



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:33 PM UTC

PDB ID : 3PIE / pdb_00003pie
Title : Crystal structure of the 5'->3' exoribonuclease Xrn1, E178Q mutant
Authors : Chang, J.H.; Xiang, S.; Tong, L.
Deposited on : 2010-11-06
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

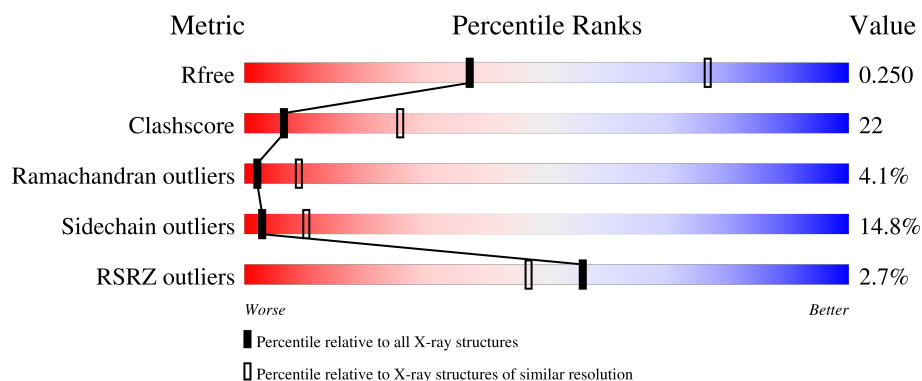
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1155	2% 52% 32% 7% 8%
1	B	1155	2% 49% 34% 7% 9%
1	C	1155	2% 52% 31% 8% 8%
1	D	1155	4% 49% 31% 7% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34009 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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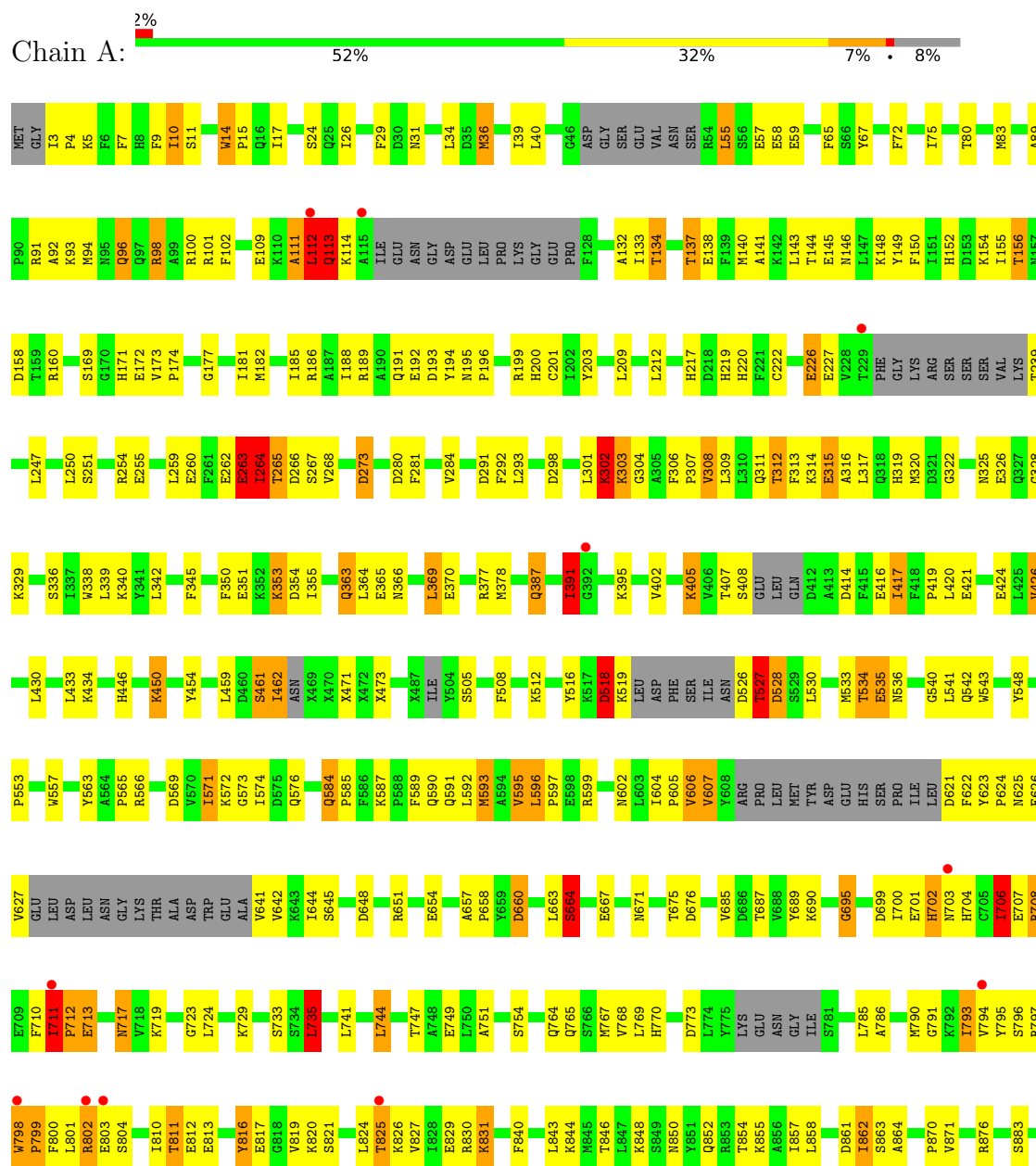
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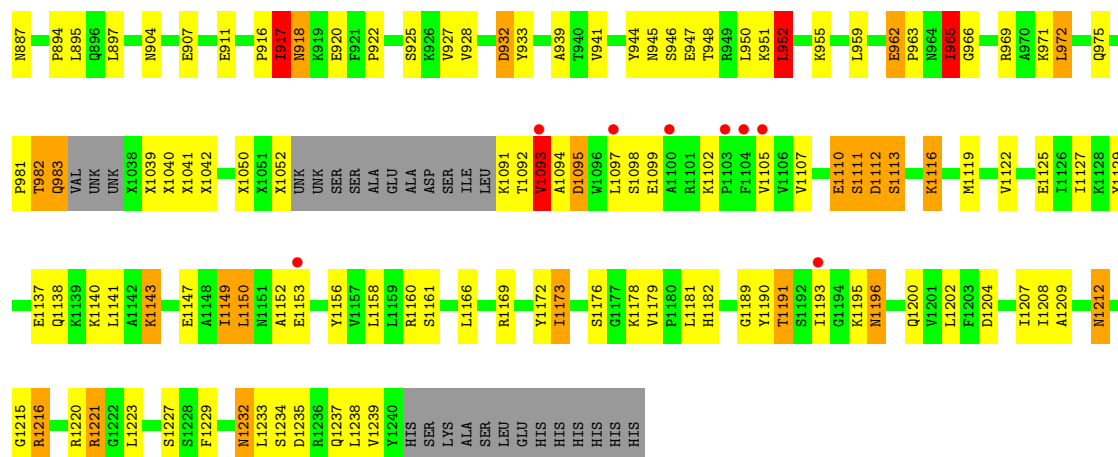
Chain	Residue	Modelled	Actual	Comment	Reference
D	474	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	475	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	476	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	477	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	478	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	479	UNK	-	SEE REMARK 999	UNP Q6CJ09
D	480	UNK	-	SEE REMARK 999	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

3 Residue-property plots

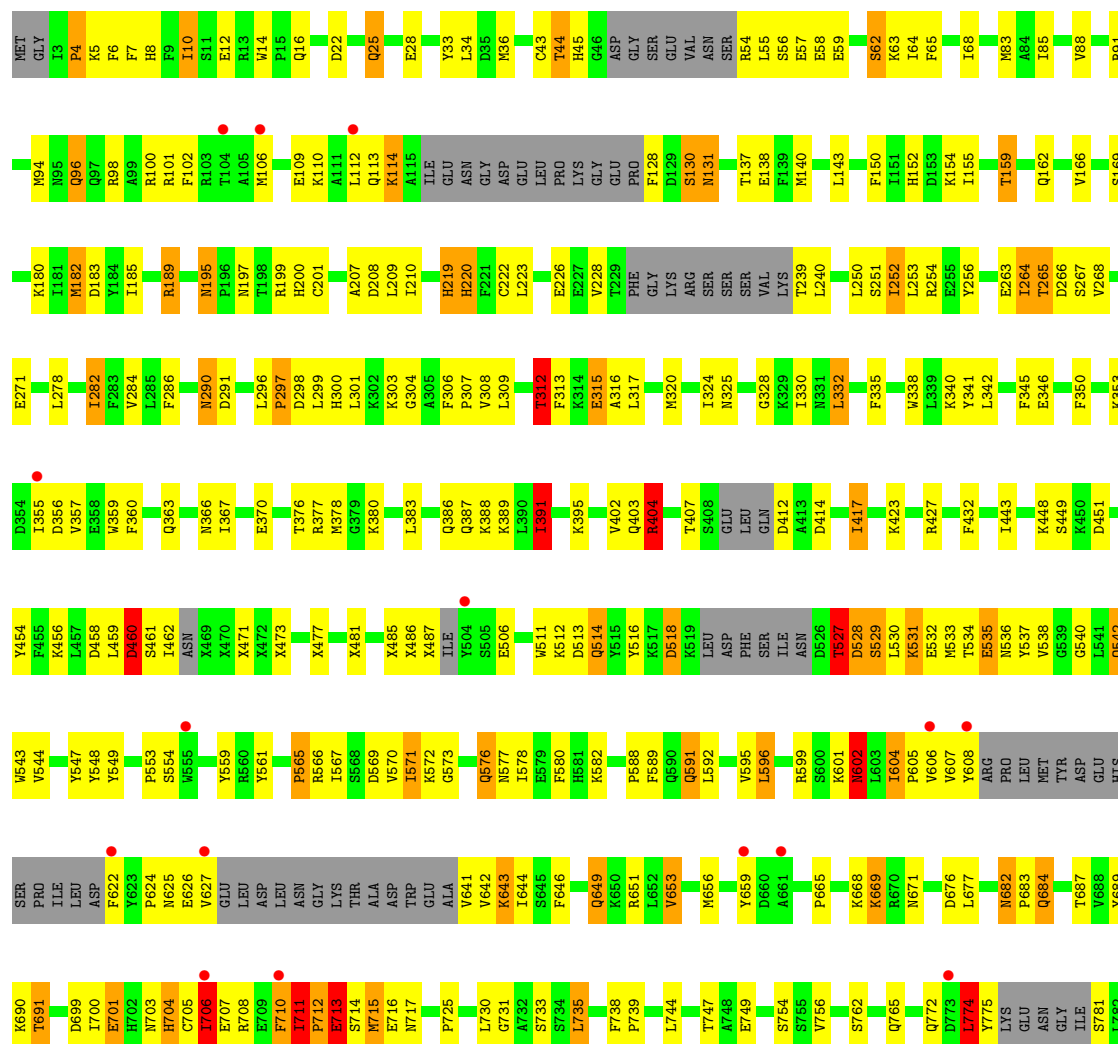
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

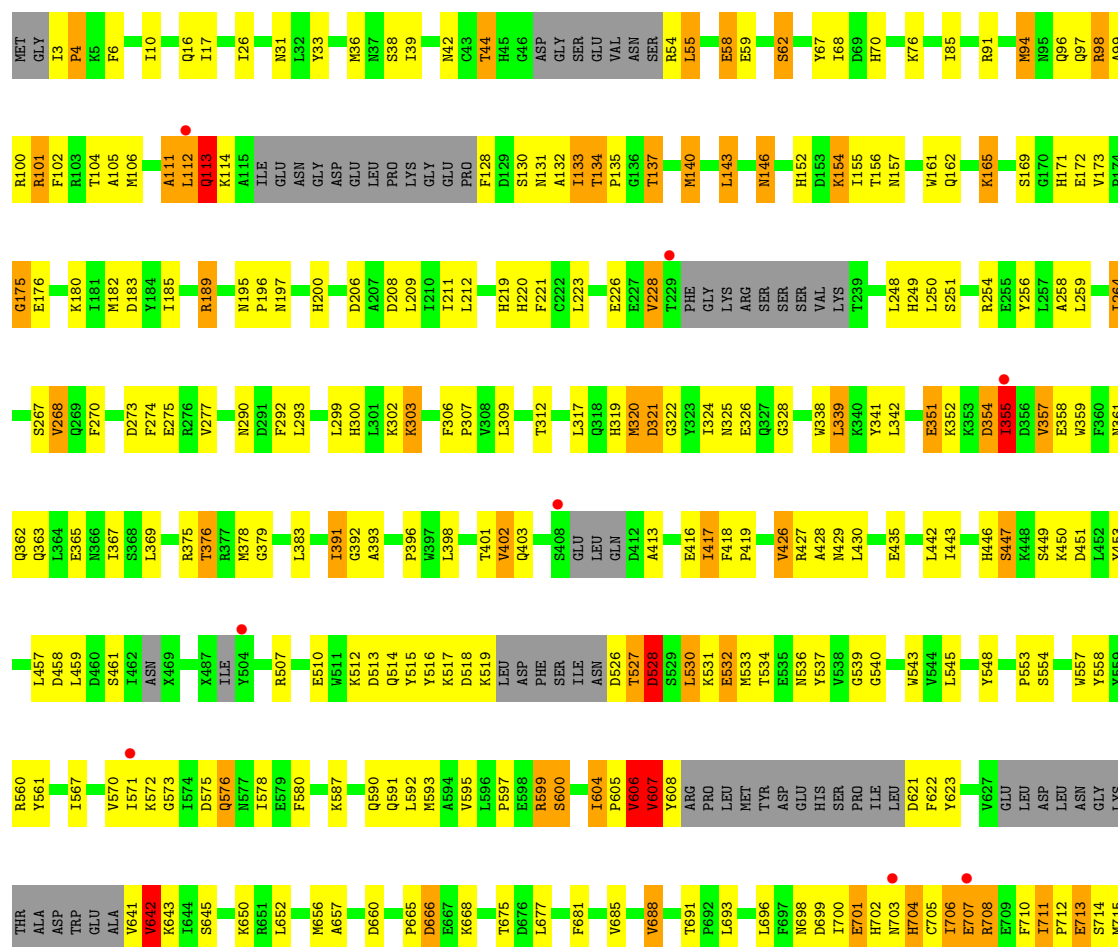
- Molecule 1: 5'→3' EXORIBONUCLEASE (Xrn1)





• Molecule 1: 5'->3' EXORIBONUCLEASE (Xrn1)









4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.72Å 132.29Å 143.89Å 110.07° 105.70° 103.75°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.90) 97.1 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.241 , 0.305 0.247 , 0.250	Depositor DCC
R_{free} test set	7868 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	34009	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.95	3/8567 (0.0%)	1.13	23/11553 (0.2%)
1	B	0.95	5/8543 (0.1%)	1.14	31/11521 (0.3%)
1	C	0.89	15/8613 (0.2%)	1.11	38/11616 (0.3%)
1	D	0.79	2/8409 (0.0%)	1.05	16/11337 (0.1%)
All	All	0.89	25/34132 (0.1%)	1.11	108/46027 (0.2%)

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 (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1086	ALA	C-O	9.93	1.35	1.24
1	C	1089	ILE	C-O	8.52	1.33	1.24
1	C	76	LYS	C-O	-8.39	1.20	1.23
1	B	711	ILE	CA-CB	7.73	1.65	1.53
1	D	711	ILE	CA-CB	7.14	1.61	1.53
1	B	1105	VAL	CA-CB	6.46	1.63	1.54
1	C	1084	ALA	N-CA	6.09	1.54	1.46
1	A	711	ILE	CA-CB	6.05	1.61	1.54
1	B	1193	ILE	CA-CB	5.79	1.62	1.54
1	C	1091	LYS	C-O	5.77	1.30	1.24
1	C	1093	VAL	CA-CB	5.76	1.60	1.54
1	C	1087	ASP	C-O	5.72	1.30	1.24
1	C	711	ILE	CA-CB	5.68	1.61	1.54
1	C	1088	SER	C-O	5.59	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1085	GLU	C-O	5.55	1.30	1.24
1	C	711	ILE	N-CA	5.46	1.52	1.46
1	D	1193	ILE	CA-CB	5.45	1.61	1.54
1	B	799	PRO	N-CA	5.44	1.54	1.47
1	C	1092	THR	C-O	5.38	1.30	1.24
1	A	825	THR	CA-CB	5.34	1.61	1.53
1	A	264	ILE	CA-CB	-5.26	1.47	1.54
1	C	1094	ALA	CA-CB	5.22	1.61	1.53
1	C	211	ILE	CA-CB	-5.08	1.48	1.54
1	B	798	TRP	CA-C	-5.05	1.46	1.52
1	C	175	GLY	N-CA	5.03	1.50	1.45

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	TRP	CA-C-N	9.42	131.62	119.84
1	A	14	TRP	C-N-CA	9.42	131.62	119.84
1	A	267	SER	N-CA-C	8.71	123.21	112.23
1	B	711	ILE	CA-C-N	8.65	130.66	119.84
1	B	711	ILE	C-N-CA	8.65	130.66	119.84
1	B	682	ASN	CA-C-N	8.46	130.41	119.84
1	B	682	ASN	C-N-CA	8.46	130.41	119.84
1	C	264	ILE	CB-CA-C	-8.31	99.28	112.16
1	B	798	TRP	CA-C-N	-8.01	109.83	119.84
1	B	798	TRP	C-N-CA	-8.01	109.83	119.84
1	B	1239	VAL	CB-CA-C	-7.98	102.51	111.45
1	C	738	PHE	CA-C-N	-7.74	112.37	120.03
1	C	738	PHE	C-N-CA	-7.74	112.37	120.03
1	C	798	TRP	CA-C-N	-7.63	110.62	119.47
1	C	798	TRP	C-N-CA	-7.63	110.62	119.47
1	D	1239	VAL	N-CA-C	7.61	120.05	109.55
1	A	664	SER	CA-C-N	-7.42	112.15	119.64
1	A	664	SER	C-N-CA	-7.42	112.15	119.64
1	D	296	LEU	CA-C-N	7.37	127.24	119.05
1	D	296	LEU	C-N-CA	7.37	127.24	119.05
1	C	599	ARG	N-CA-C	-7.28	104.00	114.12
1	C	1090	LEU	N-CA-C	-7.21	102.46	111.11
1	B	1239	VAL	N-CA-C	7.18	118.33	110.21
1	D	801	LEU	N-CA-C	7.15	119.53	110.24
1	B	1104	PHE	N-CA-C	7.01	120.61	108.76
1	C	642	VAL	N-CA-C	6.65	118.03	107.98
1	C	175	GLY	N-CA-C	6.54	118.16	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	THR	N-CA-C	-6.53	97.65	108.23
1	C	105	ALA	N-CA-C	-6.53	105.33	113.55
1	C	379	GLY	N-CA-C	-6.52	104.70	113.24
1	C	1088	SER	N-CA-C	-6.51	103.29	111.11
1	C	157	ASN	N-CA-C	6.43	121.17	112.88
1	D	1239	VAL	CB-CA-C	-6.38	102.82	111.63
1	B	528	ASP	N-CA-C	-6.38	102.90	112.54
1	A	3	ILE	CA-C-N	6.35	127.78	119.84
1	A	3	ILE	C-N-CA	6.35	127.78	119.84
1	A	134	THR	CA-C-N	-6.35	113.44	119.85
1	A	134	THR	C-N-CA	-6.35	113.44	119.85
1	C	1093	VAL	CB-CA-C	-6.27	103.67	111.70
1	C	710	PHE	N-CA-CB	-6.22	100.83	109.97
1	B	1095	ASP	N-CA-C	-6.22	105.83	113.41
1	B	827	VAL	N-CA-C	6.15	115.59	106.85
1	B	706	ILE	CB-CA-C	-6.15	102.78	111.38
1	C	913	GLU	CA-C-N	-6.10	113.39	119.92
1	C	913	GLU	C-N-CA	-6.10	113.39	119.92
1	A	281	PHE	N-CA-C	-6.08	105.35	112.89
1	D	1155	SER	N-CA-C	6.06	119.96	111.30
1	C	1089	ILE	N-CA-C	-6.01	104.65	110.42
1	B	932	ASP	N-CA-C	6.01	117.83	111.28
1	B	789	HIS	N-CA-C	6.00	121.66	113.97
1	A	264	ILE	CB-CA-C	-5.98	101.49	111.29
1	A	518	ASP	N-CA-C	5.93	123.43	110.80
1	D	3	ILE	CA-C-N	5.90	127.22	119.84
1	D	3	ILE	C-N-CA	5.90	127.22	119.84
1	C	915	LEU	CA-C-N	-5.89	113.89	120.14
1	C	915	LEU	C-N-CA	-5.89	113.89	120.14
1	B	549	TYR	N-CA-C	5.88	120.61	112.90
1	B	391	ILE	CB-CA-C	-5.82	104.28	112.14
1	C	1091	LYS	N-CA-C	-5.82	104.85	111.07
1	C	1150	LEU	N-CA-C	5.73	117.98	108.99
1	B	312	THR	N-CA-C	-5.64	105.05	111.14
1	C	965	ILE	N-CA-C	5.59	115.78	110.42
1	A	141	ALA	N-CA-C	-5.58	105.20	112.23
1	B	714	SER	N-CA-C	5.58	119.38	112.47
1	D	738	PHE	CA-C-N	5.55	125.46	119.85
1	D	738	PHE	C-N-CA	5.55	125.46	119.85
1	A	706	ILE	CB-CA-C	-5.51	102.99	111.31
1	A	625	ASN	N-CA-C	-5.50	105.19	113.89
1	C	355	ILE	CB-CA-C	-5.39	105.77	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	PRO	N-CA-C	5.38	123.56	112.47
1	D	646	PHE	N-CA-C	5.37	118.38	110.59
1	C	930	LEU	N-CA-C	-5.35	102.95	110.50
1	C	1157	VAL	CB-CA-C	-5.34	104.92	112.14
1	A	965	ILE	N-CA-C	5.34	115.54	110.42
1	B	952	LEU	N-CA-C	5.34	116.10	108.74
1	C	607	VAL	N-CA-C	5.33	120.43	109.34
1	D	421	GLU	N-CA-C	5.32	117.16	111.36
1	A	298	ASP	N-CA-C	5.32	118.78	111.54
1	B	904	ASN	N-CA-C	5.32	117.64	109.07
1	B	862	ILE	N-CA-C	5.31	114.91	107.37
1	B	704	HIS	N-CA-C	5.29	117.99	110.10
1	C	94	MET	N-CA-C	5.28	117.04	111.28
1	A	65	PHE	N-CA-C	-5.27	105.62	111.36
1	C	146	ASN	N-CA-C	5.26	116.71	110.97
1	C	869	VAL	CA-C-N	-5.22	113.31	119.84
1	C	869	VAL	C-N-CA	-5.22	113.31	119.84
1	B	814	THR	N-CA-C	5.21	117.30	109.23
1	B	25	GLN	N-CA-C	5.19	117.74	109.96
1	B	756	VAL	CB-CA-C	-5.19	105.19	111.88
1	A	145	GLU	N-CA-C	-5.18	105.08	111.40
1	C	980	TYR	N-CA-C	5.17	121.23	109.81
1	B	219	HIS	CA-C-N	-5.16	114.42	122.16
1	B	219	HIS	C-N-CA	-5.16	114.42	122.16
1	A	391	ILE	CB-CA-C	-5.15	105.11	112.22
1	A	426	VAL	CB-CA-C	-5.15	105.29	111.88
1	D	298	ASP	N-CA-C	5.15	116.62	110.44
1	D	947	GLU	N-CA-C	-5.12	107.09	113.38
1	B	529	SER	N-CA-C	-5.08	106.25	112.90
1	C	704	HIS	N-CA-C	5.07	117.58	110.23
1	B	1141	LEU	N-CA-C	5.06	116.82	110.24
1	C	44	THR	N-CA-C	5.06	117.92	111.69
1	B	711	ILE	N-CA-C	5.05	112.97	108.63
1	C	299	LEU	N-CA-C	-5.04	100.29	108.41
1	A	952	LEU	N-CA-C	5.04	116.65	109.14
1	C	173	VAL	CA-C-N	5.04	126.14	119.84
1	C	173	VAL	C-N-CA	5.04	126.14	119.84
1	D	1175	ASP	N-CA-CB	-5.04	102.73	110.44
1	D	385	LYS	N-CA-C	-5.02	107.11	113.18

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	391	0
1	B	8535	0	8385	380	0
1	C	8605	0	8450	366	0
1	D	8320	0	8233	344	0
All	All	34009	0	33472	1472	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 22.

All (1472) 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:744:LEU:HD22	1:A:798:TRP:CD1	1.67	1.28
1:D:917:ILE:H	1:D:917:ILE:CD1	1.56	1.15
1:A:798:TRP:HB3	1:A:799:PRO:CD	1.76	1.15
1:A:744:LEU:HD22	1:A:798:TRP:NE1	1.60	1.13
1:A:259:LEU:HB3	1:A:767:MET:HE3	1.28	1.12
1:D:917:ILE:HD13	1:D:917:ILE:N	1.56	1.11
1:A:595:VAL:O	1:A:596:LEU:HB2	1.49	1.11
1:A:264:ILE:HG21	1:A:268:VAL:HG13	1.19	1.10
1:B:296:LEU:HB3	1:B:297:PRO:HD3	1.33	1.10
1:D:965:ILE:HG12	1:D:1125:GLU:HG2	1.26	1.10
1:D:312:THR:HG22	1:D:338:TRP:HE1	1.14	1.10
1:A:312:THR:HG22	1:A:338:TRP:HE1	1.11	1.09
1:A:798:TRP:HB3	1:A:799:PRO:HD3	1.12	1.07
1:C:917:ILE:H	1:C:917:ILE:CD1	1.60	1.07
1:C:917:ILE:H	1:C:917:ILE:HD13	0.92	1.07
1:A:917:ILE:N	1:A:917:ILE:HD13	1.71	1.05
1:A:917:ILE:HD13	1:A:917:ILE:H	0.96	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:MET:HE3	1:D:212:LEU:HB3	1.35	1.04
1:B:152:HIS:CD2	1:B:706:ILE:HB	1.93	1.03
1:B:706:ILE:HD13	1:B:706:ILE:N	1.73	1.03
1:A:259:LEU:HB3	1:A:767:MET:CE	1.88	1.01
1:B:264:ILE:HG21	1:B:268:VAL:HG13	1.37	1.01
1:D:276:ARG:HH12	1:D:326:GLU:HA	1.23	1.01
1:A:917:ILE:H	1:A:917:ILE:CD1	1.74	1.00
1:B:325:ASN:HD21	1:B:328:GLY:H	1.03	1.00
1:C:708:ARG:HB3	1:C:708:ARG:HH11	1.28	0.99
1:C:917:ILE:HD13	1:C:917:ILE:N	1.76	0.98
1:C:708:ARG:HB2	1:C:708:ARG:NH1	1.78	0.98
1:C:708:ARG:HH11	1:C:708:ARG:CB	1.76	0.98
1:B:1204:ASP:O	1:B:1221:ARG:NH1	1.97	0.97
1:B:534:THR:HG22	1:B:573:GLY:HA3	1.47	0.96
1:D:712:PRO:O	1:D:713:GLU:HB3	1.64	0.96
1:B:296:LEU:HB3	1:B:297:PRO:CD	1.96	0.95
1:A:798:TRP:CB	1:A:799:PRO:HD3	1.96	0.94
1:B:152:HIS:HA	1:B:706:ILE:HG13	1.49	0.94
1:A:185:ILE:O	1:A:189:ARG:HG2	1.67	0.94
1:C:708:ARG:NH1	1:C:708:ARG:CB	2.31	0.94
1:B:883:SER:HA	1:B:911:GLU:HG2	1.50	0.93
1:B:934:ALA:HB2	1:B:956:LYS:HD2	1.50	0.92
1:A:264:ILE:HG21	1:A:268:VAL:CG1	1.98	0.92
1:A:264:ILE:CG2	1:A:268:VAL:HG13	1.99	0.92
1:B:965:ILE:HG12	1:B:1125:GLU:HG2	1.49	0.92
1:D:917:ILE:H	1:D:917:ILE:HD13	0.74	0.91
1:A:312:THR:CG2	1:A:338:TRP:HE1	1.82	0.91
1:A:1092:THR:O	1:A:1093:VAL:HG22	1.68	0.91
1:D:159:THR:HA	1:D:162:GLN:HG3	1.51	0.91
1:D:312:THR:HG22	1:D:338:TRP:NE1	1.86	0.91
1:B:220:HIS:HE1	1:B:735:LEU:H	1.19	0.90
1:B:16:GLN:HE22	1:B:799:PRO:CG	1.85	0.90
1:C:1102:LYS:HB2	1:C:1103:PRO:HD3	1.55	0.89
1:A:461:SER:O	1:A:462:ILE:HG13	1.72	0.89
1:A:862:ILE:HD12	1:A:862:ILE:H	1.36	0.89
1:B:689:TYR:HB2	1:B:704:HIS:CD2	2.08	0.89
1:A:887:ASN:HD21	1:A:1195:LYS:HB2	1.36	0.88
1:A:982:THR:HB	1:A:983:GLN:HE21	1.35	0.88
1:A:534:THR:HG23	1:A:573:GLY:HA3	1.53	0.88
1:C:587:LYS:H	1:C:590:GLN:HE21	1.21	0.87
1:D:687:THR:O	1:D:704:HIS:HB3	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:THR:HG22	1:A:338:TRP:NE1	1.89	0.87
1:D:303:LYS:HE3	1:D:356:ASP:HA	1.55	0.87
1:C:264:ILE:CG2	1:C:268:VAL:HG13	2.04	0.87
1:D:292:PHE:CD1	1:D:544:VAL:HG22	2.10	0.87
1:C:219:HIS:HD2	1:C:254:ARG:HH11	1.18	0.86
1:D:1107:VAL:HG22	1:D:1108:SER:H	1.39	0.86
1:C:965:ILE:HG12	1:C:1125:GLU:HG2	1.57	0.86
1:B:58:GLU:O	1:B:62:SER:HB2	1.75	0.86
1:D:527:THR:HG22	1:D:528:ASP:H	1.39	0.86
1:A:744:LEU:CD2	1:A:798:TRP:CD1	2.57	0.85
1:C:220:HIS:HE1	1:C:735:LEU:H	1.24	0.85
1:A:132:ALA:O	1:A:137:THR:HG21	1.76	0.85
1:B:36:MET:CE	1:B:83:MET:HG2	2.05	0.85
1:B:595:VAL:O	1:B:596:LEU:HB2	1.77	0.85
1:C:342:LEU:HB3	1:C:567:ILE:HG21	1.57	0.84
1:A:534:THR:HG23	1:A:573:GLY:CA	2.07	0.84
1:D:418:PHE:HB3	1:D:455:PHE:HB2	1.60	0.84
1:B:155:ILE:HD11	1:B:166:VAL:HG21	1.57	0.84
1:B:531:LYS:HB3	1:B:531:LYS:NZ	1.93	0.84
1:A:309:LEU:O	1:A:312:THR:HB	1.78	0.83
1:D:135:PRO:HG2	1:D:591:GLN:HE22	1.41	0.83
1:A:133:ILE:HA	1:A:140:MET:HE3	1.60	0.83
1:A:1052:UNK:CB	1:A:1091:LYS:O	2.26	0.83
1:C:134:THR:O	1:C:140:MET:HG3	1.77	0.83
1:C:838:LYS:HG2	1:C:842:GLU:OE2	1.79	0.82
1:A:530:LEU:O	1:A:534:THR:HB	1.78	0.82
1:B:592:LEU:O	1:B:595:VAL:O	1.97	0.82
1:C:969:ARG:HH21	1:C:972:LEU:HD22	1.44	0.82
1:C:398:LEU:HD13	1:C:442:LEU:HD21	1.60	0.82
1:D:152:HIS:CD2	1:D:706:ILE:HB	2.14	0.82
1:D:317:LEU:HA	1:D:320:MET:HE2	1.62	0.81
1:A:627:VAL:HG11	1:A:642:VAL:HG12	1.62	0.81
1:B:830:ARG:HG2	1:B:831:LYS:H	1.43	0.81
1:C:152:HIS:HD2	1:C:704:HIS:CE1	1.98	0.81
1:A:965:ILE:HG12	1:A:1125:GLU:HB3	1.61	0.81
1:A:1196:ASN:H	1:A:1196:ASN:HD22	1.28	0.81
1:B:945:ASN:ND2	1:B:1143:LYS:H	1.78	0.81
1:C:515:TYR:O	1:C:519:LYS:HG2	1.81	0.81
1:C:94:MET:HA	1:C:97:GLN:HE21	1.46	0.81
1:A:96:GLN:H	1:A:96:GLN:HE21	1.27	0.80
1:B:325:ASN:HD21	1:B:328:GLY:N	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:LEU:HB3	1:B:1118:SER:HB3	1.61	0.80
1:B:325:ASN:ND2	1:B:328:GLY:H	1.78	0.80
1:C:132:ALA:O	1:C:137:THR:HG21	1.80	0.80
1:C:152:HIS:HA	1:C:706:ILE:HG12	1.64	0.80
1:A:595:VAL:O	1:A:596:LEU:CB	2.30	0.79
1:B:918:ASN:HD21	1:D:452:LEU:HD13	1.45	0.79
1:B:1115:THR:OG1	1:B:1118:SER:HB2	1.81	0.79
1:C:969:ARG:HH21	1:C:972:LEU:CD2	1.95	0.79
1:B:16:GLN:HE22	1:B:799:PRO:HG3	1.47	0.79
1:A:621:ASP:O	1:A:622:PHE:HB2	1.83	0.79
1:A:1196:ASN:H	1:A:1196:ASN:ND2	1.78	0.79
1:C:938:GLU:HB2	1:C:1182:HIS:NE2	1.98	0.79
1:A:366:ASN:O	1:A:370:GLU:HG3	1.83	0.79
1:A:687:THR:O	1:A:704:HIS:HB3	1.83	0.78
1:B:1216:ARG:O	1:B:1216:ARG:HG3	1.83	0.78
1:D:220:HIS:HE1	1:D:735:LEU:H	1.28	0.78
1:C:516:TYR:CE2	1:C:533:MET:HE1	2.18	0.78
1:C:1038:UNK:O	1:C:1039:UNK:CB	2.32	0.78
1:A:864:ALA:HB3	1:A:895:LEU:HD12	1.65	0.78
1:A:1232:ASN:C	1:A:1232:ASN:HD22	1.92	0.78
1:D:299:LEU:HD22	1:D:309:LEU:HD11	1.64	0.78
1:B:220:HIS:CE1	1:B:735:LEU:H	2.02	0.77
1:C:961:ALA:O	1:C:1129:TYR:OH	2.01	0.77
1:D:1175:ASP:O	1:D:1175:ASP:OD1	2.03	0.77
1:C:701:GLU:O	1:C:703:ASN:N	2.13	0.77
1:B:91:ARG:HA	1:B:94:MET:HG2	1.65	0.77
1:C:593:MET:HE1	1:C:604:ILE:HD12	1.67	0.77
1:D:152:HIS:HD2	1:D:706:ILE:HB	1.50	0.77
1:B:36:MET:HE3	1:B:83:MET:HG2	1.66	0.77
1:B:303:LYS:HZ2	1:B:357:VAL:HG23	1.48	0.77
1:D:595:VAL:O	1:D:596:LEU:HB3	1.84	0.77
1:B:872:ASN:HD22	1:B:887:ASN:HD22	1.33	0.76
1:C:534:THR:HG22	1:C:573:GLY:HA3	1.68	0.76
1:D:91:ARG:HA	1:D:94:MET:HG2	1.66	0.76
1:D:574:ILE:O	1:D:574:ILE:HD12	1.85	0.76
1:C:219:HIS:HD2	1:C:254:ARG:NH1	1.82	0.76
1:A:36:MET:HG3	1:A:39:ILE:HD12	1.68	0.76
1:B:798:TRP:O	1:B:799:PRO:C	2.27	0.76
1:C:736:ALA:H	1:C:904:ASN:HD22	1.33	0.76
1:D:105:ALA:HB1	1:D:599:ARG:HD2	1.66	0.76
1:D:195:ASN:HD22	1:D:196:PRO:HD2	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ILE:HG22	1:B:265:THR:N	2.01	0.76
1:B:739:PRO:HG3	1:B:800:PHE:CE2	2.20	0.76
1:D:729:LYS:NZ	1:D:904:ASN:HD21	1.84	0.75
1:C:155:ILE:HB	1:C:706:ILE:HG13	1.69	0.75
1:D:1235:ASP:O	1:D:1237:GLN:HG3	1.87	0.75
1:D:850:ASN:O	1:D:854:THR:HB	1.87	0.75
1:C:155:ILE:HB	1:C:706:ILE:CG1	2.15	0.75
1:C:840:PHE:HD2	1:C:841:ARG:HE	1.35	0.75
1:C:101:ARG:NH1	1:C:134:THR:OG1	2.19	0.74
1:B:98:ARG:HG2	1:B:595:VAL:HA	1.69	0.74
1:B:960:ARG:NH2	1:B:1133:PRO:O	2.17	0.74
1:D:705:CYS:C	1:D:706:ILE:HD13	2.10	0.74
1:B:917:ILE:HD13	1:B:917:ILE:H	1.51	0.74
1:D:266:ASP:O	1:D:267:SER:HB3	1.86	0.74
1:D:706:ILE:HD13	1:D:706:ILE:N	2.02	0.74
1:B:534:THR:HG22	1:B:573:GLY:CA	2.17	0.74
1:A:534:THR:CG2	1:A:573:GLY:CA	2.65	0.74
1:D:155:ILE:HB	1:D:706:ILE:HG13	1.70	0.74
1:A:7:PHE:O	1:A:10:ILE:HG22	1.87	0.74
1:A:963:PRO:HD3	1:A:1129:TYR:CZ	2.22	0.74
1:A:1204:ASP:O	1:A:1221:ARG:NH1	2.20	0.74
1:D:962:GLU:HG3	1:D:1169:ARG:HE	1.53	0.74
1:A:543:TRP:CD1	1:A:553:PRO:HG2	2.23	0.73
1:C:98:ARG:NH1	1:C:645:SER:O	2.21	0.73
1:B:264:ILE:CG2	1:B:268:VAL:HG13	2.18	0.73
1:C:958:SER:HB2	1:C:1134:ASP:OD1	1.87	0.73
1:C:768:VAL:HG11	1:C:858:LEU:HD22	1.71	0.73
1:D:91:ARG:HA	1:D:94:MET:CG	2.18	0.73
1:D:676:ASP:HB2	1:D:711:ILE:HG22	1.70	0.73
1:B:16:GLN:NE2	1:B:799:PRO:HG2	2.04	0.73
1:B:152:HIS:HD2	1:B:704:HIS:CE1	2.06	0.73
1:D:334:ARG:HA	1:D:337:ILE:HD12	1.71	0.73
1:A:826:LYS:HG3	1:A:827:VAL:H	1.53	0.73
1:B:54:ARG:HD2	1:B:128:PHE:N	2.04	0.73
1:C:539:GLY:HA2	1:C:578:ILE:HD13	1.70	0.73
1:B:16:GLN:HE22	1:B:799:PRO:HG2	1.53	0.72
1:B:665:PRO:HA	1:B:668:LYS:HB2	1.71	0.72
1:D:691:THR:HG22	1:D:699:ASP:OD2	1.89	0.72
1:D:969:ARG:HD2	1:D:1121:ALA:HB3	1.70	0.72
1:A:461:SER:C	1:A:462:ILE:HG13	2.13	0.72
1:B:705:CYS:C	1:B:706:ILE:HD13	2.13	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:GLU:HG2	1:B:1138:GLN:H	1.53	0.72
1:A:606:VAL:O	1:A:607:VAL:HG23	1.89	0.72
1:D:33:TYR:OH	1:D:200:HIS:HD2	1.72	0.72
1:A:826:LYS:HG3	1:A:827:VAL:N	2.03	0.72
1:C:33:TYR:OH	1:C:200:HIS:HD2	1.71	0.72
1:C:815:VAL:HG11	1:C:830:ARG:NH1	2.04	0.72
1:D:395:LYS:HB3	1:D:396:PRO:CD	2.19	0.72
1:B:706:ILE:N	1:B:706:ILE:CD1	2.49	0.72
1:D:152:HIS:HE1	1:D:708:ARG:HE	1.38	0.72
1:B:298:ASP:HB3	1:B:300:HIS:HE1	1.55	0.72
1:C:883:SER:HA	1:C:911:GLU:HG2	1.71	0.72
1:D:299:LEU:HD22	1:D:309:LEU:CD1	2.19	0.72
1:B:1145:PRO:HB2	1:B:1147:GLU:OE1	1.89	0.71
1:D:137:THR:HG22	1:D:138:GLU:H	1.54	0.71
1:D:952:LEU:HD11	1:D:1144:VAL:HG21	1.72	0.71
1:A:797:ARG:O	1:A:798:TRP:C	2.33	0.71
1:D:292:PHE:HD1	1:D:544:VAL:HG22	1.55	0.71
1:C:707:GLU:N	1:C:707:GLU:OE1	2.24	0.71
1:B:36:MET:HE1	1:B:83:MET:HG2	1.72	0.70
1:D:276:ARG:NH1	1:D:326:GLU:HA	2.02	0.70
1:D:395:LYS:HB3	1:D:396:PRO:HD3	1.72	0.70
1:A:156:THR:HG23	1:A:703:ASN:O	1.91	0.70
1:A:1189:GLY:O	1:A:1200:GLN:HB2	1.92	0.70
1:C:152:HIS:CE1	1:C:708:ARG:HG2	2.26	0.70
1:A:952:LEU:HD13	1:A:1149:ILE:HD11	1.74	0.70
1:C:137:THR:HG22	1:C:140:MET:H	1.55	0.69
1:A:264:ILE:O	1:A:266:ASP:N	2.25	0.69
1:C:688:VAL:HG13	1:C:701:GLU:HA	1.73	0.69
1:D:701:GLU:C	1:D:703:ASN:H	2.00	0.69
1:D:756:VAL:HG23	1:D:853:ARG:HG2	1.73	0.69
1:A:1237:GLN:O	1:A:1238:LEU:HD23	1.91	0.69
1:B:195:ASN:ND2	1:B:197:ASN:H	1.89	0.69
1:A:945:ASN:ND2	1:A:1143:LYS:H	1.90	0.69
1:C:220:HIS:CE1	1:C:735:LEU:H	2.10	0.69
1:A:729:LYS:HB3	1:A:733:SER:O	1.93	0.69
1:C:212:LEU:HD21	1:C:548:TYR:CD1	2.27	0.69
1:C:514:GLN:NE2	1:C:517:LYS:HD2	2.08	0.69
1:B:626:GLU:O	1:B:627:VAL:HG23	1.92	0.69
1:D:1107:VAL:HG13	1:D:1108:SER:O	1.93	0.69
1:A:593:MET:HE3	1:A:604:ILE:HD13	1.73	0.69
1:A:96:GLN:HE21	1:A:96:GLN:N	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ASN:O	1:D:149:TYR:HB3	1.94	0.68
1:A:706:ILE:N	1:A:706:ILE:HD12	2.09	0.68
1:B:928:VAL:HG21	1:B:1173:ILE:HG22	1.74	0.68
1:B:945:ASN:HD22	1:B:1143:LYS:H	1.40	0.68
1:B:417:ILE:HG13	1:B:454:TYR:CD1	2.29	0.68
1:B:830:ARG:HG2	1:B:831:LYS:N	2.06	0.68
1:D:221:PHE:HB3	1:D:250:LEU:HD12	1.74	0.68
1:B:312:THR:HG22	1:B:338:TRP:HE1	1.56	0.68
1:A:58:GLU:HG3	1:A:59:GLU:N	2.07	0.68
1:B:531:LYS:HB3	1:B:531:LYS:HZ3	1.58	0.68
1:B:963:PRO:HD3	1:B:1129:TYR:CZ	2.28	0.68
1:C:1234:SER:O	1:C:1235:ASP:HB3	1.92	0.68
1:A:982:THR:HB	1:A:983:GLN:NE2	2.09	0.68
1:B:16:GLN:NE2	1:B:799:PRO:CG	2.57	0.68
1:C:256:TYR:HA	1:C:259:LEU:HD12	1.75	0.68
1:D:391:ILE:HG22	1:D:436:PHE:HE1	1.59	0.68
1:B:917:ILE:HG13	1:B:947:GLU:O	1.93	0.67
1:C:706:ILE:N	1:C:706:ILE:HD12	2.10	0.67
1:D:701:GLU:C	1:D:703:ASN:N	2.51	0.67
1:A:111:ALA:O	1:A:112:LEU:C	2.37	0.67
1:B:300:HIS:HB2	1:B:360:PHE:CZ	2.29	0.67
1:B:917:ILE:HD13	1:B:917:ILE:N	2.09	0.67
1:C:264:ILE:HG21	1:C:268:VAL:HG13	1.76	0.67
1:C:1160:ARG:HG3	1:C:1227:SER:OG	1.94	0.67
1:A:55:LEU:HD12	1:A:55:LEU:H	1.60	0.67
1:D:391:ILE:HG22	1:D:436:PHE:CE1	2.30	0.67
1:B:199:ARG:HG2	1:B:738:PHE:CZ	2.30	0.67
1:B:1182:HIS:O	1:B:1183:SER:C	2.37	0.67
1:C:862:ILE:HD12	1:C:862:ILE:H	1.59	0.67
1:A:535:GLU:HG2	1:A:576:GLN:CD	2.20	0.67
1:C:152:HIS:HE1	1:C:708:ARG:HG2	1.58	0.67
1:C:1213:PHE:O	1:C:1216:ARG:NH1	2.27	0.67
1:A:1093:VAL:HB	1:A:1094:ALA:HA	1.76	0.67
1:A:928:VAL:HG21	1:A:1173:ILE:HG23	1.78	0.66
1:B:918:ASN:ND2	1:D:452:LEU:HD13	2.09	0.66
1:D:807:LEU:HD11	1:D:869:VAL:HG13	1.76	0.66
1:D:1138:GLN:O	1:D:1138:GLN:HG2	1.93	0.66
1:A:262:GLU:O	1:A:264:ILE:N	2.28	0.66
1:A:798:TRP:O	1:A:799:PRO:C	2.37	0.66
1:A:199:ARG:HD3	1:A:735:LEU:HD23	1.76	0.66
1:A:627:VAL:HG11	1:A:642:VAL:CG1	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ARG:O	1:B:570:VAL:HG23	1.95	0.66
1:B:219:HIS:HD2	1:B:254:ARG:HE	1.43	0.66
1:D:156:THR:N	1:D:706:ILE:HD11	2.10	0.66
1:A:712:PRO:O	1:A:713:GLU:CB	2.44	0.66
1:B:946:SER:OG	1:B:947:GLU:N	2.26	0.66
1:D:676:ASP:HB2	1:D:711:ILE:CG2	2.25	0.66
1:C:152:HIS:O	1:C:706:ILE:CD1	2.44	0.66
1:D:171:HIS:CE1	1:D:172:GLU:OE2	2.49	0.66
1:D:195:ASN:HB3	1:D:198:THR:OG1	1.96	0.66
1:A:648:ASP:OD1	1:A:651:ARG:HB2	1.96	0.65
1:D:1232:ASN:C	1:D:1232:ASN:HD22	2.03	0.65
1:A:1232:ASN:HD22	1:A:1233:LEU:N	1.95	0.65
1:B:140:MET:HE1	1:B:143:LEU:HD13	1.78	0.65
1:B:303:LYS:NZ	1:B:357:VAL:HG23	2.11	0.65
1:A:826:LYS:CG	1:A:827:VAL:H	2.10	0.65
1:A:254:ARG:HH22	1:A:724:LEU:HD21	1.60	0.65
1:A:786:ALA:O	1:A:790:MET:HB2	1.97	0.65
1:C:840:PHE:O	1:C:844:LYS:HB2	1.97	0.65
1:D:746:LEU:CD1	1:D:769:LEU:HD22	2.26	0.65
1:C:312:THR:HG22	1:C:338:TRP:NE1	2.12	0.65
1:C:312:THR:HG22	1:C:338:TRP:CD1	2.31	0.65
1:D:512:LYS:O	1:D:516:TYR:CD1	2.49	0.65
1:D:712:PRO:O	1:D:713:GLU:CB	2.43	0.65
1:B:335:PHE:O	1:B:335:PHE:CD1	2.50	0.65
1:B:837:ARG:O	1:B:841:ARG:HG2	1.97	0.65
1:B:159:THR:OG1	1:B:1175:ASP:HB3	1.95	0.65
1:B:290:ASN:N	1:B:290:ASN:ND2	2.44	0.65
1:D:357:VAL:HG12	1:D:361:ASN:HD21	1.61	0.65
1:A:584:GLN:HG2	1:A:585:PRO:HD2	1.79	0.65
1:B:152:HIS:HA	1:B:706:ILE:CG1	2.26	0.64
1:C:96:GLN:NE2	1:C:100:ARG:HH21	1.95	0.64
1:C:708:ARG:HB2	1:C:708:ARG:CZ	2.27	0.64
1:D:330:ILE:HD12	1:D:542:GLN:HG2	1.78	0.64
1:D:729:LYS:HZ3	1:D:904:ASN:HD21	1.43	0.64
1:A:250:LEU:O	1:A:254:ARG:HG3	1.97	0.64
1:B:691:THR:HG22	1:B:699:ASP:OD1	1.97	0.64
1:C:768:VAL:CG1	1:C:858:LEU:HD22	2.27	0.64
1:D:945:ASN:ND2	1:D:1143:LYS:H	1.96	0.64
1:B:298:ASP:HB3	1:B:300:HIS:CE1	2.33	0.64
1:C:36:MET:HE1	1:C:68:ILE:CD1	2.27	0.64
1:C:165:LYS:HB3	1:C:165:LYS:HZ3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:837:ARG:HD3	1:C:841:ARG:HH22	1.62	0.64
1:C:1086:ALA:HA	1:C:1089:ILE:HD12	1.80	0.64
1:C:248:LEU:HD23	1:C:249:HIS:N	2.12	0.64
1:C:264:ILE:HG23	1:C:268:VAL:HG13	1.79	0.64
1:C:320:MET:HE1	1:C:324:ILE:HG13	1.80	0.64
1:C:701:GLU:C	1:C:703:ASN:H	2.05	0.64
1:A:155:ILE:HB	1:A:706:ILE:CG1	2.28	0.64
1:D:91:ARG:HG2	1:D:558:TYR:HB3	1.78	0.64
1:B:1147:GLU:CD	1:B:1147:GLU:H	2.06	0.64
1:C:290:ASN:HD22	1:C:292:PHE:H	1.46	0.64
1:B:278:LEU:O	1:B:282:ILE:HD12	1.98	0.63
1:B:676:ASP:HB3	1:B:711:ILE:HG22	1.80	0.63
1:B:312:THR:HG23	1:B:341:TYR:HB3	1.80	0.63
1:B:933:TYR:CE1	1:B:956:LYS:HD3	2.33	0.63
1:C:691:THR:HG22	1:C:699:ASP:OD1	1.98	0.63
1:C:1204:ASP:O	1:C:1221:ARG:NH1	2.32	0.63
1:D:25:GLN:NE2	1:D:906:ASP:OD2	2.32	0.63
1:A:156:THR:CG2	1:A:703:ASN:O	2.47	0.63
1:A:516:TYR:CE2	1:A:533:MET:HE1	2.34	0.63
1:B:290:ASN:N	1:B:290:ASN:HD22	1.95	0.63
1:B:533:MET:HA	1:B:561:TYR:CE2	2.34	0.63
1:C:815:VAL:HG11	1:C:830:ARG:HH11	1.62	0.63
1:A:802:ARG:HD2	1:A:870:PRO:HB2	1.80	0.63
1:A:922:PRO:O	1:A:925:SER:HB3	1.97	0.63
1:B:965:ILE:HD12	1:B:966:GLY:H	1.62	0.63
1:C:156:THR:N	1:C:706:ILE:HD11	2.13	0.63
1:D:312:THR:HG21	1:D:342:LEU:HD23	1.80	0.63
1:B:403:GLN:O	1:B:404:ARG:HB2	1.97	0.62
1:C:111:ALA:O	1:C:113:GLN:N	2.31	0.62
1:C:155:ILE:CG2	1:C:706:ILE:HG13	2.28	0.62
1:C:219:HIS:CD2	1:C:254:ARG:HH11	2.09	0.62
1:C:729:LYS:HD2	1:C:735:LEU:HD13	1.81	0.62
1:A:93:LYS:O	1:A:96:GLN:HG2	1.98	0.62
1:A:793:ILE:O	1:A:793:ILE:HG22	1.97	0.62
1:D:957:GLY:HA2	1:D:1136:SER:HB2	1.80	0.62
1:A:58:GLU:OE1	1:A:695:GLY:HA3	1.99	0.62
1:B:881:SER:HB3	1:B:914:PRO:HD3	1.80	0.62
1:A:1193:ILE:HB	1:A:1196:ASN:OD1	2.00	0.62
1:B:155:ILE:CG2	1:B:706:ILE:HD12	2.30	0.62
1:B:622:PHE:HD2	1:B:622:PHE:O	1.83	0.62
1:D:595:VAL:O	1:D:596:LEU:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:LEU:HD11	1:D:769:LEU:HD22	1.80	0.62
1:A:155:ILE:HB	1:A:706:ILE:HG13	1.80	0.62
1:A:219:HIS:CE1	1:A:251:SER:HB2	2.34	0.62
1:C:1084:ALA:O	1:C:1085:GLU:C	2.43	0.62
1:D:33:TYR:OH	1:D:200:HIS:CD2	2.52	0.62
1:B:423:LYS:O	1:B:427:ARG:HG2	2.00	0.62
1:C:831:LYS:O	1:C:833:GLN:N	2.26	0.62
1:B:443:ILE:HG13	1:B:458:ASP:HB2	1.81	0.62
1:C:1102:LYS:CB	1:C:1103:PRO:HD3	2.26	0.62
1:C:949:ARG:HE	1:C:1145:PRO:HB3	1.65	0.62
1:A:820:LYS:HA	1:A:825:THR:HG22	1.82	0.62
1:C:325:ASN:HD21	1:C:328:GLY:H	1.47	0.62
1:D:512:LYS:O	1:D:516:TYR:HD1	1.82	0.62
1:D:965:ILE:CG1	1:D:1125:GLU:HG2	2.16	0.61
1:A:862:ILE:HD12	1:A:862:ILE:N	2.13	0.61
1:C:309:LEU:O	1:C:312:THR:HB	1.99	0.61
1:B:312:THR:HG22	1:B:338:TRP:NE1	2.14	0.61
1:C:91:ARG:HA	1:C:94:MET:HG3	1.83	0.61
1:C:307:PRO:HG2	1:C:764:GLN:HG2	1.81	0.61
1:D:22:ASP:OD2	1:D:24:SER:HB3	2.01	0.61
1:D:879:ASP:OD1	1:D:879:ASP:N	2.32	0.61
1:A:152:HIS:HD2	1:A:704:HIS:NE2	1.98	0.61
1:D:945:ASN:OD1	1:D:951:LYS:HD2	2.00	0.61
1:A:701:GLU:O	1:A:704:HIS:N	2.34	0.61
1:B:981:PRO:HB3	1:B:1037:UNK:CB	2.31	0.61
1:D:94:MET:HE1	1:D:591:GLN:HG3	1.81	0.61
1:D:325:ASN:HD21	1:D:328:GLY:CA	2.14	0.61
1:D:390:LEU:HD11	1:D:455:PHE:HE1	1.66	0.61
1:C:97:GLN:O	1:C:101:ARG:HB2	2.01	0.61
1:A:962:GLU:HG3	1:A:1169:ARG:HE	1.66	0.61
1:B:601:LYS:O	1:B:604:ILE:HD11	2.01	0.61
1:C:228:VAL:HG12	1:C:228:VAL:O	2.01	0.61
1:A:876:ARG:NH1	1:A:920:GLU:OE2	2.34	0.60
1:A:955:LYS:HG3	1:A:1138:GLN:HG2	1.82	0.60
1:A:1208:ILE:HA	1:A:1220:ARG:HH12	1.65	0.60
1:D:929:PHE:HD1	1:D:1149:ILE:CD1	2.14	0.60
1:A:259:LEU:CB	1:A:767:MET:CE	2.72	0.60
1:A:307:PRO:HG2	1:A:764:GLN:HG2	1.82	0.60
1:B:601:LYS:O	1:B:604:ILE:CD1	2.49	0.60
1:B:785:LEU:HD23	1:B:789:HIS:HD2	1.66	0.60
1:B:1181:LEU:O	1:B:1182:HIS:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLN:NE2	1:C:799:PRO:HG3	2.16	0.60
1:C:512:LYS:C	1:C:514:GLN:H	2.09	0.60
1:C:770:HIS:CE1	1:C:858:LEU:HD23	2.37	0.60
1:C:1232:ASN:ND2	1:C:1234:SER:O	2.35	0.60
1:D:701:GLU:O	1:D:703:ASN:N	2.34	0.60
1:D:948:THR:HG22	1:D:1146:ARG:NH2	2.15	0.60
1:C:917:ILE:CD1	1:C:947:GLU:O	2.49	0.60
1:D:534:THR:HG22	1:D:573:GLY:HA3	1.82	0.60
1:A:320:MET:HE3	1:A:322:GLY:O	2.01	0.60
1:B:918:ASN:H	1:B:918:ASN:HD22	1.48	0.60
1:B:1193:ILE:CG2	1:B:1193:ILE:O	2.49	0.60
1:C:152:HIS:O	1:C:706:ILE:HD13	2.01	0.60
1:C:312:THR:HG22	1:C:338:TRP:HE1	1.64	0.60
1:C:706:ILE:HG22	1:C:707:GLU:N	2.16	0.60
1:A:301:LEU:C	1:A:303:LYS:H	2.09	0.60
1:B:320:MET:HE1	1:B:324:ILE:HG13	1.82	0.60
1:D:210:ILE:HA	1:D:223:LEU:CD1	2.32	0.60
1:A:416:GLU:HB2	1:C:951:LYS:NZ	2.17	0.60
1:B:595:VAL:O	1:B:596:LEU:CB	2.48	0.60
1:C:949:ARG:HD3	1:C:1143:LYS:O	2.01	0.60
1:C:1181:LEU:O	1:C:1182:HIS:HB2	2.00	0.60
1:A:969:ARG:NH1	1:A:972:LEU:HD23	2.17	0.60
1:A:1212:ASN:ND2	1:A:1215:GLY:H	2.00	0.60
1:B:512:LYS:HD2	1:B:566:ARG:HG3	1.83	0.60
1:C:393:ALA:HB1	1:C:418:PHE:HZ	1.67	0.60
1:D:373:ARG:O	1:D:376:THR:OG1	2.20	0.59
1:A:209:LEU:HD23	1:A:212:LEU:HD12	1.83	0.59
1:D:928:VAL:HG21	1:D:1173:ILE:HG22	1.84	0.59
1:C:1189:GLY:O	1:C:1200:GLN:HB2	2.02	0.59
1:A:516:TYR:OH	1:A:569:ASP:OD2	2.12	0.59
1:B:300:HIS:HB2	1:B:360:PHE:HZ	1.67	0.59
1:A:312:THR:CG2	1:A:338:TRP:NE1	2.54	0.59
1:A:794:VAL:HG22	1:A:804:SER:O	2.02	0.59
1:A:798:TRP:CE3	1:A:799:PRO:HD3	2.38	0.59
1:B:152:HIS:CD2	1:B:704:HIS:CE1	2.90	0.59
1:C:1169:ARG:HH11	1:C:1186:THR:HG23	1.68	0.59
1:D:3:ILE:HB	1:D:6:PHE:HB2	1.84	0.59
1:D:251:SER:O	1:D:255:GLU:HG3	2.01	0.59
1:D:264:ILE:HG22	1:D:265:THR:N	2.17	0.59
1:A:831:LYS:HD2	1:A:831:LYS:H	1.66	0.59
1:D:159:THR:CA	1:D:162:GLN:HG3	2.31	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:D:744:LEU:HD21	1:D:897:LEU:HA	1.85	0.59
1:B:1224:GLY:O	1:B:1225:LEU:HD23	2.03	0.59
1:C:873:GLY:HA2	1:C:909:TYR:HE2	1.66	0.59
1:A:304:GLY:O	1:A:307:PRO:HD2	2.03	0.59
1:B:96:GLN:NE2	1:B:100:ARG:HH21	2.01	0.59
1:D:747:THR:HG22	1:D:770:HIS:HB2	1.84	0.59
1:A:325:ASN:HD21	1:A:328:GLY:CA	2.15	0.59
1:A:751:ALA:O	1:A:765:GLN:HA	2.03	0.58
1:B:10:ILE:HG12	1:B:14:TRP:CZ3	2.38	0.58
1:B:950:LEU:HD23	1:B:1144:VAL:O	2.03	0.58
1:D:220:HIS:CE1	1:D:735:LEU:H	2.16	0.58
1:A:91:ARG:C	1:A:93:LYS:H	2.11	0.58
1:B:315:GLU:HB3	1:B:341:TYR:CZ	2.38	0.58
1:B:965:ILE:CG1	1:B:1125:GLU:HG2	2.28	0.58
1:C:219:HIS:CE1	1:C:251:SER:HB2	2.38	0.58
1:C:300:HIS:HB3	1:C:303:LYS:HB2	1.83	0.58
1:C:155:ILE:CB	1:C:706:ILE:HG13	2.33	0.58
1:D:687:THR:O	1:D:704:HIS:CB	2.50	0.58
1:D:6:PHE:CZ	1:D:10:ILE:HD12	2.39	0.58
1:A:701:GLU:C	1:A:703:ASN:H	2.10	0.58
1:A:1093:VAL:CB	1:A:1094:ALA:HA	2.32	0.58
1:C:376:THR:C	1:C:378:MET:H	2.09	0.58
1:D:259:LEU:O	1:D:260:GLU:C	2.46	0.58
1:D:516:TYR:OH	1:D:569:ASP:OD2	2.19	0.58
1:A:91:ARG:O	1:A:93:LYS:N	2.35	0.58
1:A:593:MET:CE	1:A:604:ILE:HD13	2.34	0.58
1:A:744:LEU:HD21	1:A:897:LEU:HA	1.85	0.58
1:A:1232:ASN:C	1:A:1232:ASN:ND2	2.57	0.58
1:D:181:ILE:O	1:D:185:ILE:HG13	2.04	0.58
1:D:1119:MET:HE3	1:D:1216:ARG:HE	1.69	0.58
1:B:602:ASN:OD1	1:B:602:ASN:N	2.36	0.58
1:B:774:LEU:HD12	1:B:774:LEU:H	1.68	0.58
1:C:798:TRP:O	1:C:799:PRO:C	2.45	0.58
1:A:854:THR:HG22	1:A:855:LYS:HG2	1.86	0.58
1:A:1193:ILE:H	1:A:1193:ILE:HD12	1.67	0.58
1:C:175:GLY:O	1:C:180:LYS:HE2	2.04	0.58
1:A:927:VAL:HG23	1:A:939:ALA:HB3	1.85	0.58
1:A:744:LEU:CD2	1:A:798:TRP:NE1	2.52	0.57
1:B:949:ARG:HH11	1:B:949:ARG:HG2	1.68	0.57
1:D:137:THR:HG22	1:D:138:GLU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:PHE:CE1	1:D:317:LEU:HD13	2.39	0.57
1:D:342:LEU:O	1:D:345:PHE:HB3	2.04	0.57
1:D:664:SER:HB2	1:D:667:GLU:HB2	1.86	0.57
1:A:365:GLU:OE1	1:A:369:LEU:HG	2.04	0.57
1:C:182:MET:HE2	1:C:182:MET:HA	1.85	0.57
1:C:359:TRP:CZ2	1:C:363:GLN:NE2	2.72	0.57
1:A:446:HIS:CE1	1:A:450:LYS:HE3	2.39	0.57
1:B:965:ILE:HG12	1:B:1125:GLU:CG	2.30	0.57
1:D:339:LEU:HD11	1:D:570:VAL:HB	1.86	0.57
1:D:262:GLU:HG2	1:D:263:GLU:N	2.19	0.57
1:D:335:PHE:O	1:D:339:LEU:HB2	2.04	0.57
1:D:527:THR:HG22	1:D:528:ASP:N	2.13	0.57
1:D:704:HIS:ND1	1:D:705:CYS:N	2.53	0.57
1:D:965:ILE:HG12	1:D:1125:GLU:CG	2.19	0.57
1:A:407:THR:HG22	1:A:408:SER:H	1.68	0.57
1:D:387:GLN:HG2	1:D:432:PHE:CZ	2.40	0.57
1:A:592:LEU:O	1:A:595:VAL:O	2.23	0.57
1:B:588:PRO:HD2	1:B:671:ASN:O	2.04	0.57
1:D:676:ASP:CB	1:D:711:ILE:HG22	2.35	0.57
1:C:165:LYS:NZ	1:C:165:LYS:CB	2.68	0.57
1:D:412:ASP:HB2	1:D:459:LEU:HD22	1.87	0.57
1:A:811:THR:HG22	1:A:813:GLU:H	1.70	0.57
1:D:10:ILE:HD13	1:D:14:TRP:HZ3	1.69	0.57
1:D:933:TYR:CE1	1:D:1139:LYS:HE2	2.39	0.57
1:C:36:MET:HE1	1:C:68:ILE:HD13	1.86	0.57
1:B:155:ILE:HG22	1:B:706:ILE:HD12	1.86	0.56
1:B:264:ILE:O	1:B:266:ASP:N	2.36	0.56
1:C:540:GLY:HA2	1:C:557:TRP:CZ2	2.40	0.56
1:C:593:MET:HB3	1:C:652:LEU:HD11	1.86	0.56
1:B:627:VAL:HG11	1:B:643:LYS:CB	2.35	0.56
1:C:135:PRO:HB3	1:C:171:HIS:HB2	1.87	0.56
1:D:917:ILE:HD12	1:D:947:GLU:O	2.06	0.56
1:B:689:TYR:HB3	1:B:700:ILE:HD12	1.86	0.56
1:B:182:MET:HA	1:B:182:MET:CE	2.35	0.56
1:B:789:HIS:O	1:B:792:LYS:HB2	2.05	0.56
1:C:701:GLU:C	1:C:703:ASN:N	2.64	0.56
1:D:292:PHE:HD1	1:D:544:VAL:CG2	2.18	0.56
1:A:918:ASN:HD22	1:A:918:ASN:H	1.54	0.56
1:C:518:ASP:C	1:C:519:LYS:HD3	2.29	0.56
1:D:16:GLN:HE21	1:D:855:LYS:HD2	1.69	0.56
1:A:194:TYR:OH	1:A:200:HIS:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:SER:HB3	1:C:975:GLN:NE2	2.21	0.56
1:D:715:MET:O	1:D:716:GLU:CB	2.53	0.56
1:B:28:GLU:O	1:B:199:ARG:HD2	2.05	0.56
1:D:830:ARG:NH1	1:D:836:GLU:OE2	2.38	0.56
1:D:938:GLU:HB2	1:D:1182:HIS:NE2	2.19	0.56
1:B:641:VAL:HG12	1:B:642:VAL:H	1.71	0.56
1:D:531:LYS:O	1:D:535:GLU:HG3	2.05	0.56
1:D:1171:MET:HB3	1:D:1173:ILE:HD11	1.88	0.56
1:A:259:LEU:CB	1:A:767:MET:HE3	2.20	0.55
1:A:798:TRP:CB	1:A:799:PRO:CD	2.48	0.55
1:B:342:LEU:O	1:B:345:PHE:HB3	2.05	0.55
1:B:649:GLN:O	1:B:653:VAL:HG23	2.05	0.55
1:C:514:GLN:O	1:C:517:LYS:HB3	2.06	0.55
1:A:98:ARG:NH1	1:A:644:ILE:HG12	2.21	0.55
1:A:264:ILE:HG22	1:A:265:THR:N	2.20	0.55
1:D:893:TYR:HB2	1:D:898:ILE:HD11	1.89	0.55
1:B:36:MET:HE2	1:B:68:ILE:CD1	2.36	0.55
1:D:173:VAL:HG21	1:D:676:ASP:OD1	2.07	0.55
1:D:969:ARG:HD2	1:D:1121:ALA:CB	2.35	0.55
1:D:1192:SER:HB3	1:D:1197:VAL:HG13	1.88	0.55
1:B:185:ILE:O	1:B:189:ARG:HG2	2.06	0.55
1:C:833:GLN:O	1:C:833:GLN:HG3	2.06	0.55
1:D:679:PHE:CD1	1:D:679:PHE:N	2.73	0.55
1:D:969:ARG:HD3	1:D:1118:SER:HA	1.88	0.55
1:A:505:SER:HB3	1:A:508:PHE:HB2	1.88	0.55
1:B:152:HIS:CD2	1:B:704:HIS:NE2	2.75	0.55
1:B:377:ARG:O	1:B:378:MET:C	2.50	0.55
1:B:1105:VAL:HG12	1:B:1105:VAL:O	2.07	0.55
1:C:401:THR:HG22	1:C:457:LEU:HD22	1.87	0.55
1:C:446:HIS:HD2	1:C:447:SER:O	1.90	0.55
1:A:700:ILE:HG22	1:A:704:HIS:HB2	1.89	0.55
1:B:155:ILE:O	1:B:162:GLN:NE2	2.40	0.55
1:A:102:PHE:HA	1:A:597:PRO:HG3	1.88	0.55
1:A:262:GLU:HG3	1:A:263:GLU:N	2.21	0.55
1:A:701:GLU:O	1:A:703:ASN:N	2.40	0.55
1:A:844:LYS:HB2	1:A:862:ILE:HD13	1.87	0.55
1:C:713:GLU:HG2	1:C:715:MET:H	1.71	0.55
1:C:832:PRO:O	1:C:833:GLN:C	2.50	0.55
1:A:516:TYR:CD2	1:A:533:MET:HE1	2.42	0.55
1:A:158:ASP:OD1	1:A:1176:SER:HB2	2.07	0.55
1:A:292:PHE:N	1:A:292:PHE:CD1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:ASN:HD21	1:A:1195:LYS:CB	2.13	0.55
1:C:516:TYR:HE2	1:C:533:MET:HE1	1.66	0.55
1:D:1118:SER:O	1:D:1122:VAL:HG23	2.07	0.55
1:C:248:LEU:HD23	1:C:248:LEU:C	2.33	0.54
1:A:1093:VAL:HB	1:A:1094:ALA:CA	2.36	0.54
1:C:307:PRO:CG	1:C:764:GLN:HG2	2.37	0.54
1:C:1189:GLY:O	1:C:1200:GLN:CB	2.55	0.54
1:D:756:VAL:CG2	1:D:853:ARG:HG2	2.37	0.54
1:D:1107:VAL:HG22	1:D:1108:SER:N	2.17	0.54
1:C:312:THR:HG23	1:C:341:TYR:HB2	1.88	0.54
1:D:946:SER:HB3	1:D:948:THR:H	1.73	0.54
1:A:945:ASN:HD21	1:A:951:LYS:HB3	1.73	0.54
1:B:140:MET:HE2	1:B:140:MET:HA	1.88	0.54
1:A:315:GLU:O	1:A:319:HIS:HD2	1.91	0.54
1:A:512:LYS:HG2	1:A:566:ARG:HG3	1.89	0.54
1:A:850:ASN:O	1:A:854:THR:HB	2.08	0.54
1:B:330:ILE:N	1:B:542:GLN:OE1	2.36	0.54
1:C:1111:SER:CB	1:C:1191:THR:HA	2.37	0.54
1:D:81:PHE:CE2	1:D:83:MET:HE2	2.43	0.54
1:D:786:ALA:O	1:D:790:MET:HB2	2.07	0.54
1:A:589:PHE:CE2	1:A:671:ASN:HB2	2.43	0.54
1:C:512:LYS:O	1:C:514:GLN:N	2.31	0.54
1:D:867:LYS:HG3	1:D:892:TYR:CE2	2.42	0.54
1:A:407:THR:HG22	1:A:408:SER:N	2.22	0.54
1:B:100:ARG:NH1	1:B:101:ARG:HH12	2.06	0.54
1:B:933:TYR:CZ	1:B:956:LYS:HD3	2.43	0.54
1:C:1118:SER:O	1:C:1122:VAL:HG23	2.08	0.54
1:D:352:LYS:HE2	1:D:352:LYS:HA	1.89	0.54
1:D:715:MET:O	1:D:716:GLU:HB2	2.08	0.54
1:A:293:LEU:HD11	1:A:540:GLY:HA3	1.90	0.54
1:B:114:LYS:HB2	1:B:114:LYS:NZ	2.23	0.54
1:C:916:PRO:HD2	1:C:919:LYS:HB2	1.89	0.54
1:B:312:THR:CG2	1:B:338:TRP:HE1	2.20	0.54
1:D:299:LEU:CD2	1:D:309:LEU:HD11	2.37	0.54
1:D:317:LEU:HA	1:D:320:MET:CE	2.37	0.54
1:B:303:LYS:NZ	1:B:357:VAL:H	2.06	0.54
1:C:516:TYR:HE2	1:C:533:MET:CE	2.20	0.53
1:A:417:ILE:HD13	1:C:946:SER:HA	1.90	0.53
1:B:304:GLY:O	1:B:307:PRO:HD2	2.08	0.53
1:B:332:LEU:HA	1:B:335:PHE:HB3	1.90	0.53
1:B:945:ASN:HD21	1:B:951:LYS:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:TYR:OH	1:D:697:PHE:HB3	2.08	0.53
1:D:292:PHE:HE1	1:D:544:VAL:HG13	1.72	0.53
1:C:605:PRO:O	1:C:606:VAL:C	2.51	0.53
1:D:854:THR:HG22	1:D:855:LYS:HG2	1.90	0.53
1:C:140:MET:O	1:C:171:HIS:NE2	2.41	0.53
1:C:325:ASN:ND2	1:C:328:GLY:H	2.06	0.53
1:C:450:LYS:HD3	1:C:453:TYR:OH	2.07	0.53
1:A:1110:GLU:O	1:A:1111:SER:HB3	2.07	0.53
1:B:622:PHE:HD2	1:B:622:PHE:C	2.16	0.53
1:B:781:SER:O	1:B:784:ASP:N	2.41	0.53
1:C:540:GLY:HA2	1:C:557:TRP:CH2	2.44	0.53
1:D:6:PHE:CE1	1:D:10:ILE:CD1	2.91	0.53
1:B:88:VAL:HG13	1:B:591:GLN:HG3	1.89	0.53
1:B:1223:LEU:HD21	1:B:1225:LEU:HD21	1.91	0.53
1:C:969:ARG:NH2	1:C:972:LEU:HD22	2.20	0.53
1:D:14:TRP:HB3	1:D:256:TYR:CG	2.44	0.53
1:D:55:LEU:HD22	1:D:59:GLU:HG2	1.91	0.53
1:B:516:TYR:CE2	1:B:533:MET:CE	2.91	0.53
1:B:689:TYR:HB2	1:B:704:HIS:HD2	1.68	0.53
1:B:917:ILE:H	1:B:917:ILE:CD1	2.09	0.53
1:B:1193:ILE:O	1:B:1193:ILE:HG22	2.08	0.53
1:C:264:ILE:HG21	1:C:268:VAL:CG1	2.38	0.53
1:C:312:THR:CG2	1:C:338:TRP:HE1	2.21	0.53
1:A:169:SER:CB	1:A:676:ASP:OD1	2.57	0.53
1:C:152:HIS:HD2	1:C:704:HIS:NE2	2.07	0.53
1:C:593:MET:HG3	1:C:656:MET:SD	2.49	0.53
1:D:540:GLY:O	1:D:544:VAL:HG23	2.09	0.53
1:A:965:ILE:HD13	1:A:1122:VAL:HG13	1.89	0.53
1:C:312:THR:HG23	1:C:341:TYR:CB	2.39	0.53
1:C:359:TRP:HZ2	1:C:363:GLN:HE21	1.55	0.53
1:D:533:MET:HG3	1:D:561:TYR:CG	2.44	0.53
1:B:571:ILE:C	1:B:573:GLY:H	2.18	0.52
1:C:530:LEU:C	1:C:532:GLU:H	2.16	0.52
1:D:36:MET:SD	1:D:83:MET:HB3	2.48	0.52
1:B:622:PHE:C	1:B:622:PHE:CD2	2.87	0.52
1:B:713:GLU:OE1	1:B:715:MET:HE2	2.08	0.52
1:C:339:LEU:HD21	1:C:570:VAL:HB	1.91	0.52
1:D:109:GLU:O	1:D:113:GLN:HB2	2.09	0.52
1:A:802:ARG:HD2	1:A:870:PRO:CB	2.39	0.52
1:A:864:ALA:HB3	1:A:895:LEU:CD1	2.39	0.52
1:C:963:PRO:HD3	1:C:1129:TYR:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1111:SER:HB2	1:C:1191:THR:HA	1.90	0.52
1:D:6:PHE:CE1	1:D:10:ILE:HD12	2.45	0.52
1:C:606:VAL:O	1:C:608:TYR:N	2.43	0.52
1:D:704:HIS:CE1	1:D:706:ILE:H	2.28	0.52
1:B:98:ARG:HH11	1:B:644:ILE:HG12	1.73	0.52
1:B:140:MET:CE	1:B:143:LEU:HD13	2.40	0.52
1:C:398:LEU:O	1:C:402:VAL:HB	2.10	0.52
1:A:89:ALA:O	1:A:94:MET:HE2	2.10	0.52
1:A:592:LEU:HD22	1:A:596:LEU:HD12	1.92	0.52
1:A:654:GLU:O	1:A:658:PRO:HD2	2.10	0.52
1:A:883:SER:HA	1:A:911:GLU:HG2	1.91	0.52
1:B:626:GLU:O	1:B:627:VAL:CG2	2.57	0.52
1:B:933:TYR:CD1	1:B:1139:LYS:HE2	2.45	0.52
1:B:980:TYR:HD1	1:B:980:TYR:H	1.58	0.52
1:C:98:ARG:NH2	1:C:622:PHE:O	2.43	0.52
1:D:210:ILE:HA	1:D:223:LEU:HD11	1.92	0.52
1:D:310:LEU:CD2	1:D:314:LYS:HE3	2.40	0.52
1:A:137:THR:HG22	1:A:140:MET:H	1.74	0.52
1:A:1105:VAL:HG12	1:A:1105:VAL:O	2.10	0.52
1:B:796:SER:HB2	1:B:893:TYR:CE1	2.45	0.52
1:C:844:LYS:HG3	1:C:862:ILE:HB	1.92	0.52
1:D:676:ASP:CB	1:D:711:ILE:CG2	2.88	0.52
1:A:701:GLU:C	1:A:703:ASN:N	2.68	0.52
1:C:1087:ASP:O	1:C:1088:SER:C	2.52	0.52
1:D:276:ARG:HH12	1:D:326:GLU:CA	2.10	0.52
1:D:820:LYS:HA	1:D:825:THR:HA	1.92	0.52
1:A:140:MET:O	1:A:171:HIS:NE2	2.33	0.52
1:A:325:ASN:ND2	1:A:328:GLY:H	2.07	0.52
1:C:809:LEU:C	1:C:810:ILE:HG12	2.34	0.52
1:A:606:VAL:C	1:A:607:VAL:HG23	2.34	0.51
1:B:458:ASP:OD1	1:B:461:SER:CB	2.58	0.51
1:B:592:LEU:O	1:B:596:LEU:HB2	2.09	0.51
1:C:113:GLN:O	1:C:114:LYS:C	2.53	0.51
1:A:706:ILE:N	1:A:706:ILE:CD1	2.73	0.51
1:B:1138:GLN:O	1:B:1138:GLN:HG2	2.10	0.51
1:C:1086:ALA:O	1:C:1087:ASP:C	2.52	0.51
1:B:962:GLU:HG3	1:B:1169:ARG:HE	1.75	0.51
1:C:228:VAL:O	1:C:228:VAL:CG1	2.59	0.51
1:D:159:THR:HG23	1:D:1175:ASP:OD1	2.10	0.51
1:A:1111:SER:HA	1:A:1190:TYR:CD1	2.44	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:A:1212:ASN:HD22	1:A:1215:GLY:H	1.56	0.51
1:B:201:CYS:HA	1:B:222:CYS:O	2.10	0.51
1:B:356:ASP:O	1:B:359:TRP:HB3	2.11	0.51
1:B:980:TYR:CD1	1:B:980:TYR:N	2.78	0.51
1:C:593:MET:CE	1:C:604:ILE:HD12	2.39	0.51
1:D:169:SER:OG	1:D:180:LYS:HD3	2.09	0.51
1:D:538:VAL:O	1:D:541:LEU:HB2	2.11	0.51
1:D:876:ARG:HG3	1:D:882:TYR:CE2	2.45	0.51
1:D:1111:SER:HB3	1:D:1191:THR:HA	1.92	0.51
1:A:301:LEU:O	1:A:303:LYS:N	2.42	0.51
1:C:417:ILE:O	1:C:419:PRO:HD3	2.11	0.51
1:D:395:LYS:O	1:D:396:PRO:C	2.54	0.51
1:D:589:PHE:HA	1:D:592:LEU:HB2	1.92	0.51
1:D:965:ILE:HD12	1:D:965:ILE:H	1.75	0.51
1:A:1191:THR:O	1:A:1191:THR:HG22	2.10	0.51
1:C:320:MET:HE3	1:C:322:GLY:O	2.10	0.51
1:C:969:ARG:NH2	1:C:972:LEU:CD2	2.71	0.51
1:C:979:PHE:HD2	1:C:1039:UNK:CB	2.24	0.51
1:D:170:GLY:O	1:D:180:LYS:NZ	2.44	0.51
1:D:317:LEU:HD12	1:D:320:MET:HE1	1.92	0.51
1:D:1207:ILE:O	1:D:1208:ILE:C	2.54	0.51
1:A:316:ALA:O	1:A:320:MET:HG3	2.11	0.51
1:A:1232:ASN:ND2	1:A:1235:ASP:H	2.09	0.51
1:B:102:PHE:HE1	1:B:599:ARG:NH1	2.09	0.51
1:D:91:ARG:HA	1:D:94:MET:HG3	1.91	0.51
1:B:36:MET:HE2	1:B:68:ILE:HG12	1.92	0.51
1:B:876:ARG:NH1	1:B:920:GLU:OE2	2.43	0.51
1:C:219:HIS:CD2	1:C:254:ARG:NH1	2.72	0.51
1:C:355:ILE:H	1:C:355:ILE:HD12	1.75	0.51
1:D:32:LEU:HD13	1:D:75:ILE:HG13	1.92	0.51
1:B:1188:VAL:HG11	1:B:1202:LEU:HB2	1.93	0.51
1:C:254:ARG:NH2	1:C:275:GLU:OE1	2.44	0.51
1:C:969:ARG:HH21	1:C:972:LEU:HD23	1.76	0.51
1:D:534:THR:HG22	1:D:573:GLY:CA	2.40	0.51
1:B:798:TRP:O	1:B:800:PHE:N	2.44	0.50
1:C:195:ASN:ND2	1:C:197:ASN:H	2.09	0.50
1:C:622:PHE:O	1:C:623:TYR:CD2	2.64	0.50
1:D:155:ILE:HB	1:D:706:ILE:CG1	2.41	0.50
1:B:805:LYS:HB2	1:B:886:PHE:CE2	2.46	0.50
1:C:917:ILE:HD12	1:C:947:GLU:O	2.11	0.50
1:D:871:VAL:HG22	1:D:886:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:HD21	1:A:328:GLY:N	2.09	0.50
1:A:534:THR:CG2	1:A:573:GLY:HA2	2.41	0.50
1:A:864:ALA:CB	1:A:895:LEU:HD12	2.39	0.50
1:B:34:LEU:HD12	1:B:36:MET:HE3	1.93	0.50
1:B:309:LEU:O	1:B:312:THR:HB	2.11	0.50
1:C:169:SER:O	1:C:180:LYS:NZ	2.45	0.50
1:C:543:TRP:CD1	1:C:553:PRO:HG2	2.46	0.50
1:C:558:TYR:CE1	1:C:560:ARG:HG2	2.46	0.50
1:C:665:PRO:HA	1:C:668:LYS:HB2	1.92	0.50
1:D:85:ILE:HD13	1:D:143:LEU:HD21	1.93	0.50
1:D:798:TRP:O	1:D:799:PRO:C	2.53	0.50
1:D:1212:ASN:HD22	1:D:1215:GLY:H	1.58	0.50
1:A:91:ARG:C	1:A:93:LYS:N	2.69	0.50
1:A:969:ARG:NH1	1:A:972:LEU:CD2	2.74	0.50
1:B:312:THR:HG22	1:B:338:TRP:CD1	2.47	0.50
1:D:1236:ARG:HB3	1:D:1239:VAL:HG22	1.94	0.50
1:A:768:VAL:CG1	1:A:858:LEU:HD13	2.41	0.50
1:B:948:THR:HG22	1:B:1146:ARG:NH2	2.26	0.50
1:C:798:TRP:O	1:C:801:LEU:HG	2.11	0.50
1:C:847:LEU:O	1:C:848:LYS:C	2.54	0.50
1:D:605:PRO:O	1:D:607:VAL:N	2.44	0.50
1:D:1111:SER:O	1:D:1112:ASP:HB3	2.11	0.50
1:A:1232:ASN:HD21	1:A:1235:ASP:H	1.60	0.50
1:C:554:SER:HB2	1:C:580:PHE:HB3	1.93	0.50
1:C:1171:MET:HB2	1:C:1233:LEU:HD11	1.94	0.50
1:A:770:HIS:CE1	1:A:858:LEU:HD22	2.46	0.50
1:B:589:PHE:HD1	1:B:592:LEU:HD12	1.76	0.50
1:B:677:LEU:HD13	1:B:708:ARG:HD2	1.94	0.50
1:D:310:LEU:HD21	1:D:314:LYS:HE3	1.93	0.50
1:D:542:GLN:HE21	1:D:542:GLN:HA	1.77	0.50
1:A:113:GLN:HE21	1:A:113:GLN:HA	1.76	0.50
1:B:1041:UNK:O	1:B:1042:UNK:C	2.60	0.50
1:C:666:ASP:OD1	1:C:666:ASP:N	2.32	0.50
1:D:212:LEU:HD21	1:D:548:TYR:CD1	2.46	0.50
1:D:441:GLY:HA2	1:D:462:ILE:HD13	1.93	0.50
1:A:1235:ASP:O	1:A:1237:GLN:HG3	2.12	0.50
1:C:221:PHE:HB3	1:C:250:LEU:HD12	1.94	0.50
1:A:152:HIS:HA	1:A:706:ILE:HG12	1.93	0.49
1:A:402:VAL:O	1:A:402:VAL:HG12	2.11	0.49
1:A:416:GLU:HB2	1:C:951:LYS:HZ1	1.77	0.49
1:A:417:ILE:O	1:A:419:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:GLU:HG3	1:A:947:GLU:O	2.10	0.49
1:B:22:ASP:OD2	1:B:22:ASP:C	2.55	0.49
1:B:516:TYR:HE2	1:B:533:MET:HE2	1.77	0.49
1:C:862:ILE:HD12	1:C:862:ILE:N	2.26	0.49
1:D:770:HIS:CE1	1:D:858:LEU:HD22	2.47	0.49
1:A:800:PHE:O	1:A:801:LEU:C	2.55	0.49
1:A:1112:ASP:CG	1:A:1113:SER:H	2.21	0.49
1:B:731:GLY:C	1:B:733:SER:H	2.21	0.49
1:C:965:ILE:HD12	1:C:965:ILE:H	1.76	0.49
1:D:159:THR:HA	1:D:162:GLN:CG	2.34	0.49
1:D:1173:ILE:HD11	1:D:1231:LEU:HB3	1.95	0.49
1:A:188:ILE:HG13	1:A:189:ARG:N	2.25	0.49
1:B:1115:THR:HG1	1:B:1118:SER:HB2	1.76	0.49
1:B:1203:PHE:O	1:B:1221:ARG:HD3	2.12	0.49
1:C:1210:GLY:HA2	1:C:1222:GLY:O	2.12	0.49
1:D:729:LYS:HZ1	1:D:904:ASN:HD21	1.59	0.49
1:A:144:THR:O	1:A:148:LYS:HG3	2.12	0.49
1:B:137:THR:HG22	1:B:138:GLU:N	2.27	0.49
1:B:512:LYS:NZ	1:B:569:ASP:OD1	2.45	0.49
1:B:965:ILE:O	1:B:966:GLY:C	2.56	0.49
1:C:518:ASP:O	1:C:519:LYS:HD3	2.12	0.49
1:C:928:VAL:HG21	1:C:1173:ILE:HG23	1.94	0.49
1:D:92:ALA:HA	1:D:558:TYR:HA	1.95	0.49
1:D:876:ARG:NH1	1:D:920:GLU:OE2	2.43	0.49
1:B:627:VAL:HG11	1:B:643:LYS:HB2	1.95	0.49
1:C:55:LEU:N	1:C:55:LEU:HD12	2.27	0.49
1:C:534:THR:HG21	1:C:572:LYS:C	2.38	0.49
1:D:87:GLY:C	1:D:135:PRO:HG3	2.38	0.49
1:A:72:PHE:C	1:A:72:PHE:CD2	2.91	0.49
1:A:325:ASN:HD21	1:A:328:GLY:H	1.60	0.49
1:C:152:HIS:O	1:C:706:ILE:HD11	2.10	0.49
1:C:391:ILE:HD12	1:C:392:GLY:H	1.76	0.49
1:B:210:ILE:HA	1:B:223:LEU:CD1	2.43	0.49
1:B:388:LYS:O	1:B:389:LYS:C	2.53	0.49
1:B:391:ILE:HD11	1:B:485:UNK:O	2.11	0.49
1:B:554:SER:HB2	1:B:580:PHE:HB3	1.94	0.49
1:B:954:VAL:HG21	1:B:1141:LEU:HD12	1.95	0.49
1:C:837:ARG:HD3	1:C:841:ARG:NH2	2.28	0.49
1:C:917:ILE:CD1	1:C:917:ILE:N	2.43	0.49
1:C:917:ILE:HG13	1:C:947:GLU:O	2.12	0.49
1:B:704:HIS:ND1	1:B:704:HIS:C	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:VAL:HG12	1:B:1108:SER:O	2.13	0.49
1:C:1232:ASN:HD22	1:C:1234:SER:H	1.60	0.49
1:D:219:HIS:HD2	1:D:254:ARG:NH1	2.10	0.49
1:A:797:ARG:O	1:A:798:TRP:O	2.30	0.49
1:B:154:LYS:O	1:B:155:ILE:C	2.55	0.49
1:B:704:HIS:C	1:B:704:HIS:HD1	2.21	0.49
1:C:365:GLU:O	1:C:369:LEU:HG	2.13	0.49
1:D:804:SER:HB2	1:D:868:VAL:HB	1.95	0.49
1:D:876:ARG:HG3	1:D:882:TYR:CZ	2.48	0.49
1:D:945:ASN:ND2	1:D:1143:LYS:N	2.60	0.49
1:A:146:ASN:O	1:A:149:TYR:HB3	2.12	0.48
1:B:933:TYR:CE2	1:B:1139:LYS:HB2	2.48	0.48
1:D:93:LYS:HB3	1:D:97:GLN:NE2	2.28	0.48
1:D:747:THR:CG2	1:D:770:HIS:HB2	2.43	0.48
1:D:852:GLN:HG2	1:D:857:ILE:O	2.13	0.48
1:A:302:LYS:O	1:A:303:LYS:HE2	2.13	0.48
1:A:1122:VAL:HG12	1:A:1202:LEU:HD13	1.94	0.48
1:B:33:TYR:OH	1:B:200:HIS:HD2	1.95	0.48
1:B:534:THR:CG2	1:B:573:GLY:N	2.76	0.48
1:B:744:LEU:HD22	1:B:798:TRP:CD1	2.48	0.48
1:B:965:ILE:H	1:B:965:ILE:HG13	1.44	0.48
1:C:391:ILE:HD12	1:C:392:GLY:N	2.28	0.48
1:D:507:ARG:O	1:D:511:TRP:N	2.36	0.48
1:D:965:ILE:HD12	1:D:965:ILE:N	2.28	0.48
1:B:682:ASN:O	1:B:705:CYS:HB3	2.13	0.48
1:A:969:ARG:HH12	1:A:972:LEU:HD23	1.79	0.48
1:B:1223:LEU:CD2	1:B:1225:LEU:HD21	2.43	0.48
1:C:416:GLU:HG2	1:C:417:ILE:H	1.77	0.48
1:C:597:PRO:C	1:C:599:ARG:H	2.21	0.48
1:C:1232:ASN:HD22	1:C:1232:ASN:C	2.19	0.48
1:D:933:TYR:CD1	1:D:1139:LYS:HE2	2.49	0.48
1:D:964:ASN:H	1:D:965:ILE:HD12	1.79	0.48
1:A:963:PRO:HD3	1:A:1129:TYR:CE1	2.49	0.48
1:B:152:HIS:HD2	1:B:706:ILE:HB	1.69	0.48
1:D:342:LEU:HB3	1:D:567:ILE:CG2	2.43	0.48
1:D:542:GLN:HE21	1:D:542:GLN:CA	2.26	0.48
1:A:313:PHE:CZ	1:A:317:LEU:HD22	2.49	0.48
1:A:1050:UNK:O	1:A:1091:LYS:N	2.46	0.48
1:B:182:MET:HE3	1:B:185:ILE:HD12	1.95	0.48
1:B:1137:GLU:HG2	1:B:1138:GLN:N	2.26	0.48
1:A:156:THR:N	1:A:706:ILE:HD11	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:GLU:C	1:A:264:ILE:N	2.72	0.48
1:A:426:VAL:HG13	1:A:433:LEU:HD13	1.94	0.48
1:A:535:GLU:HG2	1:A:576:GLN:OE1	2.14	0.48
1:B:131:ASN:N	1:B:131:ASN:OD1	2.45	0.48
1:B:543:TRP:CD1	1:B:553:PRO:HG2	2.49	0.48
1:B:927:VAL:HG21	1:B:1149:ILE:HG13	1.93	0.48
1:D:565:PRO:O	1:D:566:ARG:HG2	2.12	0.48
1:A:533:MET:HE3	1:A:565:PRO:HB3	1.96	0.48
1:A:816:TYR:CD1	1:A:816:TYR:N	2.80	0.48
1:B:1212:ASN:O	1:B:1213:PHE:C	2.56	0.48
1:D:61:TYR:OH	1:D:143:LEU:HD12	2.14	0.48
1:D:292:PHE:CE1	1:D:544:VAL:HG13	2.49	0.48
1:D:390:LEU:O	1:D:394:VAL:HG23	2.13	0.48
1:A:1099:GLU:OE2	1:A:1102:LYS:HE3	2.14	0.48
1:A:1112:ASP:CG	1:A:1113:SER:N	2.72	0.48
1:B:916:PRO:HD2	1:B:919:LYS:HB2	1.95	0.48
1:B:1112:ASP:OD1	1:B:1112:ASP:N	2.46	0.48
1:C:354:ASP:N	1:C:354:ASP:OD1	2.45	0.48
1:A:708:ARG:HH11	1:A:708:ARG:HB2	1.79	0.48
1:A:793:ILE:HD13	1:A:793:ILE:HA	1.75	0.48
1:A:1172:TYR:CD1	1:A:1179:VAL:HB	2.48	0.48
1:B:169:SER:OG	1:B:180:LYS:HD2	2.14	0.48
1:B:417:ILE:HG13	1:B:454:TYR:HD1	1.78	0.48
1:C:363:GLN:O	1:C:367:ILE:HD13	2.14	0.48
1:C:587:LYS:N	1:C:590:GLN:HE21	2.02	0.48
1:C:744:LEU:HD21	1:C:897:LEU:HA	1.96	0.48
1:C:873:GLY:HA2	1:C:909:TYR:CE2	2.48	0.48
1:A:336:SER:HA	1:A:339:LEU:HB2	1.94	0.47
1:A:741:LEU:HD22	1:A:769:LEU:HD11	1.95	0.47
1:A:894:PRO:HD2	1:A:897:LEU:HD12	1.96	0.47
1:B:576:GLN:HG3	1:B:577:ASN:N	2.28	0.47
1:B:918:ASN:ND2	1:B:918:ASN:H	2.10	0.47
1:C:527:THR:HB	1:C:528:ASP:H	1.44	0.47
1:D:284:VAL:HG21	1:D:313:PHE:CG	2.48	0.47
1:B:7:PHE:O	1:B:8:HIS:C	2.57	0.47
1:B:1165:HIS:O	1:B:1168:ASP:HB2	2.13	0.47
1:C:1085:GLU:O	1:C:1086:ALA:C	2.57	0.47
1:D:932:ASP:O	1:D:933:TYR:C	2.57	0.47
1:D:1175:ASP:OD1	1:D:1175:ASP:C	2.56	0.47
1:A:94:MET:O	1:A:98:ARG:HB3	2.14	0.47
1:A:526:ASP:C	1:A:527:THR:OG1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:TYR:OH	1:B:565:PRO:HD3	2.14	0.47
1:C:16:GLN:HE22	1:C:799:PRO:HG3	1.79	0.47
1:C:622:PHE:C	1:C:623:TYR:CG	2.93	0.47
1:C:730:LEU:O	1:C:731:GLY:C	2.57	0.47
1:D:142:LYS:O	1:D:146:ASN:ND2	2.46	0.47
1:D:268:VAL:C	1:D:270:PHE:H	2.21	0.47
1:D:1113:SER:HA	1:D:1189:GLY:HA2	1.96	0.47
1:B:901:ASP:CG	1:B:902:VAL:H	2.22	0.47
1:A:798:TRP:HE3	1:A:799:PRO:HD3	1.78	0.47
1:A:1212:ASN:OD1	1:A:1212:ASN:N	2.42	0.47
1:B:528:ASP:HA	1:B:531:LYS:HB2	1.96	0.47
1:B:537:TYR:O	1:B:540:GLY:N	2.47	0.47
1:D:195:ASN:HB3	1:D:198:THR:HG1	1.80	0.47
1:A:387:GLN:O	1:A:391:ILE:HG13	2.14	0.47
1:B:10:ILE:HG12	1:B:14:TRP:HZ3	1.77	0.47
1:B:676:ASP:CB	1:B:711:ILE:HG22	2.44	0.47
1:D:189:ARG:NH2	1:D:723:GLY:O	2.38	0.47
1:D:917:ILE:CD1	1:D:947:GLU:O	2.63	0.47
1:A:40:LEU:HD22	1:A:143:LEU:HD11	1.96	0.47
1:A:144:THR:HG22	1:A:148:LYS:HE3	1.97	0.47
1:A:317:LEU:HD12	1:A:320:MET:HE2	1.97	0.47
1:A:430:LEU:O	1:A:434:LYS:HG3	2.15	0.47
1:A:471:UNK:C	1:A:473:UNK:N	2.77	0.47
1:A:592:LEU:CD2	1:A:596:LEU:HD12	2.45	0.47
1:A:597:PRO:C	1:A:599:ARG:H	2.23	0.47
1:C:152:HIS:CD2	1:C:704:HIS:NE2	2.83	0.47
1:C:696:LEU:CD2	1:C:1206:GLU:HB3	2.45	0.47
1:D:220:HIS:CE1	1:D:735:LEU:HB2	2.50	0.47
1:B:544:VAL:O	1:B:547:TYR:HB3	2.15	0.47
1:C:101:ARG:HG3	1:C:131:ASN:CG	2.39	0.47
1:C:806:LEU:HA	1:C:868:VAL:HG12	1.96	0.47
1:A:182:MET:HE3	1:A:212:LEU:CB	2.45	0.47
1:A:534:THR:HG21	1:A:572:LYS:C	2.40	0.47
1:B:36:MET:HE1	1:B:83:MET:CG	2.42	0.47
1:B:531:LYS:HB3	1:B:531:LYS:HZ2	1.76	0.47
1:C:965:ILE:HD12	1:C:965:ILE:N	2.29	0.47
1:D:217:HIS:CE1	1:D:275:GLU:HB3	2.50	0.47
1:A:959:LEU:HD21	1:A:1137:GLU:OE2	2.15	0.47
1:B:367:ILE:HD12	1:B:367:ILE:H	1.80	0.47
1:B:387:GLN:HG2	1:B:432:PHE:CZ	2.49	0.47
1:B:828:ILE:O	1:B:828:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:HB3	1:C:165:LYS:NZ	2.27	0.47
1:C:1042:UNK:O	1:C:1045:UNK:N	2.48	0.47
1:D:222:CYS:SG	1:D:249:HIS:CE1	3.08	0.47
1:D:689:TYR:HB2	1:D:704:HIS:CD2	2.50	0.47
1:A:1116:LYS:HG3	1:A:1216:ARG:HG3	1.97	0.46
1:A:1195:LYS:HG2	1:A:1196:ASN:HD22	1.80	0.46
1:B:98:ARG:NH1	1:B:644:ILE:HG12	2.30	0.46
1:B:219:HIS:CE1	1:B:251:SER:HB2	2.50	0.46
1:B:830:ARG:CG	1:B:831:LYS:N	2.78	0.46
1:C:918:ASN:HA	1:C:944:TYR:CZ	2.50	0.46
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.81	0.46
1:A:622:PHE:HZ	1:A:648:ASP:HB3	1.80	0.46
1:A:826:LYS:CG	1:A:827:VAL:N	2.66	0.46
1:A:952:LEU:CD1	1:A:1149:ILE:HD11	2.44	0.46
1:A:1232:ASN:ND2	1:A:1234:SER:H	2.13	0.46
1:B:335:PHE:O	1:B:335:PHE:HD1	1.97	0.46
1:A:36:MET:HE1	1:A:83:MET:HE2	1.98	0.46
1:A:540:GLY:HA2	1:A:557:TRP:CZ2	2.50	0.46
1:B:506:GLU:CD	1:B:506:GLU:H	2.23	0.46
1:B:1163:ARG:HG3	1:B:1237:GLN:OE1	2.15	0.46
1:C:534:THR:CG2	1:C:573:GLY:HA3	2.41	0.46
1:D:589:PHE:CD1	1:D:589:PHE:N	2.84	0.46
1:D:1116:LYS:HG3	1:D:1216:ARG:CD	2.45	0.46
1:A:189:ARG:HA	1:A:194:TYR:CG	2.50	0.46
1:A:417:ILE:HG12	1:A:454:TYR:CD1	2.50	0.46
1:A:712:PRO:O	1:A:713:GLU:HB3	2.16	0.46
1:B:335:PHE:CD1	1:B:335:PHE:C	2.90	0.46
1:B:588:PRO:O	1:B:591:GLN:HB3	2.15	0.46
1:D:26:ILE:HB	1:D:27:PRO:HD2	1.98	0.46
1:A:534:THR:HG22	1:A:535:GLU:N	2.30	0.46
1:A:1181:LEU:HG	1:A:1182:HIS:CD2	2.50	0.46
1:B:43:CYS:HB2	1:B:64:ILE:HD13	1.98	0.46
1:C:128:PHE:CE2	1:C:130:SER:HA	2.50	0.46
1:C:154:LYS:HD2	1:C:154:LYS:HA	1.56	0.46
1:C:952:LEU:HD11	1:C:1144:VAL:HG21	1.98	0.46
1:A:195:ASN:HD22	1:A:196:PRO:HD2	1.79	0.46
1:A:260:GLU:O	1:A:314:LYS:HE2	2.15	0.46
1:A:303:LYS:HG2	1:A:355:ILE:O	2.16	0.46
1:B:155:ILE:HD11	1:B:166:VAL:CG2	2.37	0.46
1:B:209:LEU:HB3	1:B:223:LEU:CD2	2.46	0.46
1:D:76:LYS:HD3	1:D:160:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:VAL:HG12	1:D:361:ASN:ND2	2.30	0.46
1:A:798:TRP:O	1:A:800:PHE:N	2.49	0.46
1:A:821:SER:HB3	1:A:824:LEU:O	2.16	0.46
1:C:850:ASN:ND2	1:C:853:ARG:HH12	2.13	0.46
1:D:155:ILE:CG2	1:D:706:ILE:HD12	2.46	0.46
1:D:397:TRP:O	1:D:401:THR:OG1	2.32	0.46
1:D:1116:LYS:HG3	1:D:1216:ARG:HD2	1.98	0.46
1:A:96:GLN:H	1:A:96:GLN:NE2	2.03	0.46
1:B:1171:MET:HB3	1:B:1173:ILE:HD11	1.97	0.46
1:D:58:GLU:HG2	1:D:59:GLU:N	2.30	0.46
1:D:210:ILE:HA	1:D:223:LEU:HD13	1.97	0.46
1:D:706:ILE:N	1:D:706:ILE:CD1	2.74	0.46
1:D:927:VAL:HG21	1:D:1149:ILE:HG12	1.97	0.46
1:A:663:LEU:HB3	1:A:667:GLU:HB2	1.97	0.46
1:A:708:ARG:HH11	1:A:708:ARG:CB	2.28	0.46
1:A:798:TRP:CG	1:A:799:PRO:HD3	2.51	0.46
1:B:264:ILE:HG23	1:B:267:SER:HB2	1.98	0.46
1:B:704:HIS:CE1	1:B:706:ILE:H	2.33	0.46
1:B:798:TRP:HB3	1:B:799:PRO:HD3	1.98	0.46
1:D:325:ASN:HD21	1:D:328:GLY:HA2	1.80	0.46
1:D:340:LYS:NZ	1:D:340:LYS:HA	2.31	0.46
1:D:1204:ASP:O	1:D:1221:ARG:NH1	2.49	0.46
1:A:405:LYS:HE3	1:A:405:LYS:HB2	1.65	0.46
1:B:704:HIS:HE1	1:B:706:ILE:O	1.99	0.46
1:B:1181:LEU:O	1:B:1182:HIS:CB	2.60	0.46
1:B:1191:THR:HG23	1:B:1193:ILE:HD13	1.97	0.46
1:C:31:ASN:HB3	1:C:33:TYR:CZ	2.51	0.46
1:C:212:LEU:HD21	1:C:548:TYR:HD1	1.75	0.46
1:D:309:LEU:O	1:D:312:THR:HB	2.16	0.46
1:D:952:LEU:HD21	1:D:1149:ILE:HD13	1.96	0.46
1:A:177:GLY:O	1:A:181:ILE:HG13	2.15	0.45
1:B:296:LEU:CB	1:B:297:PRO:CD	2.79	0.45
1:B:366:ASN:O	1:B:367:ILE:C	2.58	0.45
1:C:1102:LYS:HB2	1:C:1103:PRO:CD	2.38	0.45
1:A:744:LEU:HD22	1:A:798:TRP:CE2	2.42	0.45
1:A:969:ARG:HH11	1:A:972:LEU:HD22	1.81	0.45
1:B:284:VAL:HG21	1:B:313:PHE:CG	2.50	0.45
1:B:296:LEU:HD13	1:B:567:ILE:HG12	1.97	0.45
1:B:486:UNK:O	1:B:487:UNK:C	2.63	0.45
1:C:1087:ASP:O	1:C:1090:LEU:N	2.49	0.45
1:C:1173:ILE:HG13	1:C:1231:LEU:HB2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:CD2	1:A:75:ILE:HG23	2.52	0.45
1:B:608:TYR:CE1	1:B:656:MET:HE3	2.51	0.45
1:A:303:LYS:HG2	1:A:355:ILE:HD12	1.98	0.45
1:A:811:THR:CG2	1:A:812:GLU:N	2.79	0.45
1:A:946:SER:OG	1:A:947:GLU:N	2.49	0.45
1:A:1041:UNK:O	1:A:1042:UNK:C	2.65	0.45
1:B:459:LEU:O	1:B:460:ASP:C	2.60	0.45
1:B:812:GLU:OE2	1:B:841:ARG:NH2	2.49	0.45
1:B:1210:GLY:C	1:B:1220:ARG:HG3	2.42	0.45
1:C:85:ILE:HD13	1:C:143:LEU:HD21	1.98	0.45
1:C:156:THR:OG1	1:C:705:CYS:N	2.46	0.45
1:C:264:ILE:CG2	1:C:264:ILE:O	2.64	0.45
1:C:264:ILE:O	1:C:264:ILE:HG22	2.11	0.45
1:C:875:VAL:HG12	1:C:885:SER:HB2	1.97	0.45
1:D:280:ASP:OD1	1:D:323:TYR:HB3	2.16	0.45
1:A:377:ARG:O	1:A:378:MET:C	2.57	0.45
1:A:817:GLU:O	1:A:827:VAL:HA	2.17	0.45
1:A:971:LYS:HE3	1:A:975:GLN:OE1	2.16	0.45
1:B:297:PRO:HG2	1:B:298:ASP:H	1.81	0.45
1:C:858:LEU:HD12	1:C:858:LEU:HA	1.78	0.45
1:A:795:TYR:HA	1:A:802:ARG:O	2.16	0.45
1:C:968:VAL:O	1:C:971:LYS:HB3	2.16	0.45
1:A:284:VAL:HG13	1:A:338:TRP:CZ2	2.52	0.45
1:A:417:ILE:HD13	1:C:945:ASN:O	2.16	0.45
1:A:419:PRO:HA	1:A:454:TYR:HB3	1.97	0.45
1:B:296:LEU:HB2	1:B:299:LEU:HD11	1.98	0.45
1:C:33:TYR:OH	1:C:200:HIS:CD2	2.61	0.45
1:C:140:MET:HE2	1:C:143:LEU:HD22	1.99	0.45
1:C:510:GLU:O	1:C:514:GLN:HB2	2.15	0.45
1:D:313:PHE:HE1	1:D:317:LEU:HD13	1.80	0.45
1:D:589:PHE:CE2	1:D:605:PRO:HG3	2.51	0.45
1:D:929:PHE:HD1	1:D:1149:ILE:HD12	1.80	0.45
1:D:967:LYS:O	1:D:970:ALA:HB3	2.16	0.45
1:A:624:PRO:HB2	1:A:626:GLU:O	2.17	0.45
1:A:744:LEU:HB2	1:A:798:TRP:NE1	2.32	0.45
1:A:1039:UNK:O	1:A:1040:UNK:C	2.65	0.45
1:B:264:ILE:HG22	1:B:265:THR:H	1.77	0.45
1:B:744:LEU:HD13	1:B:899:VAL:HG22	1.99	0.45
1:C:209:LEU:HB3	1:C:223:LEU:CD2	2.47	0.45
1:C:221:PHE:HB3	1:C:250:LEU:HB2	1.98	0.45
1:C:1089:ILE:O	1:C:1090:LEU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:GLU:H	1:C:1147:GLU:CD	2.24	0.45
1:D:331:ASN:OD1	1:D:334:ARG:HG2	2.16	0.45
1:D:589:PHE:N	1:D:589:PHE:HD1	2.14	0.45
1:A:571:ILE:O	1:A:574:ILE:HG12	2.17	0.45
1:A:918:ASN:HD22	1:A:918:ASN:N	2.14	0.45
1:A:1092:THR:O	1:A:1093:VAL:CG2	2.52	0.45
1:A:1093:VAL:HG12	1:A:1097:LEU:HD12	1.98	0.45
1:B:797:ARG:O	1:B:798:TRP:C	2.57	0.45
1:B:816:TYR:CD1	1:B:816:TYR:N	2.85	0.45
1:B:983:GLN:CD	1:B:983:GLN:H	2.25	0.45
1:C:112:LEU:O	1:C:113:GLN:HB2	2.17	0.45
1:C:195:ASN:HD22	1:C:196:PRO:HD2	1.81	0.45
1:C:393:ALA:O	1:C:396:PRO:HD2	2.16	0.45
1:D:754:SER:HA	1:D:762:SER:O	2.17	0.45
1:A:325:ASN:HD21	1:A:328:GLY:HA2	1.80	0.45
1:A:712:PRO:O	1:A:713:GLU:HB2	2.16	0.45
1:A:719:LYS:HZ1	1:C:716:GLU:HB3	1.82	0.45
1:A:798:TRP:O	1:A:801:LEU:N	2.49	0.45
1:A:933:TYR:OH	1:A:1137:GLU:HG2	2.16	0.45
1:C:67:TYR:O	1:C:68:ILE:C	2.60	0.45
1:D:54:ARG:HG2	1:D:55:LEU:N	2.31	0.45
1:D:140:MET:HB3	1:D:171:HIS:NE2	2.31	0.45
1:D:155:ILE:HB	1:D:706:ILE:CD1	2.47	0.45
1:A:98:ARG:HB2	1:A:595:VAL:HA	1.99	0.44
1:A:606:VAL:O	1:A:607:VAL:CG2	2.61	0.44
1:B:85:ILE:HD13	1:B:143:LEU:HD21	1.99	0.44
1:B:250:LEU:HD23	1:B:253:LEU:HD23	1.99	0.44
1:B:477:UNK:O	1:B:481:UNK:N	2.50	0.44
1:B:669:LYS:C	1:B:671:ASN:H	2.25	0.44
1:B:1111:SER:HB2	1:B:1190:TYR:O	2.17	0.44
1:C:357:VAL:O	1:C:358:GLU:C	2.60	0.44
1:C:696:LEU:HD21	1:C:1206:GLU:HB3	1.97	0.44
1:C:820:LYS:HG2	1:C:822:GLY:H	1.82	0.44
1:D:299:LEU:HD22	1:D:309:LEU:HD13	1.99	0.44
1:D:592:LEU:O	1:D:595:VAL:O	2.35	0.44
1:D:945:ASN:HD22	1:D:1143:LYS:HA	1.82	0.44
1:A:134:THR:O	1:A:140:MET:HG3	2.17	0.44
1:A:155:ILE:CG2	1:A:706:ILE:HG13	2.47	0.44
1:A:417:ILE:HG12	1:A:454:TYR:CE1	2.52	0.44
1:A:446:HIS:CD2	1:A:450:LYS:HD2	2.52	0.44
1:A:219:HIS:HA	1:A:254:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:GLY:O	1:A:541:LEU:C	2.60	0.44
1:A:965:ILE:O	1:A:966:GLY:C	2.58	0.44
1:B:700:ILE:O	1:B:701:GLU:O	2.36	0.44
1:B:1119:MET:SD	1:B:1216:ARG:HD2	2.58	0.44
1:D:178:GLN:NE2	1:D:206:ASP:OD1	2.47	0.44
1:D:412:ASP:C	1:D:414:ASP:N	2.74	0.44
1:A:342:LEU:O	1:A:345:PHE:HB3	2.17	0.44
1:A:1166:LEU:CD2	1:A:1189:GLY:HA2	2.48	0.44
1:B:315:GLU:O	1:B:316:ALA:C	2.60	0.44
1:B:451:ASP:CG	1:D:916:PRO:HG3	2.42	0.44
1:B:798:TRP:CG	1:B:799:PRO:N	2.81	0.44
1:B:931:GLY:HA2	1:B:1240:TYR:HA	1.98	0.44
1:B:1149:ILE:HD12	1:B:1149:ILE:HA	1.52	0.44
1:C:58:GLU:O	1:C:62:SER:HB2	2.17	0.44
1:C:1102:LYS:O	1:C:1104:PHE:N	2.51	0.44
1:D:14:TRP:O	1:D:17:ILE:HG23	2.18	0.44
1:D:928:VAL:CG2	1:D:1173:ILE:HG22	2.48	0.44
1:D:1139:LYS:HE3	1:D:1141:LEU:HD21	2.00	0.44
1:A:273:ASP:OD1	1:A:273:ASP:C	2.61	0.44
1:A:676:ASP:HB2	1:A:711:ILE:CG2	2.48	0.44
1:A:969:ARG:HH11	1:A:972:LEU:CD2	2.31	0.44
1:B:689:TYR:CB	1:B:704:HIS:HD2	2.29	0.44
1:B:689:TYR:CD2	1:B:690:LYS:N	2.86	0.44
1:B:774:LEU:O	1:B:775:TYR:CD2	2.71	0.44
1:B:945:ASN:ND2	1:B:951:LYS:HB3	2.33	0.44
1:C:36:MET:O	1:C:39:ILE:N	2.50	0.44
1:C:706:ILE:CG2	1:C:707:GLU:N	2.80	0.44
1:C:707:GLU:OE1	1:C:707:GLU:O	2.36	0.44
1:C:845:MET:O	1:C:849:SER:HB2	2.17	0.44
1:A:461:SER:C	1:A:462:ILE:CG1	2.88	0.44
1:B:543:TRP:NE1	1:B:553:PRO:HD2	2.33	0.44
1:C:154:LYS:HG3	1:C:161:TRP:CE2	2.53	0.44
1:C:206:ASP:OD1	1:C:208:ASP:HB2	2.17	0.44
1:C:259:LEU:HD11	1:C:741:LEU:CD1	2.47	0.44
1:C:459:LEU:C	1:C:461:SER:H	2.24	0.44
1:C:516:TYR:CE2	1:C:530:LEU:HD12	2.52	0.44
1:A:459:LEU:O	1:A:462:ILE:HD12	2.18	0.44
1:B:308:VAL:O	1:B:309:LEU:C	2.60	0.44
1:B:471:UNK:C	1:B:473:UNK:N	2.79	0.44
1:B:531:LYS:HG2	1:B:572:LYS:HB3	1.99	0.44
1:C:55:LEU:HD12	1:C:55:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLN:HG2	1:C:681:PHE:CD1	2.52	0.44
1:D:787:LYS:HA	1:D:827:VAL:HG21	2.00	0.44
1:A:264:ILE:HB	1:A:265:THR:H	1.52	0.44
1:A:593:MET:HE3	1:A:604:ILE:HG21	2.00	0.44
1:B:6:PHE:O	1:B:10:ILE:HB	2.18	0.44
1:B:250:LEU:CD2	1:B:253:LEU:HD23	2.47	0.44
1:B:391:ILE:H	1:B:391:ILE:HG13	1.60	0.44
1:B:712:PRO:O	1:B:713:GLU:CB	2.64	0.44
1:B:971:LYS:HG2	1:B:975:GLN:HE21	1.83	0.44
1:C:362:GLN:O	1:C:365:GLU:HB3	2.18	0.44
1:C:959:LEU:HD21	1:C:1137:GLU:OE2	2.18	0.44
1:D:387:GLN:O	1:D:391:ILE:HG12	2.17	0.44
1:A:981:PRO:O	1:A:982:THR:C	2.61	0.44
1:B:286:PHE:CZ	1:B:548:TYR:CD2	3.05	0.44
1:B:933:TYR:CZ	1:B:1139:LYS:HB2	2.53	0.44
1:C:293:LEU:HD21	1:C:540:GLY:HA3	2.00	0.44
1:C:530:LEU:O	1:C:534:THR:HB	2.18	0.44
1:D:56:SER:HB3	1:D:59:GLU:HB2	1.98	0.44
1:D:507:ARG:HA	1:D:510:GLU:HB3	2.00	0.44
1:D:768:VAL:HG13	1:D:858:LEU:HD13	2.00	0.44
1:A:109:GLU:O	1:A:113:GLN:HB3	2.18	0.43
1:A:1111:SER:HB2	1:A:1191:THR:HA	1.99	0.43
1:B:516:TYR:OH	1:B:569:ASP:OD2	2.36	0.43
1:C:111:ALA:O	1:C:112:LEU:C	2.60	0.43
1:C:352:LYS:HD2	1:C:354:ASP:O	2.18	0.43
1:C:429:ASN:O	1:C:430:LEU:C	2.61	0.43
1:D:762:SER:C	1:D:764:GLN:H	2.25	0.43
1:B:682:ASN:HA	1:B:683:PRO:HD2	1.49	0.43
1:C:307:PRO:HG2	1:C:764:GLN:CG	2.48	0.43
1:C:597:PRO:HD2	1:C:600:SER:HB2	2.00	0.43
1:C:876:ARG:NH1	1:C:920:GLU:OE1	2.51	0.43
1:D:1114:LEU:HD12	1:D:1188:VAL:HG12	2.00	0.43
1:A:843:LEU:HD12	1:A:843:LEU:HA	1.74	0.43
1:B:14:TRP:HB3	1:B:256:TYR:CG	2.53	0.43
1:B:534:THR:HG22	1:B:573:GLY:N	2.32	0.43
1:B:731:GLY:C	1:B:733:SER:N	2.76	0.43
1:B:781:SER:C	1:B:783:SER:N	2.75	0.43
1:B:807:LEU:O	1:B:808:SER:HB3	2.18	0.43
1:C:561:TYR:N	1:C:561:TYR:CD2	2.85	0.43
1:C:1123:GLU:O	1:C:1127:ILE:HG13	2.18	0.43
1:D:91:ARG:C	1:D:93:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:THR:CG2	1:D:338:TRP:HE1	2.03	0.43
1:D:347:TYR:O	1:D:348:LEU:C	2.60	0.43
1:D:797:ARG:O	1:D:798:TRP:C	2.61	0.43
1:D:1150:LEU:C	1:D:1150:LEU:HD12	2.43	0.43
1:A:220:HIS:CE1	1:A:735:LEU:HB2	2.53	0.43
1:A:744:LEU:HA	1:A:744:LEU:HD12	1.62	0.43
1:A:826:LYS:CD	1:A:827:VAL:H	2.31	0.43
1:B:1191:THR:HG22	1:B:1191:THR:O	2.18	0.43
1:C:426:VAL:HG12	1:C:427:ARG:N	2.33	0.43
1:D:32:LEU:HA	1:D:201:CYS:O	2.18	0.43
1:D:329:LYS:HA	1:D:542:GLN:OE1	2.18	0.43
1:D:679:PHE:N	1:D:679:PHE:HD1	2.16	0.43
1:A:11:SER:O	1:A:15:PRO:HA	2.18	0.43
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.79	0.43
1:B:533:MET:HE3	1:B:565:PRO:HA	2.00	0.43
1:C:152:HIS:CD2	1:C:706:ILE:HB	2.54	0.43
1:C:273:ASP:O	1:C:277:VAL:HG23	2.18	0.43
1:A:311:GLN:HG2	1:A:364:LEU:HD12	2.00	0.43
1:A:1111:SER:HA	1:A:1190:TYR:CE1	2.53	0.43
1:B:346:GLU:OE1	1:B:566:ARG:HB3	2.18	0.43
1:B:527:THR:HB	1:B:528:ASP:H	1.57	0.43
1:B:592:LEU:O	1:B:596:LEU:HD12	2.19	0.43
1:C:870:PRO:HD2	1:C:887:ASN:CB	2.49	0.43
1:D:103:ARG:O	1:D:106:MET:HB3	2.19	0.43
1:D:266:ASP:O	1:D:267:SER:CB	2.61	0.43
1:D:832:PRO:HA	1:D:836:GLU:OE1	2.18	0.43
1:A:589:PHE:HA	1:A:592:LEU:HB2	1.99	0.43
1:A:820:LYS:HG3	1:A:820:LYS:O	2.18	0.43
1:A:1158:LEU:O	1:A:1161:SER:OG	2.26	0.43
1:B:220:HIS:HE1	1:B:735:LEU:N	2.00	0.43
1:B:566:ARG:HB3	1:B:566:ARG:HE	1.72	0.43
1:B:684:GLN:HE21	1:B:684:GLN:HB2	1.59	0.43
1:C:156:THR:H	1:C:706:ILE:HD11	1.83	0.43
1:C:950:LEU:HD23	1:C:1144:VAL:O	2.18	0.43
1:D:303:LYS:CE	1:D:356:ASP:HA	2.36	0.43
1:D:343:SER:HA	1:D:568:SER:OG	2.18	0.43
1:B:516:TYR:HE2	1:B:533:MET:CE	2.31	0.43
1:D:61:TYR:O	1:D:65:PHE:CD2	2.72	0.43
1:D:664:SER:HB3	1:D:665:PRO:HD2	2.00	0.43
1:A:101:ARG:HD3	1:A:595:VAL:HG13	2.01	0.43
1:A:140:MET:HB3	1:A:171:HIS:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASN:ND2	1:B:195:ASN:C	2.77	0.43
1:B:303:LYS:HA	1:B:303:LYS:HD2	1.83	0.43
1:B:872:ASN:ND2	1:B:887:ASN:HD22	2.10	0.43
1:C:319:HIS:HE1	1:C:375:ARG:HG3	1.84	0.43
1:C:593:MET:CB	1:C:652:LEU:HD11	2.49	0.43
1:A:14:TRP:O	1:A:17:ILE:HG23	2.19	0.43
1:A:622:PHE:O	1:A:623:TYR:CG	2.72	0.43
1:A:1150:LEU:HD12	1:A:1150:LEU:C	2.44	0.43
1:B:159:THR:O	1:B:162:GLN:HG2	2.19	0.43
1:B:798:TRP:HA	1:B:801:LEU:HD23	2.01	0.43
1:C:355:ILE:HG22	1:C:359:TRP:CD1	2.53	0.43
1:D:604:ILE:O	1:D:606:VAL:N	2.52	0.43
1:D:713:GLU:HG3	1:D:714:SER:N	2.33	0.43
1:A:217:HIS:CG	1:A:723:GLY:HA2	2.53	0.42
1:A:461:SER:O	1:A:461:SER:OG	2.32	0.42
1:A:542:GLN:NE2	1:A:542:GLN:HA	2.34	0.42
1:B:312:THR:CG2	1:B:338:TRP:NE1	2.80	0.42
1:B:1180:PRO:O	1:B:1181:LEU:C	2.62	0.42
1:C:212:LEU:HD11	1:C:548:TYR:CE1	2.54	0.42
1:C:677:LEU:HD22	1:C:708:ARG:HH12	1.84	0.42
1:C:816:TYR:CD1	1:C:816:TYR:N	2.87	0.42
1:C:834:ASP:HA	1:C:837:ARG:HB3	2.01	0.42
1:C:949:ARG:HH21	1:C:1145:PRO:HB3	1.83	0.42
1:D:195:ASN:HD22	1:D:196:PRO:CD	2.26	0.42
1:B:417:ILE:CG1	1:B:454:TYR:CD1	2.99	0.42
1:B:1147:GLU:CD	1:B:1147:GLU:N	2.76	0.42
1:C:133:ILE:HA	1:C:140:MET:SD	2.59	0.42
1:C:351:GLU:OE2	1:C:507:ARG:NH1	2.51	0.42
1:A:36:MET:HE1	1:A:83:MET:HB3	2.02	0.42
1:A:171:HIS:CE1	1:A:172:GLU:OE2	2.72	0.42
1:A:1227:SER:O	1:A:1229:PHE:N	2.52	0.42
1:B:182:MET:HA	1:B:182:MET:HE2	2.00	0.42
1:B:1040:UNK:O	1:B:1041:UNK:C	2.67	0.42
1:C:67:TYR:O	1:C:70:HIS:N	2.52	0.42
1:C:258:ALA:HA	1:C:274:PHE:CE1	2.54	0.42
1:D:1207:ILE:HG22	1:D:1209:ALA:H	1.83	0.42
1:A:516:TYR:CE2	1:A:533:MET:CE	3.01	0.42
1:A:689:TYR:HB3	1:A:700:ILE:HB	2.00	0.42
1:A:932:ASP:OD1	1:A:932:ASP:N	2.52	0.42
1:B:209:LEU:HB3	1:B:223:LEU:HD22	2.00	0.42
1:B:928:VAL:HG21	1:B:1173:ILE:CG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1090:LEU:O	1:C:1091:LYS:C	2.62	0.42
1:D:1173:ILE:HG13	1:D:1231:LEU:HB2	2.01	0.42
1:A:98:ARG:HG3	1:A:644:ILE:HD13	2.01	0.42
1:A:950:LEU:HG	1:A:952:LEU:CD2	2.50	0.42
1:C:1191:THR:O	1:C:1191:THR:HG23	2.19	0.42
1:D:199:ARG:HG2	1:D:738:PHE:CZ	2.54	0.42
1:D:587:LYS:HG2	1:D:671:ASN:OD1	2.19	0.42
1:D:826:LYS:HA	1:D:826:LYS:HZ3	1.84	0.42
1:A:262:GLU:HG3	1:A:263:GLU:H	1.82	0.42
1:A:264:ILE:CG2	1:A:265:THR:N	2.75	0.42
1:A:657:ALA:O	1:A:660:ASP:HB2	2.20	0.42
1:A:918:ASN:O	1:A:922:PRO:HA	2.20	0.42
1:A:945:ASN:ND2	1:A:951:LYS:HB3	2.35	0.42
1:A:1152:ALA:CB	1:A:1173:ILE:HG22	2.49	0.42
1:C:152:HIS:CD2	1:C:704:HIS:CE1	2.90	0.42
1:C:270:PHE:HB3	1:C:321:ASP:O	2.19	0.42
1:C:326:GLU:O	1:C:326:GLU:HG2	2.19	0.42
1:C:357:VAL:HG12	1:C:361:ASN:HD21	1.85	0.42
1:C:833:GLN:O	1:C:835:PHE:N	2.53	0.42
1:D:537:TYR:N	1:D:559:TYR:HE1	2.17	0.42
1:D:941:VAL:HG13	1:D:950:LEU:HD12	2.02	0.42
1:D:1193:ILE:O	1:D:1195:LYS:N	2.51	0.42
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.91	0.42
1:A:690:LYS:HA	1:A:699:ASP:OD1	2.19	0.42
1:A:706:ILE:HG22	1:A:707:GLU:N	2.35	0.42
1:A:803:GLU:O	1:A:871:VAL:HG23	2.19	0.42
1:A:916:PRO:HG3	1:C:451:ASP:CG	2.45	0.42
1:A:918:ASN:HA	1:A:944:TYR:CZ	2.55	0.42
1:B:152:HIS:HD2	1:B:704:HIS:HE1	1.63	0.42
1:C:185:ILE:O	1:C:189:ARG:HG2	2.20	0.42
1:C:512:LYS:C	1:C:514:GLN:N	2.75	0.42
1:C:795:TYR:HB3	1:C:801:LEU:HD22	2.01	0.42
1:D:209:LEU:HD23	1:D:212:LEU:HD12	2.02	0.42
1:D:746:LEU:HD12	1:D:769:LEU:HB3	2.01	0.42
1:A:675:THR:HB	1:A:710:PHE:CE2	2.54	0.42
1:B:511:TRP:HH2	1:B:566:ARG:NH2	2.16	0.42
1:B:1123:GLU:OE1	1:B:1219:THR:N	2.50	0.42
1:C:102:PHE:HA	1:C:597:PRO:HG3	2.01	0.42
1:C:293:LEU:HD22	1:C:537:TYR:CD1	2.55	0.42
1:C:700:ILE:HG22	1:C:704:HIS:HB2	2.00	0.42
1:A:212:LEU:CD2	1:A:548:TYR:CD1	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:HD22	1:A:1143:LYS:H	1.66	0.42
1:B:530:LEU:C	1:B:532:GLU:H	2.27	0.42
1:B:605:PRO:C	1:B:607:VAL:N	2.78	0.42
1:B:897:LEU:HD23	1:B:897:LEU:HA	1.84	0.42
1:C:376:THR:C	1:C:378:MET:N	2.77	0.42
1:C:1199:ILE:CG2	1:C:1200:GLN:N	2.82	0.42
1:D:578:ILE:O	1:D:578:ILE:HD12	2.20	0.42
1:A:887:ASN:ND2	1:A:1195:LYS:HB2	2.19	0.42
1:B:312:THR:HG23	1:B:341:TYR:CB	2.48	0.42
1:B:534:THR:O	1:B:536:ASN:N	2.53	0.42
1:C:172:GLU:CD	1:C:172:GLU:H	2.27	0.42
1:C:320:MET:HE1	1:C:324:ILE:CG1	2.48	0.42
1:C:729:LYS:HD3	1:C:733:SER:O	2.20	0.42
1:A:67:TYR:OH	1:A:226:GLU:OE2	2.33	0.41
1:A:152:HIS:CE1	1:A:708:ARG:HG2	2.55	0.41
1:A:259:LEU:CB	1:A:767:MET:HE2	2.49	0.41
1:A:717:ASN:OD1	1:A:717:ASN:N	2.53	0.41
1:B:43:CYS:HB2	1:B:64:ILE:CD1	2.50	0.41
1:B:949:ARG:HG2	1:B:949:ARG:NH1	2.34	0.41
1:C:36:MET:CE	1:C:68:ILE:HG12	2.50	0.41
1:C:206:ASP:CG	1:C:208:ASP:HB2	2.45	0.41
1:D:81:PHE:HE2	1:D:83:MET:HE2	1.84	0.41
1:D:219:HIS:HD2	1:D:254:ARG:HH11	1.68	0.41
1:D:398:LEU:HD12	1:D:398:LEU:HA	1.83	0.41
1:A:280:ASP:O	1:A:284:VAL:HG23	2.20	0.41
1:B:182:MET:HE3	1:B:185:ILE:CD1	2.50	0.41
1:B:514:GLN:O	1:B:518:ASP:HB2	2.20	0.41
1:B:854:THR:HG22	1:B:855:LYS:HG3	2.01	0.41
1:B:876:ARG:HE	1:B:880:GLY:HA2	1.84	0.41
1:D:94:MET:O	1:D:98:ARG:HB2	2.21	0.41
1:D:394:VAL:HG22	1:D:418:PHE:CE2	2.54	0.41
1:D:586:PHE:O	1:D:587:LYS:C	2.62	0.41
1:A:830:ARG:HG3	1:A:831:LYS:O	2.20	0.41
1:B:252:ILE:HB	1:B:739:PRO:HG2	2.02	0.41
1:B:516:TYR:CE2	1:B:533:MET:HE2	2.54	0.41
1:B:701:GLU:C	1:B:703:ASN:N	2.77	0.41
1:B:703:ASN:O	1:B:705:CYS:SG	2.67	0.41
1:B:843:LEU:O	1:B:844:LYS:C	2.63	0.41
1:B:1167:GLY:O	1:B:1186:THR:HG23	2.21	0.41
1:C:128:PHE:HE2	1:C:130:SER:HA	1.85	0.41
1:C:312:THR:CG2	1:C:338:TRP:NE1	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:MET:HE2	1:C:790:MET:HB2	1.84	0.41
1:C:918:ASN:HA	1:C:944:TYR:OH	2.20	0.41
1:D:58:GLU:OE1	1:D:695:GLY:HA3	2.20	0.41
1:D:358:GLU:HA	1:D:361:ASN:HD22	1.85	0.41
1:D:704:HIS:HE1	1:D:706:ILE:HG12	1.85	0.41
1:A:848:LYS:HB2	1:A:848:LYS:HE3	1.83	0.41
1:A:862:ILE:H	1:A:862:ILE:CD1	2.13	0.41
1:B:65:PHE:CE1	1:B:150:PHE:HB2	2.56	0.41
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.83	0.41
1:B:962:GLU:CG	1:B:1169:ARG:HE	2.33	0.41
1:C:443:ILE:HD11	1:C:458:ASP:OD1	2.20	0.41
1:C:657:ALA:O	1:C:660:ASP:HB2	2.21	0.41
1:C:706:ILE:N	1:C:706:ILE:CD1	2.80	0.41
1:C:907:GLU:HA	1:C:910:ILE:HG13	2.01	0.41
1:C:929:PHE:HB2	1:C:939:ALA:HB2	2.01	0.41
1:D:155:ILE:HG22	1:D:706:ILE:HD12	2.01	0.41
1:D:565:PRO:HB2	1:D:566:ARG:H	1.64	0.41
1:D:881:SER:HB3	1:D:914:PRO:HD3	2.02	0.41
1:B:682:ASN:OD1	1:B:684:GLN:N	2.53	0.41
1:B:1118:SER:O	1:B:1122:VAL:HG23	2.20	0.41
1:C:250:LEU:O	1:C:254:ARG:HG3	2.20	0.41
1:C:514:GLN:HE21	1:C:517:LYS:HD2	1.84	0.41
1:C:787:LYS:HE3	1:C:787:LYS:HB2	1.96	0.41
1:C:831:LYS:C	1:C:833:GLN:H	2.23	0.41
1:C:918:ASN:HD22	1:C:918:ASN:N	2.17	0.41
1:C:922:PRO:O	1:C:923:LYS:C	2.62	0.41
1:C:1165:HIS:O	1:C:1166:LEU:C	2.63	0.41
1:D:294:PRO:HB2	1:D:564:ALA:HB2	2.02	0.41
1:D:323:TYR:O	1:D:324:ILE:C	2.63	0.41
1:B:12:GLU:OE1	1:B:762:SER:HB2	2.21	0.41
1:B:207:ALA:O	1:B:209:LEU:N	2.54	0.41
1:C:152:HIS:HA	1:C:706:ILE:CG1	2.41	0.41
1:C:592:LEU:HA	1:C:592:LEU:HD23	1.81	0.41
1:C:890:ILE:CG2	1:C:891:GLU:N	2.82	0.41
1:D:599:ARG:HH22	1:D:625:ASN:HD21	1.68	0.41
1:A:10:ILE:HG21	1:A:10:ILE:HD13	1.50	0.41
1:A:768:VAL:HG13	1:A:858:LEU:HD13	2.02	0.41
1:A:1223:LEU:HD12	1:A:1223:LEU:HA	1.87	0.41
1:B:5:LYS:HD2	1:B:5:LYS:HA	1.89	0.41
1:B:264:ILE:CG2	1:B:265:THR:H	2.31	0.41
1:B:330:ILE:HD12	1:B:542:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ASP:OD1	1:B:461:SER:HB3	2.19	0.41
1:C:533:MET:O	1:C:534:THR:C	2.62	0.41
1:C:917:ILE:CG1	1:C:947:GLU:O	2.69	0.41
1:C:1088:SER:O	1:C:1089:ILE:C	2.63	0.41
1:C:1111:SER:HB3	1:C:1191:THR:HA	2.02	0.41
1:D:87:GLY:O	1:D:135:PRO:HG3	2.19	0.41
1:D:928:VAL:HG21	1:D:1173:ILE:CG2	2.48	0.41
1:D:934:ALA:HB2	1:D:956:LYS:HB3	2.00	0.41
1:D:952:LEU:CD2	1:D:1149:ILE:HD13	2.51	0.41
1:D:1192:SER:O	1:D:1194:GLY:N	2.54	0.41
1:A:212:LEU:HD21	1:A:548:TYR:CE1	2.56	0.41
1:A:855:LYS:HB2	1:A:857:ILE:HG13	2.03	0.41
1:A:876:ARG:HH12	1:A:920:GLU:CD	2.28	0.41
1:B:155:ILE:HB	1:B:706:ILE:HD12	2.01	0.41
1:B:297:PRO:CG	1:B:298:ASP:H	2.34	0.41
1:B:301:LEU:HD22	1:B:306:PHE:CE2	2.56	0.41
1:C:391:ILE:H	1:C:391:ILE:HG13	1.69	0.41
1:D:934:ALA:CB	1:D:956:LYS:HB3	2.51	0.41
1:A:391:ILE:HG13	1:A:391:ILE:H	1.68	0.41
1:A:685:VAL:HG21	1:A:707:GLU:OE2	2.20	0.41
1:A:831:LYS:H	1:A:831:LYS:CD	2.28	0.41
1:A:1207:ILE:HG22	1:A:1209:ALA:H	1.86	0.41
1:B:12:GLU:CD	1:B:762:SER:HB2	2.45	0.41
1:B:45:HIS:CE1	1:B:130:SER:HB2	2.56	0.41
1:B:159:THR:HA	1:B:162:GLN:HG2	2.02	0.41
1:B:864:ALA:O	1:B:895:LEU:N	2.47	0.41
1:B:1104:PHE:HB2	1:B:1106:VAL:HG23	2.03	0.41
1:B:1188:VAL:CG1	1:B:1202:LEU:HB2	2.50	0.41
1:B:1206:GLU:HA	1:B:1221:ARG:HG2	2.02	0.41
1:C:99:ALA:HB1	1:C:642:VAL:HG12	2.02	0.41
1:C:254:ARG:HH11	1:C:254:ARG:HD3	1.72	0.41
1:C:575:ASP:O	1:C:576:GLN:HB3	2.21	0.41
1:D:221:PHE:CB	1:D:250:LEU:HD12	2.48	0.41
1:D:387:GLN:CG	1:D:432:PHE:CZ	3.04	0.41
1:D:545:LEU:HA	1:D:545:LEU:HD22	1.80	0.41
1:D:707:GLU:N	1:D:707:GLU:OE1	2.52	0.41
1:A:355:ILE:O	1:A:355:ILE:HD12	2.21	0.41
1:A:862:ILE:N	1:A:862:ILE:CD1	2.80	0.41
1:A:1127:ILE:HG12	1:A:1221:ARG:NH2	2.35	0.41
1:B:44:THR:HG22	1:B:45:HIS:CE1	2.57	0.41
1:B:412:ASP:C	1:B:414:ASP:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:MET:HE3	1:C:106:MET:O	2.20	0.41
1:C:357:VAL:O	1:C:361:ASN:ND2	2.52	0.41
1:C:378:MET:HE2	1:C:378:MET:HB3	1.86	0.41
1:C:867:LYS:HE2	1:C:890:ILE:HD13	2.02	0.41
1:A:34:LEU:CD2	1:A:203:TYR:HB3	2.51	0.40
1:A:96:GLN:O	1:A:100:ARG:HG3	2.21	0.40
1:A:173:VAL:HA	1:A:174:PRO:HD3	1.89	0.40
1:A:744:LEU:HB2	1:A:798:TRP:HE1	1.85	0.40
1:A:941:VAL:HG13	1:A:950:LEU:HD12	2.02	0.40
1:B:376:THR:O	1:B:380:LYS:HG3	2.21	0.40
1:B:710:PHE:CE2	1:B:711:ILE:O	2.74	0.40
1:C:3:ILE:HB	1:C:6:PHE:HB2	2.04	0.40
1:C:359:TRP:HZ2	1:C:363:GLN:NE2	2.18	0.40
1:C:571:ILE:C	1:C:573:GLY:H	2.29	0.40
1:D:798:TRP:CG	1:D:799:PRO:N	2.88	0.40
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.94	0.40
1:A:571:ILE:C	1:A:573:GLY:H	2.28	0.40
1:A:708:ARG:HB2	1:A:708:ARG:NH1	2.35	0.40
1:A:840:PHE:O	1:A:844:LYS:HG2	2.22	0.40
1:B:33:TYR:OH	1:B:200:HIS:CD2	2.75	0.40
1:C:536:ASN:HD22	1:C:536:ASN:HA	1.69	0.40
1:C:918:ASN:HD22	1:C:918:ASN:H	1.69	0.40
1:C:952:LEU:HD21	1:C:1149:ILE:HD13	2.03	0.40
1:D:81:PHE:O	1:D:166:VAL:HA	2.21	0.40
1:D:269:GLN:HB2	1:D:320:MET:O	2.21	0.40
1:D:391:ILE:HG13	1:D:392:GLY:N	2.36	0.40
1:D:701:GLU:O	1:D:702:HIS:C	2.65	0.40
1:A:201:CYS:HA	1:A:222:CYS:O	2.21	0.40
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.78	0.40
1:A:519:LYS:HD3	1:A:563:TYR:CE1	2.57	0.40
1:A:527:THR:HB	1:A:528:ASP:H	1.50	0.40
1:A:657:ALA:HA	1:A:660:ASP:HB2	2.03	0.40
1:A:676:ASP:CB	1:A:711:ILE:HG22	2.51	0.40
1:A:1156:TYR:O	1:A:1160:ARG:HG3	2.22	0.40
1:B:65:PHE:CZ	1:B:150:PHE:HB2	2.56	0.40
1:C:264:ILE:CG2	1:C:268:VAL:CG1	2.86	0.40
1:D:226:GLU:H	1:D:226:GLU:HG2	1.68	0.40
1:D:1189:GLY:O	1:D:1200:GLN:HB2	2.22	0.40
1:A:31:ASN:HA	1:A:80:THR:O	2.21	0.40
1:B:239:THR:O	1:B:240:LEU:C	2.64	0.40
1:B:534:THR:O	1:B:535:GLU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:THR:C	1:B:536:ASN:N	2.79	0.40
1:B:1039:UNK:O	1:B:1040:UNK:C	2.68	0.40
1:B:1213:PHE:HB3	1:B:1216:ARG:HH11	1.87	0.40
1:C:146:ASN:OD1	1:C:693:LEU:HG	2.20	0.40
1:C:815:VAL:CG1	1:C:830:ARG:HH11	2.33	0.40
1:C:1102:LYS:CB	1:C:1103:PRO:CD	2.95	0.40
1:D:527:THR:CG2	1:D:528:ASP:H	2.08	0.40
1:D:586:PHE:HB3	1:D:590:GLN:HB2	2.04	0.40
1:D:848:LYS:O	1:D:852:GLN:HG3	2.21	0.40
1:D:1226:ASP:HB3	1:D:1229:PHE:CE1	2.56	0.40
1:A:301:LEU:C	1:A:303:LYS:N	2.74	0.40
1:A:308:VAL:HG11	1:A:363:GLN:HG2	2.04	0.40
1:B:458:ASP:OD1	1:B:461:SER:HB2	2.21	0.40
1:B:656:MET:O	1:B:659:TYR:HB2	2.22	0.40
1:C:104:THR:HG22	1:C:104:THR:O	2.21	0.40
1:C:152:HIS:HD2	1:C:704:HIS:HE1	1.62	0.40
1:C:862:ILE:H	1:C:862:ILE:CD1	2.29	0.40
1:D:16:GLN:HE22	1:D:799:PRO:HG3	1.87	0.40
1:D:907:GLU:H	1:D:907:GLU:HG2	1.70	0.40
1:D:1165:HIS:O	1:D:1166:LEU:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1001/1155 (87%)	869 (87%)	95 (10%)	37 (4%)	2	11
1	B	998/1155 (86%)	842 (84%)	109 (11%)	47 (5%)	2	7
1	C	1008/1155 (87%)	866 (86%)	104 (10%)	38 (4%)	2	10
1	D	982/1155 (85%)	824 (84%)	117 (12%)	41 (4%)	2	9
All	All	3989/4620 (86%)	3401 (85%)	425 (11%)	163 (4%)	2	9

All (163) 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	702	HIS
1	A	712	PRO
1	A	798	TRP
1	A	799	PRO
1	A	861	ASP
1	A	1093	VAL
1	B	4	PRO
1	B	109	GLU
1	B	297	PRO
1	B	527	THR
1	B	596	LEU
1	B	701	GLU
1	B	712	PRO
1	B	716	GLU
1	B	798	TRP
1	B	946	SER
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
1	C	702	HIS
1	C	712	PRO
1	C	834	ASP
1	C	860	ASP
1	C	1105	VAL
1	C	1138	GLN
1	D	264	ILE
1	D	267	SER
1	D	565	PRO
1	D	702	HIS

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Mol	Chain	Res	Type
1	D	712	PRO
1	D	716	GLU
1	D	860	ASP
1	D	1193	ILE
1	D	1194	GLY
1	D	1236	ARG
1	A	92	ALA
1	A	193	ASP
1	A	518	ASP
1	A	596	LEU
1	A	713	GLU
1	A	754	SER
1	A	1095	ASP
1	B	56	SER
1	B	264	ILE
1	B	404	ARG
1	B	460	ASP
1	B	565	PRO
1	B	582	LYS
1	B	646	PHE
1	B	713	GLU
1	B	717	ASN
1	B	822	GLY
1	B	981	PRO
1	B	1108	SER
1	B	1138	GLN
1	B	1139	LYS
1	B	1213	PHE
1	C	403	GLN
1	C	513	ASP
1	C	528	ASP
1	C	713	GLU
1	C	797	ARG
1	C	833	GLN
1	C	1104	PHE
1	C	1107	VAL
1	D	92	ALA
1	D	106	MET
1	D	269	GLN
1	D	303	LYS
1	D	582	LYS
1	D	624	PRO

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Mol	Chain	Res	Type
1	D	713	GLU
1	A	191	GLN
1	A	302	LYS
1	A	461	SER
1	A	735	LEU
1	A	863	SER
1	A	917	ILE
1	A	1116	LYS
1	B	353	LYS
1	B	535	GLU
1	B	823	LYS
1	B	824	LEU
1	C	698	ASN
1	C	716	GLU
1	C	832	PRO
1	C	980	TYR
1	D	4	PRO
1	D	356	ASP
1	D	596	LEU
1	D	602	ASN
1	D	605	PRO
1	D	625	ASN
1	D	701	GLU
1	D	714	SER
1	D	1112	ASP
1	D	1195	LYS
1	A	695	GLY
1	A	791	GLY
1	A	1111	SER
1	B	265	THR
1	B	602	ASN
1	B	624	PRO
1	B	649	GLN
1	B	774	LEU
1	B	812	GLU
1	B	972	LEU
1	B	1195	LYS
1	C	576	GLN
1	C	798	TRP
1	D	438	PHE
1	D	547	TYR
1	D	588	PRO

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Mol	Chain	Res	Type
1	D	736	ALA
1	D	798	TRP
1	D	963	PRO
1	D	1143	LYS
1	A	605	PRO
1	A	606	VAL
1	B	106	MET
1	B	687	THR
1	B	861	ASP
1	C	4	PRO
1	C	413	ALA
1	C	714	SER
1	C	957	GLY
1	C	1208	ILE
1	D	265	THR
1	D	606	VAL
1	D	645	SER
1	A	113	GLN
1	A	664	SER
1	B	110	LYS
1	B	208	ASP
1	C	835	PHE
1	C	1106	VAL
1	C	1194	GLY
1	A	264	ILE
1	B	653	VAL
1	B	1194	GLY
1	D	395	LYS
1	A	395	LYS
1	B	538	VAL
1	C	133	ILE
1	C	862	ILE
1	D	133	ILE
1	D	607	VAL
1	C	917	ILE
1	C	1103	PRO
1	D	553	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	922/1004 (92%)	793 (86%)	129 (14%)	3	11
1	B	919/1004 (92%)	775 (84%)	144 (16%)	2	9
1	C	927/1004 (92%)	800 (86%)	127 (14%)	3	12
1	D	905/1004 (90%)	762 (84%)	143 (16%)	2	8
All	All	3673/4016 (92%)	3130 (85%)	543 (15%)	3	10

All (543) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	9	PHE
1	A	10	ILE
1	A	24	SER
1	A	26	ILE
1	A	36	MET
1	A	55	LEU
1	A	57	GLU
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	156	THR
1	A	160	ARG
1	A	186	ARG
1	A	192	GLU
1	A	226	GLU
1	A	227	GLU
1	A	239	THR
1	A	255	GLU
1	A	263	GLU
1	A	273	ASP
1	A	291	ASP

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Mol	Chain	Res	Type
1	A	302	LYS
1	A	303	LYS
1	A	306	PHE
1	A	308	VAL
1	A	312	THR
1	A	315	GLU
1	A	326	GLU
1	A	329	LYS
1	A	340	LYS
1	A	350	PHE
1	A	351	GLU
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	420	LEU
1	A	421	GLU
1	A	424	GLU
1	A	450	LYS
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	571	ILE
1	A	584	GLN
1	A	587	LYS
1	A	590	GLN
1	A	591	GLN
1	A	593	MET
1	A	595	VAL
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	711	ILE
1	A	717	ASN
1	A	735	LEU
1	A	744	LEU
1	A	747	THR
1	A	749	GLU
1	A	773	ASP
1	A	785	LEU
1	A	793	ILE
1	A	796	SER
1	A	802	ARG
1	A	810	ILE
1	A	811	THR
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	862	ILE
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	952	LEU
1	A	962	GLU
1	A	965	ILE
1	A	972	LEU
1	A	982	THR
1	A	983	GLN
1	A	1093	VAL
1	A	1095	ASP
1	A	1098	SER
1	A	1107	VAL
1	A	1110	GLU
1	A	1112	ASP
1	A	1113	SER

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Mol	Chain	Res	Type
1	A	1119	MET
1	A	1140	LYS
1	A	1141	LEU
1	A	1143	LYS
1	A	1147	GLU
1	A	1149	ILE
1	A	1150	LEU
1	A	1153	GLU
1	A	1173	ILE
1	A	1178	LYS
1	A	1191	THR
1	A	1196	ASN
1	A	1212	ASN
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	44	THR
1	B	55	LEU
1	B	57	GLU
1	B	59	GLU
1	B	62	SER
1	B	63	LYS
1	B	96	GLN
1	B	112	LEU
1	B	113	GLN
1	B	114	LYS
1	B	130	SER
1	B	131	ASN
1	B	159	THR
1	B	182	MET
1	B	183	ASP
1	B	189	ARG
1	B	195	ASN
1	B	220	HIS
1	B	226	GLU
1	B	228	VAL
1	B	252	ILE
1	B	263	GLU

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Mol	Chain	Res	Type
1	B	271	GLU
1	B	282	ILE
1	B	290	ASN
1	B	291	ASP
1	B	312	THR
1	B	315	GLU
1	B	332	LEU
1	B	340	LYS
1	B	350	PHE
1	B	355	ILE
1	B	363	GLN
1	B	370	GLU
1	B	383	LEU
1	B	386	GLN
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	456	LYS
1	B	460	ASP
1	B	462	ILE
1	B	513	ASP
1	B	514	GLN
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	576	GLN
1	B	578	ILE
1	B	591	GLN
1	B	602	ASN
1	B	604	ILE
1	B	606	VAL
1	B	625	ASN
1	B	643	LYS
1	B	651	ARG

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Mol	Chain	Res	Type
1	B	669	LYS
1	B	684	GLN
1	B	691	THR
1	B	706	ILE
1	B	707	GLU
1	B	710	PHE
1	B	711	ILE
1	B	713	GLU
1	B	715	MET
1	B	725	PRO
1	B	730	LEU
1	B	735	LEU
1	B	747	THR
1	B	749	GLU
1	B	754	SER
1	B	765	GLN
1	B	772	GLN
1	B	774	LEU
1	B	793	ILE
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	842	GLU
1	B	843	LEU
1	B	846	THR
1	B	850	ASN
1	B	852	GLN
1	B	853	ARG
1	B	854	THR
1	B	858	LEU
1	B	860	ASP
1	B	889	THR
1	B	890	ILE
1	B	902	VAL
1	B	903	LYS
1	B	917	ILE
1	B	918	ASN
1	B	932	ASP
1	B	952	LEU

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Mol	Chain	Res	Type
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	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	1147	GLU
1	B	1149	ILE
1	B	1150	LEU
1	B	1153	GLU
1	B	1163	ARG
1	B	1178	LYS
1	B	1191	THR
1	B	1192	SER
1	B	1193	ILE
1	B	1196	ASN
1	B	1208	ILE
1	B	1217	LEU
1	B	1232	ASN
1	B	1239	VAL
1	C	4	PRO
1	C	10	ILE
1	C	17	ILE
1	C	26	ILE
1	C	38	SER
1	C	42	ASN
1	C	44	THR

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Mol	Chain	Res	Type
1	C	54	ARG
1	C	55	LEU
1	C	58	GLU
1	C	59	GLU
1	C	62	SER
1	C	98	ARG
1	C	101	ARG
1	C	113	GLN
1	C	137	THR
1	C	140	MET
1	C	143	LEU
1	C	154	LYS
1	C	165	LYS
1	C	176	GLU
1	C	183	ASP
1	C	189	ARG
1	C	226	GLU
1	C	228	VAL
1	C	267	SER
1	C	268	VAL
1	C	302	LYS
1	C	303	LYS
1	C	306	PHE
1	C	317	LEU
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	391	ILE
1	C	402	VAL
1	C	417	ILE
1	C	426	VAL
1	C	435	GLU
1	C	447	SER
1	C	449	SER
1	C	526	ASP
1	C	527	THR

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Mol	Chain	Res	Type
1	C	528	ASP
1	C	530	LEU
1	C	531	LYS
1	C	532	GLU
1	C	545	LEU
1	C	591	GLN
1	C	595	VAL
1	C	600	SER
1	C	604	ILE
1	C	606	VAL
1	C	607	VAL
1	C	621	ASP
1	C	641	VAL
1	C	642	VAL
1	C	643	LYS
1	C	650	LYS
1	C	666	ASP
1	C	675	THR
1	C	685	VAL
1	C	688	VAL
1	C	701	GLU
1	C	706	ILE
1	C	707	GLU
1	C	708	ARG
1	C	711	ILE
1	C	730	LEU
1	C	735	LEU
1	C	744	LEU
1	C	764	GLN
1	C	772	GLN
1	C	782	LEU
1	C	785	LEU
1	C	787	LYS
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	836	GLU
1	C	841	ARG

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Mol	Chain	Res	Type
1	C	842	GLU
1	C	843	LEU
1	C	852	GLN
1	C	858	LEU
1	C	861	ASP
1	C	875	VAL
1	C	883	SER
1	C	887	ASN
1	C	907	GLU
1	C	910	ILE
1	C	912	LYS
1	C	917	ILE
1	C	918	ASN
1	C	932	ASP
1	C	940	THR
1	C	947	GLU
1	C	948	THR
1	C	949	ARG
1	C	952	LEU
1	C	968	VAL
1	C	977	LEU
1	C	1088	SER
1	C	1091	LYS
1	C	1092	THR
1	C	1097	LEU
1	C	1107	VAL
1	C	1109	LEU
1	C	1147	GLU
1	C	1149	ILE
1	C	1155	SER
1	C	1157	VAL
1	C	1173	ILE
1	C	1178	LYS
1	C	1192	SER
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

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Mol	Chain	Res	Type
1	D	66	SER
1	D	96	GLN
1	D	98	ARG
1	D	113	GLN
1	D	154	LYS
1	D	155	ILE
1	D	160	ARG
1	D	164	VAL
1	D	173	VAL
1	D	186	ARG
1	D	226	GLU
1	D	228	VAL
1	D	248	LEU
1	D	262	GLU
1	D	265	THR
1	D	266	ASP
1	D	268	VAL
1	D	280	ASP
1	D	291	ASP
1	D	293	LEU
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	358	GLU
1	D	363	GLN
1	D	378	MET
1	D	383	LEU
1	D	387	GLN
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	440	LEU
1	D	448	LYS
1	D	449	SER

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Mol	Chain	Res	Type
1	D	459	LEU
1	D	462	ILE
1	D	510	GLU
1	D	513	ASP
1	D	531	LYS
1	D	532	GLU
1	D	536	ASN
1	D	542	GLN
1	D	545	LEU
1	D	556	SER
1	D	574	ILE
1	D	578	ILE
1	D	579	GLU
1	D	580	PHE
1	D	593	MET
1	D	596	LEU
1	D	601	LYS
1	D	606	VAL
1	D	607	VAL
1	D	608	TYR
1	D	625	ASN
1	D	641	VAL
1	D	642	VAL
1	D	644	ILE
1	D	662	LYS
1	D	672	SER
1	D	679	PHE
1	D	680	ILE
1	D	699	ASP
1	D	706	ILE
1	D	707	GLU
1	D	708	ARG
1	D	709	GLU
1	D	711	ILE
1	D	713	GLU
1	D	715	MET
1	D	718	VAL
1	D	730	LEU
1	D	735	LEU
1	D	743	THR
1	D	744	LEU
1	D	746	LEU

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Mol	Chain	Res	Type
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	820	LYS
1	D	821	SER
1	D	824	LEU
1	D	825	THR
1	D	826	LYS
1	D	835	PHE
1	D	838	LYS
1	D	839	GLU
1	D	842	GLU
1	D	843	LEU
1	D	844	LYS
1	D	863	SER
1	D	876	ARG
1	D	879	ASP
1	D	907	GLU
1	D	917	ILE
1	D	918	ASN
1	D	926	LYS
1	D	930	LEU
1	D	946	SER
1	D	948	THR
1	D	949	ARG
1	D	952	LEU
1	D	962	GLU
1	D	964	ASN
1	D	968	VAL
1	D	969	ARG
1	D	972	LEU
1	D	977	LEU
1	D	1130	VAL
1	D	1131	SER
1	D	1136	SER
1	D	1138	GLN
1	D	1140	LYS

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Mol	Chain	Res	Type
1	D	1141	LEU
1	D	1143	LYS
1	D	1147	GLU
1	D	1149	ILE
1	D	1150	LEU
1	D	1155	SER
1	D	1175	ASP
1	D	1195	LYS
1	D	1217	LEU
1	D	1221	ARG
1	D	1239	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	41	HIS
1	A	73	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
1	A	325	ASN
1	A	349	ASN
1	A	363	GLN
1	A	386	GLN
1	A	446	HIS
1	A	759	ASN
1	A	770	HIS
1	A	789	HIS
1	A	833	GLN
1	A	850	ASN
1	A	877	ASN
1	A	904	ASN
1	A	918	ASN
1	A	945	ASN
1	A	983	GLN
1	A	1182	HIS

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Mol	Chain	Res	Type
1	A	1196	ASN
1	A	1232	ASN
1	B	16	GLN
1	B	19	GLN
1	B	31	ASN
1	B	73	HIS
1	B	96	GLN
1	B	113	GLN
1	B	152	HIS
1	B	157	ASN
1	B	179	HIS
1	B	195	ASN
1	B	197	ASN
1	B	200	HIS
1	B	219	HIS
1	B	220	HIS
1	B	290	ASN
1	B	311	GLN
1	B	319	HIS
1	B	325	ASN
1	B	386	GLN
1	B	576	GLN
1	B	577	ASN
1	B	591	GLN
1	B	649	GLN
1	B	684	GLN
1	B	698	ASN
1	B	703	ASN
1	B	753	ASN
1	B	852	GLN
1	B	887	ASN
1	B	918	ASN
1	B	945	ASN
1	B	964	ASN
1	B	975	GLN
1	B	1196	ASN
1	C	16	GLN
1	C	19	GLN
1	C	25	GLN
1	C	73	HIS
1	C	96	GLN
1	C	97	GLN

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Mol	Chain	Res	Type
1	C	113	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	361	ASN
1	C	362	GLN
1	C	386	GLN
1	C	387	GLN
1	C	429	ASN
1	C	446	HIS
1	C	514	GLN
1	C	576	GLN
1	C	590	GLN
1	C	591	GLN
1	C	602	ASN
1	C	703	ASN
1	C	753	ASN
1	C	759	ASN
1	C	770	HIS
1	C	850	ASN
1	C	852	GLN
1	C	877	ASN
1	C	887	ASN
1	C	904	ASN
1	C	918	ASN
1	C	975	GLN
1	C	1232	ASN
1	D	16	GLN
1	D	73	HIS
1	D	97	GLN
1	D	152	HIS
1	D	157	ASN
1	D	179	HIS
1	D	195	ASN
1	D	200	HIS

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Mol	Chain	Res	Type
1	D	219	HIS
1	D	220	HIS
1	D	269	GLN
1	D	295	ASN
1	D	325	ASN
1	D	361	ASN
1	D	362	GLN
1	D	363	GLN
1	D	576	GLN
1	D	590	GLN
1	D	591	GLN
1	D	625	ASN
1	D	702	HIS
1	D	703	ASN
1	D	753	ASN
1	D	770	HIS
1	D	772	GLN
1	D	833	GLN
1	D	904	ASN
1	D	918	ASN
1	D	945	ASN
1	D	964	ASN
1	D	1205	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1023/1155 (88%)	-0.19	19 (1%) 66 58	34, 57, 89, 110	0
1	B	1020/1155 (88%)	-0.07	22 (2%) 62 53	29, 64, 116, 133	0
1	C	1030/1155 (89%)	0.03	25 (2%) 59 50	32, 72, 100, 124	0
1	D	1004/1155 (86%)	0.25	43 (4%) 40 31	43, 79, 123, 144	0
All	All	4077/4620 (88%)	0.00	109 (2%) 56 47	29, 67, 113, 144	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1086	ALA	6.7
1	D	1106	VAL	4.7
1	D	647	VAL	4.6
1	C	1106	VAL	4.3
1	B	1093	VAL	4.3
1	A	1105	VAL	4.0
1	D	703	ASN	3.9
1	C	1105	VAL	3.9
1	B	606	VAL	3.8
1	D	529	SER	3.7
1	A	798	TRP	3.7
1	C	982	THR	3.7
1	D	594	ALA	3.5
1	C	1083	SER	3.4
1	A	1097	LEU	3.4
1	D	576	GLN	3.4
1	D	711	ILE	3.4
1	C	1094	ALA	3.3
1	D	558	TYR	3.2
1	A	711	ILE	3.2
1	B	710	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1105	VAL	3.2
1	D	570	VAL	3.1
1	C	981	PRO	3.1
1	C	1092	THR	3.0
1	C	1090	LEU	3.0
1	B	1094	ALA	3.0
1	A	1153	GLU	3.0
1	D	519	LYS	2.9
1	A	802	ARG	2.9
1	B	608	TYR	2.9
1	D	355	ILE	2.9
1	B	504	TYR	2.9
1	A	1100	ALA	2.9
1	C	408	SER	2.9
1	D	600	SER	2.9
1	D	399	LEU	2.9
1	A	112	LEU	2.9
1	D	578	ILE	2.9
1	D	665	PRO	2.8
1	C	112	LEU	2.8
1	C	1087	ASP	2.8
1	D	552	CYS	2.8
1	D	419	PRO	2.8
1	D	316	ALA	2.7
1	D	358	GLU	2.7
1	D	462	ILE	2.7
1	D	530	LEU	2.7
1	C	1097	LEU	2.7
1	A	1103	PRO	2.7
1	D	384	MET	2.6
1	B	1109	LEU	2.6
1	C	229	THR	2.6
1	C	703	ASN	2.6
1	D	319	HIS	2.6
1	C	571	ILE	2.5
1	A	115	ALA	2.5
1	B	622	PHE	2.5
1	A	803	GLU	2.5
1	A	825	THR	2.5
1	D	571	ILE	2.5
1	C	775	TYR	2.5
1	D	608	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	115	ALA	2.5
1	D	393	ALA	2.5
1	C	1085	GLU	2.5
1	D	852	GLN	2.5
1	B	661	ALA	2.4
1	D	1107	VAL	2.4
1	B	823	LYS	2.4
1	B	706	ILE	2.4
1	A	703	ASN	2.4
1	D	712	PRO	2.4
1	D	1114	LEU	2.4
1	B	355	ILE	2.3
1	D	402	VAL	2.3
1	D	556	SER	2.3
1	D	574	ILE	2.3
1	A	1104	PHE	2.2
1	B	982	THR	2.2
1	D	106	MET	2.2
1	B	112	LEU	2.2
1	D	198	THR	2.2
1	C	355	ILE	2.2
1	A	1093	VAL	2.2
1	B	106	MET	2.2
1	C	1101	ARG	2.1
1	B	627	VAL	2.1
1	D	974	SER	2.1
1	C	707	GLU	2.1
1	C	1095	ASP	2.1
1	A	229	THR	2.1
1	A	392	GLY	2.1
1	B	555	TRP	2.1
1	C	1107	VAL	2.1
1	C	813	GLU	2.1
1	D	390	LEU	2.0
1	D	573	GLY	2.0
1	A	1193	ILE	2.0
1	B	104	THR	2.0
1	B	773	ASP	2.0
1	D	661	ALA	2.0
1	C	504	TYR	2.0
1	D	659	TYR	2.0
1	A	794	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	783	SER	2.0
1	B	945	ASN	2.0
1	B	659	TYR	2.0
1	D	1240	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.