



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:24 am GMT

PDB ID : 3RPU  
Title : Crystal structure of the MukE-MukF complex  
Authors : Guarne, A.; Gloyd, M.; Ghirlando, R.  
Deposited on : 2011-04-27  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

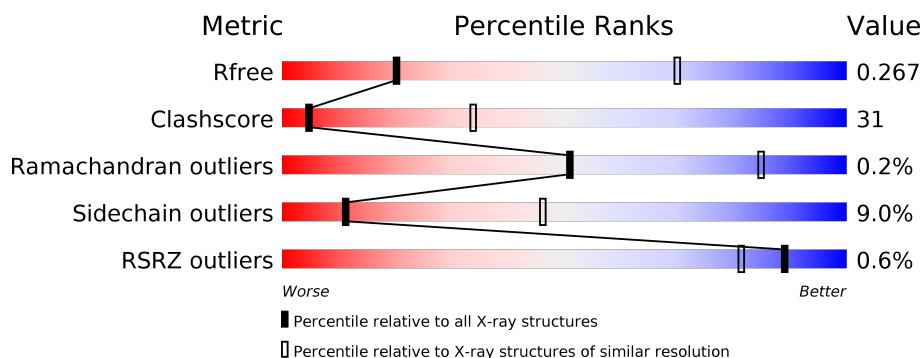
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.




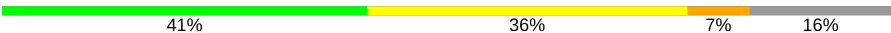
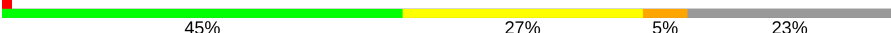
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 35%, green 30%, grey 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>35%</span> <span>30%</span> <span>•</span> <span>33%</span> </div> </div>
1	B	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 29%, green 33%, orange 1%, grey 34%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>29%</span> <span>33%</span> <span>•</span> <span>34%</span> </div> </div>
1	X	460	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 40%, yellow 25%, orange 1%, grey 33%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>40%</span> <span>25%</span> <span>•</span> <span>33%</span> </div> </div>
2	D	245	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 37%, yellow 39%, orange 7%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>37%</span> <span>39%</span> <span>7%</span> <span>17%</span> </div> </div>
2	E	245	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 44%, yellow 31%, orange 1%, grey 22%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>44%</span> <span>31%</span> <span>•</span> <span>22%</span> </div> </div>
2	G	245	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 42%, yellow 35%, orange 7%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>42%</span> <span>35%</span> <span>7%</span> <span>17%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	245	 39% 36% 22%
2	Y	245	 41% 36% 7% 16%
2	Z	245	 45% 27% 5% 23%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17083 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 Chromosome partition protein mukF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2503	1573	447	475	8			
1	B	302	Total	C	N	O	S	0	0	0
			2443	1536	438	462	7			
1	X	310	Total	C	N	O	S	0	0	0
			2504	1573	448	476	7			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P60293
A	-18	GLY	-	EXPRESSION TAG	UNP P60293
A	-17	SER	-	EXPRESSION TAG	UNP P60293
A	-16	SER	-	EXPRESSION TAG	UNP P60293
A	-15	HIS	-	EXPRESSION TAG	UNP P60293
A	-14	HIS	-	EXPRESSION TAG	UNP P60293
A	-13	HIS	-	EXPRESSION TAG	UNP P60293
A	-12	HIS	-	EXPRESSION TAG	UNP P60293
A	-11	HIS	-	EXPRESSION TAG	UNP P60293
A	-10	HIS	-	EXPRESSION TAG	UNP P60293
A	-9	SER	-	EXPRESSION TAG	UNP P60293
A	-8	SER	-	EXPRESSION TAG	UNP P60293
A	-7	GLY	-	EXPRESSION TAG	UNP P60293
A	-6	LEU	-	EXPRESSION TAG	UNP P60293
A	-5	VAL	-	EXPRESSION TAG	UNP P60293
A	-4	PRO	-	EXPRESSION TAG	UNP P60293
A	-3	ARG	-	EXPRESSION TAG	UNP P60293
A	-2	GLY	-	EXPRESSION TAG	UNP P60293
A	-1	SER	-	EXPRESSION TAG	UNP P60293
A	0	HIS	-	EXPRESSION TAG	UNP P60293
B	-19	MET	-	EXPRESSION TAG	UNP P60293
B	-18	GLY	-	EXPRESSION TAG	UNP P60293
B	-17	SER	-	EXPRESSION TAG	UNP P60293

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P60293
B	-15	HIS	-	EXPRESSION TAG	UNP P60293
B	-14	HIS	-	EXPRESSION TAG	UNP P60293
B	-13	HIS	-	EXPRESSION TAG	UNP P60293
B	-12	HIS	-	EXPRESSION TAG	UNP P60293
B	-11	HIS	-	EXPRESSION TAG	UNP P60293
B	-10	HIS	-	EXPRESSION TAG	UNP P60293
B	-9	SER	-	EXPRESSION TAG	UNP P60293
B	-8	SER	-	EXPRESSION TAG	UNP P60293
B	-7	GLY	-	EXPRESSION TAG	UNP P60293
B	-6	LEU	-	EXPRESSION TAG	UNP P60293
B	-5	VAL	-	EXPRESSION TAG	UNP P60293
B	-4	PRO	-	EXPRESSION TAG	UNP P60293
B	-3	ARG	-	EXPRESSION TAG	UNP P60293
B	-2	GLY	-	EXPRESSION TAG	UNP P60293
B	-1	SER	-	EXPRESSION TAG	UNP P60293
B	0	HIS	-	EXPRESSION TAG	UNP P60293
X	-19	MET	-	EXPRESSION TAG	UNP P60293
X	-18	GLY	-	EXPRESSION TAG	UNP P60293
X	-17	SER	-	EXPRESSION TAG	UNP P60293
X	-16	SER	-	EXPRESSION TAG	UNP P60293
X	-15	HIS	-	EXPRESSION TAG	UNP P60293
X	-14	HIS	-	EXPRESSION TAG	UNP P60293
X	-13	HIS	-	EXPRESSION TAG	UNP P60293
X	-12	HIS	-	EXPRESSION TAG	UNP P60293
X	-11	HIS	-	EXPRESSION TAG	UNP P60293
X	-10	HIS	-	EXPRESSION TAG	UNP P60293
X	-9	SER	-	EXPRESSION TAG	UNP P60293
X	-8	SER	-	EXPRESSION TAG	UNP P60293
X	-7	GLY	-	EXPRESSION TAG	UNP P60293
X	-6	LEU	-	EXPRESSION TAG	UNP P60293
X	-5	VAL	-	EXPRESSION TAG	UNP P60293
X	-4	PRO	-	EXPRESSION TAG	UNP P60293
X	-3	ARG	-	EXPRESSION TAG	UNP P60293
X	-2	GLY	-	EXPRESSION TAG	UNP P60293
X	-1	SER	-	EXPRESSION TAG	UNP P60293
X	0	HIS	-	EXPRESSION TAG	UNP P60293

- Molecule 2 is a protein called Chromosome partition protein mukE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	204	Total	C	N	O	S	0	0	0
			1656	1049	295	304	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	191	Total	C	N	O	S	0	0	0
			1561	994	277	283	7			
2	D	203	Total	C	N	O	S	0	0	0
			1649	1045	294	302	8			
2	E	191	Total	C	N	O	S	0	0	0
			1562	995	276	284	7			
2	Y	205	Total	C	N	O	S	0	0	0
			1661	1052	296	305	8			
2	Z	188	Total	C	N	O	S	0	0	0
			1542	983	272	280	7			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	MET	-	EXPRESSION TAG	UNP P22524
G	-9	GLY	-	EXPRESSION TAG	UNP P22524
G	-8	SER	-	EXPRESSION TAG	UNP P22524
G	-7	SER	-	EXPRESSION TAG	UNP P22524
G	-6	HIS	-	EXPRESSION TAG	UNP P22524
G	-5	HIS	-	EXPRESSION TAG	UNP P22524
G	-4	HIS	-	EXPRESSION TAG	UNP P22524
G	-3	HIS	-	EXPRESSION TAG	UNP P22524
G	-2	HIS	-	EXPRESSION TAG	UNP P22524
G	-1	HIS	-	EXPRESSION TAG	UNP P22524
G	0	SER	-	EXPRESSION TAG	UNP P22524
G	1	SER	-	EXPRESSION TAG	UNP P22524
G	2	GLY	-	EXPRESSION TAG	UNP P22524
G	3	LEU	-	EXPRESSION TAG	UNP P22524
G	4	VAL	-	EXPRESSION TAG	UNP P22524
G	5	PRO	-	EXPRESSION TAG	UNP P22524
G	6	ARG	-	EXPRESSION TAG	UNP P22524
G	7	GLY	-	EXPRESSION TAG	UNP P22524
G	8	SER	-	EXPRESSION TAG	UNP P22524
G	9	HIS	-	EXPRESSION TAG	UNP P22524
H	-10	MET	-	EXPRESSION TAG	UNP P22524
H	-9	GLY	-	EXPRESSION TAG	UNP P22524
H	-8	SER	-	EXPRESSION TAG	UNP P22524
H	-7	SER	-	EXPRESSION TAG	UNP P22524
H	-6	HIS	-	EXPRESSION TAG	UNP P22524
H	-5	HIS	-	EXPRESSION TAG	UNP P22524
H	-4	HIS	-	EXPRESSION TAG	UNP P22524
H	-3	HIS	-	EXPRESSION TAG	UNP P22524
H	-2	HIS	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	HIS	-	EXPRESSION TAG	UNP P22524
H	0	SER	-	EXPRESSION TAG	UNP P22524
H	1	SER	-	EXPRESSION TAG	UNP P22524
H	2	GLY	-	EXPRESSION TAG	UNP P22524
H	3	LEU	-	EXPRESSION TAG	UNP P22524
H	4	VAL	-	EXPRESSION TAG	UNP P22524
H	5	PRO	-	EXPRESSION TAG	UNP P22524
H	6	ARG	-	EXPRESSION TAG	UNP P22524
H	7	GLY	-	EXPRESSION TAG	UNP P22524
H	8	SER	-	EXPRESSION TAG	UNP P22524
H	9	HIS	-	EXPRESSION TAG	UNP P22524
D	-10	MET	-	EXPRESSION TAG	UNP P22524
D	-9	GLY	-	EXPRESSION TAG	UNP P22524
D	-8	SER	-	EXPRESSION TAG	UNP P22524
D	-7	SER	-	EXPRESSION TAG	UNP P22524
D	-6	HIS	-	EXPRESSION TAG	UNP P22524
D	-5	HIS	-	EXPRESSION TAG	UNP P22524
D	-4	HIS	-	EXPRESSION TAG	UNP P22524
D	-3	HIS	-	EXPRESSION TAG	UNP P22524
D	-2	HIS	-	EXPRESSION TAG	UNP P22524
D	-1	HIS	-	EXPRESSION TAG	UNP P22524
D	0	SER	-	EXPRESSION TAG	UNP P22524
D	1	SER	-	EXPRESSION TAG	UNP P22524
D	2	GLY	-	EXPRESSION TAG	UNP P22524
D	3	LEU	-	EXPRESSION TAG	UNP P22524
D	4	VAL	-	EXPRESSION TAG	UNP P22524
D	5	PRO	-	EXPRESSION TAG	UNP P22524
D	6	ARG	-	EXPRESSION TAG	UNP P22524
D	7	GLY	-	EXPRESSION TAG	UNP P22524
D	8	SER	-	EXPRESSION TAG	UNP P22524
D	9	HIS	-	EXPRESSION TAG	UNP P22524
E	-10	MET	-	EXPRESSION TAG	UNP P22524
E	-9	GLY	-	EXPRESSION TAG	UNP P22524
E	-8	SER	-	EXPRESSION TAG	UNP P22524
E	-7	SER	-	EXPRESSION TAG	UNP P22524
E	-6	HIS	-	EXPRESSION TAG	UNP P22524
E	-5	HIS	-	EXPRESSION TAG	UNP P22524
E	-4	HIS	-	EXPRESSION TAG	UNP P22524
E	-3	HIS	-	EXPRESSION TAG	UNP P22524
E	-2	HIS	-	EXPRESSION TAG	UNP P22524
E	-1	HIS	-	EXPRESSION TAG	UNP P22524
E	0	SER	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	SER	-	EXPRESSION TAG	UNP P22524
E	2	GLY	-	EXPRESSION TAG	UNP P22524
E	3	LEU	-	EXPRESSION TAG	UNP P22524
E	4	VAL	-	EXPRESSION TAG	UNP P22524
E	5	PRO	-	EXPRESSION TAG	UNP P22524
E	6	ARG	-	EXPRESSION TAG	UNP P22524
E	7	GLY	-	EXPRESSION TAG	UNP P22524
E	8	SER	-	EXPRESSION TAG	UNP P22524
E	9	HIS	-	EXPRESSION TAG	UNP P22524
Y	-10	MET	-	EXPRESSION TAG	UNP P22524
Y	-9	GLY	-	EXPRESSION TAG	UNP P22524
Y	-8	SER	-	EXPRESSION TAG	UNP P22524
Y	-7	SER	-	EXPRESSION TAG	UNP P22524
Y	-6	HIS	-	EXPRESSION TAG	UNP P22524
Y	-5	HIS	-	EXPRESSION TAG	UNP P22524
Y	-4	HIS	-	EXPRESSION TAG	UNP P22524
Y	-3	HIS	-	EXPRESSION TAG	UNP P22524
Y	-2	HIS	-	EXPRESSION TAG	UNP P22524
Y	-1	HIS	-	EXPRESSION TAG	UNP P22524
Y	0	SER	-	EXPRESSION TAG	UNP P22524
Y	1	SER	-	EXPRESSION TAG	UNP P22524
Y	2	GLY	-	EXPRESSION TAG	UNP P22524
Y	3	LEU	-	EXPRESSION TAG	UNP P22524
Y	4	VAL	-	EXPRESSION TAG	UNP P22524
Y	5	PRO	-	EXPRESSION TAG	UNP P22524
Y	6	ARG	-	EXPRESSION TAG	UNP P22524
Y	7	GLY	-	EXPRESSION TAG	UNP P22524
Y	8	SER	-	EXPRESSION TAG	UNP P22524
Y	9	HIS	-	EXPRESSION TAG	UNP P22524
Z	-10	MET	-	EXPRESSION TAG	UNP P22524
Z	-9	GLY	-	EXPRESSION TAG	UNP P22524
Z	-8	SER	-	EXPRESSION TAG	UNP P22524
Z	-7	SER	-	EXPRESSION TAG	UNP P22524
Z	-6	HIS	-	EXPRESSION TAG	UNP P22524
Z	-5	HIS	-	EXPRESSION TAG	UNP P22524
Z	-4	HIS	-	EXPRESSION TAG	UNP P22524
Z	-3	HIS	-	EXPRESSION TAG	UNP P22524
Z	-2	HIS	-	EXPRESSION TAG	UNP P22524
Z	-1	HIS	-	EXPRESSION TAG	UNP P22524
Z	0	SER	-	EXPRESSION TAG	UNP P22524
Z	1	SER	-	EXPRESSION TAG	UNP P22524
Z	2	GLY	-	EXPRESSION TAG	UNP P22524

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	3	LEU	-	EXPRESSION TAG	UNP P22524
Z	4	VAL	-	EXPRESSION TAG	UNP P22524
Z	5	PRO	-	EXPRESSION TAG	UNP P22524
Z	6	ARG	-	EXPRESSION TAG	UNP P22524
Z	7	GLY	-	EXPRESSION TAG	UNP P22524
Z	8	SER	-	EXPRESSION TAG	UNP P22524
Z	9	HIS	-	EXPRESSION TAG	UNP P22524

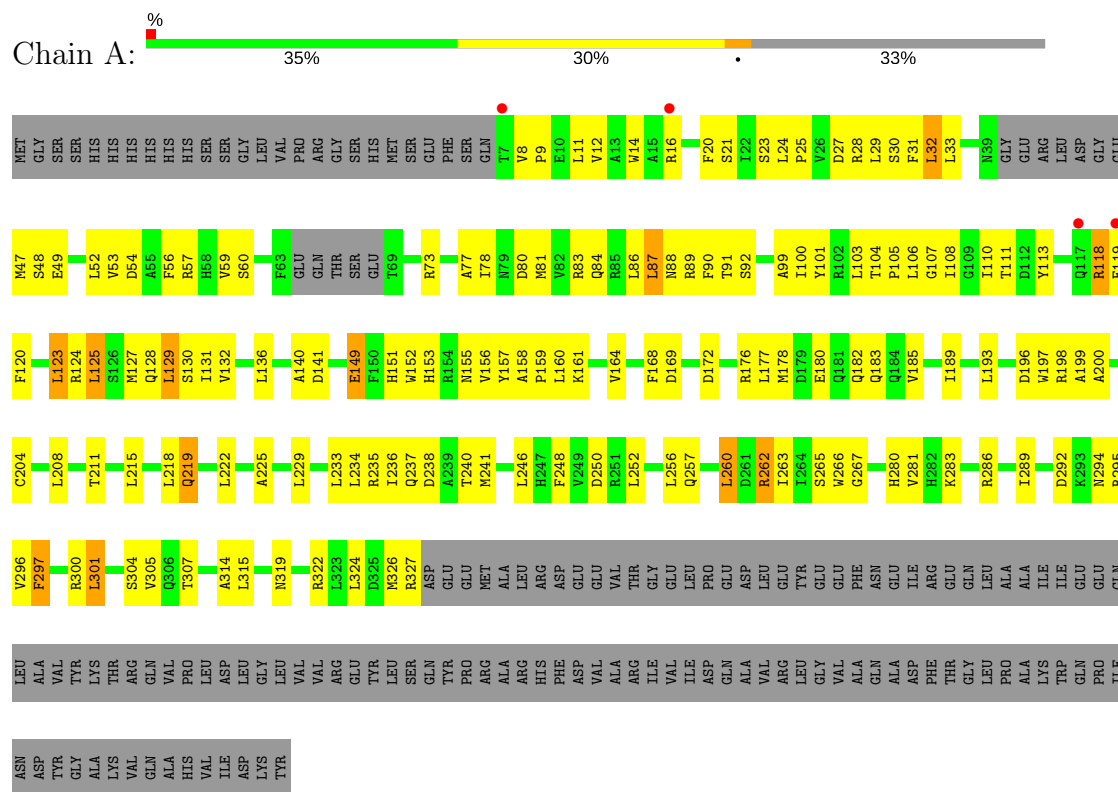
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O 1 1	0	0
3	Y	1	Total O 1 1	0	0

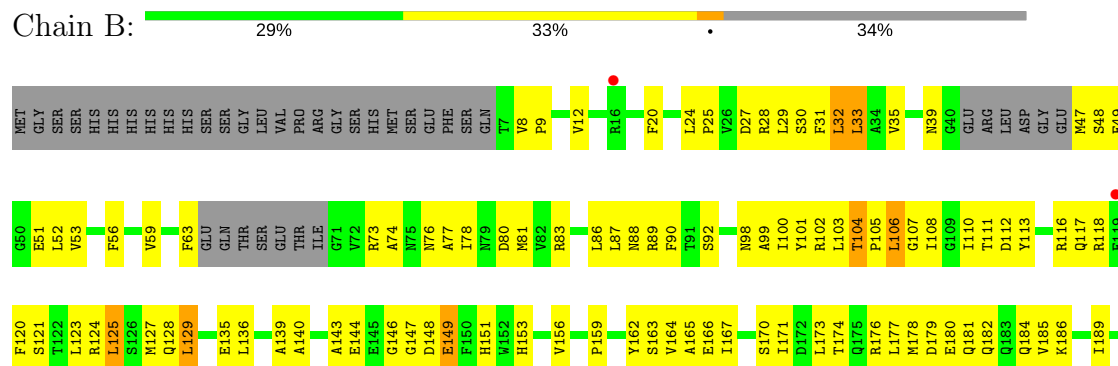
### 3 Residue-property plots

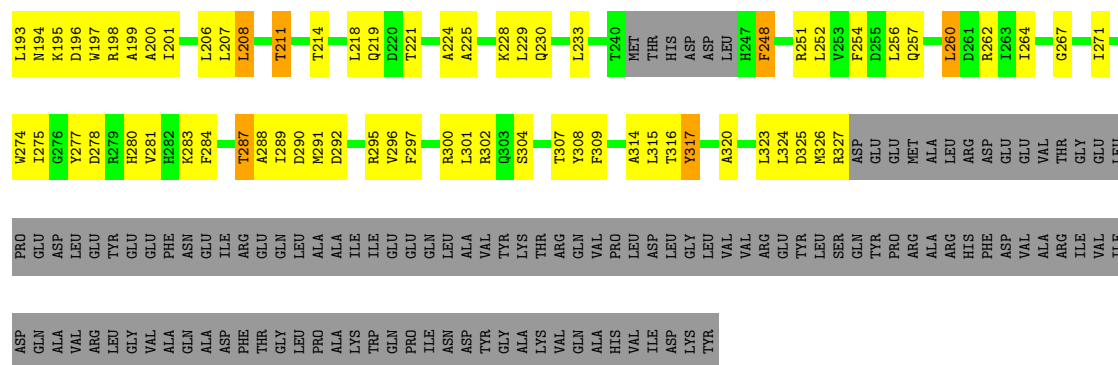
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Chromosome partition protein mukF

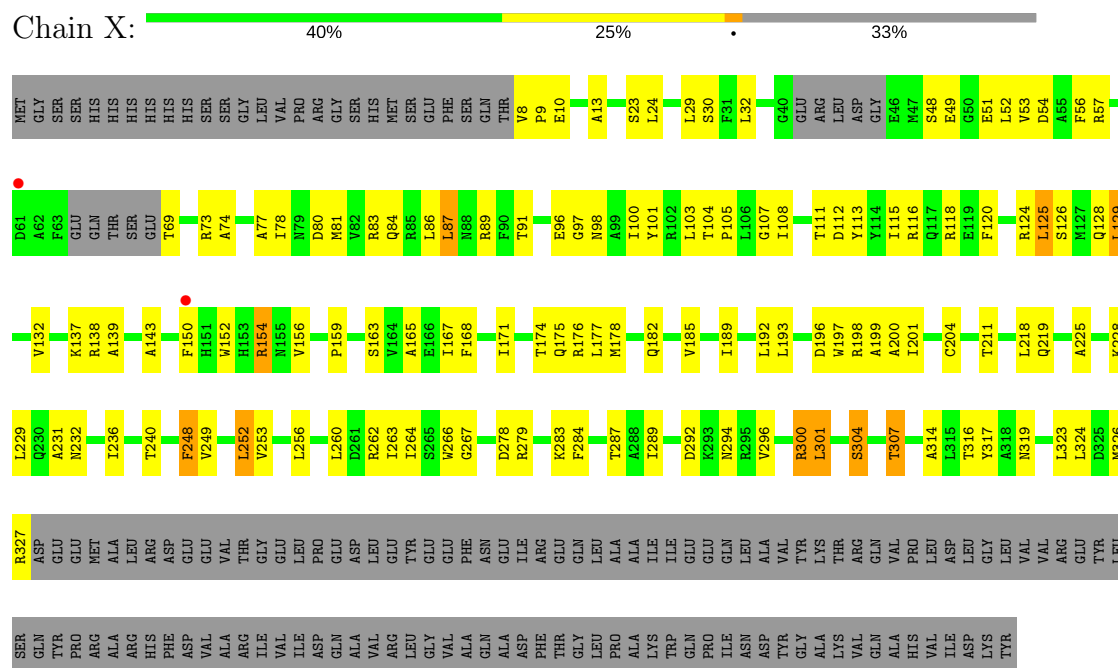


#### • Molecule 1: Chromosome partition protein mukF

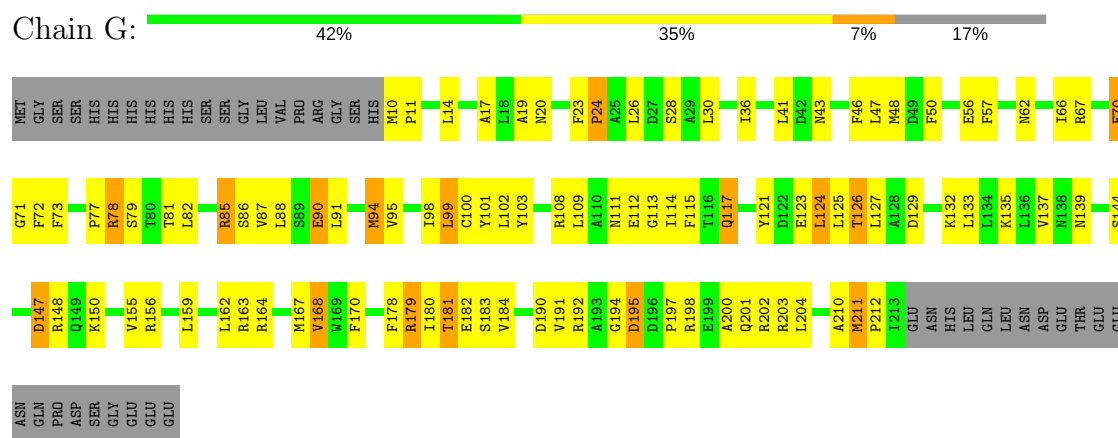




### • Molecule 1: Chromosome partition protein mukF

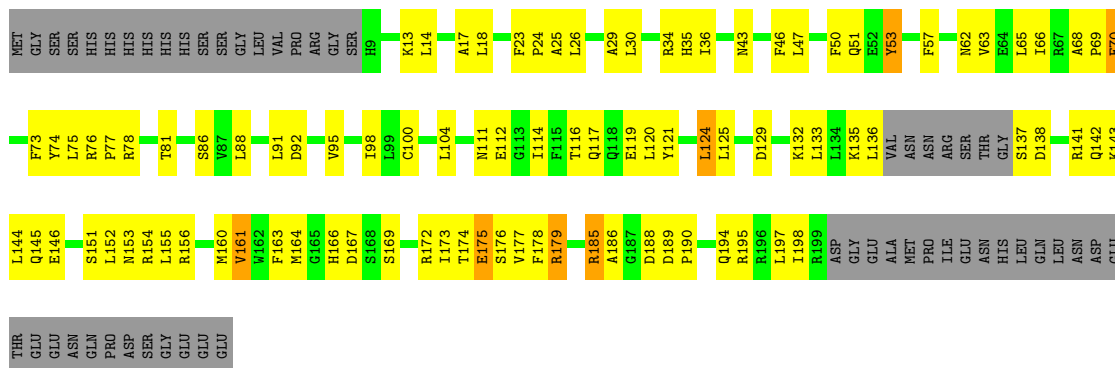
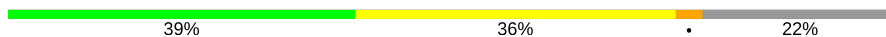


### • Molecule 2: Chromosome partition protein mukE



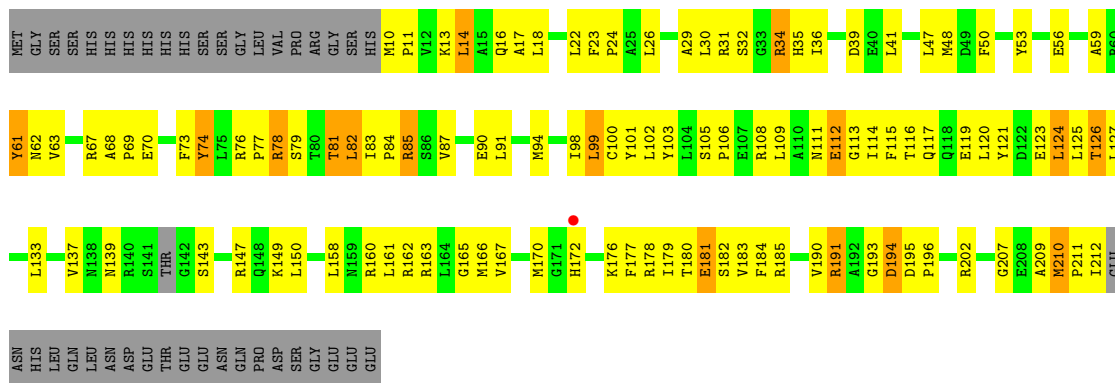
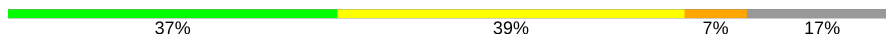
### • Molecule 2: Chromosome partition protein mukE

Chain H:



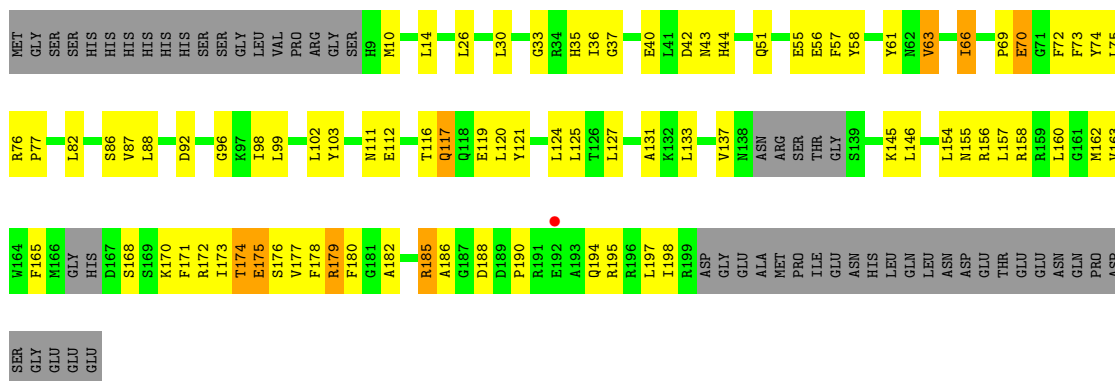
- Molecule 2: Chromosome partition protein mukE

Chain D:



- Molecule 2: Chromosome partition protein mukE

Chain E:



- Molecule 2: Chromosome partition protein mukE

Chain Y:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.89Å 149.89Å 738.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.60 19.98 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.98-3.60) 98.4 (19.98-3.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.62Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.217 , 0.274 0.204 , 0.267	Depositor DCC
$R_{free}$ test set	2888 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 79.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.65	0/2545	0.85	1/3442 (0.0%)
1	B	0.58	0/2483	0.74	0/3355
1	X	0.60	0/2546	0.82	1/3443 (0.0%)
2	D	0.70	0/1679	0.92	2/2260 (0.1%)
2	E	0.65	0/1589	0.81	1/2138 (0.0%)
2	G	0.68	0/1687	0.86	0/2273
2	H	0.62	0/1590	0.80	0/2140
2	Y	0.80	1/1692 (0.1%)	0.97	5/2280 (0.2%)
2	Z	0.71	0/1569	0.89	1/2110 (0.0%)
All	All	0.66	1/17380 (0.0%)	0.85	11/23441 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Y	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	108	ARG	CG-CD	6.25	1.67	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	41	LEU	CA-CB-CG	-6.22	101.00	115.30
2	D	81	THR	CB-CA-C	-6.13	95.05	111.60
2	Y	203	ARG	NE-CZ-NH1	-5.69	117.45	120.30
2	Y	108	ARG	CB-CG-CD	5.67	126.36	111.60
1	X	300	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	D	82	LEU	CA-CB-CG	-5.34	103.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	204	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	87	LEU	CA-CB-CG	5.29	127.47	115.30
2	Y	78	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	Y	12	VAL	CB-CA-C	-5.20	101.51	111.40
2	E	195	ARG	CG-CD-NE	-5.20	100.88	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	194	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2503	0	2463	195	0
1	B	2443	0	2405	229	0
1	X	2504	0	2453	122	0
2	D	1649	0	1652	144	0
2	E	1562	0	1571	89	0
2	G	1656	0	1660	104	0
2	H	1561	0	1567	82	0
2	Y	1661	0	1662	120	0
2	Z	1542	0	1554	75	0
3	G	1	0	0	0	0
3	Y	1	0	0	0	0
All	All	17083	0	16987	1047	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 31.

All (1047) 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:A:281:VAL:HG22	2:G:109:LEU:HD22	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:118:ARG:HB3	1:X:177:LEU:HD21	1.12	1.11
1:B:300:ARG:HH22	2:D:193:GLY:HA2	1.06	1.10
2:D:180:THR:O	2:D:183:VAL:HG23	1.51	1.09
1:X:219:GLN:HE21	1:X:267:GLY:HA3	0.98	1.09
2:Y:60:ARG:HH11	2:Y:60:ARG:HG2	1.10	1.09
2:E:63:VAL:HG22	2:E:77:PRO:HA	1.32	1.08
2:D:210:MET:HG3	2:D:211:PRO:HD2	1.38	1.05
1:A:197:TRP:CE2	1:A:289:ILE:HG12	1.92	1.03
1:A:47:MET:HG2	1:A:48:SER:H	1.25	1.01
1:B:300:ARG:NH2	2:D:193:GLY:HA2	1.76	1.00
1:X:171:ILE:HA	1:X:174:THR:HG22	1.38	0.99
2:H:154:ARG:HH21	2:H:154:ARG:HG2	1.27	0.99
1:X:283:LYS:HZ3	2:Y:108:ARG:HH12	1.10	0.96
1:A:88:ASN:ND2	1:B:179:ASP:HB3	1.78	0.96
2:H:26:LEU:HD22	2:H:43:ASN:HD22	1.30	0.96
1:A:324:LEU:HD13	2:H:88:LEU:CD2	1.96	0.95
1:A:197:TRP:NE1	1:A:289:ILE:HG12	1.82	0.95
1:X:32:LEU:HD11	1:X:86:LEU:HD13	1.45	0.95
1:A:88:ASN:HD22	1:B:179:ASP:HB3	1.32	0.93
1:X:296:VAL:HG12	1:X:300:ARG:HE	1.34	0.93
1:X:283:LYS:NZ	2:Y:108:ARG:HH12	1.67	0.93
1:X:219:GLN:NE2	1:X:267:GLY:HA3	1.84	0.92
1:B:80:ASP:HA	1:B:83:ARG:HG2	1.51	0.92
2:Y:125:LEU:HD22	2:Y:130:GLU:HG3	1.50	0.92
1:X:304:SER:HA	1:X:307:THR:HG22	1.50	0.92
1:B:124:ARG:HG2	1:B:124:ARG:HH11	1.32	0.91
1:B:32:LEU:HD11	1:B:86:LEU:HD13	1.52	0.91
1:B:300:ARG:HH11	1:B:300:ARG:HG3	1.36	0.90
1:B:118:ARG:HB3	1:B:177:LEU:HD21	1.53	0.89
2:G:126:THR:HG22	2:G:127:LEU:HD23	1.51	0.89
1:A:281:VAL:HG22	2:G:109:LEU:CD2	2.01	0.89
1:X:52:LEU:HD13	1:X:78:ILE:HD13	1.55	0.89
1:A:197:TRP:CE3	1:A:295:ARG:HD3	2.09	0.88
1:B:287:THR:HG21	2:D:108:ARG:HH22	1.38	0.88
1:X:219:GLN:HE21	1:X:267:GLY:CA	1.84	0.88
1:A:300:ARG:NH2	2:G:194:GLY:HA2	1.89	0.88
1:X:49:GLU:O	1:X:53:VAL:HG23	1.75	0.86
1:B:32:LEU:CD1	1:B:86:LEU:HD13	2.04	0.86
2:Z:104:LEU:HD13	2:Z:188:PRO:HB2	1.58	0.86
2:H:104:LEU:HD13	2:H:190:PRO:HB2	1.58	0.86
2:H:98:ILE:CD1	2:H:124:LEU:HD13	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:35:HIS:HE1	2:Z:177:ARG:HD3	1.39	0.85
1:A:241:MET:CE	2:Y:12:VAL:HG13	2.07	0.85
1:A:47:MET:HG2	1:A:48:SER:N	1.88	0.84
1:X:111:THR:O	1:X:115:ILE:HG23	1.77	0.84
2:Z:117:GLN:OE1	2:Z:152:LEU:HD23	1.77	0.84
1:B:196:ASP:HB3	1:B:199:ALA:HB3	1.60	0.83
1:X:118:ARG:CB	1:X:177:LEU:HD21	2.03	0.83
1:A:160:LEU:HB3	1:A:252:LEU:HD21	1.58	0.83
1:A:241:MET:HE1	2:Y:12:VAL:HG13	1.59	0.82
2:H:26:LEU:HD22	2:H:43:ASN:ND2	1.93	0.82
2:Y:78:ARG:HB3	2:Y:78:ARG:HH11	1.44	0.82
1:A:262:ARG:HH12	1:B:102:ARG:HH11	1.24	0.82
2:D:62:ASN:O	2:D:78:ARG:HB2	1.80	0.82
1:A:238:ASP:OD1	2:Y:12:VAL:HG23	1.79	0.82
1:B:287:THR:HG22	1:B:288:ALA:N	1.94	0.82
2:D:85:ARG:NH2	2:D:210:MET:SD	2.53	0.81
2:E:133:LEU:HG	2:E:146:LEU:HD21	1.59	0.81
2:Y:167:MET:CE	2:Y:187:PHE:HE2	1.90	0.81
2:Y:167:MET:HE3	2:Y:187:PHE:HE2	1.42	0.81
1:A:196:ASP:HB3	1:A:199:ALA:HB3	1.62	0.81
1:B:304:SER:HA	1:B:307:THR:HG22	1.60	0.81
1:B:171:ILE:HA	1:B:174:THR:HG22	1.61	0.81
2:G:46:PHE:CE1	2:G:50:PHE:HD1	1.98	0.81
1:X:167:ILE:O	1:X:171:ILE:HG13	1.79	0.81
1:X:248:PHE:HD2	1:X:248:PHE:H	1.27	0.81
1:B:314:ALA:HB2	2:D:212:ILE:HD11	1.63	0.81
1:X:171:ILE:CA	1:X:174:THR:HG22	2.13	0.79
2:Y:35:HIS:NE2	2:Y:186:ARG:NH2	2.30	0.79
1:A:262:ARG:NH1	1:B:102:ARG:HH11	1.79	0.79
2:D:78:ARG:CG	2:D:78:ARG:HH21	1.95	0.79
1:X:225:ALA:O	1:X:229:LEU:HD13	1.82	0.79
2:G:144:SER:O	2:G:148:ARG:HG3	1.82	0.79
1:A:176:ARG:NH2	1:B:39:ASN:HD21	1.80	0.79
2:Z:35:HIS:CE1	2:Z:177:ARG:HD3	2.17	0.78
1:X:287:THR:HG21	2:Y:103:TYR:CZ	2.19	0.78
2:Y:102:LEU:HD21	2:Y:123:GLU:HG2	1.65	0.78
1:A:80:ASP:HA	1:A:83:ARG:HG2	1.64	0.78
1:B:143:ALA:HA	1:B:156:VAL:HG22	1.66	0.78
1:B:106:LEU:CD2	1:B:110:ILE:HD11	2.13	0.78
1:B:300:ARG:HG3	1:B:300:ARG:NH1	1.94	0.78
2:Y:48:MET:SD	2:Y:67:ARG:NH1	2.56	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:60:ARG:NH1	2:Y:60:ARG:HG2	1.87	0.78
1:A:124:ARG:O	1:A:128:GLN:HG3	1.84	0.78
1:A:304:SER:HA	1:A:307:THR:HG22	1.65	0.78
1:B:260:LEU:O	1:B:264:ILE:HG13	1.84	0.78
2:E:63:VAL:CG1	2:E:75:LEU:HD22	2.14	0.78
1:B:185:VAL:HG21	1:B:211:THR:HG21	1.66	0.77
2:E:158:ARG:HD3	2:E:165:PHE:CE2	2.18	0.77
1:A:160:LEU:HB3	1:A:252:LEU:CD2	2.14	0.77
2:Y:167:MET:CE	2:Y:187:PHE:CE2	2.67	0.77
1:X:283:LYS:HZ3	2:Y:108:ARG:NH1	1.83	0.77
1:X:171:ILE:HA	1:X:174:THR:CG2	2.15	0.77
1:A:315:LEU:O	2:G:87:VAL:HG13	1.84	0.77
2:G:26:LEU:HD11	2:G:36:ILE:HD13	1.66	0.76
2:Z:143:LYS:HE2	2:Z:143:LYS:HA	1.67	0.76
2:G:46:PHE:CE1	2:G:50:PHE:CD1	2.74	0.76
2:H:18:LEU:HD22	2:H:23:PHE:CE2	2.20	0.76
1:A:157:TYR:CD1	1:A:248:PHE:HD1	2.04	0.76
2:D:102:LEU:HD21	2:D:123:GLU:HG2	1.66	0.76
1:A:89:ARG:HG3	1:A:101:TYR:CZ	2.21	0.76
1:X:128:GLN:O	1:X:132:VAL:HG23	1.85	0.75
2:H:154:ARG:NH2	2:H:154:ARG:HG2	1.93	0.75
2:Y:144:SER:O	2:Y:148:ARG:HG3	1.86	0.75
2:G:211:MET:HE2	2:G:211:MET:HA	1.68	0.75
1:X:80:ASP:HA	1:X:83:ARG:HG2	1.69	0.75
2:D:68:ALA:HB1	2:D:69:PRO:HD2	1.69	0.75
2:Z:63:VAL:HG22	2:Z:77:PRO:HA	1.68	0.75
1:A:300:ARG:HH22	2:G:194:GLY:HA2	1.47	0.75
1:B:283:LYS:O	1:B:287:THR:HB	1.85	0.75
1:B:143:ALA:HA	1:B:156:VAL:CG2	2.17	0.74
1:X:249:VAL:O	1:X:253:VAL:HG23	1.87	0.74
2:E:72:PHE:CE1	2:E:176:SER:HA	2.22	0.74
2:H:160:MET:O	2:H:161:VAL:HG23	1.87	0.74
1:A:157:TYR:CD2	1:A:157:TYR:C	2.61	0.74
2:Y:181:THR:O	2:Y:184:VAL:HG23	1.86	0.74
2:H:174:THR:HG22	2:H:176:SER:H	1.53	0.74
1:A:118:ARG:HD3	1:A:120:PHE:CD2	2.22	0.73
1:A:47:MET:CG	1:A:48:SER:H	2.00	0.73
1:A:113:TYR:CD2	1:B:106:LEU:HB2	2.23	0.73
2:D:99:LEU:HB3	2:D:183:VAL:HG11	1.70	0.73
2:Y:167:MET:HE3	2:Y:187:PHE:CE2	2.23	0.73
2:Z:97:LYS:HE2	2:Z:195:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HD12	1:B:113:TYR:CD2	2.23	0.73
2:Y:10:MET:CE	2:Y:14:LEU:HD13	2.19	0.73
2:E:185:ARG:O	2:E:185:ARG:HD2	1.89	0.72
1:B:24:LEU:HD13	1:B:29:LEU:HD13	1.70	0.72
2:E:63:VAL:CG2	2:E:77:PRO:HA	2.14	0.72
2:H:197:LEU:O	2:H:197:LEU:HG	1.89	0.72
1:A:297:PHE:HD1	1:A:297:PHE:O	1.72	0.72
1:B:120:PHE:CZ	1:B:218:LEU:HD21	2.24	0.72
2:G:91:LEU:O	2:G:95:VAL:HG23	1.90	0.72
2:D:78:ARG:NH2	2:D:78:ARG:CG	2.53	0.72
2:Y:61:TYR:O	2:Y:62:ASN:HB2	1.89	0.71
2:D:94:MET:HA	2:D:94:MET:HE2	1.71	0.71
1:X:225:ALA:HA	1:X:228:LYS:HE2	1.71	0.71
1:B:147:GLY:HA3	1:B:151:HIS:HB3	1.73	0.71
2:Y:196:ASP:OD1	2:Y:197:PRO:HD2	1.90	0.71
2:Z:160:MET:O	2:Z:161:VAL:HG23	1.91	0.71
2:Y:67:ARG:HB2	2:Y:73:PHE:CE1	2.25	0.71
1:X:294:ASN:HB2	1:X:296:VAL:HG23	1.71	0.71
2:D:77:PRO:HG3	2:D:85:ARG:HB2	1.73	0.70
1:A:197:TRP:CD2	1:A:295:ARG:HD3	2.25	0.70
2:Z:172:THR:HG22	2:Z:173:GLU:N	2.05	0.70
2:E:157:LEU:HD23	2:E:160:LEU:HD12	1.74	0.70
2:Y:60:ARG:CG	2:Y:60:ARG:HH11	1.97	0.70
2:H:29:ALA:HB1	2:H:34:ARG:HD3	1.74	0.70
1:B:8:VAL:HB	1:B:9:PRO:HD3	1.74	0.70
1:B:49:GLU:HB2	1:B:99:ALA:HB3	1.74	0.69
1:A:324:LEU:HD13	2:H:88:LEU:HD23	1.73	0.69
1:B:106:LEU:HD22	1:B:110:ILE:HD11	1.73	0.69
1:X:139:ALA:HB2	1:X:159:PRO:HG2	1.74	0.69
1:A:196:ASP:O	1:A:199:ALA:HB3	1.93	0.69
1:X:120:PHE:HZ	1:X:218:LEU:HD21	1.57	0.69
2:Z:42:ASP:N	2:Z:42:ASP:OD1	2.23	0.69
1:B:139:ALA:O	1:B:143:ALA:HB2	1.93	0.69
1:B:47:MET:HG2	1:B:48:SER:H	1.57	0.69
1:X:104:THR:HB	1:X:105:PRO:HD2	1.75	0.69
1:B:47:MET:HG2	1:B:48:SER:N	2.08	0.69
2:D:191:ARG:O	2:D:191:ARG:HD3	1.93	0.69
2:E:173:ILE:HG23	2:E:177:VAL:HG21	1.73	0.69
2:D:143:SER:O	2:D:147:ARG:HG3	1.93	0.69
2:Y:99:LEU:HD12	2:Y:180:ILE:HD13	1.75	0.68
2:G:211:MET:HG3	2:G:212:PRO:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD1	1:A:248:PHE:CD1	2.81	0.68
1:B:207:LEU:O	1:B:211:THR:HG23	1.93	0.68
2:Z:116:THR:OG1	2:Z:119:GLU:HG3	1.93	0.68
2:Y:167:MET:CE	2:Y:184:VAL:HA	2.24	0.68
1:A:149:GLU:HA	1:A:149:GLU:OE1	1.94	0.68
2:D:78:ARG:HG2	2:D:78:ARG:HH21	1.57	0.68
2:D:39:ASP:OD2	2:D:180:THR:HG23	1.93	0.68
1:B:287:THR:HG23	2:D:103:TYR:CE2	2.29	0.68
1:A:89:ARG:HG3	1:A:101:TYR:CE2	2.28	0.67
2:G:67:ARG:HE	2:G:71:GLY:HA2	1.60	0.67
2:H:98:ILE:HD11	2:H:124:LEU:HD13	1.75	0.67
1:X:32:LEU:CD1	1:X:86:LEU:HD13	2.22	0.67
1:B:52:LEU:HD12	1:B:101:TYR:CD2	2.30	0.67
1:X:287:THR:HG21	2:Y:103:TYR:OH	1.94	0.67
2:Y:167:MET:HE2	2:Y:187:PHE:CE2	2.29	0.67
2:G:46:PHE:HE1	2:G:50:PHE:CD1	2.13	0.66
1:X:156:VAL:O	1:X:159:PRO:HD2	1.95	0.66
2:D:126:THR:HG22	2:D:127:LEU:HD23	1.77	0.66
1:A:281:VAL:CG2	2:G:109:LEU:HD22	2.18	0.66
1:B:219:GLN:HE21	1:B:267:GLY:C	1.99	0.66
2:E:98:ILE:CD1	2:E:124:LEU:HA	2.25	0.66
1:X:232:ASN:O	1:X:236:ILE:HG13	1.96	0.66
2:Y:10:MET:HE1	2:Y:14:LEU:HD13	1.77	0.66
2:Y:167:MET:HE1	2:Y:184:VAL:HA	1.77	0.66
1:X:107:GLY:O	1:X:111:THR:HG23	1.95	0.66
2:H:121:TYR:CE2	2:H:125:LEU:HD11	2.31	0.66
2:Y:47:LEU:HD12	2:Y:73:PHE:CD2	2.31	0.66
1:B:186:LYS:HE3	1:B:274:TRP:HZ3	1.59	0.65
1:B:124:ARG:HG2	1:B:124:ARG:NH1	2.09	0.65
1:B:118:ARG:CB	1:B:177:LEU:HD21	2.26	0.65
1:B:287:THR:HG21	2:D:108:ARG:NH2	2.11	0.65
1:X:283:LYS:CE	2:Y:108:ARG:HH12	2.09	0.65
2:G:144:SER:HB3	2:G:147:ASP:HB2	1.76	0.65
1:A:219:GLN:HG3	1:A:267:GLY:O	1.97	0.65
2:D:85:ARG:O	2:D:85:ARG:HD3	1.97	0.64
2:G:113:GLY:O	2:G:179:ARG:NH2	2.31	0.64
2:H:167:ASP:OD1	2:H:169:SER:HB2	1.97	0.64
2:E:112:GLU:CG	2:E:112:GLU:O	2.46	0.64
1:B:31:PHE:HD1	1:B:59:VAL:HG21	1.61	0.64
1:X:296:VAL:HG12	1:X:300:ARG:NE	2.11	0.64
1:X:74:ALA:O	1:X:78:ILE:HG13	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ARG:NH2	2:D:78:ARG:HG3	2.12	0.64
2:D:67:ARG:HB2	2:D:73:PHE:CE1	2.32	0.64
1:X:87:LEU:HD13	1:X:103:LEU:HD23	1.79	0.64
2:H:194:GLN:O	2:H:198:ILE:HG13	1.98	0.64
2:G:117:GLN:HG2	2:G:156:ARG:CZ	2.28	0.63
2:Y:121:TYR:CE2	2:Y:125:LEU:CD1	2.82	0.63
2:Y:99:LEU:HD12	2:Y:180:ILE:CD1	2.28	0.63
1:B:287:THR:CG2	1:B:288:ALA:N	2.60	0.63
2:G:62:ASN:O	2:G:78:ARG:HB2	1.98	0.63
1:B:89:ARG:HG3	1:B:101:TYR:CE1	2.34	0.63
1:B:124:ARG:CG	1:B:124:ARG:HH11	2.05	0.63
1:A:300:ARG:CB	2:G:191:VAL:HG11	2.29	0.63
2:H:174:THR:HG22	2:H:175:GLU:N	2.14	0.63
2:D:94:MET:HA	2:D:94:MET:CE	2.29	0.63
2:G:167:MET:O	2:G:181:THR:OG1	2.13	0.63
1:B:271:ILE:O	1:B:275:ILE:HG13	1.99	0.63
1:B:291:MET:HE1	2:D:184:PHE:CE1	2.34	0.63
1:B:302:ARG:HD3	2:D:101:TYR:CZ	2.33	0.63
2:E:121:TYR:CE2	2:E:125:LEU:HD11	2.34	0.63
2:Y:121:TYR:CZ	2:Y:125:LEU:HD11	2.34	0.63
2:Y:121:TYR:CE1	2:Y:152:GLN:HG2	2.33	0.63
1:A:156:VAL:HG12	1:A:157:TYR:N	2.13	0.62
2:D:111:ASN:HB3	2:D:114:ILE:O	1.99	0.62
2:E:88:LEU:HB3	2:E:92:ASP:HB2	1.81	0.62
1:X:197:TRP:CZ2	1:X:289:ILE:HG12	2.35	0.62
1:X:197:TRP:NE1	1:X:289:ILE:HG23	2.13	0.62
1:A:14:TRP:CZ2	1:A:20:PHE:HE1	2.16	0.62
2:D:35:HIS:CE1	2:D:185:ARG:HD3	2.34	0.62
2:E:177:VAL:HG12	2:E:177:VAL:O	1.99	0.62
2:G:77:PRO:HG2	2:G:85:ARG:HB2	1.80	0.62
1:A:297:PHE:C	1:A:297:PHE:HD1	2.01	0.62
2:D:195:ASP:OD1	2:D:196:PRO:HD2	1.98	0.62
1:X:198:ARG:O	1:X:201:ILE:HG13	1.99	0.62
2:G:99:LEU:HD12	2:G:180:ILE:HD11	1.82	0.62
1:A:161:LYS:N	1:A:252:LEU:HD11	2.14	0.61
2:D:62:ASN:HB2	2:D:81:THR:HA	1.82	0.61
2:E:51:GLN:OE1	2:E:73:PHE:HE2	1.83	0.61
2:H:69:PRO:HG2	2:H:70:GLU:OE2	1.99	0.61
2:Y:102:LEU:HB3	2:Y:115:PHE:CE2	2.35	0.61
2:D:177:PHE:HD2	2:D:178:ARG:O	1.83	0.61
1:B:48:SER:HA	1:B:100:ILE:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ILE:HD11	2:H:76:ARG:CZ	2.31	0.61
1:A:196:ASP:CB	1:A:199:ALA:HB3	2.30	0.61
1:A:235:ARG:O	1:A:238:ASP:HB2	2.00	0.61
1:A:324:LEU:HD13	2:H:88:LEU:HD21	1.78	0.61
2:Z:121:TYR:O	2:Z:124:LEU:HB3	2.00	0.61
2:G:192:ARG:HD3	2:G:192:ARG:O	2.01	0.61
2:Z:87:VAL:CG1	2:Z:88:LEU:N	2.64	0.61
1:A:197:TRP:CE3	1:A:295:ARG:CD	2.83	0.61
1:X:168:PHE:HA	1:X:171:ILE:HD12	1.83	0.61
2:Z:98:ILE:HD13	2:Z:124:LEU:HA	1.82	0.61
1:B:125:LEU:HD22	1:B:129:LEU:HD22	1.82	0.61
1:B:197:TRP:CE3	1:B:295:ARG:HD2	2.35	0.61
2:H:114:ILE:HG12	2:H:172:ARG:HD3	1.83	0.61
2:Z:102:LEU:HD22	2:Z:115:PHE:CE2	2.36	0.61
2:G:99:LEU:HD12	2:G:180:ILE:CD1	2.30	0.60
2:G:41:LEU:H	2:G:41:LEU:HD12	1.66	0.60
1:X:283:LYS:HZ1	2:Y:108:ARG:HH22	1.49	0.60
1:B:230:GLN:OE1	1:B:257:GLN:HG2	2.01	0.60
2:E:116:THR:OG1	2:E:119:GLU:HG3	2.01	0.60
2:E:35:HIS:CE1	2:E:179:ARG:HD3	2.36	0.60
1:X:112:ASP:HA	1:X:115:ILE:HG12	1.82	0.60
1:A:176:ARG:NH2	1:B:39:ASN:ND2	2.50	0.60
1:A:297:PHE:C	1:A:297:PHE:CD1	2.73	0.60
1:B:49:GLU:O	1:B:53:VAL:HG23	2.02	0.60
2:D:61:TYR:HA	2:D:82:LEU:HD12	1.84	0.60
2:E:35:HIS:HE1	2:E:179:ARG:HD3	1.66	0.60
1:B:52:LEU:CD1	1:B:101:TYR:CD2	2.84	0.60
1:B:52:LEU:HB3	1:B:78:ILE:HD11	1.83	0.60
1:B:302:ARG:HG3	2:D:127:LEU:HD13	1.83	0.60
1:X:54:ASP:O	1:X:57:ARG:HB3	2.01	0.60
1:A:301:LEU:O	1:A:305:VAL:HG23	2.01	0.60
1:B:281:VAL:HG22	2:D:109:LEU:CD2	2.32	0.60
2:E:133:LEU:HG	2:E:146:LEU:CD2	2.31	0.60
2:D:74:TYR:CE1	2:D:185:ARG:NE	2.70	0.60
2:E:116:THR:HG22	2:E:170:LYS:HG2	1.83	0.60
1:X:120:PHE:CZ	1:X:218:LEU:HD21	2.37	0.60
2:Y:9:HIS:O	2:Y:11:PRO:HD3	2.01	0.60
1:X:132:VAL:HG22	1:X:167:ILE:HG21	1.83	0.60
2:G:121:TYR:CZ	2:G:125:LEU:HD11	2.37	0.59
1:A:300:ARG:HB3	2:G:191:VAL:HG11	1.83	0.59
2:H:138:ASP:OD1	2:H:138:ASP:O	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:185:VAL:HG21	1:X:211:THR:HG21	1.84	0.59
1:A:124:ARG:HD2	1:B:162:TYR:CD1	2.37	0.59
1:A:185:VAL:HG21	1:A:211:THR:HG21	1.85	0.59
1:B:124:ARG:HH12	1:B:128:GLN:NE2	2.00	0.59
1:B:301:LEU:O	1:B:304:SER:OG	2.18	0.59
1:B:324:LEU:HD13	2:E:88:LEU:HD21	1.85	0.59
2:Z:172:THR:O	2:Z:175:VAL:HB	2.03	0.59
1:B:120:PHE:HZ	1:B:218:LEU:HD21	1.67	0.59
2:D:124:LEU:HD22	2:D:133:LEU:HD21	1.85	0.59
2:G:100:CYS:HB2	2:G:184:VAL:HG12	1.83	0.59
1:B:193:LEU:HD23	1:B:200:ALA:HB3	1.85	0.59
2:Y:181:THR:HG22	2:Y:182:GLU:N	2.17	0.59
2:Y:91:LEU:O	2:Y:95:VAL:HG23	2.03	0.59
2:Z:116:THR:HG22	2:Z:168:LYS:HG2	1.83	0.59
2:D:126:THR:CG2	2:D:127:LEU:HD23	2.32	0.58
2:E:37:GLY:O	2:E:44:HIS:CD2	2.56	0.58
1:X:304:SER:HA	1:X:307:THR:CG2	2.29	0.58
2:Y:121:TYR:CE2	2:Y:125:LEU:HD11	2.38	0.58
2:E:35:HIS:CD2	2:E:162:MET:CE	2.86	0.58
2:Y:60:ARG:NH1	2:Y:60:ARG:CG	2.62	0.58
1:A:297:PHE:CD1	1:A:297:PHE:O	2.55	0.58
1:A:92:SER:H	1:A:99:ALA:HA	1.68	0.58
1:B:315:LEU:HD13	2:D:185:ARG:HG2	1.85	0.58
2:Z:87:VAL:HG12	2:Z:88:LEU:N	2.18	0.58
2:G:123:GLU:O	2:G:126:THR:HB	2.04	0.58
1:X:289:ILE:O	1:X:292:ASP:O	2.22	0.58
2:Z:98:ILE:CD1	2:Z:124:LEU:HA	2.32	0.58
2:E:10:MET:HG3	2:E:14:LEU:HD23	1.85	0.58
2:E:158:ARG:HD3	2:E:165:PHE:CD2	2.38	0.58
2:E:26:LEU:HD13	2:E:43:ASN:OD1	2.04	0.58
2:G:159:LEU:HD21	2:G:178:PHE:CE1	2.39	0.58
1:B:248:PHE:H	1:B:248:PHE:HD2	1.52	0.58
1:B:309:PHE:HE1	2:D:94:MET:SD	2.25	0.58
2:D:26:LEU:HD11	2:D:36:ILE:HD13	1.85	0.58
2:G:163:ARG:HD3	2:G:170:PHE:CD2	2.38	0.58
2:Y:163:ARG:HD2	2:Y:170:PHE:CD2	2.39	0.58
2:D:67:ARG:HB2	2:D:73:PHE:HE1	1.69	0.58
2:D:78:ARG:HD2	2:D:79:SER:H	1.68	0.58
2:E:156:ARG:HG2	2:E:156:ARG:NH2	2.18	0.58
2:Y:10:MET:CG	2:Y:10:MET:O	2.50	0.58
2:Y:14:LEU:HD22	2:Y:18:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ALA:O	1:A:229:LEU:HD13	2.04	0.58
1:B:120:PHE:CE2	1:B:218:LEU:HD21	2.38	0.58
1:A:197:TRP:HE3	1:A:295:ARG:NH1	2.02	0.57
1:B:87:LEU:CD1	1:B:103:LEU:HD23	2.34	0.57
2:G:200:ALA:O	2:G:204:LEU:HG	2.04	0.57
2:Y:116:THR:OG1	2:Y:119:GLU:HG3	2.03	0.57
1:B:292:ASP:OD2	1:B:297:PHE:HB3	2.04	0.57
2:D:105:SER:OG	2:D:106:PRO:HD2	2.04	0.57
1:X:24:LEU:HD13	1:X:29:LEU:HD13	1.87	0.57
2:Y:51:GLN:O	2:Y:55:GLU:HB2	2.03	0.57
1:X:196:ASP:HB3	1:X:199:ALA:HB3	1.86	0.57
2:Z:172:THR:HG22	2:Z:174:SER:H	1.69	0.57
2:E:182:ALA:HA	2:E:197:LEU:HD22	1.87	0.57
2:Y:191:VAL:CG1	2:Y:191:VAL:O	2.52	0.57
1:B:167:ILE:O	1:B:170:SER:HB3	2.05	0.57
2:Y:160:ASN:OD1	2:Y:163:ARG:NH1	2.37	0.57
2:E:188:ASP:O	2:E:190:PRO:HD3	2.05	0.57
2:G:197:PRO:O	2:G:201:GLN:HG3	2.04	0.57
2:G:124:LEU:HD22	2:G:133:LEU:HD21	1.87	0.57
1:X:49:GLU:HB2	1:X:101:TYR:HE2	1.70	0.57
2:Y:10:MET:HE2	2:Y:14:LEU:HD13	1.86	0.57
1:B:208:LEU:HD21	1:B:278:ASP:HA	1.86	0.57
1:X:225:ALA:HA	1:X:228:LYS:CE	2.35	0.57
2:H:174:THR:CG2	2:H:175:GLU:N	2.68	0.56
1:X:189:ILE:HG23	1:X:204:CYS:SG	2.45	0.56
1:A:118:ARG:HD2	1:A:118:ARG:O	2.05	0.56
2:H:17:ALA:HB2	2:H:50:PHE:CD2	2.39	0.56
1:X:300:ARG:O	1:X:304:SER:HB3	2.05	0.56
1:A:152:TRP:CD2	1:A:246:LEU:HD11	2.40	0.56
1:A:197:TRP:CE3	1:A:295:ARG:NH1	2.74	0.56
1:A:78:ILE:O	1:A:81:MET:HB2	2.05	0.56
1:A:29:LEU:HD23	1:B:20:PHE:O	2.05	0.56
2:H:188:ASP:O	2:H:190:PRO:HD3	2.06	0.56
2:Y:106:PRO:O	2:Y:109:LEU:HB2	2.05	0.56
2:H:133:LEU:HG	2:H:144:LEU:HD11	1.88	0.56
2:Y:159:LEU:HD21	2:Y:178:PHE:CD1	2.41	0.56
2:Y:66:ILE:O	2:Y:73:PHE:HA	2.06	0.56
2:Y:78:ARG:HH11	2:Y:78:ARG:CB	2.17	0.56
2:Y:19:ALA:HA	2:Z:60:ARG:HH22	1.70	0.56
1:A:241:MET:HE3	2:Y:12:VAL:HG13	1.86	0.56
1:B:80:ASP:CA	1:B:83:ARG:HG2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:121:TYR:CE2	2:Y:125:LEU:HD12	2.40	0.56
1:A:127:MET:HE1	1:B:159:PRO:HG3	1.88	0.56
2:Z:13:LYS:CB	2:Z:53:TYR:CE2	2.89	0.56
1:A:113:TYR:HD2	1:B:106:LEU:HG	1.70	0.56
1:A:125:LEU:HD22	1:A:129:LEU:HD22	1.86	0.56
1:A:157:TYR:O	1:A:157:TYR:CD2	2.58	0.56
1:A:30:SER:HB3	1:B:12:VAL:HG13	1.87	0.56
1:A:107:GLY:O	1:A:111:THR:HG23	2.06	0.56
1:B:297:PHE:HE1	2:D:184:PHE:CD2	2.24	0.55
1:X:236:ILE:O	1:X:240:THR:OG1	2.11	0.55
1:B:56:PHE:HE2	1:B:77:ALA:HB2	1.70	0.55
1:B:302:ARG:HD3	2:D:101:TYR:OH	2.07	0.55
1:A:90:PHE:HE1	1:B:182:GLN:NE2	2.05	0.55
2:D:61:TYR:O	2:D:62:ASN:HB2	2.05	0.55
2:E:165:PHE:CE1	2:E:168:SER:HB2	2.42	0.55
2:Y:26:LEU:O	2:Y:30:LEU:HD12	2.06	0.55
1:X:104:THR:HB	1:X:105:PRO:CD	2.36	0.55
2:D:48:MET:SD	2:D:67:ARG:NH1	2.79	0.55
2:E:112:GLU:HG2	2:E:112:GLU:O	2.07	0.55
2:G:46:PHE:CD1	2:G:50:PHE:HD1	2.24	0.55
1:B:124:ARG:NH1	1:B:128:GLN:NE2	2.54	0.55
1:B:197:TRP:CZ3	1:B:295:ARG:CZ	2.90	0.55
2:H:88:LEU:HB3	2:H:92:ASP:HB2	1.89	0.55
1:B:140:ALA:O	1:B:143:ALA:HB3	2.07	0.55
1:B:124:ARG:HH12	1:B:128:GLN:HE22	1.54	0.54
2:D:17:ALA:HB2	2:D:50:PHE:CG	2.42	0.54
2:E:157:LEU:CD2	2:E:160:LEU:HD12	2.37	0.54
2:E:162:MET:O	2:E:163:VAL:HG23	2.07	0.54
2:Z:171:ILE:HG23	2:Z:175:VAL:HG21	1.87	0.54
1:B:301:LEU:HD11	2:D:100:CYS:HB3	1.89	0.54
2:E:156:ARG:HG2	2:E:156:ARG:HH21	1.72	0.54
1:X:171:ILE:O	1:X:174:THR:HG22	2.07	0.54
1:A:182:GLN:OE1	1:A:215:LEU:HD11	2.07	0.54
1:A:28:ARG:NH1	1:A:80:ASP:OD2	2.38	0.54
1:B:167:ILE:O	1:B:171:ILE:HG13	2.07	0.54
1:B:89:ARG:NH2	1:B:101:TYR:OH	2.41	0.54
2:D:161:LEU:O	2:D:166:MET:HB2	2.07	0.54
2:D:74:TYR:N	2:D:74:TYR:CD2	2.76	0.54
2:E:72:PHE:CD1	2:E:176:SER:HA	2.41	0.54
1:X:326:MET:O	1:X:327:ARG:HD2	2.08	0.54
1:X:287:THR:HG21	2:Y:103:TYR:CE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:HIS:CD2	2:E:162:MET:HE2	2.43	0.54
2:G:26:LEU:HD11	2:G:36:ILE:CD1	2.36	0.54
1:X:248:PHE:CD2	1:X:248:PHE:N	2.70	0.54
1:B:106:LEU:HD21	1:B:110:ILE:HD11	1.90	0.54
1:B:178:MET:HE2	1:B:214:THR:HG22	1.89	0.54
2:E:63:VAL:HG11	2:E:75:LEU:HD22	1.86	0.54
1:A:60:SER:OG	1:A:73:ARG:NH2	2.41	0.54
1:B:284:PHE:HE1	2:D:105:SER:O	1.90	0.54
2:Y:125:LEU:CD2	2:Y:130:GLU:HG3	2.31	0.54
1:A:29:LEU:O	1:A:33:LEU:HD13	2.07	0.54
1:B:116:ARG:HG2	1:B:118:ARG:HD3	1.89	0.54
1:B:120:PHE:CZ	1:B:218:LEU:HD11	2.43	0.54
1:B:297:PHE:HE1	2:D:184:PHE:CE2	2.25	0.54
2:E:87:VAL:CG1	2:E:88:LEU:N	2.71	0.54
1:A:88:ASN:ND2	1:B:179:ASP:CB	2.64	0.54
1:A:103:LEU:HB2	1:B:176:ARG:NH1	2.23	0.54
1:B:52:LEU:HD13	1:B:78:ILE:HG12	1.89	0.54
2:H:174:THR:CG2	2:H:175:GLU:H	2.20	0.54
2:Y:167:MET:HE1	2:Y:183:SER:C	2.29	0.54
1:A:156:VAL:O	1:A:159:PRO:HD2	2.09	0.53
1:B:117:GLN:HG3	1:B:117:GLN:O	2.08	0.53
2:D:120:LEU:CD2	2:D:158:LEU:HD22	2.38	0.53
2:D:13:LYS:O	2:D:16:GLN:HB3	2.08	0.53
2:G:41:LEU:HD12	2:G:41:LEU:N	2.23	0.53
1:A:113:TYR:CE2	1:B:106:LEU:HB2	2.42	0.53
2:H:51:GLN:HG2	2:H:73:PHE:HE2	1.73	0.53
2:Z:117:GLN:OE1	2:Z:152:LEU:CD2	2.53	0.53
1:A:283:LYS:HG2	1:A:286:ARG:HH12	1.74	0.53
1:B:52:LEU:HD12	1:B:101:TYR:CE2	2.43	0.53
2:G:124:LEU:CD2	2:G:133:LEU:HD21	2.38	0.53
1:B:143:ALA:CA	1:B:156:VAL:HG22	2.38	0.53
2:Y:167:MET:HE1	2:Y:183:SER:O	2.09	0.53
1:B:326:MET:O	1:B:327:ARG:HB2	2.09	0.53
1:B:48:SER:O	1:B:51:GLU:HB2	2.09	0.53
2:H:132:LYS:HA	2:H:135:LYS:HB3	1.89	0.53
1:B:171:ILE:CA	1:B:174:THR:HG22	2.35	0.53
2:E:98:ILE:HD11	2:E:124:LEU:HA	1.90	0.53
1:A:157:TYR:CE1	1:A:248:PHE:HD1	2.27	0.53
1:B:287:THR:CG2	2:D:103:TYR:CE2	2.92	0.53
2:H:143:LYS:HE2	2:H:143:LYS:HA	1.91	0.53
1:X:163:SER:O	1:X:167:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:89:ARG:CZ	1:X:101:TYR:OH	2.57	0.53
2:D:191:ARG:HD3	2:D:191:ARG:C	2.29	0.53
2:H:132:LYS:O	2:H:136:LEU:HG	2.07	0.53
2:H:173:ILE:HG23	2:H:177:VAL:HG21	1.91	0.53
1:X:143:ALA:O	1:X:152:TRP:CH2	2.62	0.53
2:D:162:ARG:O	2:D:162:ARG:HG2	2.07	0.52
2:E:173:ILE:CG2	2:E:177:VAL:HG21	2.38	0.52
2:D:13:LYS:HD3	2:D:53:TYR:CE1	2.43	0.52
2:D:98:ILE:HD13	2:D:124:LEU:HA	1.91	0.52
2:E:66:ILE:CD1	2:E:76:ARG:CZ	2.87	0.52
2:G:23:PHE:O	2:G:24:PRO:C	2.46	0.52
1:X:116:ARG:HG2	1:X:118:ARG:HD3	1.90	0.52
2:Z:13:LYS:HB3	2:Z:53:TYR:CE2	2.44	0.52
1:A:158:ALA:O	1:A:159:PRO:C	2.47	0.52
2:D:98:ILE:HD12	2:D:124:LEU:HG	1.91	0.52
2:E:174:THR:HG22	2:E:175:GLU:H	1.74	0.52
2:H:68:ALA:HB1	2:H:69:PRO:HD2	1.91	0.52
1:B:162:TYR:O	1:B:166:GLU:HB2	2.09	0.52
2:G:159:LEU:HD21	2:G:178:PHE:CD1	2.45	0.52
1:X:124:ARG:O	1:X:128:GLN:HG3	2.08	0.52
2:Z:10:MET:SD	2:Z:15:ALA:HB2	2.49	0.52
1:A:151:HIS:O	1:A:155:ASN:HB2	2.10	0.52
1:B:124:ARG:NH1	1:B:124:ARG:CG	2.66	0.52
2:D:102:LEU:HB3	2:D:115:PHE:CE2	2.43	0.52
1:X:175:GLN:O	1:X:178:MET:HB3	2.09	0.52
1:B:120:PHE:CD1	1:B:120:PHE:C	2.83	0.52
1:B:248:PHE:CD2	1:B:248:PHE:N	2.77	0.52
1:A:204:CYS:O	1:A:208:LEU:HB2	2.10	0.52
1:A:292:ASP:OD2	1:A:297:PHE:HB3	2.10	0.52
1:B:219:GLN:HE21	1:B:267:GLY:CA	2.23	0.52
2:D:102:LEU:HD13	2:D:115:PHE:CE2	2.45	0.52
2:E:58:TYR:CE2	2:E:75:LEU:HD11	2.44	0.52
1:B:28:ARG:NH1	1:B:80:ASP:OD2	2.43	0.52
2:D:123:GLU:O	2:D:126:THR:HB	2.09	0.52
2:H:111:ASN:O	2:H:112:GLU:HG2	2.09	0.52
1:B:106:LEU:O	1:B:110:ILE:HG13	2.10	0.52
2:H:95:VAL:HG21	2:H:151:SER:CB	2.40	0.52
1:B:325:ASP:OD1	2:E:77:PRO:HG2	2.09	0.52
1:B:225:ALA:O	1:B:229:LEU:HD13	2.09	0.51
1:B:314:ALA:O	2:D:209:ALA:HB1	2.10	0.51
1:A:176:ARG:HH21	1:B:39:ASN:HD21	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:HA	1:B:76:ASN:ND2	2.24	0.51
2:D:99:LEU:HD13	2:D:120:LEU:HD11	1.91	0.51
2:G:26:LEU:HD13	2:G:43:ASN:CG	2.30	0.51
2:G:70:GLU:HG3	2:G:72:PHE:HE1	1.75	0.51
2:Z:155:LEU:HD22	2:Z:160:MET:HG3	1.92	0.51
2:H:23:PHE:O	2:H:24:PRO:C	2.48	0.51
1:B:260:LEU:HD22	1:B:264:ILE:HD11	1.93	0.51
2:E:51:GLN:OE1	2:E:73:PHE:CE2	2.64	0.51
2:G:99:LEU:HB3	2:G:184:VAL:HG11	1.93	0.51
1:A:197:TRP:CZ2	1:A:289:ILE:HG12	2.44	0.51
2:E:88:LEU:HD22	2:E:92:ASP:HB3	1.91	0.51
2:H:116:THR:OG1	2:H:119:GLU:HG3	2.11	0.51
1:X:91:THR:HG23	1:X:98:ASN:O	2.11	0.51
2:Y:116:THR:H	2:Y:119:GLU:HG3	1.75	0.51
1:A:260:LEU:O	1:A:260:LEU:HD23	2.11	0.51
1:B:32:LEU:HD12	1:B:86:LEU:HD13	1.90	0.51
2:H:14:LEU:HD11	2:H:57:PHE:HB2	1.93	0.51
1:A:16:ARG:NH1	1:B:63:PHE:HD1	2.09	0.51
1:B:171:ILE:O	1:B:174:THR:HG22	2.11	0.51
2:D:98:ILE:CD1	2:D:124:LEU:HA	2.40	0.51
2:Y:94:MET:HE2	2:Y:94:MET:HA	1.91	0.51
1:A:152:TRP:CE3	1:A:156:VAL:HG21	2.46	0.51
2:Y:14:LEU:CD2	2:Y:18:LEU:HG	2.40	0.51
1:X:314:ALA:HB3	2:Y:87:VAL:CG1	2.41	0.51
2:Z:129:ASP:O	2:Z:133:LEU:HB2	2.11	0.51
1:B:87:LEU:HD11	1:B:103:LEU:HD23	1.92	0.51
1:B:92:SER:O	1:B:98:ASN:HA	2.11	0.51
2:G:66:ILE:O	2:G:73:PHE:HA	2.10	0.51
2:Z:172:THR:CG2	2:Z:173:GLU:N	2.72	0.51
1:A:49:GLU:O	1:A:53:VAL:HG23	2.11	0.51
1:B:197:TRP:NE1	1:B:289:ILE:HG23	2.26	0.51
1:B:56:PHE:CD2	1:B:74:ALA:HA	2.46	0.51
2:G:48:MET:SD	2:G:67:ARG:NH1	2.84	0.51
2:H:26:LEU:HD11	2:H:36:ILE:HG13	1.92	0.51
2:Y:94:MET:CE	2:Y:94:MET:HA	2.41	0.51
1:A:159:PRO:HG3	1:B:127:MET:HE1	1.93	0.51
2:D:124:LEU:O	2:D:124:LEU:HD23	2.10	0.51
1:X:283:LYS:NZ	2:Y:108:ARG:NH1	2.47	0.51
1:B:219:GLN:NE2	1:B:267:GLY:C	2.64	0.50
1:B:197:TRP:CD1	1:B:289:ILE:HG23	2.45	0.50
2:Z:13:LYS:HB2	2:Z:53:TYR:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TRP:CE2	1:A:289:ILE:CG1	2.82	0.50
1:B:125:LEU:HD22	1:B:125:LEU:O	2.12	0.50
1:A:182:GLN:NE2	1:B:90:PHE:CE1	2.80	0.50
2:Y:26:LEU:O	2:Y:29:ALA:HB3	2.11	0.50
1:A:157:TYR:HD1	1:A:248:PHE:CD1	2.27	0.50
1:B:147:GLY:C	1:B:148:ASP:O	2.47	0.50
1:B:308:TYR:HD1	1:B:309:PHE:CD1	2.29	0.50
2:D:124:LEU:CD2	2:D:133:LEU:HD21	2.41	0.50
2:E:56:GLU:O	2:E:57:PHE:C	2.48	0.50
2:G:81:THR:HG23	2:G:81:THR:O	2.12	0.50
2:Y:206:ARG:O	2:Y:206:ARG:HG2	2.12	0.50
1:A:106:LEU:CD2	1:A:110:ILE:HD11	2.41	0.50
1:B:106:LEU:HD22	1:B:110:ILE:CD1	2.40	0.50
1:B:121:SER:O	1:B:124:ARG:HB3	2.11	0.50
1:X:112:ASP:O	1:X:116:ARG:HB3	2.12	0.50
1:A:88:ASN:HD21	1:B:179:ASP:C	2.14	0.50
1:B:300:ARG:CG	1:B:300:ARG:NH1	2.68	0.50
2:D:116:THR:OG1	2:D:119:GLU:HG3	2.10	0.50
1:X:324:LEU:HD13	2:Z:88:LEU:HD21	1.93	0.50
1:A:197:TRP:CD1	1:A:198:ARG:N	2.80	0.50
2:E:63:VAL:HG22	2:E:77:PRO:CA	2.23	0.50
1:B:280:HIS:NE2	2:D:113:GLY:CA	2.74	0.50
2:D:81:THR:OG1	2:D:81:THR:O	2.29	0.50
1:A:196:ASP:O	1:A:199:ALA:CB	2.58	0.50
1:B:31:PHE:CD1	1:B:59:VAL:HG21	2.46	0.50
2:D:63:VAL:HG22	2:D:77:PRO:HA	1.93	0.50
2:H:154:ARG:NH2	2:H:154:ARG:CG	2.65	0.50
2:D:47:LEU:HB3	2:D:73:PHE:CE2	2.47	0.50
2:E:163:VAL:HG13	2:E:171:PHE:HB2	1.94	0.50
1:B:107:GLY:O	1:B:111:THR:HG23	2.12	0.49
2:E:66:ILE:HD11	2:E:76:ARG:NH2	2.27	0.49
2:H:100:CYS:HA	2:H:177:VAL:HG11	1.93	0.49
2:H:70:GLU:HG3	2:H:178:PHE:CD1	2.47	0.49
2:Y:116:THR:OG1	2:Y:119:GLU:CG	2.60	0.49
2:D:124:LEU:HD22	2:D:133:LEU:CD2	2.42	0.49
2:D:74:TYR:HD2	2:D:74:TYR:N	2.10	0.49
2:Y:137:VAL:HG23	2:Y:151:LEU:HD13	1.94	0.49
2:Y:26:LEU:HG	2:Y:30:LEU:HD12	1.94	0.49
2:Y:38:LEU:HG	2:Y:182:GLU:OE2	2.12	0.49
1:A:193:LEU:HD23	1:A:200:ALA:HB3	1.94	0.49
1:A:48:SER:HA	1:A:100:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:THR:HG22	2:D:181:GLU:N	2.28	0.49
2:E:158:ARG:HD3	2:E:165:PHE:HE2	1.75	0.49
2:H:153:ASN:OD1	2:H:156:ARG:NH1	2.45	0.49
2:Z:35:HIS:CE1	2:Z:177:ARG:CD	2.92	0.49
1:B:149:GLU:HB2	1:B:153:HIS:HD1	1.78	0.49
1:B:219:GLN:NE2	1:B:267:GLY:HA3	2.27	0.49
2:E:155:ASN:OD1	2:E:158:ARG:NH1	2.46	0.49
2:G:129:ASP:O	2:G:133:LEU:HB2	2.12	0.49
1:X:115:ILE:HG13	1:X:116:ARG:N	2.28	0.49
1:X:116:ARG:HG2	1:X:118:ARG:CD	2.42	0.49
1:X:125:LEU:HD12	1:X:218:LEU:CD2	2.41	0.49
1:A:140:ALA:HA	1:A:236:ILE:HG12	1.94	0.49
1:B:144:GLU:O	1:B:146:GLY:N	2.45	0.49
2:G:150:LYS:HA	2:G:150:LYS:HE2	1.94	0.49
1:X:125:LEU:HD22	1:X:129:LEU:HD22	1.95	0.49
1:A:52:LEU:HD13	1:A:78:ILE:CD1	2.43	0.49
2:E:185:ARG:O	2:E:186:ALA:HB3	2.12	0.49
2:G:103:TYR:HD1	2:G:180:ILE:HG22	1.77	0.49
1:X:104:THR:O	1:X:108:ILE:HB	2.13	0.49
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.50	0.49
2:E:158:ARG:CD	2:E:165:PHE:CD2	2.96	0.49
2:G:163:ARG:HG3	2:G:168:VAL:O	2.13	0.49
1:X:137:LYS:O	1:X:138:ARG:C	2.50	0.49
1:X:283:LYS:HE2	2:Y:108:ARG:HH12	1.78	0.49
1:A:149:GLU:CA	1:A:149:GLU:OE1	2.59	0.48
1:A:240:THR:O	1:A:240:THR:HG22	2.11	0.48
1:X:228:LYS:O	1:X:231:ALA:HB3	2.13	0.48
2:Y:178:PHE:CD2	2:Y:178:PHE:C	2.87	0.48
1:A:118:ARG:HD2	1:A:118:ARG:C	2.34	0.48
1:A:196:ASP:HB3	1:A:199:ALA:CB	2.38	0.48
1:B:136:LEU:HD13	1:B:164:VAL:HG21	1.95	0.48
1:A:177:LEU:HD12	1:B:105:PRO:HG2	1.96	0.48
2:D:137:VAL:HG11	2:D:149:LYS:HB2	1.94	0.48
2:H:50:PHE:O	2:H:51:GLN:C	2.52	0.48
2:H:91:LEU:O	2:H:92:ASP:C	2.50	0.48
1:X:8:VAL:HB	1:X:9:PRO:HD3	1.95	0.48
1:A:304:SER:HA	1:A:307:THR:CG2	2.41	0.48
2:G:98:ILE:O	2:G:101:TYR:N	2.47	0.48
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.62	0.48
2:D:99:LEU:HD12	2:D:179:ILE:CD1	2.44	0.48
1:X:314:ALA:HB2	2:Y:213:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:O	1:A:84:GLN:HG2	2.14	0.48
1:B:309:PHE:CE1	2:D:94:MET:SD	3.07	0.48
2:H:13:LYS:HB3	2:H:53:TYR:CE2	2.48	0.48
1:A:158:ALA:HB3	1:A:159:PRO:HD3	1.94	0.48
1:A:169:ASP:OD1	1:B:116:ARG:NH2	2.46	0.48
2:D:179:ILE:CG2	2:D:183:VAL:HG21	2.44	0.48
2:H:164:MET:CE	2:H:164:MET:HA	2.44	0.48
2:Z:133:LEU:HG	2:Z:144:LEU:HD11	1.95	0.48
1:A:326:MET:O	1:A:327:ARG:HB2	2.13	0.48
1:B:225:ALA:HA	1:B:228:LYS:HE3	1.94	0.48
1:A:266:TRP:CH2	1:B:102:ARG:HD2	2.48	0.48
2:D:78:ARG:H	2:D:81:THR:HG22	1.79	0.48
2:D:99:LEU:HD13	2:D:120:LEU:CD1	2.43	0.48
2:E:37:GLY:O	2:E:44:HIS:HD2	1.97	0.48
2:E:66:ILE:HG22	2:E:74:TYR:CE2	2.48	0.48
1:X:197:TRP:CE2	1:X:289:ILE:HG12	2.49	0.48
1:B:291:MET:CE	2:D:184:PHE:CE1	2.96	0.48
2:E:42:ASP:OD1	2:E:42:ASP:N	2.47	0.48
1:X:150:PHE:O	1:X:154:ARG:HB3	2.14	0.47
1:X:301:LEU:HD11	2:Y:100:CYS:HB3	1.96	0.47
1:A:113:TYR:CD2	1:B:106:LEU:HG	2.49	0.47
1:A:159:PRO:HG3	1:B:127:MET:CE	2.45	0.47
1:B:297:PHE:O	1:B:301:LEU:HB2	2.15	0.47
2:G:113:GLY:O	2:G:179:ARG:HB2	2.14	0.47
2:G:14:LEU:O	2:G:17:ALA:HB3	2.13	0.47
2:Y:145:ASP:OD1	2:Y:145:ASP:O	2.31	0.47
1:A:106:LEU:HD23	1:A:106:LEU:O	2.13	0.47
1:A:23:SER:O	1:A:24:LEU:HD23	2.14	0.47
2:D:99:LEU:HD12	2:D:179:ILE:HD11	1.96	0.47
2:E:117:GLN:OE1	2:E:154:LEU:HD23	2.13	0.47
1:X:81:MET:HE2	1:X:81:MET:HA	1.96	0.47
1:X:284:PHE:CE2	1:X:289:ILE:HG13	2.49	0.47
1:X:304:SER:CA	1:X:307:THR:HG22	2.32	0.47
1:X:314:ALA:O	2:Y:210:ALA:HB1	2.14	0.47
2:Y:103:TYR:CE2	2:Y:182:GLU:HA	2.49	0.47
2:Y:103:TYR:CD1	2:Y:108:ARG:HD2	2.50	0.47
2:Y:111:ASN:HB3	2:Y:114:ILE:O	2.15	0.47
2:Z:10:MET:HA	2:Z:11:PRO:HD3	1.75	0.47
1:A:160:LEU:HB3	1:A:252:LEU:HD22	1.96	0.47
1:B:197:TRP:CZ3	1:B:295:ARG:NE	2.83	0.47
2:H:74:TYR:CE1	2:H:179:ARG:CZ	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:167:MET:HE3	2:Y:184:VAL:HA	1.96	0.47
2:Y:54:LEU:HD23	2:Y:54:LEU:HA	1.60	0.47
2:Z:14:LEU:HB2	2:Z:53:TYR:HB3	1.96	0.47
2:D:62:ASN:CB	2:D:81:THR:HA	2.44	0.47
2:E:66:ILE:HD11	2:E:76:ARG:CZ	2.44	0.47
2:H:137:SER:O	2:H:141:ARG:HG3	2.15	0.47
1:B:86:LEU:HD23	1:B:106:LEU:HD13	1.97	0.47
2:Y:10:MET:HA	2:Y:11:PRO:HD2	1.70	0.47
1:B:219:GLN:HE21	1:B:267:GLY:HA3	1.78	0.47
1:B:56:PHE:CE2	1:B:77:ALA:HB2	2.50	0.47
1:A:123:LEU:O	1:A:127:MET:HG3	2.15	0.47
1:B:189:ILE:CD1	1:B:208:LEU:HD13	2.45	0.47
2:D:177:PHE:CD2	2:D:177:PHE:O	2.68	0.47
2:E:33:GLY:O	2:E:160:LEU:HD22	2.15	0.47
2:G:30:LEU:HA	2:G:30:LEU:HD23	1.70	0.47
2:H:167:ASP:OD2	2:H:167:ASP:C	2.53	0.47
2:D:194:ASP:OD2	2:D:202:ARG:NH2	2.48	0.46
2:D:23:PHE:N	2:D:24:PRO:HD2	2.29	0.46
2:E:155:ASN:O	2:E:156:ARG:C	2.51	0.46
2:G:211:MET:CE	2:G:211:MET:HA	2.40	0.46
1:X:284:PHE:HE2	1:X:289:ILE:HG13	1.80	0.46
1:X:323:LEU:C	1:X:323:LEU:HD23	2.36	0.46
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.67	0.46
1:B:206:LEU:HD12	1:B:206:LEU:HA	1.80	0.46
2:E:96:GLY:HA3	2:E:180:PHE:CD1	2.49	0.46
2:H:35:HIS:NE2	2:H:179:ARG:HD3	2.30	0.46
2:Y:115:PHE:N	2:Y:115:PHE:CD1	2.83	0.46
2:Y:157:SER:O	2:Y:160:ASN:N	2.48	0.46
2:Y:205:ILE:HG22	2:Y:206:ARG:N	2.30	0.46
2:Y:211:MET:HE3	2:Y:212:PRO:HD2	1.98	0.46
1:A:136:LEU:HD13	1:A:164:VAL:HG21	1.96	0.46
2:G:111:ASN:HB3	2:G:114:ILE:O	2.16	0.46
2:G:121:TYR:CE2	2:G:125:LEU:HD11	2.50	0.46
1:X:171:ILE:C	1:X:174:THR:HG22	2.35	0.46
2:Z:83:ILE:HG23	2:Z:84:PRO:HD2	1.97	0.46
1:A:14:TRP:CZ2	1:A:20:PHE:CE1	3.02	0.46
1:A:56:PHE:CD1	1:A:56:PHE:O	2.69	0.46
1:A:32:LEU:CD1	1:A:86:LEU:HD13	2.46	0.46
1:B:280:HIS:NE2	2:D:113:GLY:N	2.63	0.46
1:A:197:TRP:NE1	1:A:289:ILE:HG23	2.31	0.46
2:D:68:ALA:HB1	2:D:69:PRO:CD	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:192:ARG:C	2:G:192:ARG:HD3	2.36	0.46
2:H:156:ARG:HD3	2:H:163:PHE:CD2	2.51	0.46
1:X:283:LYS:NZ	2:Y:108:ARG:HH22	2.12	0.46
1:A:177:LEU:CD1	1:B:105:PRO:HG2	2.45	0.46
2:D:127:LEU:HD23	2:D:127:LEU:N	2.30	0.46
1:B:314:ALA:HB1	2:D:87:VAL:HG13	1.96	0.46
2:Z:35:HIS:ND1	2:Z:74:TYR:HB3	2.31	0.46
1:B:194:ASN:HD22	1:B:195:LYS:HE2	1.80	0.46
1:B:197:TRP:HZ3	1:B:295:ARG:CZ	2.28	0.46
1:A:197:TRP:CE3	1:A:295:ARG:CZ	2.99	0.46
2:D:41:LEU:HD12	2:D:41:LEU:H	1.80	0.46
2:E:87:VAL:HG12	2:E:88:LEU:N	2.31	0.46
2:H:13:LYS:HD2	2:H:53:TYR:OH	2.16	0.46
1:X:10:GLU:O	1:X:13:ALA:HB3	2.16	0.46
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.49	0.45
1:B:171:ILE:HA	1:B:174:THR:CG2	2.39	0.45
1:B:186:LYS:HG2	1:B:277:TYR:CZ	2.50	0.45
2:H:88:LEU:HB3	2:H:92:ASP:CB	2.46	0.45
1:A:234:LEU:HD12	1:A:237:GLN:HB3	1.97	0.45
1:B:221:THR:O	1:B:224:ALA:HB3	2.16	0.45
2:G:181:THR:HB	2:G:183:SER:HB2	1.98	0.45
2:H:121:TYR:CE1	2:H:145:GLN:HG2	2.52	0.45
2:H:167:ASP:CG	2:H:169:SER:H	2.20	0.45
2:Z:88:LEU:HB3	2:Z:92:ASP:HB2	1.98	0.45
1:A:119:GLU:HB2	1:A:124:ARG:CZ	2.46	0.45
1:A:233:LEU:HD13	1:A:257:GLN:HG3	1.98	0.45
2:D:120:LEU:HD22	2:D:158:LEU:HD22	1.99	0.45
1:A:300:ARG:HB2	2:G:191:VAL:HG11	1.98	0.45
2:Y:165:LEU:HD12	2:Y:165:LEU:HA	1.74	0.45
1:B:292:ASP:CG	1:B:297:PHE:HB3	2.36	0.45
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.42	0.45
2:E:137:VAL:HG11	2:E:145:LYS:HB2	1.98	0.45
2:E:51:GLN:O	2:E:55:GLU:HB2	2.17	0.45
2:G:198:ARG:O	2:G:202:ARG:HG3	2.17	0.45
2:Z:117:GLN:O	2:Z:120:LEU:HB3	2.14	0.45
1:B:35:VAL:CG1	1:B:103:LEU:HD21	2.47	0.45
1:B:25:PRO:HB2	1:B:27:ASP:OD1	2.16	0.45
2:D:41:LEU:HD12	2:D:41:LEU:N	2.32	0.45
2:E:99:LEU:CD2	2:E:120:LEU:HD13	2.46	0.45
2:E:88:LEU:HB3	2:E:92:ASP:CB	2.45	0.45
2:G:85:ARG:NH2	2:G:211:MET:SD	2.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:103:TYR:HE2	2:Y:182:GLU:HA	1.81	0.45
1:A:189:ILE:CD1	1:A:208:LEU:HD13	2.47	0.45
2:E:177:VAL:O	2:E:177:VAL:CG1	2.65	0.45
2:Y:31:ARG:HA	2:Y:75:LEU:HD12	1.98	0.45
2:Z:152:LEU:HD12	2:Z:152:LEU:HA	1.43	0.45
1:A:152:TRP:CE3	1:A:246:LEU:CD1	2.99	0.45
2:G:117:GLN:CA	2:G:117:GLN:HE21	2.30	0.45
2:G:126:THR:CG2	2:G:127:LEU:HD23	2.34	0.45
2:H:177:VAL:CG1	2:H:177:VAL:O	2.63	0.45
1:A:104:THR:O	1:A:105:PRO:C	2.55	0.45
1:A:294:ASN:O	1:A:295:ARG:HB3	2.17	0.45
1:B:35:VAL:HG11	1:B:103:LEU:HD21	1.99	0.45
2:D:14:LEU:HD22	2:D:18:LEU:CD1	2.47	0.45
2:Z:102:LEU:HA	2:Z:102:LEU:HD23	1.53	0.45
1:B:280:HIS:CD2	2:D:112:GLU:O	2.70	0.45
2:D:137:VAL:HG21	2:D:150:LEU:HA	1.99	0.45
2:D:74:TYR:HE1	2:D:185:ARG:NE	2.13	0.45
2:E:96:GLY:HA3	2:E:180:PHE:CE1	2.52	0.45
2:G:195:ASP:OD2	2:G:203:ARG:NH2	2.49	0.45
2:Z:187:ASP:O	2:Z:188:PRO:C	2.54	0.45
2:Z:51:GLN:O	2:Z:55:GLU:HB2	2.17	0.45
1:A:197:TRP:HE1	1:A:289:ILE:HG23	1.82	0.45
2:D:170:MET:HB2	2:D:176:LYS:O	2.17	0.45
2:D:61:TYR:CD1	2:D:61:TYR:N	2.83	0.45
2:G:102:LEU:HB3	2:G:115:PHE:CE2	2.52	0.45
2:G:94:MET:CE	2:G:94:MET:HA	2.46	0.45
2:Y:196:ASP:OD1	2:Y:197:PRO:CD	2.63	0.45
2:Z:41:LEU:HA	2:Z:41:LEU:HD23	1.71	0.45
1:A:314:ALA:HB1	2:G:87:VAL:HG12	1.99	0.44
2:D:190:VAL:HG12	2:D:191:ARG:N	2.30	0.44
2:G:132:LYS:O	2:G:135:LYS:N	2.49	0.44
2:Z:92:ASP:OD1	2:Z:154:ARG:HD2	2.17	0.44
2:Z:35:HIS:HE1	2:Z:177:ARG:CD	2.19	0.44
1:B:112:ASP:O	1:B:116:ARG:CB	2.66	0.44
2:D:100:CYS:O	2:D:103:TYR:N	2.50	0.44
2:D:62:ASN:O	2:D:81:THR:HG22	2.17	0.44
2:G:82:LEU:HD13	2:H:25:ALA:HA	1.98	0.44
1:X:266:TRP:CG	1:X:266:TRP:O	2.69	0.44
1:A:152:TRP:CE2	1:A:246:LEU:HD11	2.52	0.44
2:D:160:ARG:O	2:D:163:ARG:N	2.51	0.44
2:D:30:LEU:HA	2:D:30:LEU:HD23	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:TYR:HB2	2:E:173:ILE:HG21	1.98	0.44
1:X:219:GLN:NE2	1:X:264:ILE:O	2.50	0.44
2:Y:26:LEU:CD1	2:Y:36:ILE:CD1	2.96	0.44
1:A:106:LEU:O	1:A:110:ILE:HG13	2.18	0.44
1:B:165:ALA:HB2	1:B:256:LEU:HD21	1.99	0.44
2:E:30:LEU:HD23	2:E:30:LEU:HA	1.63	0.44
2:E:61:TYR:HA	2:E:82:LEU:HD12	1.98	0.44
1:X:96:GLU:HG2	1:X:97:GLY:N	2.31	0.44
2:Z:100:CYS:HA	2:Z:175:VAL:CG1	2.47	0.44
2:Z:70:GLU:CD	2:Z:70:GLU:H	2.19	0.44
1:A:108:ILE:HD13	1:A:108:ILE:HA	1.70	0.44
1:A:153:HIS:HA	1:A:157:TYR:HB3	1.99	0.44
2:G:90:GLU:H	2:G:90:GLU:HG2	1.43	0.44
2:Y:103:TYR:HD1	2:Y:108:ARG:HD2	1.82	0.44
1:A:31:PHE:HB2	1:A:59:VAL:HG11	2.00	0.44
1:B:173:LEU:HA	1:B:173:LEU:HD12	1.85	0.44
1:B:195:LYS:HD3	1:B:195:LYS:HA	1.79	0.44
1:B:198:ARG:O	1:B:201:ILE:HG13	2.18	0.44
1:B:289:ILE:O	1:B:290:ASP:C	2.55	0.44
2:G:117:GLN:HG2	2:G:156:ARG:NH1	2.33	0.44
2:Y:10:MET:HG2	2:Y:10:MET:O	2.18	0.44
1:A:222:LEU:HD13	1:A:263:ILE:HG22	1.99	0.44
1:B:180:GLU:OE2	1:B:180:GLU:HA	2.17	0.44
1:B:28:ARG:NH1	1:B:80:ASP:CG	2.71	0.44
1:A:81:MET:HB3	1:A:87:LEU:HD22	2.00	0.44
2:H:95:VAL:HG12	2:H:155:LEU:HD12	2.00	0.44
1:A:315:LEU:O	2:G:87:VAL:CG1	2.62	0.44
1:B:89:ARG:HG2	1:B:90:PHE:N	2.32	0.44
2:D:17:ALA:HB2	2:D:50:PHE:CD1	2.52	0.44
2:H:63:VAL:HG22	2:H:77:PRO:HA	2.00	0.44
2:Y:121:TYR:CZ	2:Y:152:GLN:HG2	2.53	0.44
2:Y:47:LEU:HB3	2:Y:73:PHE:CE2	2.53	0.44
1:A:12:VAL:HG13	1:B:30:SER:HB3	2.00	0.43
2:G:98:ILE:CD1	2:G:124:LEU:HA	2.48	0.43
2:G:168:VAL:HG22	2:G:179:ARG:O	2.18	0.43
1:X:324:LEU:HA	1:X:324:LEU:HD23	1.38	0.43
1:A:157:TYR:HD2	1:A:157:TYR:C	2.19	0.43
2:D:76:ARG:HD2	2:D:207:GLY:O	2.17	0.43
1:A:113:TYR:CD2	1:B:106:LEU:CB	2.98	0.43
1:B:128:GLN:NE2	1:B:170:SER:OG	2.52	0.43
2:D:34:ARG:HH12	2:D:165:GLY:HA2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:LEU:HA	2:D:82:LEU:HD23	1.71	0.43
2:G:163:ARG:O	2:G:164:ARG:C	2.55	0.43
1:A:118:ARG:HB2	1:A:120:PHE:CE2	2.53	0.43
1:A:88:ASN:N	1:A:104:THR:HG23	2.34	0.43
2:D:22:LEU:O	2:D:23:PHE:C	2.56	0.43
2:G:26:LEU:HD21	2:G:47:LEU:HD21	1.99	0.43
2:H:174:THR:HG22	2:H:175:GLU:H	1.79	0.43
2:H:62:ASN:O	2:H:78:ARG:HB2	2.18	0.43
1:X:48:SER:HA	1:X:100:ILE:HA	2.01	0.43
2:Y:98:ILE:HD13	2:Y:124:LEU:HA	1.99	0.43
2:Z:97:LYS:HD3	2:Z:195:LEU:HD23	2.00	0.43
1:A:28:ARG:O	1:A:31:PHE:HB3	2.18	0.43
2:H:142:GLN:O	2:H:146:GLU:HG3	2.19	0.43
1:X:252:LEU:HD22	1:X:256:LEU:HD12	2.01	0.43
2:G:108:ARG:HG3	2:G:115:PHE:CE1	2.54	0.43
2:H:18:LEU:HD22	2:H:23:PHE:CZ	2.53	0.43
2:Y:38:LEU:HD23	2:Y:38:LEU:HA	1.73	0.43
2:Y:67:ARG:HB2	2:Y:73:PHE:HE1	1.78	0.43
2:Z:14:LEU:O	2:Z:18:LEU:HG	2.18	0.43
1:A:118:ARG:CD	1:A:118:ARG:C	2.87	0.43
1:B:284:PHE:CE1	2:D:105:SER:O	2.70	0.43
2:D:102:LEU:CD2	2:D:123:GLU:HG2	2.43	0.43
2:E:76:ARG:HA	2:E:77:PRO:HD3	1.79	0.43
2:G:91:LEU:HD11	2:G:155:VAL:HG22	2.01	0.43
2:Y:129:ASP:C	2:Y:131:ALA:N	2.72	0.43
2:Y:167:MET:HE1	2:Y:184:VAL:CA	2.46	0.43
1:B:129:LEU:HD12	1:B:129:LEU:HA	1.65	0.43
2:E:70:GLU:HG3	2:E:178:PHE:HD1	1.84	0.43
1:X:323:LEU:O	1:X:323:LEU:HD23	2.18	0.43
2:Z:111:ASN:O	2:Z:112:GLU:HB3	2.19	0.43
2:D:103:TYR:CE1	2:D:108:ARG:NH2	2.87	0.43
2:D:181:GLU:O	2:D:182:SER:C	2.57	0.43
2:E:127:LEU:HA	2:E:127:LEU:HD23	1.75	0.43
2:G:14:LEU:O	2:G:14:LEU:HD23	2.19	0.43
2:Y:184:VAL:O	2:Y:186:ARG:N	2.52	0.43
2:Y:205:ILE:CD1	2:Y:212:PRO:HD3	2.49	0.43
2:Z:124:LEU:HG	2:Z:133:LEU:HD21	2.00	0.43
1:B:104:THR:HG22	1:B:105:PRO:HD2	2.01	0.43
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.74	0.43
1:B:317:TYR:N	1:B:317:TYR:CD2	2.87	0.43
1:B:315:LEU:CD1	2:D:185:ARG:HG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:LEU:CB	2:D:73:PHE:CE2	3.02	0.43
1:B:314:ALA:CB	2:D:87:VAL:HG13	2.49	0.43
1:X:323:LEU:HB2	2:Z:31:ARG:O	2.19	0.43
1:A:105:PRO:O	1:A:108:ILE:HB	2.19	0.42
1:A:32:LEU:HD11	1:A:86:LEU:HD13	2.00	0.42
1:B:254:PHE:O	1:B:257:GLN:HB2	2.19	0.42
2:D:14:LEU:HD22	2:D:18:LEU:HD11	2.00	0.42
2:G:47:LEU:HD23	2:G:47:LEU:N	2.34	0.42
1:X:120:PHE:HZ	1:X:218:LEU:CD2	2.27	0.42
2:Y:133:LEU:HG	2:Y:151:LEU:HD11	2.01	0.42
1:A:131:ILE:HD11	1:B:135:GLU:OE2	2.18	0.42
1:A:152:TRP:CE3	1:A:246:LEU:HD11	2.54	0.42
1:B:316:THR:HG23	2:D:209:ALA:HA	2.00	0.42
2:E:69:PRO:HG2	2:E:70:GLU:OE2	2.20	0.42
2:G:162:LEU:O	2:G:167:MET:HB2	2.19	0.42
2:Z:100:CYS:HB3	2:Z:192:GLN:NE2	2.34	0.42
2:Z:21:PRO:O	2:Z:24:PRO:HD2	2.19	0.42
2:Z:92:ASP:HA	2:Z:151:SER:OG	2.20	0.42
1:A:11:LEU:O	1:A:14:TRP:N	2.52	0.42
1:A:54:ASP:O	1:A:57:ARG:HB3	2.20	0.42
1:A:8:VAL:HB	1:A:9:PRO:HD3	2.02	0.42
1:A:91:THR:HB	2:D:112:GLU:OE2	2.19	0.42
1:B:325:ASP:OD2	1:B:326:MET:N	2.40	0.42
1:A:266:TRP:CZ2	1:B:102:ARG:HD2	2.55	0.42
2:D:100:CYS:O	2:D:101:TYR:C	2.57	0.42
2:H:143:LYS:CE	2:H:143:LYS:HA	2.49	0.42
2:H:152:LEU:HA	2:H:152:LEU:HD12	1.59	0.42
2:H:198:ILE:O	2:H:198:ILE:HG22	2.20	0.42
2:Y:181:THR:CG2	2:Y:182:GLU:N	2.81	0.42
2:Z:98:ILE:HG22	2:Z:120:LEU:HD11	2.01	0.42
2:Z:134:LEU:HD21	2:Z:141:ARG:HG2	2.01	0.42
2:Z:26:LEU:HD21	2:Z:47:LEU:HG	2.01	0.42
1:A:81:MET:HE2	1:A:81:MET:HA	2.02	0.42
2:D:10:MET:HA	2:D:11:PRO:HD3	1.87	0.42
2:G:210:ALA:O	2:G:211:MET:HE3	2.19	0.42
2:G:70:GLU:HG3	2:G:72:PHE:CE1	2.55	0.42
1:X:316:THR:HG23	2:Y:210:ALA:HA	2.00	0.42
2:Z:100:CYS:HA	2:Z:175:VAL:HG11	2.01	0.42
1:B:149:GLU:HB2	1:B:153:HIS:ND1	2.34	0.42
1:B:186:LYS:HE3	1:B:274:TRP:CZ3	2.47	0.42
1:B:251:ARG:HD3	1:B:251:ARG:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.57	0.42
1:B:77:ALA:O	1:B:81:MET:HG2	2.19	0.42
2:D:76:ARG:HD2	2:D:207:GLY:C	2.40	0.42
2:D:77:PRO:CG	2:D:85:ARG:HB2	2.48	0.42
2:H:161:VAL:HG22	2:H:172:ARG:O	2.19	0.42
1:A:106:LEU:HD21	1:A:110:ILE:HD11	1.99	0.42
1:B:28:ARG:NH1	1:B:80:ASP:OD1	2.53	0.42
2:G:133:LEU:HD12	2:G:133:LEU:HA	1.90	0.42
1:A:314:ALA:HB3	2:G:87:VAL:HG11	2.02	0.42
2:H:185:ARG:O	2:H:186:ALA:HB3	2.20	0.42
1:X:81:MET:HA	1:X:81:MET:CE	2.50	0.42
2:Y:184:VAL:C	2:Y:186:ARG:H	2.22	0.42
2:Y:190:ASP:N	2:Y:190:ASP:OD2	2.53	0.42
2:Y:191:VAL:HG13	2:Y:191:VAL:O	2.20	0.42
1:A:140:ALA:O	1:A:141:ASP:C	2.57	0.42
1:B:112:ASP:O	1:B:113:TYR:C	2.57	0.42
1:B:28:ARG:HH12	1:B:80:ASP:CG	2.23	0.42
2:E:194:GLN:O	2:E:198:ILE:HG13	2.20	0.42
1:X:236:ILE:O	1:X:240:THR:CB	2.67	0.42
2:Z:115:PHE:CD1	2:Z:115:PHE:N	2.88	0.42
1:A:119:GLU:H	1:A:119:GLU:HG2	1.70	0.42
2:G:109:LEU:HA	2:G:109:LEU:HD23	1.78	0.42
2:H:156:ARG:HD3	2:H:163:PHE:CE2	2.54	0.42
2:H:30:LEU:HB3	2:H:75:LEU:HG	2.02	0.42
1:A:125:LEU:HD12	1:A:218:LEU:HD22	2.02	0.42
1:B:291:MET:HE2	1:B:291:MET:HB2	1.71	0.42
1:B:297:PHE:CE1	2:D:184:PHE:CD2	3.06	0.42
2:D:26:LEU:O	2:D:29:ALA:HB3	2.19	0.42
2:D:31:ARG:HD3	2:D:83:ILE:CD1	2.50	0.42
2:E:125:LEU:HD23	2:E:125:LEU:N	2.34	0.42
2:G:108:ARG:HG3	2:G:115:PHE:CZ	2.55	0.42
2:G:56:GLU:O	2:G:57:PHE:C	2.57	0.42
2:H:65:LEU:HA	2:H:75:LEU:HD23	2.00	0.42
1:X:317:TYR:N	1:X:317:TYR:CD2	2.88	0.42
2:Y:27:ASP:O	2:Y:31:ARG:HG3	2.19	0.42
1:A:182:GLN:O	1:A:183:GLN:C	2.57	0.41
1:A:294:ASN:HB2	1:A:296:VAL:HG23	2.02	0.41
2:D:210:MET:HG3	2:D:211:PRO:CD	2.28	0.41
2:G:87:VAL:HG12	2:G:88:LEU:N	2.35	0.41
2:H:100:CYS:HA	2:H:177:VAL:CG1	2.50	0.41
1:X:263:ILE:HG22	1:X:264:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:48:SER:OG	1:X:51:GLU:HG3	2.20	0.41
2:Y:117:GLN:HB2	2:Y:117:GLN:HE21	1.63	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.68	0.41
1:B:326:MET:O	1:B:327:ARG:CB	2.68	0.41
2:D:121:TYR:CZ	2:D:125:LEU:HD11	2.55	0.41
2:E:121:TYR:CZ	2:E:125:LEU:HD11	2.55	0.41
2:G:178:PHE:C	2:G:178:PHE:CD2	2.93	0.41
2:H:76:ARG:HA	2:H:77:PRO:HD3	1.73	0.41
2:Z:41:LEU:O	2:Z:42:ASP:C	2.58	0.41
1:A:90:PHE:CE1	1:B:182:GLN:NE2	2.87	0.41
1:B:181:GLN:O	1:B:184:GLN:HB3	2.20	0.41
1:X:278:ASP:O	1:X:279:ARG:C	2.59	0.41
1:A:113:TYR:OH	1:A:180:GLU:OE2	2.30	0.41
1:B:291:MET:HB3	1:B:291:MET:HE3	1.68	0.41
1:B:323:LEU:HD23	1:B:323:LEU:C	2.40	0.41
2:D:36:ILE:HG22	2:D:36:ILE:O	2.20	0.41
2:E:111:ASN:O	2:E:112:GLU:HB3	2.20	0.41
1:X:193:LEU:HD23	1:X:200:ALA:HB3	2.02	0.41
1:X:56:PHE:HE2	1:X:77:ALA:CB	2.34	0.41
2:Z:155:LEU:O	2:Z:160:MET:HB2	2.20	0.41
2:Z:173:GLU:HG3	2:Z:173:GLU:H	1.29	0.41
1:A:113:TYR:CD2	1:B:106:LEU:CG	3.04	0.41
1:A:295:ARG:HG3	1:A:295:ARG:O	2.21	0.41
1:B:296:VAL:O	1:B:300:ARG:HG2	2.21	0.41
2:E:117:GLN:HE21	2:E:117:GLN:HB2	1.58	0.41
2:E:35:HIS:CD2	2:E:162:MET:HE1	2.54	0.41
1:X:115:ILE:CG1	1:X:116:ARG:N	2.84	0.41
1:X:23:SER:N	1:X:84:GLN:OE1	2.46	0.41
2:Z:118:GLN:O	2:Z:119:GLU:C	2.59	0.41
1:A:322:ARG:HD2	2:H:86:SER:OG	2.20	0.41
1:B:248:PHE:HD2	1:B:248:PHE:N	2.15	0.41
2:G:19:ALA:O	2:G:20:ASN:C	2.58	0.41
1:A:319:ASN:ND2	1:A:319:ASN:C	2.73	0.41
2:H:46:PHE:C	2:H:46:PHE:CD2	2.94	0.41
1:X:193:LEU:HA	1:X:193:LEU:HD23	1.73	0.41
2:Z:117:GLN:NE2	2:Z:166:SER:O	2.51	0.41
1:B:320:ALA:HA	2:D:84:PRO:HD2	2.02	0.41
2:E:117:GLN:O	2:E:120:LEU:HB3	2.21	0.41
2:H:47:LEU:HA	2:H:47:LEU:HD23	1.89	0.41
1:X:112:ASP:O	1:X:113:TYR:C	2.59	0.41
2:Y:184:VAL:C	2:Y:186:ARG:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:136:LEU:N	2:Z:136:LEU:HD23	2.35	0.41
1:A:25:PRO:HB2	1:A:27:ASP:OD1	2.21	0.41
1:A:314:ALA:HB1	2:G:88:LEU:O	2.20	0.41
1:A:80:ASP:OD1	1:A:81:MET:HE3	2.20	0.41
2:D:56:GLU:O	2:D:59:ALA:HB3	2.20	0.41
2:E:163:VAL:HA	2:E:172:ARG:O	2.20	0.41
1:X:193:LEU:HD12	2:Y:109:LEU:CD1	2.51	0.41
2:Z:54:LEU:HA	2:Z:54:LEU:HD23	1.67	0.41
1:A:178:MET:HB2	1:A:178:MET:HE2	1.88	0.41
1:A:240:THR:O	1:A:240:THR:CG2	2.68	0.41
1:A:152:TRP:CZ3	1:A:246:LEU:CD1	3.04	0.41
1:B:284:PHE:O	1:B:284:PHE:CD2	2.74	0.41
2:G:126:THR:HG22	2:G:127:LEU:N	2.35	0.41
1:A:158:ALA:O	1:A:160:LEU:N	2.53	0.41
1:A:16:ARG:NH1	1:B:63:PHE:CD1	2.87	0.41
1:A:172:ASP:OD2	1:A:172:ASP:C	2.59	0.41
1:B:177:LEU:O	1:B:180:GLU:HB2	2.21	0.41
1:B:178:MET:CE	1:B:214:THR:HG22	2.49	0.41
2:E:102:LEU:HA	2:E:102:LEU:HD23	1.92	0.41
2:E:175:GLU:H	2:E:175:GLU:HG3	1.31	0.41
1:X:56:PHE:HE2	1:X:77:ALA:HB2	1.86	0.41
1:A:197:TRP:CZ2	1:A:289:ILE:CG1	3.04	0.40
2:D:137:VAL:HG21	2:D:150:LEU:CA	2.51	0.40
2:D:77:PRO:CB	2:D:81:THR:HG21	2.51	0.40
2:G:163:ARG:HD3	2:G:170:PHE:CE2	2.56	0.40
2:G:190:ASP:OD2	2:G:191:VAL:N	2.54	0.40
2:H:117:GLN:O	2:H:120:LEU:HB3	2.22	0.40
2:Z:132:LYS:O	2:Z:135:LYS:HB3	2.20	0.40
1:A:132:VAL:HG11	1:A:168:PHE:HE1	1.86	0.40
1:B:280:HIS:CD2	2:D:112:GLU:C	2.94	0.40
2:D:26:LEU:HA	2:D:26:LEU:HD12	1.88	0.40
2:D:91:LEU:HD12	2:D:91:LEU:HA	1.87	0.40
2:E:36:ILE:HG23	2:E:36:ILE:HD12	1.80	0.40
2:G:99:LEU:HD12	2:G:180:ILE:HD13	2.00	0.40
2:H:177:VAL:HG12	2:H:177:VAL:O	2.21	0.40
1:X:182:GLN:O	1:X:185:VAL:N	2.54	0.40
2:Z:98:ILE:CG2	2:Z:120:LEU:CD1	3.00	0.40
2:Z:13:LYS:HD2	2:Z:53:TYR:OH	2.21	0.40
1:B:124:ARG:O	1:B:128:GLN:HG3	2.20	0.40
2:D:94:MET:CA	2:D:94:MET:CE	2.97	0.40
2:E:75:LEU:HD23	2:E:75:LEU:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:HIS:CE1	2:G:108:ARG:HD2	2.56	0.40
2:G:10:MET:HA	2:G:11:PRO:HD3	1.99	0.40
2:G:191:VAL:O	2:G:192:ARG:C	2.59	0.40
2:H:73:PHE:CD1	2:H:73:PHE:N	2.90	0.40
1:X:165:ALA:HA	1:X:256:LEU:HD21	2.03	0.40
2:Z:117:GLN:HB2	2:Z:117:GLN:HE21	1.70	0.40
2:Z:87:VAL:CG1	2:Z:88:LEU:H	2.34	0.40
1:A:77:ALA:O	1:A:81:MET:HG2	2.21	0.40
1:B:289:ILE:C	1:B:291:MET:N	2.75	0.40
1:B:89:ARG:HB2	1:B:101:TYR:CE1	2.57	0.40
2:D:179:ILE:HG23	2:D:183:VAL:HG21	2.03	0.40
2:E:121:TYR:O	2:E:124:LEU:HB3	2.22	0.40
2:G:179:ARG:HH21	2:G:179:ARG:HB2	1.85	0.40
1:X:171:ILE:O	1:X:174:THR:CG2	2.69	0.40
2:Z:57:PHE:O	2:Z:60:ARG:HG3	2.22	0.40
1:A:118:ARG:NE	1:A:120:PHE:HB2	2.37	0.40
1:B:56:PHE:CG	1:B:74:ALA:HA	2.56	0.40
2:D:18:LEU:HD23	2:D:23:PHE:CE2	2.56	0.40
2:G:103:TYR:HD1	2:G:180:ILE:CG2	2.34	0.40
2:Y:78:ARG:CG	2:Y:78:ARG:HH11	2.34	0.40
2:Z:81:THR:O	2:Z:81:THR:HG23	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	303/460 (66%)	284 (94%)	19 (6%)	0	100	100
1	B	294/460 (64%)	277 (94%)	17 (6%)	0	100	100
1	X	304/460 (66%)	286 (94%)	18 (6%)	0	100	100
2	D	199/245 (81%)	190 (96%)	8 (4%)	1 (0%)	32	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	185/245 (76%)	167 (90%)	17 (9%)	1 (0%)	32	73
2	G	202/245 (82%)	189 (94%)	11 (5%)	2 (1%)	18	62
2	H	187/245 (76%)	181 (97%)	6 (3%)	0	100	100
2	Y	203/245 (83%)	191 (94%)	12 (6%)	0	100	100
2	Z	182/245 (74%)	171 (94%)	11 (6%)	0	100	100
All	All	2059/2850 (72%)	1936 (94%)	119 (6%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	126	THR
2	E	131	ALA
2	G	126	THR
2	G	137	VAL

### 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	268/397 (68%)	254 (95%)	14 (5%)	27	65
1	B	260/397 (66%)	241 (93%)	19 (7%)	16	54
1	X	266/397 (67%)	248 (93%)	18 (7%)	18	57
2	D	177/215 (82%)	157 (89%)	20 (11%)	7	35
2	E	168/215 (78%)	158 (94%)	10 (6%)	22	62
2	G	178/215 (83%)	157 (88%)	21 (12%)	6	33
2	H	167/215 (78%)	155 (93%)	12 (7%)	17	55
2	Y	178/215 (83%)	145 (82%)	33 (18%)	2	12
2	Z	166/215 (77%)	149 (90%)	17 (10%)	8	40
All	All	1828/2481 (74%)	1664 (91%)	164 (9%)	11	46

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	118	ARG
1	A	123	LEU
1	A	125	LEU
1	A	129	LEU
1	A	130	SER
1	A	149	GLU
1	A	219	GLN
1	A	250	ASP
1	A	260	LEU
1	A	262	ARG
1	A	265	SER
1	A	297	PHE
1	A	301	LEU
2	G	24	PRO
2	G	28	SER
2	G	70	GLU
2	G	78	ARG
2	G	79	SER
2	G	85	ARG
2	G	86	SER
2	G	90	GLU
2	G	94	MET
2	G	99	LEU
2	G	112	GLU
2	G	117	GLN
2	G	124	LEU
2	G	139	ASN
2	G	147	ASP
2	G	168	VAL
2	G	179	ARG
2	G	181	THR
2	G	182	GLU
2	G	195	ASP
2	G	211	MET
2	H	53	TYR
2	H	70	GLU
2	H	81	THR
2	H	124	LEU
2	H	129	ASP
2	H	161	VAL
2	H	166	HIS
2	H	175	GLU

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Mol	Chain	Res	Type
2	H	179	ARG
2	H	185	ARG
2	H	189	ASP
2	H	195	ARG
1	B	32	LEU
1	B	33	LEU
1	B	88	ASN
1	B	104	THR
1	B	106	LEU
1	B	108	ILE
1	B	123	LEU
1	B	125	LEU
1	B	129	LEU
1	B	149	GLU
1	B	163	SER
1	B	208	LEU
1	B	211	THR
1	B	248	PHE
1	B	252	LEU
1	B	260	LEU
1	B	262	ARG
1	B	287	THR
1	B	317	TYR
2	D	14	LEU
2	D	32	SER
2	D	34	ARG
2	D	61	TYR
2	D	70	GLU
2	D	74	TYR
2	D	78	ARG
2	D	85	ARG
2	D	90	GLU
2	D	99	LEU
2	D	112	GLU
2	D	117	GLN
2	D	124	LEU
2	D	139	ASN
2	D	167	VAL
2	D	172	HIS
2	D	181	GLU
2	D	191	ARG
2	D	194	ASP

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Mol	Chain	Res	Type
2	D	210	MET
2	E	40	GLU
2	E	63	VAL
2	E	66	ILE
2	E	70	GLU
2	E	86	SER
2	E	117	GLN
2	E	174	THR
2	E	175	GLU
2	E	179	ARG
2	E	185	ARG
1	X	30	SER
1	X	69	THR
1	X	73	ARG
1	X	87	LEU
1	X	125	LEU
1	X	126	SER
1	X	129	LEU
1	X	154	ARG
1	X	176	ARG
1	X	192	LEU
1	X	248	PHE
1	X	252	LEU
1	X	260	LEU
1	X	262	ARG
1	X	301	LEU
1	X	304	SER
1	X	307	THR
1	X	319	ASN
2	Y	10	MET
2	Y	11	PRO
2	Y	14	LEU
2	Y	30	LEU
2	Y	32	SER
2	Y	39	ASP
2	Y	60	ARG
2	Y	70	GLU
2	Y	78	ARG
2	Y	79	SER
2	Y	89	SER
2	Y	90	GLU
2	Y	98	ILE

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Mol	Chain	Res	Type
2	Y	99	LEU
2	Y	112	GLU
2	Y	115	PHE
2	Y	124	LEU
2	Y	126	THR
2	Y	139	ASN
2	Y	147	ASP
2	Y	156	ARG
2	Y	157	SER
2	Y	163	ARG
2	Y	165	LEU
2	Y	168	VAL
2	Y	173	HIS
2	Y	174	ASP
2	Y	186	ARG
2	Y	192	ARG
2	Y	195	ASP
2	Y	202	ARG
2	Y	203	ARG
2	Y	205	ILE
2	Z	21	PRO
2	Z	28	SER
2	Z	48	MET
2	Z	60	ARG
2	Z	70	GLU
2	Z	81	THR
2	Z	102	LEU
2	Z	117	GLN
2	Z	123	GLU
2	Z	164	MET
2	Z	165	ASP
2	Z	166	SER
2	Z	173	GLU
2	Z	175	VAL
2	Z	177	ARG
2	Z	183	ARG
2	Z	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	232	ASN
1	A	243	HIS
1	A	280	HIS
1	A	319	ASN
2	G	117	GLN
2	H	43	ASN
2	H	62	ASN
1	B	39	ASN
1	B	76	ASN
1	B	128	GLN
1	B	219	GLN
1	B	319	ASN
2	D	35	HIS
2	D	117	GLN
2	E	35	HIS
1	X	219	GLN
2	Y	117	GLN
2	Z	35	HIS
2	Z	43	ASN
2	Z	62	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	309/460 (67%)	-0.53	4 (1%) 77 64	75, 131, 215, 275	0
1	B	302/460 (65%)	-0.52	2 (0%) 87 78	81, 149, 217, 294	0
1	X	310/460 (67%)	-0.52	2 (0%) 89 81	61, 141, 209, 280	0
2	D	203/245 (82%)	-0.62	1 (0%) 90 84	73, 113, 175, 222	0
2	E	191/245 (77%)	-0.60	1 (0%) 90 84	72, 110, 184, 244	0
2	G	204/245 (83%)	-0.67	0 100 100	75, 110, 178, 217	0
2	H	191/245 (77%)	-0.62	0 100 100	79, 111, 171, 222	0
2	Y	205/245 (83%)	-0.73	0 100 100	57, 94, 168, 205	0
2	Z	188/245 (76%)	-0.60	3 (1%) 72 59	64, 108, 169, 264	0
All	All	2103/2850 (73%)	-0.59	13 (0%) 89 81	57, 123, 200, 294	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ARG	4.1
1	A	117	GLN	3.0
1	A	7	THR	2.8
1	A	119	GLU	2.5
2	Z	141	ARG	2.4
1	X	150	PHE	2.4
1	B	16	ARG	2.2
2	Z	166	SER	2.2
2	E	192	GLU	2.2
2	Z	140	ASP	2.2
2	D	172	HIS	2.1
1	B	119	GLU	2.1
1	X	61	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.