	157	ARG
2	C	168	ARG
2	C	177	GLU
2	C	182	VAL
2	C	196	LEU
2	C	216	GLU
2	C	218	VAL
2	C	221	LEU
2	C	223	ASP

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Mol	Chain	Res	Type
2	C	229	MET
2	C	230	ARG
2	C	232	GLU
2	C	233	GLU
2	C	251	ASP
2	C	325	ILE
2	C	353	ARG
2	C	359	MET
2	C	361	MET
2	C	372	LEU
2	C	402	SER
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	527	GLU
2	C	575	GLN
2	C	584	GLU
2	C	585	GLU
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	640	ARG
2	C	650	ARG
2	C	670	GLN
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	807	ARG
2	C	815	LEU
2	C	845	ASN
2	C	848	VAL
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	36	THR
3	D	38	LYS
3	D	40	GLU
3	D	67	ARG
3	D	68	PHE

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Mol	Chain	Res	Type
3	D	69	GLU
3	D	78	VAL
3	D	81	THR
3	D	106	LYS
3	D	141	ILE
3	D	154	THR
3	D	184	GLU
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	335	LEU
3	D	354	VAL
3	D	372	ASP
3	D	374	GLU
3	D	411	THR
3	D	445	ARG
3	D	486	ARG
3	D	488	ARG
3	D	525	ARG
3	D	534	ARG
3	D	596	SER
3	D	623	VAL
3	D	637	LEU
3	D	640	HIS
3	D	709	HIS
3	D	717	GLN
3	D	754	PHE
3	D	784	ASP
3	D	785	ILE
3	D	817	GLU
3	D	829	VAL
3	D	832	ARG
3	D	833	GLU
3	D	858	VAL
3	D	867	ARG
3	D	894	LYS

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Mol	Chain	Res	Type
3	D	922	LEU
3	D	924	MET
3	D	940	THR
3	D	943	THR
3	D	969	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1046	GLN
3	D	1083	ASP
3	D	1100	ASP
3	D	1128	VAL
3	D	1130	ARG
3	D	1132	LEU
3	D	1133	ARG
3	D	1152	GLU
3	D	1208	ASP
3	D	1219	GLU
3	D	1234	THR
3	D	1283	ILE
3	D	1284	GLU
3	D	1287	GLU
3	D	1288	GLU
3	D	1289	LYS
3	D	1290	LEU
3	D	1305	LEU
3	D	1308	GLU
3	D	1310	ARG
3	D	1311	LEU
3	D	1312	LEU
3	D	1317	ASP
3	D	1373	ARG
3	D	1382	THR
3	D	1383	ASP
3	D	1389	LEU
3	D	1393	GLN
3	D	1406	ARG
3	D	1456	LYS
3	D	1468	LEU
4	E	50	THR
4	E	92	LEU
4	E	95	VAL
5	F	88	ILE

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Mol	Chain	Res	Type
5	F	117	SER
5	F	125	ASP
5	F	186	HIS
5	F	203	THR
5	F	205	ARG
5	F	218	GLN
5	F	259	ARG
5	F	287	THR
5	F	295	MET
5	F	315	VAL
5	F	325	LYS
5	F	376	ILE
5	F	377	ASP
1	K	6	LEU
1	K	58	ILE
1	K	86	VAL
1	K	87	VAL
1	K	126	ASP
1	K	142	VAL
1	K	184	THR
1	K	185	ARG
1	K	188	GLN
1	K	215	VAL
1	L	5	LYS
1	L	54	THR
1	L	96	THR
1	L	191	ASP
1	L	192	LEU
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	38	LYS
2	M	50	GLU
2	M	81	ASP
2	M	85	GLU
2	M	103	LYS
2	M	105	THR
2	M	107	LEU
2	M	133	ASP

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Mol	Chain	Res	Type
2	M	141	HIS
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	182	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	230	ARG
2	M	233	GLU
2	M	237	ARG
2	M	238	LEU
2	M	240	THR
2	M	297	GLU
2	M	299	LYS
2	M	325	ILE
2	M	353	ARG
2	M	359	MET
2	M	361	MET
2	M	372	LEU
2	M	427	VAL
2	M	434	HIS
2	M	454	SER
2	M	490	GLU
2	M	493	ARG
2	M	527	GLU
2	M	575	GLN
2	M	584	GLU
2	M	585	GLU
2	M	610	ARG
2	M	617	ASP
2	M	633	GLN
2	M	640	ARG
2	M	650	ARG
2	M	670	GLN

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Mol	Chain	Res	Type
2	M	781	LYS
2	M	807	ARG
2	M	815	LEU
2	M	816	LYS
2	M	845	ASN
2	M	848	VAL
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	48	ARG
3	N	106	LYS
3	N	107	ASP
3	N	141	ILE
3	N	154	THR
3	N	184	GLU
3	N	199	LEU
3	N	230	TRP
3	N	264	LEU
3	N	266	GLU
3	N	270	LEU
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	315	ARG
3	N	354	VAL
3	N	411	THR
3	N	434	ARG
3	N	445	ARG
3	N	486	ARG
3	N	488	ARG
3	N	518	PRO
3	N	525	ARG
3	N	587	ARG
3	N	591	VAL

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Mol	Chain	Res	Type
3	N	597	ASP
3	N	598	ARG
3	N	623	VAL
3	N	637	LEU
3	N	640	HIS
3	N	709	HIS
3	N	717	GLN
3	N	754	PHE
3	N	817	GLU
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	867	ARG
3	N	894	LYS
3	N	940	THR
3	N	943	THR
3	N	1020	LEU
3	N	1041	LEU
3	N	1044	LEU
3	N	1046	GLN
3	N	1083	ASP
3	N	1100	ASP
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	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	1301	LYS
3	N	1305	LEU

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Mol	Chain	Res	Type
3	N	1308	GLU
3	N	1311	LEU
3	N	1312	LEU
3	N	1317	ASP
3	N	1373	ARG
3	N	1382	THR
3	N	1383	ASP
3	N	1389	LEU
3	N	1393	GLN
3	N	1413	THR
3	N	1418	LYS
3	N	1459	LEU
4	O	50	THR
4	O	93	TYR
5	P	77	THR
5	P	82	ARG
5	P	123	ASP
5	P	140	ARG
5	P	186	HIS
5	P	205	ARG
5	P	222	ARG
5	P	244	ARG
5	P	287	THR
5	P	315	VAL
5	P	325	LYS
5	P	361	LEU
5	P	362	SER
5	P	377	ASP
5	P	379	ARG
5	P	383	LEU
5	P	386	VAL
5	P	393	THR
5	P	414	ARG
5	P	416	ARG
5	P	417	LYS
5	P	418	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	187	ASN
2	C	330	ASN

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Mol	Chain	Res	Type
2	C	845	ASN
2	C	884	GLN
3	D	483	HIS
3	D	1046	GLN
3	D	1172	HIS
1	L	221	HIS
2	M	187	ASN
2	M	330	ASN
2	M	845	ASN
2	M	884	GLN
3	N	483	HIS
3	N	1046	GLN
3	N	1195	GLN
3	N	1202	GLN
3	N	1441	GLN
5	P	381	HIS

5.3.3 RNA

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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, 95^{th} 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%)	-0.27	0 100 100	47, 67, 98, 118	0
1	B	222/315 (70%)	-0.17	2 (0%) 85 64	50, 79, 119, 142	0
1	K	226/315 (71%)	-0.21	0 100 100	49, 73, 103, 122	0
1	L	225/315 (71%)	-0.14	3 (1%) 79 53	51, 81, 126, 148	0
2	C	1111/1119 (99%)	-0.02	29 (2%) 59 29	34, 62, 122, 168	0
2	M	1111/1119 (99%)	0.26	84 (7%) 17 6	38, 76, 142, 179	0
3	D	1482/1524 (97%)	0.03	50 (3%) 49 21	32, 66, 130, 178	1 (0%)
3	N	1489/1524 (97%)	0.07	57 (3%) 44 18	34, 69, 129, 201	1 (0%)
4	E	94/99 (94%)	-0.07	3 (3%) 51 23	44, 66, 113, 121	0
4	O	94/99 (94%)	-0.09	3 (3%) 51 23	49, 72, 116, 130	0
5	F	346/443 (78%)	-0.14	6 (1%) 73 45	42, 70, 124, 147	0
5	P	347/443 (78%)	0.05	17 (4%) 33 13	46, 83, 156, 214	0
6	G	16/21 (76%)	-0.45	0 100 100	42, 78, 172, 179	0
6	Q	16/21 (76%)	-0.60	0 100 100	53, 80, 182, 183	0
7	H	24/27 (88%)	-0.35	0 100 100	67, 95, 146, 201	0
7	R	24/27 (88%)	-0.35	0 100 100	65, 106, 160, 210	0
8	I	2/2 (100%)	-0.37	0 100 100	50, 50, 50, 55	0
8	S	2/2 (100%)	-0.35	0 100 100	62, 62, 62, 63	0
All	All	7057/7730 (91%)	0.02	254 (3%) 46 20	32, 71, 132, 214	2 (0%)

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	363	SER	6.6
5	P	392	VAL	6.1
5	P	411	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
2	M	191	PHE	6.0
5	P	375	LEU	5.7
2	M	196	LEU	5.5
2	M	367	LEU	5.5
2	M	200	LEU	5.4
2	M	362	GLY	5.3
3	D	241	ILE	5.1
5	P	389	PHE	5.0
3	N	1247	ALA	4.9
2	M	311	PHE	4.9
3	D	991	GLN	4.8
5	P	410	TYR	4.8
2	M	211	LEU	4.5
3	N	1246	VAL	4.4
5	P	415	THR	4.3
2	M	199	VAL	4.3
2	M	296	GLY	4.3
2	M	226	VAL	4.3
5	P	393	THR	4.3
3	D	980	MET	4.3
2	M	221	LEU	4.2
5	P	373	LYS	4.2
2	M	778	PHE	4.2
2	C	364	GLU	4.2
2	C	365	ASP	4.2
2	M	364	GLU	4.2
3	N	355	VAL	4.1
3	N	367	ILE	4.0
3	D	1297	GLU	4.0
5	P	423	ASP	3.9
3	D	335	LEU	3.9
3	N	978	TYR	3.9
3	N	311	LEU	3.8
2	M	295	ASP	3.8
5	F	423	ASP	3.8
2	M	207	LEU	3.7
3	N	191	LEU	3.7
2	C	188	LYS	3.7
3	N	378	ILE	3.7
3	N	1128	VAL	3.7
2	M	368	THR	3.7
2	M	231	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	M	64	LEU	3.7
2	C	176	VAL	3.7
3	D	995	LEU	3.7
2	C	366	SER	3.7
3	D	367	ILE	3.7
2	M	172	ILE	3.6
2	M	181	VAL	3.6
5	P	391	GLY	3.6
2	M	184	MET	3.6
3	D	1279	GLY	3.6
2	M	777	ILE	3.6
2	M	188	LYS	3.6
2	M	109	LYS	3.6
2	M	68	PHE	3.6
3	D	1128	VAL	3.5
5	P	390	PHE	3.5
2	M	649	VAL	3.5
3	N	202	VAL	3.5
2	M	365	ASP	3.5
3	D	343	LYS	3.5
3	D	203	ALA	3.5
2	C	219	GLN	3.4
3	D	982	PHE	3.4
4	O	85	LEU	3.4
3	N	1250	ALA	3.4
3	N	1249	ALA	3.3
3	D	371	ILE	3.3
1	L	65	PHE	3.3
2	M	107	LEU	3.3
3	N	177	ALA	3.3
3	N	371	ILE	3.3
2	M	104	ASP	3.3
3	D	976	GLN	3.2
2	M	98	LEU	3.2
2	C	814	GLU	3.2
2	M	297	GLU	3.2
3	N	1129	THR	3.2
2	M	222	MET	3.2
2	C	101	ILE	3.2
2	M	764	GLU	3.2
3	D	977	ALA	3.1
2	M	769	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	257	VAL	3.1
3	N	232	GLU	3.1
2	M	300	ASP	3.1
2	C	616	GLU	3.1
5	P	414	ARG	3.1
4	O	84	ARG	3.1
3	D	1130	ARG	3.1
2	C	811	PRO	3.1
3	N	974	ILE	3.0
2	M	152	PRO	3.0
3	N	406	ASP	3.0
3	N	394	LEU	3.0
3	N	1304	LYS	3.0
2	M	201	GLY	3.0
2	M	344	PHE	3.0
5	P	359	SER	3.0
3	N	1408	ILE	2.9
3	D	1318	TYR	2.9
3	D	213	VAL	2.9
2	M	762	LYS	2.9
3	D	1495	ILE	2.9
3	N	213	VAL	2.9
5	P	386	VAL	2.9
2	M	44	ILE	2.9
3	N	1409	ALA	2.9
2	M	30	LEU	2.9
2	M	811	PRO	2.9
2	M	175	GLU	2.8
2	M	766	GLU	2.8
3	D	988	ARG	2.8
3	D	309	GLY	2.8
3	N	352	ASN	2.8
2	C	181	VAL	2.8
3	N	388	HIS	2.8
3	N	1281	VAL	2.8
2	M	307	LEU	2.8
4	E	52	GLU	2.8
2	M	219	GLN	2.8
3	D	983	LEU	2.8
3	D	360	ARG	2.8
2	M	655	LEU	2.7
5	P	416	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	645	VAL	2.7
2	M	102	HIS	2.7
3	D	406	ASP	2.7
3	D	198	ARG	2.7
2	M	66	LEU	2.7
3	N	426	LYS	2.7
3	N	971	LEU	2.7
2	M	111	ASP	2.7
2	C	815	LEU	2.7
3	N	1497	GLU	2.7
3	N	1299	PHE	2.7
2	M	108	ILE	2.7
3	D	345	TYR	2.6
5	P	406	ARG	2.6
3	D	310	LEU	2.6
2	M	265	ARG	2.6
2	M	254	VAL	2.6
3	N	353	VAL	2.6
3	D	973	GLN	2.6
3	N	1251	ASP	2.6
3	D	388	HIS	2.6
3	N	1319	VAL	2.6
3	D	839	LEU	2.6
2	M	153	ALA	2.6
2	M	48	PHE	2.6
2	M	595	LEU	2.6
3	D	322	VAL	2.6
2	M	197	LEU	2.6
2	C	650	ARG	2.6
3	N	212	ARG	2.6
3	N	197	SER	2.6
3	N	1313	VAL	2.5
2	M	372	LEU	2.5
3	N	218	LYS	2.5
3	D	1294	VAL	2.5
3	N	68	PHE	2.5
2	M	101	ILE	2.5
3	D	992	ILE	2.5
2	M	106	GLY	2.5
2	M	354	GLY	2.5
2	M	1	MET	2.5
2	C	65	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	594	ALA	2.4
2	C	55	GLU	2.4
3	D	197	SER	2.4
2	M	190	LYS	2.4
3	D	212	ARG	2.4
3	N	236	TYR	2.4
4	O	95	VAL	2.4
3	N	1248	GLY	2.4
3	N	396	VAL	2.4
2	C	66	LEU	2.4
2	M	629	TYR	2.4
3	D	355	VAL	2.4
3	N	1495	ILE	2.3
2	M	235	LEU	2.3
3	D	76	CYS	2.3
3	N	63	TYR	2.3
2	M	644	VAL	2.3
2	C	764	GLU	2.3
2	C	729	LEU	2.3
2	M	65	VAL	2.3
3	N	407	VAL	2.3
2	C	629	TYR	2.3
5	F	422	LEU	2.3
3	N	1314	LYS	2.3
2	M	176	VAL	2.3
3	D	339	TRP	2.3
2	M	371	LYS	2.3
3	D	161	LEU	2.3
2	M	293	PHE	2.2
3	D	1498	ALA	2.2
2	M	351	LEU	2.2
3	D	470	LEU	2.2
3	N	235	ALA	2.2
2	C	254	VAL	2.2
2	M	785	VAL	2.2
3	N	316	GLN	2.2
2	C	778	PHE	2.2
2	C	157	ARG	2.2
5	F	388	ALA	2.2
2	C	69	LEU	2.2
2	C	170	PRO	2.2
2	M	614	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1319	VAL	2.2
1	L	4	SER	2.2
3	N	1253	THR	2.2
2	M	220	GLY	2.1
3	N	1493	LYS	2.1
5	P	382	THR	2.1
3	N	807	ALA	2.1
2	M	814	GLU	2.1
5	F	380	GLU	2.1
3	N	279	VAL	2.1
4	E	51	LEU	2.1
2	C	771	GLU	2.1
2	M	294	GLU	2.1
1	L	165	ILE	2.1
3	N	393	ILE	2.1
3	D	321	GLN	2.1
3	D	409	VAL	2.1
2	C	92	ALA	2.1
3	N	203	ALA	2.1
4	E	87	LYS	2.1
3	N	133	ILE	2.1
3	N	318	ARG	2.1
2	C	100	LEU	2.1
3	D	165	LYS	2.1
5	F	232	ARG	2.1
3	D	666	ILE	2.1
1	B	64	GLU	2.1
2	M	170	PRO	2.1
3	D	1041	LEU	2.1
3	N	1292	VAL	2.1
2	M	203	ASP	2.1
3	D	365	ASP	2.1
5	F	379	ARG	2.1
1	B	66	SER	2.0
2	M	621	VAL	2.0
2	C	172	ILE	2.0
3	D	1408	ILE	2.0
3	D	1312	LEU	2.0
2	M	225	SER	2.0
3	N	405	ASP	2.0
2	M	314	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	MG	K	1001	1/1	0.89	0.66	11.75	69,69,69,69	0
10	MG	N	2004	1/1	0.83	0.37	2.41	65,65,65,65	0
10	MG	D	2004	1/1	0.97	0.44	1.92	63,63,63,63	0
9	ZN	N	2001	1/1	0.98	0.20	1.27	62,62,62,62	0
9	ZN	D	2001	1/1	0.99	0.13	-0.59	62,62,62,62	0
9	ZN	N	2002	1/1	0.99	0.05	-1.45	107,107,107,107	0
9	ZN	D	2002	1/1	0.98	0.08	-1.85	83,83,83,83	0
10	MG	D	2003	1/1	0.94	0.24	-	40,40,40,40	0
10	MG	N	2003	1/1	0.79	0.20	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.