



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:38 am BST

PDB ID : 3PIF  
Title : Crystal structure of the 5'->3' exoribonuclease Xrn1, E178Q mutant in Complex with Manganese  
Authors : Chang, J.H.; Xiang, S.; Tong, L.  
Deposited on : 2010-11-06  
Resolution : 2.92 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

<https://www.wwpdb.org/validation/2017/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)	:	1.13
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

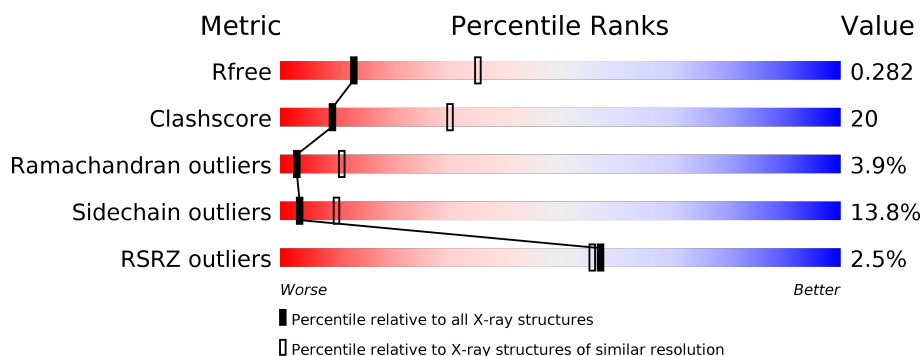
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	1155	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>27%</div> <div>7%</div> <div>8%</div> </div> </div>
1	B	1155	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>32%</div> <div>7%</div> <div>9%</div> </div> </div>
1	C	1155	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>30%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	1155	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>30%</div> <div>6%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34013 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 5'->3' EXORIBONUCLEASE (xrn1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0	0
			8549	5509	1438	1579	23			
1	B	1056	Total	C	N	O	S	0	0	0
			8535	5501	1436	1575	23			
1	C	1066	Total	C	N	O	S	0	0	0
			8605	5543	1446	1593	23			
1	D	1023	Total	C	N	O	S	0	0	0
			8320	5365	1397	1535	23			

There are 188 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
A	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
A	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
A	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
A	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
A	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
B	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	483	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
B	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
B	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
B	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
B	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
C	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	473	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	478	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
C	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
C	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
C	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
C	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
C	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	178	GLN	GLU	ENGINEERED MUTATION	UNP Q6CJ09
D	469	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	470	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	471	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	472	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	473	UNK	-	SEE REMARK 999	UNP Q6CJ09

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Chain	Residue	Modelled	Actual	Comment	Reference
D	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	480	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	481	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	482	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	483	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	484	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	485	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	486	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	487	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1036	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1037	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1038	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1039	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1040	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1041	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1042	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1043	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1044	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1045	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1046	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1047	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1048	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1049	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1050	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1051	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1052	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1053	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1054	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	1246	LEU	-	EXPRESSION TAG	UNP Q6CJ09
D	1247	GLU	-	EXPRESSION TAG	UNP Q6CJ09
D	1248	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1249	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1250	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1251	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1252	HIS	-	EXPRESSION TAG	UNP Q6CJ09
D	1253	HIS	-	EXPRESSION TAG	UNP Q6CJ09

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

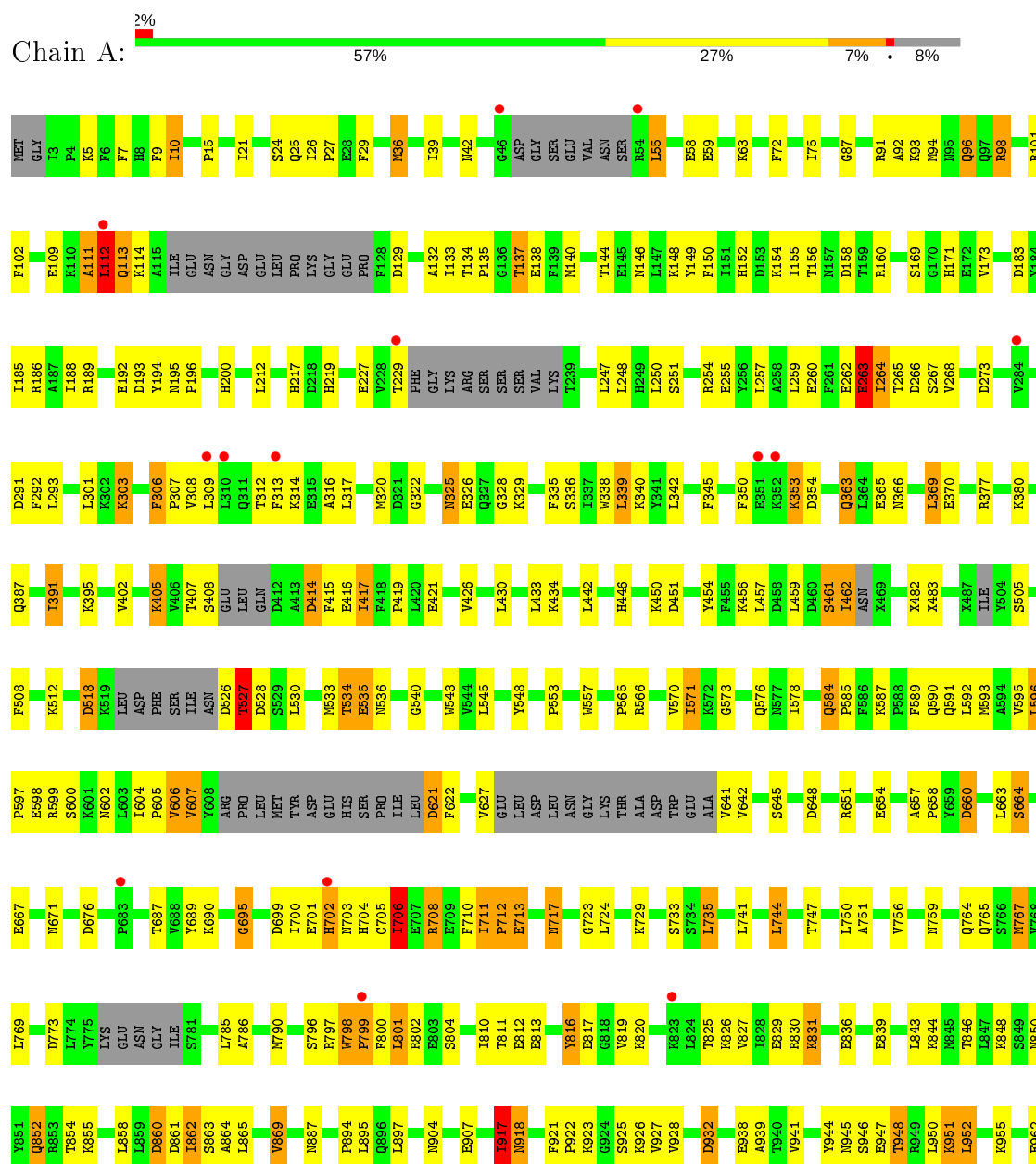
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

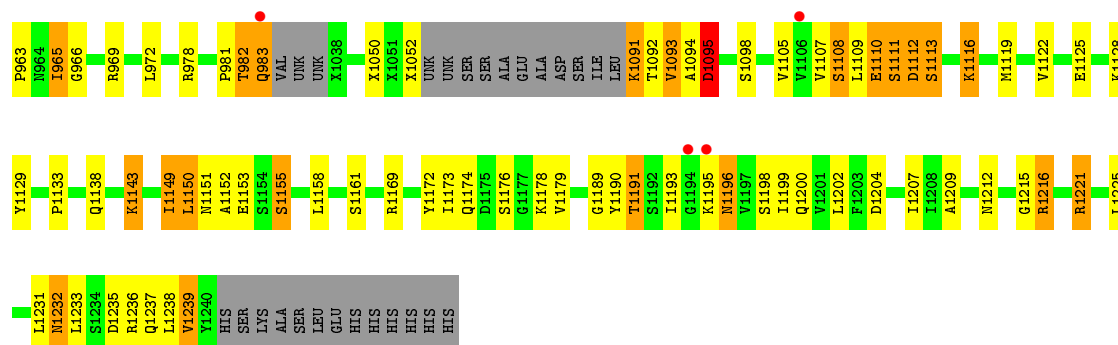


### 3 Residue-property plots [i](#)

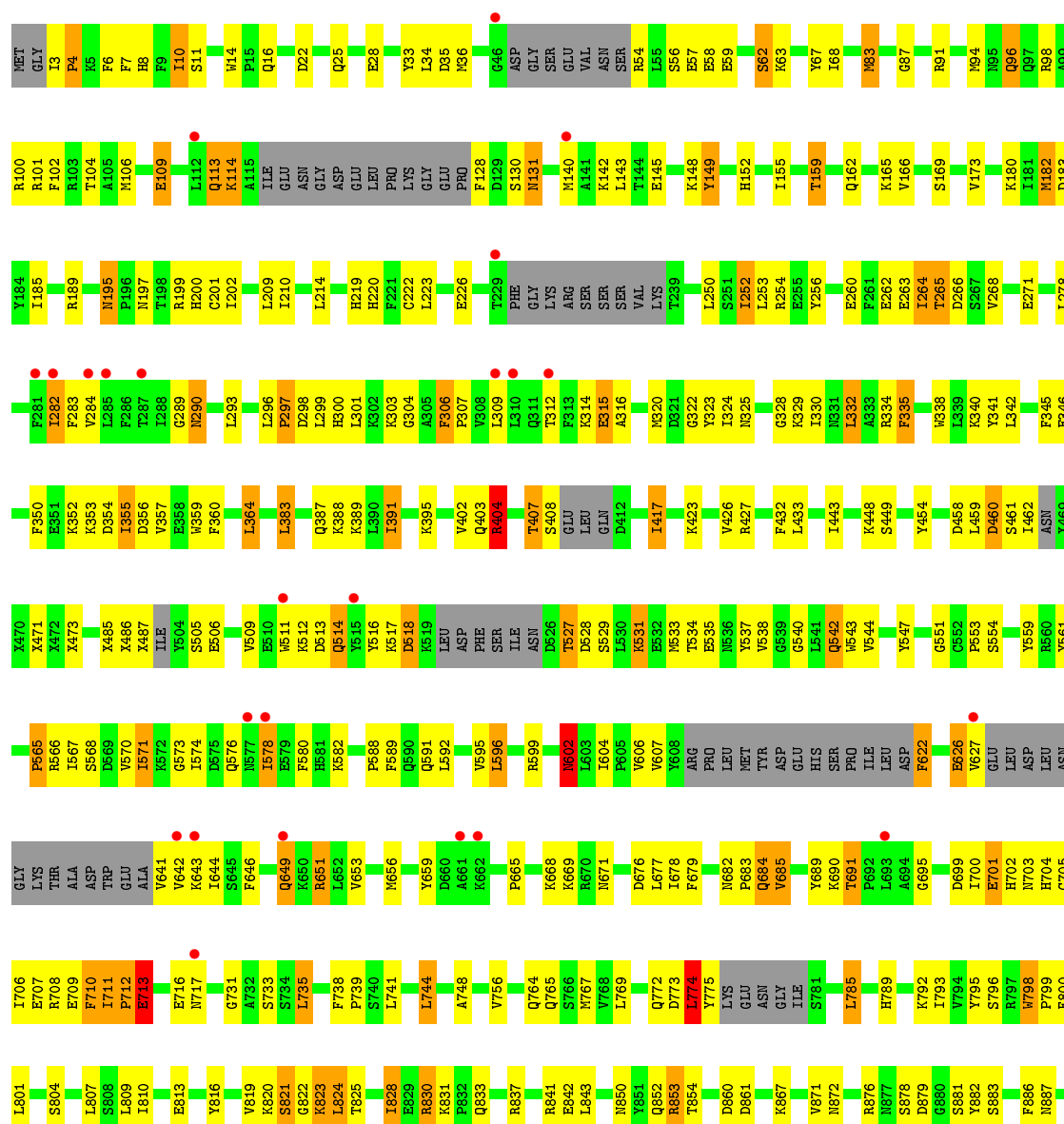
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 5'->3' EXORIBONUCLEASE (xrn1)

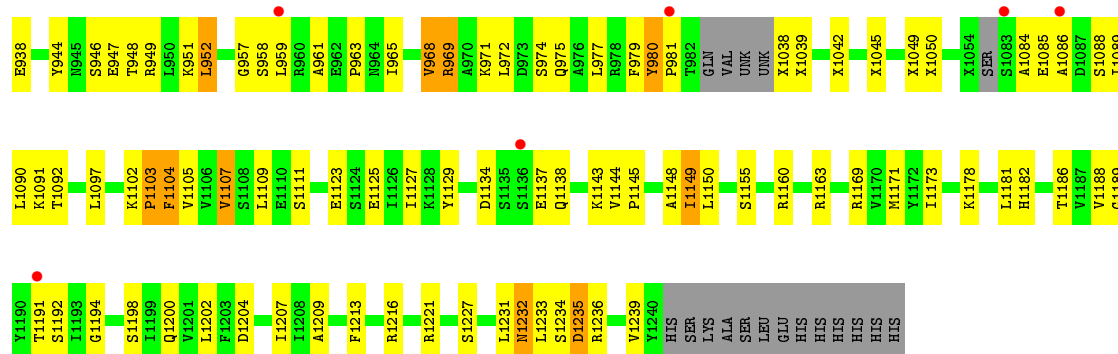


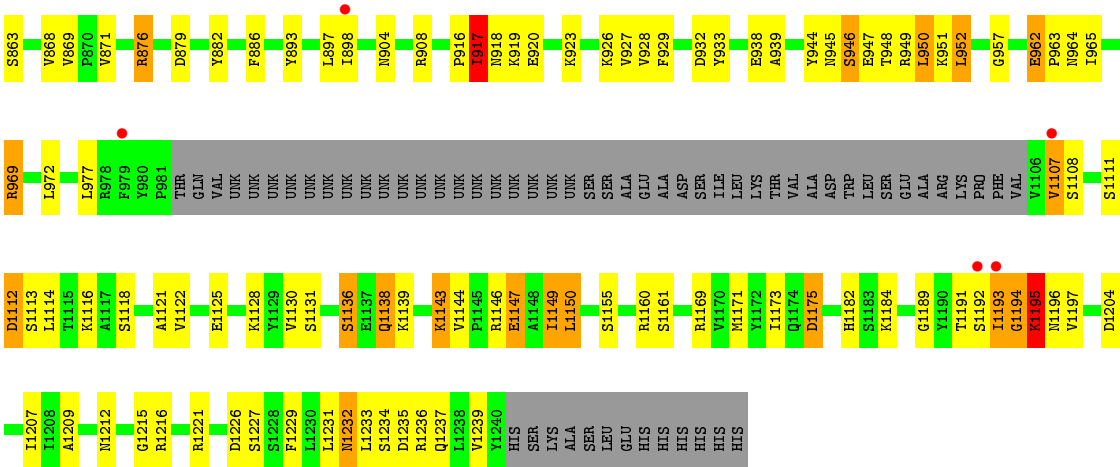


• Molecule 1: 5'->3' EXORIBONUCLEASE (xrn1)









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.27Å 132.58Å 144.07Å 109.92° 105.81° 104.00°	Depositor
Resolution (Å)	30.00 – 2.92 29.05 – 2.92	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-2.92) 96.1 (29.05-2.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.248 , 0.284 0.245 , 0.282	Depositor DCC
$R_{free}$ test set	7614 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.6	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,h+k+l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	34013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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

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

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	0.85	3/8567 (0.0%)	0.88	5/11553 (0.0%)
1	B	0.84	2/8543 (0.0%)	0.89	4/11521 (0.0%)
1	C	0.77	0/8613	0.81	7/11616 (0.1%)
1	D	0.70	1/8409 (0.0%)	0.80	4/11337 (0.0%)
All	All	0.79	6/34132 (0.0%)	0.84	20/46027 (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
1	C	0	2
1	D	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	598	GLU	CG-CD	7.86	1.63	1.51
1	A	598	GLU	CB-CG	7.25	1.66	1.52
1	A	705	CYS	CB-SG	7.23	1.94	1.82
1	B	709	GLU	CB-CG	7.18	1.65	1.52
1	B	1153	GLU	CG-CD	5.90	1.60	1.51
1	D	262	GLU	CB-CG	5.35	1.62	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	774	LEU	CA-CB-CG	7.08	131.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	950	LEU	CA-CB-CG	6.76	130.86	115.30
1	B	35	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	865	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	706	ILE	CB-CA-C	-6.13	99.34	111.60
1	C	299	LEU	CA-CB-CG	5.82	128.68	115.30
1	C	240	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	824	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	293	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	112	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	950	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	744	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	112	LEU	CA-CB-CG	5.41	127.74	115.30
1	D	247	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	189	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	100	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	134	THR	N-CA-C	-5.30	96.70	111.00
1	C	710	PHE	N-CA-CB	-5.29	101.08	110.60
1	D	923	LYS	CD-CE-NZ	5.23	123.72	111.70
1	A	621	ASP	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	797	ARG	Peptide
1	C	980	TYR	Peptide
1	D	860	ASP	Peptide

## 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	8549	0	8404	346	0
1	B	8535	0	8385	367	0
1	C	8605	0	8452	314	0
1	D	8320	0	8233	315	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	34013	0	33474	1333	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 20.

All (1333) 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:798:TRP:HB3	1:A:799:PRO:CD	1.73	1.19
1:C:917:ILE:H	1:C:917:ILE:CD1	1.51	1.18
1:B:36:MET:HE3	1:B:83:MET:HG2	1.21	1.17
1:C:917:ILE:N	1:C:917:ILE:HD13	1.61	1.14
1:B:264:ILE:HG21	1:B:268:VAL:HG13	1.23	1.14
1:A:312:THR:HG22	1:A:338:TRP:HE1	1.12	1.13
1:D:182:MET:HE3	1:D:212:LEU:HB3	1.27	1.13
1:A:917:ILE:HD13	1:A:917:ILE:H	1.02	1.13
1:D:917:ILE:CD1	1:D:917:ILE:H	1.55	1.12
1:D:917:ILE:N	1:D:917:ILE:HD13	1.53	1.12
1:A:264:ILE:HG21	1:A:268:VAL:HG13	1.18	1.11
1:A:798:TRP:HB3	1:A:799:PRO:HD3	1.13	1.10
1:B:965:ILE:HG12	1:B:1125:GLU:HG2	1.30	1.10
1:D:965:ILE:HG12	1:D:1125:GLU:HG2	1.24	1.09
1:D:312:THR:HG22	1:D:338:TRP:HE1	1.13	1.09
1:A:259:LEU:HB3	1:A:767:MET:HE3	1.15	1.09
1:A:259:LEU:HB3	1:A:767:MET:CE	1.83	1.08
1:A:595:VAL:O	1:A:596:LEU:HB2	1.52	1.07
1:B:152:HIS:CD2	1:B:706:ILE:HB	1.91	1.06
1:B:36:MET:CE	1:B:83:MET:HG2	1.86	1.06
1:B:296:LEU:HB3	1:B:297:PRO:HD3	1.34	1.05
1:A:744:LEU:HD22	1:A:798:TRP:CD1	1.95	1.01
1:B:16:GLN:HE22	1:B:799:PRO:CG	1.71	1.01
1:C:965:ILE:HG12	1:C:1125:GLU:HG2	1.43	1.01
1:B:1204:ASP:O	1:B:1221:ARG:NH1	1.93	1.00
1:D:712:PRO:O	1:D:713:GLU:HB3	1.61	1.00
1:B:155:ILE:CG2	1:B:706:ILE:HD12	1.91	1.00
1:A:798:TRP:CB	1:A:799:PRO:HD3	1.92	0.98
1:B:883:SER:HA	1:B:911:GLU:HG2	1.43	0.98
1:B:534:THR:HG22	1:B:573:GLY:HA3	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:PRO:HG3	1:B:800:PHE:CE2	1.98	0.98
1:C:219:HIS:HD2	1:C:254:ARG:HH11	1.02	0.97
1:A:1052:UNK:CB	1:A:1091:LYS:O	2.12	0.97
1:A:982:THR:HB	1:A:983:GLN:HE21	1.25	0.97
1:C:1086:ALA:HA	1:C:1089:ILE:HD12	1.46	0.96
1:B:934:ALA:HB2	1:B:956:LYS:HD2	1.48	0.95
1:A:798:TRP:CB	1:A:799:PRO:CD	2.44	0.95
1:C:917:ILE:H	1:C:917:ILE:HD13	0.78	0.94
1:A:55:LEU:HD12	1:A:55:LEU:H	1.31	0.94
1:B:264:ILE:CG2	1:B:268:VAL:HG13	1.96	0.94
1:A:917:ILE:H	1:A:917:ILE:CD1	1.79	0.93
1:C:708:ARG:HB3	1:C:708:ARG:HH11	1.34	0.92
1:A:264:ILE:CG2	1:A:268:VAL:HG13	1.98	0.92
1:B:592:LEU:O	1:B:595:VAL:O	1.87	0.92
1:B:830:ARG:HG2	1:B:831:LYS:H	1.34	0.92
1:B:16:GLN:HE22	1:B:799:PRO:HG2	1.33	0.91
1:B:325:ASN:HD21	1:B:328:GLY:H	0.97	0.91
1:B:58:GLU:O	1:B:62:SER:HB2	1.71	0.90
1:D:312:THR:HG22	1:D:338:TRP:NE1	1.87	0.90
1:B:296:LEU:HB3	1:B:297:PRO:CD	2.02	0.89
1:A:264:ILE:HG21	1:A:268:VAL:CG1	2.01	0.89
1:A:917:ILE:HD13	1:A:917:ILE:N	1.86	0.89
1:D:152:HIS:CD2	1:D:706:ILE:HB	2.06	0.89
1:B:91:ARG:HA	1:B:94:MET:HG2	1.52	0.89
1:B:220:HIS:HE1	1:B:735:LEU:H	1.19	0.88
1:A:1092:THR:O	1:A:1093:VAL:HG22	1.71	0.88
1:A:96:GLN:H	1:A:96:GLN:HE21	1.20	0.88
1:C:587:LYS:H	1:C:590:GLN:HE21	1.15	0.88
1:D:746:LEU:HD11	1:D:769:LEU:HD22	1.55	0.88
1:A:862:ILE:H	1:A:862:ILE:HD12	1.39	0.88
1:D:135:PRO:HG2	1:D:591:GLN:HE22	1.36	0.88
1:A:132:ALA:O	1:A:137:THR:HG21	1.73	0.88
1:D:917:ILE:H	1:D:917:ILE:HD13	0.74	0.88
1:B:16:GLN:NE2	1:B:799:PRO:HG2	1.89	0.87
1:D:292:PHE:CD1	1:D:544:VAL:HG22	2.09	0.87
1:A:312:THR:CG2	1:A:338:TRP:HE1	1.86	0.87
1:A:887:ASN:HD21	1:A:1195:LYS:HB2	1.38	0.87
1:B:325:ASN:ND2	1:B:328:GLY:H	1.72	0.87
1:B:1216:ARG:O	1:B:1216:ARG:HG3	1.73	0.87
1:B:917:ILE:HD13	1:B:917:ILE:H	1.40	0.86
1:B:36:MET:HE3	1:B:83:MET:CG	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ASN:HD22	1:A:1232:ASN:C	1.79	0.86
1:A:312:THR:HG22	1:A:338:TRP:NE1	1.90	0.86
1:C:264:ILE:HG23	1:C:268:VAL:HG13	1.56	0.86
1:C:708:ARG:NH1	1:C:708:ARG:CB	2.39	0.85
1:D:1192:SER:HB3	1:D:1197:VAL:HG13	1.58	0.85
1:C:969:ARG:HH21	1:C:972:LEU:HD22	1.42	0.85
1:B:689:TYR:HB2	1:B:704:HIS:CD2	2.12	0.84
1:A:744:LEU:HD22	1:A:798:TRP:NE1	1.91	0.84
1:D:152:HIS:HD2	1:D:706:ILE:HB	1.38	0.84
1:C:132:ALA:O	1:C:137:THR:HG21	1.77	0.84
1:C:98:ARG:NH1	1:C:645:SER:O	2.10	0.83
1:B:965:ILE:HG12	1:B:1125:GLU:CG	2.07	0.83
1:C:708:ARG:HH11	1:C:708:ARG:CB	1.91	0.83
1:D:952:LEU:HD11	1:D:1144:VAL:HG21	1.59	0.83
1:B:199:ARG:HG2	1:B:738:PHE:CZ	2.12	0.83
1:C:736:ALA:H	1:C:904:ASN:HD22	1.26	0.83
1:D:687:THR:O	1:D:704:HIS:HB3	1.78	0.83
1:B:325:ASN:HD21	1:B:328:GLY:N	1.75	0.82
1:A:1189:GLY:O	1:A:1200:GLN:HB2	1.79	0.82
1:A:534:THR:HG23	1:A:573:GLY:HA3	1.62	0.82
1:B:531:LYS:HB3	1:B:531:LYS:NZ	1.95	0.82
1:C:838:LYS:HG2	1:C:842:GLU:OE2	1.79	0.82
1:C:220:HIS:HE1	1:C:735:LEU:H	1.25	0.82
1:A:1093:VAL:HB	1:A:1094:ALA:HA	1.60	0.82
1:C:101:ARG:NH1	1:C:134:THR:OG1	2.12	0.82
1:C:708:ARG:HB2	1:C:708:ARG:NH1	1.95	0.82
1:A:706:ILE:HD12	1:A:706:ILE:N	1.92	0.81
1:B:219:HIS:HD2	1:B:254:ARG:HE	1.28	0.81
1:B:264:ILE:HG22	1:B:265:THR:N	1.96	0.81
1:C:219:HIS:CD2	1:C:254:ARG:HH11	1.95	0.81
1:B:152:HIS:HA	1:B:706:ILE:HG13	1.63	0.81
1:C:701:GLU:O	1:C:703:ASN:N	2.13	0.81
1:D:527:THR:HG22	1:D:528:ASP:H	1.46	0.80
1:C:815:VAL:HG11	1:C:830:ARG:NH1	1.97	0.80
1:D:159:THR:HA	1:D:162:GLN:HG3	1.62	0.79
1:C:152:HIS:HD2	1:C:704:HIS:CE1	2.00	0.79
1:D:220:HIS:HE1	1:D:735:LEU:H	1.31	0.79
1:D:352:LYS:HA	1:D:352:LYS:HE2	1.64	0.79
1:C:219:HIS:HD2	1:C:254:ARG:NH1	1.80	0.79
1:A:309:LEU:O	1:A:312:THR:HB	1.83	0.78
1:C:221:PHE:HB3	1:C:250:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:MET:HA	1:C:97:GLN:HE21	1.49	0.78
1:D:311:GLN:HA	1:D:311:GLN:OE1	1.83	0.78
1:A:945:ASN:ND2	1:A:1143:LYS:H	1.82	0.78
1:A:687:THR:O	1:A:704:HIS:HB3	1.84	0.78
1:A:844:LYS:HB2	1:A:862:ILE:HD13	1.64	0.78
1:D:299:LEU:HD22	1:D:309:LEU:HD11	1.64	0.78
1:B:534:THR:HG22	1:B:573:GLY:CA	2.14	0.78
1:D:1235:ASP:O	1:D:1237:GLN:HG3	1.84	0.77
1:B:1114:LEU:HB3	1:B:1118:SER:HB3	1.64	0.77
1:D:850:ASN:O	1:D:854:THR:HB	1.85	0.77
1:A:1196:ASN:H	1:A:1196:ASN:ND2	1.83	0.77
1:B:300:HIS:HB2	1:B:360:PHE:HZ	1.48	0.77
1:D:969:ARG:HD2	1:D:1121:ALA:HB3	1.67	0.77
1:A:133:ILE:HG23	1:A:140:MET:HE3	1.66	0.77
1:B:595:VAL:O	1:B:596:LEU:HB2	1.83	0.77
1:B:155:ILE:HG21	1:B:706:ILE:HD12	1.66	0.77
1:B:16:GLN:HE22	1:B:799:PRO:HG3	1.49	0.77
1:A:264:ILE:O	1:A:266:ASP:N	2.17	0.77
1:D:676:ASP:HB2	1:D:711:ILE:HG22	1.66	0.76
1:D:91:ARG:HA	1:D:94:MET:HG2	1.66	0.76
1:A:366:ASN:O	1:A:370:GLU:HG3	1.86	0.76
1:D:595:VAL:O	1:D:596:LEU:HB3	1.84	0.76
1:A:963:PRO:HD3	1:A:1129:TYR:CZ	2.20	0.76
1:C:264:ILE:CG2	1:C:268:VAL:HG13	2.16	0.76
1:D:266:ASP:O	1:D:267:SER:HB3	1.84	0.76
1:B:16:GLN:NE2	1:B:799:PRO:CG	2.47	0.76
1:B:706:ILE:N	1:B:706:ILE:HD13	1.98	0.76
1:D:292:PHE:HD1	1:D:544:VAL:HG22	1.51	0.76
1:D:264:ILE:HG22	1:D:265:THR:N	2.01	0.75
1:A:407:THR:HG22	1:A:408:SER:H	1.49	0.75
1:A:543:TRP:CD1	1:A:553:PRO:HG2	2.22	0.75
1:C:938:GLU:HB2	1:C:1182:HIS:NE2	2.02	0.75
1:B:963:PRO:HD3	1:B:1129:TYR:CZ	2.22	0.75
1:C:961:ALA:O	1:C:1129:TYR:OH	2.04	0.74
1:D:395:LYS:HB3	1:D:396:PRO:HD3	1.68	0.74
1:B:155:ILE:HB	1:B:706:ILE:CD1	2.17	0.74
1:D:303:LYS:HE3	1:D:356:ASP:HA	1.68	0.74
1:A:982:THR:HB	1:A:983:GLN:NE2	2.03	0.74
1:B:220:HIS:CE1	1:B:735:LEU:H	2.03	0.74
1:B:945:ASN:ND2	1:B:1143:LYS:H	1.86	0.74
1:B:152:HIS:HD2	1:B:704:HIS:CE1	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:ASP:O	1:A:1221:ARG:NH1	2.20	0.73
1:B:98:ARG:HG2	1:B:595:VAL:HA	1.69	0.73
1:C:534:THR:HG22	1:C:573:GLY:HA3	1.70	0.73
1:D:391:ILE:HG22	1:D:436:PHE:HE1	1.53	0.73
1:A:627:VAL:HG11	1:A:642:VAL:HG12	1.69	0.73
1:C:398:LEU:HD13	1:C:442:LEU:HD21	1.71	0.73
1:B:155:ILE:CG2	1:B:706:ILE:CD1	2.66	0.73
1:A:36:MET:HG3	1:A:39:ILE:HD12	1.70	0.72
1:D:1175:ASP:O	1:D:1175:ASP:OD1	2.07	0.72
1:A:712:PRO:O	1:A:713:GLU:CB	2.37	0.72
1:A:927:VAL:HG23	1:A:939:ALA:HB3	1.69	0.72
1:C:515:TYR:O	1:C:519:LYS:HG2	1.89	0.72
1:A:1212:ASN:ND2	1:A:1215:GLY:H	1.86	0.72
1:B:264:ILE:HG21	1:B:268:VAL:CG1	2.13	0.72
1:B:312:THR:HG23	1:B:341:TYR:HB3	1.71	0.72
1:D:317:LEU:HA	1:D:320:MET:HE1	1.72	0.72
1:A:595:VAL:O	1:A:596:LEU:CB	2.32	0.72
1:B:155:ILE:HD11	1:B:166:VAL:HG21	1.71	0.72
1:C:152:HIS:HA	1:C:706:ILE:HG12	1.72	0.72
1:D:418:PHE:HB3	1:D:455:PHE:HB2	1.71	0.72
1:D:746:LEU:CD1	1:D:769:LEU:HD22	2.20	0.72
1:B:300:HIS:HB2	1:B:360:PHE:CZ	2.24	0.72
1:C:248:LEU:HD23	1:C:249:HIS:N	2.05	0.72
1:D:173:VAL:HG21	1:D:676:ASP:OD1	1.90	0.72
1:D:395:LYS:HB3	1:D:396:PRO:CD	2.20	0.72
1:A:1232:ASN:HD22	1:A:1233:LEU:N	1.88	0.71
1:A:965:ILE:HG12	1:A:1125:GLU:HB3	1.70	0.71
1:C:840:PHE:HD2	1:C:841:ARG:HE	1.36	0.71
1:D:105:ALA:HB1	1:D:599:ARG:HD2	1.70	0.71
1:A:259:LEU:CB	1:A:767:MET:CE	2.67	0.71
1:D:391:ILE:HG22	1:D:436:PHE:CE1	2.24	0.71
1:A:1237:GLN:O	1:A:1238:LEU:HD23	1.90	0.71
1:B:391:ILE:HD11	1:B:485:UNK:O	1.89	0.71
1:C:312:THR:HG22	1:C:338:TRP:CD1	2.26	0.71
1:C:342:LEU:HB3	1:C:567:ILE:HG21	1.72	0.71
1:B:918:ASN:HD22	1:B:918:ASN:H	1.37	0.71
1:A:584:GLN:HG2	1:A:585:PRO:HD2	1.72	0.70
1:C:883:SER:HA	1:C:911:GLU:HG2	1.71	0.70
1:B:872:ASN:HD22	1:B:887:ASN:HD22	1.39	0.70
1:A:96:GLN:N	1:A:96:GLN:HE21	1.87	0.70
1:C:96:GLN:NE2	1:C:100:ARG:HH21	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:THR:CG2	1:A:573:GLY:HA3	2.21	0.70
1:B:691:THR:HG22	1:B:699:ASP:OD1	1.92	0.70
1:D:195:ASN:HD22	1:D:196:PRO:HD2	1.55	0.70
1:B:830:ARG:HG2	1:B:831:LYS:N	2.07	0.70
1:A:1196:ASN:H	1:A:1196:ASN:HD22	1.39	0.70
1:D:729:LYS:NZ	1:D:904:ASN:HD21	1.89	0.70
1:A:530:LEU:O	1:A:534:THR:HB	1.92	0.70
1:A:798:TRP:CE3	1:A:799:PRO:HD3	2.27	0.70
1:C:768:VAL:CG1	1:C:858:LEU:HD22	2.22	0.70
1:D:574:ILE:HD12	1:D:574:ILE:O	1.91	0.70
1:B:96:GLN:NE2	1:B:100:ARG:HH21	1.89	0.69
1:D:595:VAL:O	1:D:596:LEU:CB	2.40	0.69
1:C:516:TYR:CE2	1:C:533:MET:HE1	2.27	0.69
1:D:276:ARG:HH12	1:D:326:GLU:HA	1.55	0.69
1:D:756:VAL:HG23	1:D:853:ARG:HG2	1.73	0.69
1:A:417:ILE:HG12	1:A:454:TYR:CD1	2.27	0.69
1:D:1138:GLN:HG2	1:D:1138:GLN:O	1.91	0.69
1:D:16:GLN:HE22	1:D:799:PRO:HG3	1.57	0.69
1:C:152:HIS:HE1	1:C:708:ARG:HG2	1.56	0.69
1:C:593:MET:HB3	1:C:652:LEU:HD11	1.74	0.69
1:D:342:LEU:O	1:D:345:PHE:HB3	1.93	0.69
1:C:815:VAL:HG11	1:C:830:ARG:HH11	1.56	0.69
1:A:534:THR:CG2	1:A:573:GLY:CA	2.71	0.69
1:C:979:PHE:HD2	1:C:1039:UNK:CB	2.06	0.69
1:C:706:ILE:HD12	1:C:706:ILE:N	2.08	0.69
1:D:676:ASP:HB2	1:D:711:ILE:CG2	2.22	0.69
1:A:414:ASP:OD1	1:C:1143:LYS:NZ	2.25	0.69
1:A:648:ASP:OD1	1:A:651:ARG:HB2	1.93	0.69
1:B:917:ILE:HD13	1:B:917:ILE:N	2.07	0.69
1:D:1107:VAL:HG13	1:D:1108:SER:O	1.93	0.68
1:A:1212:ASN:HD22	1:A:1215:GLY:H	1.40	0.68
1:D:691:THR:HG22	1:D:699:ASP:OD2	1.94	0.68
1:C:768:VAL:HG11	1:C:858:LEU:HD22	1.74	0.68
1:D:312:THR:HG21	1:D:342:LEU:HD23	1.74	0.68
1:D:712:PRO:O	1:D:713:GLU:CB	2.39	0.68
1:A:1105:VAL:HG12	1:A:1105:VAL:O	1.93	0.68
1:A:58:GLU:OE1	1:A:695:GLY:HA3	1.93	0.68
1:C:155:ILE:HB	1:C:706:ILE:HG13	1.76	0.68
1:C:137:THR:HG22	1:C:140:MET:H	1.58	0.68
1:D:16:GLN:NE2	1:D:799:PRO:HG3	2.08	0.68
1:C:134:THR:O	1:C:140:MET:HG3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:NZ	1:C:165:LYS:CB	2.57	0.68
1:C:16:GLN:NE2	1:C:799:PRO:HG3	2.09	0.68
1:C:514:GLN:O	1:C:517:LYS:HB3	1.93	0.68
1:D:101:ARG:NH2	1:D:134:THR:HG23	2.09	0.68
1:C:1181:LEU:O	1:C:1182:HIS:HB2	1.92	0.67
1:C:220:HIS:CE1	1:C:735:LEU:H	2.11	0.67
1:C:155:ILE:HB	1:C:706:ILE:CG1	2.23	0.67
1:A:188:ILE:HG13	1:A:189:ARG:N	2.09	0.67
1:C:831:LYS:O	1:C:833:GLN:N	2.22	0.67
1:D:146:ASN:O	1:D:149:TYR:HB3	1.94	0.67
1:C:1213:PHE:O	1:C:1216:ARG:NH1	2.28	0.67
1:A:627:VAL:HG11	1:A:642:VAL:CG1	2.24	0.67
1:A:307:PRO:HG2	1:A:764:GLN:HG2	1.76	0.67
1:B:828:ILE:HG22	1:B:828:ILE:O	1.94	0.67
1:C:1169:ARG:HH11	1:C:1186:THR:HG23	1.60	0.67
1:B:1115:THR:OG1	1:B:1118:SER:HB2	1.95	0.67
1:C:837:ARG:HD3	1:C:841:ARG:HH22	1.58	0.67
1:D:152:HIS:HE1	1:D:708:ARG:HE	1.43	0.67
1:D:1107:VAL:HG22	1:D:1108:SER:H	1.60	0.67
1:D:664:SER:HB2	1:D:667:GLU:HB2	1.75	0.67
1:A:185:ILE:O	1:A:189:ARG:HG2	1.94	0.66
1:C:300:HIS:HB3	1:C:303:LYS:HB2	1.75	0.66
1:A:259:LEU:CB	1:A:767:MET:HE3	2.10	0.66
1:A:1093:VAL:CB	1:A:1094:ALA:HA	2.26	0.66
1:B:342:LEU:O	1:B:345:PHE:HB3	1.95	0.66
1:C:1102:LYS:HB2	1:C:1103:PRO:HD3	1.77	0.66
1:C:587:LYS:H	1:C:590:GLN:NE2	1.91	0.66
1:A:250:LEU:O	1:A:254:ARG:HG3	1.94	0.66
1:A:407:THR:HG22	1:A:408:SER:N	2.09	0.66
1:C:1038:UNK:O	1:C:1039:UNK:CB	2.44	0.66
1:D:137:THR:HG22	1:D:138:GLU:H	1.60	0.66
1:B:54:ARG:HD2	1:B:128:PHE:N	2.10	0.66
1:C:706:ILE:HG22	1:C:707:GLU:N	2.11	0.66
1:C:958:SER:HB2	1:C:1134:ASP:OD1	1.96	0.66
1:C:152:HIS:CE1	1:C:708:ARG:HG2	2.31	0.66
1:C:969:ARG:HH21	1:C:972:LEU:CD2	2.09	0.66
1:D:182:MET:CE	1:D:212:LEU:HB3	2.17	0.66
1:A:320:MET:HE3	1:A:322:GLY:O	1.94	0.66
1:B:641:VAL:HG12	1:B:642:VAL:H	1.61	0.66
1:D:10:ILE:HD13	1:D:14:TRP:HZ3	1.61	0.66
1:A:621:ASP:O	1:A:622:PHE:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LYS:HD2	1:B:566:ARG:HG3	1.77	0.66
1:D:91:ARG:HA	1:D:94:MET:CG	2.25	0.65
1:D:317:LEU:HA	1:D:320:MET:CE	2.26	0.65
1:B:284:VAL:HG13	1:B:338:TRP:CZ2	2.31	0.65
1:D:221:PHE:HB3	1:D:250:LEU:HD12	1.77	0.65
1:D:299:LEU:HD22	1:D:309:LEU:CD1	2.26	0.65
1:A:134:THR:HG22	1:A:135:PRO:HD2	1.78	0.65
1:A:798:TRP:HA	1:A:801:LEU:HD21	1.78	0.65
1:A:113:GLN:HA	1:A:113:GLN:HE21	1.61	0.65
1:A:798:TRP:O	1:A:800:PHE:N	2.30	0.65
1:A:592:LEU:HD22	1:A:596:LEU:HD12	1.78	0.65
1:B:665:PRO:HA	1:B:668:LYS:HB2	1.79	0.65
1:C:401:THR:HG22	1:C:457:LEU:HD22	1.79	0.65
1:D:946:SER:HB3	1:D:948:THR:H	1.61	0.65
1:D:1232:ASN:C	1:D:1232:ASN:HD22	1.99	0.65
1:A:1232:ASN:ND2	1:A:1232:ASN:C	2.47	0.64
1:A:606:VAL:O	1:A:607:VAL:HG23	1.97	0.64
1:C:606:VAL:O	1:C:608:TYR:N	2.30	0.64
1:D:276:ARG:HH12	1:D:326:GLU:HG3	1.62	0.64
1:A:826:LYS:HG3	1:A:827:VAL:N	2.12	0.64
1:C:1173:ILE:HG13	1:C:1231:LEU:HB2	1.78	0.64
1:A:854:THR:HG22	1:A:855:LYS:HG2	1.78	0.64
1:B:159:THR:OG1	1:B:1175:ASP:HB3	1.97	0.64
1:B:798:TRP:O	1:B:799:PRO:C	2.32	0.64
1:C:1234:SER:O	1:C:1235:ASP:HB3	1.97	0.64
1:B:933:TYR:CE1	1:B:956:LYS:HD3	2.31	0.64
1:A:712:PRO:O	1:A:713:GLU:HB2	1.98	0.64
1:C:688:VAL:HG13	1:C:701:GLU:HA	1.80	0.64
1:C:155:ILE:CG2	1:C:706:ILE:HG13	2.28	0.64
1:B:1182:HIS:O	1:B:1183:SER:C	2.36	0.64
1:A:1122:VAL:HG12	1:A:1202:LEU:HD13	1.78	0.63
1:C:840:PHE:O	1:C:844:LYS:HB2	1.98	0.63
1:A:58:GLU:HG3	1:A:59:GLU:N	2.13	0.63
1:B:458:ASP:OD1	1:B:461:SER:HB3	1.98	0.63
1:D:1207:ILE:HG22	1:D:1209:ALA:H	1.63	0.63
1:C:307:PRO:HG2	1:C:764:GLN:HG2	1.79	0.63
1:B:155:ILE:HG22	1:B:706:ILE:CD1	2.28	0.63
1:A:1193:ILE:HD12	1:A:1193:ILE:H	1.61	0.63
1:A:797:ARG:O	1:A:798:TRP:C	2.37	0.63
1:A:922:PRO:O	1:A:925:SER:HB3	1.98	0.63
1:A:592:LEU:O	1:A:595:VAL:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:GLU:O	1:B:199:ARG:HD2	1.98	0.62
1:B:298:ASP:HB3	1:B:300:HIS:HE1	1.64	0.62
1:B:155:ILE:HG22	1:B:706:ILE:HD12	1.78	0.62
1:A:111:ALA:O	1:A:112:LEU:C	2.37	0.62
1:B:1137:GLU:HG2	1:B:1138:GLN:H	1.64	0.62
1:A:169:SER:CB	1:A:676:ASP:OD1	2.47	0.62
1:B:417:ILE:HG13	1:B:454:TYR:CD1	2.33	0.62
1:A:1235:ASP:O	1:A:1237:GLN:HG3	1.99	0.62
1:B:335:PHE:CD1	1:B:335:PHE:O	2.53	0.62
1:C:1189:GLY:O	1:C:1200:GLN:HB2	2.00	0.62
1:B:278:LEU:O	1:B:282:ILE:HD12	2.00	0.62
1:D:512:LYS:O	1:D:516:TYR:CD1	2.52	0.62
1:A:461:SER:O	1:A:462:ILE:HG13	1.99	0.62
1:A:744:LEU:HD21	1:A:897:LEU:HA	1.81	0.62
1:B:881:SER:HB3	1:B:914:PRO:HD3	1.81	0.62
1:A:365:GLU:OE1	1:A:369:LEU:HG	2.00	0.62
1:C:708:ARG:CZ	1:C:708:ARG:HB2	2.29	0.62
1:B:202:ILE:HG21	1:B:209:LEU:HD22	1.80	0.61
1:D:1111:SER:HB3	1:D:1191:THR:HA	1.82	0.61
1:A:430:LEU:O	1:A:434:LYS:HG3	2.00	0.61
1:A:982:THR:CB	1:A:983:GLN:HE21	2.08	0.61
1:D:1118:SER:O	1:D:1122:VAL:HG23	2.00	0.61
1:C:539:GLY:HA2	1:C:578:ILE:HD13	1.83	0.61
1:D:512:LYS:O	1:D:516:TYR:HD1	1.82	0.61
1:D:957:GLY:HA2	1:D:1136:SER:HB2	1.82	0.61
1:C:1160:ARG:HG3	1:C:1227:SER:OG	2.00	0.61
1:D:293:LEU:HD21	1:D:540:GLY:HA3	1.81	0.61
1:A:1093:VAL:HB	1:A:1094:ALA:CA	2.29	0.61
1:B:22:ASP:OD2	1:B:22:ASP:C	2.39	0.61
1:D:715:MET:O	1:D:716:GLU:HB2	2.01	0.61
1:A:1191:THR:O	1:A:1191:THR:HG22	2.00	0.61
1:A:7:PHE:O	1:A:10:ILE:HG22	2.00	0.61
1:D:169:SER:OG	1:D:180:LYS:HD3	1.99	0.61
1:D:534:THR:HG22	1:D:573:GLY:HA3	1.83	0.61
1:A:826:LYS:HG3	1:A:827:VAL:H	1.65	0.61
1:D:212:LEU:HD21	1:D:548:TYR:CD1	2.36	0.61
1:A:134:THR:CG2	1:A:135:PRO:HD2	2.30	0.60
1:A:293:LEU:HD11	1:A:540:GLY:HA3	1.82	0.60
1:D:962:GLU:HG3	1:D:1169:ARG:HE	1.66	0.60
1:A:928:VAL:HG21	1:A:1173:ILE:HG23	1.82	0.60
1:A:706:ILE:CD1	1:A:706:ILE:N	2.62	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:TRP:O	1:A:799:PRO:C	2.38	0.60
1:B:798:TRP:HB3	1:B:799:PRO:HD3	1.83	0.60
1:C:33:TYR:OH	1:C:200:HIS:HD2	1.83	0.60
1:C:798:TRP:O	1:C:799:PRO:C	2.38	0.60
1:C:917:ILE:HG13	1:C:947:GLU:O	2.00	0.60
1:D:701:GLU:C	1:D:703:ASN:N	2.53	0.60
1:C:290:ASN:HD22	1:C:292:PHE:H	1.48	0.60
1:C:91:ARG:HA	1:C:94:MET:HG3	1.83	0.60
1:D:565:PRO:O	1:D:566:ARG:HG2	2.00	0.60
1:B:58:GLU:OE2	1:B:695:GLY:HA3	2.01	0.60
1:B:588:PRO:HD2	1:B:671:ASN:O	2.01	0.60
1:C:949:ARG:HE	1:C:1145:PRO:HB3	1.67	0.60
1:D:441:GLY:HA2	1:D:462:ILE:HD13	1.84	0.60
1:B:312:THR:HG22	1:B:338:TRP:HE1	1.66	0.60
1:D:701:GLU:C	1:D:703:ASN:H	2.05	0.60
1:C:325:ASN:HD21	1:C:328:GLY:H	1.46	0.60
1:A:156:THR:HG23	1:A:703:ASN:O	2.01	0.60
1:C:111:ALA:O	1:C:113:GLN:N	2.34	0.60
1:C:293:LEU:HD21	1:C:540:GLY:HA3	1.84	0.60
1:C:152:HIS:O	1:C:706:ILE:HD13	2.01	0.60
1:B:1118:SER:O	1:B:1122:VAL:HG23	2.02	0.60
1:D:1196:ASN:ND2	1:D:1226:ASP:OD2	2.29	0.60
1:B:965:ILE:CG1	1:B:1125:GLU:HG2	2.19	0.60
1:B:297:PRO:HG2	1:B:298:ASP:H	1.67	0.60
1:D:22:ASP:OD2	1:D:24:SER:HB3	2.02	0.60
1:D:299:LEU:CD2	1:D:309:LEU:HD11	2.32	0.60
1:A:535:GLU:HG2	1:A:576:GLN:CD	2.22	0.59
1:B:114:LYS:NZ	1:B:114:LYS:HB2	2.17	0.59
1:B:949:ARG:HD2	1:B:1143:LYS:O	2.02	0.59
1:D:159:THR:HG23	1:D:1175:ASP:OD1	2.02	0.59
1:D:334:ARG:HA	1:D:337:ILE:HD12	1.84	0.59
1:A:446:HIS:CE1	1:A:450:LYS:HE3	2.36	0.59
1:B:152:HIS:CD2	1:B:704:HIS:CE1	2.90	0.59
1:C:357:VAL:O	1:C:361:ASN:ND2	2.33	0.59
1:C:963:PRO:HD3	1:C:1129:TYR:CZ	2.37	0.59
1:B:949:ARG:HG2	1:B:949:ARG:HH11	1.66	0.59
1:C:691:THR:HG22	1:C:699:ASP:OD1	2.02	0.59
1:B:152:HIS:HD2	1:B:706:ILE:HB	1.62	0.59
1:D:715:MET:O	1:D:716:GLU:CB	2.50	0.59
1:B:533:MET:HA	1:B:561:TYR:CE2	2.37	0.59
1:C:312:THR:HG22	1:C:338:TRP:NE1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:THR:CG2	1:D:338:TRP:NE1	2.63	0.59
1:C:248:LEU:C	1:C:248:LEU:HD23	2.23	0.59
1:D:412:ASP:HB2	1:D:459:LEU:HD22	1.85	0.59
1:A:336:SER:HA	1:A:339:LEU:HB2	1.84	0.59
1:A:505:SER:HB3	1:A:508:PHE:HB2	1.84	0.59
1:D:701:GLU:O	1:D:703:ASN:N	2.36	0.59
1:C:398:LEU:O	1:C:402:VAL:HB	2.03	0.59
1:C:152:HIS:O	1:C:706:ILE:CD1	2.50	0.59
1:D:6:PHE:CE1	1:D:10:ILE:CD1	2.86	0.59
1:A:137:THR:HG22	1:A:140:MET:H	1.68	0.58
1:A:831:LYS:H	1:A:831:LYS:HD2	1.68	0.58
1:B:155:ILE:CB	1:B:706:ILE:CD1	2.81	0.58
1:C:969:ARG:NH2	1:C:972:LEU:HD22	2.14	0.58
1:C:540:GLY:HA2	1:C:557:TRP:CH2	2.39	0.58
1:A:729:LYS:HB3	1:A:733:SER:O	2.03	0.58
1:B:774:LEU:H	1:B:774:LEU:HD12	1.68	0.58
1:D:929:PHE:HB2	1:D:939:ALA:HB2	1.85	0.58
1:A:798:TRP:CG	1:A:799:PRO:HD3	2.38	0.58
1:D:56:SER:HB3	1:D:59:GLU:HB2	1.84	0.58
1:B:1193:ILE:O	1:B:1193:ILE:CG2	2.50	0.58
1:B:649:GLN:O	1:B:653:VAL:HG23	2.02	0.58
1:C:156:THR:N	1:C:706:ILE:HD11	2.17	0.58
1:D:171:HIS:CE1	1:D:172:GLU:OE2	2.57	0.58
1:A:798:TRP:HA	1:A:801:LEU:CD2	2.33	0.58
1:B:152:HIS:HA	1:B:706:ILE:CG1	2.33	0.58
1:D:101:ARG:HH21	1:D:134:THR:HG23	1.68	0.58
1:D:173:VAL:HG12	1:D:180:LYS:HE2	1.84	0.58
1:D:262:GLU:HG2	1:D:263:GLU:N	2.17	0.58
1:D:3:ILE:HB	1:D:6:PHE:HB2	1.84	0.58
1:A:91:ARG:O	1:A:93:LYS:N	2.36	0.58
1:B:195:ASN:ND2	1:B:197:ASN:H	2.02	0.58
1:C:93:LYS:NZ	1:C:100:ARG:HH22	2.02	0.58
1:D:16:GLN:HE21	1:D:855:LYS:HD2	1.69	0.58
1:C:219:HIS:CE1	1:C:251:SER:HB2	2.39	0.58
1:C:514:GLN:HE22	1:C:517:LYS:NZ	2.02	0.58
1:D:687:THR:O	1:D:704:HIS:CB	2.51	0.58
1:D:91:ARG:HG2	1:D:558:TYR:HB3	1.84	0.58
1:D:210:ILE:HA	1:D:223:LEU:CD1	2.34	0.57
1:A:534:THR:HG23	1:A:573:GLY:CA	2.32	0.57
1:D:357:VAL:HG12	1:D:361:ASN:HD21	1.68	0.57
1:D:946:SER:HB3	1:D:949:ARG:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ASN:O	1:A:854:THR:HB	2.05	0.57
1:B:744:LEU:HD13	1:B:899:VAL:HG22	1.86	0.57
1:C:918:ASN:HA	1:C:944:TYR:CZ	2.40	0.57
1:D:706:ILE:HD13	1:D:706:ILE:N	2.19	0.57
1:D:220:HIS:CE1	1:D:735:LEU:H	2.19	0.57
1:D:747:THR:HG22	1:D:770:HIS:HB2	1.86	0.57
1:A:152:HIS:HD2	1:A:704:HIS:NE2	2.03	0.57
1:B:677:LEU:HD13	1:B:708:ARG:HH11	1.69	0.57
1:C:512:LYS:C	1:C:514:GLN:H	2.08	0.57
1:D:154:LYS:HE2	1:D:158:ASP:CB	2.35	0.57
1:B:264:ILE:O	1:B:266:ASP:N	2.35	0.57
1:B:155:ILE:CB	1:B:706:ILE:HD12	2.34	0.57
1:C:1232:ASN:ND2	1:C:1234:SER:O	2.38	0.57
1:C:165:LYS:HZ2	1:C:165:LYS:HB2	1.69	0.57
1:C:256:TYR:HA	1:C:259:LEU:HD12	1.85	0.57
1:D:159:THR:HA	1:D:162:GLN:CG	2.34	0.57
1:D:705:CYS:C	1:D:706:ILE:HD13	2.25	0.57
1:D:969:ARG:HD2	1:D:1121:ALA:CB	2.33	0.57
1:B:315:GLU:HB3	1:B:341:TYR:CZ	2.40	0.56
1:C:165:LYS:NZ	1:C:165:LYS:HB3	2.20	0.56
1:C:390:LEU:O	1:C:394:VAL:HG23	2.05	0.56
1:D:76:LYS:HD3	1:D:160:ARG:CZ	2.35	0.56
1:C:354:ASP:OD1	1:C:354:ASP:N	2.38	0.56
1:D:33:TYR:OH	1:D:200:HIS:HD2	1.88	0.56
1:C:1102:LYS:CB	1:C:1103:PRO:HD3	2.34	0.56
1:C:516:TYR:HE2	1:C:533:MET:HE1	1.68	0.56
1:C:677:LEU:HD22	1:C:708:ARG:HH12	1.71	0.56
1:D:534:THR:HG22	1:D:573:GLY:CA	2.36	0.56
1:B:296:LEU:CB	1:B:297:PRO:CD	2.81	0.56
1:B:298:ASP:HB3	1:B:300:HIS:CE1	2.40	0.56
1:C:729:LYS:HD2	1:C:735:LEU:HD13	1.88	0.56
1:D:276:ARG:NH1	1:D:326:GLU:HA	2.20	0.56
1:A:535:GLU:HG2	1:A:576:GLN:OE1	2.06	0.56
1:B:960:ARG:NH2	1:B:1133:PRO:O	2.24	0.56
1:A:533:MET:HE3	1:A:565:PRO:HB3	1.87	0.56
1:B:312:THR:HG22	1:B:338:TRP:NE1	2.21	0.56
1:C:917:ILE:CD1	1:C:947:GLU:O	2.54	0.56
1:A:416:GLU:HB2	1:C:951:LYS:NZ	2.20	0.56
1:D:933:TYR:CE1	1:D:1139:LYS:HE2	2.41	0.56
1:D:945:ASN:OD1	1:D:951:LYS:HD2	2.05	0.56
1:A:826:LYS:CG	1:A:827:VAL:H	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:GLY:O	1:B:1186:THR:HG23	2.06	0.56
1:B:443:ILE:HG13	1:B:458:ASP:HB2	1.87	0.56
1:A:155:ILE:HB	1:A:706:ILE:HG13	1.87	0.56
1:B:531:LYS:HB3	1:B:531:LYS:HZ2	1.66	0.56
1:B:626:GLU:O	1:B:627:VAL:HG23	2.06	0.56
1:C:873:GLY:HA2	1:C:909:TYR:HE2	1.70	0.56
1:D:945:ASN:ND2	1:D:1143:LYS:H	2.04	0.56
1:A:786:ALA:O	1:A:790:MET:HB2	2.06	0.55
1:A:918:ASN:HD22	1:A:918:ASN:H	1.55	0.55
1:B:1109:LEU:O	1:B:1110:GLU:HG2	2.05	0.55
1:B:290:ASN:ND2	1:B:290:ASN:N	2.51	0.55
1:B:785:LEU:HD23	1:B:789:HIS:HD2	1.71	0.55
1:C:58:GLU:O	1:C:62:SER:HB2	2.06	0.55
1:C:307:PRO:CG	1:C:764:GLN:HG2	2.36	0.55
1:D:1212:ASN:HD22	1:D:1215:GLY:H	1.52	0.55
1:A:312:THR:CG2	1:A:338:TRP:NE1	2.56	0.55
1:A:512:LYS:HG2	1:A:566:ARG:HG3	1.88	0.55
1:A:708:ARG:HB2	1:A:708:ARG:HH11	1.70	0.55
1:B:152:HIS:CD2	1:B:704:HIS:NE2	2.75	0.55
1:C:1189:GLY:O	1:C:1200:GLN:CB	2.54	0.55
1:D:704:HIS:CE1	1:D:706:ILE:H	2.24	0.55
1:A:91:ARG:C	1:A:93:LYS:H	2.10	0.55
1:D:770:HIS:CE1	1:D:858:LEU:CD2	2.90	0.55
1:A:1193:ILE:HD12	1:A:1193:ILE:N	2.20	0.55
1:C:543:TRP:CD1	1:C:553:PRO:HG2	2.41	0.55
1:D:1173:ILE:HG13	1:D:1231:LEU:HB2	1.89	0.55
1:D:137:THR:HG22	1:D:138:GLU:N	2.21	0.55
1:A:864:ALA:HB3	1:A:895:LEU:HD12	1.89	0.55
1:C:36:MET:HE2	1:C:39:ILE:HD12	1.88	0.55
1:C:540:GLY:HA2	1:C:557:TRP:CZ2	2.42	0.55
1:C:593:MET:HG3	1:C:656:MET:SD	2.47	0.55
1:C:918:ASN:HA	1:C:944:TYR:OH	2.07	0.55
1:C:135:PRO:HB3	1:C:171:HIS:HB2	1.89	0.55
1:A:1174:GLN:HA	1:A:1174:GLN:OE1	2.06	0.55
1:A:1191:THR:CG2	1:A:1191:THR:O	2.55	0.55
1:A:219:HIS:HD2	1:A:254:ARG:NH1	2.05	0.55
1:A:55:LEU:CD1	1:A:55:LEU:H	2.07	0.55
1:B:602:ASN:OD1	1:B:602:ASN:N	2.39	0.55
1:B:705:CYS:C	1:B:706:ILE:HD13	2.27	0.55
1:C:325:ASN:ND2	1:C:328:GLY:H	2.05	0.55
1:D:195:ASN:HB3	1:D:198:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PHE:HA	1:A:597:PRO:HG3	1.88	0.55
1:A:158:ASP:OD1	1:A:1176:SER:HB2	2.07	0.55
1:C:165:LYS:HZ3	1:C:165:LYS:HB3	1.72	0.55
1:C:312:THR:HG23	1:C:341:TYR:HB2	1.87	0.55
1:A:262:GLU:O	1:A:264:ILE:N	2.40	0.54
1:D:390:LEU:HD11	1:D:455:PHE:HE1	1.72	0.54
1:C:965:ILE:CG1	1:C:1125:GLU:HG2	2.30	0.54
1:D:58:GLU:HG2	1:D:59:GLU:N	2.22	0.54
1:A:152:HIS:HA	1:A:706:ILE:HG12	1.88	0.54
1:A:816:TYR:N	1:A:816:TYR:CD1	2.74	0.54
1:B:927:VAL:HG21	1:B:1149:ILE:HG13	1.88	0.54
1:B:933:TYR:CE2	1:B:1139:LYS:HB2	2.43	0.54
1:B:182:MET:HE3	1:B:185:ILE:HD12	1.88	0.54
1:B:214:LEU:CD2	1:B:250:LEU:HD22	2.37	0.54
1:B:531:LYS:HB3	1:B:531:LYS:HZ3	1.71	0.54
1:B:330:ILE:N	1:B:542:GLN:OE1	2.37	0.54
1:B:559:TYR:OH	1:B:565:PRO:HD3	2.07	0.54
1:D:871:VAL:HG22	1:D:886:PHE:CE2	2.43	0.54
1:A:969:ARG:HH11	1:A:972:LEU:HD22	1.72	0.54
1:B:626:GLU:O	1:B:627:VAL:CG2	2.55	0.54
1:A:219:HIS:CE1	1:A:251:SER:HB2	2.42	0.54
1:A:676:ASP:CB	1:A:711:ILE:HG22	2.38	0.54
1:B:309:LEU:O	1:B:312:THR:HB	2.08	0.54
1:B:516:TYR:CE2	1:B:533:MET:CE	2.91	0.54
1:D:93:LYS:HB3	1:D:97:GLN:NE2	2.23	0.54
1:A:741:LEU:HD22	1:A:769:LEU:HD11	1.90	0.54
1:D:155:ILE:HB	1:D:706:ILE:HG13	1.90	0.54
1:A:887:ASN:HD21	1:A:1195:LYS:CB	2.16	0.54
1:B:1193:ILE:O	1:B:1193:ILE:HG22	2.07	0.54
1:B:304:GLY:O	1:B:307:PRO:HD2	2.08	0.54
1:B:918:ASN:H	1:B:918:ASN:ND2	2.05	0.54
1:C:833:GLN:HG3	1:C:833:GLN:O	2.08	0.54
1:A:417:ILE:HD13	1:C:946:SER:HA	1.89	0.54
1:A:1173:ILE:HG13	1:A:1231:LEU:HB2	1.90	0.53
1:A:91:ARG:HA	1:A:94:MET:HG3	1.90	0.53
1:B:801:LEU:HD11	1:B:899:VAL:HG21	1.90	0.53
1:D:704:HIS:ND1	1:D:705:CYS:N	2.56	0.53
1:B:290:ASN:HD22	1:B:290:ASN:N	2.07	0.53
1:B:537:TYR:O	1:B:540:GLY:N	2.41	0.53
1:B:330:ILE:HD12	1:B:542:GLN:HG2	1.90	0.53
1:C:587:LYS:N	1:C:590:GLN:HE21	1.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:786:ALA:O	1:D:790:MET:HB2	2.07	0.53
1:B:945:ASN:HD22	1:B:1143:LYS:H	1.57	0.53
1:B:210:ILE:HA	1:B:223:LEU:CD1	2.37	0.53
1:B:712:PRO:O	1:B:713:GLU:CB	2.56	0.53
1:D:756:VAL:CG2	1:D:853:ARG:HG2	2.39	0.53
1:A:1111:SER:HB2	1:A:1191:THR:HA	1.90	0.53
1:C:312:THR:HG23	1:C:341:TYR:CB	2.38	0.53
1:D:6:PHE:CE1	1:D:10:ILE:HD11	2.44	0.53
1:C:376:THR:C	1:C:378:MET:H	2.10	0.53
1:C:55:LEU:HD12	1:C:55:LEU:N	2.24	0.53
1:C:99:ALA:HB1	1:C:642:VAL:HG12	1.91	0.53
1:D:729:LYS:HZ2	1:D:904:ASN:HD21	1.53	0.53
1:B:322:GLY:HA3	1:B:334:ARG:CZ	2.38	0.53
1:C:98:ARG:NH2	1:C:622:PHE:O	2.42	0.53
1:B:303:LYS:NZ	1:B:357:VAL:H	2.07	0.53
1:C:182:MET:HE2	1:C:185:ILE:HD12	1.90	0.53
1:C:312:THR:HG22	1:C:338:TRP:HE1	1.74	0.53
1:D:531:LYS:O	1:D:535:GLU:HG3	2.08	0.53
1:A:1232:ASN:HD21	1:A:1235:ASP:H	1.56	0.53
1:A:461:SER:C	1:A:462:ILE:HG13	2.29	0.53
1:B:387:GLN:HG2	1:B:432:PHE:CZ	2.43	0.53
1:B:622:PHE:HD2	1:B:622:PHE:O	1.92	0.53
1:B:1188:VAL:HG11	1:B:1202:LEU:HB2	1.90	0.53
1:C:112:LEU:O	1:C:113:GLN:HB2	2.09	0.53
1:D:927:VAL:HG21	1:D:1149:ILE:HG12	1.91	0.53
1:A:301:LEU:C	1:A:303:LYS:H	2.12	0.52
1:A:589:PHE:HA	1:A:592:LEU:HB2	1.89	0.52
1:C:558:TYR:CE1	1:C:560:ARG:HG2	2.45	0.52
1:A:417:ILE:HG12	1:A:454:TYR:CE1	2.44	0.52
1:A:534:THR:HG22	1:A:535:GLU:N	2.22	0.52
1:B:981:PRO:HB3	1:B:1037:UNK:CB	2.39	0.52
1:B:6:PHE:O	1:B:10:ILE:HB	2.10	0.52
1:C:1171:MET:O	1:C:1173:ILE:HG12	2.08	0.52
1:C:228:VAL:O	1:C:228:VAL:HG12	2.09	0.52
1:D:335:PHE:O	1:D:339:LEU:HB2	2.09	0.52
1:D:744:LEU:HD21	1:D:897:LEU:HA	1.91	0.52
1:A:144:THR:HG22	1:A:148:LYS:HE3	1.91	0.52
1:A:419:PRO:HA	1:A:454:TYR:HB3	1.91	0.52
1:B:201:CYS:HA	1:B:222:CYS:O	2.09	0.52
1:B:627:VAL:HG11	1:B:643:LYS:CB	2.38	0.52
1:B:744:LEU:HD22	1:B:798:TRP:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:770:HIS:CE1	1:D:858:LEU:HD23	2.44	0.52
1:A:597:PRO:C	1:A:599:ARG:H	2.12	0.52
1:C:264:ILE:CG2	1:C:268:VAL:CG1	2.86	0.52
1:B:1236:ARG:HB3	1:B:1239:VAL:HG13	1.91	0.52
1:B:945:ASN:HD21	1:B:951:LYS:HB3	1.75	0.52
1:C:152:HIS:HD2	1:C:704:HIS:NE2	2.08	0.52
1:D:325:ASN:HD21	1:D:328:GLY:CA	2.23	0.52
1:C:1111:SER:CB	1:C:1191:THR:HA	2.40	0.52
1:D:284:VAL:HG21	1:D:313:PHE:CG	2.44	0.52
1:A:701:GLU:O	1:A:704:HIS:N	2.42	0.52
1:B:1138:GLN:HG2	1:B:1138:GLN:O	2.08	0.52
1:B:566:ARG:O	1:B:570:VAL:HG23	2.09	0.52
1:D:276:ARG:NH1	1:D:326:GLU:HG3	2.25	0.52
1:B:332:LEU:HA	1:B:335:PHE:HB3	1.91	0.52
1:B:809:LEU:O	1:B:810:ILE:HG12	2.10	0.52
1:B:871:VAL:HG22	1:B:886:PHE:CE2	2.44	0.52
1:A:1111:SER:HA	1:A:1190:TYR:CD1	2.44	0.52
1:B:710:PHE:CE2	1:B:711:ILE:O	2.63	0.52
1:B:796:SER:HB2	1:B:893:TYR:CE1	2.45	0.52
1:B:199:ARG:HG2	1:B:738:PHE:HZ	1.69	0.51
1:A:1232:ASN:ND2	1:A:1235:ASP:H	2.08	0.51
1:A:140:MET:O	1:A:171:HIS:NE2	2.36	0.51
1:B:458:ASP:OD1	1:B:461:SER:CB	2.58	0.51
1:C:155:ILE:CB	1:C:706:ILE:HG13	2.40	0.51
1:D:155:ILE:HB	1:D:706:ILE:CD1	2.40	0.51
1:C:172:GLU:H	1:C:172:GLU:CD	2.13	0.51
1:C:221:PHE:CB	1:C:250:LEU:HD12	2.39	0.51
1:D:277:VAL:O	1:D:280:ASP:N	2.43	0.51
1:A:101:ARG:HD3	1:A:595:VAL:CG1	2.39	0.51
1:B:595:VAL:O	1:B:596:LEU:CB	2.53	0.51
1:C:97:GLN:O	1:C:101:ARG:HB2	2.10	0.51
1:C:707:GLU:N	1:C:707:GLU:OE1	2.44	0.51
1:A:96:GLN:H	1:A:96:GLN:NE2	1.97	0.51
1:B:677:LEU:HD13	1:B:708:ARG:HD2	1.92	0.51
1:C:516:TYR:CE2	1:C:530:LEU:HD12	2.46	0.51
1:D:527:THR:CG2	1:D:528:ASP:H	2.15	0.51
1:A:657:ALA:HA	1:A:660:ASP:HB2	1.93	0.51
1:A:798:TRP:HE3	1:A:799:PRO:HD3	1.72	0.51
1:B:739:PRO:HG3	1:B:800:PHE:CZ	2.42	0.51
1:C:309:LEU:O	1:C:312:THR:HB	2.09	0.51
1:D:360:PHE:HA	1:D:363:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:HG22	1:D:528:ASP:N	2.19	0.51
1:D:36:MET:SD	1:D:83:MET:HB3	2.51	0.51
1:A:589:PHE:CE2	1:A:671:ASN:HB2	2.46	0.51
1:A:804:SER:HB2	1:A:869:VAL:O	2.11	0.51
1:B:250:LEU:HD23	1:B:253:LEU:HD23	1.92	0.51
1:B:332:LEU:HD12	1:B:332:LEU:H	1.75	0.51
1:C:16:GLN:HE22	1:C:799:PRO:HG3	1.76	0.51
1:D:292:PHE:HD1	1:D:544:VAL:CG2	2.21	0.51
1:D:358:GLU:HA	1:D:361:ASN:HD22	1.75	0.51
1:B:918:ASN:ND2	1:D:452:LEU:HD13	2.26	0.51
1:A:798:TRP:CD2	1:A:799:PRO:HD3	2.45	0.51
1:B:505:SER:O	1:B:509:VAL:HG23	2.11	0.51
1:B:283:PHE:CE2	1:B:324:ILE:HG21	2.46	0.51
1:B:689:TYR:CB	1:B:704:HIS:CD2	2.91	0.51
1:D:599:ARG:HH22	1:D:625:ASN:HD21	1.58	0.51
1:B:423:LYS:O	1:B:427:ARG:HG2	2.11	0.50
1:B:773:ASP:O	1:B:775:TYR:N	2.44	0.50
1:B:7:PHE:O	1:B:8:HIS:C	2.49	0.50
1:D:1160:ARG:HA	1:D:1227:SER:OG	2.11	0.50
1:A:1150:LEU:O	1:A:1150:LEU:HD12	2.11	0.50
1:A:1199:ILE:N	1:A:1225:LEU:O	2.42	0.50
1:D:1107:VAL:HG13	1:D:1108:SER:N	2.27	0.50
1:D:587:LYS:HG2	1:D:671:ASN:OD1	2.11	0.50
1:D:820:LYS:HA	1:D:825:THR:HA	1.93	0.50
1:A:134:THR:HG22	1:A:135:PRO:CD	2.42	0.50
1:B:10:ILE:HG12	1:B:14:TRP:CZ3	2.47	0.50
1:B:388:LYS:O	1:B:389:LYS:C	2.49	0.50
1:B:486:UNK:O	1:B:487:UNK:C	2.58	0.50
1:B:36:MET:HE1	1:B:83:MET:HG2	1.84	0.50
1:B:917:ILE:HG13	1:B:947:GLU:O	2.11	0.50
1:C:154:LYS:HG3	1:C:161:TRP:CE2	2.47	0.50
1:B:1223:LEU:HD21	1:B:1225:LEU:HD21	1.92	0.50
1:D:1116:LYS:HG3	1:D:1216:ARG:HD2	1.93	0.50
1:D:1232:ASN:HD22	1:D:1233:LEU:N	2.09	0.50
1:B:210:ILE:HA	1:B:223:LEU:HD13	1.93	0.50
1:B:547:TYR:HA	1:B:551:GLY:O	2.11	0.50
1:D:142:LYS:O	1:D:146:ASN:ND2	2.44	0.50
1:C:1102:LYS:O	1:C:1104:PHE:N	2.45	0.50
1:C:959:LEU:HD21	1:C:1137:GLU:OE2	2.12	0.50
1:D:762:SER:C	1:D:764:GLN:H	2.15	0.50
1:D:852:GLN:HG2	1:D:858:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:MET:HE2	1:A:604:ILE:HD13	1.94	0.50
1:A:690:LYS:HA	1:A:699:ASP:OD1	2.11	0.50
1:C:175:GLY:O	1:C:180:LYS:HE2	2.12	0.50
1:D:1193:ILE:HG22	1:D:1193:ILE:O	2.12	0.50
1:A:1173:ILE:O	1:A:1173:ILE:HG22	2.12	0.50
1:B:679:PHE:CE2	1:B:708:ARG:HG2	2.47	0.50
1:D:713:GLU:HG3	1:D:714:SER:N	2.26	0.50
1:A:798:TRP:O	1:A:801:LEU:N	2.44	0.50
1:A:817:GLU:O	1:A:827:VAL:HA	2.12	0.50
1:A:820:LYS:HA	1:A:825:THR:HG22	1.94	0.50
1:B:10:ILE:HG12	1:B:14:TRP:HZ3	1.76	0.50
1:B:356:ASP:O	1:B:359:TRP:HB3	2.12	0.50
1:D:1150:LEU:HD12	1:D:1150:LEU:C	2.32	0.50
1:D:533:MET:HG3	1:D:561:TYR:CG	2.46	0.50
1:A:29:PHE:CD2	1:A:75:ILE:HG23	2.46	0.49
1:A:826:LYS:CG	1:A:827:VAL:N	2.74	0.49
1:B:1223:LEU:CD2	1:B:1225:LEU:HD21	2.42	0.49
1:B:516:TYR:HE2	1:B:533:MET:HE2	1.77	0.49
1:C:393:ALA:O	1:C:396:PRO:HD2	2.11	0.49
1:C:597:PRO:C	1:C:599:ARG:H	2.14	0.49
1:C:626:GLU:O	1:C:627:VAL:HB	2.12	0.49
1:D:156:THR:N	1:D:706:ILE:HD11	2.27	0.49
1:A:155:ILE:CG2	1:A:706:ILE:HG13	2.42	0.49
1:B:214:LEU:HD23	1:B:250:LEU:HD22	1.93	0.49
1:C:393:ALA:HB1	1:C:418:PHE:HZ	1.78	0.49
1:D:339:LEU:HD11	1:D:570:VAL:HB	1.94	0.49
1:C:446:HIS:HD2	1:C:447:SER:O	1.95	0.49
1:D:331:ASN:OD1	1:D:334:ARG:HG2	2.12	0.49
1:A:1212:ASN:HD22	1:A:1215:GLY:N	2.10	0.49
1:A:94:MET:O	1:A:98:ARG:HB3	2.13	0.49
1:A:93:LYS:O	1:A:96:GLN:HG2	2.12	0.49
1:A:982:THR:CB	1:A:983:GLN:NE2	2.71	0.49
1:B:543:TRP:NE1	1:B:553:PRO:HD2	2.27	0.49
1:B:543:TRP:CD1	1:B:553:PRO:HG2	2.48	0.49
1:D:1171:MET:HB3	1:D:1173:ILE:HD11	1.95	0.49
1:D:938:GLU:HB2	1:D:1182:HIS:NE2	2.26	0.49
1:A:377:ARG:HA	1:A:380:LYS:HZ2	1.76	0.49
1:C:1171:MET:HB2	1:C:1233:LEU:HD11	1.95	0.49
1:C:312:THR:CG2	1:C:338:TRP:HE1	2.26	0.49
1:A:26:ILE:HB	1:A:27:PRO:HD2	1.95	0.49
1:A:947:GLU:HG3	1:A:947:GLU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:GLU:C	1:C:703:ASN:N	2.66	0.49
1:D:826:LYS:HZ2	1:D:827:VAL:H	1.60	0.49
1:D:876:ARG:NH1	1:D:920:GLU:OE2	2.45	0.49
1:A:963:PRO:HD3	1:A:1129:TYR:CE1	2.47	0.49
1:D:679:PHE:N	1:D:679:PHE:CD1	2.79	0.49
1:A:155:ILE:HB	1:A:706:ILE:CG1	2.43	0.49
1:B:676:ASP:HB3	1:B:711:ILE:HG22	1.94	0.49
1:A:1105:VAL:CG1	1:A:1105:VAL:O	2.60	0.49
1:A:798:TRP:CE3	1:A:799:PRO:CD	2.96	0.49
1:B:837:ARG:O	1:B:841:ARG:HG2	2.12	0.49
1:B:876:ARG:NH1	1:B:920:GLU:OE2	2.46	0.49
1:B:933:TYR:CZ	1:B:1139:LYS:HB2	2.48	0.49
1:D:586:PHE:HD1	1:D:590:GLN:HE21	1.61	0.49
1:D:676:ASP:CB	1:D:711:ILE:HG22	2.38	0.49
1:B:264:ILE:HG22	1:B:265:THR:H	1.72	0.49
1:B:589:PHE:HD1	1:B:592:LEU:HD12	1.78	0.49
1:C:510:GLU:O	1:C:514:GLN:HB2	2.13	0.49
1:C:561:TYR:N	1:C:561:TYR:CD2	2.80	0.49
1:D:155:ILE:CG2	1:D:706:ILE:HD12	2.43	0.49
1:A:1092:THR:O	1:A:1093:VAL:CG2	2.54	0.48
1:A:1195:LYS:HG2	1:A:1196:ASN:HD22	1.78	0.48
1:A:217:HIS:CG	1:A:723:GLY:HA2	2.47	0.48
1:B:312:THR:HG22	1:B:338:TRP:CD1	2.48	0.48
1:C:209:LEU:HB3	1:C:223:LEU:HD22	1.94	0.48
1:C:809:LEU:C	1:C:810:ILE:HG12	2.32	0.48
1:D:170:GLY:O	1:D:180:LYS:NZ	2.46	0.48
1:A:1172:TYR:CD1	1:A:1179:VAL:HB	2.48	0.48
1:A:415:PHE:CE1	1:A:459:LEU:HD13	2.48	0.48
1:B:1171:MET:HB3	1:B:1173:ILE:HD11	1.95	0.48
1:B:320:MET:CE	1:B:324:ILE:HG13	2.43	0.48
1:B:627:VAL:HG11	1:B:643:LYS:HB3	1.95	0.48
1:C:365:GLU:O	1:C:369:LEU:HG	2.13	0.48
1:B:830:ARG:CG	1:B:831:LYS:H	2.17	0.48
1:C:1084:ALA:O	1:C:1085:GLU:C	2.51	0.48
1:D:969:ARG:HD3	1:D:1118:SER:HA	1.95	0.48
1:A:676:ASP:HB2	1:A:711:ILE:HG22	1.96	0.48
1:C:605:PRO:O	1:C:606:VAL:C	2.52	0.48
1:C:876:ARG:NH1	1:C:920:GLU:OE1	2.46	0.48
1:D:210:ILE:HA	1:D:223:LEU:HD11	1.96	0.48
1:A:534:THR:CG2	1:A:573:GLY:N	2.77	0.48
1:B:297:PRO:CG	1:B:298:ASP:H	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:GLN:O	1:B:518:ASP:HB2	2.13	0.48
1:C:928:VAL:HG21	1:C:1173:ILE:HG23	1.96	0.48
1:D:917:ILE:HD12	1:D:947:GLU:O	2.13	0.48
1:B:830:ARG:CG	1:B:831:LYS:N	2.75	0.48
1:B:933:TYR:CZ	1:B:956:LYS:HD3	2.48	0.48
1:A:945:ASN:O	1:C:417:ILE:HD12	2.14	0.48
1:A:308:VAL:HG11	1:A:363:GLN:HG2	1.95	0.48
1:B:332:LEU:CD1	1:B:332:LEU:H	2.24	0.48
1:D:14:TRP:HB3	1:D:256:TYR:CG	2.49	0.48
1:D:395:LYS:O	1:D:396:PRO:C	2.52	0.48
1:A:417:ILE:O	1:A:419:PRO:HD3	2.13	0.48
1:A:969:ARG:NH1	1:A:972:LEU:CD2	2.77	0.48
1:C:1188:VAL:HG11	1:C:1202:LEU:HB2	1.96	0.48
1:C:815:VAL:CG1	1:C:830:ARG:HH11	2.26	0.48
1:A:918:ASN:HD22	1:A:918:ASN:N	2.12	0.48
1:B:689:TYR:HB2	1:B:704:HIS:HD2	1.76	0.48
1:C:206:ASP:OD1	1:C:208:ASP:HB2	2.13	0.48
1:C:219:HIS:CD2	1:C:254:ARG:NH1	2.68	0.48
1:D:1232:ASN:ND2	1:D:1234:SER:H	2.12	0.48
1:A:339:LEU:HD13	1:A:571:ILE:HD13	1.95	0.48
1:B:155:ILE:HB	1:B:706:ILE:HD11	1.95	0.48
1:B:155:ILE:HB	1:B:706:ILE:HD12	1.93	0.48
1:C:398:LEU:CD1	1:C:442:LEU:HD21	2.42	0.48
1:D:159:THR:CA	1:D:162:GLN:HG3	2.37	0.48
1:B:307:PRO:HG3	1:B:764:GLN:HG3	1.95	0.47
1:B:931:GLY:HA2	1:B:1240:TYR:HA	1.96	0.47
1:D:1173:ILE:HG22	1:D:1173:ILE:O	2.14	0.47
1:B:98:ARG:HH11	1:B:644:ILE:HG12	1.79	0.47
1:C:952:LEU:HD11	1:C:1144:VAL:HG21	1.95	0.47
1:D:312:THR:CG2	1:D:338:TRP:HE1	2.02	0.47
1:D:605:PRO:O	1:D:607:VAL:N	2.47	0.47
1:A:862:ILE:HD12	1:A:862:ILE:N	2.19	0.47
1:B:933:TYR:CD1	1:B:1139:LYS:HE2	2.49	0.47
1:D:1169:ARG:HH21	1:D:1184:LYS:HD2	1.79	0.47
1:D:264:ILE:HG22	1:D:265:THR:H	1.78	0.47
1:D:312:THR:HG21	1:D:342:LEU:CD2	2.41	0.47
1:A:1195:LYS:CG	1:A:1196:ASN:HD22	2.27	0.47
1:A:102:PHE:CE2	1:A:627:VAL:HB	2.49	0.47
1:B:1112:ASP:N	1:B:1112:ASP:OD1	2.48	0.47
1:B:516:TYR:HE2	1:B:533:MET:CE	2.27	0.47
1:C:785:LEU:HD23	1:C:789:HIS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:GLN:NE2	1:D:206:ASP:OD1	2.42	0.47
1:D:33:TYR:OH	1:D:200:HIS:CD2	2.67	0.47
1:A:1110:GLU:O	1:A:1111:SER:HB3	2.15	0.47
1:A:194:TYR:OH	1:A:200:HIS:HE1	1.98	0.47
1:B:169:SER:CB	1:B:676:ASP:OD1	2.62	0.47
1:B:965:ILE:HG13	1:B:965:ILE:H	1.44	0.47
1:C:198:THR:HG22	1:C:200:HIS:CE1	2.50	0.47
1:C:258:ALA:HA	1:C:274:PHE:CE1	2.50	0.47
1:D:807:LEU:HD11	1:D:869:VAL:HG13	1.95	0.47
1:A:156:THR:CG2	1:A:703:ASN:O	2.62	0.47
1:B:689:TYR:HB3	1:B:700:ILE:HD12	1.95	0.47
1:C:706:ILE:CD1	1:C:706:ILE:N	2.77	0.47
1:C:770:HIS:CE1	1:C:858:LEU:HD23	2.49	0.47
1:D:538:VAL:O	1:D:541:LEU:HB2	2.15	0.47
1:D:729:LYS:NZ	1:D:904:ASN:ND2	2.60	0.47
1:D:92:ALA:HA	1:D:558:TYR:HA	1.97	0.47
1:A:260:GLU:O	1:A:314:LYS:HE2	2.15	0.47
1:A:962:GLU:HG3	1:A:1169:ARG:HE	1.79	0.47
1:B:1181:LEU:HG	1:B:1182:HIS:CD2	2.50	0.47
1:B:284:VAL:HG13	1:B:338:TRP:CH2	2.50	0.47
1:D:1116:LYS:HG3	1:D:1216:ARG:CD	2.45	0.47
1:D:770:HIS:CE1	1:D:858:LEU:HD22	2.50	0.47
1:A:1092:THR:OG1	1:A:1093:VAL:N	2.48	0.47
1:A:140:MET:HB3	1:A:171:HIS:NE2	2.30	0.47
1:A:717:ASN:N	1:A:717:ASN:OD1	2.48	0.47
1:A:797:ARG:HD3	1:A:802:ARG:NE	2.30	0.47
1:A:923:LYS:HA	1:A:941:VAL:HG12	1.96	0.47
1:A:969:ARG:NH1	1:A:972:LEU:HD22	2.28	0.47
1:B:87:GLY:HA3	1:B:173:VAL:O	2.14	0.47
1:D:729:LYS:HZ3	1:D:904:ASN:ND2	2.12	0.47
1:D:747:THR:CG2	1:D:770:HIS:HB2	2.44	0.47
1:B:301:LEU:HD22	1:B:306:PHE:CE2	2.50	0.47
1:C:182:MET:CE	1:C:185:ILE:HD12	2.45	0.47
1:C:195:ASN:ND2	1:C:197:ASN:H	2.13	0.47
1:A:751:ALA:O	1:A:765:GLN:HA	2.15	0.47
1:B:1109:LEU:C	1:B:1110:GLU:HG2	2.35	0.47
1:C:974:SER:HB3	1:C:975:GLN:NE2	2.30	0.47
1:D:76:LYS:HD3	1:D:160:ARG:NE	2.30	0.47
1:D:271:GLU:HG3	1:D:271:GLU:O	2.13	0.47
1:D:876:ARG:HG3	1:D:882:TYR:CE2	2.50	0.47
1:D:893:TYR:HB2	1:D:898:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:HA2	1:A:557:TRP:CZ2	2.50	0.47
1:A:894:PRO:HD2	1:A:897:LEU:HD12	1.97	0.47
1:B:323:TYR:H	1:B:334:ARG:NH1	2.12	0.47
1:C:832:PRO:O	1:C:833:GLN:C	2.53	0.47
1:D:854:THR:HG22	1:D:855:LYS:HG2	1.97	0.47
1:A:741:LEU:HD22	1:A:769:LEU:CD1	2.44	0.46
1:B:1147:GLU:CD	1:B:1147:GLU:H	2.19	0.46
1:B:149:TYR:HB2	1:B:689:TYR:CE2	2.50	0.46
1:C:31:ASN:HB3	1:C:33:TYR:CZ	2.50	0.46
1:C:417:ILE:HG12	1:C:454:TYR:CD1	2.49	0.46
1:C:162:GLN:HG2	1:C:681:PHE:CD1	2.51	0.46
1:D:55:LEU:HD22	1:D:59:GLU:HG2	1.97	0.46
1:A:1158:LEU:O	1:A:1161:SER:OG	2.22	0.46
1:A:952:LEU:HD13	1:A:1149:ILE:HD11	1.98	0.46
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.83	0.46
1:C:706:ILE:CG2	1:C:707:GLU:N	2.76	0.46
1:D:158:ASP:O	1:D:162:GLN:HG3	2.15	0.46
1:A:708:ARG:NH1	1:A:708:ARG:HB2	2.30	0.46
1:A:955:LYS:HG3	1:A:1138:GLN:HG2	1.97	0.46
1:B:1105:VAL:HG12	1:B:1105:VAL:O	2.15	0.46
1:B:1145:PRO:HB2	1:B:1147:GLU:OE1	2.14	0.46
1:B:928:VAL:HG21	1:B:1173:ILE:HG22	1.97	0.46
1:C:1207:ILE:HG22	1:C:1209:ALA:H	1.80	0.46
1:D:330:ILE:HD12	1:D:542:GLN:HG2	1.97	0.46
1:A:156:THR:N	1:A:706:ILE:HD11	2.30	0.46
1:B:948:THR:HG22	1:B:1146:ARG:NH2	2.30	0.46
1:B:36:MET:CE	1:B:83:MET:CG	2.76	0.46
1:B:731:GLY:C	1:B:733:SER:H	2.19	0.46
1:B:789:HIS:O	1:B:792:LYS:HB2	2.15	0.46
1:B:828:ILE:CG2	1:B:828:ILE:O	2.63	0.46
1:C:873:GLY:HA2	1:C:909:TYR:CE2	2.49	0.46
1:A:96:GLN:N	1:A:96:GLN:NE2	2.60	0.46
1:B:296:LEU:HD13	1:B:567:ILE:HG12	1.96	0.46
1:C:1232:ASN:HD22	1:C:1234:SER:H	1.63	0.46
1:D:589:PHE:CD1	1:D:589:PHE:N	2.84	0.46
1:A:965:ILE:O	1:A:966:GLY:C	2.52	0.46
1:B:102:PHE:HE1	1:B:599:ARG:NH1	2.14	0.46
1:C:1111:SER:HB2	1:C:1191:THR:HA	1.97	0.46
1:C:867:LYS:HE2	1:C:890:ILE:HD13	1.98	0.46
1:D:329:LYS:HA	1:D:542:GLN:OE1	2.15	0.46
1:A:1050:UNK:O	1:A:1091:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:GLU:CG	1:A:576:GLN:OE1	2.64	0.46
1:A:918:ASN:HA	1:A:944:TYR:CZ	2.51	0.46
1:B:342:LEU:HB3	1:B:567:ILE:HG21	1.98	0.46
1:B:798:TRP:CG	1:B:799:PRO:N	2.81	0.46
1:B:756:VAL:HG23	1:B:853:ARG:HG2	1.98	0.46
1:C:1089:ILE:O	1:C:1090:LEU:C	2.53	0.46
1:A:926:LYS:NZ	1:A:938:GLU:OE1	2.44	0.46
1:B:100:ARG:NH1	1:B:101:ARG:HH12	2.14	0.46
1:B:335:PHE:CD1	1:B:335:PHE:C	2.90	0.46
1:B:807:LEU:HB2	1:B:867:LYS:O	2.16	0.46
1:C:657:ALA:O	1:C:660:ASP:HB2	2.15	0.46
1:D:711:ILE:HA	1:D:712:PRO:HD3	1.83	0.46
1:D:749:GLU:HG3	1:D:749:GLU:O	2.16	0.46
1:A:442:LEU:HD23	1:A:457:LEU:HA	1.98	0.46
1:B:417:ILE:HG22	1:D:944:TYR:HB2	1.98	0.46
1:C:1204:ASP:O	1:C:1221:ARG:NH1	2.49	0.46
1:C:140:MET:O	1:C:171:HIS:NE2	2.49	0.46
1:C:922:PRO:O	1:C:923:LYS:C	2.54	0.46
1:A:416:GLU:HB2	1:C:951:LYS:HZ1	1.80	0.46
1:D:280:ASP:OD2	1:D:324:ILE:N	2.48	0.46
1:A:831:LYS:H	1:A:831:LYS:CD	2.29	0.45
1:C:530:LEU:C	1:C:532:GLU:H	2.19	0.45
1:C:917:ILE:N	1:C:917:ILE:CD1	2.32	0.45
1:C:91:ARG:HA	1:C:94:MET:CG	2.46	0.45
1:D:220:HIS:CE1	1:D:735:LEU:HB2	2.51	0.45
1:D:210:ILE:HA	1:D:223:LEU:HD13	1.97	0.45
1:D:214:LEU:HG	1:D:250:LEU:HD22	1.97	0.45
1:D:342:LEU:HB3	1:D:567:ILE:CG2	2.46	0.45
1:D:541:LEU:O	1:D:545:LEU:HB2	2.16	0.45
1:D:746:LEU:HD12	1:D:769:LEU:HB3	1.98	0.45
1:A:219:HIS:CD2	1:A:254:ARG:NH1	2.84	0.45
1:B:303:LYS:HZ2	1:B:357:VAL:H	1.65	0.45
1:B:511:TRP:HH2	1:B:566:ARG:NH2	2.13	0.45
1:C:152:HIS:CD2	1:C:704:HIS:NE2	2.84	0.45
1:C:85:ILE:HD12	1:C:168:PHE:CE2	2.52	0.45
1:D:927:VAL:HG21	1:D:1149:ILE:CG1	2.46	0.45
1:D:1173:ILE:HD11	1:D:1231:LEU:HB3	1.98	0.45
1:A:189:ARG:HA	1:A:194:TYR:CG	2.51	0.45
1:A:262:GLU:HG3	1:A:263:GLU:H	1.82	0.45
1:A:946:SER:OG	1:A:948:THR:HG23	2.17	0.45
1:B:1188:VAL:CG1	1:B:1202:LEU:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:HD23	1:B:578:ILE:HD11	1.99	0.45
1:B:592:LEU:O	1:B:596:LEU:HB2	2.17	0.45
1:C:1042:UNK:O	1:C:1045:UNK:N	2.50	0.45
1:C:505:SER:OG	1:C:508:PHE:HB3	2.17	0.45
1:C:810:ILE:HG23	1:C:815:VAL:HG22	1.98	0.45
1:C:949:ARG:HD3	1:C:1143:LYS:O	2.17	0.45
1:A:798:TRP:CE3	1:A:799:PRO:HG3	2.51	0.45
1:B:641:VAL:HG12	1:B:642:VAL:N	2.29	0.45
1:B:684:GLN:HB2	1:B:684:GLN:HE21	1.62	0.45
1:D:929:PHE:HD1	1:D:1149:ILE:CD1	2.30	0.45
1:D:309:LEU:O	1:D:312:THR:HB	2.16	0.45
1:C:144:THR:O	1:C:148:LYS:HG3	2.15	0.45
1:D:347:TYR:O	1:D:348:LEU:C	2.54	0.45
1:A:101:ARG:HD3	1:A:595:VAL:HG13	1.98	0.45
1:C:321:ASP:N	1:C:321:ASP:OD1	2.49	0.45
1:A:91:ARG:C	1:A:93:LYS:N	2.70	0.45
1:C:1049:UNK:O	1:C:1050:UNK:C	2.64	0.45
1:D:965:ILE:CG1	1:D:1125:GLU:HG2	2.17	0.45
1:D:575:ASP:O	1:D:576:GLN:HB3	2.16	0.45
1:A:1150:LEU:C	1:A:1150:LEU:HD12	2.37	0.45
1:A:262:GLU:HG3	1:A:263:GLU:N	2.32	0.45
1:A:335:PHE:CD1	1:A:335:PHE:O	2.70	0.45
1:B:1149:ILE:HD12	1:B:1149:ILE:HA	1.58	0.45
1:C:1148:ALA:O	1:C:1149:ILE:HD12	2.17	0.45
1:C:159:THR:O	1:C:162:GLN:HB2	2.17	0.45
1:C:383:LEU:HA	1:C:383:LEU:HD23	1.81	0.45
1:C:442:LEU:HD13	1:C:455:PHE:HB3	1.98	0.45
1:C:527:THR:HB	1:C:528:ASP:H	1.43	0.45
1:D:387:GLN:HG2	1:D:432:PHE:CZ	2.52	0.45
1:D:537:TYR:N	1:D:559:TYR:HE1	2.15	0.45
1:D:601:LYS:O	1:D:604:ILE:HG13	2.16	0.45
1:A:1111:SER:O	1:A:1111:SER:OG	2.35	0.45
1:A:426:VAL:HG13	1:A:433:LEU:HD13	1.98	0.45
1:B:3:ILE:HG12	1:B:289:GLY:HA3	1.98	0.45
1:B:534:THR:HG22	1:B:573:GLY:N	2.32	0.45
1:C:729:LYS:HD2	1:C:735:LEU:CD1	2.47	0.45
1:D:154:LYS:HD2	1:D:154:LYS:HA	1.72	0.45
1:A:456:LYS:O	1:A:456:LYS:HG3	2.16	0.45
1:B:917:ILE:CD1	1:B:917:ILE:H	1.96	0.45
1:C:554:SER:HB2	1:C:580:PHE:HB3	1.99	0.45
1:D:589:PHE:N	1:D:589:PHE:HD1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:SER:HB3	1:D:665:PRO:HD2	1.97	0.45
1:A:811:THR:HG22	1:A:813:GLU:H	1.82	0.44
1:B:950:LEU:HD23	1:B:1144:VAL:O	2.17	0.44
1:B:10:ILE:HG22	1:B:11:SER:N	2.32	0.44
1:B:1203:PHE:O	1:B:1221:ARG:HD3	2.17	0.44
1:B:169:SER:OG	1:B:180:LYS:HD2	2.17	0.44
1:B:296:LEU:HB2	1:B:299:LEU:HD11	1.98	0.44
1:B:793:ILE:HA	1:B:804:SER:O	2.16	0.44
1:C:1089:ILE:O	1:C:1092:THR:HB	2.16	0.44
1:C:250:LEU:O	1:C:254:ARG:HG3	2.17	0.44
1:C:518:ASP:C	1:C:519:LYS:HD3	2.36	0.44
1:D:1113:SER:OG	1:D:1114:LEU:N	2.51	0.44
1:D:1232:ASN:HD22	1:D:1234:SER:H	1.65	0.44
1:D:589:PHE:HA	1:D:592:LEU:HB2	1.99	0.44
1:B:1181:LEU:O	1:B:1182:HIS:HB2	2.16	0.44
1:B:293:LEU:HD13	1:B:537:TYR:CE1	2.53	0.44
1:B:748:ALA:HB1	1:B:767:MET:SD	2.58	0.44
1:C:212:LEU:HD21	1:C:548:TYR:CD1	2.52	0.44
1:D:540:GLY:O	1:D:544:VAL:HG23	2.17	0.44
1:D:798:TRP:O	1:D:799:PRO:C	2.55	0.44
1:A:254:ARG:HH22	1:A:724:LEU:HD21	1.82	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.72	0.44
1:B:364:LEU:O	1:B:364:LEU:HG	2.16	0.44
1:B:704:HIS:CE1	1:B:706:ILE:H	2.35	0.44
1:B:883:SER:CA	1:B:911:GLU:HG2	2.31	0.44
1:C:917:ILE:CG1	1:C:947:GLU:O	2.64	0.44
1:A:109:GLU:O	1:A:113:GLN:HB3	2.17	0.44
1:A:701:GLU:C	1:A:703:ASN:H	2.20	0.44
1:B:155:ILE:O	1:B:162:GLN:NE2	2.50	0.44
1:B:264:ILE:CG2	1:B:265:THR:H	2.26	0.44
1:B:297:PRO:CG	1:B:298:ASP:N	2.80	0.44
1:B:332:LEU:HD12	1:B:332:LEU:N	2.32	0.44
1:B:971:LYS:HG2	1:B:975:GLN:HE21	1.82	0.44
1:C:806:LEU:HA	1:C:868:VAL:HG12	1.99	0.44
1:A:932:ASP:OD1	1:A:932:ASP:N	2.51	0.44
1:B:1163:ARG:HG3	1:B:1237:GLN:OE1	2.16	0.44
1:C:113:GLN:O	1:C:114:LYS:C	2.55	0.44
1:C:708:ARG:HB3	1:C:708:ARG:NH1	2.06	0.44
1:C:744:LEU:HD22	1:C:798:TRP:CD1	2.53	0.44
1:D:1111:SER:O	1:D:1112:ASP:HB3	2.17	0.44
1:A:1150:LEU:C	1:A:1150:LEU:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ILE:HB	1:A:1196:ASN:OD1	2.18	0.44
1:A:461:SER:O	1:A:461:SER:OG	2.32	0.44
1:A:798:TRP:HB3	1:A:799:PRO:HD2	1.82	0.44
1:B:335:PHE:HD1	1:B:335:PHE:O	1.98	0.44
1:C:198:THR:CG2	1:C:200:HIS:CE1	3.01	0.44
1:D:830:ARG:NH1	1:D:836:GLU:OE2	2.43	0.44
1:D:876:ARG:NH1	1:D:920:GLU:OE1	2.51	0.44
1:A:402:VAL:HG12	1:A:402:VAL:O	2.18	0.44
1:A:945:ASN:HD21	1:A:951:LYS:HB3	1.83	0.44
1:B:948:THR:HG22	1:B:1146:ARG:HH21	1.82	0.44
1:B:323:TYR:N	1:B:334:ARG:NH1	2.66	0.44
1:B:980:TYR:CD1	1:B:980:TYR:N	2.85	0.44
1:C:138:GLU:OE2	1:C:670:ARG:NH1	2.46	0.44
1:C:816:TYR:N	1:C:816:TYR:CD1	2.86	0.44
1:D:507:ARG:HA	1:D:510:GLU:HB3	1.99	0.44
1:A:1207:ILE:HG22	1:A:1209:ALA:H	1.82	0.44
1:A:981:PRO:O	1:A:982:THR:C	2.55	0.44
1:B:312:THR:HG23	1:B:341:TYR:CB	2.43	0.44
1:B:704:HIS:C	1:B:704:HIS:ND1	2.71	0.44
1:B:946:SER:OG	1:B:947:GLU:N	2.51	0.44
1:D:401:THR:CG2	1:D:457:LEU:HD11	2.47	0.44
1:A:622:PHE:HZ	1:A:648:ASP:HB3	1.82	0.44
1:A:921:PHE:O	1:A:941:VAL:HG11	2.18	0.44
1:B:1135:SER:OG	1:B:1136:SER:N	2.50	0.44
1:C:206:ASP:CG	1:C:208:ASP:HB2	2.39	0.44
1:C:32:LEU:HB3	1:C:77:PRO:HG3	2.00	0.44
1:C:862:ILE:H	1:C:862:ILE:HD12	1.82	0.44
1:D:1193:ILE:O	1:D:1195:LYS:N	2.49	0.44
1:B:152:HIS:HD2	1:B:704:HIS:HE1	1.62	0.43
1:C:708:ARG:CZ	1:C:708:ARG:CB	2.92	0.43
1:B:1212:ASN:O	1:B:1213:PHE:C	2.57	0.43
1:B:352:LYS:HD2	1:B:354:ASP:O	2.18	0.43
1:B:407:THR:OG1	1:B:408:SER:N	2.50	0.43
1:B:528:ASP:HA	1:B:531:LYS:HB2	2.00	0.43
1:B:571:ILE:C	1:B:573:GLY:H	2.21	0.43
1:B:934:ALA:HB2	1:B:956:LYS:CD	2.34	0.43
1:D:1113:SER:HA	1:D:1189:GLY:HA2	1.99	0.43
1:D:388:LYS:NZ	1:D:486:UNK:O	2.51	0.43
1:D:578:ILE:HD12	1:D:578:ILE:O	2.18	0.43
1:A:259:LEU:CB	1:A:767:MET:HE2	2.48	0.43
1:A:534:THR:HG21	1:A:573:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLU:O	1:B:316:ALA:C	2.56	0.43
1:A:169:SER:HB2	1:A:676:ASP:OD1	2.19	0.43
1:A:152:HIS:CE1	1:A:708:ARG:HG2	2.54	0.43
1:C:1173:ILE:HA	1:C:1173:ILE:HD13	1.85	0.43
1:C:363:GLN:O	1:C:367:ILE:HD13	2.18	0.43
1:D:928:VAL:HG21	1:D:1173:ILE:CG2	2.49	0.43
1:B:918:ASN:HD21	1:D:452:LEU:HD13	1.82	0.43
1:D:542:GLN:HE21	1:D:542:GLN:CA	2.32	0.43
1:D:294:PRO:HB2	1:D:564:ALA:HB2	2.01	0.43
1:A:864:ALA:HB3	1:A:895:LEU:CD1	2.48	0.43
1:B:114:LYS:HZ2	1:B:114:LYS:HB2	1.82	0.43
1:B:544:VAL:O	1:B:547:TYR:HB3	2.19	0.43
1:C:730:LEU:O	1:C:731:GLY:C	2.57	0.43
1:C:739:PRO:HB3	1:C:800:PHE:CE2	2.53	0.43
1:D:266:ASP:O	1:D:267:SER:CB	2.58	0.43
1:B:34:LEU:HD12	1:B:36:MET:CE	2.48	0.43
1:B:391:ILE:CD1	1:B:485:UNK:O	2.65	0.43
1:B:682:ASN:HA	1:B:683:PRO:HD2	1.51	0.43
1:B:816:TYR:N	1:B:816:TYR:CD1	2.87	0.43
1:C:154:LYS:HA	1:C:154:LYS:HD2	1.59	0.43
1:C:166:VAL:O	1:C:678:ILE:HA	2.19	0.43
1:C:795:TYR:CZ	1:C:803:GLU:HG2	2.54	0.43
1:A:195:ASN:HD22	1:A:196:PRO:HD2	1.83	0.43
1:A:446:HIS:CD2	1:A:450:LYS:HD2	2.54	0.43
1:A:5:LYS:HA	1:A:5:LYS:HD3	1.92	0.43
1:A:811:THR:CG2	1:A:812:GLU:N	2.81	0.43
1:A:839:GLU:O	1:A:843:LEU:HB2	2.19	0.43
1:B:1112:ASP:HB2	1:B:1113:SER:H	1.66	0.43
1:B:260:GLU:O	1:B:314:LYS:HE2	2.18	0.43
1:B:303:LYS:HG2	1:B:355:ILE:O	2.18	0.43
1:B:58:GLU:CD	1:B:695:GLY:HA3	2.39	0.43
1:B:876:ARG:HG3	1:B:882:TYR:CE2	2.53	0.43
1:D:54:ARG:HG2	1:D:55:LEU:N	2.32	0.43
1:D:932:ASP:O	1:D:933:TYR:C	2.57	0.43
1:A:325:ASN:HD21	1:A:328:GLY:CA	2.31	0.43
1:B:403:GLN:O	1:B:404:ARG:HB2	2.18	0.43
1:B:534:THR:CG2	1:B:573:GLY:N	2.81	0.43
1:D:201:CYS:HA	1:D:222:CYS:O	2.19	0.43
1:D:58:GLU:OE1	1:D:695:GLY:HA3	2.18	0.43
1:A:945:ASN:HD22	1:A:1143:LYS:H	1.62	0.43
1:A:1236:ARG:HB3	1:A:1239:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:HG2	1:A:380:LYS:NZ	2.34	0.43
1:B:704:HIS:C	1:B:704:HIS:HD1	2.22	0.43
1:C:152:HIS:CD2	1:C:706:ILE:HB	2.54	0.43
1:C:895:LEU:HG	1:C:895:LEU:O	2.19	0.43
1:A:301:LEU:O	1:A:303:LYS:N	2.51	0.43
1:A:72:PHE:C	1:A:72:PHE:CD2	2.93	0.43
1:B:1171:MET:O	1:B:1230:LEU:HA	2.19	0.43
1:B:329:LYS:HA	1:B:542:GLN:OE1	2.19	0.43
1:B:252:ILE:HB	1:B:739:PRO:HG2	2.01	0.43
1:B:68:ILE:HG21	1:B:83:MET:HE3	2.01	0.43
1:D:744:LEU:HD22	1:D:798:TRP:CD1	2.54	0.43
1:A:293:LEU:HD11	1:A:540:GLY:CA	2.46	0.42
1:A:676:ASP:HB2	1:A:711:ILE:CG2	2.50	0.42
1:A:744:LEU:HD12	1:A:744:LEU:HA	1.54	0.42
1:C:786:ALA:HB2	1:C:809:LEU:HD12	2.01	0.42
1:C:834:ASP:HA	1:C:837:ARG:HB3	2.01	0.42
1:C:843:LEU:O	1:C:844:LYS:C	2.57	0.42
1:C:916:PRO:HB2	1:C:918:ASN:ND2	2.33	0.42
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.84	0.42
1:D:651:ARG:O	1:D:655:ALA:HB3	2.19	0.42
1:D:916:PRO:HD2	1:D:919:LYS:HB2	2.00	0.42
1:D:94:MET:O	1:D:98:ARG:HB2	2.19	0.42
1:A:1116:LYS:HG3	1:A:1216:ARG:HG3	2.00	0.42
1:B:346:GLU:OE2	1:B:568:SER:OG	2.27	0.42
1:C:362:GLN:O	1:C:365:GLU:HB3	2.19	0.42
1:C:55:LEU:HD12	1:C:55:LEU:H	1.84	0.42
1:C:648:ASP:OD1	1:C:651:ARG:HB2	2.19	0.42
1:D:945:ASN:HD21	1:D:1143:LYS:H	1.67	0.42
1:A:1111:SER:HA	1:A:1190:TYR:CE1	2.54	0.42
1:A:248:LEU:C	1:A:248:LEU:HD23	2.40	0.42
1:A:292:PHE:N	1:A:292:PHE:CD1	2.87	0.42
1:A:212:LEU:HD21	1:A:548:TYR:CD1	2.54	0.42
1:B:148:LYS:HD3	1:B:708:ARG:HD3	2.01	0.42
1:C:128:PHE:CE2	1:C:130:SER:HA	2.54	0.42
1:C:14:TRP:CD1	1:C:256:TYR:HB3	2.54	0.42
1:C:281:PHE:HE1	1:C:310:LEU:HD13	1.84	0.42
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.95	0.42
1:B:471:UNK:C	1:B:473:UNK:N	2.81	0.42
1:B:685:VAL:O	1:B:704:HIS:O	2.38	0.42
1:B:704:HIS:HE1	1:B:706:ILE:O	2.03	0.42
1:C:93:LYS:HZ3	1:C:100:ARG:HH22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:LYS:HB2	1:C:886:PHE:CE2	2.54	0.42
1:C:844:LYS:HG3	1:C:862:ILE:HB	2.01	0.42
1:D:140:MET:HB3	1:D:171:HIS:NE2	2.34	0.42
1:D:804:SER:HB2	1:D:868:VAL:HB	1.99	0.42
1:D:945:ASN:ND2	1:D:1143:LYS:N	2.67	0.42
1:A:260:GLU:OE1	1:A:750:LEU:HD11	2.19	0.42
1:B:1160:ARG:HA	1:B:1227:SER:OG	2.19	0.42
1:B:131:ASN:OD1	1:B:131:ASN:N	2.53	0.42
1:B:140:MET:CE	1:B:143:LEU:HD13	2.50	0.42
1:B:142:LYS:HD2	1:B:145:GLU:OE1	2.20	0.42
1:B:14:TRP:HB3	1:B:256:TYR:CG	2.54	0.42
1:B:516:TYR:CE2	1:B:533:MET:HE2	2.53	0.42
1:B:622:PHE:HD2	1:B:622:PHE:C	2.22	0.42
1:B:741:LEU:HD22	1:B:769:LEU:HD11	2.01	0.42
1:B:965:ILE:O	1:B:966:GLY:C	2.58	0.42
1:C:1102:LYS:CB	1:C:1103:PRO:CD	2.97	0.42
1:C:870:PRO:HD2	1:C:887:ASN:CB	2.50	0.42
1:C:968:VAL:O	1:C:971:LYS:HB3	2.18	0.42
1:D:1192:SER:O	1:D:1194:GLY:N	2.52	0.42
1:D:91:ARG:HB2	1:D:586:PHE:HE2	1.84	0.42
1:B:169:SER:HB2	1:B:676:ASP:OD1	2.20	0.42
1:B:689:TYR:CB	1:B:704:HIS:HD2	2.31	0.42
1:C:1111:SER:HB3	1:C:1191:THR:HA	2.01	0.42
1:C:32:LEU:HD22	1:C:75:ILE:HB	2.01	0.42
1:C:820:LYS:HG2	1:C:822:GLY:H	1.84	0.42
1:D:952:LEU:CD1	1:D:1144:VAL:HG21	2.41	0.42
1:D:394:VAL:HG22	1:D:418:PHE:CE2	2.54	0.42
1:A:338:TRP:CZ2	1:A:342:LEU:HD11	2.54	0.42
1:D:1226:ASP:O	1:D:1229:PHE:HD1	2.03	0.42
1:D:317:LEU:HG	1:D:317:LEU:O	2.20	0.42
1:D:446:HIS:HB3	1:D:453:TYR:CE2	2.55	0.42
1:A:1173:ILE:O	1:A:1173:ILE:CG2	2.68	0.42
1:A:592:LEU:HD22	1:A:596:LEU:CD1	2.47	0.42
1:A:596:LEU:HA	1:A:597:PRO:HD3	1.84	0.42
1:B:209:LEU:HB3	1:B:223:LEU:CD2	2.49	0.42
1:B:388:LYS:HD2	1:B:388:LYS:HA	1.88	0.42
1:B:774:LEU:O	1:B:775:TYR:CD2	2.73	0.42
1:C:156:THR:OG1	1:C:705:CYS:N	2.50	0.42
1:C:355:ILE:H	1:C:355:ILE:HD12	1.84	0.42
1:A:451:ASP:OD1	1:C:916:PRO:HG3	2.19	0.42
1:D:1169:ARG:HA	1:D:1169:ARG:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:C	1:A:527:THR:OG1	2.58	0.42
1:A:654:GLU:O	1:A:658:PRO:HD2	2.20	0.42
1:A:848:LYS:HB2	1:A:848:LYS:HE3	1.81	0.42
1:B:656:MET:O	1:B:659:TYR:HB2	2.20	0.42
1:B:945:ASN:ND2	1:B:951:LYS:HB3	2.35	0.42
1:C:1188:VAL:CG1	1:C:1202:LEU:HB2	2.50	0.42
1:C:14:TRP:O	1:C:17:ILE:HG23	2.20	0.42
1:D:264:ILE:CG2	1:D:265:THR:H	2.32	0.42
1:B:897:LEU:HA	1:B:897:LEU:HD23	1.86	0.42
1:C:713:GLU:HG2	1:C:715:MET:H	1.85	0.42
1:D:217:HIS:CG	1:D:723:GLY:HA2	2.55	0.42
1:D:189:ARG:NH2	1:D:723:GLY:O	2.46	0.42
1:A:146:ASN:O	1:A:149:TYR:HB3	2.20	0.41
1:A:301:LEU:HD22	1:A:306:PHE:CD2	2.55	0.41
1:A:316:ALA:O	1:A:320:MET:HG3	2.20	0.41
1:C:417:ILE:O	1:C:419:PRO:HD3	2.19	0.41
1:C:534:THR:CG2	1:C:573:GLY:HA3	2.46	0.41
1:C:837:ARG:HD3	1:C:841:ARG:NH2	2.29	0.41
1:D:917:ILE:HG23	1:D:1146:ARG:HD3	2.02	0.41
1:D:1147:GLU:CD	1:D:1147:GLU:H	2.23	0.41
1:D:962:GLU:HA	1:D:963:PRO:HD2	1.91	0.41
1:A:21:ILE:HD11	1:A:247:LEU:HG	2.01	0.41
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.87	0.41
1:A:852:GLN:HG3	1:A:858:LEU:HD12	2.02	0.41
1:B:433:LEU:HA	1:B:433:LEU:HD23	1.93	0.41
1:B:417:ILE:CG1	1:B:454:TYR:CD1	3.02	0.41
1:B:651:ARG:HG3	1:B:651:ARG:O	2.20	0.41
1:B:689:TYR:CD2	1:B:690:LYS:N	2.88	0.41
1:B:807:LEU:HA	1:B:807:LEU:HD23	1.79	0.41
1:C:111:ALA:O	1:C:112:LEU:C	2.58	0.41
1:C:512:LYS:O	1:C:514:GLN:N	2.40	0.41
1:C:858:LEU:HD12	1:C:858:LEU:HA	1.81	0.41
1:D:952:LEU:CD2	1:D:1149:ILE:HD13	2.50	0.41
1:A:391:ILE:H	1:A:391:ILE:HG13	1.66	0.41
1:B:33:TYR:OH	1:B:200:HIS:HD2	2.03	0.41
1:B:34:LEU:HD12	1:B:36:MET:HE3	2.02	0.41
1:C:75:ILE:HD11	1:C:224:LEU:HD22	2.01	0.41
1:C:36:MET:O	1:C:39:ILE:N	2.53	0.41
1:C:744:LEU:HD21	1:C:897:LEU:HA	2.02	0.41
1:D:1204:ASP:O	1:D:1221:ARG:NH1	2.52	0.41
1:D:1232:ASN:C	1:D:1232:ASN:ND2	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:ARG:O	1:D:798:TRP:C	2.58	0.41
1:D:849:SER:O	1:D:850:ASN:C	2.59	0.41
1:A:87:GLY:HA3	1:A:173:VAL:O	2.21	0.41
1:A:459:LEU:O	1:A:462:ILE:HD12	2.21	0.41
1:A:756:VAL:O	1:A:756:VAL:HG12	2.21	0.41
1:B:622:PHE:C	1:B:622:PHE:CD2	2.94	0.41
1:C:182:MET:HA	1:C:182:MET:HE2	2.02	0.41
1:C:725:PRO:HG2	1:C:728:ALA:HB2	2.01	0.41
1:C:949:ARG:HH21	1:C:1145:PRO:HB3	1.85	0.41
1:A:1112:ASP:CG	1:A:1113:SER:H	2.24	0.41
1:B:1191:THR:O	1:B:1191:THR:HG22	2.20	0.41
1:B:293:LEU:HD13	1:B:537:TYR:CD1	2.55	0.41
1:B:682:ASN:HD21	1:B:684:GLN:NE2	2.18	0.41
1:C:381:LYS:O	1:C:384:MET:HB2	2.21	0.41
1:C:3:ILE:HB	1:C:6:PHE:HB2	2.01	0.41
1:C:706:ILE:HD12	1:C:706:ILE:H	1.80	0.41
1:C:847:LEU:O	1:C:848:LYS:C	2.59	0.41
1:D:154:LYS:HG2	1:D:161:TRP:CE2	2.56	0.41
1:D:357:VAL:HG12	1:D:361:ASN:ND2	2.35	0.41
1:D:591:GLN:HE21	1:D:591:GLN:HB3	1.69	0.41
1:D:927:VAL:CG2	1:D:1149:ILE:HG13	2.49	0.41
1:A:1095:ASP:N	1:A:1095:ASP:OD2	2.53	0.41
1:A:1152:ALA:CB	1:A:1173:ILE:HG22	2.51	0.41
1:A:1212:ASN:N	1:A:1212:ASN:OD1	2.50	0.41
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.84	0.41
1:A:301:LEU:C	1:A:303:LYS:N	2.74	0.41
1:A:690:LYS:HD2	1:A:699:ASP:OD1	2.20	0.41
1:B:315:GLU:OE1	1:B:315:GLU:CA	2.69	0.41
1:B:426:VAL:HG13	1:B:433:LEU:HD13	2.02	0.41
1:C:657:ALA:N	1:C:658:PRO:HD2	2.36	0.41
1:D:27:PRO:HA	1:D:908:ARG:HH22	1.86	0.41
1:A:405:LYS:HE3	1:A:405:LYS:HB2	1.81	0.41
1:A:129:ASP:OD2	1:A:600:SER:HB2	2.21	0.41
1:A:169:SER:OG	1:A:676:ASP:OD1	2.35	0.41
1:B:346:GLU:OE1	1:B:566:ARG:HB3	2.21	0.41
1:C:807:LEU:HA	1:C:807:LEU:HD23	1.52	0.41
1:C:85:ILE:HD12	1:C:168:PHE:HE2	1.86	0.41
1:D:149:TYR:OH	1:D:697:PHE:HB3	2.21	0.41
1:A:313:PHE:CZ	1:A:317:LEU:HD22	2.55	0.41
1:A:811:THR:HG22	1:A:812:GLU:N	2.35	0.41
1:B:540:GLY:O	1:B:543:TRP:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:TRP:HB3	1:B:799:PRO:CD	2.49	0.41
1:D:6:PHE:HE1	1:D:10:ILE:HD11	1.84	0.41
1:A:1151:ASN:O	1:A:1155:SER:OG	2.34	0.41
1:A:342:LEU:O	1:A:345:PHE:HB3	2.21	0.41
1:A:689:TYR:HB3	1:A:700:ILE:HD12	2.02	0.41
1:A:701:GLU:C	1:A:703:ASN:N	2.74	0.41
1:B:701:GLU:HB3	1:B:702:HIS:H	1.74	0.41
1:B:798:TRP:HA	1:B:801:LEU:HD23	2.03	0.41
1:B:916:PRO:HD2	1:B:919:LYS:HB2	2.02	0.41
1:C:1191:THR:O	1:C:1191:THR:HG23	2.20	0.41
1:C:395:LYS:HB3	1:C:396:PRO:HD3	2.03	0.41
1:C:459:LEU:C	1:C:461:SER:H	2.24	0.41
1:D:1212:ASN:ND2	1:D:1215:GLY:H	2.18	0.41
1:D:32:LEU:HD13	1:D:75:ILE:HG13	2.02	0.41
1:D:437:ALA:O	1:D:439:ASP:N	2.53	0.41
1:B:165:LYS:HG2	1:B:678:ILE:HD11	2.02	0.41
1:C:312:THR:CG2	1:C:338:TRP:NE1	2.83	0.41
1:C:34:LEU:HD22	1:C:203:TYR:HB3	2.02	0.41
1:C:54:ARG:HG3	1:C:128:PHE:HB2	2.02	0.41
1:D:308:VAL:O	1:D:311:GLN:N	2.54	0.41
1:B:1212:ASN:O	1:B:1214:GLY:N	2.54	0.41
1:C:40:LEU:O	1:C:44:THR:HB	2.21	0.41
1:C:98:ARG:HG3	1:C:595:VAL:HA	2.03	0.41
1:C:711:ILE:HA	1:C:712:PRO:HD3	1.87	0.41
1:D:109:GLU:O	1:D:113:GLN:HB2	2.21	0.41
1:D:134:THR:O	1:D:140:MET:HG3	2.21	0.41
1:D:61:TYR:OH	1:D:143:LEU:HD12	2.21	0.41
1:D:210:ILE:HG13	1:D:223:LEU:HD13	2.02	0.41
1:A:663:LEU:HB3	1:A:667:GLU:HB2	2.03	0.40
1:A:712:PRO:O	1:A:713:GLU:HB3	2.19	0.40
1:A:918:ASN:HA	1:A:944:TYR:OH	2.21	0.40
1:B:312:THR:CG2	1:B:338:TRP:HE1	2.32	0.40
1:B:383:LEU:HD23	1:B:383:LEU:HA	2.00	0.40
1:B:554:SER:HB2	1:B:580:PHE:HB3	2.02	0.40
1:B:735:LEU:HA	1:B:735:LEU:HD12	1.96	0.40
1:C:206:ASP:O	1:C:209:LEU:HB2	2.20	0.40
1:D:507:ARG:O	1:D:511:TRP:N	2.41	0.40
1:A:826:LYS:CD	1:A:827:VAL:H	2.34	0.40
1:B:109:GLU:O	1:B:113:GLN:HB3	2.21	0.40
1:B:1224:GLY:O	1:B:1225:LEU:HD23	2.22	0.40
1:B:426:VAL:HG13	1:B:433:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1123:GLU:O	1:C:1127:ILE:HG13	2.20	0.40
1:C:228:VAL:O	1:C:228:VAL:CG1	2.69	0.40
1:C:426:VAL:HG12	1:C:427:ARG:N	2.36	0.40
1:D:545:LEU:HA	1:D:545:LEU:HD22	1.83	0.40
1:D:783:SER:O	1:D:787:LYS:HG3	2.21	0.40
1:A:482:UNK:O	1:A:483:UNK:C	2.69	0.40
1:A:830:ARG:NH2	1:A:836:GLU:OE1	2.54	0.40
1:B:1123:GLU:O	1:B:1127:ILE:HG13	2.22	0.40
1:B:954:VAL:HG21	1:B:1141:LEU:HD12	2.03	0.40
1:B:182:MET:HE3	1:B:185:ILE:CD1	2.52	0.40
1:B:795:TYR:HB3	1:B:801:LEU:HD22	2.02	0.40
1:B:821:SER:O	1:B:823:LYS:N	2.54	0.40
1:B:962:GLU:HG3	1:B:1169:ARG:HE	1.86	0.40
1:C:969:ARG:NH2	1:C:972:LEU:CD2	2.80	0.40
1:D:310:LEU:HD21	1:D:314:LYS:HE3	2.04	0.40
1:D:317:LEU:HD12	1:D:320:MET:HE1	2.04	0.40
1:D:73:HIS:HE1	1:D:158:ASP:OD2	2.04	0.40
1:D:81:PHE:O	1:D:166:VAL:HA	2.22	0.40
1:A:1173:ILE:HA	1:A:1173:ILE:HD13	1.86	0.40
1:A:576:GLN:HG3	1:A:578:ILE:HG12	2.03	0.40
1:A:91:ARG:HA	1:A:94:MET:CG	2.51	0.40
1:B:96:GLN:HE22	1:B:100:ARG:HH21	1.66	0.40
1:B:1179:VAL:HA	1:B:1180:PRO:HD3	1.96	0.40
1:C:1232:ASN:HD22	1:C:1232:ASN:C	2.23	0.40
1:C:152:HIS:CD2	1:C:704:HIS:CE1	2.92	0.40
1:D:6:PHE:CE1	1:D:10:ILE:HD12	2.55	0.40
1:A:965:ILE:HD13	1:A:1122:VAL:HG13	2.04	0.40
1:A:264:ILE:HG23	1:A:267:SER:OG	2.22	0.40
1:A:339:LEU:HD11	1:A:570:VAL:HB	2.04	0.40
1:A:676:ASP:CB	1:A:711:ILE:CG2	2.99	0.40
1:C:591:GLN:HG2	1:C:591:GLN:O	2.20	0.40
1:D:81:PHE:HE2	1:D:161:TRP:CH2	2.40	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	1001/1155 (87%)	867 (87%)	98 (10%)	36 (4%)	3	13
1	B	998/1155 (86%)	839 (84%)	113 (11%)	46 (5%)	2	8
1	C	1008/1155 (87%)	855 (85%)	118 (12%)	35 (4%)	3	13
1	D	982/1155 (85%)	827 (84%)	117 (12%)	38 (4%)	3	11
All	All	3989/4620 (86%)	3388 (85%)	446 (11%)	155 (4%)	3	11

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	112	LEU
1	A	263	GLU
1	A	265	THR
1	A	353	LYS
1	A	527	THR
1	A	528	ASP
1	A	607	VAL
1	A	712	PRO
1	A	798	TRP
1	A	1093	VAL
1	A	1095	ASP
1	B	264	ILE
1	B	297	PRO
1	B	460	ASP
1	B	527	THR
1	B	596	LEU
1	B	701	GLU
1	B	712	PRO
1	B	716	GLU
1	B	1193	ILE
1	B	1235	ASP
1	C	111	ALA
1	C	112	LEU
1	C	113	GLN
1	C	428	ALA
1	C	606	VAL
1	C	607	VAL

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Mol	Chain	Res	Type
1	C	702	HIS
1	C	713	GLU
1	C	798	TRP
1	C	860	ASP
1	C	1138	GLN
1	D	264	ILE
1	D	267	SER
1	D	269	GLN
1	D	565	PRO
1	D	702	HIS
1	D	712	PRO
1	D	713	GLU
1	D	716	GLU
1	D	860	ASP
1	D	1193	ILE
1	D	1194	GLY
1	A	92	ALA
1	A	518	ASP
1	A	702	HIS
1	A	713	GLU
1	A	799	PRO
1	B	4	PRO
1	B	109	GLU
1	B	353	LYS
1	B	535	GLU
1	B	565	PRO
1	B	602	ASN
1	B	713	GLU
1	B	774	LEU
1	B	822	GLY
1	B	823	LYS
1	B	946	SER
1	B	981	PRO
1	B	1195	LYS
1	B	1213	PHE
1	C	528	ASP
1	C	712	PRO
1	C	715	MET
1	C	833	GLN
1	C	834	ASP
1	C	957	GLY
1	C	1105	VAL

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Mol	Chain	Res	Type
1	C	1107	VAL
1	D	106	MET
1	D	438	PHE
1	D	582	LYS
1	D	602	ASN
1	D	645	SER
1	D	1112	ASP
1	D	1236	ARG
1	A	193	ASP
1	A	596	LEU
1	A	735	LEU
1	A	860	ASP
1	A	861	ASP
1	B	262	GLU
1	B	404	ARG
1	B	538	VAL
1	B	607	VAL
1	B	717	ASN
1	B	798	TRP
1	B	824	LEU
1	B	972	LEU
1	B	1194	GLY
1	C	403	GLN
1	C	513	ASP
1	C	698	ASN
1	C	716	GLU
1	C	797	ARG
1	C	832	PRO
1	C	917	ILE
1	C	980	TYR
1	C	1104	PHE
1	C	1194	GLY
1	D	356	ASP
1	D	576	GLN
1	D	596	LEU
1	D	624	PRO
1	D	701	GLU
1	A	461	SER
1	A	664	SER
1	A	1108	SER
1	A	1111	SER
1	A	1116	LYS

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Mol	Chain	Res	Type
1	B	265	THR
1	B	646	PHE
1	B	861	ASP
1	B	878	SER
1	B	973	ASP
1	B	1138	GLN
1	C	1103	PRO
1	D	265	THR
1	D	605	PRO
1	D	798	TRP
1	D	1195	LYS
1	A	395	LYS
1	A	605	PRO
1	A	606	VAL
1	A	801	LEU
1	A	863	SER
1	B	106	MET
1	B	582	LYS
1	B	649	GLN
1	B	833	GLN
1	B	1111	SER
1	B	1217	LEU
1	C	714	SER
1	C	1235	ASP
1	D	4	PRO
1	D	92	ALA
1	D	303	LYS
1	D	714	SER
1	A	695	GLY
1	B	685	VAL
1	C	460	ASP
1	C	835	PHE
1	D	625	ASN
1	D	395	LYS
1	D	606	VAL
1	A	15	PRO
1	D	553	PRO
1	D	607	VAL
1	A	264	ILE
1	A	917	ILE
1	D	588	PRO
1	C	981	PRO

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Mol	Chain	Res	Type
1	D	917	ILE

### 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	922/1004 (92%)	799 (87%)	123 (13%)	4	11
1	B	919/1004 (92%)	787 (86%)	132 (14%)	3	9
1	C	927/1004 (92%)	804 (87%)	123 (13%)	4	11
1	D	905/1004 (90%)	775 (86%)	130 (14%)	3	9
All	All	3673/4016 (92%)	3165 (86%)	508 (14%)	3	10

All (508) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	10	ILE
1	A	24	SER
1	A	25	GLN
1	A	36	MET
1	A	42	ASN
1	A	55	LEU
1	A	63	LYS
1	A	96	GLN
1	A	98	ARG
1	A	112	LEU
1	A	113	GLN
1	A	114	LYS
1	A	137	THR
1	A	138	GLU
1	A	150	PHE
1	A	154	LYS
1	A	160	ARG
1	A	183	ASP
1	A	186	ARG

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Mol	Chain	Res	Type
1	A	192	GLU
1	A	227	GLU
1	A	229	THR
1	A	255	GLU
1	A	263	GLU
1	A	273	ASP
1	A	291	ASP
1	A	303	LYS
1	A	306	PHE
1	A	325	ASN
1	A	326	GLU
1	A	329	LYS
1	A	339	LEU
1	A	340	LYS
1	A	350	PHE
1	A	353	LYS
1	A	354	ASP
1	A	363	GLN
1	A	369	LEU
1	A	387	GLN
1	A	391	ILE
1	A	405	LYS
1	A	414	ASP
1	A	417	ILE
1	A	421	GLU
1	A	462	ILE
1	A	518	ASP
1	A	527	THR
1	A	534	THR
1	A	535	GLU
1	A	536	ASN
1	A	545	LEU
1	A	571	ILE
1	A	584	GLN
1	A	587	LYS
1	A	590	GLN
1	A	591	GLN
1	A	602	ASN
1	A	641	VAL
1	A	645	SER
1	A	660	ASP
1	A	664	SER

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Mol	Chain	Res	Type
1	A	702	HIS
1	A	706	ILE
1	A	708	ARG
1	A	710	PHE
1	A	711	ILE
1	A	717	ASN
1	A	735	LEU
1	A	744	LEU
1	A	747	THR
1	A	759	ASN
1	A	767	MET
1	A	773	ASP
1	A	785	LEU
1	A	796	SER
1	A	810	ILE
1	A	816	TYR
1	A	819	VAL
1	A	829	GLU
1	A	831	LYS
1	A	846	THR
1	A	852	GLN
1	A	860	ASP
1	A	862	ILE
1	A	869	VAL
1	A	904	ASN
1	A	907	GLU
1	A	917	ILE
1	A	918	ASN
1	A	932	ASP
1	A	948	THR
1	A	951	LYS
1	A	952	LEU
1	A	965	ILE
1	A	978	ARG
1	A	982	THR
1	A	983	GLN
1	A	1091	LYS
1	A	1095	ASP
1	A	1098	SER
1	A	1107	VAL
1	A	1108	SER
1	A	1109	LEU

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Mol	Chain	Res	Type
1	A	1110	GLU
1	A	1112	ASP
1	A	1113	SER
1	A	1119	MET
1	A	1128	LYS
1	A	1133	PRO
1	A	1143	LYS
1	A	1149	ILE
1	A	1150	LEU
1	A	1153	GLU
1	A	1155	SER
1	A	1178	LYS
1	A	1191	THR
1	A	1196	ASN
1	A	1198	SER
1	A	1216	ARG
1	A	1221	ARG
1	A	1232	ASN
1	A	1239	VAL
1	B	4	PRO
1	B	10	ILE
1	B	25	GLN
1	B	56	SER
1	B	57	GLU
1	B	59	GLU
1	B	62	SER
1	B	63	LYS
1	B	67	TYR
1	B	83	MET
1	B	96	GLN
1	B	104	THR
1	B	113	GLN
1	B	114	LYS
1	B	130	SER
1	B	131	ASN
1	B	149	TYR
1	B	159	THR
1	B	182	MET
1	B	183	ASP
1	B	195	ASN
1	B	226	GLU
1	B	252	ILE

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Mol	Chain	Res	Type
1	B	263	GLU
1	B	271	GLU
1	B	282	ILE
1	B	290	ASN
1	B	306	PHE
1	B	315	GLU
1	B	332	LEU
1	B	335	PHE
1	B	340	LYS
1	B	350	PHE
1	B	355	ILE
1	B	364	LEU
1	B	383	LEU
1	B	391	ILE
1	B	395	LYS
1	B	402	VAL
1	B	404	ARG
1	B	407	THR
1	B	417	ILE
1	B	448	LYS
1	B	449	SER
1	B	459	LEU
1	B	460	ASP
1	B	462	ILE
1	B	506	GLU
1	B	513	ASP
1	B	514	GLN
1	B	517	LYS
1	B	518	ASP
1	B	527	THR
1	B	529	SER
1	B	531	LYS
1	B	542	GLN
1	B	571	ILE
1	B	574	ILE
1	B	576	GLN
1	B	578	ILE
1	B	591	GLN
1	B	602	ASN
1	B	604	ILE
1	B	606	VAL
1	B	622	PHE

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Mol	Chain	Res	Type
1	B	626	GLU
1	B	651	ARG
1	B	669	LYS
1	B	684	GLN
1	B	691	THR
1	B	703	ASN
1	B	707	GLU
1	B	710	PHE
1	B	711	ILE
1	B	713	GLU
1	B	735	LEU
1	B	765	GLN
1	B	772	GLN
1	B	774	LEU
1	B	785	LEU
1	B	813	GLU
1	B	819	VAL
1	B	820	LYS
1	B	821	SER
1	B	825	THR
1	B	828	ILE
1	B	830	ARG
1	B	842	GLU
1	B	843	LEU
1	B	850	ASN
1	B	852	GLN
1	B	853	ARG
1	B	854	THR
1	B	860	ASP
1	B	879	ASP
1	B	890	ILE
1	B	903	LYS
1	B	917	ILE
1	B	918	ASN
1	B	932	ASP
1	B	953	THR
1	B	956	LYS
1	B	965	ILE
1	B	969	ARG
1	B	974	SER
1	B	978	ARG
1	B	979	PHE

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Mol	Chain	Res	Type
1	B	980	TYR
1	B	983	GLN
1	B	1093	VAL
1	B	1097	LEU
1	B	1098	SER
1	B	1109	LEU
1	B	1110	GLU
1	B	1112	ASP
1	B	1113	SER
1	B	1116	LYS
1	B	1118	SER
1	B	1128	LYS
1	B	1130	VAL
1	B	1139	LYS
1	B	1143	LYS
1	B	1149	ILE
1	B	1153	GLU
1	B	1163	ARG
1	B	1178	LYS
1	B	1191	THR
1	B	1193	ILE
1	B	1196	ASN
1	B	1197	VAL
1	B	1232	ASN
1	B	1239	VAL
1	C	4	PRO
1	C	17	ILE
1	C	25	GLN
1	C	26	ILE
1	C	38	SER
1	C	44	THR
1	C	54	ARG
1	C	55	LEU
1	C	58	GLU
1	C	59	GLU
1	C	62	SER
1	C	67	TYR
1	C	98	ARG
1	C	101	ARG
1	C	113	GLN
1	C	137	THR
1	C	143	LEU

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Mol	Chain	Res	Type
1	C	154	LYS
1	C	164	VAL
1	C	176	GLU
1	C	183	ASP
1	C	189	ARG
1	C	195	ASN
1	C	226	GLU
1	C	299	LEU
1	C	303	LYS
1	C	306	PHE
1	C	320	MET
1	C	321	ASP
1	C	339	LEU
1	C	351	GLU
1	C	354	ASP
1	C	355	ILE
1	C	357	VAL
1	C	376	THR
1	C	383	LEU
1	C	389	LYS
1	C	391	ILE
1	C	400	LYS
1	C	402	VAL
1	C	412	ASP
1	C	417	ILE
1	C	427	ARG
1	C	435	GLU
1	C	449	SER
1	C	513	ASP
1	C	526	ASP
1	C	527	THR
1	C	528	ASP
1	C	530	LEU
1	C	531	LYS
1	C	532	GLU
1	C	533	MET
1	C	536	ASN
1	C	591	GLN
1	C	595	VAL
1	C	602	ASN
1	C	604	ILE
1	C	606	VAL

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Mol	Chain	Res	Type
1	C	607	VAL
1	C	621	ASP
1	C	641	VAL
1	C	642	VAL
1	C	643	LYS
1	C	666	ASP
1	C	675	THR
1	C	688	VAL
1	C	699	ASP
1	C	701	GLU
1	C	706	ILE
1	C	707	GLU
1	C	708	ARG
1	C	710	PHE
1	C	711	ILE
1	C	715	MET
1	C	730	LEU
1	C	735	LEU
1	C	766	SER
1	C	772	GLN
1	C	782	LEU
1	C	784	ASP
1	C	785	LEU
1	C	810	ILE
1	C	814	THR
1	C	823	LYS
1	C	824	LEU
1	C	825	THR
1	C	826	LYS
1	C	830	ARG
1	C	833	GLN
1	C	836	GLU
1	C	841	ARG
1	C	842	GLU
1	C	852	GLN
1	C	858	LEU
1	C	859	LEU
1	C	861	ASP
1	C	887	ASN
1	C	907	GLU
1	C	917	ILE
1	C	918	ASN

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Mol	Chain	Res	Type
1	C	923	LYS
1	C	932	ASP
1	C	948	THR
1	C	952	LEU
1	C	968	VAL
1	C	969	ARG
1	C	977	LEU
1	C	1088	SER
1	C	1091	LYS
1	C	1097	LEU
1	C	1107	VAL
1	C	1109	LEU
1	C	1149	ILE
1	C	1150	LEU
1	C	1155	SER
1	C	1163	ARG
1	C	1178	LYS
1	C	1192	SER
1	C	1198	SER
1	C	1232	ASN
1	C	1236	ARG
1	C	1239	VAL
1	D	4	PRO
1	D	10	ILE
1	D	26	ILE
1	D	31	ASN
1	D	42	ASN
1	D	58	GLU
1	D	66	SER
1	D	96	GLN
1	D	98	ARG
1	D	113	GLN
1	D	154	LYS
1	D	160	ARG
1	D	164	VAL
1	D	186	ARG
1	D	195	ASN
1	D	221	PHE
1	D	228	VAL
1	D	254	ARG
1	D	262	GLU
1	D	265	THR

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Mol	Chain	Res	Type
1	D	268	VAL
1	D	280	ASP
1	D	291	ASP
1	D	306	PHE
1	D	312	THR
1	D	315	GLU
1	D	329	LYS
1	D	339	LEU
1	D	340	LYS
1	D	352	LYS
1	D	353	LYS
1	D	358	GLU
1	D	363	GLN
1	D	378	MET
1	D	383	LEU
1	D	389	LYS
1	D	402	VAL
1	D	405	LYS
1	D	406	VAL
1	D	412	ASP
1	D	417	ILE
1	D	423	LYS
1	D	427	ARG
1	D	438	PHE
1	D	440	LEU
1	D	448	LYS
1	D	449	SER
1	D	459	LEU
1	D	462	ILE
1	D	510	GLU
1	D	513	ASP
1	D	532	GLU
1	D	536	ASN
1	D	542	GLN
1	D	545	LEU
1	D	550	ARG
1	D	574	ILE
1	D	579	GLU
1	D	580	PHE
1	D	589	PHE
1	D	593	MET
1	D	596	LEU

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Mol	Chain	Res	Type
1	D	601	LYS
1	D	606	VAL
1	D	608	TYR
1	D	625	ASN
1	D	642	VAL
1	D	651	ARG
1	D	662	LYS
1	D	672	SER
1	D	679	PHE
1	D	680	ILE
1	D	703	ASN
1	D	707	GLU
1	D	709	GLU
1	D	710	PHE
1	D	711	ILE
1	D	713	GLU
1	D	715	MET
1	D	718	VAL
1	D	719	LYS
1	D	730	LEU
1	D	735	LEU
1	D	746	LEU
1	D	747	THR
1	D	764	GLN
1	D	772	GLN
1	D	774	LEU
1	D	784	ASP
1	D	797	ARG
1	D	803	GLU
1	D	813	GLU
1	D	821	SER
1	D	826	LYS
1	D	835	PHE
1	D	838	LYS
1	D	839	GLU
1	D	843	LEU
1	D	844	LYS
1	D	845	MET
1	D	863	SER
1	D	876	ARG
1	D	879	ASP
1	D	917	ILE

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Mol	Chain	Res	Type
1	D	918	ASN
1	D	926	LYS
1	D	946	SER
1	D	950	LEU
1	D	952	LEU
1	D	962	GLU
1	D	964	ASN
1	D	969	ARG
1	D	972	LEU
1	D	977	LEU
1	D	1107	VAL
1	D	1128	LYS
1	D	1130	VAL
1	D	1131	SER
1	D	1136	SER
1	D	1138	GLN
1	D	1143	LYS
1	D	1147	GLU
1	D	1149	ILE
1	D	1150	LEU
1	D	1155	SER
1	D	1161	SER
1	D	1175	ASP
1	D	1195	LYS
1	D	1232	ASN
1	D	1239	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	19	GLN
1	A	25	GLN
1	A	41	HIS
1	A	96	GLN
1	A	97	GLN
1	A	113	GLN
1	A	152	HIS
1	A	195	ASN
1	A	200	HIS
1	A	219	HIS
1	A	220	HIS

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Mol	Chain	Res	Type
1	A	311	GLN
1	A	319	HIS
1	A	325	ASN
1	A	327	GLN
1	A	362	GLN
1	A	363	GLN
1	A	366	ASN
1	A	386	GLN
1	A	387	GLN
1	A	446	HIS
1	A	590	GLN
1	A	625	ASN
1	A	759	ASN
1	A	770	HIS
1	A	833	GLN
1	A	850	ASN
1	A	918	ASN
1	A	945	ASN
1	A	983	GLN
1	A	1196	ASN
1	A	1212	ASN
1	A	1232	ASN
1	B	16	GLN
1	B	19	GLN
1	B	96	GLN
1	B	113	GLN
1	B	152	HIS
1	B	162	GLN
1	B	195	ASN
1	B	200	HIS
1	B	219	HIS
1	B	220	HIS
1	B	290	ASN
1	B	319	HIS
1	B	325	ASN
1	B	386	GLN
1	B	576	GLN
1	B	591	GLN
1	B	684	GLN
1	B	887	ASN
1	B	918	ASN
1	B	945	ASN

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Mol	Chain	Res	Type
1	B	964	ASN
1	B	975	GLN
1	B	1196	ASN
1	B	1232	ASN
1	C	16	GLN
1	C	19	GLN
1	C	25	GLN
1	C	96	GLN
1	C	97	GLN
1	C	152	HIS
1	C	195	ASN
1	C	200	HIS
1	C	219	HIS
1	C	220	HIS
1	C	269	GLN
1	C	290	ASN
1	C	311	GLN
1	C	319	HIS
1	C	325	ASN
1	C	386	GLN
1	C	387	GLN
1	C	429	ASN
1	C	446	HIS
1	C	514	GLN
1	C	590	GLN
1	C	591	GLN
1	C	702	HIS
1	C	770	HIS
1	C	850	ASN
1	C	852	GLN
1	C	887	ASN
1	C	904	ASN
1	C	918	ASN
1	C	945	ASN
1	C	975	GLN
1	C	1196	ASN
1	C	1232	ASN
1	D	16	GLN
1	D	19	GLN
1	D	25	GLN
1	D	73	HIS
1	D	97	GLN

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Mol	Chain	Res	Type
1	D	152	HIS
1	D	195	ASN
1	D	200	HIS
1	D	219	HIS
1	D	220	HIS
1	D	295	ASN
1	D	300	HIS
1	D	325	ASN
1	D	361	ASN
1	D	363	GLN
1	D	403	GLN
1	D	446	HIS
1	D	576	GLN
1	D	590	GLN
1	D	591	GLN
1	D	625	ASN
1	D	702	HIS
1	D	753	ASN
1	D	770	HIS
1	D	904	ASN
1	D	918	ASN
1	D	945	ASN
1	D	964	ASN
1	D	1212	ASN
1	D	1232	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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1023/1155 (88%)	-0.28	18 (1%) 68 67	44, 66, 97, 117	0
1	B	1020/1155 (88%)	-0.16	27 (2%) 56 53	36, 72, 124, 140	0
1	C	1030/1155 (89%)	-0.11	19 (1%) 68 67	51, 81, 109, 133	0
1	D	1004/1155 (86%)	0.01	39 (3%) 39 36	51, 87, 131, 151	0
All	All	4077/4620 (88%)	-0.14	103 (2%) 57 56	36, 76, 121, 151	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	LEU	6.0
1	B	627	VAL	5.8
1	A	229	THR	4.2
1	B	662	LYS	4.2
1	C	823	LYS	4.0
1	D	663	LEU	3.9
1	B	643	LYS	3.9
1	B	577	ASN	3.8
1	D	459	LEU	3.7
1	C	981	PRO	3.6
1	C	959	LEU	3.6
1	C	703	ASN	3.5
1	D	1107	VAL	3.5
1	C	284	VAL	3.4
1	C	694	ALA	3.4
1	D	460	ASP	3.4
1	D	284	VAL	3.3
1	A	823	LYS	3.3
1	A	702	HIS	3.3
1	D	979	PHE	3.2
1	B	46	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	229	THR	3.2
1	A	1195	LYS	3.2
1	B	578	ILE	3.1
1	D	46	GLY	3.1
1	A	351	GLU	3.1
1	B	661	ALA	3.0
1	D	399	LEU	3.0
1	A	1194	GLY	2.9
1	B	511	TRP	2.9
1	D	515	TYR	2.9
1	D	1193	ILE	2.9
1	B	285	LEU	2.9
1	D	662	LYS	2.9
1	B	983	GLN	2.8
1	C	822	GLY	2.8
1	A	46	GLY	2.8
1	C	1083	SER	2.8
1	B	312	THR	2.8
1	C	229	THR	2.8
1	A	983	GLN	2.8
1	D	688	VAL	2.7
1	B	649	GLN	2.7
1	D	338	TRP	2.7
1	D	353	LYS	2.7
1	C	309	LEU	2.6
1	D	112	LEU	2.6
1	B	642	VAL	2.6
1	D	600	SER	2.6
1	C	310	LEU	2.6
1	B	229	THR	2.6
1	C	1086	ALA	2.6
1	B	980	TYR	2.6
1	A	683	PRO	2.6
1	D	384	MET	2.5
1	D	419	PRO	2.5
1	A	309	LEU	2.5
1	A	284	VAL	2.4
1	D	288	ILE	2.4
1	B	287	THR	2.4
1	B	284	VAL	2.4
1	C	1191	THR	2.4
1	D	309	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	354	ASP	2.4
1	B	717	ASN	2.4
1	B	309	LEU	2.4
1	D	287	THR	2.3
1	D	823	LYS	2.3
1	C	681	PHE	2.3
1	A	310	LEU	2.3
1	D	281	PHE	2.3
1	B	140	MET	2.3
1	C	702	HIS	2.3
1	D	377	ARG	2.3
1	D	822	GLY	2.2
1	D	1192	SER	2.2
1	A	799	PRO	2.2
1	B	281	PHE	2.2
1	B	282	ILE	2.2
1	A	313	PHE	2.2
1	D	651	ARG	2.2
1	C	825	THR	2.2
1	B	310	LEU	2.1
1	A	352	LYS	2.1
1	B	112	LEU	2.1
1	D	113	GLN	2.1
1	B	693	LEU	2.1
1	D	310	LEU	2.1
1	D	282	ILE	2.1
1	D	285	LEU	2.1
1	A	54	ARG	2.1
1	B	515	TYR	2.1
1	D	898	ILE	2.1
1	D	307	PRO	2.1
1	B	1104	PHE	2.1
1	D	598	GLU	2.1
1	C	1136	SER	2.0
1	C	112	LEU	2.0
1	D	799	PRO	2.0
1	D	819	VAL	2.0
1	A	1106	VAL	2.0
1	C	687	THR	2.0
1	D	106	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MN	A	1254	1/1	0.97	0.16	67,67,67,67	0
2	MN	B	1254	1/1	0.97	0.14	67,67,67,67	0
2	MN	D	1254	1/1	0.98	0.21	75,75,75,75	0
2	MN	C	1254	1/1	0.99	0.17	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.