



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:22 am BST

PDB ID : 6AP4
Title : Crystal structure of the DNA polymerase III subunit beta from *Acinetobacter baumannii*
Authors : McGrath, A.E.; Oakley, A.J.
Deposited on : 2017-08-16
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

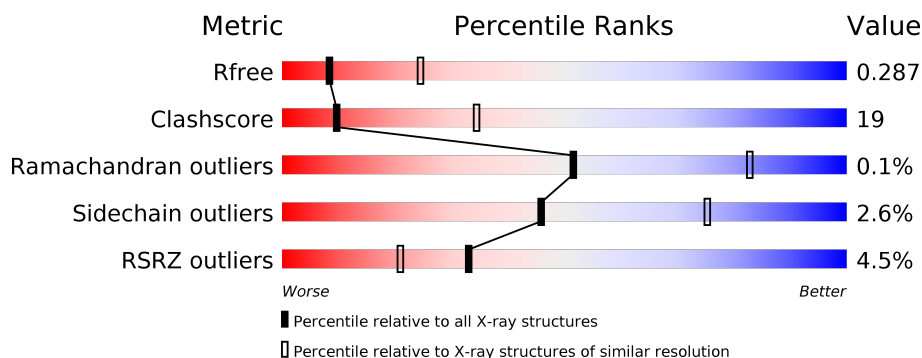
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>29%</div> <div></div> </div> <div>.</div> </div>
1	B	388	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div></div> </div> <div>..</div> </div>
1	C	388	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div></div> </div> <div>..</div> </div>
1	D	388	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div></div> </div> <div>..</div> </div>
1	E	388	<div> <div></div> <div> <div></div> <div>73%</div> <div>24%</div> <div></div> </div> <div>..</div> </div>
1	F	388	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div></div> </div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	388	
1	H	388	
1	I	388	
1	J	388	
1	K	388	
1	L	388	
1	M	388	
1	N	388	
1	O	388	
1	P	388	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 46780 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 polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2938	1836	515	575	12			
1	B	382	Total	C	N	O	S	0	0	0
			2964	1852	518	582	12			
1	C	379	Total	C	N	O	S	0	0	0
			2942	1842	514	574	12			
1	D	382	Total	C	N	O	S	0	0	0
			2962	1853	520	578	11			
1	E	382	Total	C	N	O	S	0	0	0
			2965	1852	519	582	12			
1	F	379	Total	C	N	O	S	0	0	0
			2942	1839	515	576	12			
1	G	378	Total	C	N	O	S	0	0	0
			2941	1840	516	573	12			
1	H	383	Total	C	N	O	S	0	0	0
			2957	1848	517	580	12			
1	I	370	Total	C	N	O	S	0	0	0
			2874	1804	503	555	12			
1	J	384	Total	C	N	O	S	0	0	0
			2981	1862	525	582	12			
1	K	365	Total	C	N	O	S	0	1	0
			2830	1773	497	547	13			
1	L	356	Total	C	N	O	S	0	0	0
			2735	1710	476	537	12			
1	M	378	Total	C	N	O	S	0	0	0
			2929	1833	510	574	12			
1	N	372	Total	C	N	O	S	0	0	0
			2891	1812	507	560	12			
1	O	357	Total	C	N	O	S	0	0	0
			2768	1741	486	530	11			
1	P	377	Total	C	N	O	S	0	0	0
			2914	1823	508	571	12			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP V5V7W3
A	-4	HIS	-	expression tag	UNP V5V7W3
A	-3	HIS	-	expression tag	UNP V5V7W3
A	-2	HIS	-	expression tag	UNP V5V7W3
A	-1	HIS	-	expression tag	UNP V5V7W3
A	0	HIS	-	expression tag	UNP V5V7W3
B	-5	HIS	-	expression tag	UNP V5V7W3
B	-4	HIS	-	expression tag	UNP V5V7W3
B	-3	HIS	-	expression tag	UNP V5V7W3
B	-2	HIS	-	expression tag	UNP V5V7W3
B	-1	HIS	-	expression tag	UNP V5V7W3
B	0	HIS	-	expression tag	UNP V5V7W3
C	-5	HIS	-	expression tag	UNP V5V7W3
C	-4	HIS	-	expression tag	UNP V5V7W3
C	-3	HIS	-	expression tag	UNP V5V7W3
C	-2	HIS	-	expression tag	UNP V5V7W3
C	-1	HIS	-	expression tag	UNP V5V7W3
C	0	HIS	-	expression tag	UNP V5V7W3
D	-5	HIS	-	expression tag	UNP V5V7W3
D	-4	HIS	-	expression tag	UNP V5V7W3
D	-3	HIS	-	expression tag	UNP V5V7W3
D	-2	HIS	-	expression tag	UNP V5V7W3
D	-1	HIS	-	expression tag	UNP V5V7W3
D	0	HIS	-	expression tag	UNP V5V7W3
E	-5	HIS	-	expression tag	UNP V5V7W3
E	-4	HIS	-	expression tag	UNP V5V7W3
E	-3	HIS	-	expression tag	UNP V5V7W3
E	-2	HIS	-	expression tag	UNP V5V7W3
E	-1	HIS	-	expression tag	UNP V5V7W3
E	0	HIS	-	expression tag	UNP V5V7W3
F	-5	HIS	-	expression tag	UNP V5V7W3
F	-4	HIS	-	expression tag	UNP V5V7W3
F	-3	HIS	-	expression tag	UNP V5V7W3
F	-2	HIS	-	expression tag	UNP V5V7W3
F	-1	HIS	-	expression tag	UNP V5V7W3
F	0	HIS	-	expression tag	UNP V5V7W3
G	-5	HIS	-	expression tag	UNP V5V7W3
G	-4	HIS	-	expression tag	UNP V5V7W3
G	-3	HIS	-	expression tag	UNP V5V7W3
G	-2	HIS	-	expression tag	UNP V5V7W3
G	-1	HIS	-	expression tag	UNP V5V7W3
G	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP V5V7W3
H	-4	HIS	-	expression tag	UNP V5V7W3
H	-3	HIS	-	expression tag	UNP V5V7W3
H	-2	HIS	-	expression tag	UNP V5V7W3
H	-1	HIS	-	expression tag	UNP V5V7W3
H	0	HIS	-	expression tag	UNP V5V7W3
I	-5	HIS	-	expression tag	UNP V5V7W3
I	-4	HIS	-	expression tag	UNP V5V7W3
I	-3	HIS	-	expression tag	UNP V5V7W3
I	-2	HIS	-	expression tag	UNP V5V7W3
I	-1	HIS	-	expression tag	UNP V5V7W3
I	0	HIS	-	expression tag	UNP V5V7W3
J	-5	HIS	-	expression tag	UNP V5V7W3
J	-4	HIS	-	expression tag	UNP V5V7W3
J	-3	HIS	-	expression tag	UNP V5V7W3
J	-2	HIS	-	expression tag	UNP V5V7W3
J	-1	HIS	-	expression tag	UNP V5V7W3
J	0	HIS	-	expression tag	UNP V5V7W3
K	-5	HIS	-	expression tag	UNP V5V7W3
K	-4	HIS	-	expression tag	UNP V5V7W3
K	-3	HIS	-	expression tag	UNP V5V7W3
K	-2	HIS	-	expression tag	UNP V5V7W3
K	-1	HIS	-	expression tag	UNP V5V7W3
K	0	HIS	-	expression tag	UNP V5V7W3
L	-5	HIS	-	expression tag	UNP V5V7W3
L	-4	HIS	-	expression tag	UNP V5V7W3
L	-3	HIS	-	expression tag	UNP V5V7W3
L	-2	HIS	-	expression tag	UNP V5V7W3
L	-1	HIS	-	expression tag	UNP V5V7W3
L	0	HIS	-	expression tag	UNP V5V7W3
M	-5	HIS	-	expression tag	UNP V5V7W3
M	-4	HIS	-	expression tag	UNP V5V7W3
M	-3	HIS	-	expression tag	UNP V5V7W3
M	-2	HIS	-	expression tag	UNP V5V7W3
M	-1	HIS	-	expression tag	UNP V5V7W3
M	0	HIS	-	expression tag	UNP V5V7W3
N	-5	HIS	-	expression tag	UNP V5V7W3
N	-4	HIS	-	expression tag	UNP V5V7W3
N	-3	HIS	-	expression tag	UNP V5V7W3
N	-2	HIS	-	expression tag	UNP V5V7W3
N	-1	HIS	-	expression tag	UNP V5V7W3
N	0	HIS	-	expression tag	UNP V5V7W3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	HIS	-	expression tag	UNP V5V7W3
O	-4	HIS	-	expression tag	UNP V5V7W3
O	-3	HIS	-	expression tag	UNP V5V7W3
O	-2	HIS	-	expression tag	UNP V5V7W3
O	-1	HIS	-	expression tag	UNP V5V7W3
O	0	HIS	-	expression tag	UNP V5V7W3
P	-5	HIS	-	expression tag	UNP V5V7W3
P	-4	HIS	-	expression tag	UNP V5V7W3
P	-3	HIS	-	expression tag	UNP V5V7W3
P	-2	HIS	-	expression tag	UNP V5V7W3
P	-1	HIS	-	expression tag	UNP V5V7W3
P	0	HIS	-	expression tag	UNP V5V7W3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	J	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	14	Total O 14 14	0	0
3	B	14	Total O 14 14	0	0
3	C	15	Total O 15 15	0	0
3	D	30	Total O 30 30	0	0
3	E	47	Total O 47 47	0	0
3	F	11	Total O 11 11	0	0
3	G	22	Total O 22 22	0	0
3	H	8	Total O 8 8	0	0
3	I	5	Total O 5 5	0	0

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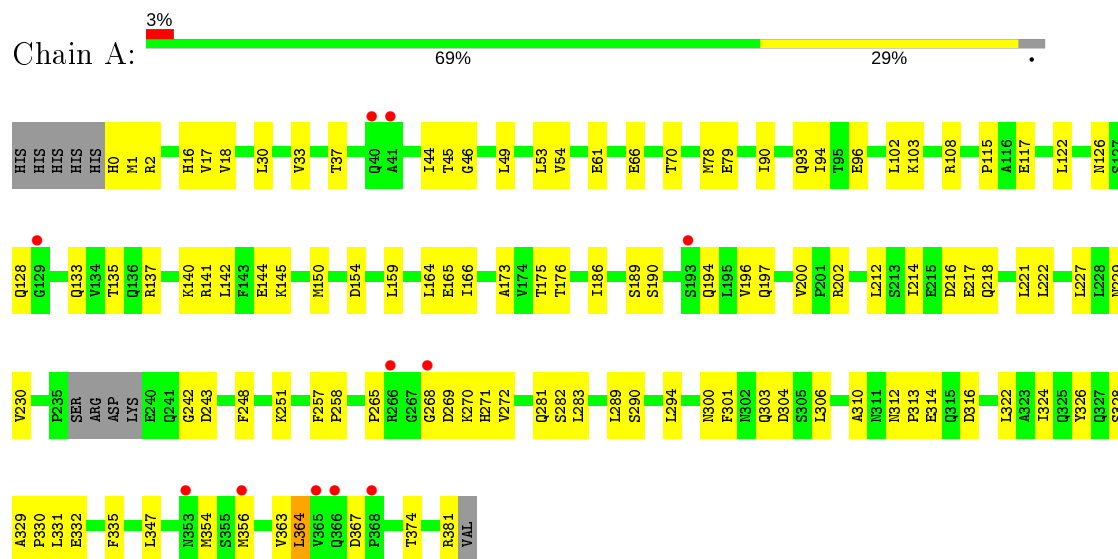
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	17	Total 17	O 17	0	0
3	K	9	Total 9	O 9	0	0
3	L	10	Total 10	O 10	0	0
3	M	18	Total 18	O 18	0	0
3	N	9	Total 9	O 9	0	0
3	O	6	Total 6	O 6	0	0
3	P	10	Total 10	O 10	0	0

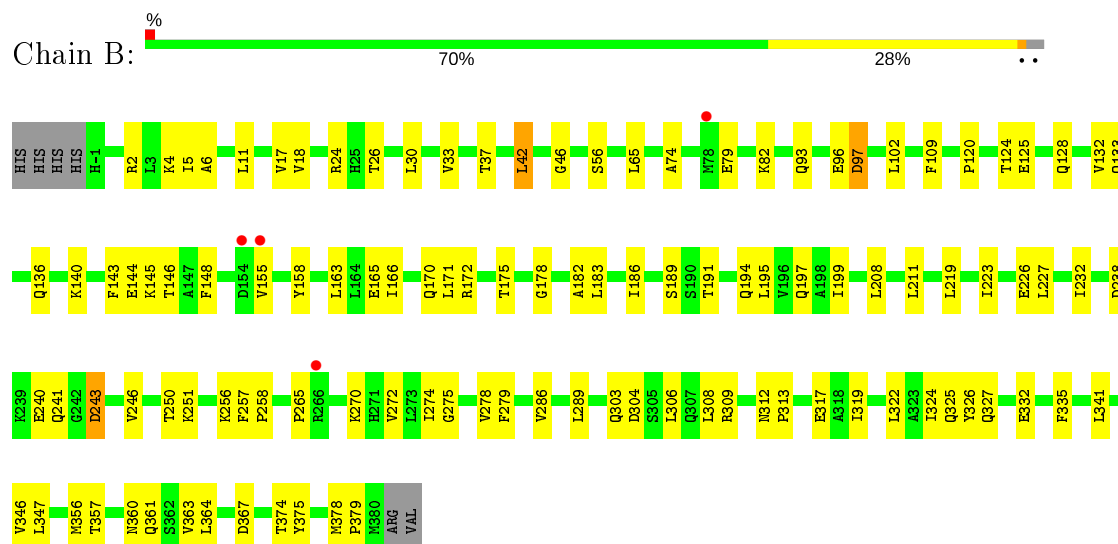
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 polymerase III subunit beta

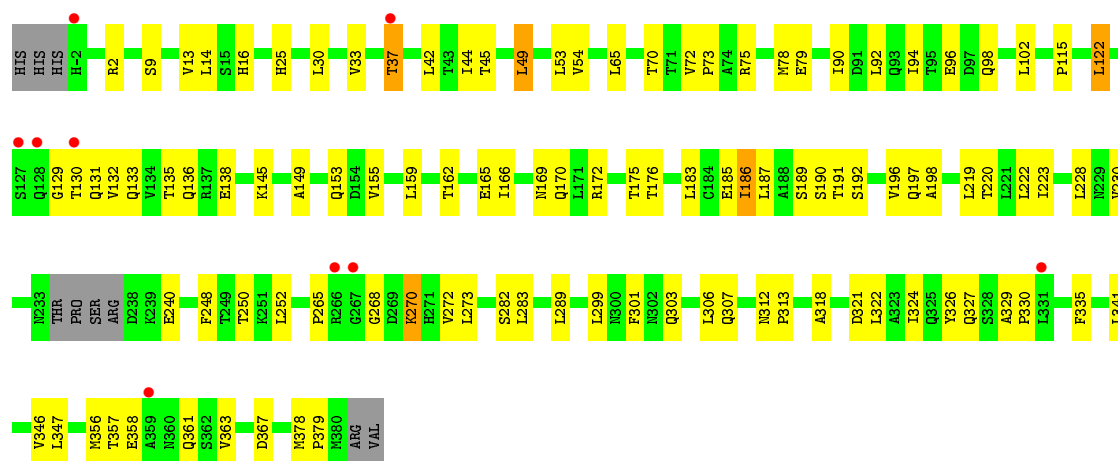


• Molecule 1: DNA polymerase III subunit beta

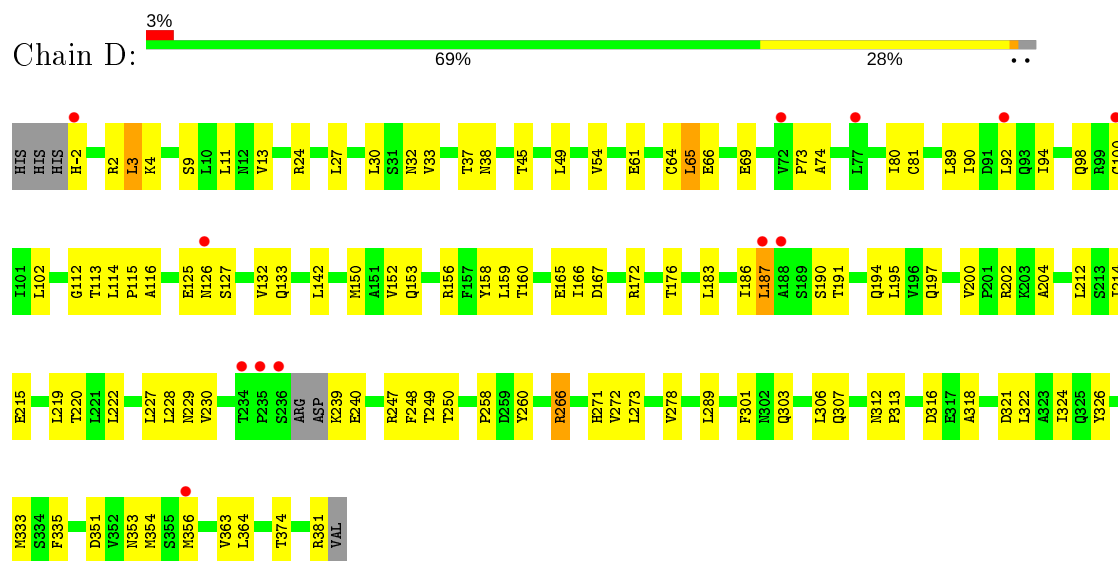


• Molecule 1: DNA polymerase III subunit beta

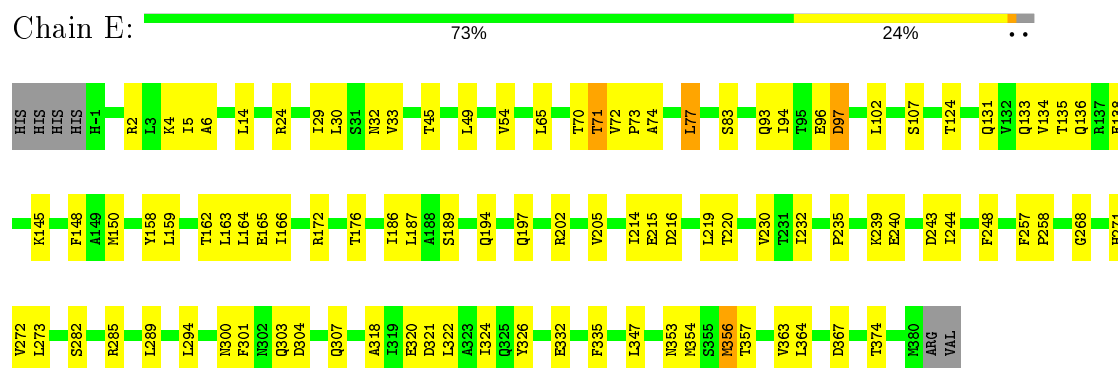




• Molecule 1: DNA polymerase III subunit beta

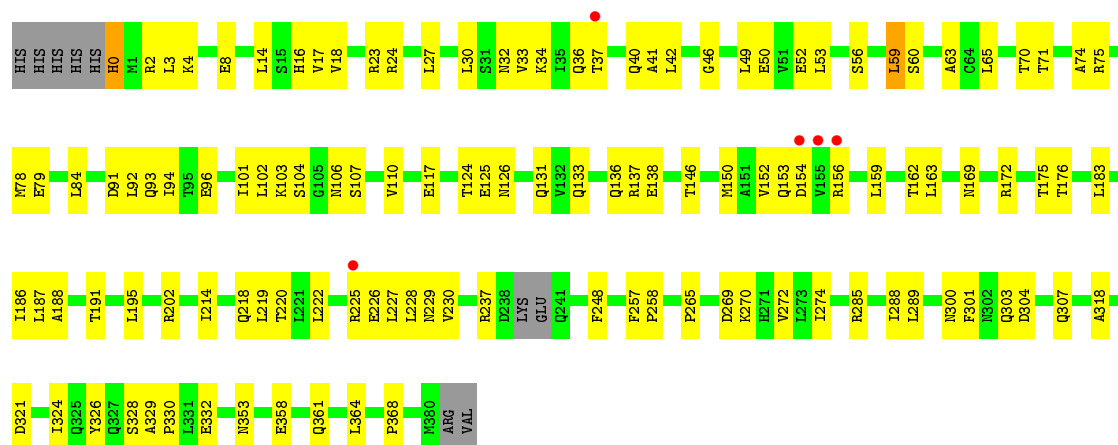


• Molecule 1: DNA polymerase III subunit beta

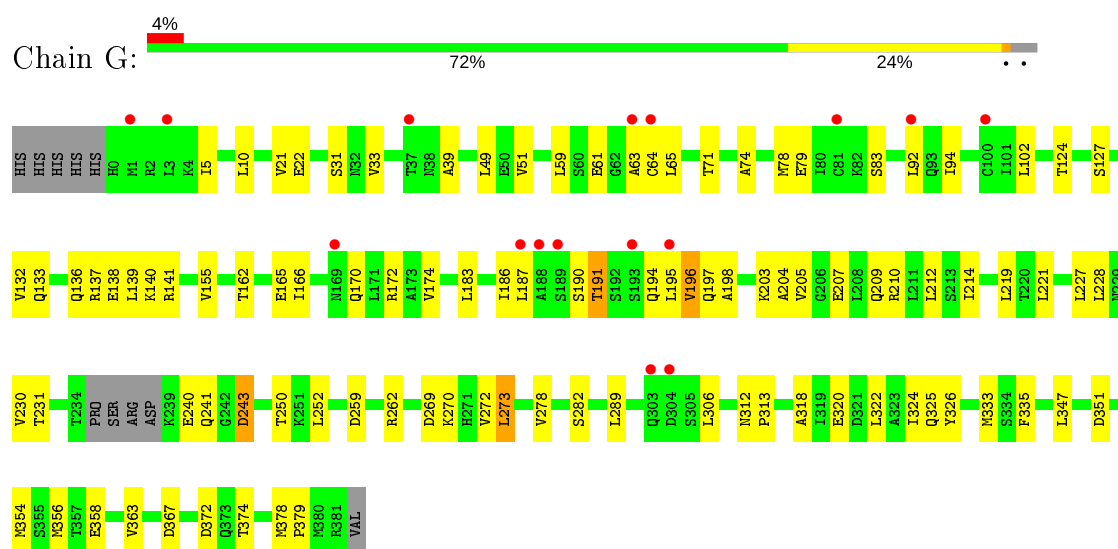


• Molecule 1: DNA polymerase III subunit beta

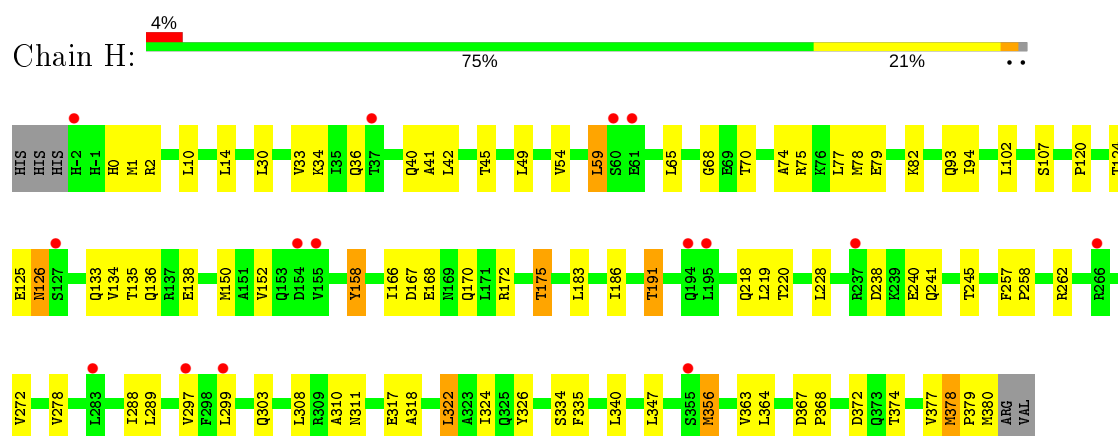




• Molecule 1: DNA polymerase III subunit beta

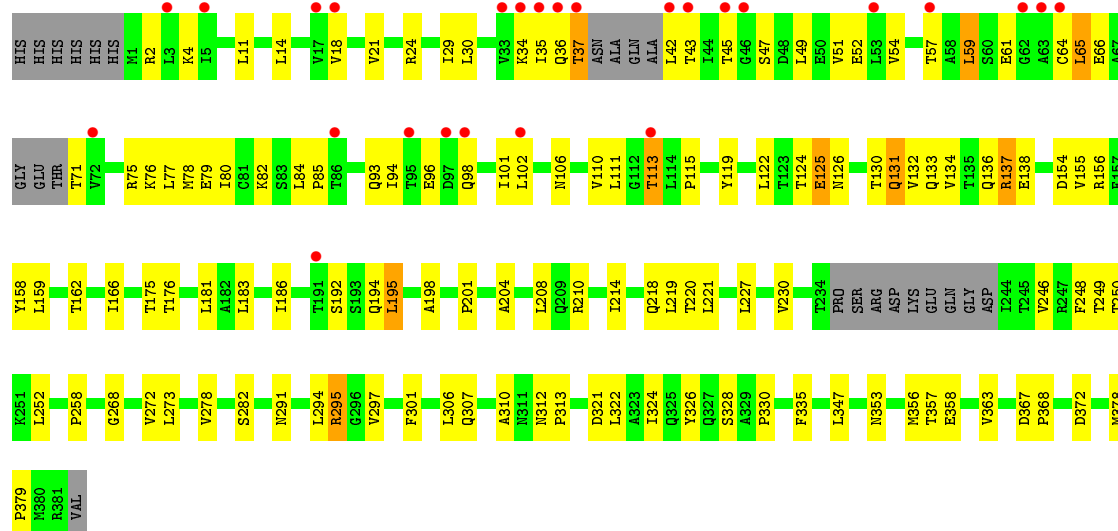


• Molecule 1: DNA polymerase III subunit beta

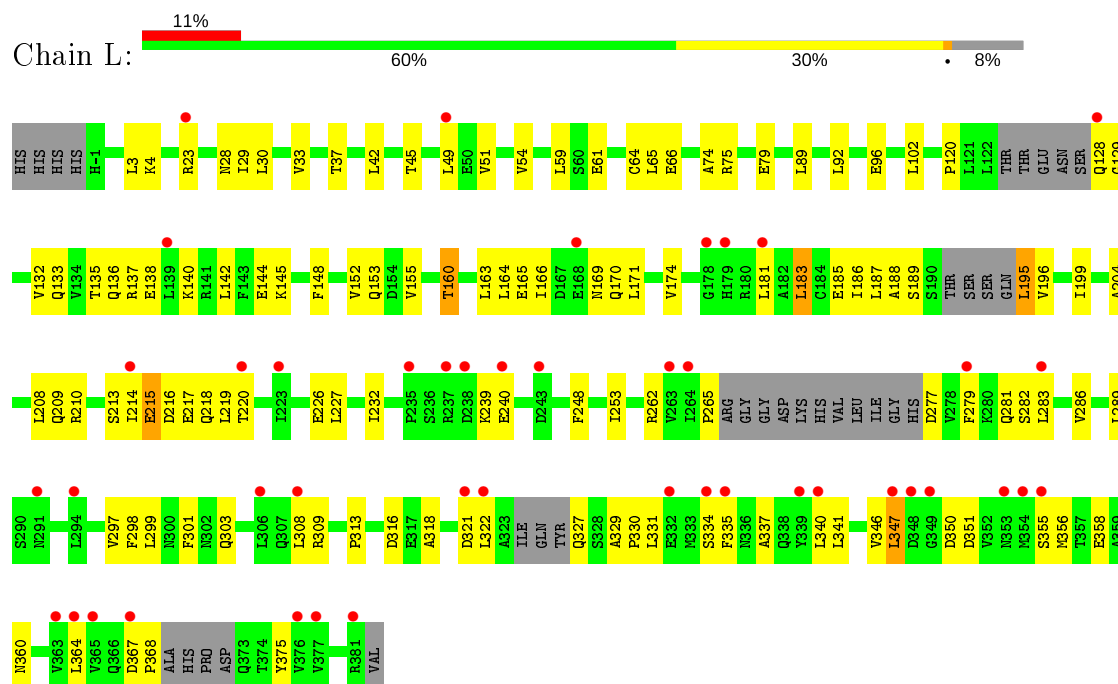


• Molecule 1: DNA polymerase III subunit beta

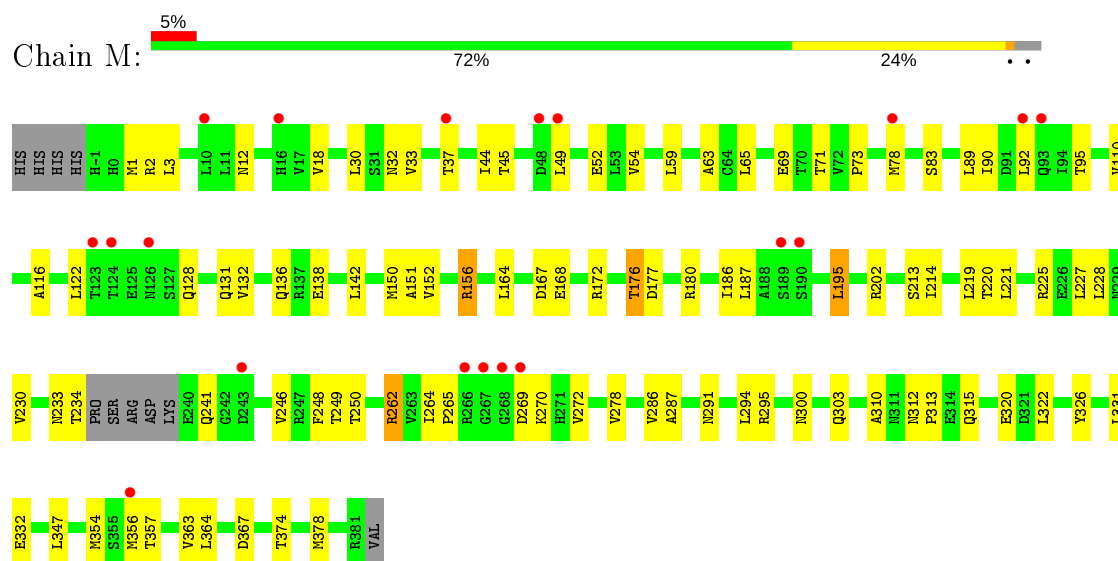




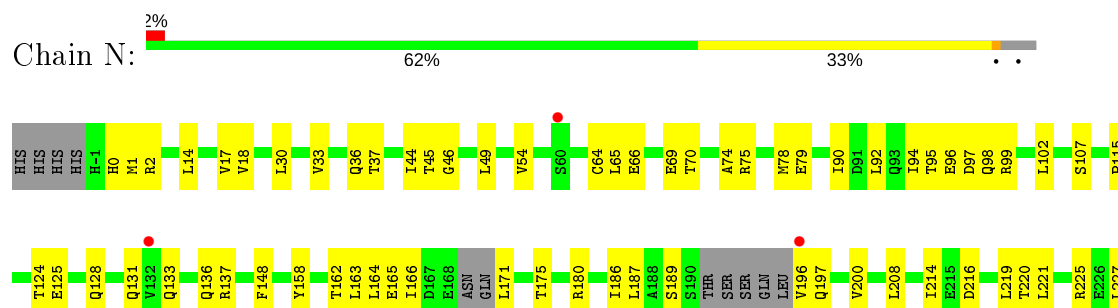
- Molecule 1: DNA polymerase III subunit beta

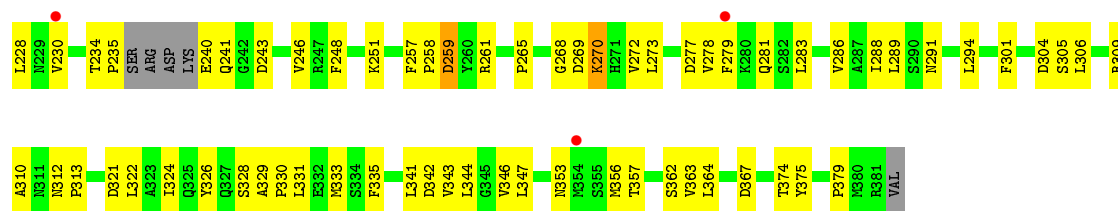


- Molecule 1: DNA polymerase III subunit beta

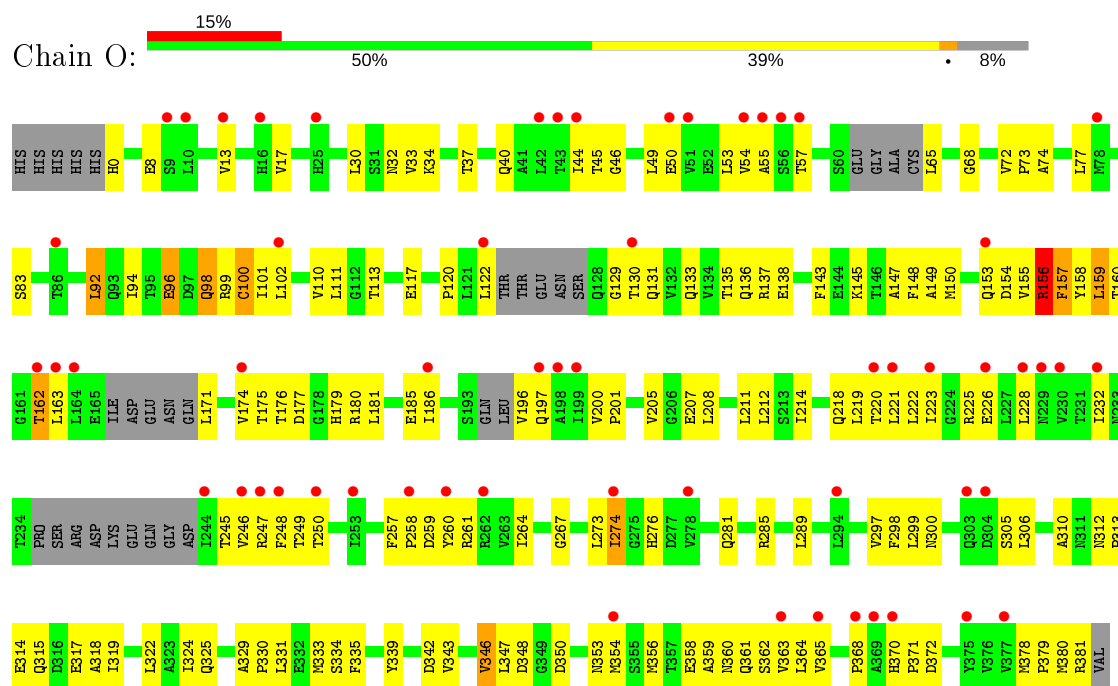


- Molecule 1: DNA polymerase III subunit beta

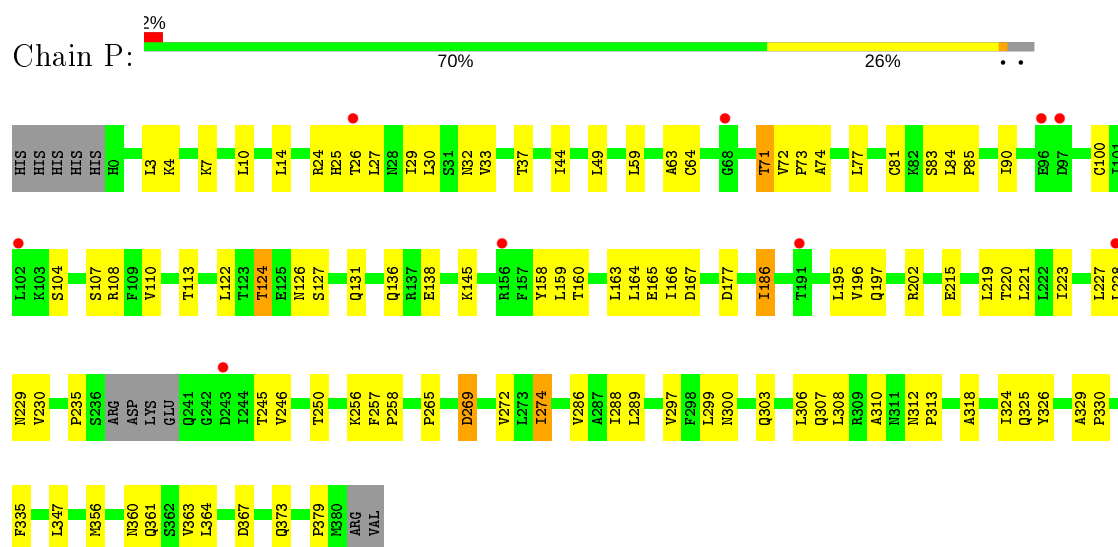




• Molecule 1: DNA polymerase III subunit beta



• Molecule 1: DNA polymerase III subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.71 Å 328.60 Å 147.50 Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	164.30 – 2.95 49.06 – 2.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (164.30-2.95) 85.5 (49.06-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.248 , 0.287 0.243 , 0.287	Depositor DCC
R_{free} test set	6719 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 10.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46780	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2972	0.73	0/4029
1	B	0.52	0/3000	0.75	0/4070
1	C	0.48	0/2977	0.73	0/4035
1	D	0.53	0/2998	0.74	0/4066
1	E	0.60	0/3001	0.79	0/4070
1	F	0.51	0/2976	0.72	0/4035
1	G	0.49	0/2974	0.75	0/4030
1	H	0.46	0/2994	0.70	0/4064
1	I	0.49	0/2907	0.72	0/3940
1	J	0.48	0/3018	0.71	0/4094
1	K	0.51	0/2860	0.75	0/3876
1	L	0.47	0/2759	0.73	0/3736
1	M	0.48	0/2963	0.72	0/4018
1	N	0.47	0/2924	0.71	0/3961
1	O	0.40	0/2797	0.71	1/3786 (0.0%)
1	P	0.45	0/2948	0.70	0/3999
All	All	0.49	0/47068	0.73	1/63809 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	156	ARG	N-CA-C	-5.06	97.34	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2938	0	2992	114	0
1	B	2964	0	3009	117	0
1	C	2942	0	2990	101	0
1	D	2962	0	3006	111	0
1	E	2965	0	3011	89	0
1	F	2942	0	2998	119	0
1	G	2941	0	3001	96	0
1	H	2957	0	2986	108	0
1	I	2874	0	2939	110	0
1	J	2981	0	3025	98	0
1	K	2830	0	2874	131	0
1	L	2735	0	2772	158	0
1	M	2929	0	2975	102	0
1	N	2891	0	2948	149	0
1	O	2768	0	2839	185	0
1	P	2914	0	2963	95	0
2	C	1	0	0	0	0
2	J	1	0	0	0	0
3	A	14	0	0	0	0
3	B	14	0	0	1	0
3	C	15	0	0	0	0
3	D	30	0	0	0	0
3	E	47	0	0	2	0
3	F	11	0	0	1	0
3	G	22	0	0	1	0
3	H	8	0	0	0	0
3	I	5	0	0	0	0
3	J	17	0	0	0	0
3	K	9	0	0	1	0
3	L	10	0	0	0	0
3	M	18	0	0	0	0
3	N	9	0	0	1	0
3	O	6	0	0	0	0
3	P	10	0	0	0	0
All	All	46780	0	47328	1816	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1816) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:276:HIS:CD2	1:O:347:LEU:HD11	1.53	1.40
1:G:92:LEU:HG	1:G:102:LEU:CD2	1.62	1.28
1:O:276:HIS:CD2	1:O:347:LEU:CD1	2.23	1.19
1:H:1:MET:CE	1:H:70:THR:HG22	1.73	1.19
1:C:162:THR:HG22	1:C:175:THR:CG2	1.72	1.18
1:D:4:LYS:NZ	1:D:89:LEU:HB3	1.60	1.17
1:J:308:LEU:HD11	1:J:322:LEU:HD21	1.22	1.16
1:O:98:GLN:HG2	1:O:113:THR:O	1.44	1.15
1:I:4:LYS:HE2	1:I:91:ASP:OD2	1.43	1.15
1:L:137:ARG:HB2	1:L:215:GLU:HA	1.28	1.15
1:L:303:GLN:OE1	1:L:327:GLN:HA	1.46	1.15
1:I:166:ILE:CG2	1:I:196:VAL:HG22	1.77	1.14
1:B:346:VAL:HG11	1:B:375:TYR:OH	1.45	1.13
1:H:1:MET:HE1	1:H:70:THR:HG22	1.20	1.13
1:P:7:LYS:CD	1:P:84:LEU:HB2	1.81	1.11
1:K:14:LEU:CD1	1:K:78:MET:SD	2.39	1.10
1:K:132:VAL:HG21	1:K:166:ILE:HD11	1.15	1.10
1:I:5:ILE:HD12	1:I:10:LEU:HB2	1.33	1.10
1:L:367:ASP:OD1	1:L:368:PRO:HD2	1.50	1.09
1:G:92:LEU:HG	1:G:102:LEU:HD23	1.19	1.09
1:C:162:THR:HG22	1:C:175:THR:HG22	1.30	1.08
1:N:36:GLN:HG2	1:N:69:GLU:HG2	1.27	1.08
1:M:262:ARG:HH11	1:M:262:ARG:HB2	1.18	1.07
1:J:312:ASN:HB2	1:J:313:PRO:HD2	1.32	1.06
1:C:136:GLN:HG2	1:C:219:LEU:HD11	1.35	1.06
1:K:14:LEU:HD13	1:K:78:MET:SD	1.95	1.06
1:G:172:ARG:HD3	1:G:183:LEU:HD11	1.38	1.05
1:K:132:VAL:HG21	1:K:166:ILE:CD1	1.86	1.05
1:N:36:GLN:HG2	1:N:69:GLU:CG	1.86	1.04
1:I:166:ILE:HG21	1:I:196:VAL:HG22	1.37	1.04
1:K:378[A]:MET:SD	1:K:379:PRO:HD2	1.97	1.04
1:P:167:ASP:HB2	1:P:195:LEU:HD23	1.39	1.04
1:G:221:LEU:HD23	1:G:230:VAL:CG2	1.87	1.03
1:B:143:PHE:CE2	1:B:208:LEU:HD23	1.94	1.02
1:J:312:ASN:HB2	1:J:313:PRO:CD	1.88	1.02
1:N:33:VAL:HG23	1:N:74:ALA:HB2	1.41	1.01
1:N:279:PHE:CE1	1:N:283:LEU:HD21	1.94	1.01
1:C:312:ASN:HB2	1:C:313:PRO:HD2	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LYS:H	1:C:270:LYS:HD2	1.17	1.01
1:K:132:VAL:CG2	1:K:166:ILE:CD1	2.39	1.01
1:H:133:GLN:HB3	1:H:218:GLN:HE21	1.21	1.00
1:H:33:VAL:HG13	1:H:74:ALA:HB2	1.44	0.99
1:J:273:LEU:HD21	1:J:351:ASP:HB3	1.40	0.99
1:K:132:VAL:CG2	1:K:166:ILE:HD11	1.92	0.99
1:N:98:GLN:HE22	1:N:115:PRO:HD3	1.25	0.99
1:B:257:PHE:CD2	1:B:258:PRO:HD2	1.97	0.98
1:H:133:GLN:HB3	1:H:218:GLN:NE2	1.77	0.98
1:O:135:THR:HG23	1:O:138:GLU:H	1.26	0.97
1:J:308:LEU:HD11	1:J:322:LEU:CD2	1.95	0.97
1:M:1:MET:SD	1:M:37:THR:HG22	2.04	0.97
1:I:195:LEU:H	1:I:195:LEU:CD1	1.77	0.97
1:O:276:HIS:NE2	1:O:347:LEU:HD11	1.78	0.97
1:P:312:ASN:HB2	1:P:313:PRO:HD2	1.44	0.96
1:L:350:ASP:O	1:L:351:ASP:OD1	1.81	0.96
1:E:300:ASN:OD1	1:E:332:GLU:HG3	1.64	0.96
1:H:378:MET:HB3	1:H:379:PRO:HD2	1.48	0.96
1:C:145:LYS:HD2	1:C:346:VAL:HG22	1.44	0.96
1:M:156:ARG:HG2	1:M:156:ARG:HH11	1.31	0.96
1:L:265:PRO:HG2	1:L:364:LEU:HD23	1.43	0.95
1:O:133:GLN:HB3	1:O:218:GLN:HE21	1.30	0.95
1:P:7:LYS:HD3	1:P:84:LEU:HB2	1.47	0.95
1:C:166:ILE:CG2	1:C:196:VAL:HG22	1.96	0.95
1:I:70:THR:HG21	1:I:94:ILE:HD11	1.48	0.95
1:P:312:ASN:HB2	1:P:313:PRO:CD	1.97	0.95
1:O:180:ARG:HD3	1:O:339:TYR:CD1	2.00	0.94
1:L:136:GLN:NE2	1:L:213:SER:HB3	1.82	0.94
1:M:312:ASN:HB2	1:M:313:PRO:HD2	1.50	0.94
1:H:1:MET:CE	1:H:70:THR:CG2	2.45	0.94
1:I:5:ILE:CD1	1:I:10:LEU:HB2	1.98	0.94
1:O:136:GLN:HG2	1:O:219:LEU:HD11	1.50	0.94
1:D:312:ASN:HB2	1:D:313:PRO:CD	1.97	0.94
1:P:7:LYS:HD2	1:P:84:LEU:HB2	1.45	0.94
1:K:4:LYS:HB3	1:K:64:CYS:HB2	1.50	0.94
1:O:335:PHE:HZ	1:O:363:VAL:HG21	1.30	0.93
1:O:145:LYS:HD3	1:O:346:VAL:HG22	1.49	0.93
1:J:33:VAL:HG13	1:J:74:ALA:HB2	1.51	0.93
1:D:150:MET:HE3	1:D:160:THR:O	1.68	0.93
1:I:138:GLU:HB3	1:I:186:ILE:HG21	1.50	0.93
1:I:195:LEU:HD22	1:I:195:LEU:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:VAL:HG23	1:B:356:MET:CE	1.99	0.92
1:H:136:GLN:HG2	1:H:219:LEU:HD11	1.51	0.92
1:K:14:LEU:HD12	1:K:78:MET:SD	2.07	0.92
1:O:33:VAL:HG13	1:O:74:ALA:HB2	1.48	0.92
1:J:308:LEU:CD1	1:J:322:LEU:CD2	2.47	0.92
1:G:132:VAL:HA	1:G:191:THR:HG22	1.51	0.91
1:L:142:LEU:CD1	1:L:171:LEU:HD22	2.00	0.91
1:K:138:GLU:HB3	1:K:186:ILE:HD12	1.49	0.91
1:O:137:ARG:NH1	1:O:137:ARG:HB3	1.85	0.91
1:M:312:ASN:HB2	1:M:313:PRO:CD	2.00	0.91
1:C:145:LYS:HA	1:C:346:VAL:HG21	1.50	0.91
1:F:59:LEU:HD12	1:F:60:SER:H	1.35	0.91
1:H:2:ARG:HD3	1:H:65:LEU:HD22	1.53	0.91
1:G:92:LEU:CG	1:G:102:LEU:CD2	2.48	0.91
1:O:276:HIS:HD2	1:O:347:LEU:HD11	1.19	0.91
1:F:59:LEU:HD11	1:F:63:ALA:HB1	1.52	0.90
1:D:4:LYS:HZ3	1:D:89:LEU:HB3	1.25	0.90
1:E:243:ASP:OD1	1:E:243:ASP:O	1.88	0.90
1:P:136:GLN:HG2	1:P:219:LEU:HD11	1.50	0.90
1:M:142:LEU:HD21	1:M:186:ILE:HB	1.51	0.90
1:H:262:ARG:HB3	1:H:262:ARG:NH1	1.86	0.90
1:F:59:LEU:HD11	1:F:63:ALA:CB	2.02	0.90
1:O:378:MET:SD	1:O:379:PRO:HD2	2.12	0.90
1:C:166:ILE:HG21	1:C:196:VAL:HG22	1.55	0.90
1:G:269:ASP:OD1	1:G:270:LYS:HG3	1.72	0.90
1:L:135:THR:HB	1:L:138:GLU:HG2	1.52	0.90
1:J:126:ASN:OD1	1:J:226:GLU:HG3	1.72	0.89
1:D:150:MET:CE	1:D:160:THR:O	2.20	0.89
1:L:138:GLU:HB3	1:L:186:ILE:HG12	1.55	0.89
1:O:305:SER:O	1:O:324:ILE:HD11	1.72	0.89
1:G:132:VAL:HG13	1:G:191:THR:CG2	2.03	0.89
1:I:166:ILE:CG2	1:I:196:VAL:CG2	2.50	0.89
1:A:49:LEU:HD23	1:A:122:LEU:HD12	1.54	0.89
1:G:221:LEU:HD23	1:G:230:VAL:HG22	1.52	0.89
1:C:131:GLN:HG3	1:C:220:THR:CG2	2.03	0.88
1:B:274:ILE:HG12	1:B:324:ILE:HG22	1.55	0.88
1:N:98:GLN:NE2	1:N:115:PRO:HD3	1.88	0.88
1:F:4:LYS:HG3	1:F:65:LEU:HD11	1.54	0.88
1:P:299:LEU:HD22	1:P:308:LEU:HD22	1.55	0.88
1:H:1:MET:HE1	1:H:70:THR:CG2	2.03	0.88
1:G:172:ARG:CD	1:G:183:LEU:HD11	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ILE:HG22	1:I:196:VAL:HG22	1.53	0.88
1:F:23:ARG:HG2	1:F:24:ARG:HG3	1.54	0.88
1:J:308:LEU:CD1	1:J:322:LEU:HD21	2.01	0.88
1:G:138:GLU:HB3	1:G:186:ILE:HD12	1.55	0.88
1:I:32:ASN:OD1	1:I:73:PRO:HA	1.74	0.88
1:N:95:THR:HG22	1:N:97:ASP:H	1.39	0.88
1:F:154:ASP:OD1	1:F:154:ASP:O	1.92	0.87
1:M:262:ARG:CB	1:M:262:ARG:HH11	1.87	0.87
1:O:136:GLN:CG	1:O:219:LEU:HD11	2.03	0.87
1:A:312:ASN:HB2	1:A:313:PRO:HD2	1.55	0.87
1:I:5:ILE:HD11	1:I:10:LEU:HD22	1.55	0.87
1:O:163:LEU:HD23	1:O:174:VAL:CG1	2.05	0.87
1:C:312:ASN:HB2	1:C:313:PRO:CD	2.03	0.87
1:H:322:LEU:HD12	1:H:322:LEU:H	1.40	0.87
1:L:301:PHE:HE2	1:L:356:MET:CE	1.87	0.87
1:A:166:ILE:CG2	1:A:196:VAL:HG22	2.04	0.87
1:H:257:PHE:CD2	1:H:258:PRO:HD2	2.09	0.87
1:O:133:GLN:HB3	1:O:218:GLN:NE2	1.89	0.87
1:B:124:THR:O	1:B:124:THR:OG1	1.88	0.86
1:B:312:ASN:HB2	1:B:313:PRO:HD2	1.57	0.86
1:O:137:ARG:HB3	1:O:137:ARG:HH11	1.38	0.86
1:I:70:THR:HG21	1:I:94:ILE:CD1	2.04	0.86
1:N:353:ASN:OD1	1:N:353:ASN:O	1.93	0.86
1:P:335:PHE:HZ	1:P:363:VAL:HG21	1.40	0.86
1:E:135:THR:OG1	1:E:138:GLU:HG3	1.75	0.86
1:O:276:HIS:NE2	1:O:347:LEU:CD1	2.37	0.85
1:G:136:GLN:HG2	1:G:219:LEU:HD11	1.58	0.85
1:L:301:PHE:CE2	1:L:356:MET:CE	2.58	0.85
1:C:329:ALA:HB1	1:C:330:PRO:HD2	1.56	0.85
1:H:272:VAL:HG23	1:H:356:MET:HE1	1.58	0.85
1:J:280:LYS:O	1:J:284:GLN:HG3	1.76	0.85
1:D:4:LYS:HZ1	1:D:89:LEU:HB3	1.37	0.85
1:A:166:ILE:HG21	1:A:196:VAL:HG22	1.57	0.84
1:B:346:VAL:CG1	1:B:375:TYR:OH	2.24	0.84
1:L:37:THR:HG22	1:L:42:LEU:HD12	1.57	0.84
1:I:59:LEU:HD23	1:I:59:LEU:O	1.76	0.84
1:B:346:VAL:HG11	1:B:375:TYR:CZ	2.12	0.84
1:G:132:VAL:HG13	1:G:191:THR:HG21	1.59	0.84
1:N:279:PHE:O	1:N:283:LEU:HD23	1.75	0.84
1:D:356:MET:HG2	1:D:363:VAL:HG22	1.58	0.84
1:F:137:ARG:HB2	1:F:214:ILE:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:VAL:HG21	1:I:166:ILE:HD13	1.59	0.84
1:L:301:PHE:HE2	1:L:356:MET:SD	2.01	0.84
1:O:136:GLN:HA	1:O:219:LEU:HD11	1.60	0.84
1:A:90:ILE:HG23	1:A:102:LEU:HD21	1.58	0.83
1:A:331:LEU:HD23	1:A:356:MET:SD	2.18	0.83
1:P:165:GLU:HG2	1:P:195:LEU:HD21	1.58	0.83
1:N:0:HIS:CE1	1:N:96:GLU:HA	2.12	0.83
1:L:301:PHE:O	1:L:330:PRO:HA	1.77	0.83
1:D:312:ASN:HB2	1:D:313:PRO:HD2	1.60	0.83
1:I:166:ILE:HG21	1:I:196:VAL:CG2	2.08	0.83
1:O:129:GLY:HA2	1:O:223:ILE:O	1.78	0.83
1:L:33:VAL:HG13	1:L:74:ALA:HB2	1.59	0.82
1:O:163:LEU:HB3	1:O:174:VAL:HG13	1.61	0.82
1:B:258:PRO:HB3	1:O:156:ARG:HE	1.43	0.82
1:I:335:PHE:HZ	1:I:363:VAL:HG21	1.44	0.82
1:I:195:LEU:N	1:I:195:LEU:CD1	2.41	0.82
1:K:35:ILE:CG2	1:K:37:THR:HG22	2.09	0.82
1:B:33:VAL:HG13	1:B:74:ALA:HB2	1.62	0.82
1:P:84:LEU:HD12	1:P:90:ILE:HD11	1.60	0.82
1:A:164:LEU:HD23	1:A:200:VAL:HG23	1.62	0.82
1:D:167:ASP:HB2	1:D:195:LEU:HD13	1.60	0.82
1:F:300:ASN:OD1	1:F:332:GLU:HG3	1.79	0.82
1:P:7:LYS:HD3	1:P:84:LEU:CB	2.09	0.82
1:B:312:ASN:HB2	1:B:313:PRO:CD	2.10	0.81
1:D:333:MET:SD	1:D:356:MET:SD	2.78	0.81
1:L:136:GLN:NE2	1:L:213:SER:CB	2.43	0.81
1:P:3:LEU:HD13	1:P:37:THR:HG21	1.61	0.81
1:B:166:ILE:HD11	1:B:223:ILE:HD12	1.62	0.81
1:B:143:PHE:HE2	1:B:208:LEU:HD23	1.39	0.81
1:M:90:ILE:HG22	1:M:92:LEU:CD1	2.11	0.81
1:A:49:LEU:HD23	1:A:122:LEU:CD1	2.10	0.81
1:O:364:LEU:O	1:O:364:LEU:HD12	1.80	0.81
1:B:243:ASP:OD1	1:B:243:ASP:N	2.13	0.81
1:K:65:LEU:HD13	1:K:65:LEU:O	1.79	0.81
1:H:2:ARG:HG3	1:H:93:GLN:NE2	1.96	0.80
1:F:136:GLN:HG2	1:F:219:LEU:HD11	1.63	0.80
1:L:215:GLU:OE1	1:L:215:GLU:N	2.12	0.80
1:L:301:PHE:CE2	1:L:356:MET:SD	2.75	0.80
1:K:378[A]:MET:SD	1:K:379:PRO:CD	2.70	0.80
1:C:378:MET:SD	1:C:379:PRO:HD2	2.22	0.80
1:I:195:LEU:H	1:I:195:LEU:HD12	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:319:ILE:HD12	1:P:108:ARG:HD3	1.64	0.80
1:I:195:LEU:HD13	1:I:195:LEU:N	1.97	0.80
1:A:312:ASN:HB2	1:A:313:PRO:CD	2.10	0.79
1:E:354:MET:HE2	1:E:363:VAL:HG11	1.64	0.79
1:I:312:ASN:HB2	1:I:313:PRO:HD2	1.63	0.79
1:G:33:VAL:HG13	1:G:74:ALA:HB2	1.64	0.79
1:N:64:CYS:SG	1:N:66:GLU:O	2.40	0.79
1:P:30:LEU:HD11	1:P:49:LEU:HG	1.64	0.79
1:N:186:ILE:O	1:N:186:ILE:HD12	1.83	0.78
1:F:307:GLN:HG3	1:F:321:ASP:OD1	1.82	0.78
1:G:312:ASN:HB2	1:G:313:PRO:CD	2.12	0.78
1:M:214:ILE:HD12	1:M:214:ILE:H	1.48	0.78
1:O:133:GLN:CB	1:O:218:GLN:HE21	1.96	0.78
1:P:138:GLU:HG2	1:P:186:ILE:HD12	1.65	0.78
1:F:353:ASN:ND2	1:F:368:PRO:HD3	1.98	0.78
1:L:142:LEU:CD1	1:L:171:LEU:CD2	2.61	0.78
1:P:269:ASP:OD1	1:P:269:ASP:N	2.12	0.78
1:C:270:LYS:N	1:C:270:LYS:HD2	1.99	0.78
1:M:269:ASP:OD1	1:M:270:LYS:HG3	1.84	0.78
1:N:278:VAL:HG12	1:N:322:LEU:HD11	1.65	0.78
1:O:163:LEU:HD23	1:O:174:VAL:HG11	1.64	0.78
1:B:143:PHE:HE2	1:B:208:LEU:CD2	1.97	0.77
1:B:272:VAL:HG23	1:B:356:MET:HE1	1.65	0.77
1:P:33:VAL:HG13	1:P:74:ALA:HB2	1.66	0.77
1:G:312:ASN:HB2	1:G:313:PRO:HD2	1.67	0.77
1:L:283:LEU:HD22	1:L:341:LEU:HG	1.67	0.77
1:O:136:GLN:CA	1:O:219:LEU:HD11	2.15	0.77
1:O:136:GLN:HA	1:O:219:LEU:CD1	2.15	0.77
1:O:353:ASN:ND2	1:O:368:PRO:HG3	2.00	0.77
1:P:4:LYS:HE2	1:P:63:ALA:HA	1.67	0.77
1:C:75:ARG:HD2	1:C:79:GLU:OE2	1.85	0.76
1:D:4:LYS:HZ1	1:D:89:LEU:CB	1.98	0.76
1:I:132:VAL:HG21	1:I:166:ILE:CD1	2.14	0.76
1:I:312:ASN:HB2	1:I:313:PRO:CD	2.15	0.76
1:L:45:THR:HG23	1:L:54:VAL:HG22	1.67	0.76
1:O:347:LEU:O	1:O:347:LEU:HD12	1.85	0.76
1:E:30:LEU:HD11	1:E:49:LEU:HG	1.65	0.76
1:D:61:GLU:OE1	1:D:61:GLU:N	2.17	0.76
1:I:166:ILE:HG22	1:I:196:VAL:CG2	2.15	0.76
1:D:166:ILE:HG13	1:D:191:THR:HG21	1.67	0.76
1:G:243:ASP:OD1	1:G:243:ASP:N	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:273:LEU:HB2	1:O:325:GLN:HB2	1.66	0.76
1:N:33:VAL:HG23	1:N:74:ALA:CB	2.15	0.76
1:B:272:VAL:HG23	1:B:356:MET:HE3	1.68	0.76
1:C:162:THR:HG22	1:C:175:THR:HG21	1.67	0.75
1:G:5:ILE:HD13	1:G:10:LEU:HB2	1.68	0.75
1:N:166:ILE:HD12	1:N:196:VAL:HG22	1.67	0.75
1:G:136:GLN:HG2	1:G:219:LEU:CD1	2.17	0.75
1:N:234:THR:N	1:N:235:PRO:HD2	2.02	0.75
1:H:262:ARG:HB3	1:H:262:ARG:HH11	1.49	0.75
1:P:84:LEU:CD1	1:P:90:ILE:HD11	2.15	0.75
1:D:166:ILE:CG1	1:D:191:THR:HG21	2.16	0.75
1:D:354:MET:HE3	1:D:363:VAL:HG11	1.69	0.75
1:H:322:LEU:HD12	1:H:322:LEU:N	2.00	0.75
1:H:367:ASP:OD1	1:H:368:PRO:HD2	1.86	0.75
1:K:137:ARG:HG3	1:K:214:ILE:O	1.86	0.75
1:O:331:LEU:HD11	1:O:359:ALA:HB2	1.68	0.75
1:E:303:GLN:OE1	1:E:303:GLN:N	2.18	0.75
1:K:132:VAL:HG22	1:K:166:ILE:CD1	2.17	0.75
1:M:156:ARG:HG2	1:M:156:ARG:NH1	1.99	0.75
1:C:166:ILE:HG22	1:C:196:VAL:HG22	1.68	0.74
1:O:135:THR:HG22	1:O:138:GLU:CB	2.17	0.74
1:E:214:ILE:HD12	1:E:214:ILE:N	2.02	0.74
1:O:129:GLY:CA	1:O:223:ILE:O	2.36	0.74
1:O:40:GLN:NE2	1:O:40:GLN:H	1.85	0.74
1:O:260:TYR:O	1:O:264:ILE:HD12	1.88	0.74
1:P:272:VAL:HG23	1:P:356:MET:CE	2.17	0.74
1:L:136:GLN:HE21	1:L:213:SER:HB3	1.52	0.74
1:M:272:VAL:HG22	1:M:326:TYR:CD1	2.22	0.74
1:F:18:VAL:HG21	1:F:78:MET:HE3	1.68	0.74
1:M:214:ILE:HD12	1:M:214:ILE:N	2.03	0.74
1:O:335:PHE:CZ	1:O:363:VAL:HG21	2.20	0.74
1:L:185:GLU:N	1:L:185:GLU:OE1	2.20	0.74
1:P:167:ASP:CB	1:P:195:LEU:HD23	2.16	0.74
1:B:18:VAL:O	1:B:18:VAL:HG22	1.88	0.73
1:P:272:VAL:HG23	1:P:356:MET:HE2	1.70	0.73
1:K:356:MET:HG2	1:K:363:VAL:HG22	1.70	0.73
1:M:303:GLN:OE1	1:M:303:GLN:N	2.16	0.73
1:L:136:GLN:HE22	1:L:213:SER:CB	2.00	0.73
1:O:135:THR:CG2	1:O:138:GLU:H	2.02	0.73
1:B:286:VAL:HG21	1:B:308:LEU:HB2	1.70	0.73
1:C:131:GLN:HG3	1:C:220:THR:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:CD	1:C:346:VAL:HG22	2.19	0.73
1:E:33:VAL:HG13	1:E:74:ALA:HB2	1.70	0.73
1:O:360:ASN:HB2	1:O:381:ARG:HD2	1.69	0.73
1:L:136:GLN:HG2	1:L:219:LEU:CD1	2.19	0.73
1:G:166:ILE:HG23	1:G:196:VAL:HG13	1.70	0.73
1:O:306:LEU:HB2	1:O:324:ILE:HD13	1.71	0.73
1:D:222:LEU:HB2	1:J:194:GLN:HE22	1.54	0.73
1:M:225:ARG:O	1:M:225:ARG:HD2	1.88	0.73
1:H:1:MET:HE2	1:H:70:THR:HG22	1.70	0.72
1:K:132:VAL:CG2	1:K:166:ILE:HD13	2.19	0.72
1:C:270:LYS:HB3	1:C:326:TYR:HE1	1.52	0.72
1:G:174:VAL:HG22	1:G:183:LEU:HD13	1.70	0.72
1:H:126:ASN:H	1:H:126:ASN:ND2	1.83	0.72
1:D:194:GLN:OE1	1:D:194:GLN:N	2.20	0.72
1:I:107:SER:HB3	1:J:320:GLU:OE1	1.88	0.72
1:K:132:VAL:HG22	1:K:166:ILE:HD13	1.70	0.72
1:L:137:ARG:HB2	1:L:215:GLU:CA	2.15	0.72
1:L:364:LEU:HD12	1:L:364:LEU:O	1.90	0.72
1:C:149:ALA:HB3	1:C:175:THR:OG1	1.89	0.72
1:N:33:VAL:CG2	1:N:74:ALA:HB2	2.16	0.72
1:F:59:LEU:CD1	1:F:63:ALA:CB	2.67	0.72
1:B:303:GLN:N	1:B:303:GLN:OE1	2.23	0.72
1:E:356:MET:HG3	1:E:363:VAL:HG13	1.71	0.72
1:H:134:VAL:HG23	1:H:138:GLU:OE1	1.89	0.72
1:F:65:LEU:H	1:F:65:LEU:HD12	1.53	0.72
1:G:92:LEU:HG	1:G:102:LEU:HD21	1.69	0.72
1:O:335:PHE:HZ	1:O:363:VAL:CG2	2.02	0.72
1:D:303:GLN:N	1:D:303:GLN:OE1	2.23	0.72
1:H:347:LEU:HD22	1:H:367:ASP:HB2	1.70	0.72
1:L:37:THR:HG22	1:L:42:LEU:CD1	2.20	0.72
1:M:262:ARG:NH1	1:M:262:ARG:HB2	2.01	0.71
1:B:146:THR:O	1:B:175:THR:HG21	1.91	0.71
1:K:4:LYS:HB3	1:K:64:CYS:CB	2.20	0.71
1:L:65:LEU:N	1:L:65:LEU:HD12	2.04	0.71
1:H:10:LEU:O	1:H:10:LEU:HD23	1.91	0.71
1:H:1:MET:HB2	1:H:68:GLY:HA3	1.73	0.71
1:O:261:ARG:H	1:O:261:ARG:HD2	1.55	0.71
1:L:144:GLU:HG3	1:L:145:LYS:HD3	1.73	0.71
1:C:45:THR:HG23	1:C:54:VAL:HG22	1.73	0.71
1:M:278:VAL:CG1	1:M:322:LEU:HD22	2.21	0.71
1:C:136:GLN:HG2	1:C:219:LEU:CD1	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LEU:HD22	1:C:367:ASP:HB2	1.72	0.71
1:I:156:ARG:HH11	1:L:262:ARG:HH21	1.39	0.71
1:H:75:ARG:HD2	1:H:79:GLU:OE1	1.89	0.70
1:K:4:LYS:O	1:K:64:CYS:HB2	1.91	0.70
1:L:239:LYS:HG2	1:L:239:LYS:O	1.90	0.70
1:P:303:GLN:OE1	1:P:303:GLN:N	2.23	0.70
1:B:148:PHE:CE1	1:B:346:VAL:HG21	2.26	0.70
1:E:271:HIS:HD2	1:J:216:ASP:HB3	1.56	0.70
1:K:133:GLN:HB3	1:K:218:GLN:HE21	1.54	0.70
1:L:30:LEU:HD21	1:L:49:LEU:HG	1.72	0.70
1:C:131:GLN:CG	1:C:220:THR:CG2	2.69	0.70
1:G:172:ARG:HD3	1:G:183:LEU:CD1	2.19	0.70
1:H:136:GLN:HG2	1:H:219:LEU:CD1	2.20	0.70
1:H:311:ASN:HB3	1:H:317:GLU:HG3	1.72	0.70
1:D:165:GLU:HG2	1:D:195:LEU:HD11	1.73	0.70
1:F:153:GLN:HA	1:F:153:GLN:HE21	1.56	0.70
1:I:132:VAL:CG2	1:I:166:ILE:HD11	2.22	0.70
1:L:289:LEU:HD12	1:L:318:ALA:HB2	1.74	0.70
1:A:1:MET:HE3	1:A:94:ILE:CD1	2.22	0.70
1:I:132:VAL:CG2	1:I:166:ILE:CD1	2.70	0.70
1:I:281:GLN:HA	1:I:281:GLN:NE2	2.06	0.70
1:N:131:GLN:CG	1:N:220:THR:HG23	2.22	0.70
1:O:276:HIS:HD2	1:O:347:LEU:CD1	1.81	0.70
1:P:289:LEU:HD12	1:P:318:ALA:HB2	1.73	0.69
1:C:96:GLU:CD	1:C:96:GLU:H	1.95	0.69
1:J:273:LEU:CD2	1:J:351:ASP:HB3	2.17	0.69
1:N:279:PHE:CE1	1:N:283:LEU:CD2	2.75	0.69
1:N:98:GLN:HE22	1:N:115:PRO:CD	2.04	0.69
1:G:61:GLU:H	1:G:61:GLU:CD	1.95	0.69
1:G:132:VAL:HA	1:G:191:THR:CG2	2.21	0.69
1:K:42:LEU:N	1:K:42:LEU:HD12	2.08	0.69
1:C:169:ASN:H	1:C:191:THR:HG21	1.57	0.69
1:H:257:PHE:CG	1:H:258:PRO:HD2	2.27	0.69
1:N:312:ASN:HB2	1:N:313:PRO:HD2	1.73	0.69
1:O:339:TYR:O	1:O:343:VAL:HG23	1.92	0.69
1:P:124:THR:CG2	1:P:227:LEU:HD12	2.21	0.69
1:I:170:GLN:HE21	1:I:172:ARG:HH21	1.40	0.69
1:L:142:LEU:HD13	1:L:171:LEU:CD2	2.22	0.69
1:G:141:ARG:NH1	1:G:372:ASP:OD2	2.23	0.69
1:I:281:GLN:HE21	1:I:281:GLN:HA	1.58	0.69
1:P:124:THR:HG22	1:P:227:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:ASP:HA	1:E:324:ILE:O	1.92	0.69
1:L:3:LEU:CD1	1:L:37:THR:HG21	2.23	0.69
1:N:163:LEU:HD22	1:N:257:PHE:CD2	2.27	0.69
1:A:217:GLU:OE2	1:A:218:GLN:O	2.10	0.68
1:F:34:LYS:HE2	1:F:36:GLN:NE2	2.08	0.68
1:H:2:ARG:HG3	1:H:93:GLN:HE21	1.58	0.68
1:J:23:ARG:HH22	1:J:75:ARG:NH1	1.92	0.68
1:N:148:PHE:CE1	1:N:346:VAL:HG11	2.29	0.68
1:A:1:MET:HE3	1:A:94:ILE:HD11	1.73	0.68
1:J:45:THR:HG23	1:J:54:VAL:HG22	1.75	0.68
1:N:90:ILE:HG23	1:N:102:LEU:HD21	1.75	0.68
1:E:273:LEU:HD21	1:J:187:LEU:HD12	1.75	0.68
1:H:2:ARG:CD	1:H:65:LEU:HD22	2.23	0.68
1:K:230:VAL:HG12	1:K:248:PHE:HB3	1.75	0.68
1:N:187:LEU:HD12	1:N:187:LEU:C	2.14	0.68
1:C:240:GLU:HA	1:C:240:GLU:OE1	1.92	0.68
1:N:187:LEU:O	1:N:187:LEU:HD12	1.94	0.68
1:B:272:VAL:CG2	1:B:356:MET:CE	2.70	0.68
1:L:142:LEU:HD11	1:L:171:LEU:HD22	1.75	0.68
1:P:257:PHE:CD2	1:P:258:PRO:HD2	2.28	0.68
1:G:133:GLN:HB2	1:G:190:SER:CB	2.24	0.68
1:I:353:ASN:HD21	1:I:366:GLN:HB2	1.57	0.67
1:C:145:LYS:HD2	1:C:346:VAL:CG2	2.19	0.67
1:C:37:THR:HG23	1:C:42:LEU:HD12	1.75	0.67
1:H:135:THR:OG1	1:H:138:GLU:HG3	1.93	0.67
1:O:305:SER:O	1:O:324:ILE:CD1	2.41	0.67
1:D:278:VAL:HG12	1:D:322:LEU:HD11	1.76	0.67
1:I:32:ASN:OD1	1:I:73:PRO:CA	2.42	0.67
1:N:166:ILE:HD12	1:N:196:VAL:CG2	2.24	0.67
1:N:165:GLU:HG3	1:N:197:GLN:HG2	1.75	0.67
1:J:195:LEU:HD23	1:J:195:LEU:C	2.14	0.67
1:F:304:ASP:HA	1:F:324:ILE:O	1.94	0.67
1:K:4:LYS:O	1:K:64:CYS:SG	2.52	0.67
1:O:180:ARG:HD3	1:O:339:TYR:CE1	2.29	0.67
1:O:299:LEU:HD12	1:O:299:LEU:N	2.10	0.67
1:P:257:PHE:CG	1:P:258:PRO:HD2	2.29	0.67
1:F:237:ARG:HD2	1:F:237:ARG:O	1.95	0.67
1:M:364:LEU:HD11	1:M:374:THR:HG23	1.77	0.67
1:N:136:GLN:HG2	1:N:219:LEU:HD11	1.77	0.67
1:K:77:LEU:O	1:K:77:LEU:HD23	1.95	0.67
1:A:303:GLN:N	1:A:303:GLN:OE1	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:VAL:CG2	1:B:356:MET:HE1	2.25	0.67
1:I:2:ARG:HG2	1:I:65:LEU:HD12	1.78	0.67
1:N:227:LEU:HD23	1:N:251:LYS:HA	1.76	0.67
1:O:162:THR:HG23	1:O:205:VAL:HG21	1.76	0.67
1:O:176:THR:HB	1:O:181:LEU:HD13	1.77	0.67
1:A:90:ILE:HG23	1:A:102:LEU:CD2	2.23	0.66
1:B:79:GLU:HA	1:B:79:GLU:OE2	1.95	0.66
1:D:266:ARG:CG	1:D:266:ARG:HH11	2.08	0.66
1:H:150:MET:HG3	1:H:175:THR:HG22	1.77	0.66
1:C:145:LYS:HA	1:C:346:VAL:CG2	2.22	0.66
1:I:132:VAL:HG22	1:I:166:ILE:HD11	1.76	0.66
1:F:153:GLN:HA	1:F:153:GLN:NE2	2.11	0.66
1:C:145:LYS:CD	1:C:346:VAL:CG2	2.73	0.66
1:M:136:GLN:NE2	1:M:213:SER:OG	2.29	0.66
1:O:33:VAL:HG13	1:O:74:ALA:CB	2.25	0.66
1:A:186:ILE:O	1:A:186:ILE:HG13	1.96	0.66
1:H:134:VAL:HG21	1:H:186:ILE:CD1	2.26	0.66
1:H:272:VAL:HG22	1:H:326:TYR:CD1	2.30	0.66
1:H:14:LEU:HD11	1:H:77:LEU:HD23	1.76	0.66
1:J:289:LEU:HD22	1:J:316:ASP:CB	2.26	0.66
1:L:136:GLN:HE22	1:L:213:SER:HB2	1.61	0.66
1:L:217:GLU:HA	1:L:217:GLU:OE1	1.96	0.66
1:N:124:THR:HB	1:N:227:LEU:HD12	1.78	0.66
1:O:135:THR:CG2	1:O:138:GLU:CB	2.74	0.66
1:M:195:LEU:HD12	1:M:195:LEU:O	1.95	0.66
1:N:279:PHE:CD1	1:N:283:LEU:CD2	2.79	0.66
1:O:276:HIS:HE2	1:O:347:LEU:CD1	2.09	0.66
1:F:358:GLU:HB2	1:F:361:GLN:HG3	1.76	0.66
1:A:142:LEU:HD13	1:A:186:ILE:HG23	1.78	0.66
1:A:133:GLN:HB3	1:A:189:SER:HB3	1.77	0.66
1:J:78:MET:CE	1:J:82:LYS:HE3	2.26	0.66
1:B:360:ASN:O	1:B:379:PRO:HG3	1.96	0.66
1:F:154:ASP:CG	1:F:154:ASP:O	2.34	0.66
1:F:59:LEU:HG	1:F:63:ALA:HB3	1.76	0.66
1:J:356:MET:HG2	1:J:363:VAL:HG22	1.77	0.66
1:M:315:GLN:HE21	1:N:99:ARG:NH1	1.94	0.66
1:E:271:HIS:CD2	1:J:216:ASP:HB3	2.30	0.65
1:H:70:THR:HG21	1:H:94:ILE:HD11	1.77	0.65
1:L:33:VAL:HG13	1:L:74:ALA:CB	2.26	0.65
1:O:17:VAL:HG21	1:O:46:GLY:N	2.11	0.65
1:O:17:VAL:HG23	1:O:53:LEU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:NZ	1:A:212:LEU:O	2.29	0.65
1:D:3:LEU:HD12	1:D:3:LEU:O	1.96	0.65
1:M:89:LEU:N	1:M:89:LEU:HD12	2.12	0.65
1:P:3:LEU:CD1	1:P:37:THR:HG21	2.27	0.65
1:A:2:ARG:HG3	1:A:93:GLN:OE1	1.97	0.65
1:C:283:LEU:HD23	1:C:341:LEU:HG	1.77	0.65
1:G:132:VAL:HG22	1:G:191:THR:HG21	1.77	0.65
1:G:92:LEU:CD2	1:G:102:LEU:HD21	2.25	0.65
1:I:185:GLU:O	1:I:186:ILE:HD13	1.96	0.65
1:J:312:ASN:CB	1:J:313:PRO:CD	2.62	0.65
1:L:199:ILE:CG2	1:L:253:ILE:HB	2.27	0.65
1:L:282:SER:O	1:L:286:VAL:HG12	1.95	0.65
1:L:65:LEU:N	1:L:65:LEU:CD1	2.60	0.65
1:G:278:VAL:HG12	1:G:322:LEU:HD11	1.79	0.65
1:H:33:VAL:HG13	1:H:74:ALA:CB	2.24	0.65
1:J:289:LEU:HD22	1:J:316:ASP:HB2	1.77	0.65
1:O:17:VAL:CG2	1:O:46:GLY:H	2.10	0.65
1:E:307:GLN:HG3	1:E:321:ASP:OD1	1.96	0.65
1:F:18:VAL:HG21	1:F:78:MET:CE	2.25	0.65
1:J:33:VAL:HG13	1:J:74:ALA:CB	2.26	0.65
1:K:137:ARG:CG	1:K:214:ILE:O	2.44	0.65
1:A:300:ASN:OD1	1:A:332:GLU:HG3	1.96	0.65
1:L:164:LEU:HD22	1:L:171:LEU:HD21	1.79	0.65
1:L:61:GLU:H	1:L:61:GLU:CD	1.99	0.65
1:C:187:LEU:HD12	1:C:187:LEU:O	1.97	0.65
1:C:9:SER:O	1:C:13:VAL:HG23	1.97	0.65
1:D:187:LEU:HD13	1:D:187:LEU:C	2.18	0.65
1:G:306:LEU:HB2	1:G:324:ILE:HD13	1.78	0.65
1:M:168:GLU:OE1	1:M:168:GLU:HA	1.97	0.65
1:N:259:ASP:OD1	1:N:259:ASP:N	2.13	0.65
1:O:259:ASP:OD1	1:O:259:ASP:O	2.15	0.65
1:G:221:LEU:CD2	1:G:230:VAL:CG2	2.70	0.65
1:I:134:VAL:HG12	1:I:188:ALA:CB	2.27	0.64
1:A:165:GLU:HG3	1:A:197:GLN:HG2	1.79	0.64
1:A:166:ILE:CG2	1:A:196:VAL:CG2	2.75	0.64
1:F:269:ASP:OD1	1:F:270:LYS:HG3	1.97	0.64
1:A:17:VAL:CG2	1:A:46:GLY:N	2.61	0.64
1:D:194:GLN:CD	1:D:194:GLN:H	1.99	0.64
1:D:239:LYS:O	1:D:239:LYS:HG3	1.98	0.64
1:N:131:GLN:NE2	1:N:220:THR:CG2	2.60	0.64
1:F:59:LEU:HD12	1:F:60:SER:N	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:MET:HE3	1:H:82:LYS:HE3	1.80	0.64
1:K:138:GLU:HB3	1:K:186:ILE:CD1	2.23	0.64
1:J:330:PRO:HG2	1:N:329:ALA:HB1	1.78	0.64
1:E:303:GLN:HA	1:E:326:TYR:O	1.98	0.64
1:M:83:SER:HB3	1:N:288:ILE:HD11	1.79	0.64
1:O:222:LEU:C	1:O:222:LEU:HD23	2.18	0.64
1:O:149:ALA:HB3	1:O:175:THR:OG1	1.98	0.64
1:B:238:ASP:HB2	1:B:241:GLN:HB2	1.80	0.64
1:I:3:LEU:N	1:I:3:LEU:HD23	2.13	0.64
1:M:278:VAL:HG12	1:M:322:LEU:HD22	1.80	0.64
1:O:257:PHE:CD2	1:O:258:PRO:HD2	2.32	0.64
1:A:314:GLU:OE2	1:A:314:GLU:N	2.30	0.64
1:E:83:SER:HB3	1:F:288:ILE:HD11	1.79	0.64
1:I:59:LEU:HD23	1:I:59:LEU:C	2.18	0.64
1:L:137:ARG:HD3	1:L:215:GLU:HB3	1.80	0.64
1:M:262:ARG:HH11	1:M:262:ARG:CG	2.10	0.64
1:D:272:VAL:HG22	1:D:326:TYR:CD1	2.32	0.63
1:O:281:GLN:HB3	1:O:285:ARG:HH12	1.62	0.63
1:O:37:THR:HG22	1:O:68:GLY:O	1.98	0.63
1:A:164:LEU:HD23	1:A:200:VAL:CG2	2.28	0.63
1:K:47:SER:HB3	1:K:52:GLU:HA	1.81	0.63
1:K:42:LEU:HG	1:K:57:THR:O	1.98	0.63
1:E:214:ILE:HD12	1:E:214:ILE:H	1.61	0.63
1:J:136:GLN:HG2	1:J:219:LEU:HD11	1.79	0.63
1:L:135:THR:CB	1:L:138:GLU:HG2	2.25	0.63
1:P:27:LEU:HG	1:P:29:ILE:HG22	1.79	0.63
1:A:49:LEU:CD2	1:A:122:LEU:HD12	2.27	0.63
1:F:300:ASN:CG	1:F:332:GLU:HG3	2.19	0.63
1:J:263:VAL:HG11	1:K:155:VAL:HG13	1.80	0.63
1:K:98:GLN:HA	1:K:113:THR:HG22	1.80	0.63
1:M:33:VAL:CG2	1:M:44:ILE:HG22	2.29	0.63
1:C:289:LEU:HD12	1:C:318:ALA:HB2	1.80	0.63
1:C:307:GLN:HG3	1:C:321:ASP:OD1	1.99	0.63
1:J:30:LEU:HD21	1:J:120:PRO:HG2	1.79	0.63
1:M:2:ARG:HG2	1:M:65:LEU:HD13	1.81	0.63
1:A:269:ASP:O	1:A:271:HIS:CD2	2.51	0.63
1:D:100:CYS:HB2	1:D:113:THR:CG2	2.29	0.63
1:H:30:LEU:HD11	1:H:49:LEU:HG	1.81	0.63
1:A:269:ASP:OD1	1:A:270:LYS:N	2.32	0.63
1:B:125:GLU:HA	1:D:187:LEU:HD21	1.80	0.63
1:F:2:ARG:HG3	1:F:65:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:134:VAL:HG21	1:H:186:ILE:HD11	1.81	0.63
1:M:221:LEU:HD22	1:M:230:VAL:HG22	1.80	0.63
1:G:140:LYS:NZ	1:G:209:GLN:O	2.32	0.63
1:B:191:THR:O	1:J:222:LEU:HD21	1.98	0.63
1:M:303:GLN:CD	1:M:303:GLN:H	2.01	0.63
1:N:180:ARG:NH1	1:N:342:ASP:OD2	2.28	0.63
1:P:272:VAL:CG2	1:P:356:MET:HE1	2.29	0.63
1:C:270:LYS:HB3	1:C:326:TYR:CE1	2.34	0.62
1:M:269:ASP:OD1	1:M:270:LYS:N	2.31	0.62
1:G:162:THR:HG23	1:G:205:VAL:HG21	1.81	0.62
1:I:47:SER:HB2	1:I:52:GLU:HA	1.81	0.62
1:H:378:MET:SD	1:H:378:MET:N	2.71	0.62
1:H:79:GLU:OE2	1:H:79:GLU:HA	1.99	0.62
1:M:315:GLN:HE21	1:N:99:ARG:HH12	1.45	0.62
1:M:30:LEU:HD11	1:M:49:LEU:HG	1.81	0.62
1:N:312:ASN:HB2	1:N:313:PRO:CD	2.30	0.62
1:O:17:VAL:CG2	1:O:46:GLY:N	2.63	0.62
1:C:268:GLY:HA2	1:C:357:THR:HG22	1.82	0.62
1:D:100:CYS:HB2	1:D:113:THR:HG21	1.80	0.62
1:E:322:LEU:HD12	1:E:322:LEU:N	2.14	0.62
1:H:45:THR:HG23	1:H:54:VAL:HG22	1.81	0.62
1:K:14:LEU:HB3	1:K:78:MET:SD	2.39	0.62
1:N:36:GLN:CG	1:N:69:GLU:CG	2.73	0.62
1:D:266:ARG:HH22	1:O:300:ASN:CG	2.03	0.62
1:A:17:VAL:HG21	1:A:46:GLY:N	2.15	0.62
1:C:335:PHE:HZ	1:C:363:VAL:HG21	1.64	0.62
1:G:259:ASP:O	1:G:262:ARG:HG2	1.99	0.62
1:I:41:ALA:HA	1:I:59:LEU:HD22	1.80	0.62
1:K:306:LEU:HB2	1:K:324:ILE:HD13	1.81	0.62
1:E:24:ARG:HA	1:E:24:ARG:HE	1.64	0.62
1:N:98:GLN:NE2	1:N:115:PRO:CD	2.62	0.62
1:O:0:HIS:NE2	1:O:96:GLU:HB2	2.13	0.62
1:P:335:PHE:CZ	1:P:363:VAL:HG21	2.29	0.62
1:I:270:LYS:NZ	1:I:357:THR:O	2.32	0.62
1:E:2:ARG:HG2	1:E:65:LEU:HD12	1.82	0.62
1:G:59:LEU:HG	1:G:63:ALA:HB3	1.82	0.62
1:H:77:LEU:CD1	1:H:102:LEU:HD21	2.30	0.62
1:I:142:LEU:HD21	1:I:186:ILE:HG12	1.82	0.62
1:K:301:PHE:O	1:K:330:PRO:HA	2.00	0.62
1:E:294:LEU:HD12	1:E:294:LEU:N	2.15	0.62
1:O:155:VAL:HG21	1:O:159:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:GLU:N	1:F:8:GLU:OE2	2.30	0.62
1:N:235:PRO:HG3	1:N:243:ASP:HB2	1.81	0.62
1:A:221:LEU:HD12	1:A:230:VAL:HB	1.82	0.61
1:A:281:GLN:OE1	1:A:281:GLN:HA	2.00	0.61
1:K:11:LEU:HD11	1:K:82:LYS:HG2	1.80	0.61
1:L:301:PHE:HE2	1:L:356:MET:HE1	1.64	0.61
1:P:166:ILE:O	1:P:166:ILE:HG23	2.00	0.61
1:J:314:GLU:N	1:J:314:GLU:OE2	2.33	0.61
1:O:117:GLU:OE1	1:O:117:GLU:N	2.20	0.61
1:A:96:GLU:H	1:A:96:GLU:CD	2.02	0.61
1:B:128:GLN:OE1	1:B:128:GLN:HA	2.01	0.61
1:F:32:ASN:CB	1:F:71:THR:HG22	2.30	0.61
1:M:278:VAL:HG12	1:M:322:LEU:CD2	2.31	0.61
1:N:131:GLN:NE2	1:N:220:THR:HG21	2.15	0.61
1:G:207:GLU:OE2	1:G:210:ARG:NH2	2.24	0.61
1:K:96:GLU:O	1:K:96:GLU:HG2	1.98	0.61
1:M:1:MET:SD	1:M:37:THR:CG2	2.86	0.61
1:N:277:ASP:O	1:N:281:GLN:HG2	2.01	0.61
1:E:158:TYR:CE1	1:E:258:PRO:HD3	2.36	0.61
1:H:191:THR:O	1:H:191:THR:HG23	2.00	0.61
1:L:3:LEU:HD13	1:L:37:THR:HG21	1.82	0.61
1:A:364:LEU:HD21	1:A:374:THR:CG2	2.30	0.61
1:K:136:GLN:HG2	1:K:219:LEU:HD11	1.81	0.61
1:B:166:ILE:HD11	1:B:223:ILE:CD1	2.31	0.61
1:L:169:ASN:HA	1:L:188:ALA:O	2.01	0.61
1:O:273:LEU:HD22	1:O:325:GLN:OE1	2.01	0.61
1:K:96:GLU:N	1:K:96:GLU:OE1	2.34	0.61
1:K:162:THR:HG22	1:K:175:THR:CG2	2.31	0.61
1:B:265:PRO:HG2	1:B:364:LEU:HB2	1.83	0.60
1:B:4:LYS:HG3	1:B:65:LEU:HD21	1.82	0.60
1:J:78:MET:HE2	1:J:82:LYS:HE3	1.82	0.60
1:O:135:THR:HG23	1:O:138:GLU:N	2.09	0.60
1:O:137:ARG:CB	1:O:137:ARG:HH11	2.12	0.60
1:B:33:VAL:HG13	1:B:74:ALA:CB	2.31	0.60
1:G:273:LEU:CD2	1:G:351:ASP:HB3	2.32	0.60
1:H:238:ASP:HB2	1:H:241:GLN:HB2	1.82	0.60
1:H:372:ASP:N	1:H:372:ASP:OD1	2.28	0.60
1:J:330:PRO:HG2	1:N:329:ALA:CB	2.31	0.60
1:L:135:THR:HB	1:L:138:GLU:CG	2.27	0.60
1:O:122:LEU:HD12	1:O:249:THR:HG22	1.83	0.60
1:P:272:VAL:CG2	1:P:356:MET:CE	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:HG22	1:A:46:GLY:HA3	1.83	0.60
1:D:364:LEU:HD11	1:D:374:THR:HG23	1.83	0.60
1:P:274:ILE:HG23	1:P:324:ILE:HG22	1.83	0.60
1:B:272:VAL:CG2	1:B:356:MET:HE3	2.31	0.60
1:H:70:THR:HG21	1:H:94:ILE:CD1	2.31	0.60
1:M:152:VAL:O	1:M:202:ARG:NH2	2.34	0.60
1:N:279:PHE:CD1	1:N:283:LEU:HD21	2.37	0.60
1:D:152:VAL:HG12	1:D:153:GLN:HG2	1.84	0.60
1:F:125:GLU:OE2	1:F:125:GLU:N	2.33	0.60
1:F:30:LEU:HD11	1:F:49:LEU:HG	1.84	0.60
1:L:301:PHE:CE2	1:L:356:MET:HE1	2.36	0.60
1:M:228:LEU:HD23	1:M:228:LEU:C	2.22	0.60
1:O:214:ILE:O	1:O:214:ILE:HG22	2.00	0.60
1:B:274:ILE:HG21	1:B:279:PHE:HB2	1.84	0.60
1:B:270:LYS:HD3	1:B:326:TYR:OH	2.01	0.60
1:D:165:GLU:CG	1:D:195:LEU:HD11	2.31	0.60
1:H:303:GLN:OE1	1:H:303:GLN:N	2.34	0.60
1:C:230:VAL:HG12	1:C:248:PHE:HB3	1.84	0.60
1:C:358:GLU:HB2	1:C:361:GLN:HG2	1.82	0.60
1:G:356:MET:HG2	1:G:363:VAL:HG22	1.84	0.60
1:L:283:LEU:HD21	1:L:337:ALA:HB1	1.84	0.60
1:N:17:VAL:CG2	1:N:46:GLY:N	2.65	0.60
1:L:298:PHE:C	1:L:299:LEU:HD12	2.22	0.59
1:N:214:ILE:HG12	1:N:214:ILE:O	2.02	0.59
1:A:166:ILE:HG21	1:A:196:VAL:CG2	2.31	0.59
1:B:278:VAL:HB	1:B:322:LEU:HD11	1.84	0.59
1:K:137:ARG:HG3	1:K:214:ILE:C	2.22	0.59
1:L:335:PHE:HB3	1:L:340:LEU:HD11	1.83	0.59
1:N:326:TYR:CE1	1:N:328:SER:HB2	2.37	0.59
1:L:166:ILE:HG12	1:L:196:VAL:HG22	1.83	0.59
1:N:291:ASN:HB3	1:N:294:LEU:HB2	1.84	0.59
1:B:97:ASP:N	1:B:97:ASP:OD1	2.27	0.59
1:K:18:VAL:O	1:K:21:VAL:HG12	2.02	0.59
1:E:5:ILE:HG13	1:E:6:ALA:N	2.17	0.59
1:F:169:ASN:O	1:F:188:ALA:O	2.20	0.59
1:O:207:GLU:OE2	1:O:207:GLU:HA	2.01	0.59
1:B:171:LEU:HB3	1:B:186:ILE:HD11	1.83	0.59
1:O:133:GLN:CB	1:O:218:GLN:NE2	2.62	0.59
1:B:30:LEU:HD21	1:B:120:PRO:HG2	1.84	0.59
1:N:131:GLN:HG3	1:N:220:THR:HG23	1.85	0.59
1:A:269:ASP:O	1:A:271:HIS:HD2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.02	0.59
1:H:278:VAL:HG12	1:H:322:LEU:HD23	1.84	0.59
1:H:378:MET:HB3	1:H:379:PRO:CD	2.28	0.59
1:K:35:ILE:HG22	1:K:37:THR:HG22	1.84	0.59
1:N:30:LEU:HD11	1:N:49:LEU:HG	1.85	0.59
1:F:270:LYS:HD3	1:F:326:TYR:OH	2.03	0.59
1:G:51:VAL:HG22	1:G:204:ALA:HB2	1.84	0.59
1:K:134:VAL:HG21	1:K:186:ILE:HD11	1.83	0.59
1:F:133:GLN:HB3	1:F:218:GLN:HE21	1.68	0.59
1:K:347:LEU:HD22	1:K:367:ASP:HB2	1.85	0.59
1:N:131:GLN:HG3	1:N:220:THR:CG2	2.33	0.59
1:O:196:VAL:HG12	1:O:197:GLN:N	2.16	0.59
1:L:135:THR:HG22	1:L:137:ARG:H	1.68	0.58
1:I:39:ALA:HB1	1:I:61:GLU:HG2	1.85	0.58
1:K:357:THR:OG1	1:K:358:GLU:N	2.33	0.58
1:K:43:THR:HG22	1:K:43:THR:O	2.02	0.58
1:M:286:VAL:HG12	1:M:310:ALA:HB2	1.86	0.58
1:C:283:LEU:CD2	1:C:341:LEU:HG	2.32	0.58
1:O:133:GLN:CG	1:O:218:GLN:NE2	2.67	0.58
1:F:228:LEU:HD23	1:F:228:LEU:C	2.23	0.58
1:P:138:GLU:HB3	1:P:186:ILE:HG21	1.84	0.58
1:I:168:GLU:HG3	1:I:168:GLU:O	2.04	0.58
1:J:158:TYR:CE1	1:J:258:PRO:CD	2.86	0.58
1:O:159:LEU:HD13	1:O:177:ASP:HA	1.84	0.58
1:B:145:LYS:HD2	1:B:346:VAL:HG13	1.85	0.58
1:G:165:GLU:HG3	1:G:197:GLN:HG2	1.86	0.58
1:H:30:LEU:HD21	1:H:120:PRO:HG2	1.85	0.58
1:K:4:LYS:O	1:K:64:CYS:CB	2.51	0.58
1:N:186:ILE:C	1:N:186:ILE:HD12	2.24	0.58
1:O:317:GLU:HB3	1:P:110:VAL:HG22	1.85	0.58
1:C:132:VAL:HG22	1:C:166:ILE:HD12	1.84	0.58
1:J:23:ARG:HH22	1:J:75:ARG:HH11	1.52	0.58
1:L:64:CYS:SG	1:L:66:GLU:O	2.61	0.58
1:O:273:LEU:HG	1:O:353:ASN:OD1	2.04	0.58
1:P:223:ILE:HD12	1:P:228:LEU:HD13	1.84	0.58
1:A:96:GLU:N	1:A:96:GLU:OE1	2.23	0.58
1:D:90:ILE:HG22	1:D:92:LEU:CD1	2.34	0.58
1:H:364:LEU:HD11	1:H:374:THR:CG2	2.33	0.58
1:N:133:GLN:HB2	1:N:189:SER:HB2	1.85	0.58
1:N:128:GLN:HE22	1:N:225:ARG:HE	1.50	0.58
1:H:335:PHE:HZ	1:H:363:VAL:HG21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:180:ARG:NH1	1:I:339:TYR:CE1	2.72	0.58
1:M:33:VAL:HG22	1:M:44:ILE:HG22	1.85	0.58
1:I:134:VAL:HG12	1:I:188:ALA:HB1	1.85	0.58
1:K:291:ASN:HB3	1:K:294:LEU:HB2	1.86	0.58
1:P:136:GLN:HG2	1:P:219:LEU:CD1	2.29	0.58
1:D:381:ARG:CZ	1:D:381:ARG:HB2	2.33	0.57
1:M:167:ASP:HB3	1:M:172:ARG:HH12	1.68	0.57
1:B:289:LEU:N	1:B:289:LEU:HD22	2.19	0.57
1:D:381:ARG:NH2	1:D:381:ARG:HB2	2.19	0.57
1:M:12:ASN:ND2	1:M:241:GLN:NE2	2.51	0.57
1:M:214:ILE:CD1	1:M:214:ILE:H	2.16	0.57
1:O:17:VAL:HG21	1:O:46:GLY:H	1.66	0.57
1:E:97:ASP:OD1	1:E:97:ASP:N	2.38	0.57
1:J:304:ASP:HA	1:J:324:ILE:O	2.04	0.57
1:J:335:PHE:HZ	1:J:363:VAL:HG21	1.69	0.57
1:J:23:ARG:HH12	1:J:75:ARG:NH1	2.02	0.57
1:O:276:HIS:NE2	1:O:347:LEU:HD12	2.17	0.57
1:B:5:ILE:HG13	1:B:6:ALA:N	2.18	0.57
1:D:240:GLU:OE2	1:D:240:GLU:HA	2.04	0.57
1:D:266:ARG:HH22	1:O:300:ASN:ND2	2.03	0.57
1:F:152:VAL:HG12	1:F:152:VAL:O	2.04	0.57
1:H:299:LEU:HD13	1:H:335:PHE:HD2	1.69	0.57
1:K:85:PRO:HB3	1:L:281:GLN:HE22	1.69	0.57
1:L:283:LEU:HD22	1:L:341:LEU:CG	2.35	0.57
1:A:304:ASP:HA	1:A:324:ILE:O	2.05	0.57
1:G:273:LEU:HD13	1:G:325:GLN:OE1	2.04	0.57
1:J:210:ARG:NH1	1:J:210:ARG:HB3	2.20	0.57
1:K:378[A]:MET:CE	1:K:379:PRO:HD2	2.35	0.57
1:N:17:VAL:HG22	1:N:17:VAL:O	2.03	0.57
1:N:301:PHE:O	1:N:330:PRO:HA	2.05	0.57
1:B:166:ILE:CD1	1:B:223:ILE:HD12	2.32	0.57
1:B:11:LEU:HD11	1:B:82:LYS:HG2	1.86	0.57
1:J:58:ALA:HB3	1:J:241:GLN:HG3	1.87	0.57
1:P:122:LEU:N	1:P:122:LEU:HD12	2.19	0.57
1:E:347:LEU:HD22	1:E:367:ASP:HB2	1.85	0.57
1:F:17:VAL:HG22	1:F:46:GLY:HA3	1.87	0.57
1:K:29:ILE:HG13	1:K:71:THR:HG21	1.87	0.57
1:N:95:THR:HG22	1:N:96:GLU:N	2.19	0.57
1:O:136:GLN:CA	1:O:219:LEU:CD1	2.80	0.57
1:O:138:GLU:CB	1:O:186:ILE:HG12	2.35	0.57
1:P:347:LEU:HD22	1:P:367:ASP:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ASN:CB	1:D:313:PRO:CD	2.71	0.56
1:F:27:LEU:N	1:F:27:LEU:HD12	2.20	0.56
1:G:272:VAL:HG23	1:G:326:TYR:HB2	1.87	0.56
1:I:268:GLY:HA2	1:I:357:THR:HG22	1.85	0.56
1:J:156:ARG:HH12	1:K:154:ASP:HB2	1.70	0.56
1:P:165:GLU:HG3	1:P:197:GLN:HG2	1.87	0.56
1:P:131:GLN:HG3	1:P:220:THR:HG23	1.87	0.56
1:B:56:SER:HB3	1:E:194:GLN:HE22	1.69	0.56
1:D:220:THR:HG1	1:J:193:SER:HG	1.53	0.56
1:M:331:LEU:HD23	1:M:356:MET:SD	2.45	0.56
1:O:55:ALA:HB2	1:O:246:VAL:HG22	1.87	0.56
1:P:145:LYS:HD2	1:P:373:GLN:OE1	2.05	0.56
1:A:166:ILE:HG22	1:A:196:VAL:CG2	2.35	0.56
1:B:327:GLN:O	1:B:327:GLN:HG3	2.04	0.56
1:D:4:LYS:NZ	1:D:89:LEU:CB	2.48	0.56
1:E:136:GLN:HG2	1:E:219:LEU:HD11	1.87	0.56
1:F:272:VAL:HG22	1:F:326:TYR:CD1	2.40	0.56
1:P:245:THR:O	1:P:245:THR:HG23	2.05	0.56
1:K:208:LEU:HD13	1:K:248:PHE:CD2	2.40	0.56
1:M:287:ALA:HB1	1:M:295:ARG:HH21	1.71	0.56
1:M:214:ILE:HG22	1:M:214:ILE:O	2.05	0.56
1:M:227:LEU:HD22	1:M:249:THR:HG22	1.87	0.56
1:E:273:LEU:CD2	1:J:187:LEU:HD12	2.35	0.56
1:I:136:GLN:HG2	1:I:219:LEU:HD11	1.88	0.56
1:K:227:LEU:HD23	1:K:249:THR:CG2	2.35	0.56
1:D:37:THR:HG22	1:D:64:CYS:SG	2.46	0.56
1:L:136:GLN:HG2	1:L:219:LEU:HG	1.87	0.56
1:A:354:MET:HE3	1:A:363:VAL:HG11	1.86	0.56
1:E:162:THR:HG23	1:E:205:VAL:HG21	1.87	0.56
1:G:347:LEU:HD22	1:G:367:ASP:HB2	1.87	0.56
1:J:24:ARG:HH11	1:J:24:ARG:HB2	1.70	0.56
1:K:93:GLN:NE2	1:K:93:GLN:HA	2.20	0.56
1:I:24:ARG:NH1	1:L:313:PRO:HG2	2.20	0.56
1:P:32:ASN:HB3	1:P:71:THR:HG22	1.86	0.56
1:A:94:ILE:HD12	1:A:94:ILE:N	2.19	0.56
1:G:65:LEU:N	1:G:65:LEU:HD12	2.21	0.56
1:L:133:GLN:HB2	1:L:189:SER:HB2	1.87	0.56
1:O:163:LEU:HB3	1:O:174:VAL:CG1	2.33	0.56
1:D:220:THR:HG21	1:J:194:GLN:HG3	1.88	0.56
1:M:90:ILE:HG22	1:M:92:LEU:HD12	1.86	0.56
1:N:162:THR:HB	1:N:200:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:CG2	1:B:46:GLY:N	2.69	0.56
1:N:324:ILE:CD1	1:N:326:TYR:HB2	2.36	0.56
1:N:36:GLN:HA	1:N:69:GLU:HG3	1.88	0.56
1:A:166:ILE:HG22	1:A:196:VAL:HG22	1.85	0.55
1:B:143:PHE:CE2	1:B:208:LEU:CD2	2.75	0.55
1:D:126:ASN:OD1	1:D:127:SER:N	2.39	0.55
1:G:132:VAL:CG1	1:G:191:THR:HG21	2.35	0.55
1:L:297:VAL:CG1	1:L:337:ALA:HB2	2.36	0.55
1:N:125:GLU:HB2	1:N:128:GLN:HG3	1.87	0.55
1:O:158:TYR:CE1	1:O:258:PRO:HD3	2.40	0.55
1:A:1:MET:SD	1:A:37:THR:HG22	2.47	0.55
1:B:148:PHE:HE1	1:B:346:VAL:HG21	1.72	0.55
1:D:271:HIS:NE2	1:D:353:ASN:HB2	2.21	0.55
1:O:17:VAL:HG22	1:O:17:VAL:O	2.06	0.55
1:C:98:GLN:NE2	1:C:115:PRO:HD3	2.22	0.55
1:F:17:VAL:CG2	1:F:46:GLY:N	2.70	0.55
1:H:262:ARG:CB	1:H:262:ARG:HH11	2.19	0.55
1:J:30:LEU:HD11	1:J:49:LEU:HG	1.87	0.55
1:N:234:THR:N	1:N:235:PRO:CD	2.69	0.55
1:C:133:GLN:HG2	1:C:190:SER:HB2	1.88	0.55
1:E:136:GLN:NE2	1:E:232:ILE:HG23	2.21	0.55
1:I:172:ARG:HD2	1:I:260:TYR:OH	2.06	0.55
1:I:99:ARG:HH11	1:I:110:VAL:HG12	1.71	0.55
1:C:14:LEU:HD22	1:C:78:MET:HE1	1.88	0.55
1:H:125:GLU:H	1:H:125:GLU:CD	2.09	0.55
1:N:362:SER:HA	1:N:379:PRO:HD3	1.89	0.55
1:C:172:ARG:HG2	1:C:185:GLU:HG2	1.89	0.55
1:D:3:LEU:HD12	1:D:3:LEU:C	2.26	0.55
1:K:59:LEU:N	1:K:59:LEU:HD12	2.20	0.55
1:P:124:THR:HG22	1:P:227:LEU:CD1	2.36	0.55
1:C:329:ALA:CB	1:C:330:PRO:HD2	2.30	0.55
1:D:54:VAL:HG11	1:D:247:ARG:HH21	1.72	0.55
1:K:111:LEU:HD23	1:L:316:ASP:CG	2.27	0.55
1:L:23:ARG:HB2	1:L:23:ARG:HH11	1.72	0.55
1:P:312:ASN:CB	1:P:313:PRO:CD	2.70	0.55
1:C:187:LEU:HD12	1:C:187:LEU:C	2.27	0.55
1:E:159:LEU:HD22	1:E:176:THR:HG23	1.87	0.55
1:N:326:TYR:CZ	1:N:328:SER:HB2	2.42	0.55
1:A:242:GLY:O	1:A:243:ASP:OD1	2.24	0.55
1:I:269:ASP:OD1	1:I:270:LYS:HG3	2.06	0.55
1:K:208:LEU:HD13	1:K:248:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:306:LEU:HB2	1:N:324:ILE:HG21	1.89	0.55
1:P:14:LEU:HD23	1:P:44:ILE:HG21	1.88	0.55
1:D:54:VAL:HG11	1:D:247:ARG:NH2	2.23	0.54
1:G:230:VAL:HG12	1:G:231:THR:N	2.23	0.54
1:N:240:GLU:OE1	1:N:240:GLU:HA	2.07	0.54
1:N:75:ARG:O	1:N:79:GLU:HG2	2.07	0.54
1:A:103:LYS:HE3	1:A:108:ARG:HH11	1.72	0.54
1:A:49:LEU:HA	1:A:122:LEU:HD11	1.89	0.54
1:B:364:LEU:HD11	1:B:374:THR:CG2	2.37	0.54
1:K:77:LEU:C	1:K:77:LEU:HD23	2.28	0.54
1:L:301:PHE:N	1:L:331:LEU:O	2.31	0.54
1:O:133:GLN:CG	1:O:218:GLN:HE21	2.18	0.54
1:O:285:ARG:HG2	1:P:83:SER:HB2	1.89	0.54
1:C:131:GLN:CG	1:C:220:THR:HG23	2.37	0.54
1:E:321:ASP:C	1:E:322:LEU:HD12	2.28	0.54
1:J:195:LEU:O	1:J:195:LEU:HD23	2.07	0.54
1:K:335:PHE:HZ	1:K:363:VAL:HG21	1.72	0.54
1:P:223:ILE:CD1	1:P:228:LEU:HD13	2.37	0.54
1:E:150:MET:HE2	1:E:202:ARG:HD2	1.88	0.54
1:L:298:PHE:CE1	1:L:334:SER:HB3	2.42	0.54
1:O:261:ARG:HD2	1:O:261:ARG:N	2.21	0.54
1:F:33:VAL:HG13	1:F:74:ALA:HB2	1.89	0.54
1:K:45:THR:CG2	1:K:54:VAL:HG22	2.38	0.54
1:L:355:SER:HB2	1:L:364:LEU:HG	1.89	0.54
1:M:52:GLU:OE1	1:M:122:LEU:HD13	2.07	0.54
1:I:309:ARG:HG3	1:I:319:ILE:HG12	1.89	0.54
1:P:7:LYS:HE2	1:P:85:PRO:O	2.06	0.54
1:L:199:ILE:HG21	1:L:253:ILE:HB	1.88	0.54
1:C:33:VAL:HG22	1:C:44:ILE:CG2	2.38	0.54
1:L:335:PHE:CB	1:L:340:LEU:HD11	2.38	0.54
1:O:298:PHE:HD1	1:O:334:SER:HB2	1.73	0.54
1:B:286:VAL:HG21	1:B:308:LEU:CB	2.38	0.54
1:B:17:VAL:HG22	1:B:46:GLY:HA3	1.89	0.54
1:D:230:VAL:HG12	1:D:248:PHE:HB3	1.88	0.54
1:F:14:LEU:HB3	1:F:78:MET:SD	2.47	0.54
1:H:1:MET:HE2	1:H:70:THR:CG2	2.31	0.54
1:L:329:ALA:HB1	1:L:330:PRO:HD2	1.88	0.54
1:O:196:VAL:CG1	1:O:197:GLN:N	2.70	0.54
1:O:362:SER:OG	1:O:378:MET:CE	2.56	0.54
1:B:257:PHE:CG	1:B:258:PRO:HD2	2.40	0.54
1:C:335:PHE:HZ	1:C:363:VAL:CG2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:LEU:N	1:F:65:LEU:HD12	2.23	0.54
1:G:172:ARG:CG	1:G:183:LEU:HD11	2.37	0.54
1:L:166:ILE:HG13	1:L:166:ILE:O	2.08	0.54
1:L:299:LEU:N	1:L:299:LEU:HD12	2.24	0.54
1:L:65:LEU:H	1:L:65:LEU:CD1	2.21	0.54
1:C:79:GLU:HA	1:C:79:GLU:OE1	2.08	0.53
1:D:9:SER:O	1:D:13:VAL:HG23	2.08	0.53
1:H:377:VAL:HG23	1:H:377:VAL:O	2.08	0.53
1:M:131:GLN:HG3	1:M:220:THR:HG23	1.90	0.53
1:O:130:THR:N	1:O:223:ILE:O	2.41	0.53
1:O:361:GLN:HA	1:O:361:GLN:OE1	2.07	0.53
1:E:94:ILE:HD12	1:E:94:ILE:N	2.22	0.53
1:F:131:GLN:HG3	1:F:220:THR:HG23	1.91	0.53
1:F:52:GLU:C	1:F:53:LEU:HD12	2.28	0.53
1:M:150:MET:HE1	1:M:202:ARG:HA	1.90	0.53
1:N:90:ILE:HG23	1:N:102:LEU:CD2	2.39	0.53
1:A:61:GLU:N	1:A:61:GLU:OE2	2.25	0.53
1:B:172:ARG:HD3	1:B:183:LEU:HD11	1.91	0.53
1:C:49:LEU:HD13	1:C:122:LEU:HD11	1.90	0.53
1:C:16:HIS:O	1:C:53:LEU:HD13	2.08	0.53
1:H:183:LEU:HD23	1:H:183:LEU:C	2.28	0.53
1:I:285:ARG:NH2	1:I:320:GLU:OE2	2.36	0.53
1:E:96:GLU:HA	1:E:96:GLU:OE1	2.08	0.53
1:F:150:MET:HE1	1:F:202:ARG:HA	1.91	0.53
1:J:158:TYR:CE1	1:J:258:PRO:HD3	2.44	0.53
1:N:131:GLN:NE2	1:N:220:THR:HG23	2.24	0.53
1:A:364:LEU:HD21	1:A:374:THR:HG23	1.90	0.53
1:I:156:ARG:HH11	1:L:262:ARG:NH2	2.05	0.53
1:I:353:ASN:HD22	1:I:353:ASN:C	2.10	0.53
1:A:335:PHE:HZ	1:A:363:VAL:HG21	1.73	0.53
1:J:3:LEU:HD12	1:J:63:ALA:O	2.09	0.53
1:M:320:GLU:OE1	1:N:107:SER:HB3	2.08	0.53
1:N:235:PRO:HG3	1:N:243:ASP:CB	2.37	0.53
1:A:301:PHE:O	1:A:330:PRO:HA	2.09	0.53
1:B:155:VAL:HB	1:O:153:GLN:HE21	1.73	0.53
1:E:2:ARG:HG2	1:E:65:LEU:HB2	1.91	0.53
1:F:18:VAL:CG2	1:F:78:MET:CE	2.87	0.53
1:B:274:ILE:CG2	1:B:279:PHE:HB2	2.39	0.53
1:C:33:VAL:CG2	1:C:44:ILE:CG2	2.86	0.53
1:E:271:HIS:HD2	1:J:216:ASP:CB	2.19	0.53
1:E:77:LEU:HD21	1:E:102:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:LYS:HE2	1:H:36:GLN:HE21	1.74	0.53
1:I:78:MET:HE2	1:I:82:LYS:HD2	1.91	0.53
1:F:124:THR:CG2	1:F:227:LEU:HD12	2.38	0.53
1:L:3:LEU:HD11	1:L:37:THR:HG21	1.90	0.53
1:M:312:ASN:CB	1:M:313:PRO:CD	2.72	0.53
1:N:131:GLN:HE21	1:N:220:THR:HG23	1.73	0.53
1:O:57:THR:HG23	1:O:57:THR:O	2.08	0.53
1:G:372:ASP:OD1	1:G:372:ASP:N	2.33	0.53
1:M:347:LEU:HD22	1:M:367:ASP:HB2	1.91	0.53
1:N:171:LEU:HB3	1:N:186:ILE:HD11	1.91	0.53
1:O:334:SER:OG	1:O:380:MET:HE2	2.10	0.53
1:E:285:ARG:HD3	1:F:84:LEU:HD23	1.90	0.52
1:M:176:THR:HG23	1:M:180:ARG:O	2.09	0.52
1:N:18:VAL:HG11	1:N:78:MET:HE3	1.91	0.52
1:A:17:VAL:CG2	1:A:46:GLY:HA3	2.39	0.52
1:A:1:MET:HE1	1:A:70:THR:HG22	1.90	0.52
1:B:335:PHE:CZ	1:B:363:VAL:HG21	2.45	0.52
1:B:361:GLN:HA	1:B:361:GLN:OE1	2.10	0.52
1:B:37:THR:HG22	1:B:42:LEU:HD12	1.91	0.52
1:N:268:GLY:HA2	1:N:357:THR:HG22	1.92	0.52
1:C:129:GLY:HA3	1:C:222:LEU:HD11	1.91	0.52
1:C:272:VAL:HG21	1:C:301:PHE:CE1	2.44	0.52
1:D:183:LEU:HD23	1:D:183:LEU:C	2.29	0.52
1:I:228:LEU:HB3	1:I:250:THR:HG22	1.91	0.52
1:L:301:PHE:CE2	1:L:356:MET:HE3	2.43	0.52
1:P:361:GLN:HA	1:P:361:GLN:OE1	2.09	0.52
1:C:282:SER:OG	1:C:322:LEU:CD1	2.57	0.52
1:F:59:LEU:CD1	1:F:63:ALA:HB3	2.38	0.52
1:G:272:VAL:HG12	1:G:354:MET:HB2	1.91	0.52
1:G:65:LEU:CD1	1:G:65:LEU:N	2.72	0.52
1:I:272:VAL:HG22	1:I:326:TYR:CD1	2.44	0.52
1:K:59:LEU:O	1:K:59:LEU:HD12	2.09	0.52
1:O:147:ALA:O	1:O:150:MET:HE2	2.09	0.52
1:E:214:ILE:O	1:E:214:ILE:HG22	2.09	0.52
1:E:235:PRO:HD3	3:E:418:HOH:O	2.09	0.52
1:E:4:LYS:CB	1:E:4:LYS:NZ	2.73	0.52
1:G:378:MET:SD	1:G:379:PRO:HD2	2.50	0.52
1:H:228:LEU:HD23	1:H:228:LEU:C	2.30	0.52
1:J:28:ASN:CG	1:L:28:ASN:HB3	2.30	0.52
1:N:36:GLN:CG	1:N:69:GLU:HG2	2.19	0.52
1:O:179:HIS:C	1:O:180:ARG:HG3	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG23	1:A:54:VAL:HG22	1.91	0.52
1:I:282:SER:OG	1:I:322:LEU:HD11	2.10	0.52
1:I:353:ASN:ND2	1:I:353:ASN:O	2.43	0.52
1:M:291:ASN:HB3	1:M:294:LEU:HB2	1.91	0.52
1:P:122:LEU:N	1:P:122:LEU:CD1	2.73	0.52
1:A:166:ILE:HD11	1:A:190:SER:HB3	1.91	0.52
1:B:274:ILE:HG22	1:B:275:GLY:O	2.10	0.52
1:H:2:ARG:CG	1:H:93:GLN:NE2	2.71	0.52
1:I:285:ARG:HG2	1:J:83:SER:HB2	1.92	0.52
1:L:226:GLU:C	1:L:227:LEU:HD12	2.30	0.52
1:M:356:MET:HG2	1:M:363:VAL:HG22	1.91	0.52
1:H:77:LEU:HD11	1:H:102:LEU:HD21	1.91	0.52
1:J:241:GLN:HA	1:J:241:GLN:OE1	2.09	0.52
1:L:210:ARG:HG2	1:L:210:ARG:HH11	1.74	0.52
1:N:246:VAL:O	1:N:246:VAL:HG13	2.10	0.52
1:B:132:VAL:HG21	1:B:166:ILE:HG12	1.91	0.52
1:C:75:ARG:O	1:C:79:GLU:HG2	2.10	0.52
1:F:50:GLU:HG3	1:F:156:ARG:HH21	1.75	0.52
1:F:59:LEU:CG	1:F:63:ALA:HB3	2.40	0.52
1:M:272:VAL:HG22	1:M:326:TYR:HD1	1.69	0.52
1:O:358:GLU:HA	1:O:358:GLU:OE2	2.09	0.52
1:O:372:ASP:N	1:O:372:ASP:OD1	2.36	0.52
1:P:195:LEU:C	1:P:195:LEU:HD13	2.30	0.52
1:F:14:LEU:HD13	1:F:78:MET:SD	2.50	0.52
1:J:24:ARG:NH1	1:J:24:ARG:HB2	2.24	0.52
1:L:23:ARG:NH1	1:L:23:ARG:HB2	2.25	0.52
1:L:299:LEU:N	1:L:299:LEU:CD1	2.73	0.52
1:A:257:PHE:CG	1:A:258:PRO:HD2	2.44	0.51
1:E:72:VAL:CG1	1:E:73:PRO:HD2	2.39	0.51
1:F:18:VAL:CG2	1:F:78:MET:HE3	2.39	0.51
1:K:195:LEU:N	1:K:195:LEU:CD1	2.73	0.51
1:N:235:PRO:HG3	1:N:243:ASP:CA	2.40	0.51
1:O:257:PHE:CG	1:O:258:PRO:HD2	2.44	0.51
1:O:313:PRO:C	1:O:315:GLN:H	2.14	0.51
1:P:25:HIS:CE1	1:P:30:LEU:HD12	2.44	0.51
1:A:347:LEU:HD22	1:A:367:ASP:HB2	1.92	0.51
1:B:325:GLN:HG2	1:B:325:GLN:O	2.10	0.51
1:F:172:ARG:HD3	1:F:183:LEU:HD11	1.91	0.51
1:G:22:GLU:HG3	1:G:203:LYS:NZ	2.25	0.51
1:A:294:LEU:N	1:A:294:LEU:HD12	2.26	0.51
1:A:306:LEU:HB2	1:A:324:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LEU:HD22	1:D:176:THR:HG23	1.93	0.51
1:E:239:LYS:HG3	1:E:239:LYS:O	2.10	0.51
1:L:136:GLN:HG2	1:L:219:LEU:CG	2.41	0.51
1:M:122:LEU:HD23	1:M:227:LEU:HD21	1.92	0.51
1:C:145:LYS:HD3	1:C:346:VAL:CG2	2.40	0.51
1:F:146:THR:HG22	1:F:175:THR:HG23	1.91	0.51
1:F:138:GLU:HB3	1:F:186:ILE:HG12	1.93	0.51
1:J:126:ASN:OD1	1:J:226:GLU:CG	2.53	0.51
1:K:65:LEU:N	1:K:65:LEU:CD1	2.73	0.51
1:N:333:MET:HE3	1:N:335:PHE:HE2	1.76	0.51
1:N:45:THR:HG23	1:N:54:VAL:HG22	1.92	0.51
1:E:294:LEU:N	1:E:294:LEU:CD1	2.73	0.51
1:I:1:MET:HE2	1:I:70:THR:HG22	1.92	0.51
1:K:312:ASN:HB2	1:K:313:PRO:HD2	1.92	0.51
1:M:18:VAL:HG22	1:M:18:VAL:O	2.11	0.51
1:B:211:LEU:HD21	1:B:246:VAL:HG11	1.92	0.51
1:B:346:VAL:HG11	1:B:375:TYR:HH	1.67	0.51
1:L:186:ILE:HD12	1:L:187:LEU:H	1.75	0.51
1:L:96:GLU:H	1:L:96:GLU:CD	2.13	0.51
1:N:131:GLN:HE21	1:N:220:THR:CG2	2.24	0.51
1:B:18:VAL:O	1:B:18:VAL:CG2	2.59	0.51
1:D:98:GLN:NE2	1:D:115:PRO:HD3	2.26	0.51
1:E:165:GLU:HG3	1:E:197:GLN:HG2	1.93	0.51
1:K:35:ILE:HG21	1:K:37:THR:HG22	1.90	0.51
1:N:268:GLY:HA2	1:N:357:THR:CG2	2.41	0.51
1:O:8:GLU:OE1	1:O:8:GLU:N	2.37	0.51
1:A:289:LEU:HD22	1:A:316:ASP:HB3	1.93	0.51
1:A:33:VAL:CG2	1:A:44:ILE:HG22	2.40	0.51
1:A:18:VAL:HG11	1:A:78:MET:HG3	1.91	0.51
1:D:156:ARG:CZ	1:D:159:LEU:HD11	2.41	0.51
1:E:320:GLU:HG3	1:F:106:ASN:O	2.11	0.51
1:K:248:PHE:CE1	1:K:250:THR:OG1	2.62	0.51
1:P:228:LEU:HD12	1:P:229:ASN:N	2.26	0.51
1:A:257:PHE:CD2	1:A:258:PRO:HD2	2.46	0.50
1:E:268:GLY:HA2	1:E:357:THR:HG23	1.93	0.50
1:J:136:GLN:NE2	1:J:232:ILE:HG23	2.25	0.50
1:O:32:ASN:HB3	1:O:72:VAL:O	2.10	0.50
1:O:333:MET:HG2	1:O:359:ALA:HA	1.92	0.50
1:P:297:VAL:HG22	1:P:310:ALA:HB2	1.93	0.50
1:G:92:LEU:HD21	1:G:102:LEU:HD21	1.93	0.50
1:G:166:ILE:O	1:G:166:ILE:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:MET:HE2	1:G:335:PHE:CZ	2.46	0.50
1:L:163:LEU:HD23	1:L:199:ILE:HG12	1.93	0.50
1:N:286:VAL:HG12	1:N:310:ALA:HB2	1.94	0.50
1:G:139:LEU:HD23	1:G:212:LEU:HD11	1.93	0.50
1:I:158:TYR:CE1	1:I:258:PRO:HD3	2.46	0.50
1:L:79:GLU:HA	1:L:79:GLU:OE1	2.11	0.50
1:F:126:ASN:ND2	1:F:126:ASN:N	2.60	0.50
1:I:98:GLN:HE22	1:I:114:LEU:C	2.14	0.50
1:K:42:LEU:CD1	1:K:42:LEU:N	2.73	0.50
1:M:138:GLU:HB3	1:M:186:ILE:HG12	1.94	0.50
1:B:257:PHE:CG	1:B:258:PRO:CD	2.95	0.50
1:C:306:LEU:HB2	1:C:324:ILE:HD13	1.92	0.50
1:K:273:LEU:HG	1:K:353:ASN:OD1	2.11	0.50
1:L:364:LEU:HD12	1:L:364:LEU:C	2.31	0.50
1:N:158:TYR:CE1	1:N:258:PRO:HD3	2.47	0.50
1:B:191:THR:O	1:J:222:LEU:CD2	2.59	0.50
1:B:272:VAL:HG22	1:B:326:TYR:CD1	2.47	0.50
1:B:165:GLU:HG3	1:B:197:GLN:HG2	1.93	0.50
1:B:2:ARG:NH1	1:B:93:GLN:OE1	2.44	0.50
1:D:312:ASN:HB2	1:D:313:PRO:HD3	1.87	0.50
1:H:134:VAL:CG2	1:H:186:ILE:CD1	2.90	0.50
1:N:36:GLN:HG2	1:N:69:GLU:CD	2.31	0.50
1:O:145:LYS:HD3	1:O:346:VAL:CG2	2.30	0.50
1:G:10:LEU:HD12	1:G:10:LEU:O	2.12	0.50
1:K:272:VAL:HG22	1:K:326:TYR:CD1	2.46	0.50
1:N:17:VAL:HG22	1:N:46:GLY:HA3	1.93	0.50
1:N:272:VAL:O	1:N:353:ASN:HA	2.12	0.50
1:D:133:GLN:HB2	1:D:190:SER:HB2	1.93	0.50
1:D:150:MET:HE1	1:D:160:THR:O	2.11	0.50
1:E:166:ILE:O	1:E:166:ILE:HG23	2.11	0.50
1:H:42:LEU:CB	1:H:59:LEU:HD11	2.42	0.50
1:I:268:GLY:O	1:I:271:HIS:NE2	2.45	0.50
1:I:347:LEU:HD22	1:I:367:ASP:HB2	1.94	0.50
1:K:101:ILE:HD13	1:K:110:VAL:HG13	1.92	0.50
1:L:133:GLN:OE1	1:L:218:GLN:OE1	2.29	0.50
1:L:135:THR:HG22	1:L:137:ARG:N	2.27	0.50
1:M:228:LEU:HB3	1:M:250:THR:HG22	1.94	0.50
1:I:1:MET:HG2	1:I:3:LEU:HD22	1.94	0.49
1:J:260:TYR:CE1	1:J:261:ARG:HD2	2.47	0.49
1:K:111:LEU:HD23	1:L:316:ASP:OD2	2.12	0.49
1:N:33:VAL:CG2	1:N:74:ALA:CB	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:O	1:A:271:HIS:NE2	2.44	0.49
1:B:158:TYR:CD1	1:B:158:TYR:C	2.85	0.49
1:E:94:ILE:CD1	1:E:94:ILE:N	2.75	0.49
1:G:312:ASN:CB	1:G:313:PRO:CD	2.83	0.49
1:H:158:TYR:CD1	1:H:158:TYR:C	2.85	0.49
1:J:150:MET:HB2	1:J:202:ARG:NH1	2.27	0.49
1:L:301:PHE:CD2	1:L:356:MET:SD	3.05	0.49
1:O:145:LYS:CD	1:O:346:VAL:HG22	2.31	0.49
1:O:34:LYS:HB3	1:O:45:THR:HG22	1.93	0.49
1:C:282:SER:OG	1:C:322:LEU:HD11	2.12	0.49
1:E:214:ILE:CD1	1:E:214:ILE:N	2.73	0.49
1:F:41:ALA:HB2	1:H:40:GLN:HB3	1.93	0.49
1:K:201:PRO:HG2	1:K:250:THR:CG2	2.43	0.49
1:A:282:SER:CB	1:A:322:LEU:HD11	2.42	0.49
1:G:214:ILE:HG13	1:G:214:ILE:O	2.12	0.49
1:N:131:GLN:CG	1:N:220:THR:CG2	2.89	0.49
1:B:317:GLU:OE2	1:B:319:ILE:HD11	2.12	0.49
1:C:335:PHE:CZ	1:C:363:VAL:HG21	2.46	0.49
1:E:243:ASP:OD1	1:E:243:ASP:C	2.51	0.49
1:F:3:LEU:HD12	1:F:63:ALA:O	2.12	0.49
1:F:75:ARG:O	1:F:79:GLU:HG3	2.13	0.49
1:N:235:PRO:HG3	1:N:243:ASP:HA	1.94	0.49
1:N:335:PHE:HZ	1:N:363:VAL:CG1	2.25	0.49
1:O:289:LEU:HD12	1:O:318:ALA:HB2	1.94	0.49
1:O:34:LYS:HB3	1:O:45:THR:CG2	2.43	0.49
1:B:335:PHE:CE1	1:B:363:VAL:HG21	2.47	0.49
1:D:266:ARG:NH1	1:D:266:ARG:CG	2.72	0.49
1:L:51:VAL:HG22	1:L:204:ALA:HB2	1.94	0.49
1:L:248:PHE:CD1	1:L:248:PHE:C	2.85	0.49
1:O:131:GLN:HA	1:O:221:LEU:O	2.11	0.49
1:D:202:ARG:HD2	1:D:202:ARG:O	2.12	0.49
1:I:172:ARG:HG3	1:I:185:GLU:HG2	1.93	0.49
1:K:122:LEU:HB3	1:K:227:LEU:HD21	1.95	0.49
1:L:137:ARG:HB2	1:L:214:ILE:O	2.12	0.49
1:B:26:THR:HB	1:O:314:GLU:CD	2.33	0.49
1:I:166:ILE:HG22	1:I:196:VAL:H	1.78	0.49
1:I:230:VAL:HG12	1:I:248:PHE:HB3	1.95	0.49
1:K:204:ALA:CB	1:K:250:THR:HG21	2.42	0.49
1:L:163:LEU:HB3	1:L:174:VAL:HG13	1.94	0.49
1:L:136:GLN:HG2	1:L:219:LEU:HD11	1.95	0.49
1:B:274:ILE:HG12	1:B:324:ILE:CG2	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ASN:ND2	1:D:114:LEU:HD12	2.27	0.49
1:F:93:GLN:HG3	1:F:101:ILE:HB	1.95	0.49
1:H:134:VAL:HG22	1:H:138:GLU:HB2	1.95	0.49
1:K:59:LEU:HD12	1:K:59:LEU:H	1.78	0.49
1:L:24:ARG:HH12	1:L:313:PRO:HG2	1.77	0.49
1:M:59:LEU:HD22	1:M:63:ALA:CB	2.43	0.49
1:P:59:LEU:HD13	1:P:64:CYS:HB2	1.95	0.49
1:A:217:GLU:CD	1:A:218:GLN:O	2.51	0.48
1:A:306:LEU:HB3	1:A:322:LEU:HB2	1.95	0.48
1:D:150:MET:HE3	1:D:160:THR:C	2.31	0.48
1:F:32:ASN:HB2	1:F:71:THR:CG2	2.42	0.48
1:O:92:LEU:HG	1:O:102:LEU:HD22	1.95	0.48
1:A:102:LEU:HD23	1:A:102:LEU:C	2.34	0.48
1:B:227:LEU:HD23	1:B:251:LYS:HA	1.95	0.48
1:D:306:LEU:HB2	1:D:324:ILE:HD13	1.95	0.48
1:K:80:ILE:HG21	1:K:102:LEU:HD21	1.95	0.48
1:K:75:ARG:NH1	1:K:79:GLU:HG3	2.28	0.48
1:N:312:ASN:CB	1:N:313:PRO:CD	2.90	0.48
1:C:2:ARG:HG2	1:C:65:LEU:HD12	1.94	0.48
1:F:32:ASN:HB3	1:F:71:THR:HG22	1.94	0.48
1:H:150:MET:HG3	1:H:175:THR:CG2	2.42	0.48
1:H:1:MET:CE	1:H:70:THR:HG21	2.40	0.48
1:J:367:ASP:OD2	1:J:370:HIS:CD2	2.66	0.48
1:M:90:ILE:CG2	1:M:92:LEU:HD11	2.43	0.48
1:B:136:GLN:HG2	1:B:219:LEU:CD1	2.44	0.48
1:K:45:THR:HG22	1:K:54:VAL:HG22	1.95	0.48
1:L:350:ASP:O	1:L:351:ASP:CG	2.48	0.48
1:A:16:HIS:O	1:A:53:LEU:HD23	2.14	0.48
1:A:282:SER:HB3	1:A:322:LEU:HD11	1.96	0.48
1:D:289:LEU:HD12	1:D:289:LEU:N	2.29	0.48
1:L:297:VAL:HG13	1:L:337:ALA:HB2	1.95	0.48
1:O:298:PHE:CD1	1:O:334:SER:HB2	2.48	0.48
1:C:33:VAL:CG2	1:C:44:ILE:HG22	2.43	0.48
1:D:2:ARG:HA	1:D:92:LEU:O	2.13	0.48
1:E:273:LEU:HG	1:E:353:ASN:OD1	2.13	0.48
1:E:4:LYS:NZ	1:E:4:LYS:HB2	2.29	0.48
1:H:322:LEU:CD1	1:H:322:LEU:N	2.75	0.48
1:J:181:LEU:HD13	1:J:263:VAL:HG21	1.96	0.48
1:J:37:THR:HG22	1:J:42:LEU:HD12	1.94	0.48
1:O:145:LYS:HA	1:O:346:VAL:HG21	1.95	0.48
1:P:360:ASN:O	1:P:379:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LEU:HD12	3:B:409:HOH:O	2.14	0.48
1:K:159:LEU:HD22	1:K:176:THR:HG23	1.96	0.48
1:O:353:ASN:HD22	1:O:368:PRO:HG3	1.78	0.48
1:A:17:VAL:O	1:A:17:VAL:HG22	2.14	0.48
1:A:290:SER:HB3	1:A:310:ALA:HB1	1.95	0.48
1:B:304:ASP:HA	1:B:324:ILE:O	2.14	0.48
1:E:272:VAL:HG21	1:E:301:PHE:CE1	2.48	0.48
1:I:136:GLN:HG2	1:I:219:LEU:CD1	2.44	0.48
1:A:222:LEU:HD12	1:A:229:ASN:HB3	1.96	0.48
1:B:309:ARG:NH2	1:B:332:GLU:OE2	2.46	0.48
1:C:169:ASN:H	1:C:191:THR:CG2	2.25	0.48
1:C:49:LEU:HD13	1:C:49:LEU:O	2.14	0.48
1:D:132:VAL:HA	1:D:190:SER:O	2.12	0.48
1:H:240:GLU:OE1	1:H:240:GLU:HA	2.13	0.48
1:J:78:MET:HE3	1:J:82:LYS:HE3	1.94	0.48
1:L:163:LEU:CD2	1:L:199:ILE:HG12	2.44	0.48
1:M:262:ARG:NH1	1:M:262:ARG:CG	2.73	0.48
1:O:226:GLU:HG2	1:O:226:GLU:O	2.13	0.48
1:O:99:ARG:HA	1:O:111:LEU:O	2.13	0.48
1:D:165:GLU:HG3	1:D:197:GLN:HG2	1.96	0.48
1:E:230:VAL:HG12	1:E:248:PHE:HB3	1.96	0.48
1:J:27:LEU:HG	1:J:29:ILE:HG22	1.94	0.48
1:K:210:ARG:HG3	1:K:210:ARG:HH11	1.79	0.48
1:K:297:VAL:HG12	1:K:310:ALA:HB2	1.95	0.48
1:N:2:ARG:HG2	1:N:65:LEU:HB3	1.95	0.48
1:O:143:PHE:HE2	1:O:208:LEU:HD13	1.79	0.48
1:D:266:ARG:NH2	1:O:300:ASN:ND2	2.61	0.48
1:O:77:LEU:CD1	1:O:102:LEU:HD11	2.44	0.48
1:F:257:PHE:CG	1:F:258:PRO:HD2	2.49	0.47
1:K:183:LEU:C	1:K:183:LEU:HD23	2.35	0.47
1:A:154:ASP:OD1	1:P:158:TYR:OH	2.31	0.47
1:K:312:ASN:HB2	1:K:313:PRO:CD	2.44	0.47
1:E:32:ASN:HB3	1:E:71:THR:HG22	1.96	0.47
1:F:153:GLN:HE21	1:F:153:GLN:CA	2.19	0.47
1:L:303:GLN:HA	1:L:303:GLN:NE2	2.30	0.47
1:N:343:VAL:HG23	1:N:375:TYR:CD2	2.48	0.47
1:O:83:SER:HB3	1:P:288:ILE:HD11	1.96	0.47
1:E:93:GLN:HG3	1:E:93:GLN:O	2.14	0.47
1:F:92:LEU:HD23	1:F:102:LEU:HG	1.95	0.47
1:H:152:VAL:O	1:H:152:VAL:HG23	2.14	0.47
1:J:372:ASP:N	1:J:372:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:330:PRO:CG	1:O:267:GLY:HA3	2.44	0.47
1:K:84:LEU:HB3	1:K:85:PRO:HD2	1.95	0.47
1:N:230:VAL:HG13	1:N:248:PHE:HB3	1.96	0.47
1:O:98:GLN:HG3	1:O:113:THR:OG1	2.14	0.47
1:P:167:ASP:HB2	1:P:195:LEU:CD2	2.27	0.47
1:B:24:ARG:NH2	1:P:26:THR:HA	2.29	0.47
1:E:134:VAL:HG21	1:E:186:ILE:HD11	1.96	0.47
1:I:312:ASN:CB	1:I:313:PRO:CD	2.84	0.47
1:I:98:GLN:NE2	1:I:114:LEU:CA	2.78	0.47
1:J:308:LEU:CD1	1:J:322:LEU:HD22	2.41	0.47
1:L:92:LEU:HD23	1:L:102:LEU:HG	1.95	0.47
1:N:148:PHE:HE1	1:N:346:VAL:HG11	1.76	0.47
1:N:1:MET:HE3	1:N:70:THR:HG22	1.96	0.47
1:O:212:LEU:HD23	1:O:232:ILE:HD13	1.97	0.47
1:C:270:LYS:H	1:C:270:LYS:CD	2.01	0.47
1:D:33:VAL:HG13	1:D:74:ALA:HB2	1.96	0.47
1:F:163:LEU:HD22	1:F:257:PHE:CD1	2.50	0.47
1:G:94:ILE:HD12	1:G:94:ILE:N	2.29	0.47
1:H:138:GLU:HB3	1:H:186:ILE:CD1	2.43	0.47
1:K:322:LEU:HD23	3:K:405:HOH:O	2.13	0.47
1:L:289:LEU:CD1	1:L:318:ALA:HB2	2.41	0.47
1:M:89:LEU:N	1:M:89:LEU:CD1	2.77	0.47
1:P:300:ASN:HB3	1:P:307:GLN:HB3	1.96	0.47
1:D:266:ARG:HG3	1:D:266:ARG:HH11	1.79	0.47
1:K:36:GLN:HB2	1:K:43:THR:HG21	1.97	0.47
1:O:314:GLU:N	1:O:314:GLU:OE1	2.43	0.47
1:E:145:LYS:O	1:E:148:PHE:HE1	1.98	0.47
1:J:4:LYS:HG3	1:J:4:LYS:O	2.15	0.47
1:O:94:ILE:CD1	1:O:100:CYS:HB2	2.45	0.47
1:B:96:GLU:HA	1:B:96:GLU:OE1	2.14	0.47
1:C:358:GLU:HB2	1:C:361:GLN:CG	2.44	0.47
1:M:3:LEU:HD13	1:M:37:THR:HG21	1.97	0.47
1:N:364:LEU:HD11	1:N:374:THR:HG23	1.96	0.47
1:D:307:GLN:HG3	1:D:321:ASP:OD1	2.14	0.47
1:D:37:THR:HG22	1:D:38:ASN:N	2.29	0.47
1:J:11:LEU:HD12	1:J:78:MET:SD	2.55	0.47
1:M:128:GLN:H	1:M:128:GLN:HG3	1.50	0.47
1:P:272:VAL:CG1	1:P:324:ILE:HD12	2.45	0.47
1:P:72:VAL:CG1	1:P:73:PRO:HD2	2.44	0.47
1:B:194:GLN:H	1:B:194:GLN:CD	2.18	0.47
1:B:306:LEU:HB2	1:B:324:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:98:GLN:NE2	1:I:114:LEU:HA	2.30	0.47
1:J:221:LEU:HD23	1:J:230:VAL:HB	1.96	0.47
1:P:100:CYS:HB2	1:P:113:THR:CG2	2.45	0.47
1:B:278:VAL:HB	1:B:322:LEU:CD1	2.44	0.46
1:F:126:ASN:N	1:F:126:ASN:HD22	2.13	0.46
1:F:230:VAL:HG12	1:F:248:PHE:HB3	1.97	0.46
1:G:194:GLN:HB3	1:G:195:LEU:HD12	1.96	0.46
1:G:273:LEU:HB3	1:G:325:GLN:OE1	2.16	0.46
1:I:335:PHE:CZ	1:I:363:VAL:HG21	2.36	0.46
1:L:137:ARG:CB	1:L:215:GLU:HA	2.21	0.46
1:O:225:ARG:HG3	1:O:225:ARG:O	2.15	0.46
1:A:289:LEU:HD22	1:A:316:ASP:CB	2.46	0.46
1:B:158:TYR:HB2	1:B:199:ILE:HD13	1.97	0.46
1:C:346:VAL:O	1:C:346:VAL:HG22	2.15	0.46
1:E:364:LEU:HD11	1:E:374:THR:CG2	2.45	0.46
1:F:230:VAL:CG1	1:F:248:PHE:HB3	2.45	0.46
1:G:21:VAL:HG11	1:G:31:SER:O	2.14	0.46
1:H:10:LEU:C	1:H:10:LEU:HD23	2.32	0.46
1:H:334:SER:C	1:H:380:MET:HG2	2.35	0.46
1:I:5:ILE:HD11	1:I:10:LEU:CD2	2.37	0.46
1:K:204:ALA:HB2	1:K:250:THR:HG21	1.97	0.46
1:L:174:VAL:HG23	1:L:181:LEU:HD21	1.96	0.46
1:L:174:VAL:HB	1:L:183:LEU:CD2	2.45	0.46
1:L:298:PHE:HB2	1:L:309:ARG:HG3	1.97	0.46
1:B:155:VAL:H	1:O:153:GLN:NE2	2.13	0.46
1:O:211:LEU:HD13	1:O:246:VAL:HG11	1.97	0.46
1:O:228:LEU:HB3	1:O:250:THR:HG22	1.97	0.46
1:P:163:LEU:HD22	1:P:257:PHE:CD2	2.50	0.46
1:P:221:LEU:HD23	1:P:230:VAL:HB	1.98	0.46
1:B:175:THR:HG22	1:B:182:ALA:HB3	1.96	0.46
1:E:187:LEU:HD23	1:E:187:LEU:C	2.36	0.46
1:E:289:LEU:HD12	1:E:318:ALA:HB2	1.97	0.46
1:F:222:LEU:HB3	1:F:229:ASN:HB2	1.96	0.46
1:G:221:LEU:HD23	1:G:230:VAL:HG23	1.91	0.46
1:G:320:GLU:OE1	1:H:107:SER:HB3	2.15	0.46
1:H:168:GLU:HG3	1:H:168:GLU:O	2.14	0.46
1:K:134:VAL:HG12	1:K:221:LEU:CD1	2.46	0.46
1:K:301:PHE:CE1	1:K:306:LEU:HD13	2.50	0.46
1:L:358:GLU:HG3	1:L:360:ASN:H	1.79	0.46
1:N:304:ASP:HA	1:N:324:ILE:O	2.15	0.46
1:C:183:LEU:HD21	1:C:185:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:THR:HG21	1:F:94:ILE:HG12	1.96	0.46
1:J:128:GLN:NE2	1:J:225:ARG:HG3	2.30	0.46
1:L:331:LEU:HD23	1:L:356:MET:SD	2.56	0.46
1:O:179:HIS:O	1:O:180:ARG:HG3	2.15	0.46
1:A:90:ILE:CG2	1:A:102:LEU:HD21	2.38	0.46
1:A:17:VAL:CG2	1:A:46:GLY:CA	2.93	0.46
1:A:272:VAL:HG13	1:A:324:ILE:HD12	1.96	0.46
1:C:135:THR:HG23	1:C:138:GLU:H	1.79	0.46
1:D:187:LEU:HD13	1:D:187:LEU:O	2.15	0.46
1:D:335:PHE:HZ	1:D:363:VAL:HG21	1.80	0.46
1:I:220:THR:HG23	1:I:220:THR:O	2.15	0.46
1:L:174:VAL:HG23	1:L:183:LEU:HG	1.97	0.46
1:D:125:GLU:OE2	1:D:227:LEU:N	2.48	0.46
1:F:154:ASP:OD1	1:F:154:ASP:C	2.47	0.46
1:I:227:LEU:HD23	1:I:251:LYS:HA	1.98	0.46
1:I:264:ILE:HG13	1:I:376:VAL:HG21	1.98	0.46
1:K:162:THR:HG22	1:K:175:THR:HG21	1.96	0.46
1:O:378:MET:CG	1:O:379:PRO:HD2	2.45	0.46
1:O:94:ILE:O	1:O:94:ILE:HG22	2.15	0.46
1:C:70:THR:HG21	1:C:94:ILE:CD1	2.46	0.46
1:H:78:MET:CE	1:H:82:LYS:HE3	2.46	0.46
1:J:156:ARG:HB2	1:J:159:LEU:HD23	1.98	0.46
1:L:322:LEU:C	1:L:322:LEU:HD12	2.36	0.46
1:N:272:VAL:HG23	1:N:356:MET:HE2	1.98	0.46
1:N:279:PHE:CD1	1:N:283:LEU:HD23	2.50	0.46
1:N:33:VAL:CG1	1:N:44:ILE:HG22	2.46	0.46
1:O:312:ASN:HB2	1:O:313:PRO:HD2	1.98	0.46
1:A:326:TYR:CE1	1:A:328:SER:HB2	2.51	0.46
1:K:134:VAL:HG21	1:K:186:ILE:CD1	2.44	0.46
1:L:29:ILE:HG23	1:L:30:LEU:HD12	1.97	0.46
1:B:163:LEU:HD22	1:B:257:PHE:CD2	2.51	0.46
1:C:299:LEU:HD12	1:C:299:LEU:N	2.31	0.46
1:G:124:THR:HB	1:G:227:LEU:HD12	1.97	0.46
1:M:176:THR:CG2	1:M:180:ARG:O	2.64	0.46
1:M:30:LEU:CD1	1:M:49:LEU:HG	2.44	0.46
1:A:141:ARG:O	1:A:145:LYS:HG2	2.16	0.46
1:A:1:MET:CE	1:A:70:THR:HG22	2.46	0.46
1:B:256:LYS:HB3	1:B:256:LYS:HE2	1.79	0.46
1:C:329:ALA:HB1	1:C:330:PRO:CD	2.38	0.46
1:F:117:GLU:CD	1:F:117:GLU:H	2.19	0.46
1:F:126:ASN:ND2	1:F:126:ASN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:TYR:CZ	1:F:328:SER:HB2	2.51	0.46
1:G:59:LEU:HG	1:G:63:ALA:CB	2.46	0.46
1:H:134:VAL:CG2	1:H:186:ILE:HD12	2.46	0.46
1:J:333:MET:HG2	1:J:359:ALA:HA	1.98	0.46
1:N:1:MET:HG3	1:N:37:THR:HG22	1.98	0.46
1:P:160:THR:O	1:P:202:ARG:HB2	2.16	0.46
1:F:307:GLN:NE2	3:F:401:HOH:O	2.49	0.45
1:F:265:PRO:HG2	1:F:364:LEU:HB2	1.98	0.45
1:J:289:LEU:HD22	1:J:316:ASP:HB3	1.97	0.45
1:K:248:PHE:HE1	1:K:250:THR:HG1	1.55	0.45
1:K:34:LYS:HD2	1:K:119:TYR:CG	2.51	0.45
1:L:30:LEU:HD11	1:L:120:PRO:CG	2.46	0.45
1:L:142:LEU:HD13	1:L:171:LEU:HD23	1.96	0.45
1:B:136:GLN:HG2	1:B:219:LEU:HD11	1.97	0.45
1:D:133:GLN:CG	1:D:190:SER:HB2	2.47	0.45
1:D:228:LEU:HB3	1:D:250:THR:HG22	1.98	0.45
1:F:153:GLN:NE2	1:F:153:GLN:CA	2.73	0.45
1:H:14:LEU:HD11	1:H:77:LEU:CD2	2.45	0.45
1:L:163:LEU:HB3	1:L:174:VAL:CG1	2.46	0.45
1:N:346:VAL:HG21	1:N:375:TYR:CZ	2.51	0.45
1:E:14:LEU:HD11	1:E:77:LEU:HD12	1.98	0.45
1:G:49:LEU:HD23	1:G:49:LEU:HA	1.73	0.45
1:I:69:GLU:HG3	1:I:116:ALA:HB3	1.99	0.45
1:N:70:THR:HG21	1:N:94:ILE:CD1	2.47	0.45
1:P:159:LEU:HD23	1:P:177:ASP:HA	1.99	0.45
1:D:301:PHE:CD2	1:D:356:MET:HE1	2.51	0.45
1:H:262:ARG:HB3	1:H:262:ARG:CZ	2.45	0.45
1:A:142:LEU:HG	1:A:173:ALA:HB2	1.99	0.45
1:C:159:LEU:HD22	1:C:176:THR:HG23	1.98	0.45
1:I:72:VAL:CG1	1:I:73:PRO:HD2	2.46	0.45
1:I:78:MET:HE3	1:I:78:MET:HB2	1.72	0.45
1:N:347:LEU:HD22	1:N:367:ASP:HB2	1.99	0.45
1:O:98:GLN:CG	1:O:113:THR:OG1	2.65	0.45
1:A:381:ARG:HG2	1:A:381:ARG:O	2.15	0.45
1:C:228:LEU:HB2	1:C:252:LEU:HD21	1.99	0.45
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.70	0.45
1:I:54:VAL:HG21	1:I:247:ARG:NH2	2.32	0.45
1:I:3:LEU:H	1:I:3:LEU:HD23	1.80	0.45
1:K:307:GLN:HG3	1:K:321:ASP:OD1	2.16	0.45
1:K:65:LEU:C	1:K:65:LEU:HD13	2.37	0.45
1:M:270:LYS:HE3	1:M:357:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HD23	1:B:232:ILE:HD12	1.97	0.45
1:D:167:ASP:HB2	1:D:195:LEU:CD1	2.37	0.45
1:L:136:GLN:NE2	1:L:213:SER:H	2.15	0.45
1:L:277:ASP:C	1:L:279:PHE:N	2.70	0.45
1:P:37:THR:HG22	1:P:64:CYS:SG	2.57	0.45
1:D:301:PHE:CE2	1:D:356:MET:CE	2.99	0.45
1:F:274:ILE:HG12	1:F:324:ILE:HG22	1.99	0.45
1:J:133:GLN:HB3	1:J:218:GLN:NE2	2.32	0.45
1:M:33:VAL:HG22	1:M:44:ILE:CG2	2.47	0.45
1:O:260:TYR:HD1	1:O:264:ILE:CD1	2.30	0.45
1:P:223:ILE:HD12	1:P:223:ILE:N	2.32	0.45
1:D:158:TYR:CE1	1:D:258:PRO:HD3	2.52	0.45
1:E:235:PRO:CD	3:E:418:HOH:O	2.64	0.45
1:G:335:PHE:HZ	1:G:363:VAL:HG21	1.82	0.45
1:I:230:VAL:CG1	1:I:248:PHE:HB3	2.46	0.45
1:I:7:LYS:HA	1:I:90:ILE:HD11	1.99	0.45
1:J:183:LEU:HD23	1:J:183:LEU:C	2.36	0.45
1:K:76:LYS:HD3	1:K:111:LEU:HD21	1.97	0.45
1:K:158:TYR:CE1	1:K:258:PRO:HD3	2.51	0.45
1:L:210:ARG:HG2	1:L:210:ARG:NH1	2.32	0.45
1:L:335:PHE:HB3	1:L:340:LEU:CD1	2.47	0.45
1:M:248:PHE:C	1:M:248:PHE:CD1	2.89	0.45
1:M:90:ILE:CG2	1:M:92:LEU:CD1	2.90	0.45
1:O:40:GLN:N	1:O:40:GLN:NE2	2.60	0.45
1:C:283:LEU:HD23	1:C:341:LEU:CG	2.46	0.45
1:F:257:PHE:CD1	1:F:258:PRO:HD2	2.51	0.45
1:G:166:ILE:HD12	1:G:170:GLN:O	2.17	0.45
1:K:77:LEU:C	1:K:77:LEU:CD2	2.85	0.45
1:M:122:LEU:HD12	1:M:122:LEU:N	2.31	0.45
1:N:70:THR:HG21	1:N:94:ILE:HD11	1.99	0.45
1:B:178:GLY:O	1:O:154:ASP:OD2	2.35	0.45
1:O:157:PHE:HD2	1:O:157:PHE:O	2.00	0.45
1:D:229:ASN:OD1	1:D:249:THR:HG23	2.17	0.44
1:G:33:VAL:O	1:G:71:THR:HA	2.16	0.44
1:J:70:THR:HG21	1:J:94:ILE:CD1	2.47	0.44
1:N:221:LEU:HD23	1:N:230:VAL:HB	1.98	0.44
1:O:13:VAL:HG23	1:O:44:ILE:HD12	1.99	0.44
1:P:124:THR:HG21	1:P:227:LEU:HD12	2.00	0.44
1:A:1:MET:HE3	1:A:94:ILE:HD13	1.99	0.44
1:C:301:PHE:HB3	1:C:326:TYR:CE2	2.52	0.44
1:C:326:TYR:CG	1:C:326:TYR:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:THR:O	1:F:191:THR:OG1	2.27	0.44
1:L:128:GLN:HB3	1:L:129:GLY:H	1.54	0.44
1:M:45:THR:HG23	1:M:54:VAL:HG22	1.99	0.44
1:N:240:GLU:O	1:N:240:GLU:HG3	2.17	0.44
1:N:301:PHE:N	1:N:331:LEU:O	2.38	0.44
1:O:222:LEU:CD2	1:O:222:LEU:C	2.85	0.44
1:O:30:LEU:HD21	1:O:49:LEU:HG	1.98	0.44
1:P:215:GLU:OE2	1:P:235:PRO:HG3	2.17	0.44
1:P:10:LEU:HD23	1:P:81:CYS:SG	2.57	0.44
1:A:326:TYR:CZ	1:A:328:SER:HB2	2.53	0.44
1:B:170:GLN:NE2	1:B:172:ARG:NH2	2.66	0.44
1:C:283:LEU:HD23	1:C:341:LEU:CD2	2.47	0.44
1:E:24:ARG:HA	1:E:24:ARG:NE	2.30	0.44
1:F:0:HIS:HE1	1:F:96:GLU:HG2	1.81	0.44
1:F:162:THR:HA	1:F:175:THR:HG22	1.99	0.44
1:F:16:HIS:O	1:F:53:LEU:HD23	2.18	0.44
1:F:37:THR:HG22	1:F:42:LEU:HA	1.99	0.44
1:L:153:GLN:HA	1:L:160:THR:HG21	2.00	0.44
1:M:354:MET:CE	1:M:363:VAL:HG11	2.47	0.44
1:O:346:VAL:O	1:O:346:VAL:HG13	2.18	0.44
1:D:3:LEU:CD1	1:D:3:LEU:C	2.85	0.44
1:E:257:PHE:CG	1:E:258:PRO:HD2	2.53	0.44
1:E:72:VAL:HG12	1:E:73:PRO:HD2	1.98	0.44
1:G:39:ALA:HA	1:G:64:CYS:SG	2.58	0.44
1:F:56:SER:CB	1:H:40:GLN:OE1	2.66	0.44
1:N:309:ARG:NH2	3:N:401:HOH:O	2.50	0.44
1:O:370:HIS:HA	1:O:371:PRO:HD2	1.85	0.44
1:D:172:ARG:HD2	1:D:260:TYR:OH	2.18	0.44
1:F:301:PHE:O	1:F:330:PRO:HA	2.17	0.44
1:G:273:LEU:HD23	1:G:351:ASP:HB3	1.99	0.44
1:H:42:LEU:HB3	1:H:59:LEU:HD11	1.98	0.44
1:I:132:VAL:HG22	1:I:166:ILE:CD1	2.43	0.44
1:K:282:SER:OG	1:K:322:LEU:HD11	2.18	0.44
1:K:353:ASN:ND2	1:K:368:PRO:HG3	2.32	0.44
1:N:90:ILE:HG22	1:N:92:LEU:HD12	1.98	0.44
1:B:186:ILE:C	1:B:186:ILE:HD12	2.38	0.44
1:C:98:GLN:HE21	1:C:115:PRO:HD3	1.82	0.44
1:D:187:LEU:C	1:D:187:LEU:CD1	2.85	0.44
1:N:95:THR:HG22	1:N:97:ASP:N	2.20	0.44
1:O:101:ILE:HG23	1:O:110:VAL:HG22	2.00	0.44
1:P:167:ASP:CA	1:P:195:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:HIS:O	1:A:66:GLU:HB3	2.18	0.44
1:B:194:GLN:OE1	1:B:194:GLN:N	2.40	0.44
1:B:364:LEU:HD11	1:B:374:THR:HG23	1.98	0.44
1:D:-2:HIS:O	1:D:-2:HIS:CG	2.70	0.44
1:F:40:GLN:HE22	1:H:245:THR:HG23	1.82	0.44
1:H:308:LEU:N	1:H:308:LEU:HD12	2.33	0.44
1:L:136:GLN:OE1	1:L:232:ILE:HG23	2.18	0.44
1:L:148:PHE:CE2	1:L:346:VAL:HG21	2.52	0.44
1:M:300:ASN:OD1	1:M:332:GLU:HG3	2.17	0.44
1:N:1:MET:SD	1:N:37:THR:HG22	2.58	0.44
1:O:136:GLN:CB	1:O:219:LEU:HD11	2.47	0.44
1:B:24:ARG:HB3	1:P:24:ARG:HG2	1.99	0.44
1:D:69:GLU:HG3	1:D:116:ALA:HB3	2.00	0.44
1:E:354:MET:HB3	1:E:356:MET:HE3	1.99	0.44
1:H:10:LEU:C	1:H:10:LEU:CD2	2.86	0.44
1:M:241:GLN:HA	1:M:241:GLN:OE1	2.17	0.44
1:C:90:ILE:CG2	1:C:102:LEU:HD23	2.48	0.44
1:E:322:LEU:CD1	1:E:322:LEU:N	2.80	0.44
1:F:17:VAL:HG23	1:F:53:LEU:O	2.17	0.44
1:P:7:LYS:CD	1:P:84:LEU:CB	2.68	0.44
1:E:4:LYS:HG3	1:E:65:LEU:HD11	2.00	0.43
1:G:358:GLU:OE1	1:G:358:GLU:HA	2.18	0.43
1:I:281:GLN:CA	1:I:281:GLN:NE2	2.73	0.43
1:K:201:PRO:HG2	1:K:250:THR:HG21	1.98	0.43
1:L:164:LEU:HA	1:L:164:LEU:HD23	1.76	0.43
1:L:358:GLU:HG2	1:L:360:ASN:OD1	2.18	0.43
1:L:75:ARG:O	1:L:79:GLU:HG2	2.17	0.43
1:B:175:THR:CG2	1:B:182:ALA:HB3	2.48	0.43
1:D:266:ARG:HG2	1:D:266:ARG:NH1	2.33	0.43
1:E:335:PHE:HZ	1:E:363:VAL:HG21	1.84	0.43
1:I:289:LEU:HD12	1:I:318:ALA:HB2	2.00	0.43
1:I:353:ASN:C	1:I:353:ASN:ND2	2.72	0.43
1:J:25:HIS:CE1	1:J:30:LEU:HD12	2.53	0.43
1:L:4:LYS:HE3	1:L:89:LEU:CD2	2.49	0.43
1:A:159:LEU:HD22	1:A:176:THR:HG23	2.01	0.43
1:B:140:LYS:O	1:B:144:GLU:HG3	2.18	0.43
1:B:171:LEU:HB3	1:B:186:ILE:CD1	2.48	0.43
1:C:183:LEU:HD23	1:C:183:LEU:C	2.39	0.43
1:D:80:ILE:HG21	1:D:102:LEU:HD12	2.00	0.43
1:E:163:LEU:HD11	1:E:197:GLN:HB3	2.00	0.43
1:E:240:GLU:O	1:E:240:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:GLN:HG3	1:G:187:LEU:HD13	2.00	0.43
1:N:305:SER:N	1:N:324:ILE:HG13	2.33	0.43
1:O:148:PHE:CD2	1:O:342:ASP:HB3	2.53	0.43
1:O:297:VAL:HG12	1:O:310:ALA:HB2	2.00	0.43
1:O:299:LEU:N	1:O:299:LEU:CD1	2.80	0.43
1:D:65:LEU:HA	1:D:65:LEU:HD13	1.58	0.43
1:F:101:ILE:HG12	1:F:110:VAL:HG22	2.01	0.43
1:G:127:SER:HB2	3:G:417:HOH:O	2.19	0.43
1:F:56:SER:HB3	1:H:40:GLN:OE1	2.18	0.43
1:K:125:GLU:O	1:K:125:GLU:HG2	2.19	0.43
1:L:163:LEU:HD13	1:L:163:LEU:C	2.38	0.43
1:M:269:ASP:OD1	1:M:270:LYS:CG	2.61	0.43
1:N:257:PHE:CG	1:N:258:PRO:HD2	2.53	0.43
1:O:145:LYS:HA	1:O:346:VAL:CG2	2.49	0.43
1:D:172:ARG:HE	1:D:172:ARG:HB2	1.53	0.43
1:D:65:LEU:HB3	1:D:66:GLU:H	1.61	0.43
1:L:135:THR:CG2	1:L:137:ARG:HB3	2.48	0.43
1:L:297:VAL:HG11	1:L:337:ALA:HB2	2.00	0.43
1:M:187:LEU:HA	1:M:187:LEU:HD23	1.78	0.43
1:M:136:GLN:HE21	1:M:213:SER:H	1.65	0.43
1:N:65:LEU:HD13	1:N:66:GLU:HG2	2.01	0.43
1:O:155:VAL:HB	1:O:156:ARG:CZ	2.48	0.43
1:O:356:MET:N	1:O:356:MET:SD	2.92	0.43
1:A:1:MET:HG3	1:A:37:THR:CG2	2.49	0.43
1:A:294:LEU:N	1:A:294:LEU:CD1	2.81	0.43
1:C:133:GLN:HB2	1:C:189:SER:HB3	2.00	0.43
1:C:356:MET:HG3	1:C:363:VAL:HG13	2.00	0.43
1:D:142:LEU:HD11	1:D:186:ILE:HD13	2.01	0.43
1:D:273:LEU:HD21	1:D:351:ASP:OD1	2.18	0.43
1:H:378:MET:CB	1:H:379:PRO:CD	2.92	0.43
1:M:227:LEU:HD22	1:M:249:THR:CG2	2.49	0.43
1:O:260:TYR:HD1	1:O:264:ILE:HD13	1.84	0.43
1:O:50:GLU:HG2	1:O:50:GLU:O	2.18	0.43
1:P:303:GLN:N	1:P:303:GLN:CD	2.72	0.43
1:B:347:LEU:HD22	1:B:367:ASP:HB2	2.00	0.43
1:E:136:GLN:HE22	1:E:232:ILE:HG23	1.83	0.43
1:J:2:ARG:NH1	1:J:93:GLN:OE1	2.51	0.43
1:M:264:ILE:HA	1:M:265:PRO:HD3	1.92	0.43
1:M:32:ASN:CB	1:M:71:THR:HG22	2.49	0.43
1:P:329:ALA:HA	1:P:330:PRO:HD3	1.87	0.43
1:E:164:LEU:HD12	1:E:164:LEU:HA	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:ARG:HE	1:E:24:ARG:CA	2.29	0.43
1:F:17:VAL:HG22	1:F:46:GLY:CA	2.49	0.43
1:I:100:CYS:HB2	1:I:113:THR:CG2	2.49	0.43
1:K:134:VAL:HG12	1:K:221:LEU:HD13	2.01	0.43
1:K:65:LEU:H	1:K:65:LEU:CD1	2.31	0.43
1:L:37:THR:CG2	1:L:42:LEU:CD1	2.95	0.43
1:M:278:VAL:CG1	1:M:322:LEU:CD2	2.91	0.43
1:M:32:ASN:HB3	1:M:71:THR:HG22	2.00	0.43
1:M:59:LEU:HD22	1:M:63:ALA:HB1	1.99	0.43
1:N:228:LEU:C	1:N:228:LEU:HD23	2.39	0.43
1:G:289:LEU:HD12	1:G:318:ALA:HB2	2.01	0.43
1:H:135:THR:HA	1:H:218:GLN:HA	2.01	0.43
1:I:142:LEU:CD2	1:I:186:ILE:HG12	2.48	0.43
1:I:83:SER:HB2	1:J:285:ARG:HG2	2.00	0.43
1:M:312:ASN:HB2	1:M:313:PRO:HD3	1.96	0.43
1:M:33:VAL:CG2	1:M:44:ILE:CG2	2.97	0.43
1:N:166:ILE:CD1	1:N:196:VAL:CG2	2.96	0.43
1:P:272:VAL:HG22	1:P:326:TYR:CD1	2.53	0.43
1:D:45:THR:HG23	1:D:54:VAL:HG22	2.00	0.43
1:F:32:ASN:CB	1:F:71:THR:CG2	2.95	0.43
1:H:303:GLN:N	1:H:303:GLN:CD	2.72	0.43
1:J:306:LEU:HB2	1:J:324:ILE:HG21	2.01	0.43
1:J:3:LEU:HD22	1:J:37:THR:HG21	2.01	0.43
1:J:71:THR:O	1:J:113:THR:HB	2.18	0.43
1:N:208:LEU:HA	1:N:208:LEU:HD12	1.87	0.43
1:A:248:PHE:C	1:A:248:PHE:CD1	2.92	0.42
1:A:33:VAL:CG2	1:A:44:ILE:CG2	2.96	0.42
1:C:131:GLN:CD	1:C:220:THR:HG21	2.39	0.42
1:D:289:LEU:HD23	1:D:316:ASP:HB3	2.01	0.42
1:E:272:VAL:HG13	1:E:324:ILE:HD12	2.01	0.42
1:F:30:LEU:HD23	1:F:30:LEU:HA	1.79	0.42
1:G:198:ALA:HB1	1:G:252:LEU:HD13	2.01	0.42
1:I:49:LEU:HA	1:I:49:LEU:HD12	1.43	0.42
1:L:283:LEU:HA	1:L:286:VAL:CG1	2.49	0.42
1:N:162:THR:HA	1:N:175:THR:HG22	2.01	0.42
1:N:65:LEU:C	1:N:65:LEU:HD13	2.38	0.42
1:B:155:VAL:H	1:O:153:GLN:HE21	1.66	0.42
1:O:248:PHE:CD1	1:O:248:PHE:C	2.92	0.42
1:O:13:VAL:CG2	1:O:44:ILE:HD12	2.48	0.42
1:P:256:LYS:HB3	1:P:256:LYS:HE2	1.91	0.42
1:P:59:LEU:CD1	1:P:64:CYS:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLN:HA	1:A:326:TYR:O	2.19	0.42
1:B:133:GLN:HB2	1:B:189:SER:HB3	2.01	0.42
1:D:142:LEU:CD1	1:D:186:ILE:HD13	2.49	0.42
1:D:200:VAL:HG12	1:D:204:ALA:HB3	2.01	0.42
1:D:27:LEU:HD12	1:D:30:LEU:HD12	2.01	0.42
1:D:30:LEU:HD11	1:D:49:LEU:HG	2.01	0.42
1:D:94:ILE:HD12	1:D:94:ILE:N	2.35	0.42
1:E:124:THR:O	1:E:124:THR:HG23	2.18	0.42
1:F:17:VAL:HG21	1:F:46:GLY:N	2.35	0.42
1:G:83:SER:HB3	1:H:288:ILE:HD11	2.01	0.42
1:L:163:LEU:HD12	1:L:165:GLU:HB2	2.00	0.42
1:N:171:LEU:HB3	1:N:186:ILE:CD1	2.49	0.42
1:N:289:LEU:O	1:N:312:ASN:HB3	2.18	0.42
1:O:281:GLN:HB3	1:O:285:ARG:NH1	2.31	0.42
1:F:2:ARG:HG3	1:F:65:LEU:HB2	2.01	0.42
1:J:258:PRO:HB3	1:K:156:ARG:CZ	2.49	0.42
1:K:208:LEU:HA	1:K:208:LEU:HD12	1.77	0.42
1:K:326:TYR:CE1	1:K:328:SER:HB2	2.55	0.42
1:L:163:LEU:CD1	1:L:165:GLU:HB2	2.49	0.42
1:L:174:VAL:HB	1:L:183:LEU:HD21	2.01	0.42
1:L:195:LEU:HB3	1:L:196:VAL:H	1.61	0.42
1:L:289:LEU:HD22	1:L:316:ASP:HB3	2.00	0.42
1:L:42:LEU:HB2	1:L:59:LEU:HD13	2.01	0.42
1:N:272:VAL:HG23	1:N:356:MET:CE	2.50	0.42
1:O:135:THR:C	1:O:219:LEU:HD12	2.39	0.42
1:A:33:VAL:HG22	1:A:44:ILE:CG2	2.49	0.42
1:B:132:VAL:CG2	1:B:166:ILE:HG12	2.49	0.42
1:B:5:ILE:HG13	1:B:6:ALA:H	1.83	0.42
1:D:27:LEU:HD12	1:D:30:LEU:CD1	2.49	0.42
1:E:29:ILE:O	1:E:32:ASN:HB2	2.19	0.42
1:K:11:LEU:HD11	1:K:82:LYS:CG	2.47	0.42
1:K:131:GLN:HG3	1:K:220:THR:HG23	2.01	0.42
1:L:152:VAL:O	1:L:153:GLN:HG3	2.20	0.42
1:N:124:THR:HB	1:N:227:LEU:CD1	2.47	0.42
1:N:305:SER:C	1:N:324:ILE:HG12	2.39	0.42
1:N:1:MET:CE	1:N:70:THR:HG22	2.49	0.42
1:O:30:LEU:HD11	1:O:120:PRO:CG	2.49	0.42
1:A:272:VAL:HG22	1:A:326:TYR:CD1	2.54	0.42
1:J:158:TYR:CZ	1:J:258:PRO:HD3	2.55	0.42
1:L:148:PHE:CD2	1:L:346:VAL:HG21	2.53	0.42
1:L:137:ARG:CB	1:L:214:ILE:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:299:LEU:HG	1:L:308:LEU:CD2	2.49	0.42
1:M:132:VAL:HB	1:M:221:LEU:HB2	2.01	0.42
1:P:306:LEU:HB2	1:P:324:ILE:HD13	2.02	0.42
1:A:312:ASN:CB	1:A:313:PRO:CD	2.83	0.42
1:B:303:GLN:CD	1:B:303:GLN:N	2.72	0.42
1:C:165:GLU:HG3	1:C:197:GLN:HG2	2.00	0.42
1:C:186:ILE:HD12	1:C:187:LEU:H	1.85	0.42
1:C:25:HIS:CE1	1:C:30:LEU:HD12	2.54	0.42
1:C:327:GLN:H	1:C:327:GLN:CD	2.23	0.42
1:F:237:ARG:HG3	1:F:237:ARG:HH11	1.83	0.42
1:O:186:ILE:HA	1:O:186:ILE:HD12	1.95	0.42
1:A:115:PRO:HB3	1:A:117:GLU:HG2	2.01	0.42
1:B:102:LEU:HB2	1:B:109:PHE:HB2	2.02	0.42
1:D:64:CYS:SG	1:D:64:CYS:O	2.77	0.42
1:E:49:LEU:HD23	1:E:49:LEU:HA	1.82	0.42
1:F:32:ASN:HB2	1:F:71:THR:HG22	2.02	0.42
1:G:269:ASP:OD1	1:G:270:LYS:N	2.52	0.42
1:I:294:LEU:N	1:I:294:LEU:HD12	2.35	0.42
1:J:293:LYS:HD3	1:J:293:LYS:N	2.34	0.42
1:J:329:ALA:HA	1:J:330:PRO:HD3	1.77	0.42
1:K:295:ARG:HA	1:K:295:ARG:HD2	1.87	0.42
1:K:2:ARG:HG2	1:K:94:ILE:N	2.34	0.42
1:K:64:CYS:O	1:K:64:CYS:SG	2.78	0.42
1:N:1:MET:HG3	1:N:37:THR:CG2	2.50	0.42
1:O:305:SER:C	1:O:324:ILE:HG12	2.40	0.42
1:O:354:MET:HG2	1:O:365:VAL:HG22	2.02	0.42
1:P:14:LEU:HD11	1:P:77:LEU:CD2	2.50	0.42
1:P:228:LEU:HB3	1:P:250:THR:HG22	2.01	0.42
1:B:195:LEU:O	1:B:195:LEU:HD12	2.19	0.42
1:D:289:LEU:HD13	1:D:318:ALA:HB2	2.02	0.42
1:H:299:LEU:HD13	1:H:335:PHE:CD2	2.51	0.42
1:K:198:ALA:HB1	1:K:252:LEU:HD13	2.02	0.42
1:K:75:ARG:CZ	1:K:79:GLU:HG3	2.50	0.42
1:M:122:LEU:CD1	1:M:122:LEU:N	2.82	0.42
1:N:17:VAL:CG2	1:N:17:VAL:O	2.68	0.42
1:O:364:LEU:C	1:O:364:LEU:HD12	2.39	0.42
1:O:380:MET:HE2	1:O:380:MET:HB2	1.68	0.42
1:H:297:VAL:HG22	1:H:310:ALA:HB2	2.02	0.42
1:I:295:ARG:HA	1:I:295:ARG:HD2	1.71	0.42
1:J:150:MET:HB2	1:J:202:ARG:HH12	1.85	0.42
1:K:30:LEU:HD11	1:K:49:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:208:LEU:HA	1:O:208:LEU:HD23	1.90	0.42
1:O:222:LEU:HD23	1:O:223:ILE:N	2.35	0.42
1:A:329:ALA:HA	1:A:330:PRO:HD3	1.89	0.42
1:F:303:GLN:O	1:F:303:GLN:HG2	2.17	0.42
1:G:282:SER:OG	1:G:322:LEU:HD13	2.20	0.42
1:H:220:THR:O	1:H:220:THR:HG23	2.20	0.42
1:I:162:THR:HA	1:I:175:THR:HG22	2.02	0.42
1:I:2:ARG:CG	1:I:65:LEU:HD12	2.47	0.42
1:J:37:THR:HG22	1:J:42:LEU:CD1	2.50	0.42
1:J:70:THR:HG21	1:J:94:ILE:HD12	2.02	0.42
1:K:131:GLN:CG	1:K:220:THR:HG23	2.49	0.42
1:K:268:GLY:HA2	1:K:357:THR:HG22	2.00	0.42
1:K:61:GLU:HA	1:K:64:CYS:SG	2.60	0.42
1:L:145:LYS:HD2	1:L:346:VAL:HG12	2.01	0.42
1:L:132:VAL:HG11	1:L:171:LEU:HD12	2.00	0.42
1:M:228:LEU:HD23	1:M:228:LEU:O	2.20	0.42
1:N:14:LEU:HB3	1:N:78:MET:CE	2.50	0.42
1:A:33:VAL:HG22	1:A:44:ILE:HG22	2.03	0.41
1:C:327:GLN:N	1:C:327:GLN:CD	2.73	0.41
1:D:73:PRO:HD3	1:D:112:GLY:O	2.20	0.41
1:D:312:ASN:CB	1:D:313:PRO:HD3	2.46	0.41
1:F:125:GLU:N	1:F:125:GLU:CD	2.73	0.41
1:H:138:GLU:HB3	1:H:186:ILE:HD12	2.02	0.41
1:J:364:LEU:HD11	1:J:374:THR:CG2	2.50	0.41
1:K:162:THR:HA	1:K:175:THR:HG22	2.02	0.41
1:M:354:MET:HB3	1:M:354:MET:HE2	1.91	0.41
1:N:234:THR:HB	1:N:235:PRO:HD3	2.01	0.41
1:O:72:VAL:CG1	1:O:73:PRO:HD2	2.50	0.41
1:D:322:LEU:HD12	1:D:322:LEU:HA	1.78	0.41
1:E:45:THR:HG23	1:E:54:VAL:HG22	2.02	0.41
1:F:225:ARG:NH1	1:F:226:GLU:OE1	2.52	0.41
1:H:364:LEU:HD11	1:H:374:THR:HG23	2.02	0.41
1:M:110:VAL:O	1:M:110:VAL:HG23	2.20	0.41
1:C:198:ALA:HB2	1:C:223:ILE:CG2	2.51	0.41
1:C:49:LEU:HD13	1:C:122:LEU:CD1	2.50	0.41
1:E:135:THR:HG1	1:E:138:GLU:HG3	1.80	0.41
1:G:137:ARG:HG2	1:G:137:ARG:NH1	2.35	0.41
1:G:241:GLN:N	1:G:241:GLN:CD	2.73	0.41
1:I:166:ILE:O	1:I:166:ILE:HG23	2.20	0.41
1:I:166:ILE:HD12	1:I:171:LEU:HD13	2.02	0.41
1:J:263:VAL:HG11	1:K:155:VAL:CG1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:333:MET:CE	1:N:335:PHE:HE2	2.33	0.41
1:N:95:THR:CG2	1:N:96:GLU:N	2.82	0.41
1:P:265:PRO:HG2	1:P:364:LEU:HB2	2.00	0.41
1:A:140:LYS:O	1:A:144:GLU:HG3	2.19	0.41
1:C:72:VAL:CG1	1:C:73:PRO:HD2	2.51	0.41
1:F:27:LEU:N	1:F:27:LEU:CD1	2.83	0.41
1:G:78:MET:CE	1:G:79:GLU:HG3	2.51	0.41
1:H:134:VAL:HG23	1:H:186:ILE:HD12	2.01	0.41
1:I:24:ARG:HH12	1:L:313:PRO:CG	2.33	0.41
1:K:51:VAL:HG22	1:K:204:ALA:HB2	2.03	0.41
1:K:4:LYS:CB	1:K:64:CYS:HB2	2.34	0.41
1:L:140:LYS:NZ	1:L:209:GLN:O	2.53	0.41
1:A:150:MET:HG2	1:A:175:THR:HG22	2.02	0.41
1:A:227:LEU:HD23	1:A:251:LYS:HA	2.03	0.41
1:A:303:GLN:H	1:A:303:GLN:CD	2.14	0.41
1:A:303:GLN:N	1:A:303:GLN:CD	2.73	0.41
1:C:162:THR:CG2	1:C:175:THR:HG22	2.22	0.41
1:D:301:PHE:CE2	1:D:356:MET:HE1	2.56	0.41
1:D:37:THR:CG2	1:D:38:ASN:N	2.83	0.41
1:G:136:GLN:HG2	1:G:219:LEU:CG	2.49	0.41
1:I:30:LEU:HA	1:I:30:LEU:HD23	1.71	0.41
1:J:28:ASN:CB	1:L:28:ASN:HB3	2.50	0.41
1:M:83:SER:CB	1:N:288:ILE:HD11	2.49	0.41
1:N:17:VAL:HG21	1:N:46:GLY:N	2.34	0.41
1:P:104:SER:O	1:P:107:SER:HB2	2.20	0.41
1:B:2:ARG:NH1	1:B:93:GLN:HB2	2.36	0.41
1:E:172:ARG:HE	1:E:172:ARG:HB2	1.61	0.41
1:H:125:GLU:CD	1:H:125:GLU:N	2.73	0.41
1:J:195:LEU:CD2	1:J:195:LEU:C	2.85	0.41
1:M:151:ALA:HB2	1:M:177:ASP:HB2	2.03	0.41
1:O:226:GLU:O	1:O:226:GLU:CG	2.68	0.41
1:O:274:ILE:HG21	1:O:322:LEU:HD23	2.01	0.41
1:P:164:LEU:HD23	1:P:164:LEU:HA	1.91	0.41
1:F:0:HIS:N	1:F:0:HIS:ND1	2.63	0.41
1:H:289:LEU:HD12	1:H:318:ALA:HB2	2.03	0.41
1:K:278:VAL:CG1	1:K:322:LEU:HD22	2.51	0.41
1:N:241:GLN:OE1	1:N:241:GLN:HA	2.21	0.41
1:N:343:VAL:HG23	1:N:375:TYR:CG	2.56	0.41
1:O:77:LEU:HD12	1:O:102:LEU:HD11	2.02	0.41
1:O:329:ALA:HA	1:O:330:PRO:HD3	1.90	0.41
1:A:142:LEU:HG	1:A:173:ALA:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:MET:HE3	1:A:78:MET:O	2.20	0.41
1:B:250:THR:HG23	1:B:250:THR:O	2.21	0.41
1:E:107:SER:OG	1:F:285:ARG:HD2	2.21	0.41
1:F:289:LEU:HD12	1:F:318:ALA:HB2	2.03	0.41
1:I:278:VAL:CG1	1:I:322:LEU:HD22	2.51	0.41
1:I:367:ASP:HA	1:I:368:PRO:HD2	1.90	0.41
1:L:208:LEU:HA	1:L:208:LEU:HD12	1.91	0.41
1:L:145:LYS:HA	1:L:346:VAL:CG1	2.50	0.41
1:L:347:LEU:HD11	1:L:375:TYR:CD2	2.56	0.41
1:A:214:ILE:HG23	1:A:214:ILE:O	2.20	0.41
1:D:212:LEU:CD2	1:D:219:LEU:HD11	2.51	0.41
1:E:133:GLN:HB2	1:E:189:SER:HB2	2.03	0.41
1:G:228:LEU:HB3	1:G:250:THR:HG22	2.03	0.41
1:J:301:PHE:O	1:J:330:PRO:HB3	2.21	0.41
1:K:124:THR:C	1:K:126:ASN:H	2.24	0.41
1:K:130:THR:HG23	1:K:192:SER:HB2	2.02	0.41
1:L:135:THR:HG22	1:L:137:ARG:HB3	2.03	0.41
1:M:233:ASN:O	1:M:234:THR:HG22	2.21	0.41
1:O:137:ARG:HG3	1:O:214:ILE:HG23	2.01	0.41
1:O:248:PHE:CD1	1:O:248:PHE:O	2.73	0.41
1:A:194:GLN:O	1:A:194:GLN:HG2	2.21	0.41
1:B:226:GLU:O	1:B:226:GLU:HG2	2.21	0.41
1:C:33:VAL:HG22	1:C:44:ILE:HG23	2.02	0.41
1:F:91:ASP:HB3	1:F:103:LYS:HB2	2.03	0.41
1:F:329:ALA:HA	1:F:330:PRO:HD3	1.89	0.41
1:G:21:VAL:CG1	1:G:31:SER:O	2.69	0.41
1:I:3:LEU:N	1:I:3:LEU:CD2	2.83	0.41
1:M:54:VAL:O	1:M:246:VAL:HA	2.21	0.41
1:M:69:GLU:HB3	1:M:116:ALA:CB	2.51	0.41
1:N:230:VAL:CG1	1:N:248:PHE:HB3	2.50	0.41
1:O:174:VAL:HG23	1:O:181:LEU:HD11	2.03	0.41
1:O:200:VAL:HA	1:O:201:PRO:HD3	1.87	0.41
1:A:49:LEU:HA	1:A:49:LEU:HD23	1.89	0.41
1:F:104:SER:O	1:F:107:SER:HB2	2.21	0.41
1:F:300:ASN:ND2	1:F:332:GLU:HG3	2.36	0.41
1:G:183:LEU:HB3	1:G:374:THR:HB	2.03	0.41
1:G:162:THR:CG2	1:G:205:VAL:HG21	2.49	0.41
1:H:272:VAL:CG1	1:H:324:ILE:HD12	2.51	0.41
1:J:322:LEU:HD23	1:J:322:LEU:N	2.36	0.41
1:K:93:GLN:CA	1:K:93:GLN:NE2	2.82	0.41
1:K:106:ASN:ND2	1:L:321:ASP:O	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:164:LEU:HD23	1:N:164:LEU:HA	1.93	0.41
1:N:341:LEU:HD23	1:N:344:LEU:HD12	2.03	0.41
1:A:30:LEU:HD11	1:A:49:LEU:HG	2.02	0.40
1:D:214:ILE:HG12	1:E:216:ASP:HB3	2.03	0.40
1:G:59:LEU:HD12	1:G:59:LEU:HA	1.82	0.40
1:G:94:ILE:CD1	1:G:94:ILE:N	2.84	0.40
1:H:49:LEU:HD23	1:H:49:LEU:HA	1.73	0.40
1:M:136:GLN:HG2	1:M:219:LEU:HD11	2.02	0.40
1:P:49:LEU:HA	1:P:49:LEU:HD23	1.79	0.40
1:B:17:VAL:HG21	1:B:46:GLY:N	2.36	0.40
1:F:152:VAL:O	1:F:152:VAL:CG1	2.70	0.40
1:J:289:LEU:HD12	1:J:318:ALA:HB2	2.02	0.40
1:J:293:LYS:HG3	1:K:24:ARG:NE	2.36	0.40
1:N:269:ASP:OD1	1:N:269:ASP:N	2.49	0.40
1:O:136:GLN:N	1:O:219:LEU:HD12	2.35	0.40
1:A:135:THR:CG2	1:A:216:ASP:HA	2.51	0.40
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.94	0.40
1:C:130:THR:HG23	1:C:192:SER:HB2	2.03	0.40
1:G:132:VAL:CG1	1:G:191:THR:CG2	2.89	0.40
1:G:65:LEU:CD1	1:G:65:LEU:H	2.34	0.40
1:H:334:SER:O	1:H:380:MET:HG2	2.20	0.40
1:H:2:ARG:NE	1:H:65:LEU:HD22	2.35	0.40
1:J:2:ARG:HG3	1:J:65:LEU:HD12	2.04	0.40
1:L:61:GLU:N	1:L:61:GLU:CD	2.72	0.40
1:M:286:VAL:HG12	1:M:310:ALA:CB	2.51	0.40
1:N:278:VAL:HG23	1:N:278:VAL:H	1.67	0.40
1:O:171:LEU:C	1:O:171:LEU:HD12	2.42	0.40
1:A:96:GLU:N	1:A:96:GLU:CD	2.72	0.40
1:C:228:LEU:HB3	1:C:250:THR:HG22	2.02	0.40
1:D:11:LEU:HD13	1:D:81:CYS:CB	2.51	0.40
1:F:136:GLN:HG2	1:F:219:LEU:CD1	2.41	0.40
1:G:124:THR:O	1:G:124:THR:HG23	2.20	0.40
1:G:230:VAL:CG1	1:G:231:THR:N	2.83	0.40
1:F:40:GLN:HB3	1:H:41:ALA:HB2	2.02	0.40
1:I:195:LEU:HD22	1:I:195:LEU:C	2.36	0.40
1:L:92:LEU:CD2	1:L:102:LEU:HG	2.52	0.40
1:N:335:PHE:HZ	1:N:363:VAL:HG11	1.85	0.40
1:P:286:VAL:HG21	1:P:308:LEU:HB2	2.02	0.40
1:A:102:LEU:HD23	1:A:103:LYS:N	2.36	0.40
1:A:137:ARG:NH1	1:A:216:ASP:OD1	2.49	0.40
1:B:96:GLU:CA	1:B:96:GLU:OE1	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:GLN:HG2	1:E:220:THR:HG23	2.03	0.40
1:E:70:THR:HG21	1:E:94:ILE:HG12	2.02	0.40
1:F:92:LEU:CD2	1:F:102:LEU:HG	2.51	0.40
1:F:159:LEU:CD2	1:F:176:THR:HG23	2.51	0.40
1:H:170:GLN:HG3	1:H:170:GLN:O	2.21	0.40
1:H:340:LEU:N	1:H:340:LEU:HD12	2.37	0.40
1:K:248:PHE:C	1:K:248:PHE:CD1	2.95	0.40
1:L:145:LYS:HD2	1:L:346:VAL:CG1	2.51	0.40
1:L:240:GLU:HA	1:L:240:GLU:OE2	2.22	0.40
1:M:164:LEU:HA	1:M:164:LEU:HD23	1.96	0.40
1:N:137:ARG:HD3	1:N:214:ILE:HG12	2.03	0.40
1:N:270:LYS:HG2	1:N:270:LYS:H	1.58	0.40
1:O:356:MET:HG3	1:O:363:VAL:HG13	2.02	0.40
1:O:54:VAL:HB	1:O:247:ARG:HB2	2.03	0.40
1:P:195:LEU:HD22	1:P:196:VAL:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	374/388 (96%)	367 (98%)	6 (2%)	1 (0%)	41	73
1	B	380/388 (98%)	375 (99%)	5 (1%)	0	100	100
1	C	375/388 (97%)	365 (97%)	9 (2%)	1 (0%)	41	73
1	D	378/388 (97%)	370 (98%)	8 (2%)	0	100	100
1	E	380/388 (98%)	371 (98%)	9 (2%)	0	100	100
1	F	375/388 (97%)	369 (98%)	6 (2%)	0	100	100
1	G	374/388 (96%)	366 (98%)	8 (2%)	0	100	100
1	H	381/388 (98%)	375 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	364/388 (94%)	352 (97%)	11 (3%)	1 (0%)	41	73
1	J	382/388 (98%)	372 (97%)	10 (3%)	0	100	100
1	K	358/388 (92%)	344 (96%)	12 (3%)	2 (1%)	25	60
1	L	344/388 (89%)	336 (98%)	7 (2%)	1 (0%)	41	73
1	M	374/388 (96%)	368 (98%)	5 (1%)	1 (0%)	41	73
1	N	364/388 (94%)	360 (99%)	3 (1%)	1 (0%)	41	73
1	O	345/388 (89%)	334 (97%)	11 (3%)	0	100	100
1	P	373/388 (96%)	359 (96%)	14 (4%)	0	100	100
All	All	5921/6208 (95%)	5783 (98%)	130 (2%)	8 (0%)	51	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	125	GLU
1	A	265	PRO
1	L	160	THR
1	N	265	PRO
1	K	115	PRO
1	C	265	PRO
1	I	234	THR
1	M	73	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	330/341 (97%)	326 (99%)	4 (1%)	71	88
1	B	333/341 (98%)	326 (98%)	7 (2%)	53	80
1	C	329/341 (96%)	318 (97%)	11 (3%)	38	70
1	D	331/341 (97%)	325 (98%)	6 (2%)	59	82
1	E	333/341 (98%)	326 (98%)	7 (2%)	53	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	331/341 (97%)	327 (99%)	4 (1%)	71	88
1	G	329/341 (96%)	323 (98%)	6 (2%)	59	82
1	H	330/341 (97%)	317 (96%)	13 (4%)	32	65
1	I	321/341 (94%)	312 (97%)	9 (3%)	43	74
1	J	334/341 (98%)	328 (98%)	6 (2%)	59	82
1	K	314/341 (92%)	301 (96%)	13 (4%)	30	64
1	L	304/341 (89%)	296 (97%)	8 (3%)	46	75
1	M	328/341 (96%)	321 (98%)	7 (2%)	53	80
1	N	323/341 (95%)	317 (98%)	6 (2%)	57	81
1	O	309/341 (91%)	292 (94%)	17 (6%)	21	53
1	P	327/341 (96%)	318 (97%)	9 (3%)	43	74
All	All	5206/5456 (95%)	5073 (97%)	133 (3%)	46	75

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	128	GLN
1	A	202	ARG
1	A	364	LEU
1	B	42	LEU
1	B	97	ASP
1	B	240	GLU
1	B	243	ASP
1	B	341	LEU
1	B	357	THR
1	B	378	MET
1	C	37	THR
1	C	49	LEU
1	C	92	LEU
1	C	122	LEU
1	C	153	GLN
1	C	155	VAL
1	C	170	GLN
1	C	186	ILE
1	C	270	LYS
1	C	273	LEU
1	C	303	GLN

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Mol	Chain	Res	Type
1	D	3	LEU
1	D	24	ARG
1	D	65	LEU
1	D	187	LEU
1	D	215	GLU
1	D	266	ARG
1	E	71	THR
1	E	77	LEU
1	E	97	ASP
1	E	215	GLU
1	E	244	ILE
1	E	282	SER
1	E	356	MET
1	F	0	HIS
1	F	59	LEU
1	F	187	LEU
1	F	195	LEU
1	G	155	VAL
1	G	191	THR
1	G	196	VAL
1	G	240	GLU
1	G	243	ASP
1	G	273	LEU
1	H	0	HIS
1	H	59	LEU
1	H	124	THR
1	H	126	ASN
1	H	158	TYR
1	H	166	ILE
1	H	167	ASP
1	H	172	ARG
1	H	175	THR
1	H	191	THR
1	H	322	LEU
1	H	356	MET
1	H	378	MET
1	I	33	VAL
1	I	59	LEU
1	I	111	LEU
1	I	167	ASP
1	I	195	LEU
1	I	295	ARG

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Mol	Chain	Res	Type
1	I	353	ASN
1	I	356	MET
1	I	381	ARG
1	J	-2	HIS
1	J	158	TYR
1	J	170	GLN
1	J	191	THR
1	J	195	LEU
1	J	269	ASP
1	K	37	THR
1	K	59	LEU
1	K	65	LEU
1	K	66	GLU
1	K	113	THR
1	K	131	GLN
1	K	137	ARG
1	K	181	LEU
1	K	194	GLN
1	K	195	LEU
1	K	246	VAL
1	K	295	ARG
1	K	372	ASP
1	L	155	VAL
1	L	170	GLN
1	L	183	LEU
1	L	195	LEU
1	L	215	GLU
1	L	216	ASP
1	L	220	THR
1	L	347	LEU
1	M	78	MET
1	M	95	THR
1	M	156	ARG
1	M	176	THR
1	M	195	LEU
1	M	262	ARG
1	M	378	MET
1	N	216	ASP
1	N	259	ASP
1	N	261	ARG
1	N	270	LYS
1	N	273	LEU

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Mol	Chain	Res	Type
1	N	321	ASP
1	O	65	LEU
1	O	92	LEU
1	O	96	GLU
1	O	98	GLN
1	O	100	CYS
1	O	156	ARG
1	O	157	PHE
1	O	159	LEU
1	O	160	THR
1	O	162	THR
1	O	185	GLU
1	O	220	THR
1	O	245	THR
1	O	274	ILE
1	O	346	VAL
1	O	348	ASP
1	O	350	ASP
1	P	71	THR
1	P	124	THR
1	P	126	ASN
1	P	127	SER
1	P	186	ILE
1	P	246	VAL
1	P	269	ASP
1	P	274	ILE
1	P	325	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	271	HIS
1	A	373	GLN
1	B	126	ASN
1	B	271	HIS
1	B	302	ASN
1	C	98	GLN
1	C	128	GLN
1	C	131	GLN
1	C	133	GLN
1	C	303	GLN

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Mol	Chain	Res	Type
1	D	98	GLN
1	D	284	GLN
1	D	302	ASN
1	D	373	GLN
1	E	194	GLN
1	E	218	GLN
1	E	361	GLN
1	F	36	GLN
1	F	126	ASN
1	F	131	GLN
1	F	133	GLN
1	F	153	GLN
1	F	218	GLN
1	F	233	ASN
1	F	373	GLN
1	G	0	HIS
1	G	233	ASN
1	G	307	GLN
1	G	361	GLN
1	G	373	GLN
1	H	0	HIS
1	H	36	GLN
1	H	93	GLN
1	H	126	ASN
1	H	131	GLN
1	H	133	GLN
1	H	218	GLN
1	H	361	GLN
1	H	373	GLN
1	I	98	GLN
1	I	133	GLN
1	I	153	GLN
1	I	170	GLN
1	I	218	GLN
1	I	281	GLN
1	I	353	ASN
1	I	373	GLN
1	J	128	GLN
1	J	133	GLN
1	J	153	GLN
1	J	194	GLN
1	J	209	GLN

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Mol	Chain	Res	Type
1	J	366	GLN
1	K	126	ASN
1	K	131	GLN
1	K	133	GLN
1	K	197	GLN
1	K	218	GLN
1	L	-1	HIS
1	L	128	GLN
1	L	136	GLN
1	L	281	GLN
1	L	284	GLN
1	L	303	GLN
1	M	12	ASN
1	M	136	GLN
1	M	170	GLN
1	M	315	GLN
1	M	327	GLN
1	M	353	ASN
1	M	366	GLN
1	M	373	GLN
1	N	0	HIS
1	N	36	GLN
1	N	98	GLN
1	N	128	GLN
1	N	131	GLN
1	N	133	GLN
1	O	40	GLN
1	O	98	GLN
1	O	133	GLN
1	O	153	GLN
1	O	218	GLN
1	O	291	ASN
1	O	327	GLN
1	P	302	ASN
1	P	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	378/388 (97%)	0.14	11 (2%) 51 35	27, 56, 94, 134	0
1	B	382/388 (98%)	-0.01	4 (1%) 82 68	18, 44, 86, 118	0
1	C	379/388 (97%)	0.21	9 (2%) 59 42	30, 54, 92, 114	1 (0%)
1	D	382/388 (98%)	0.07	12 (3%) 49 32	15, 39, 72, 101	1 (0%)
1	E	382/388 (98%)	-0.09	0 100 100	12, 32, 63, 132	0
1	F	379/388 (97%)	0.04	5 (1%) 77 61	26, 46, 76, 121	1 (0%)
1	G	378/388 (97%)	0.22	16 (4%) 36 23	21, 50, 89, 128	2 (0%)
1	H	383/388 (98%)	0.20	15 (3%) 39 25	30, 59, 95, 128	0
1	I	370/388 (95%)	0.49	32 (8%) 10 6	28, 65, 98, 148	3 (0%)
1	J	384/388 (98%)	0.04	7 (1%) 68 51	22, 52, 85, 108	1 (0%)
1	K	365/388 (94%)	0.41	26 (7%) 16 9	22, 51, 110, 134	3 (0%)
1	L	356/388 (91%)	0.62	44 (12%) 4 2	29, 78, 116, 149	1 (0%)
1	M	378/388 (97%)	0.24	19 (5%) 28 18	20, 53, 96, 118	0
1	N	372/388 (95%)	0.27	6 (1%) 72 55	30, 64, 98, 120	2 (0%)
1	O	357/388 (92%)	0.91	58 (16%) 1 1	39, 81, 108, 136	0
1	P	377/388 (97%)	0.25	9 (2%) 59 42	30, 63, 105, 132	0
All	All	6002/6208 (96%)	0.25	273 (4%) 33 21	12, 55, 101, 149	15 (0%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	PRO	8.2
1	K	63	ALA	7.3
1	L	354	MET	7.1
1	O	55	ALA	6.5
1	I	235	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	O	244	ILE	6.4
1	O	228	LEU	6.1
1	D	187	LEU	5.9
1	H	237	ARG	5.7
1	K	62	GLY	5.7
1	L	353	ASN	5.6
1	O	247	ARG	5.4
1	K	102	LEU	5.2
1	O	42	LEU	5.1
1	I	25	HIS	5.0
1	O	153	GLN	5.0
1	O	230	VAL	4.8
1	L	377	VAL	4.7
1	M	37	THR	4.7
1	L	128	GLN	4.7
1	L	214	ILE	4.6
1	I	55	ALA	4.5
1	G	188	ALA	4.5
1	O	221	LEU	4.4
1	H	-2	HIS	4.4
1	L	283	LEU	4.4
1	M	190	SER	4.4
1	K	35	ILE	4.3
1	A	40	GLN	4.3
1	L	279	PHE	4.3
1	G	37	THR	4.2
1	G	304	ASP	4.2
1	B	155	VAL	4.1
1	F	156	ARG	4.0
1	O	248	PHE	4.0
1	K	64	CYS	4.0
1	L	139	LEU	3.9
1	O	78	MET	3.8
1	P	68	GLY	3.7
1	O	197	GLN	3.7
1	L	339	TYR	3.7
1	F	155	VAL	3.7
1	A	268	GLY	3.7
1	I	42	LEU	3.7
1	O	43	THR	3.7
1	O	44	ILE	3.7
1	K	5	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	269	ASP	3.6
1	M	126	ASN	3.6
1	C	359	ALA	3.6
1	I	186	ILE	3.6
1	M	268	GLY	3.6
1	N	279	PHE	3.6
1	L	347	LEU	3.5
1	L	381	ARG	3.5
1	N	196	VAL	3.5
1	O	304	ASP	3.5
1	L	340	LEU	3.4
1	O	57	THR	3.4
1	I	61	GLU	3.4
1	K	86	THR	3.4
1	H	61	GLU	3.4
1	G	100	CYS	3.4
1	M	92	LEU	3.3
1	K	46	GLY	3.3
1	K	98	GLN	3.3
1	O	56	SER	3.3
1	O	199	ILE	3.3
1	I	50	GLU	3.3
1	K	53	LEU	3.3
1	L	349	GLY	3.3
1	F	225	ARG	3.2
1	D	126	ASN	3.2
1	L	355	SER	3.2
1	O	9	SER	3.2
1	I	200	VAL	3.2
1	I	198	ALA	3.2
1	H	60	SER	3.2
1	M	49	LEU	3.2
1	I	228	LEU	3.1
1	D	100	CYS	3.1
1	I	211	LEU	3.1
1	L	235	PRO	3.1
1	H	127	SER	3.1
1	H	155	VAL	3.1
1	O	354	MET	3.1
1	O	363	VAL	3.0
1	O	54	VAL	3.0
1	O	377	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	194	GLN	3.0
1	O	122	LEU	3.0
1	O	303	GLN	3.0
1	I	9	SER	3.0
1	O	253	ILE	3.0
1	K	33	VAL	3.0
1	G	193	SER	3.0
1	N	60	SER	3.0
1	I	27	LEU	3.0
1	L	294	LEU	3.0
1	G	187	LEU	3.0
1	M	124	THR	3.0
1	N	354	MET	3.0
1	L	322	LEU	2.9
1	L	335	PHE	2.9
1	L	237	ARG	2.9
1	M	266	ARG	2.9
1	M	267	GLY	2.9
1	C	331	LEU	2.9
1	I	22	GLU	2.9
1	O	369	ALA	2.9
1	C	266	ARG	2.9
1	G	169	ASN	2.9
1	I	28	ASN	2.9
1	H	297	VAL	2.9
1	O	198	ALA	2.9
1	P	243	ASP	2.8
1	L	365	VAL	2.8
1	D	188	ALA	2.8
1	D	356	MET	2.8
1	A	353	ASN	2.8
1	A	41	ALA	2.8
1	H	355	SER	2.8
1	A	129	GLY	2.8
1	H	266	ARG	2.8
1	L	348	ASP	2.8
1	K	42	LEU	2.8
1	K	113	THR	2.8
1	I	233	ASN	2.7
1	O	25	HIS	2.7
1	L	181	LEU	2.7
1	I	197	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	154	ASP	2.7
1	L	364	LEU	2.7
1	O	164	LEU	2.7
1	C	267	GLY	2.7
1	G	303	GLN	2.7
1	K	36	GLN	2.7
1	I	23	ARG	2.7
1	G	63	ALA	2.7
1	K	95	THR	2.7
1	L	240	GLU	2.7
1	D	236	SER	2.7
1	O	50	GLU	2.7
1	O	51	VAL	2.7
1	O	258	PRO	2.7
1	F	154	ASP	2.6
1	J	154	ASP	2.6
1	K	97	ASP	2.6
1	C	37	THR	2.6
1	O	163	LEU	2.6
1	O	375	TYR	2.6
1	M	16	HIS	2.6
1	L	306	LEU	2.6
1	K	72	VAL	2.6
1	L	263	VAL	2.6
1	L	49	LEU	2.6
1	O	223	ILE	2.5
1	L	264	ILE	2.5
1	I	26	THR	2.5
1	L	376	VAL	2.5
1	L	367	ASP	2.5
1	G	64	CYS	2.5
1	O	16	HIS	2.5
1	O	86	THR	2.5
1	G	92	LEU	2.5
1	A	266	ARG	2.5
1	L	238	ASP	2.5
1	A	193	SER	2.5
1	J	348	ASP	2.5
1	L	178	GLY	2.5
1	O	102	LEU	2.5
1	O	186	ILE	2.5
1	M	189	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	174	VAL	2.4
1	L	321	ASP	2.4
1	D	234	THR	2.4
1	O	250	THR	2.4
1	I	102	LEU	2.4
1	B	78	MET	2.4
1	I	24	ARG	2.4
1	K	57	THR	2.4
1	K	191	THR	2.4
1	I	49	LEU	2.4
1	P	97	ASP	2.4
1	J	243	ASP	2.4
1	G	195	LEU	2.4
1	I	138	GLU	2.4
1	I	303	GLN	2.4
1	O	162	THR	2.4
1	K	17	VAL	2.4
1	A	366	GLN	2.3
1	I	53	LEU	2.3
1	I	164	LEU	2.3
1	K	34	LYS	2.3
1	I	81	CYS	2.3
1	O	232	ILE	2.3
1	O	262	ARG	2.3
1	L	332	GLU	2.3
1	G	81	CYS	2.3
1	C	128	GLN	2.3
1	I	51	VAL	2.3
1	L	168	GLU	2.3
1	O	226	GLU	2.3
1	I	223	ILE	2.3
1	O	229	ASN	2.3
1	I	16	HIS	2.2
1	M	78	MET	2.2
1	B	266	ARG	2.2
1	D	72	VAL	2.2
1	L	243	ASP	2.2
1	H	195	LEU	2.2
1	M	356	MET	2.2
1	G	189	SER	2.2
1	O	365	VAL	2.2
1	F	37	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	220	THR	2.2
1	P	228	LEU	2.2
1	A	368	PRO	2.2
1	O	260	TYR	2.2
1	M	93	GLN	2.2
1	I	221	LEU	2.2
1	H	283	LEU	2.2
1	C	-2	HIS	2.2
1	O	368	PRO	2.2
1	K	3	LEU	2.2
1	P	26	THR	2.2
1	O	13	VAL	2.2
1	L	223	ILE	2.1
1	K	18	VAL	2.1
1	D	92	LEU	2.1
1	M	10	LEU	2.1
1	O	294	LEU	2.1
1	P	96	GLU	2.1
1	J	155	VAL	2.1
1	K	43	THR	2.1
1	L	308	LEU	2.1
1	A	365	VAL	2.1
1	H	37	THR	2.1
1	P	191	THR	2.1
1	L	23	ARG	2.1
1	O	274	ILE	2.1
1	G	1	MET	2.1
1	N	230	VAL	2.1
1	K	45	THR	2.1
1	G	3	LEU	2.1
1	M	243	ASP	2.1
1	H	299	LEU	2.1
1	I	195	LEU	2.1
1	K	37	THR	2.1
1	H	154	ASP	2.1
1	O	220	THR	2.1
1	L	291	ASN	2.1
1	J	331	LEU	2.1
1	O	246	VAL	2.1
1	D	77	LEU	2.0
1	O	10	LEU	2.0
1	C	130	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	49	LEU	2.0
1	L	179	HIS	2.0
1	C	127	SER	2.0
1	N	132	VAL	2.0
1	P	102	LEU	2.0
1	L	334	SER	2.0
1	J	78	MET	2.0
1	L	363	VAL	2.0
1	P	156	ARG	2.0
1	D	-2	HIS	2.0
1	M	48	ASP	2.0
1	O	370	HIS	2.0
1	M	123	THR	2.0
1	O	130	THR	2.0
1	O	278	VAL	2.0
1	A	356	MET	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	401	1/1	0.92	0.14	30,30,30,30	0
2	MG	J	401	1/1	0.96	0.09	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.