



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:14 am GMT

PDB ID : 2NVY
Title : RNA Polymerase II form II in 150 mM Mn+2
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on : 2006-11-13
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

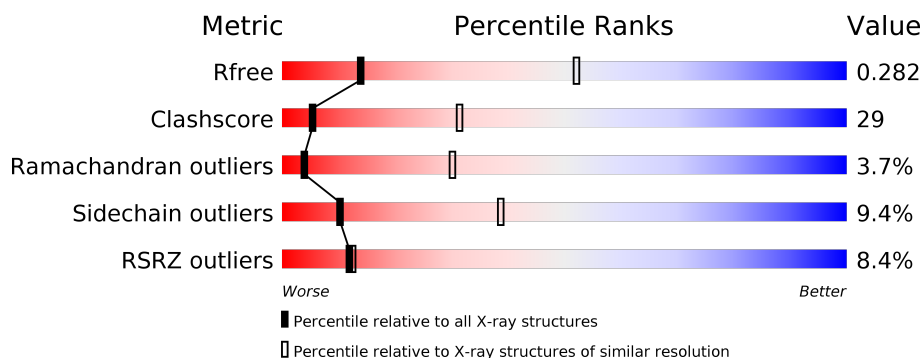
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1733	<div> <div>7%</div> <div> <div>39%</div> <div>37%</div> <div>6%</div> <div>18%</div> </div> </div>
2	B	1224	<div> <div>8%</div> <div> <div>44%</div> <div>41%</div> <div>•</div> <div>11%</div> </div> </div>
3	C	318	<div> <div>2%</div> <div> <div>35%</div> <div>42%</div> <div>6%</div> <div>16%</div> </div> </div>
4	E	215	<div> <div>4%</div> <div> <div>58%</div> <div>39%</div> <div>•</div> </div> </div>
5	F	155	<div> <div>3%</div> <div> <div>21%</div> <div>30%</div> <div>•</div> <div>46%</div> </div> </div>
6	H	146	<div> <div>18%</div> <div> <div>50%</div> <div>36%</div> <div>5%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	I	122	<div><div></div><div>21%61%37%</div><div></div></div>
8	J	70	<div><div></div><div>31%51%10%7%</div><div></div></div>
9	K	120	<div><div></div><div>5%42%44%9%5%</div><div></div></div>
10	L	70	<div><div></div><div>7%24%30%10%34%</div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28289 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0	0
			11154	7023	1952	2118	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1094	Total	C	N	O	S	0	0	0
			8711	5525	1519	1614	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		
11	A	2	Total	Zn	0	0
			2	2		
11	L	1	Total	Zn	0	0
			1	1		

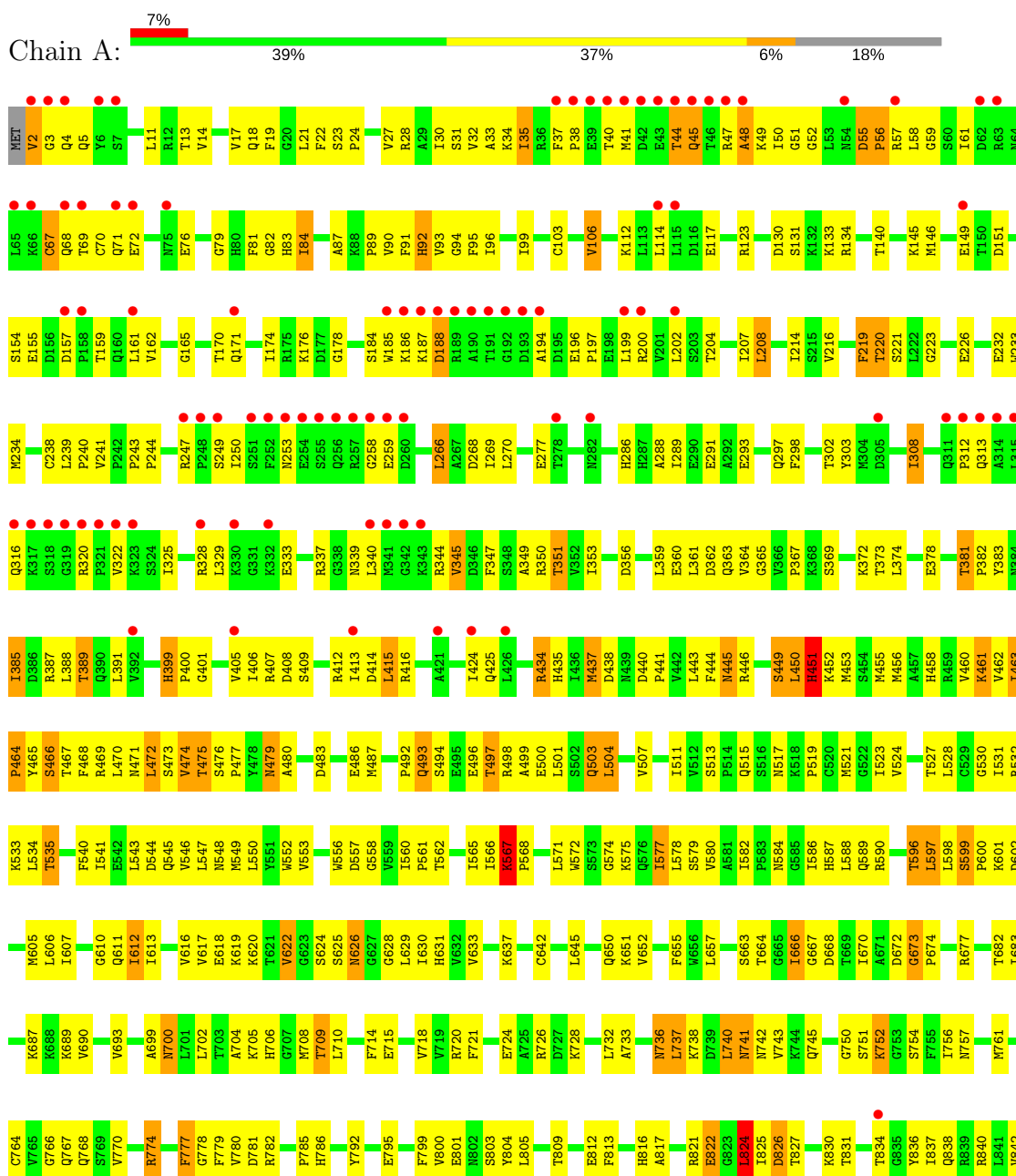
- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total 2	Mn 2	0	0

3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II largest subunit



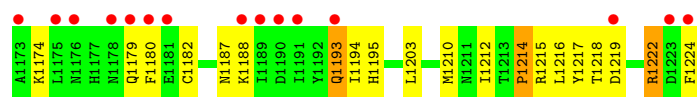
SER	TYR	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	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● Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

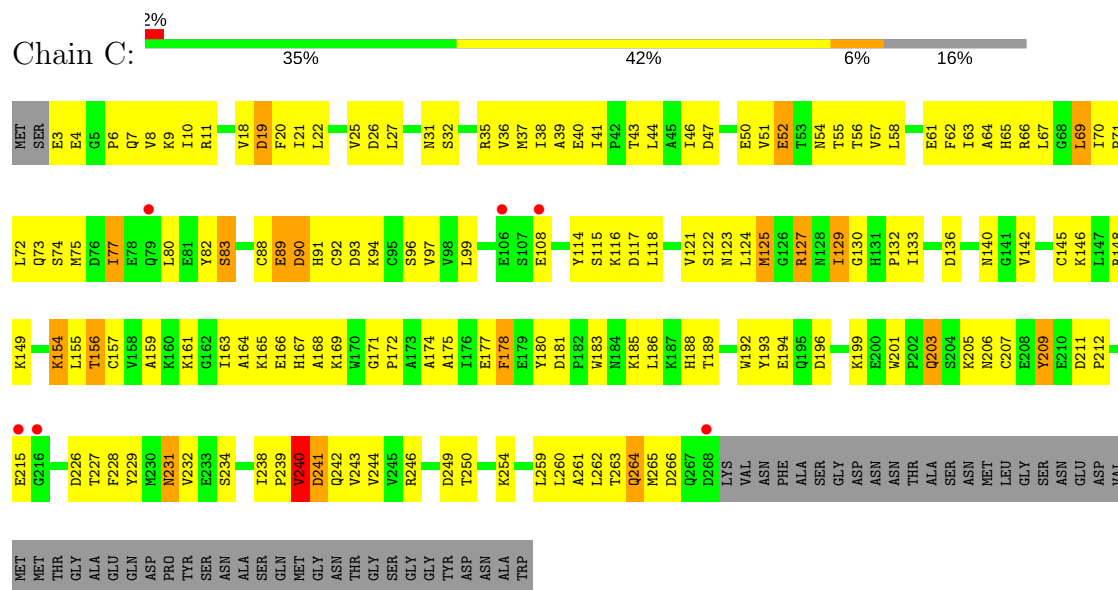


MET	SER	ASP	LEU	ALA	ASN	SER	GLY	LYS	TYR	THR	ASP	ASP	PRO	GLY	F18	E19	D20	S21	S22	I25	D29	S30	W31	A32	V33	I34	S35	A36	R39	E40	L43	Q46	Q47	Q53	F54	Y57	I62	I63	C64	E65	D66	S67	T68	L69	I70	LEU	GLU	GLN	LEU
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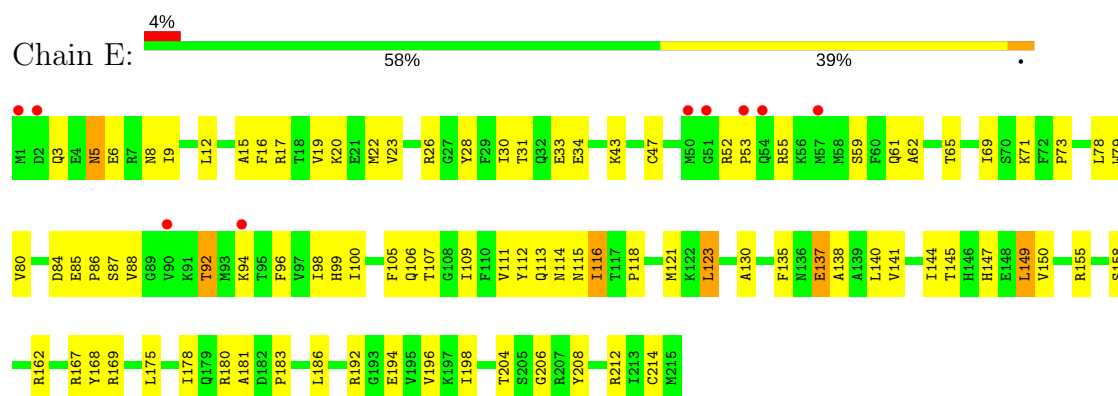
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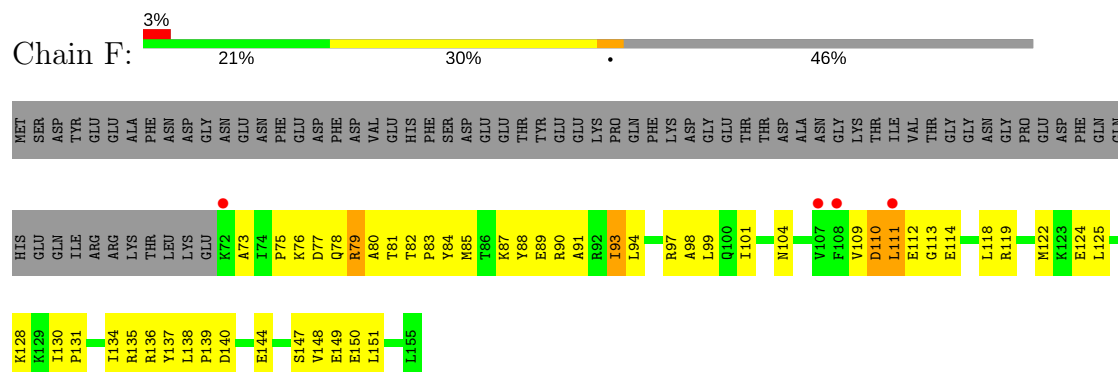
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



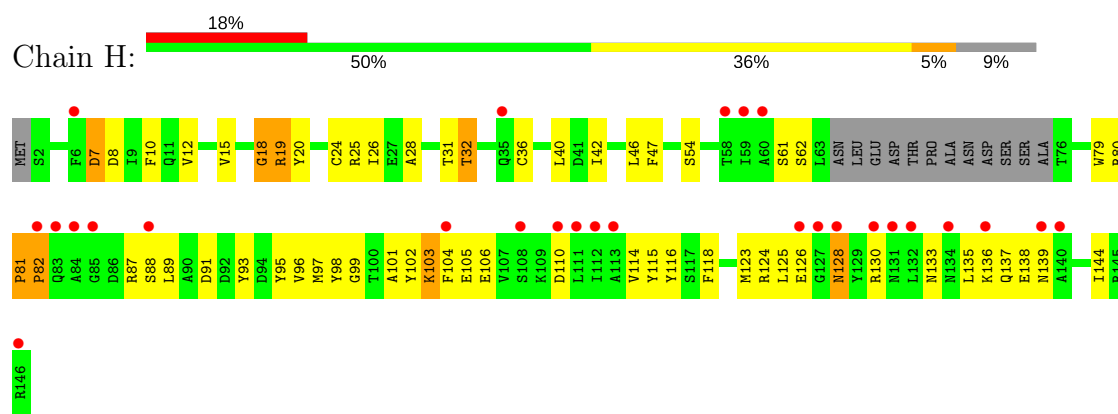
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



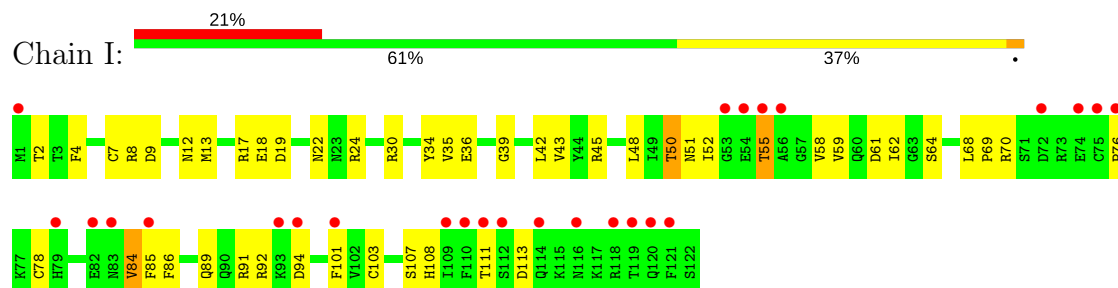
• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



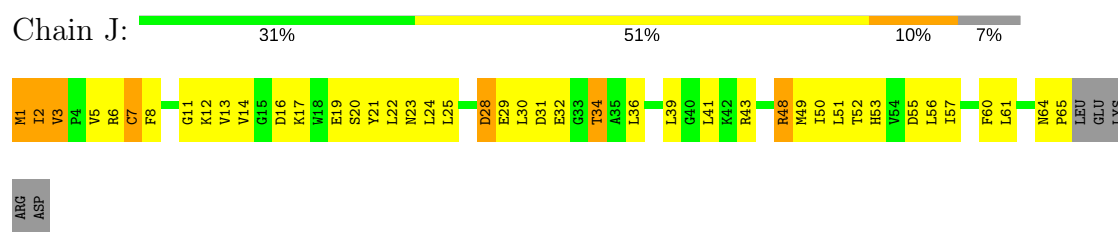
• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



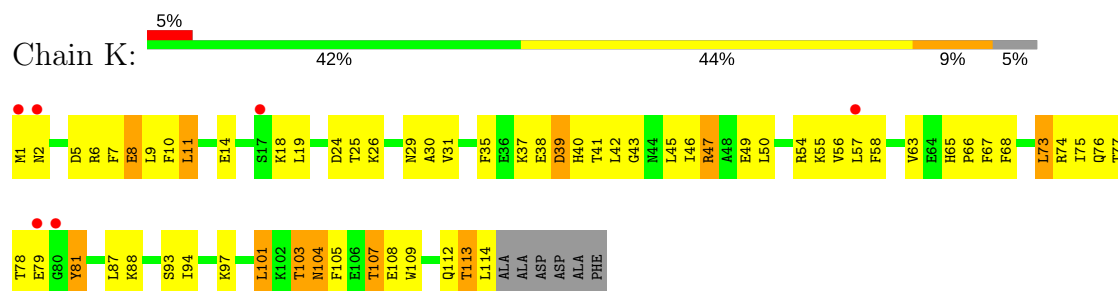
• Molecule 7: DNA-directed RNA polymerase II subunit 9



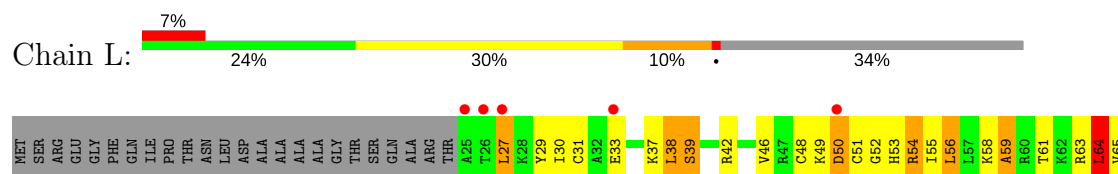
• Molecule 8: DNA-directed RNA polymerases I/II/III subunit 10



• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



• Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



Q66
F67
E68
A69
R70

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.04Å 218.91Å 369.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 39.71 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.40) 97.8 (39.71-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.249 , 0.323 0.229 , 0.282	Depositor DCC
R_{free} test set	1970 reflections (3.14%)	DCC
Wilson B-factor (Å ²)	89.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28289	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	2/11352 (0.0%)	0.71	1/15352 (0.0%)
2	B	0.58	0/8882	0.69	0/11976
3	C	0.58	0/2133	0.70	0/2891
4	E	0.57	0/1796	0.70	0/2416
5	F	0.61	0/691	0.71	0/933
6	H	0.47	0/1086	0.65	0/1470
7	I	0.52	0/1016	0.64	0/1365
8	J	0.62	0/541	0.76	0/727
9	K	0.56	0/937	0.71	0/1265
10	L	0.54	0/366	0.73	0/485
All	All	0.58	2/28800 (0.0%)	0.70	1/38880 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1449	SER	CB-OG	12.62	1.58	1.42
1	A	1421	CYS	CB-SG	-5.25	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	LEU	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	11154	0	11225	712	0
2	B	8711	0	8737	561	0
3	C	2095	0	2051	161	0
4	E	1760	0	1788	74	0
5	F	679	0	701	54	0
6	H	1068	0	1040	74	0
7	I	997	0	955	40	0
8	J	532	0	542	59	0
9	K	919	0	929	81	0
10	L	364	0	388	35	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
All	All	28289	0	28356	1637	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 29.

All (1637) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	8:J:52:THR:CG2	1.63	1.25
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.66	1.21
1:A:672:ASP:HB2	1:A:736:ASN:ND2	1.60	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	0.98	1.14
1:A:672:ASP:CB	1:A:736:ASN:HD21	1.59	1.14
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.06	1.14
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.25	1.12
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.18	1.09
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.24	1.09
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.30	1.08
3:C:148:ARG:NH1	8:J:64:ASN:HA	1.68	1.07
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.36	1.07
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.12	1.06
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.56	1.05
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.39	1.05
1:A:535:THR:HG21	1:A:617:VAL:H	1.24	1.02
1:A:774:ARG:HG3	1:A:774:ARG:HH11	1.25	1.02
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.02	1.02
1:A:855:THR:CG2	1:A:857:ARG:HE	1.74	1.01
6:H:95:TYR:CE2	6:H:97:MET:HG3	1.96	1.01
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.90	1.00
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.24	1.00
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.43	0.99
1:A:470:LEU:HD11	1:A:487:MET:CE	1.94	0.97
1:A:444:PHE:CE2	1:A:470:LEU:HD21	2.00	0.97
1:A:849:MET:HE1	1:A:1436:ILE:HA	1.43	0.97
6:H:130:ARG:HA	6:H:133:ASN:HB2	1.47	0.97
2:B:29:ASP:HB3	2:B:658:ILE:CD1	1.95	0.96
1:A:855:THR:HG21	1:A:857:ARG:NE	1.79	0.96
2:B:644:GLU:HG3	2:B:654:ARG:NH2	1.80	0.96
2:B:800:GLN:CB	8:J:52:THR:HG22	1.94	0.96
1:A:472:LEU:O	1:A:475:THR:HB	1.66	0.96
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.65	0.94
5:F:81:THR:HG22	5:F:136:ARG:NH1	1.84	0.93
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.48	0.93
2:B:824:ILE:HG12	8:J:48:ARG:NH1	1.83	0.92
1:A:913:LEU:HD11	1:A:981:LEU:O	1.70	0.92
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.50	0.92
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.66	0.92
3:C:40:GLU:HA	3:C:163:ILE:HG23	1.51	0.92
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.33	0.92
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.11	0.91
1:A:869:GLY:O	4:E:204:THR:HG21	1.71	0.91
2:B:542:MET:HG3	2:B:747:MET:HE3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:65:HIS:HD2	9:K:67:PHE:H	0.97	0.91
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.00	0.91
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.85	0.91
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.53	0.91
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.52	0.91
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.18	0.91
1:A:313:GLN:HG2	1:A:322:VAL:HB	1.52	0.90
1:A:672:ASP:HB2	1:A:736:ASN:HD21	0.77	0.90
9:K:65:HIS:CD2	9:K:67:PHE:H	1.88	0.90
3:C:166:GLU:HG2	10:L:70:ARG:HH12	1.37	0.90
1:A:470:LEU:HD11	1:A:487:MET:HE3	1.53	0.88
2:B:705:MET:HE1	2:B:742:GLU:HG3	1.56	0.88
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.08	0.88
1:A:55:ASP:H	1:A:56:PRO:HD2	1.36	0.87
2:B:1081:LEU:CD1	2:B:1085:ILE:HD11	2.03	0.87
5:F:81:THR:HB	5:F:144:GLU:OE1	1.74	0.87
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.75	0.87
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.55	0.87
1:A:134:ARG:HD2	1:A:221:SER:O	1.75	0.87
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.39	0.87
3:C:66:ARG:NH2	8:J:3:VAL:O	2.09	0.85
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.41	0.85
1:A:519:PRO:HG2	1:A:624:SER:O	1.77	0.85
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.74	0.85
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.89	0.85
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.59	0.85
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.07	0.84
1:A:1398:MET:HG3	1:A:1426:GLU:HG2	1.58	0.84
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.78	0.84
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.59	0.84
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.42	0.84
1:A:567:LYS:HB3	6:H:96:VAL:N	1.93	0.84
3:C:166:GLU:HG2	10:L:70:ARG:NH1	1.92	0.84
2:B:801:LYS:O	8:J:52:THR:HG23	1.77	0.83
2:B:324:ILE:HD11	2:B:333:PHE:HB2	1.58	0.83
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.41	0.83
1:A:302:THR:HG21	1:A:312:PRO:HG2	1.61	0.83
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.13	0.83
2:B:705:MET:CE	2:B:745:PRO:HB3	2.08	0.83
2:B:648:HIS:HE1	2:B:712:PRO:HD3	1.43	0.82
1:A:548:ASN:HD21	9:K:47:ARG:HH21	1.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.15	0.82
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.38	0.82
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.63	0.82
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.62	0.81
1:A:2:VAL:HG21	2:B:1157:ALA:O	1.80	0.81
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.63	0.81
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.15	0.81
2:B:35:SER:HA	2:B:811:TYR:HE2	1.43	0.81
3:C:54:ASN:OD1	3:C:56:THR:HG22	1.80	0.81
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.21	0.80
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.63	0.80
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.61	0.80
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.64	0.80
4:E:180:ARG:HH21	4:E:192:ARG:HB2	1.47	0.80
1:A:770:VAL:HG13	1:A:822:GLU:HG3	1.63	0.80
1:A:353:ILE:HD13	1:A:487:MET:CE	2.07	0.79
1:A:535:THR:CG2	1:A:616:VAL:HA	2.11	0.79
3:C:32:SER:O	3:C:36:VAL:HG23	1.82	0.79
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.61	0.79
1:A:757:ASN:HA	2:B:1021:MET:CE	2.12	0.79
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.30	0.79
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.64	0.79
2:B:954:VAL:O	10:L:55:ILE:O	2.01	0.79
1:A:567:LYS:HB3	6:H:96:VAL:H	1.46	0.79
2:B:515:HIS:H	2:B:518:HIS:HD2	1.30	0.79
3:C:74:SER:HB2	3:C:238:ILE:HG13	1.63	0.79
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.65	0.78
1:A:535:THR:HG21	1:A:617:VAL:N	1.99	0.78
2:B:210:LYS:HE3	2:B:461:LEU:O	1.84	0.78
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.47	0.78
3:C:57:VAL:HG11	8:J:60:PHE:CB	2.14	0.78
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.18	0.78
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.14	0.77
5:F:81:THR:HG21	5:F:136:ARG:CD	2.14	0.77
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.14	0.77
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.67	0.77
1:A:399:HIS:O	1:A:401:GLY:N	2.16	0.77
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.85	0.76
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.76
4:E:118:PRO:HA	4:E:121:MET:HB2	1.67	0.76
10:L:51:CYS:HB3	10:L:53:HIS:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.18	0.76
6:H:26:ILE:HD13	6:H:42:ILE:HD12	1.66	0.76
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.66	0.76
2:B:685:LEU:HD11	2:B:692:TYR:CE1	2.21	0.76
6:H:95:TYR:HE2	6:H:97:MET:CG	1.94	0.76
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.50	0.76
2:B:341:LEU:O	2:B:341:LEU:HD12	1.86	0.76
2:B:1081:LEU:HD12	2:B:1085:ILE:CD1	2.15	0.75
2:B:25:ILE:HD12	2:B:653:VAL:HB	1.67	0.75
2:B:43:LEU:HD11	2:B:811:TYR:O	1.84	0.75
1:A:470:LEU:HD11	1:A:487:MET:HE1	1.69	0.75
1:A:494:SER:OG	1:A:497:THR:HB	1.87	0.75
1:A:911:SER:O	1:A:978:PRO:HB3	1.87	0.75
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.67	0.75
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.67	0.75
1:A:984:LYS:O	1:A:988:LEU:HB2	1.85	0.75
6:H:81:PRO:CB	6:H:82:PRO:HD3	2.12	0.75
1:A:668:ASP:OD2	1:A:742:ASN:HB2	1.86	0.75
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.65	0.75
1:A:683:ILE:HD11	1:A:764:CYS:HB2	1.68	0.75
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.20	0.75
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.52	0.75
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.01	0.75
1:A:571:LEU:HD22	6:H:46:LEU:HD11	1.69	0.74
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.50	0.74
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.16	0.74
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.69	0.74
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.69	0.74
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.17	0.74
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.22	0.74
1:A:492:PRO:HG3	1:A:501:LEU:CD1	2.18	0.74
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.68	0.74
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.74
2:B:766:ARG:NH1	2:B:985:GLY:O	2.20	0.74
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.68	0.74
2:B:311:LEU:HB3	7:I:4:PHE:CZ	2.22	0.74
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.50	0.74
9:K:65:HIS:HD2	9:K:67:PHE:N	1.80	0.73
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.70	0.73
4:E:147:HIS:HD2	4:E:149:LEU:H	1.37	0.73
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:OG	2:B:236:HIS:HD2	1.72	0.73
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.36	0.73
2:B:35:SER:HA	2:B:811:TYR:CE2	2.23	0.73
4:E:94:LYS:HG3	4:E:123:LEU:HD11	1.69	0.73
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.23	0.73
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.54	0.72
1:A:1438:THR:HG22	2:B:1144:ALA:H	1.55	0.72
1:A:34:LYS:HA	1:A:83:HIS:HD2	1.53	0.72
1:A:499:ALA:O	1:A:503:GLN:HB2	1.89	0.72
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.51	0.72
1:A:899:VAL:HG12	1:A:929:LEU:HD13	1.72	0.72
2:B:986:GLN:HE21	2:B:987:LYS:N	1.87	0.72
4:E:147:HIS:CD2	4:E:149:LEU:H	2.08	0.72
8:J:24:LEU:O	8:J:30:LEU:HB2	1.89	0.72
2:B:680:THR:HG22	2:B:682:SER:N	2.05	0.72
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.71	0.72
3:C:93:ASP:O	3:C:127:ARG:NH2	2.21	0.72
1:A:548:ASN:ND2	9:K:47:ARG:HH21	1.85	0.72
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.72	0.71
1:A:33:ALA:O	1:A:83:HIS:HB3	1.90	0.71
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.71	0.71
9:K:30:ALA:HB2	9:K:76:GLN:HG3	1.72	0.71
1:A:903:ASN:HD22	1:A:905:ASP:H	1.39	0.71
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.72	0.71
1:A:754:SER:H	1:A:757:ASN:HD22	1.38	0.71
1:A:761:MET:O	1:A:803:SER:HB2	1.90	0.71
1:A:579:SER:HB3	1:A:611:GLN:HA	1.71	0.71
2:B:238:ALA:HB2	2:B:385:LEU:HB2	1.73	0.70
2:B:542:MET:HG3	2:B:747:MET:CE	2.20	0.70
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.06	0.70
1:A:353:ILE:HG21	1:A:487:MET:CE	2.21	0.70
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.72	0.70
6:H:10:PHE:O	6:H:54:SER:HA	1.91	0.70
1:A:1166:ASP:HA	1:A:1169:ILE:HG23	1.71	0.70
2:B:185:THR:HG23	2:B:188:ASP:OD2	1.90	0.70
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.89	0.70
1:A:774:ARG:HH11	1:A:774:ARG:CG	2.02	0.70
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.73	0.70
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.73	0.70
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.73	0.70
1:A:548:ASN:HD21	9:K:47:ARG:NH2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.92	0.70
1:A:374:LEU:HD23	2:B:1107:ALA:HB2	1.74	0.70
1:A:1206:ASP:HB2	1:A:1274:ARG:HH12	1.57	0.69
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.74	0.69
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.75	0.69
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.04	0.69
2:B:914:LYS:HB3	2:B:937:ALA:O	1.93	0.69
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.75	0.69
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.74	0.69
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.57	0.69
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.74	0.69
1:A:567:LYS:HD3	6:H:95:TYR:CG	2.27	0.69
1:A:44:THR:O	1:A:45:GLN:HB2	1.93	0.69
6:H:12:VAL:HG13	6:H:26:ILE:HG23	1.74	0.69
2:B:205:ILE:HD12	2:B:461:LEU:HB3	1.74	0.69
5:F:109:VAL:HG12	5:F:110:ASP:N	2.07	0.69
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.74	0.68
2:B:515:HIS:H	2:B:518:HIS:CD2	2.11	0.68
2:B:642:ASP:HB3	2:B:649:LYS:HE2	1.73	0.68
1:A:567:LYS:CB	6:H:96:VAL:H	2.05	0.68
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.24	0.68
2:B:899:ILE:O	2:B:952:VAL:HG21	1.93	0.68
2:B:610:ASN:HB3	2:B:613:VAL:HG23	1.76	0.68
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.76	0.68
6:H:103:LYS:HA	6:H:115:TYR:HB2	1.76	0.68
1:A:1434:ALA:HB3	1:A:1436:ILE:HG12	1.75	0.68
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.73	0.68
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.75	0.68
1:A:92:HIS:HD2	1:A:94:GLY:H	1.41	0.68
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.73	0.68
1:A:345:VAL:HG12	2:B:1150:ARG:HH22	1.59	0.68
1:A:565:ILE:HG23	1:A:567:LYS:HG3	1.77	0.68
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.24	0.68
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.76	0.67
1:A:1329:THR:HG22	1:A:1335:ILE:HG13	1.77	0.67
4:E:112:TYR:CE1	4:E:115:ASN:HA	2.29	0.67
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	2.09	0.67
2:B:324:ILE:CD1	2:B:333:PHE:HB2	2.25	0.67
2:B:1060:ARG:HB2	2:B:1066:SER:HB3	1.76	0.67
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.30	0.67
6:H:103:LYS:HG2	6:H:115:TYR:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.76	0.67
1:A:1063:MET:HG3	2:B:1139:ILE:HG22	1.76	0.67
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.77	0.67
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.25	0.66
2:B:1152:MET:CE	2:B:1152:MET:HA	2.25	0.66
2:B:996:ARG:NH2	3:C:174:ALA:O	2.27	0.66
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.31	0.66
1:A:858:ASN:HD22	1:A:858:ASN:C	1.99	0.66
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.25	0.66
7:I:111:THR:HG22	7:I:113:ASP:H	1.58	0.66
1:A:849:MET:CE	1:A:1436:ILE:HA	2.21	0.66
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.30	0.66
3:C:18:VAL:O	3:C:18:VAL:HG12	1.96	0.66
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.77	0.66
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.78	0.66
1:A:1282:VAL:HG22	1:A:1308:THR:HG22	1.76	0.66
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.66
1:A:131:SER:HB2	1:A:223:GLY:HA2	1.77	0.66
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.77	0.66
7:I:59:VAL:HG12	7:I:61:ASP:H	1.59	0.66
1:A:302:THR:HG21	1:A:312:PRO:CG	2.25	0.66
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.78	0.66
1:A:1398:MET:HG3	1:A:1426:GLU:CG	2.24	0.65
9:K:6:ARG:O	9:K:9:LEU:HG	1.96	0.65
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.78	0.65
3:C:261:ALA:O	3:C:265:MET:HB2	1.96	0.65
1:A:824:LEU:HD21	2:B:765:PRO:HB3	1.78	0.65
2:B:816:GLU:O	8:J:56:LEU:HD21	1.95	0.65
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.77	0.65
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.31	0.65
2:B:1008:PRO:HB3	2:B:1087:PHE:CE1	2.31	0.65
1:A:553:VAL:CG2	1:A:652:VAL:CG2	2.75	0.65
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.78	0.65
1:A:258:GLY:O	1:A:259:GLU:HG3	1.96	0.65
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	1.92	0.65
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.31	0.65
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.77	0.65
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.37	0.65
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.48	0.65
2:B:195:CYS:SG	2:B:783:THR:OG1	2.49	0.65
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:O	1:A:416:ARG:N	2.30	0.65
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.27	0.65
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.25	0.65
3:C:89:GLU:O	3:C:90:ASP:CB	2.45	0.65
1:A:785:PRO:HD2	1:A:786:HIS:HD2	1.62	0.64
1:A:1336:MET:HE1	1:A:1381:LEU:HG	1.79	0.64
2:B:805:THR:HG21	2:B:815:ARG:HE	1.63	0.64
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.43	0.64
2:B:311:LEU:HB3	7:I:4:PHE:HZ	1.63	0.64
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.79	0.64
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.32	0.64
2:B:884:ARG:O	2:B:936:ASP:HB3	1.98	0.64
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.79	0.64
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.33	0.64
2:B:276:ILE:HG21	2:B:280:ILE:CD1	2.27	0.64
5:F:118:LEU:O	5:F:122:MET:HG3	1.98	0.64
10:L:58:LYS:O	10:L:59:ALA:O	2.16	0.64
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.33	0.64
2:B:1212:ILE:O	2:B:1214:PRO:HD3	1.98	0.64
2:B:684:LEU:HD23	2:B:689:LEU:CD1	2.27	0.64
10:L:38:LEU:O	10:L:39:SER:HB3	1.97	0.64
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.62	0.64
2:B:841:MET:O	2:B:993:THR:HA	1.98	0.64
2:B:994:TYR:HB2	2:B:999:MET:CE	2.27	0.64
10:L:61:THR:HB	10:L:63:ARG:HG2	1.80	0.64
10:L:33:GLU:HB2	10:L:53:HIS:CD2	2.33	0.64
1:A:626:ASN:O	1:A:631:HIS:HD2	1.82	0.63
5:F:75:PRO:O	5:F:77:ASP:O	2.16	0.63
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.63	0.63
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.80	0.63
1:A:1315:GLU:O	1:A:1318:THR:HG22	1.98	0.63
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.79	0.63
1:A:528:LEU:O	1:A:531:ILE:HG22	1.98	0.63
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.33	0.63
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.80	0.63
1:A:1199:ARG:HA	1:A:1202:MET:HB2	1.81	0.63
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.79	0.63
3:C:242:GLN:O	3:C:246:ARG:HG3	1.99	0.63
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.34	0.63
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.80	0.63
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HG12	1:A:412:ARG:HG2	1.81	0.63
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.29	0.63
3:C:73:GLN:HE21	3:C:75:MET:H	1.46	0.63
3:C:166:GLU:CG	10:L:70:ARG:HH12	2.10	0.63
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.81	0.63
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.31	0.63
2:B:451:LYS:O	2:B:455:SER:HB2	1.97	0.63
3:C:163:ILE:HG22	3:C:165:LYS:H	1.64	0.62
10:L:46:VAL:O	10:L:54:ARG:HA	1.99	0.62
1:A:477:PRO:HG3	1:A:521:MET:HG2	1.82	0.62
1:A:982:THR:O	1:A:985:ASP:HB2	1.98	0.62
4:E:19:VAL:HG22	4:E:140:LEU:HD13	1.81	0.62
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.81	0.62
1:A:901:LEU:HA	1:A:907:THR:HG23	1.80	0.62
3:C:40:GLU:HA	3:C:163:ILE:CG2	2.25	0.62
9:K:42:LEU:HG	9:K:46:ILE:HD11	1.78	0.62
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.82	0.62
1:A:642:CYS:O	1:A:645:LEU:HB3	1.98	0.62
2:B:1016:ALA:O	2:B:1020:ARG:HG2	2.00	0.62
2:B:906:SER:HB2	2:B:946:ASN:HB2	1.82	0.62
1:A:1398:MET:CG	1:A:1426:GLU:HG2	2.28	0.62
1:A:89:PRO:HB3	1:A:208:LEU:HD12	1.81	0.62
9:K:55:LYS:CB	9:K:81:TYR:HD1	2.13	0.62
1:A:567:LYS:CG	6:H:96:VAL:H	2.12	0.62
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.81	0.62
1:A:1268:LEU:HD13	7:I:48:LEU:HD21	1.80	0.62
1:A:1062:GLU:O	1:A:1064:VAL:N	2.32	0.62
1:A:1289:ARG:O	1:A:1300:LYS:HA	2.00	0.62
1:A:553:VAL:HG22	1:A:652:VAL:HG23	1.82	0.62
1:A:382:PRO:HD2	5:F:104:ASN:OD1	1.99	0.62
9:K:1:MET:HG3	9:K:2:ASN:N	2.15	0.62
2:B:1222:ARG:H	2:B:1222:ARG:HD2	1.64	0.62
4:E:88:VAL:HG13	4:E:92:THR:HB	1.82	0.62
1:A:329:LEU:O	1:A:333:GLU:HG2	2.00	0.62
1:A:535:THR:HG21	1:A:616:VAL:HA	1.81	0.62
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.35	0.62
2:B:509:ALA:O	2:B:511:PRO:HD3	1.99	0.62
1:A:504:LEU:CD1	5:F:91:ALA:HB2	2.29	0.62
1:A:597:LEU:O	6:H:102:TYR:OH	2.14	0.61
2:B:1053:GLU:OE1	2:B:1053:GLU:HA	2.00	0.61
2:B:430:ARG:HB3	2:B:434:ARG:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:HB2	2:B:612:GLU:HG3	1.80	0.61
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.35	0.61
1:A:1222:ASN:O	1:A:1224:LEU:N	2.33	0.61
1:A:883:LEU:O	1:A:886:ILE:HG22	2.00	0.61
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.81	0.61
1:A:23:SER:O	1:A:27:VAL:HG23	2.00	0.61
3:C:58:LEU:HD11	8:J:2:ILE:CD1	2.29	0.61
3:C:57:VAL:HG11	8:J:60:PHE:HB2	1.81	0.61
2:B:773:MET:CE	2:B:985:GLY:HA2	2.30	0.61
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.83	0.61
2:B:241:ARG:HG2	2:B:251:ILE:HG23	1.82	0.61
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.33	0.61
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.81	0.61
1:A:391:LEU:HD22	1:A:400:PRO:O	2.00	0.61
1:A:720:ARG:NH2	1:A:721:PHE:CE2	2.69	0.61
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.65	0.61
1:A:1001:ARG:HB2	5:F:80:ALA:O	2.01	0.61
1:A:465:TYR:HA	9:K:2:ASN:HB3	1.82	0.61
9:K:78:THR:HG22	9:K:79:GLU:N	2.16	0.61
2:B:728:ARG:HD2	2:B:730:ARG:HE	1.64	0.61
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.12	0.61
2:B:237:VAL:HG22	2:B:257:LYS:HG2	1.82	0.61
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.82	0.60
1:A:553:VAL:HG22	1:A:652:VAL:HG21	1.82	0.60
6:H:130:ARG:CA	6:H:133:ASN:HB2	2.26	0.60
1:A:3:GLY:O	1:A:5:GLN:N	2.34	0.60
2:B:1065:GLN:HE21	2:B:1069:PHE:N	1.98	0.60
2:B:1166:CYS:O	2:B:1168:LEU:N	2.30	0.60
2:B:190:TYR:OH	2:B:196:PRO:HG3	2.01	0.60
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.82	0.60
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.01	0.60
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.04	0.60
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.82	0.60
2:B:776:GLN:O	2:B:1095:LEU:HA	2.01	0.60
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.36	0.60
5:F:109:VAL:CG1	5:F:110:ASP:N	2.63	0.60
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.90	0.60
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.01	0.60
1:A:1398:MET:HA	1:A:1425:SER:HB2	1.84	0.60
1:A:269:ILE:HD11	1:A:303:TYR:HB2	1.83	0.60
1:A:535:THR:HG22	1:A:616:VAL:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:CB	2:B:946:ASN:HB2	2.32	0.60
9:K:113:THR:O	9:K:114:LEU:HB2	2.00	0.60
1:A:1222:ASN:C	1:A:1224:LEU:H	2.03	0.60
1:A:303:TYR:CZ	1:A:325:ILE:HD11	2.37	0.60
3:C:116:LYS:HG2	3:C:117:ASP:OD1	2.01	0.60
6:H:101:ALA:HB1	6:H:103:LYS:HG3	1.82	0.60
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.34	0.60
3:C:121:VAL:HG12	3:C:121:VAL:O	2.01	0.60
2:B:172:ILE:CD1	2:B:178:ASN:HB3	2.31	0.60
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.37	0.60
4:E:65:THR:O	4:E:69:ILE:HG13	2.00	0.60
3:C:58:LEU:HD11	8:J:2:ILE:HD11	1.84	0.60
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.37	0.59
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.84	0.59
3:C:41:ILE:HG21	3:C:172:PRO:HG3	1.83	0.59
2:B:351:TYR:CE2	2:B:355:ILE:HD11	2.37	0.59
2:B:648:HIS:CE1	2:B:712:PRO:HD3	2.30	0.59
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.67	0.59
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.67	0.59
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.84	0.59
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.83	0.59
1:A:349:ALA:HB2	1:A:374:LEU:HD21	1.84	0.59
1:A:476:SER:N	1:A:477:PRO:HD2	2.16	0.59
1:A:587:HIS:HA	1:A:607:ILE:O	2.01	0.59
3:C:142:VAL:HG11	8:J:5:VAL:HG22	1.83	0.59
3:C:37:MET:HA	3:C:41:ILE:HD12	1.84	0.59
10:L:48:CYS:HB3	10:L:51:CYS:O	2.01	0.59
1:A:523:ILE:CD1	1:A:622:VAL:HG22	2.32	0.59
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.37	0.59
3:C:241:ASP:CB	9:K:109:TRP:CE2	2.85	0.59
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.14	0.59
1:A:329:LEU:HB3	1:A:333:GLU:HB3	1.84	0.59
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.32	0.59
8:J:21:TYR:HB2	8:J:39:LEU:HD11	1.83	0.59
9:K:24:ASP:OD2	9:K:74:ARG:NH1	2.31	0.59
4:E:28:TYR:CZ	4:E:78:LEU:HG	2.38	0.59
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.36	0.59
1:A:777:PHE:HE1	1:A:792:TYR:CZ	2.19	0.59
9:K:8:GLU:O	9:K:37:LYS:HD2	2.02	0.59
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.84	0.59
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLN:NE2	1:A:493:GLN:HA	2.18	0.59
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.59
2:B:980:PHE:CE1	2:B:1094:ARG:HG3	2.37	0.59
2:B:973:ILE:O	2:B:975:GLN:HG3	2.02	0.59
4:E:9:ILE:HG21	4:E:43:LYS:HE3	1.84	0.59
5:F:111:LEU:O	5:F:113:GLY:N	2.32	0.59
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.85	0.59
1:A:1313:LEU:O	1:A:1317:MET:HB2	2.02	0.58
1:A:55:ASP:O	1:A:57:ARG:N	2.36	0.58
3:C:167:HIS:HD2	3:C:169:LYS:N	2.00	0.58
2:B:294:ASP:H	7:I:12:ASN:ND2	2.01	0.58
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.67	0.58
2:B:586:TRP:NE1	2:B:588:GLY:O	2.36	0.58
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.36	0.58
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.84	0.58
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.33	0.58
1:A:532:ARG:HH12	1:A:745:GLN:HE21	1.51	0.58
2:B:1152:MET:HE2	2:B:1152:MET:HA	1.85	0.58
2:B:872:GLU:HG2	2:B:916:THR:OG1	2.03	0.58
2:B:950:ASP:OD2	2:B:969:ARG:HD3	2.02	0.58
9:K:29:ASN:ND2	9:K:79:GLU:HA	2.19	0.58
1:A:470:LEU:CD1	1:A:487:MET:CE	2.75	0.58
1:A:540:PHE:C	1:A:541:ILE:HD12	2.23	0.58
2:B:130:VAL:HG12	2:B:131:ASP:H	1.68	0.58
2:B:276:ILE:HG23	2:B:337:ARG:HB2	1.85	0.58
2:B:604:ARG:HH22	2:B:697:GLU:CD	2.07	0.58
1:A:567:LYS:HG2	6:H:96:VAL:H	1.68	0.58
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.38	0.58
2:B:120:ARG:HG3	2:B:955:THR:HG21	1.85	0.58
2:B:796:LEU:O	2:B:799:PRO:HD3	2.03	0.58
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.49	0.58
5:F:99:LEU:HG	5:F:99:LEU:O	2.03	0.58
6:H:82:PRO:HG2	9:K:54:ARG:HG2	1.86	0.58
1:A:470:LEU:CD1	1:A:487:MET:HE3	2.29	0.58
2:B:370:PHE:CD1	2:B:370:PHE:N	2.71	0.58
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.86	0.58
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.86	0.58
1:A:1199:ARG:HG3	1:A:1236:LEU:CD1	2.31	0.58
1:A:903:ASN:C	1:A:903:ASN:HD22	2.06	0.58
10:L:30:ILE:HG13	10:L:59:ALA:HB2	1.86	0.58
1:A:626:ASN:O	1:A:631:HIS:CD2	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.51	0.58
2:B:593:PRO:O	2:B:596:LEU:N	2.37	0.58
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.19	0.58
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.85	0.58
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.85	0.58
10:L:30:ILE:HG22	10:L:31:CYS:N	2.19	0.58
2:B:239:GLU:HG3	2:B:255:GLN:HG2	1.85	0.58
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.18	0.58
2:B:602:THR:O	2:B:606:LYS:HG3	2.04	0.58
10:L:38:LEU:O	10:L:39:SER:CB	2.51	0.58
1:A:493:GLN:CA	1:A:493:GLN:HE21	2.17	0.57
6:H:103:LYS:NZ	6:H:114:VAL:HB	2.18	0.57
1:A:1107:VAL:HG12	1:A:1333:ILE:HD11	1.84	0.57
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.25	0.57
2:B:228:LYS:O	2:B:261:ARG:NH2	2.36	0.57
2:B:36:ALA:HA	2:B:39:ARG:CZ	2.34	0.57
5:F:111:LEU:C	5:F:113:GLY:H	2.07	0.57
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.34	0.57
7:I:70:ARG:HG2	7:I:84:VAL:HG23	1.87	0.57
2:B:235:SER:HA	2:B:261:ARG:NH2	2.19	0.57
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.87	0.57
10:L:51:CYS:HB3	10:L:53:HIS:NE2	2.19	0.57
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.86	0.57
2:B:701:ILE:HB	2:B:739:THR:OG1	2.04	0.57
1:A:849:MET:HE2	1:A:1063:MET:SD	2.44	0.57
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.86	0.57
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.39	0.57
4:E:180:ARG:HH21	4:E:192:ARG:CB	2.16	0.57
4:E:78:LEU:HD23	4:E:107:THR:HB	1.86	0.57
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.86	0.57
1:A:689:LYS:O	1:A:693:VAL:HG23	2.04	0.57
1:A:34:LYS:HA	1:A:83:HIS:CD2	2.37	0.57
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.85	0.57
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.85	0.57
5:F:83:PRO:HD2	5:F:84:TYR:HD1	1.69	0.57
6:H:103:LYS:CE	6:H:114:VAL:HB	2.35	0.57
9:K:1:MET:HG3	9:K:2:ASN:H	1.70	0.57
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.87	0.57
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.87	0.57
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.40	0.57
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:LYS:O	1:A:1106:ASN:HB2	2.05	0.57
1:A:471:ASN:O	1:A:474:VAL:HG12	2.05	0.57
1:A:579:SER:HA	1:A:582:ILE:HD12	1.87	0.57
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.86	0.57
1:A:347:PHE:H	2:B:1107:ALA:HA	1.70	0.57
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.20	0.57
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.87	0.57
2:B:1079:LYS:CA	3:C:27:LEU:HD21	2.35	0.57
6:H:91:ASP:C	6:H:93:TYR:H	2.08	0.57
4:E:94:LYS:O	4:E:98:ILE:HB	2.05	0.56
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.86	0.56
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.05	0.56
1:A:337:ARG:HA	1:A:340:LEU:HB2	1.85	0.56
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.40	0.56
2:B:1072:MET:HE3	2:B:1087:PHE:CD1	2.40	0.56
2:B:54:PHE:HE2	2:B:170:LEU:HD21	1.71	0.56
1:A:1063:MET:HG3	2:B:1139:ILE:CG2	2.35	0.56
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.56
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.05	0.56
1:A:1116:LEU:HD13	1:A:1311:VAL:HA	1.86	0.56
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.40	0.56
7:I:103:CYS:O	7:I:107:SER:HA	2.05	0.56
8:J:6:ARG:HD3	8:J:11:GLY:O	2.06	0.56
1:A:446:ARG:HB2	1:A:487:MET:SD	2.46	0.56
1:A:850:VAL:O	1:A:1060:PRO:HA	2.06	0.56
2:B:242:SER:OG	2:B:362:PRO:HD2	2.05	0.56
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.87	0.56
1:A:40:THR:HG22	1:A:41:MET:HG3	1.88	0.56
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.45	0.56
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.21	0.56
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.88	0.56
9:K:29:ASN:HB3	9:K:77:THR:O	2.05	0.56
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.04	0.56
1:A:824:LEU:CD2	2:B:765:PRO:HB3	2.35	0.56
2:B:408:LEU:HD23	2:B:409:ALA:H	1.69	0.56
2:B:63:ILE:HD13	2:B:95:ILE:HD11	1.88	0.56
2:B:772:ALA:O	2:B:775:LYS:HB2	2.05	0.56
1:A:1208:THR:HB	1:A:1211:GLN:H	1.71	0.56
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	1.87	0.56
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.36	0.56
4:E:22:MET:O	4:E:26:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HA	6:H:28:ALA:HA	1.87	0.56
3:C:124:LEU:O	3:C:127:ARG:HG3	2.06	0.56
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.71	0.56
1:A:1264:GLU:HA	1:A:1267:MET:HE2	1.88	0.56
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.36	0.56
2:B:890:TYR:CD2	2:B:893:LEU:HD11	2.41	0.56
3:C:209:TYR:N	3:C:209:TYR:CD1	2.74	0.56
3:C:19:ASP:HA	3:C:231:ASN:HA	1.87	0.56
3:C:246:ARG:HA	3:C:249:ASP:HB3	1.87	0.56
1:A:1115:SER:HA	1:A:1308:THR:O	2.07	0.55
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.39	0.55
1:A:96:ILE:HG22	1:A:176:LYS:HD2	1.89	0.55
1:A:785:PRO:HD2	1:A:786:HIS:CD2	2.41	0.55
1:A:903:ASN:O	1:A:905:ASP:N	2.38	0.55
1:A:738:LYS:HA	6:H:19:ARG:HH22	1.70	0.55
1:A:1295:THR:HB	1:A:1297:GLU:OE1	2.06	0.55
1:A:1376:THR:HG23	4:E:212:ARG:NH2	2.19	0.55
1:A:451:HIS:CG	1:A:1074:GLU:HG3	2.41	0.55
2:B:25:ILE:CD1	2:B:658:ILE:HD11	2.37	0.55
1:A:503:GLN:NE2	5:F:90:ARG:HH21	2.04	0.55
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.88	0.55
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.36	0.55
1:A:847:ASP:N	1:A:847:ASP:OD1	2.31	0.55
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.88	0.55
4:E:155:ARG:HD2	4:E:194:GLU:CD	2.27	0.55
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.37	0.55
1:A:458:HIS:HE1	1:A:474:VAL:HG21	1.70	0.55
1:A:843:LYS:NZ	1:A:1386:ARG:HB3	2.21	0.55
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.86	0.55
3:C:209:TYR:N	3:C:209:TYR:HD1	2.05	0.55
1:A:870:GLU:HG2	4:E:208:TYR:CG	2.41	0.55
7:I:55:THR:O	7:I:58:VAL:HG23	2.06	0.55
8:J:8:PHE:HB2	8:J:48:ARG:NH2	2.20	0.55
1:A:534:LEU:HG	1:A:534:LEU:O	2.07	0.55
1:A:809:THR:O	1:A:813:PHE:N	2.35	0.55
2:B:1222:ARG:C	2:B:1224:PHE:H	2.10	0.55
2:B:685:LEU:HD11	2:B:692:TYR:CZ	2.41	0.55
1:A:572:TRP:H	1:A:572:TRP:HE3	1.53	0.55
1:A:774:ARG:HG3	1:A:774:ARG:NH1	2.06	0.55
1:A:92:HIS:CD2	1:A:94:GLY:H	2.21	0.55
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:LYS:HE2	6:H:116:TYR:CZ	2.42	0.55
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.88	0.55
1:A:469:ARG:NH2	2:B:991:GLY:O	2.39	0.55
1:A:586:ILE:HD11	1:A:637:LYS:HG3	1.89	0.55
1:A:852:TYR:CD2	5:F:136:ARG:HD3	2.42	0.55
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.65	0.55
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.87	0.55
5:F:101:ILE:HD11	5:F:124:GLU:OE1	2.07	0.55
5:F:76:LYS:O	5:F:79:ARG:HD3	2.06	0.55
2:B:995:ARG:HD3	9:K:6:ARG:HH12	1.71	0.55
1:A:35:ILE:HB	1:A:83:HIS:O	2.06	0.55
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.87	0.55
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.70	0.55
2:B:558:LEU:HB3	2:B:563:MET:HE2	1.88	0.55
8:J:8:PHE:HB2	8:J:48:ARG:HH21	1.71	0.55
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.81	0.55
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.27	0.55
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.88	0.55
9:K:56:VAL:HG22	9:K:77:THR:HG22	1.89	0.55
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.89	0.54
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.42	0.54
1:A:535:THR:O	1:A:575:LYS:HE3	2.07	0.54
1:A:527:THR:CG2	1:A:650:GLN:HA	2.37	0.54
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.89	0.54
9:K:42:LEU:HG	9:K:46:ILE:CD1	2.36	0.54
10:L:51:CYS:C	10:L:53:HIS:H	2.10	0.54
1:A:1111:MET:HE1	1:A:1331:SER:HB2	1.89	0.54
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.42	0.54
2:B:955:THR:HG23	10:L:55:ILE:HA	1.90	0.54
3:C:71:PRO:HG3	8:J:13:VAL:HG21	1.88	0.54
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.90	0.54
2:B:104:GLU:HG3	10:L:54:ARG:NH1	2.23	0.54
2:B:652:LYS:HE3	2:B:688:GLY:O	2.08	0.54
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.54
6:H:103:LYS:HD3	6:H:114:VAL:HB	1.89	0.54
7:I:78:CYS:SG	7:I:103:CYS:SG	3.06	0.54
1:A:31:SER:CB	1:A:83:HIS:HB2	2.38	0.54
1:A:589:GLN:HB2	1:A:961:ARG:NH2	2.23	0.54
4:E:61:GLN:HG3	4:E:105:PHE:CE2	2.42	0.54
1:A:935:GLN:HG3	1:A:1023:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.89	0.54
2:B:999:MET:HE2	2:B:1011:ILE:HD12	1.88	0.54
2:B:1180:PHE:O	2:B:1188:LYS:HA	2.08	0.54
3:C:239:PRO:O	3:C:242:GLN:HB2	2.08	0.54
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.89	0.54
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.89	0.54
2:B:521:LEU:CD2	2:B:635:ARG:HD3	2.37	0.54
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.90	0.54
2:B:903:VAL:HG22	10:L:63:ARG:HD3	1.89	0.54
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.37	0.54
1:A:668:ASP:CG	1:A:742:ASN:HB2	2.27	0.54
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.54
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.08	0.54
1:A:1219:THR:HG21	1:A:1271:ILE:HG12	1.90	0.54
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.90	0.54
2:B:751:VAL:HG13	2:B:812:LEU:HD13	1.90	0.54
2:B:950:ASP:OD2	2:B:969:ARG:NH1	2.31	0.54
6:H:36:CYS:HA	6:H:126:GLU:O	2.08	0.54
1:A:975:HIS:H	6:H:136:LYS:NZ	2.05	0.54
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.54
1:A:545:GLN:HG2	1:A:549:MET:CE	2.36	0.54
2:B:1053:GLU:OE1	2:B:1067:ARG:NH1	2.41	0.54
2:B:870:ILE:O	2:B:870:ILE:HG22	2.08	0.54
3:C:229:TYR:N	3:C:229:TYR:CD1	2.75	0.54
6:H:126:GLU:N	6:H:130:ARG:HH12	2.06	0.54
9:K:55:LYS:HB2	9:K:81:TYR:HE1	1.66	0.54
1:A:588:LEU:O	1:A:606:LEU:HA	2.08	0.54
1:A:903:ASN:ND2	1:A:905:ASP:H	2.04	0.54
2:B:531:GLN:H	2:B:531:GLN:CD	2.11	0.54
2:B:315:LYS:HE2	7:I:13:MET:SD	2.48	0.54
7:I:8:ARG:HB3	7:I:34:TYR:CE1	2.42	0.54
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.90	0.53
1:A:479:ASN:HD22	1:A:479:ASN:C	2.12	0.53
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.73	0.53
2:B:1084:GLN:HE22	3:C:192:TRP:H	0.81	0.53
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.90	0.53
2:B:69:LEU:HD12	2:B:90:ILE:HB	1.90	0.53
1:A:740:LEU:HD21	3:C:193:TYR:CE2	2.43	0.53
4:E:106:GLN:O	4:E:130:ALA:HA	2.08	0.53
1:A:1329:THR:CG2	1:A:1335:ILE:HG13	2.38	0.53
1:A:1359:ASP:C	1:A:1361:SER:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:O	1:A:48:ALA:HB2	2.08	0.53
1:A:1438:THR:HG22	2:B:1142:GLY:O	2.08	0.53
2:B:1160:VAL:HG12	2:B:1161:HIS:H	1.72	0.53
2:B:1168:LEU:HB3	2:B:1170:THR:HG23	1.90	0.53
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.39	0.53
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.55	0.53
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.03	0.53
1:A:914:GLU:O	1:A:916:GLY:N	2.34	0.53
2:B:116:GLU:HG3	10:L:55:ILE:HD11	1.89	0.53
2:B:521:LEU:HD21	2:B:635:ARG:HD3	1.91	0.53
2:B:565:PRO:HG2	2:B:568:ASP:HB2	1.90	0.53
2:B:583:ASN:OD1	2:B:628:THR:N	2.41	0.53
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.90	0.53
3:C:114:TYR:HB3	3:C:140:ASN:O	2.08	0.53
1:A:84:ILE:HG22	1:A:241:VAL:HG23	1.90	0.53
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.90	0.53
2:B:40:GLU:OE1	2:B:680:THR:HG23	2.08	0.53
3:C:18:VAL:O	3:C:19:ASP:C	2.46	0.53
1:A:470:LEU:CD1	1:A:487:MET:HE1	2.37	0.53
2:B:996:ARG:CZ	3:C:38:ILE:HG23	2.39	0.53
3:C:40:GLU:OE2	3:C:254:LYS:NZ	2.34	0.53
1:A:907:THR:HG22	1:A:908:LEU:N	2.24	0.53
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.91	0.53
2:B:541:LEU:HD11	2:B:808:ALA:HB1	1.91	0.53
1:A:369:SER:OG	9:K:2:ASN:ND2	2.41	0.53
1:A:444:PHE:HE2	1:A:470:LEU:HD21	1.64	0.53
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.90	0.53
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.89	0.53
4:E:88:VAL:HB	4:E:116:ILE:HG23	1.91	0.53
1:A:1341:ILE:HD11	1:A:1376:THR:O	2.09	0.53
1:A:1384:VAL:O	1:A:1386:ARG:N	2.42	0.53
1:A:690:VAL:HG13	1:A:718:VAL:HG13	1.89	0.53
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.90	0.53
3:C:31:ASN:O	3:C:35:ARG:HG3	2.08	0.53
1:A:1265:ASN:HD21	2:B:263:GLY:HA2	1.73	0.53
1:A:401:GLY:O	1:A:435:HIS:ND1	2.42	0.53
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.90	0.53
1:A:872:GLY:HA3	1:A:999:VAL:HG11	1.91	0.52
2:B:121:ASN:HA	2:B:207:GLY:CA	2.39	0.52
2:B:185:THR:N	2:B:188:ASP:HB2	2.24	0.52
2:B:120:ARG:HG3	2:B:955:THR:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:NH1	2:B:1091:TYR:CB	2.72	0.52
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.91	0.52
3:C:7:GLN:HG2	9:K:104:ASN:ND2	2.24	0.52
1:A:866:PHE:HZ	4:E:175:LEU:HD23	1.74	0.52
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.92	0.52
10:L:51:CYS:O	10:L:53:HIS:N	2.35	0.52
1:A:443:LEU:HG	1:A:455:MET:CE	2.40	0.52
2:B:408:LEU:HD12	2:B:545:ILE:HD12	1.91	0.52
2:B:898:LEU:CD2	2:B:964:VAL:HG11	2.40	0.52
3:C:71:PRO:O	3:C:72:LEU:HD23	2.10	0.52
1:A:511:ILE:O	1:A:519:PRO:HA	2.09	0.52
2:B:1167:GLY:H	2:B:1217:TYR:HE2	1.57	0.52
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.90	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.21	0.52
4:E:15:ALA:O	4:E:19:VAL:HG23	2.09	0.52
1:A:1333:ILE:HG12	1:A:1381:LEU:HD13	1.92	0.52
1:A:286:HIS:C	1:A:288:ALA:H	2.13	0.52
1:A:49:LYS:CB	1:A:55:ASP:HB2	2.38	0.52
3:C:183:TRP:O	3:C:185:LYS:N	2.43	0.52
1:A:364:VAL:CG1	1:A:364:VAL:O	2.57	0.52
2:B:130:VAL:HG12	2:B:131:ASP:N	2.23	0.52
3:C:11:ARG:HE	3:C:209:TYR:HE2	1.55	0.52
10:L:31:CYS:HA	10:L:56:LEU:HA	1.92	0.52
1:A:1265:ASN:HD21	2:B:263:GLY:CA	2.23	0.52
1:A:1293:SER:CB	1:A:1294:PRO:HD2	2.39	0.52
1:A:90:VAL:HG13	1:A:297:GLN:NE2	2.25	0.52
2:B:361:LEU:HB3	2:B:364:ILE:HD12	1.92	0.52
2:B:36:ALA:HB2	2:B:661:LEU:HD22	1.92	0.52
4:E:6:GLU:OE2	4:E:43:LYS:NZ	2.40	0.52
1:A:23:SER:CB	1:A:233:TRP:CE2	2.93	0.52
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.17	0.52
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.40	0.52
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.52
2:B:230:ALA:N	2:B:231:PRO:HD2	2.25	0.52
2:B:43:LEU:O	2:B:496:ARG:HD2	2.10	0.52
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.36	0.52
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.91	0.52
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.91	0.52
2:B:370:PHE:HD1	2:B:370:PHE:N	2.08	0.52
8:J:23:ASN:O	8:J:25:LEU:N	2.43	0.52
1:A:1025:ARG:O	1:A:1035:TYR:HE1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:OD2	1:A:362:ASP:N	2.41	0.52
1:A:72:GLU:HB3	1:A:76:GLU:CB	2.37	0.52
1:A:399:HIS:O	1:A:435:HIS:ND1	2.43	0.51
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.45	0.51
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.92	0.51
1:A:19:PHE:O	1:A:1416:ALA:HA	2.11	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HE2	1.92	0.51
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.46	0.51
2:B:1162:ILE:HD13	2:B:1216:LEU:HB2	1.92	0.51
2:B:239:GLU:CG	2:B:255:GLN:HG2	2.40	0.51
2:B:287:ARG:NH1	2:B:324:ILE:O	2.43	0.51
2:B:550:ASP:OD1	2:B:552:MET:HG3	2.11	0.51
2:B:561:TRP:O	2:B:590:HIS:HE1	1.93	0.51
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.40	0.51
1:A:103:CYS:HB3	1:A:174:ILE:HD13	1.92	0.51
1:A:367:PRO:HB3	1:A:465:TYR:O	2.11	0.51
2:B:710:LEU:HD23	2:B:738:PHE:CD1	2.45	0.51
1:A:30:ILE:HB	2:B:1170:THR:HG21	1.92	0.51
2:B:310:MET:O	2:B:313:MET:HB2	2.10	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.93	0.51
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.41	0.51
9:K:18:LYS:NZ	9:K:38:GLU:HG2	2.25	0.51
1:A:445:ASN:HD21	1:A:449:SER:HB3	1.75	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.93	0.51
1:A:385:ILE:O	1:A:389:THR:HB	2.10	0.51
1:A:47:ARG:O	1:A:48:ALA:CB	2.59	0.51
2:B:526:GLU:HG3	2:B:752:ALA:HB3	1.92	0.51
3:C:91:HIS:HB2	3:C:96:SER:OG	2.11	0.51
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.23	0.51
1:A:219:PHE:CD1	1:A:219:PHE:C	2.84	0.51
10:L:29:TYR:CE2	10:L:58:LYS:HG2	2.45	0.51
1:A:486:GLU:OE2	2:B:1102:LYS:HB3	2.11	0.51
1:A:567:LYS:HB3	6:H:95:TYR:HA	1.91	0.51
2:B:333:PHE:O	2:B:337:ARG:HG2	2.11	0.51
2:B:217:ARG:HD3	2:B:407:ASP:OD2	2.09	0.51
1:A:868:TYR:CZ	1:A:1064:VAL:HG22	2.46	0.51
1:A:1433:MET:HE2	2:B:1144:ALA:HB3	1.92	0.51
2:B:18:PHE:N	2:B:18:PHE:CD2	2.77	0.51
2:B:845:SER:HB3	2:B:850:LEU:CD2	2.40	0.51
3:C:35:ARG:HD3	9:K:41:THR:HA	1.93	0.51
5:F:138:LEU:HB3	5:F:139:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:TYR:O	1:A:1349:TYR:CD2	2.64	0.51
1:A:868:TYR:CE2	1:A:1366:ARG:HD3	2.46	0.51
2:B:487:THR:HG22	2:B:490:SER:H	1.75	0.51
2:B:62:ILE:HA	2:B:65:GLU:OE1	2.11	0.51
2:B:858:SER:HA	2:B:966:VAL:O	2.11	0.51
3:C:180:TYR:HB3	3:C:228:PHE:HD2	1.76	0.51
3:C:43:THR:HG22	3:C:44:LEU:N	2.25	0.51
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.26	0.51
9:K:47:ARG:HB3	9:K:47:ARG:NH1	2.26	0.51
9:K:58:PHE:HB3	9:K:76:GLN:CB	2.41	0.51
1:A:1206:ASP:CB	1:A:1274:ARG:HH12	2.24	0.50
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.46	0.50
1:A:673:GLY:N	1:A:674:PRO:HD2	2.25	0.50
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.94	0.50
2:B:680:THR:CG2	2:B:682:SER:HB2	2.41	0.50
1:A:1376:THR:O	4:E:212:ARG:NH2	2.43	0.50
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.46	0.50
6:H:7:ASP:O	6:H:8:ASP:HB2	2.11	0.50
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.45	0.50
1:A:1015:VAL:O	1:A:1015:VAL:CG1	2.59	0.50
1:A:145:LYS:HD2	1:A:149:GLU:OE1	2.12	0.50
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.93	0.50
1:A:185:TRP:O	1:A:197:PRO:HA	2.11	0.50
1:A:817:ALA:HA	2:B:764:SER:OG	2.12	0.50
2:B:1027:ILE:HG12	2:B:1052:VAL:HG22	1.93	0.50
2:B:1004:GLU:OE2	2:B:1064:TYR:CE2	2.65	0.50
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.94	0.50
2:B:654:ARG:H	2:B:657:HIS:HD2	1.58	0.50
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.46	0.50
5:F:114:GLU:CD	5:F:119:ARG:HG2	2.32	0.50
5:F:85:MET:HE1	5:F:93:ILE:CD1	2.41	0.50
1:A:1072:ILE:HG23	1:A:1356:ILE:CD1	2.41	0.50
1:A:1139:GLU:HA	1:A:1279:ILE:HG22	1.93	0.50
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.11	0.50
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.46	0.50
1:A:350:ARG:HA	1:A:487:MET:O	2.10	0.50
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.93	0.50
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.47	0.50
5:F:109:VAL:CG1	5:F:110:ASP:H	2.24	0.50
1:A:1392:SER:O	1:A:1393:ASN:HB2	2.12	0.50
1:A:451:HIS:CE1	1:A:453:MET:HE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:HG23	1:A:728:LYS:HG3	1.92	0.50
2:B:241:ARG:HH21	2:B:251:ILE:HD11	1.77	0.50
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.94	0.50
9:K:78:THR:CG2	9:K:79:GLU:N	2.74	0.50
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.93	0.50
2:B:744:HIS:HD2	2:B:746:SER:OG	1.94	0.50
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.44	0.50
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.15	0.50
1:A:112:LYS:HD2	1:A:165:GLY:HA3	1.94	0.50
1:A:1395:GLY:H	1:A:1398:MET:HE2	1.77	0.50
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.93	0.50
2:B:89:GLU:N	2:B:137:TYR:HB2	2.27	0.50
2:B:120:ARG:HH21	2:B:956:THR:HB	1.76	0.50
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.94	0.50
1:A:1359:ASP:O	1:A:1361:SER:N	2.44	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
2:B:408:LEU:CD1	2:B:545:ILE:HD12	2.41	0.50
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.26	0.50
1:A:987:VAL:HG23	1:A:1028:THR:OG1	2.11	0.50
1:A:757:ASN:CA	2:B:1021:MET:HE1	2.21	0.50
2:B:125:SER:HA	2:B:171:PRO:HA	1.92	0.50
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.12	0.50
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.92	0.50
3:C:89:GLU:O	3:C:90:ASP:HB2	2.12	0.50
7:I:69:PRO:HG2	7:I:85:PHE:O	2.12	0.50
1:A:1198:ASP:O	1:A:1202:MET:HB2	2.12	0.49
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.47	0.49
1:A:361:LEU:HG	1:A:361:LEU:O	2.11	0.49
1:A:465:TYR:CD1	1:A:465:TYR:N	2.77	0.49
1:A:562:THR:HG23	6:H:79:TRP:CD1	2.46	0.49
2:B:1037:LEU:HD13	2:B:1062:HIS:HB3	1.94	0.49
2:B:604:ARG:NH2	2:B:697:GLU:OE1	2.39	0.49
4:E:158:SER:O	4:E:162:ARG:HG3	2.12	0.49
8:J:32:GLU:CD	8:J:32:GLU:H	2.14	0.49
9:K:39:ASP:OD1	9:K:40:HIS:N	2.45	0.49
1:A:130:ASP:HB3	1:A:133:LYS:HB2	1.92	0.49
1:A:381:THR:HG23	1:A:383:TYR:CD1	2.47	0.49
1:A:441:PRO:HG2	1:A:498:ARG:HG2	1.93	0.49
1:A:527:THR:HG21	1:A:650:GLN:HA	1.93	0.49
1:A:557:ASP:HA	9:K:26:LYS:HD2	1.94	0.49
1:A:55:ASP:H	1:A:56:PRO:CD	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.49
3:C:263:THR:C	3:C:265:MET:H	2.16	0.49
3:C:62:PHE:O	3:C:66:ARG:HG3	2.12	0.49
7:I:103:CYS:HB3	7:I:108:HIS:H	1.77	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.94	0.49
1:A:460:VAL:CG1	1:A:461:LYS:N	2.75	0.49
1:A:92:HIS:C	1:A:92:HIS:CD2	2.86	0.49
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.13	0.49
2:B:103:ASN:HB2	2:B:169:ARG:HH12	1.77	0.49
2:B:63:ILE:O	2:B:63:ILE:HG23	2.12	0.49
2:B:684:LEU:HD23	2:B:689:LEU:HD13	1.93	0.49
2:B:704:ALA:HB3	2:B:741:CYS:HB2	1.94	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
4:E:31:THR:C	4:E:33:GLU:N	2.66	0.49
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.47	0.49
1:A:864:ILE:HD13	1:A:1374:VAL:HG22	1.95	0.49
2:B:235:SER:HB3	2:B:261:ARG:HA	1.93	0.49
2:B:770:GLN:HG2	2:B:983:ARG:O	2.12	0.49
2:B:806:THR:HG22	2:B:808:ALA:N	2.27	0.49
1:A:493:GLN:CA	1:A:493:GLN:NE2	2.74	0.49
1:A:741:ASN:HD22	1:A:741:ASN:C	2.15	0.49
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.45	0.49
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.94	0.49
2:B:25:ILE:HD12	2:B:653:VAL:CB	2.38	0.49
1:A:782:ARG:NH2	2:B:701:ILE:O	2.40	0.49
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	1.94	0.49
1:A:1151:GLU:HG2	7:I:42:LEU:HD11	1.95	0.49
2:B:120:ARG:CZ	10:L:54:ARG:HH11	2.26	0.49
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.94	0.49
1:A:1293:SER:HB3	1:A:1299:VAL:CG2	2.42	0.49
1:A:50:ILE:C	1:A:52:GLY:H	2.16	0.49
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.42	0.49
4:E:23:VAL:CG1	4:E:30:ILE:HD11	2.43	0.49
1:A:572:TRP:CE3	1:A:572:TRP:N	2.80	0.49
1:A:532:ARG:HH12	1:A:745:GLN:NE2	2.10	0.49
1:A:781:ASP:OD2	7:I:91:ARG:NH2	2.46	0.49
2:B:251:ILE:HG22	2:B:251:ILE:O	2.11	0.49
5:F:111:LEU:H	5:F:111:LEU:HD12	1.77	0.49
6:H:47:PHE:HD2	6:H:47:PHE:O	1.96	0.49
1:A:1111:MET:CE	1:A:1331:SER:HB2	2.43	0.49
2:B:167:ILE:HG22	2:B:167:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:HH21	2:B:614:SER:HA	1.76	0.49
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.49
3:C:43:THR:CG2	3:C:44:LEU:N	2.75	0.49
5:F:134:ILE:HD12	5:F:151:LEU:HD12	1.93	0.49
1:A:709:THR:CG2	7:I:94:ASP:HA	2.43	0.49
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.93	0.49
1:A:534:LEU:O	1:A:574:GLY:HA3	2.13	0.49
1:A:530:GLY:HA2	1:A:657:LEU:HD13	1.93	0.49
2:B:283:VAL:HG21	2:B:318:VAL:HA	1.95	0.49
2:B:648:HIS:N	2:B:648:HIS:CD2	2.80	0.49
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.81	0.49
4:E:12:LEU:HD22	4:E:55:ARG:CZ	2.43	0.49
9:K:18:LYS:HZ2	9:K:38:GLU:HG2	1.78	0.49
1:A:666:ILE:HD12	2:B:1030:LEU:HD22	1.94	0.48
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.40	0.48
2:B:879:ARG:HB3	2:B:883:LEU:HD22	1.94	0.48
2:B:890:TYR:HD2	2:B:893:LEU:HD11	1.77	0.48
4:E:62:ALA:HB3	4:E:78:LEU:HB2	1.93	0.48
5:F:81:THR:HG21	5:F:136:ARG:HD2	1.92	0.48
9:K:58:PHE:HE2	9:K:74:ARG:HB3	1.78	0.48
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.95	0.48
4:E:5:ASN:HD21	4:E:53:PRO:HD3	1.77	0.48
9:K:7:PHE:C	9:K:9:LEU:H	2.16	0.48
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.48
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.48
2:B:918:ILE:HD12	2:B:935:ARG:HH11	1.78	0.48
4:E:113:GLN:HG2	4:E:137:GLU:OE1	2.13	0.48
1:A:103:CYS:SG	1:A:207:ILE:HG23	2.53	0.48
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.94	0.48
1:A:879:GLU:CD	1:A:962:ARG:HH22	2.17	0.48
2:B:1163:CYS:HB2	2:B:1182:CYS:SG	2.53	0.48
7:I:84:VAL:CG1	7:I:84:VAL:O	2.61	0.48
9:K:87:LEU:O	9:K:88:LYS:C	2.52	0.48
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.96	0.48
2:B:986:GLN:NE2	2:B:986:GLN:HA	2.27	0.48
3:C:65:HIS:CE1	3:C:69:LEU:HD11	2.48	0.48
2:B:893:LEU:HD21	2:B:910:VAL:HG12	1.93	0.48
2:B:227:LYS:HD3	2:B:236:HIS:CE1	2.49	0.48
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.49	0.48
3:C:99:LEU:HD23	3:C:118:LEU:HB3	1.95	0.48
1:A:1154:TYR:OH	7:I:18:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:TRP:CE2	1:A:1048:ASN:ND2	2.82	0.48
1:A:1077:THR:O	1:A:1078:GLN:NE2	2.46	0.48
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.14	0.48
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.48
4:E:23:VAL:HG11	4:E:30:ILE:HD11	1.96	0.48
1:A:838:GLN:HE22	1:A:1070:GLN:HG2	1.79	0.48
1:A:1277:GLU:O	1:A:1278:ASN:CB	2.62	0.48
1:A:562:THR:HB	6:H:98:TYR:CE2	2.48	0.48
1:A:67:CYS:O	1:A:68:GLN:HB2	2.14	0.48
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.79	0.48
2:B:564:GLU:N	2:B:589:VAL:O	2.45	0.48
2:B:680:THR:HG22	2:B:682:SER:H	1.78	0.48
4:E:109:ILE:HG23	4:E:135:PHE:HD1	1.79	0.48
6:H:47:PHE:CD2	6:H:47:PHE:O	2.67	0.48
9:K:7:PHE:HB2	9:K:11:LEU:CD2	2.44	0.48
1:A:1164:PRO:C	1:A:1166:ASP:H	2.17	0.48
1:A:360:GLU:OE2	1:A:651:LYS:NZ	2.46	0.48
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.49	0.48
4:E:145:THR:HA	4:E:150:VAL:HG11	1.96	0.48
1:A:353:ILE:HG21	1:A:487:MET:HE2	1.95	0.47
1:A:598:LEU:O	1:A:599:SER:C	2.52	0.47
1:A:523:ILE:HD12	1:A:622:VAL:HG22	1.94	0.47
2:B:801:LYS:O	8:J:52:THR:CG2	2.55	0.47
7:I:62:ILE:O	7:I:68:LEU:HD12	2.13	0.47
9:K:7:PHE:O	9:K:9:LEU:N	2.47	0.47
1:A:1062:GLU:C	1:A:1064:VAL:N	2.67	0.47
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.13	0.47
1:A:339:ASN:HD21	1:A:344:ARG:CZ	2.27	0.47
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.44	0.47
2:B:1004:GLU:OE2	2:B:1064:TYR:HE2	1.97	0.47
2:B:705:MET:CE	2:B:742:GLU:HG3	2.36	0.47
3:C:50:GLU:OE1	3:C:156:THR:HB	2.14	0.47
1:A:836:TYR:CE2	1:A:1385:THR:HG22	2.49	0.47
1:A:967:ALA:HB1	1:A:1041:ALA:HB1	1.96	0.47
2:B:1072:MET:HE3	2:B:1087:PHE:CG	2.50	0.47
3:C:97:VAL:CG2	3:C:129:ILE:CG2	2.92	0.47
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.32	0.47
1:A:874:ASP:HB2	1:A:1058:VAL:HA	1.96	0.47
1:A:868:TYR:CZ	1:A:1064:VAL:CG2	2.97	0.47
1:A:186:LYS:HE2	1:A:197:PRO:HD3	1.96	0.47
1:A:333:GLU:HG3	1:A:337:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.45	0.47
1:A:825:ILE:HG22	1:A:826:ASP:N	2.29	0.47
2:B:523:CYS:HB2	2:B:750:GLY:N	2.29	0.47
9:K:58:PHE:O	9:K:75:ILE:HA	2.15	0.47
1:A:55:ASP:N	1:A:56:PRO:HD2	2.15	0.47
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.15	0.47
1:A:91:PHE:CD1	1:A:99:ILE:HD13	2.49	0.47
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.50	0.47
2:B:406:LEU:CD1	2:B:498:THR:OG1	2.62	0.47
4:E:168:TYR:C	4:E:169:ARG:HG3	2.33	0.47
5:F:90:ARG:HG3	5:F:125:LEU:HD21	1.96	0.47
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.79	0.47
8:J:23:ASN:C	8:J:25:LEU:N	2.63	0.47
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.97	0.47
2:B:890:TYR:C	2:B:892:LYS:H	2.18	0.47
3:C:115:SER:O	3:C:118:LEU:HB2	2.14	0.47
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.97	0.47
1:A:848:ILE:CD1	1:A:1374:VAL:HG21	2.42	0.47
1:A:1438:THR:CG2	2:B:1144:ALA:H	2.26	0.47
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.50	0.47
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.50	0.47
8:J:48:ARG:O	8:J:52:THR:HB	2.14	0.47
3:C:146:LYS:O	8:J:61:LEU:HD21	2.14	0.47
1:A:1199:ARG:CA	1:A:1202:MET:HB2	2.45	0.47
1:A:672:ASP:CB	1:A:736:ASN:ND2	2.41	0.47
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.45	0.47
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.47
2:B:546:SER:CB	2:B:612:GLU:HG3	2.44	0.47
4:E:114:ASN:OD1	4:E:115:ASN:N	2.48	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.50	0.47
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.14	0.47
1:A:629:LEU:O	1:A:633:VAL:HG23	2.15	0.47
2:B:787:VAL:O	2:B:787:VAL:HG12	2.15	0.47
3:C:40:GLU:HG2	3:C:163:ILE:HG21	1.97	0.47
1:A:706:HIS:NE2	1:A:1139:GLU:OE1	2.48	0.47
1:A:313:GLN:HE21	1:A:322:VAL:HG12	1.80	0.47
1:A:32:VAL:HG23	1:A:58:LEU:HD23	1.96	0.47
1:A:364:VAL:O	1:A:364:VAL:HG13	2.15	0.47
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.97	0.47
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.15	0.47
2:B:211:VAL:O	2:B:480:SER:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:PHE:CZ	2:B:517:THR:HA	2.50	0.47
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.96	0.47
2:B:836:GLU:O	2:B:837:ASP:HB2	2.14	0.47
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.95	0.47
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.15	0.47
1:A:329:LEU:HD12	1:A:1406:VAL:HG22	1.96	0.47
2:B:130:VAL:HB	2:B:167:ILE:HD12	1.96	0.47
2:B:842:ASN:O	2:B:846:ILE:HG13	2.15	0.47
2:B:800:GLN:CB	8:J:52:THR:CG2	2.60	0.47
1:A:345:VAL:HG11	2:B:1129:ARG:HA	1.97	0.46
1:A:437:MET:O	1:A:438:ASP:C	2.53	0.46
1:A:445:ASN:ND2	1:A:449:SER:HB3	2.31	0.46
1:A:579:SER:OG	1:A:612:ILE:HG23	2.15	0.46
1:A:600:PRO:C	1:A:602:ASP:H	2.18	0.46
1:A:855:THR:HG21	1:A:857:ARG:CZ	2.44	0.46
2:B:343:ILE:HG22	2:B:348:ARG:HG3	1.97	0.46
4:E:84:ASP:O	4:E:113:GLN:NE2	2.48	0.46
7:I:2:THR:HG22	7:I:2:THR:O	2.15	0.46
1:A:1276:VAL:CG1	1:A:1279:ILE:HD13	2.45	0.46
1:A:22:PHE:HB3	1:A:27:VAL:HG22	1.97	0.46
1:A:620:LYS:O	1:A:625:SER:OG	2.34	0.46
2:B:422:LYS:HA	2:B:422:LYS:HD2	1.74	0.46
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.45	0.46
3:C:142:VAL:CG1	8:J:5:VAL:HG22	2.45	0.46
3:C:70:ILE:HG21	3:C:115:SER:HB3	1.97	0.46
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.47	0.46
1:A:32:VAL:HG22	1:A:81:PHE:O	2.16	0.46
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.80	0.46
1:A:778:GLY:HA3	2:B:516:ASN:ND2	2.30	0.46
3:C:246:ARG:HA	3:C:249:ASP:CB	2.46	0.46
1:A:1191:TRP:CZ3	7:I:43:VAL:HG21	2.51	0.46
1:A:914:GLU:C	1:A:916:GLY:H	2.15	0.46
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.80	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.50	0.46
3:C:10:ILE:HG21	9:K:112:GLN:HG3	1.96	0.46
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.97	0.46
6:H:99:GLY:HA3	6:H:118:PHE:CD2	2.50	0.46
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.45	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.96	0.46
2:B:408:LEU:O	2:B:409:ALA:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:O	2:B:65:GLU:HG2	2.15	0.46
3:C:240:VAL:O	3:C:243:VAL:N	2.48	0.46
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.35	0.46
1:A:1215:ARG:HA	1:A:1218:GLN:HE21	1.80	0.46
1:A:736:ASN:O	1:A:737:LEU:C	2.54	0.46
1:A:868:TYR:CD1	1:A:1064:VAL:HG11	2.50	0.46
2:B:47:GLN:NE2	2:B:408:LEU:HD21	2.31	0.46
2:B:770:GLN:HB2	2:B:985:GLY:H	1.80	0.46
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.50	0.46
6:H:87:ARG:O	6:H:89:LEU:N	2.44	0.46
7:I:19:ASP:OD1	7:I:22:ASN:HB2	2.16	0.46
9:K:45:LEU:HG	9:K:94:ILE:CD1	2.45	0.46
2:B:841:MET:HB2	2:B:990:ILE:HG12	1.98	0.46
3:C:167:HIS:CD2	3:C:169:LYS:HB3	2.51	0.46
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.98	0.46
3:C:44:LEU:CD2	3:C:130:GLY:HA2	2.46	0.46
6:H:103:LYS:CD	6:H:114:VAL:HB	2.46	0.46
1:A:1164:PRO:O	1:A:1166:ASP:N	2.49	0.46
1:A:590:ARG:HG2	1:A:605:MET:HB3	1.97	0.46
1:A:87:ALA:HB2	1:A:277:GLU:HG3	1.97	0.46
2:B:515:HIS:CD2	2:B:517:THR:H	2.33	0.46
2:B:597:MET:HE1	2:B:615:MET:HB2	1.97	0.46
8:J:2:ILE:HG12	8:J:57:ILE:HG21	1.97	0.46
1:A:1116:LEU:HD23	1:A:1316:VAL:HG11	1.96	0.46
1:A:456:MET:HB3	1:A:507:VAL:HG22	1.98	0.46
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.41	0.46
2:B:823:ALA:O	2:B:1089:PRO:HA	2.15	0.46
2:B:173:MET:HE1	2:B:409:ALA:CB	2.46	0.46
2:B:25:ILE:HD12	2:B:653:VAL:CG2	2.46	0.46
3:C:262:LEU:HD21	9:K:87:LEU:HD23	1.98	0.46
3:C:57:VAL:CG1	8:J:60:PHE:HB3	2.45	0.46
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.97	0.46
1:A:500:GLU:CD	1:A:1438:THR:HG21	2.35	0.46
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.98	0.46
2:B:306:ASN:O	2:B:308:TRP:N	2.43	0.46
2:B:322:PHE:CE1	7:I:30:ARG:HG3	2.51	0.46
2:B:657:HIS:O	2:B:660:LYS:HB2	2.15	0.46
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.15	0.46
1:A:567:LYS:CB	6:H:95:TYR:HA	2.46	0.46
8:J:1:MET:O	8:J:57:ILE:HG22	2.16	0.46
1:A:1187:GLN:CG	1:A:1188:GLN:H	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:O	1:A:742:ASN:HB3	2.16	0.45
2:B:1020:ARG:O	2:B:1021:MET:HB2	2.16	0.45
2:B:291:ILE:HD12	2:B:300:HIS:CE1	2.51	0.45
2:B:416:LEU:O	2:B:420:LEU:N	2.50	0.45
2:B:816:GLU:OE1	2:B:816:GLU:N	2.49	0.45
3:C:175:ALA:HB2	8:J:43:ARG:CZ	2.46	0.45
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.36	0.45
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.77	0.45
8:J:31:ASP:OD1	8:J:34:THR:OG1	2.32	0.45
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.98	0.45
1:A:848:ILE:HD13	1:A:1370:LEU:HD11	1.98	0.45
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.46	0.45
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.17	0.45
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.47	0.45
1:A:1220:PHE:CE1	1:A:1271:ILE:HD11	2.51	0.45
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.98	0.45
2:B:515:HIS:O	2:B:518:HIS:HB2	2.16	0.45
1:A:1341:ILE:HD13	4:E:212:ARG:NH2	2.32	0.45
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.45
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.29	0.45
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.98	0.45
2:B:1065:GLN:NE2	2:B:1069:PHE:H	2.05	0.45
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.97	0.45
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.98	0.45
1:A:27:VAL:HB	1:A:238:CYS:SG	2.56	0.45
1:A:329:LEU:HD21	2:B:1203:LEU:HD13	1.98	0.45
2:B:515:HIS:O	2:B:516:ASN:C	2.55	0.45
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.45
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.79	0.45
2:B:89:GLU:HB2	2:B:137:TYR:CD1	2.52	0.45
2:B:911:ILE:HG23	2:B:966:VAL:HG11	1.98	0.45
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.47	0.45
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.45	0.45
4:E:147:HIS:HD2	4:E:149:LEU:N	2.09	0.45
7:I:34:TYR:HE2	7:I:36:GLU:HG2	1.81	0.45
1:A:1434:ALA:C	1:A:1436:ILE:H	2.19	0.45
1:A:391:LEU:HD12	1:A:434:ARG:HB3	1.99	0.45
1:A:405:VAL:HB	1:A:413:ILE:HD12	1.99	0.45
1:A:553:VAL:CG2	1:A:652:VAL:HG21	2.43	0.45
1:A:556:TRP:HD1	1:A:580:VAL:HG11	1.81	0.45
1:A:848:ILE:HD11	1:A:1374:VAL:CG2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:LYS:HG3	1:A:955:PRO:HD3	1.98	0.45
2:B:361:LEU:HD21	2:B:381:MET:HE1	1.98	0.45
1:A:1340:GLY:HA2	4:E:183:PRO:HD2	1.98	0.45
4:E:71:LYS:O	4:E:73:PRO:HD3	2.17	0.45
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.21	0.45
1:A:456:MET:SD	1:A:521:MET:HE1	2.57	0.45
1:A:565:ILE:CG2	1:A:567:LYS:HE2	2.46	0.45
1:A:838:GLN:NE2	1:A:1070:GLN:HG2	2.31	0.45
1:A:17:VAL:HA	2:B:1215:ARG:O	2.17	0.45
2:B:808:ALA:O	2:B:812:LEU:HG	2.15	0.45
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.17	0.45
3:C:259:LEU:HD21	9:K:88:LYS:HA	1.99	0.45
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.51	0.45
1:A:325:ILE:HA	1:A:328:ARG:HB2	1.99	0.45
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.77	0.45
1:A:858:ASN:ND2	1:A:858:ASN:C	2.68	0.45
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.48	0.45
2:B:318:VAL:HG21	7:I:13:MET:HE3	1.97	0.45
2:B:890:TYR:HD2	2:B:893:LEU:CD1	2.30	0.45
1:A:11:LEU:HD11	2:B:1195:HIS:NE2	2.32	0.45
1:A:699:ALA:O	1:A:700:ASN:CB	2.65	0.45
2:B:801:LYS:HG2	8:J:52:THR:O	2.17	0.45
2:B:859:TYR:OH	2:B:942:ARG:HG3	2.16	0.45
1:A:1276:VAL:HG12	1:A:1279:ILE:HD13	1.97	0.45
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.77	0.45
1:A:809:THR:HG22	2:B:730:ARG:HG2	1.99	0.45
2:B:783:THR:HG23	2:B:817:LEU:HD21	1.99	0.45
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.17	0.45
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.99	0.44
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.98	0.44
2:B:406:LEU:HD13	2:B:498:THR:OG1	2.17	0.44
1:A:780:VAL:HG23	2:B:699:GLU:OE2	2.17	0.44
3:C:56:THR:HG23	3:C:58:LEU:H	1.82	0.44
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.44
1:A:911:SER:O	1:A:978:PRO:CB	2.63	0.44
2:B:234:ILE:HG22	2:B:236:HIS:O	2.18	0.44
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.66	0.44
2:B:623:GLU:OE1	2:B:625:LYS:HE3	2.17	0.44
2:B:405:ARG:NE	2:B:632:ARG:HG3	2.33	0.44
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.82	0.44
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:CYS:SG	3:C:146:LYS:N	2.90	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.99	0.44
1:A:1222:ASN:C	1:A:1224:LEU:N	2.68	0.44
1:A:445:ASN:HB2	1:A:455:MET:HE3	1.99	0.44
2:B:350:GLN:O	2:B:354:ASP:OD2	2.35	0.44
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.99	0.44
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.98	0.44
2:B:882:THR:HG21	2:B:935:ARG:HG3	2.00	0.44
2:B:99:LYS:HB3	2:B:180:TYR:CE2	2.53	0.44
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	2.00	0.44
1:A:443:LEU:HD21	1:A:455:MET:HE2	1.98	0.44
1:A:523:ILE:HG23	1:A:527:THR:HB	2.00	0.44
1:A:560:ILE:HD11	9:K:58:PHE:HD1	1.81	0.44
1:A:600:PRO:O	1:A:602:ASP:N	2.50	0.44
1:A:777:PHE:CE1	1:A:792:TYR:CZ	3.04	0.44
2:B:322:PHE:HE1	7:I:30:ARG:HG3	1.82	0.44
6:H:135:LEU:HD13	6:H:137:GLN:HB2	1.99	0.44
6:H:15:VAL:HG13	6:H:24:CYS:HB3	1.99	0.44
1:A:1153:TYR:CZ	7:I:42:LEU:HD13	2.53	0.44
3:C:6:PRO:HG2	9:K:97:LYS:O	2.18	0.44
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.33	0.44
1:A:596:THR:HG22	1:A:597:LEU:H	1.83	0.44
2:B:1001:PHE:CZ	2:B:1073:TYR:CB	2.99	0.44
2:B:1002:THR:HG22	2:B:1006:ILE:HB	2.00	0.44
2:B:229:ALA:C	2:B:231:PRO:HD2	2.38	0.44
2:B:235:SER:HB3	2:B:260:GLY:O	2.18	0.44
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.99	0.44
2:B:53:GLN:NE2	2:B:57:TYR:HB2	2.33	0.44
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.82	0.44
1:A:1215:ARG:HD2	1:A:1218:GLN:HE21	1.82	0.44
1:A:617:VAL:CG1	1:A:622:VAL:HB	2.48	0.44
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.64	0.44
2:B:1031:LEU:O	2:B:1032:SER:C	2.56	0.44
2:B:680:THR:HG21	2:B:682:SER:HB2	1.99	0.44
3:C:18:VAL:O	3:C:20:PHE:N	2.50	0.44
3:C:226:ASP:O	3:C:227:THR:HB	2.17	0.44
4:E:144:ILE:HG13	4:E:145:THR:N	2.32	0.44
1:A:913:LEU:HD12	1:A:914:GLU:H	1.83	0.44
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.17	0.44
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.51	0.44
2:B:170:LEU:HD13	2:B:457:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:CYS:HB3	2:B:782:LEU:HD22	2.00	0.44
3:C:205:LYS:HB3	3:C:206:ASN:OD1	2.18	0.44
3:C:80:LEU:HD12	3:C:94:LYS:O	2.18	0.44
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.42	0.44
1:A:523:ILE:HB	1:A:622:VAL:HG13	2.00	0.44
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.18	0.44
2:B:360:PHE:CE2	2:B:374:LYS:HB3	2.52	0.44
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.99	0.44
2:B:651:LEU:CD2	2:B:741:CYS:HB3	2.47	0.44
2:B:826:ALA:HB2	2:B:1087:PHE:HE1	1.81	0.44
4:E:178:ILE:HG23	4:E:214:CYS:HA	2.00	0.44
5:F:151:LEU:HD23	5:F:151:LEU:HA	1.78	0.44
9:K:107:THR:HG22	9:K:108:GLU:N	2.33	0.44
9:K:40:HIS:O	9:K:41:THR:C	2.56	0.44
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.99	0.44
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.18	0.44
1:A:843:LYS:HZ3	1:A:1386:ARG:HB3	1.81	0.44
1:A:687:LYS:NZ	1:A:795:GLU:HG3	2.33	0.44
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.18	0.44
2:B:1163:CYS:SG	2:B:1187:ASN:ND2	2.91	0.44
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.58	0.44
4:E:20:LYS:HE3	4:E:34:GLU:HG2	2.00	0.44
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	0.43
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.32	0.43
1:A:1064:VAL:HG13	1:A:1370:LEU:CD2	2.48	0.43
1:A:329:LEU:O	1:A:333:GLU:N	2.39	0.43
1:A:474:VAL:HG13	1:A:474:VAL:O	2.17	0.43
1:A:704:ALA:HB1	1:A:708:MET:O	2.18	0.43
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.50	0.43
1:A:914:GLU:C	1:A:916:GLY:N	2.70	0.43
2:B:99:LYS:HB3	2:B:180:TYR:CZ	2.53	0.43
2:B:287:ARG:NH1	2:B:321:GLY:O	2.50	0.43
1:A:1006:ILE:HB	4:E:167:ARG:HG3	1.98	0.43
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.33	0.43
4:E:17:ARG:O	4:E:20:LYS:HB2	2.18	0.43
6:H:26:ILE:CD1	6:H:42:ILE:HB	2.48	0.43
8:J:23:ASN:C	8:J:25:LEU:H	2.22	0.43
1:A:566:ILE:HD11	6:H:98:TYR:HB2	2.00	0.43
1:A:909:ASP:O	1:A:911:SER:N	2.51	0.43
2:B:195:CYS:SG	2:B:782:LEU:HD22	2.58	0.43
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:SER:HB2	3:C:240:VAL:HG13	2.00	0.43
1:A:1134:ILE:HG22	1:A:1306:LEU:CD1	2.48	0.43
1:A:1281:ARG:HB2	1:A:1309:ASP:HB2	2.00	0.43
1:A:1422:ARG:HA	1:A:1435:PRO:CG	2.49	0.43
1:A:367:PRO:HB3	1:A:466:SER:HA	2.00	0.43
1:A:41:MET:HG2	1:A:48:ALA:O	2.17	0.43
1:A:528:LEU:HD23	1:A:751:SER:N	2.33	0.43
1:A:549:MET:SD	1:A:577:ILE:CD1	3.06	0.43
1:A:724:GLU:O	1:A:728:LYS:HG2	2.18	0.43
1:A:805:LEU:O	1:A:805:LEU:HG	2.18	0.43
1:A:497:THR:HG21	2:B:1149:GLU:CD	2.38	0.43
2:B:120:ARG:NH2	10:L:54:ARG:HD2	2.33	0.43
2:B:212:LEU:HD21	2:B:461:LEU:HG	1.99	0.43
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.99	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.83	0.43
4:E:198:ILE:CD1	4:E:212:ARG:HG3	2.48	0.43
5:F:93:ILE:CG2	5:F:130:ILE:HD13	2.48	0.43
6:H:18:GLY:O	6:H:20:TYR:N	2.50	0.43
6:H:31:THR:O	6:H:32:THR:CB	2.65	0.43
6:H:89:LEU:C	6:H:91:ASP:H	2.22	0.43
1:A:830:LYS:HG2	1:A:1079:MET:O	2.17	0.43
1:A:917:SER:C	1:A:919:ILE:H	2.21	0.43
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.19	0.43
2:B:384:ARG:HB3	2:B:384:ARG:HE	1.60	0.43
2:B:593:PRO:O	2:B:596:LEU:HB3	2.18	0.43
2:B:597:MET:HG3	2:B:601:ARG:NH1	2.33	0.43
2:B:904:ARG:NH2	2:B:948:ILE:HD11	2.33	0.43
3:C:41:ILE:HG22	3:C:172:PRO:HG3	1.95	0.43
6:H:125:LEU:HB3	6:H:130:ARG:NH1	2.34	0.43
6:H:12:VAL:HG22	6:H:28:ALA:HB2	2.00	0.43
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.82	0.43
1:A:187:LYS:O	1:A:188:ASP:HB2	2.18	0.43
1:A:239:LEU:HD23	1:A:240:PRO:O	2.19	0.43
1:A:664:THR:HA	1:A:668:ASP:OD2	2.19	0.43
1:A:672:ASP:O	1:A:673:GLY:C	2.57	0.43
2:B:620:ARG:NH2	7:I:86:PHE:CB	2.81	0.43
3:C:108:GLU:HG2	3:C:149:LYS:CD	2.49	0.43
3:C:121:VAL:O	3:C:121:VAL:CG1	2.65	0.43
2:B:847:ASP:O	3:C:65:HIS:HE1	2.01	0.43
7:I:50:THR:HB	7:I:92:ARG:NH2	2.34	0.43
1:A:1438:THR:HA	5:F:88:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.00	0.43
1:A:48:ALA:O	1:A:49:LYS:HG3	2.19	0.43
1:A:845:LEU:HB3	1:A:848:ILE:HD12	2.01	0.43
3:C:263:THR:O	3:C:265:MET:N	2.52	0.43
9:K:113:THR:O	9:K:114:LEU:CB	2.67	0.43
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.18	0.43
1:A:541:ILE:N	1:A:541:ILE:HD12	2.33	0.43
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.99	0.43
1:A:974:ASP:HA	6:H:136:LYS:HE2	2.01	0.43
2:B:681:TRP:HE1	2:B:692:TYR:HH	1.64	0.43
2:B:31:TRP:CZ2	2:B:744:HIS:CD2	3.06	0.43
2:B:955:THR:HG22	2:B:956:THR:H	1.83	0.43
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.75	0.43
8:J:14:VAL:HG13	8:J:50:ILE:CD1	2.44	0.43
1:A:387:ARG:O	1:A:391:LEU:HG	2.19	0.43
1:A:741:ASN:ND2	1:A:741:ASN:C	2.72	0.43
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.34	0.43
2:B:120:ARG:HH11	2:B:122:LEU:HD11	1.83	0.43
2:B:336:ARG:HG2	2:B:348:ARG:HD2	2.01	0.43
1:A:483:ASP:HB3	2:B:837:ASP:HB3	2.00	0.43
2:B:1080:LYS:HG3	3:C:180:TYR:CZ	2.54	0.43
3:C:82:TYR:O	3:C:83:SER:C	2.54	0.43
9:K:18:LYS:O	9:K:35:PHE:HA	2.19	0.43
9:K:49:GLU:HG3	9:K:94:ILE:HG13	2.00	0.43
1:A:473:SER:C	1:A:475:THR:H	2.23	0.43
1:A:596:THR:HB	1:A:598:LEU:H	1.83	0.43
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.87	0.43
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.59	0.43
1:A:847:ASP:OD2	1:A:859:SER:OG	2.33	0.43
3:C:115:SER:HB2	3:C:132:PRO:HB3	2.00	0.43
4:E:19:VAL:HG11	4:E:80:VAL:CG1	2.41	0.43
5:F:134:ILE:HD12	5:F:151:LEU:CD1	2.48	0.43
8:J:30:LEU:HD22	8:J:34:THR:HB	2.00	0.43
10:L:49:LYS:O	10:L:50:ASP:HB2	2.19	0.43
1:A:663:SER:OG	1:A:664:THR:N	2.52	0.43
1:A:870:GLU:HG2	4:E:208:TYR:CD2	2.53	0.43
2:B:280:ILE:HA	2:B:281:PRO:HD2	1.87	0.43
2:B:29:ASP:CB	2:B:658:ILE:HD12	2.41	0.43
3:C:56:THR:HG1	3:C:145:CYS:HG	1.65	0.43
4:E:111:VAL:HA	4:E:135:PHE:O	2.19	0.43
4:E:31:THR:C	4:E:33:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:SER:O	5:F:150:GLU:N	2.50	0.43
5:F:77:ASP:O	5:F:78:GLN:HB2	2.19	0.43
6:H:110:ASP:O	6:H:128:ASN:ND2	2.52	0.43
8:J:21:TYR:HB2	8:J:39:LEU:CD1	2.47	0.43
9:K:31:VAL:O	9:K:74:ARG:HA	2.19	0.43
1:A:1293:SER:HB3	1:A:1299:VAL:HG21	2.00	0.42
1:A:493:GLN:HE21	1:A:493:GLN:HA	1.80	0.42
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.48	0.42
1:A:619:LYS:HD2	1:A:750:GLY:HA3	2.00	0.42
1:A:781:ASP:O	1:A:782:ARG:HB3	2.19	0.42
2:B:1010:LEU:HA	2:B:1010:LEU:HD12	1.82	0.42
2:B:1072:MET:HE1	2:B:1087:PHE:CZ	2.54	0.42
2:B:515:HIS:N	2:B:518:HIS:HD2	2.07	0.42
3:C:175:ALA:HB2	8:J:43:ARG:NE	2.33	0.42
9:K:57:LEU:N	9:K:76:GLN:O	2.52	0.42
1:A:1104:ILE:HG22	1:A:1105:LEU:N	2.33	0.42
1:A:1201:ALA:HB1	1:A:1205:LYS:NZ	2.34	0.42
2:B:234:ILE:HG21	2:B:257:LYS:HB3	2.00	0.42
2:B:578:THR:HA	2:B:622:LYS:O	2.18	0.42
2:B:653:VAL:HG13	2:B:689:LEU:HB3	2.00	0.42
2:B:651:LEU:CD1	2:B:707:PRO:HB3	2.39	0.42
2:B:890:TYR:O	2:B:892:LYS:N	2.52	0.42
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.33	0.42
1:A:123:ARG:HH22	1:A:155:GLU:HG2	1.83	0.42
1:A:1137:ALA:HB2	1:A:1274:ARG:HH21	1.84	0.42
1:A:445:ASN:ND2	1:A:455:MET:HG2	2.34	0.42
1:A:619:LYS:O	1:A:620:LYS:C	2.58	0.42
1:A:741:ASN:HD22	1:A:743:VAL:N	2.17	0.42
3:C:56:THR:HG21	3:C:63:ILE:HD11	2.01	0.42
8:J:24:LEU:HD23	8:J:24:LEU:HA	1.83	0.42
1:A:837:ILE:HD12	1:A:1098:VAL:HG13	2.01	0.42
1:A:925:LEU:O	1:A:928:LEU:N	2.52	0.42
1:A:928:LEU:HD11	1:A:984:LYS:HG2	2.00	0.42
1:A:350:ARG:HD2	2:B:1128:LEU:HB2	2.02	0.42
2:B:1182:CYS:HB3	2:B:1187:ASN:HB2	2.01	0.42
2:B:728:ARG:HD2	2:B:730:ARG:HH21	1.84	0.42
5:F:97:ARG:HE	5:F:124:GLU:CD	2.22	0.42
6:H:125:LEU:C	6:H:130:ARG:HH12	2.23	0.42
6:H:80:ARG:HG2	9:K:57:LEU:HD22	2.02	0.42
8:J:48:ARG:O	8:J:52:THR:CB	2.68	0.42
1:A:463:ILE:HD13	1:A:469:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.54	0.42
2:B:104:GLU:HG3	10:L:54:ARG:CZ	2.50	0.42
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.34	0.42
2:B:287:ARG:HG2	2:B:292:ILE:HA	2.01	0.42
3:C:91:HIS:HB2	3:C:96:SER:CB	2.49	0.42
4:E:85:GLU:HA	4:E:86:PRO:HD3	1.85	0.42
7:I:50:THR:HG22	7:I:51:ASN:N	2.35	0.42
1:A:1124:HIS:HB2	1:A:1130:GLN:OE1	2.20	0.42
1:A:1289:ARG:HB3	1:A:1301:GLU:O	2.19	0.42
1:A:1067:LEU:HD23	1:A:1367:HIS:HE1	1.85	0.42
1:A:535:THR:HG21	1:A:616:VAL:CA	2.49	0.42
1:A:566:ILE:O	1:A:567:LYS:O	2.38	0.42
1:A:715:GLU:OE1	1:A:774:ARG:NH1	2.53	0.42
1:A:751:SER:O	1:A:752:LYS:C	2.58	0.42
1:A:782:ARG:NH2	2:B:699:GLU:O	2.52	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:46:GLN:NE2	2:B:496:ARG:HA	2.32	0.42
2:B:515:HIS:HB3	2:B:518:HIS:CD2	2.55	0.42
2:B:558:LEU:HB3	2:B:563:MET:CE	2.49	0.42
2:B:572:HIS:C	2:B:572:HIS:CD2	2.93	0.42
3:C:180:TYR:HD1	3:C:181:ASP:HB2	1.84	0.42
3:C:61:GLU:HB3	10:L:67:PHE:CE2	2.55	0.42
1:A:1199:ARG:O	1:A:1200:ALA:C	2.58	0.42
1:A:1215:ARG:HH11	1:A:1218:GLN:NE2	2.17	0.42
1:A:298:PHE:HE2	1:A:312:PRO:HG3	1.85	0.42
1:A:562:THR:HG23	6:H:79:TRP:HD1	1.85	0.42
1:A:567:LYS:HB3	6:H:95:TYR:CA	2.50	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.42
2:B:973:ILE:O	2:B:974:PRO:C	2.57	0.42
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.99	0.42
4:E:96:PHE:CE2	4:E:100:ILE:HD11	2.53	0.42
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.60	0.42
1:A:365:GLY:O	1:A:468:PHE:HA	2.20	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.89	0.42
2:B:204:ILE:O	2:B:205:ILE:HG12	2.19	0.42
2:B:36:ALA:CB	2:B:661:LEU:HD22	2.50	0.42
2:B:770:GLN:HA	2:B:773:MET:HE2	2.02	0.42
2:B:953:LEU:O	2:B:964:VAL:HA	2.20	0.42
3:C:99:LEU:HD12	3:C:99:LEU:N	2.35	0.42
8:J:16:ASP:OD1	8:J:17:LYS:CG	2.67	0.42
1:A:1080:THR:O	1:A:1081:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:HA	1:A:1169:ILE:CG2	2.43	0.42
1:A:151:ASP:HB3	1:A:161:LEU:HB3	2.02	0.42
1:A:329:LEU:O	1:A:333:GLU:CG	2.68	0.42
1:A:704:ALA:HB2	1:A:710:LEU:CD1	2.44	0.42
1:A:733:ALA:O	1:A:737:LEU:HG	2.20	0.42
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.02	0.42
1:A:975:HIS:H	6:H:136:LYS:HZ1	1.65	0.42
1:A:993:LEU:O	1:A:996:ASN:HB2	2.20	0.42
2:B:899:ILE:HD12	2:B:911:ILE:HA	2.02	0.42
7:I:101:PHE:N	7:I:101:PHE:CD1	2.88	0.42
9:K:103:THR:O	9:K:104:ASN:C	2.58	0.42
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.55	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.20	0.42
2:B:1084:GLN:HE21	3:C:201:TRP:HZ2	1.65	0.42
2:B:314:LEU:O	2:B:315:LYS:C	2.59	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.02	0.42
2:B:890:TYR:CZ	2:B:910:VAL:HG21	2.54	0.42
2:B:770:GLN:HB2	2:B:985:GLY:N	2.35	0.42
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.34	0.42
1:A:1436:ILE:HG13	2:B:1144:ALA:HB2	2.00	0.41
1:A:705:LYS:HB2	1:A:708:MET:HE3	2.02	0.41
2:B:571:PRO:C	2:B:573:GLN:N	2.72	0.41
1:A:994:GLN:HE22	1:A:1023:ARG:HH21	1.68	0.41
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.33	0.41
1:A:741:ASN:ND2	1:A:743:VAL:H	2.18	0.41
2:B:1162:ILE:HD11	2:B:1216:LEU:HD12	2.01	0.41
2:B:185:THR:H	2:B:188:ASP:HB2	1.84	0.41
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.55	0.41
5:F:114:GLU:OE2	5:F:119:ARG:HG2	2.20	0.41
6:H:103:LYS:HZ1	6:H:114:VAL:HB	1.85	0.41
1:A:567:LYS:NZ	6:H:95:TYR:CZ	2.69	0.41
8:J:2:ILE:HG22	8:J:3:VAL:H	1.85	0.41
9:K:65:HIS:HB3	9:K:68:PHE:CD1	2.55	0.41
3:C:169:LYS:HZ2	10:L:69:ALA:HB3	1.85	0.41
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.35	0.41
1:A:451:HIS:CE1	1:A:453:MET:CE	3.03	0.41
1:A:804:TYR:HH	1:A:816:HIS:CE1	2.37	0.41
1:A:842:VAL:O	1:A:843:LYS:C	2.58	0.41
2:B:1072:MET:SD	2:B:1085:ILE:HD12	2.60	0.41
2:B:224:GLN:HB3	2:B:226:PHE:CZ	2.56	0.41
2:B:906:SER:O	2:B:907:GLY:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:128:LYS:NZ	5:F:148:VAL:O	2.48	0.41
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.55	0.41
1:A:216:VAL:O	1:A:220:THR:HB	2.20	0.41
2:B:1167:GLY:N	2:B:1217:TYR:HE2	2.17	0.41
2:B:335:GLY:O	2:B:339:THR:HB	2.21	0.41
2:B:63:ILE:HB	2:B:95:ILE:HD11	2.01	0.41
3:C:56:THR:CG2	3:C:63:ILE:HD11	2.49	0.41
1:A:95:PHE:HB3	1:A:234:MET:SD	2.60	0.41
2:B:1002:THR:HG23	2:B:1004:GLU:HB2	2.01	0.41
2:B:557:PHE:CD2	2:B:557:PHE:C	2.94	0.41
2:B:809:MET:CG	2:B:814:PHE:HB3	2.51	0.41
7:I:61:ASP:O	7:I:64:SER:N	2.49	0.41
8:J:5:VAL:O	8:J:14:VAL:N	2.46	0.41
9:K:5:ASP:HB3	9:K:7:PHE:CE2	2.56	0.41
1:A:21:LEU:HD21	1:A:95:PHE:CZ	2.55	0.41
1:A:32:VAL:CG2	1:A:58:LEU:HD23	2.51	0.41
1:A:834:THR:HG21	1:A:1077:THR:HA	2.02	0.41
1:A:91:PHE:HB3	1:A:96:ILE:HG12	2.02	0.41
2:B:420:LEU:HD13	2:B:453:ILE:HA	2.02	0.41
2:B:842:ASN:HB3	2:B:1009:ASP:HA	2.02	0.41
3:C:243:VAL:O	3:C:244:VAL:C	2.59	0.41
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.02	0.41
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.89	0.41
1:A:849:MET:CE	1:A:1063:MET:SD	3.07	0.41
1:A:1276:VAL:HG11	1:A:1312:ASN:HB3	2.01	0.41
1:A:550:LEU:HD11	1:A:561:PRO:HD2	2.02	0.41
1:A:584:ASN:O	1:A:637:LYS:HE3	2.20	0.41
2:B:654:ARG:H	2:B:657:HIS:CD2	2.38	0.41
2:B:680:THR:HG22	2:B:682:SER:HB2	2.03	0.41
3:C:21:ILE:HD11	3:C:209:TYR:HD2	1.85	0.41
4:E:112:TYR:HE1	4:E:115:ASN:HA	1.82	0.41
4:E:138:ALA:HA	4:E:141:VAL:HG23	2.03	0.41
5:F:124:GLU:HB3	5:F:130:ILE:HG13	2.03	0.41
8:J:28:ASP:N	8:J:28:ASP:OD1	2.54	0.41
1:A:1122:PRO:HD3	1:A:1323:ASP:OD2	2.21	0.41
1:A:1104:ILE:HD11	1:A:1351:GLU:HB3	2.03	0.41
1:A:452:LYS:HB2	1:A:452:LYS:HE2	1.86	0.41
1:A:345:VAL:HA	2:B:1150:ARG:HH12	1.86	0.41
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.03	0.41
9:K:19:LEU:HD21	9:K:35:PHE:CE2	2.56	0.41
1:A:909:ASP:C	1:A:911:SER:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:VAL:HA	2:B:1010:LEU:O	2.21	0.41
2:B:600:LEU:HD23	2:B:600:LEU:HA	1.88	0.41
2:B:779:GLY:O	2:B:795:ILE:HA	2.21	0.41
2:B:786:ASN:O	2:B:967:ARG:NH2	2.54	0.41
2:B:950:ASP:O	2:B:951:GLN:HG3	2.20	0.41
4:E:5:ASN:HD21	4:E:52:ARG:HA	1.86	0.41
5:F:93:ILE:O	5:F:94:LEU:C	2.58	0.41
6:H:15:VAL:HG22	6:H:26:ILE:HG13	2.02	0.41
1:A:852:TYR:HA	1:A:1060:PRO:CG	2.51	0.41
2:B:203:PHE:O	2:B:209:GLU:HA	2.20	0.41
2:B:393:LYS:HA	2:B:393:LYS:HD3	1.71	0.41
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.54	0.41
2:B:546:SER:HA	2:B:634:TYR:HE2	1.85	0.41
4:E:52:ARG:HA	4:E:53:PRO:HD3	1.88	0.41
10:L:30:ILE:HG22	10:L:31:CYS:H	1.83	0.41
1:A:1163:ILE:HA	1:A:1164:PRO:HD2	1.84	0.41
1:A:313:GLN:O	1:A:320:ARG:HA	2.21	0.41
1:A:55:ASP:N	1:A:56:PRO:CD	2.82	0.41
1:A:871:ASP:OD1	1:A:873:MET:HB2	2.21	0.41
2:B:983:ARG:CD	2:B:1091:TYR:HD2	2.34	0.41
2:B:20:ASP:C	2:B:22:SER:H	2.24	0.41
1:A:817:ALA:HB1	2:B:524:PRO:HB2	2.02	0.41
2:B:539:LEU:HD22	2:B:543:SER:HB2	2.03	0.41
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.51	0.41
2:B:786:ASN:OD1	2:B:967:ARG:NH2	2.54	0.41
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.91	0.41
7:I:4:PHE:HE1	7:I:13:MET:CE	2.34	0.41
8:J:6:ARG:HB3	8:J:11:GLY:HA2	2.03	0.41
1:A:249:SER:HB2	1:A:258:GLY:O	2.21	0.40
1:A:367:PRO:HA	1:A:463:ILE:O	2.21	0.40
1:A:582:ILE:HG21	1:A:610:GLY:HA2	2.03	0.40
1:A:840:ARG:HA	1:A:840:ARG:HD3	1.93	0.40
1:A:902:LEU:HD23	1:A:921:GLY:HA2	2.02	0.40
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.21	0.40
2:B:806:THR:CG2	2:B:807:ARG:N	2.84	0.40
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	2.03	0.40
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.20	0.40
5:F:98:ALA:HB2	5:F:118:LEU:HA	2.03	0.40
1:A:1076:ALA:C	1:A:1078:GLN:H	2.25	0.40
1:A:289:ILE:O	1:A:293:GLU:N	2.48	0.40
1:A:35:ILE:HD13	1:A:241:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:HD21	1:A:424:ILE:HD12	2.03	0.40
1:A:460:VAL:HG12	1:A:461:LYS:N	2.37	0.40
1:A:531:ILE:CD1	1:A:578:LEU:HD21	2.47	0.40
1:A:858:ASN:HD22	1:A:861:GLY:H	1.68	0.40
2:B:1002:THR:O	2:B:1003:ALA:C	2.60	0.40
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.42	0.40
2:B:173:MET:HE1	2:B:409:ALA:HB2	2.02	0.40
2:B:408:LEU:CD2	2:B:409:ALA:H	2.30	0.40
2:B:519:TRP:CD1	2:B:519:TRP:C	2.95	0.40
3:C:250:THR:O	3:C:254:LYS:HG3	2.21	0.40
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.51	0.40
1:A:767:GLN:HG3	1:A:768:GLN:O	2.21	0.40
1:A:846:GLU:OE1	2:B:1135:ARG:NH2	2.52	0.40
1:A:879:GLU:O	1:A:955:PRO:HA	2.22	0.40
2:B:120:ARG:HB3	2:B:122:LEU:HG	2.01	0.40
2:B:830:TYR:CE1	2:B:1000:PRO:HB3	2.56	0.40
2:B:901:PRO:HD2	10:L:59:ALA:O	2.21	0.40
1:A:1327:ILE:O	4:E:147:HIS:HE1	2.04	0.40
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.99	0.40
6:H:12:VAL:CG1	6:H:26:ILE:HG23	2.48	0.40
8:J:57:ILE:O	8:J:60:PHE:N	2.52	0.40
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.56	0.40
1:A:1424:VAL:HG21	2:B:1139:ILE:HG12	2.02	0.40
1:A:170:THR:HG21	1:A:186:LYS:O	2.21	0.40
1:A:359:LEU:HB3	1:A:363:GLN:HB2	2.03	0.40
2:B:892:LYS:HD2	2:B:909:ASP:OD2	2.22	0.40
6:H:104:PHE:O	6:H:106:GLU:N	2.54	0.40
1:A:858:ASN:ND2	1:A:861:GLY:H	2.19	0.40
2:B:1098:MET:O	2:B:1099:VAL:C	2.60	0.40
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.21	0.40
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.42	0.40
1:A:1433:MET:HE3	2:B:1145:SER:N	2.36	0.40
2:B:1210:MET:O	2:B:1212:ILE:HG13	2.21	0.40
2:B:701:ILE:HB	2:B:739:THR:HG1	1.87	0.40
3:C:8:VAL:HG23	9:K:101:LEU:HD23	2.04	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	1411/1733 (81%)	1182 (84%)	174 (12%)	55 (4%)	3	28
2	B	1074/1224 (88%)	924 (86%)	122 (11%)	28 (3%)	6	38
3	C	264/318 (83%)	221 (84%)	34 (13%)	9 (3%)	4	32
4	E	213/215 (99%)	179 (84%)	30 (14%)	4 (2%)	9	45
5	F	82/155 (53%)	68 (83%)	11 (13%)	3 (4%)	4	30
6	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	1	8
7	I	120/122 (98%)	96 (80%)	21 (18%)	3 (2%)	6	39
8	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	5	34
9	K	112/120 (93%)	92 (82%)	14 (12%)	6 (5%)	2	19
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0	2
All	All	3512/4173 (84%)	2935 (84%)	448 (13%)	129 (4%)	4	30

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	415	LEU
1	A	464	PRO
1	A	567	LYS
1	A	752	LYS
1	A	1223	ASP
1	A	1386	ARG
1	A	1393	ASN
3	C	90	ASP
3	C	231	ASN
6	H	18	GLY
6	H	32	THR

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Mol	Chain	Res	Type
10	L	39	SER
10	L	59	ALA
10	L	64	LEU
1	A	188	ASP
1	A	226	GLU
1	A	601	LYS
1	A	628	GLY
1	A	736	ASN
1	A	915	SER
1	A	958	VAL
1	A	1063	MET
1	A	1127	ASP
1	A	1165	GLU
1	A	1200	ALA
1	A	1360	GLY
1	A	1385	THR
1	A	1391	ARG
1	A	1392	SER
1	A	1399	ARG
1	A	1400	CYS
2	B	165	VAL
2	B	266	ALA
2	B	864	LYS
2	B	884	ARG
2	B	891	ASP
2	B	1099	VAL
3	C	4	GLU
3	C	19	ASP
3	C	88	CYS
4	E	3	GLN
4	E	59	SER
4	E	137	GLU
5	F	112	GLU
6	H	19	ARG
6	H	81	PRO
6	H	88	SER
6	H	103	LYS
6	H	105	GLU
6	H	128	ASN
8	J	29	GLU
9	K	8	GLU
1	A	45	GLN

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Mol	Chain	Res	Type
1	A	67	CYS
1	A	408	ASP
1	A	409	SER
1	A	517	ASN
1	A	737	LEU
1	A	926	GLN
2	B	304	ASP
6	H	82	PRO
6	H	138	GLU
9	K	103	THR
9	K	104	ASN
10	L	56	LEU
1	A	56	PRO
1	A	196	GLU
1	A	451	HIS
1	A	466	SER
1	A	467	THR
1	A	777	PHE
1	A	904	THR
2	B	249	ARG
2	B	383	ASN
2	B	907	GLY
2	B	1222	ARG
3	C	168	ALA
3	C	241	ASP
4	E	5	ASN
6	H	61	SER
8	J	41	LEU
9	K	107	THR
10	L	38	LEU
1	A	35	ILE
1	A	79	GLY
1	A	154	SER
1	A	673	GLY
1	A	700	ASN
1	A	986	ILE
2	B	90	ILE
2	B	303	TYR
2	B	307	ASP
2	B	367	LEU
2	B	369	GLY
2	B	541	LEU

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Mol	Chain	Res	Type
2	B	648	HIS
2	B	708	GLU
2	B	879	ARG
2	B	883	LEU
2	B	1104	HIS
2	B	1167	GLY
3	C	264	GLN
5	F	73	ALA
6	H	139	ASN
7	I	9	ASP
7	I	76	PRO
10	L	54	ARG
1	A	253	ASN
1	A	599	SER
2	B	711	GLU
3	C	240	VAL
7	I	39	GLY
9	K	93	SER
10	L	52	GLY
1	A	955	PRO
2	B	743	ILE
1	A	51	GLY
1	A	308	ILE
2	B	901	PRO
5	F	93	ILE
9	K	43	GLY
1	A	178	GLY
1	A	399	HIS
1	A	910	PRO
2	B	1214	PRO
2	B	571	PRO

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1239/1520 (82%)	1108 (89%)	131 (11%)	8 33
2	B	950/1061 (90%)	867 (91%)	83 (9%)	12 43
3	C	234/274 (85%)	208 (89%)	26 (11%)	7 31
4	E	197/197 (100%)	188 (95%)	9 (5%)	31 68
5	F	74/137 (54%)	68 (92%)	6 (8%)	14 47
6	H	117/128 (91%)	115 (98%)	2 (2%)	66 86
7	I	116/116 (100%)	108 (93%)	8 (7%)	18 55
8	J	60/65 (92%)	49 (82%)	11 (18%)	2 9
9	K	99/102 (97%)	88 (89%)	11 (11%)	7 31
10	L	40/57 (70%)	34 (85%)	6 (15%)	3 18
All	All	3126/3657 (86%)	2833 (91%)	293 (9%)	10 39

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	44	THR
1	A	61	ILE
1	A	69	THR
1	A	70	CYS
1	A	71	GLN
1	A	84	ILE
1	A	92	HIS
1	A	93	VAL
1	A	106	VAL
1	A	117	GLU
1	A	140	THR
1	A	146	MET
1	A	157	ASP
1	A	159	THR
1	A	162	VAL
1	A	200	ARG
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR

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Mol	Chain	Res	Type
1	A	232	GLU
1	A	247	ARG
1	A	250	ILE
1	A	266	LEU
1	A	268	ASP
1	A	291	GLU
1	A	308	ILE
1	A	316	GLN
1	A	345	VAL
1	A	351	THR
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	389	THR
1	A	425	GLN
1	A	434	ARG
1	A	437	MET
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	461	LYS
1	A	463	ILE
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	493	GLN
1	A	496	GLU
1	A	497	THR
1	A	503	GLN
1	A	504	LEU
1	A	513	SER
1	A	515	GLN
1	A	524	VAL
1	A	535	THR
1	A	543	LEU
1	A	544	ASP
1	A	567	LYS
1	A	577	ILE
1	A	596	THR
1	A	597	LEU

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Mol	Chain	Res	Type
1	A	612	ILE
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	666	ILE
1	A	677	ARG
1	A	702	LEU
1	A	709	THR
1	A	740	LEU
1	A	741	ASN
1	A	756	ILE
1	A	774	ARG
1	A	821	ARG
1	A	822	GLU
1	A	824	LEU
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	855	THR
1	A	858	ASN
1	A	873	MET
1	A	885	THR
1	A	903	ASN
1	A	913	LEU
1	A	919	ILE
1	A	920	LEU
1	A	988	LEU
1	A	1006	ILE
1	A	1030	ARG
1	A	1043	ASP
1	A	1064	VAL
1	A	1095	THR
1	A	1118	VAL
1	A	1133	LEU
1	A	1141	THR
1	A	1146	VAL
1	A	1169	ILE
1	A	1204	ASP
1	A	1233	ASP
1	A	1237	ILE
1	A	1240	CYS

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Mol	Chain	Res	Type
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1359	ASP
1	A	1361	SER
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1382	THR
1	A	1383	SER
1	A	1385	THR
1	A	1387	HIS
1	A	1399	ARG
1	A	1417	GLU
1	A	1419	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1449	SER
2	B	18	PHE
2	B	19	GLU
2	B	20	ASP
2	B	22	SER
2	B	40	GLU
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	98	THR
2	B	102	VAL
2	B	136	THR
2	B	170	LEU
2	B	179	CYS
2	B	183	GLU
2	B	194	GLU
2	B	199	MET
2	B	208	SER

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Mol	Chain	Res	Type
2	B	217	ARG
2	B	261	ARG
2	B	277	LYS
2	B	291	ILE
2	B	337	ARG
2	B	339	THR
2	B	365	THR
2	B	367	LEU
2	B	370	PHE
2	B	408	LEU
2	B	424	LEU
2	B	455	SER
2	B	466	TRP
2	B	485	ARG
2	B	487	THR
2	B	496	ARG
2	B	498	THR
2	B	513	GLN
2	B	531	GLN
2	B	540	SER
2	B	543	SER
2	B	547	VAL
2	B	556	THR
2	B	572	HIS
2	B	579	ARG
2	B	592	ASN
2	B	599	THR
2	B	615	MET
2	B	619	ILE
2	B	628	THR
2	B	646	LEU
2	B	648	HIS
2	B	653	VAL
2	B	691	GLU
2	B	706	GLN
2	B	737	THR
2	B	741	CYS
2	B	783	THR
2	B	790	ASP
2	B	801	LYS
2	B	831	SER
2	B	857	ARG

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Mol	Chain	Res	Type
2	B	864	LYS
2	B	873	THR
2	B	889	THR
2	B	915	THR
2	B	946	ASN
2	B	955	THR
2	B	971	THR
2	B	996	ARG
2	B	999	MET
2	B	1019	SER
2	B	1045	SER
2	B	1049	ASP
2	B	1060	ARG
2	B	1087	PHE
2	B	1099	VAL
2	B	1101	ASP
2	B	1150	ARG
2	B	1152	MET
2	B	1153	GLU
2	B	1159	ARG
2	B	1169	MET
2	B	1193	GLN
2	B	1218	THR
2	B	1219	ASP
3	C	3	GLU
3	C	9	LYS
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	55	THR
3	C	69	LEU
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	136	ASP
3	C	154	LYS
3	C	156	THR
3	C	178	PHE
3	C	189	THR

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Mol	Chain	Res	Type
3	C	203	GLN
3	C	209	TYR
3	C	211	ASP
3	C	215	GLU
3	C	240	VAL
3	C	260	LEU
3	C	264	GLN
3	C	266	ASP
4	E	8	ASN
4	E	47	CYS
4	E	87	SER
4	E	92	THR
4	E	99	HIS
4	E	116	ILE
4	E	123	LEU
4	E	149	LEU
4	E	196	VAL
5	F	79	ARG
5	F	82	THR
5	F	110	ASP
5	F	111	LEU
5	F	140	ASP
5	F	149	GLU
6	H	7	ASP
6	H	62	SER
7	I	7	CYS
7	I	17	ARG
7	I	24	ARG
7	I	35	VAL
7	I	50	THR
7	I	52	ILE
7	I	55	THR
7	I	84	VAL
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	12	LYS
8	J	19	GLU
8	J	20	SER
8	J	22	LEU
8	J	28	ASP

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Mol	Chain	Res	Type
8	J	34	THR
8	J	48	ARG
9	K	11	LEU
9	K	14	GLU
9	K	25	THR
9	K	39	ASP
9	K	47	ARG
9	K	63	VAL
9	K	66	PRO
9	K	73	LEU
9	K	81	TYR
9	K	101	LEU
9	K	113	THR
10	L	27	LEU
10	L	42	ARG
10	L	50	ASP
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	313	GLN
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	548	ASN
1	A	587	HIS
1	A	631	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	768	GLN
1	A	858	ASN
1	A	862	ASN

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Mol	Chain	Res	Type
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	966	ASN
1	A	994	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1140	HIS
1	A	1173	HIS
1	A	1218	GLN
1	A	1265	ASN
1	A	1364	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	53	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	300	HIS
2	B	325	GLN
2	B	383	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	590	HIS
2	B	648	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	881	ASN
2	B	958	GLN
2	B	986	GLN
2	B	1065	GLN
2	B	1084	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	17	ASN
3	C	24	ASN
3	C	31	ASN
3	C	65	HIS
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	102	GLN
3	C	112	ASN
3	C	167	HIS
3	C	203	GLN
3	C	242	GLN
4	E	5	ASN
4	E	101	GLN
4	E	113	GLN
4	E	147	HIS
6	H	11	GLN
6	H	128	ASN
7	I	12	ASN
7	I	46	HIS
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN
10	L	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1419/1733 (81%)	0.40	119 (8%)	12 12	41, 79, 162, 188	0
2	B	1094/1224 (89%)	0.39	98 (8%)	10 11	47, 80, 140, 167	0
3	C	266/318 (83%)	0.13	6 (2%)	61 56	58, 78, 111, 133	0
4	E	215/215 (100%)	0.20	9 (4%)	37 34	51, 98, 130, 145	0
5	F	84/155 (54%)	0.20	4 (4%)	31 28	52, 71, 92, 98	0
6	H	133/146 (91%)	1.02	27 (20%)	1 1	103, 119, 147, 149	0
7	I	122/122 (100%)	1.07	26 (21%)	1 1	75, 107, 129, 150	0
8	J	65/70 (92%)	-0.05	0	100 100	58, 70, 91, 94	0
9	K	114/120 (95%)	0.33	6 (5%)	27 25	58, 85, 107, 126	0
10	L	46/70 (65%)	0.76	5 (10%)	6 7	87, 137, 144, 145	0
All	All	3558/4173 (85%)	0.40	300 (8%)	12 12	41, 82, 146, 188	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1110	PRO	9.7
1	A	1390	ASN	9.1
1	A	323	LYS	9.0
1	A	188	ASP	8.2
2	B	919	SER	8.1
2	B	733	HIS	8.1
2	B	1104	HIS	8.1
2	B	1105	ALA	7.8
6	H	131	ASN	7.8
1	A	189	ARG	7.7
2	B	1109	GLY	7.1
1	A	255	SER	7.1
1	A	318	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	6.9
1	A	341	MET	6.7
2	B	247	GLY	6.7
2	B	248	SER	6.7
1	A	1446	ASP	6.7
1	A	253	ASN	6.4
2	B	726	ALA	6.3
1	A	312	PRO	6.3
1	A	69	THR	6.3
1	A	1175	SER	6.2
4	E	1	MET	6.1
1	A	248	PRO	6.0
2	B	90	ILE	5.9
2	B	1103	ILE	5.9
2	B	725	PRO	5.8
2	B	722	ASP	5.7
2	B	732	SER	5.7
2	B	1106	ARG	5.5
1	A	314	ALA	5.4
10	L	50	ASP	5.4
2	B	882	THR	5.4
2	B	918	ILE	5.3
1	A	319	GLY	5.3
1	A	249	SER	5.3
1	A	44	THR	5.3
3	C	268	ASP	5.2
2	B	136	THR	5.1
6	H	127	GLY	5.1
1	A	1402	PHE	5.1
2	B	915	THR	4.9
1	A	251	SER	4.9
1	A	1387	HIS	4.9
10	L	25	ALA	4.9
2	B	1223	ASP	4.8
2	B	435	THR	4.8
2	B	89	GLU	4.8
1	A	1449	SER	4.8
1	A	1389	PHE	4.8
1	A	40	THR	4.8
1	A	322	VAL	4.8
6	H	139	ASN	4.7
10	L	26	THR	4.6

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Mol	Chain	Res	Type	RSRZ
6	H	111	LEU	4.5
1	A	316	GLN	4.5
2	B	734	HIS	4.5
1	A	321	PRO	4.5
1	A	1188	GLN	4.4
2	B	69	LEU	4.4
2	B	66	ASP	4.4
7	I	111	THR	4.4
1	A	315	LEU	4.4
7	I	76	PRO	4.3
2	B	916	THR	4.2
2	B	935	ARG	4.2
1	A	62	ASP	4.2
2	B	936	ASP	4.2
1	A	343	LYS	4.2
2	B	727	LYS	4.1
1	A	252	PHE	4.1
9	K	1	MET	4.1
2	B	1188	LYS	4.1
6	H	132	LEU	4.1
1	A	342	GLY	4.1
1	A	1388	GLY	4.1
6	H	134	ASN	4.0
1	A	1448	GLU	4.0
7	I	101	PHE	4.0
7	I	121	PHE	4.0
1	A	171	GLN	3.9
6	H	83	GLN	3.9
1	A	330	LYS	3.9
1	A	38	PRO	3.9
1	A	193	ASP	3.9
2	B	883	LEU	3.8
2	B	1189	ILE	3.8
1	A	3	GLY	3.8
1	A	1092	LYS	3.8
7	I	110	PHE	3.8
7	I	55	THR	3.8
1	A	186	LYS	3.7
9	K	2	ASN	3.7
2	B	134	LYS	3.7
2	B	871	THR	3.7
2	B	1176	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	1101	ASP	3.7
2	B	1193	GLN	3.7
2	B	246	LYS	3.7
1	A	340	LEU	3.7
1	A	1176	LEU	3.7
2	B	428	ILE	3.7
1	A	45	GLN	3.7
2	B	92	PHE	3.6
2	B	729	ILE	3.6
7	I	74	GLU	3.6
2	B	724	ASP	3.6
2	B	1180	PHE	3.6
2	B	436	VAL	3.5
10	L	27	LEU	3.5
2	B	1100	ASP	3.5
7	I	82	GLU	3.5
2	B	885	MET	3.5
1	A	42	ASP	3.5
7	I	118	ARG	3.5
7	I	54	GLU	3.5
1	A	75	ASN	3.5
2	B	1224	PHE	3.5
6	H	35	GLN	3.5
9	K	17	SER	3.5
1	A	39	GLU	3.4
7	I	114	GLN	3.4
2	B	866	TYR	3.4
1	A	194	ALA	3.4
2	B	933	SER	3.4
7	I	116	ASN	3.4
2	B	137	TYR	3.4
4	E	51	GLY	3.4
2	B	870	ILE	3.4
2	B	1098	MET	3.3
1	A	63	ARG	3.3
7	I	94	ASP	3.3
1	A	191	THR	3.3
2	B	432	MET	3.3
6	H	126	GLU	3.3
2	B	1191	ILE	3.3
1	A	332	LYS	3.3
6	H	112	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
7	I	112	SER	3.3
1	A	185	TRP	3.2
7	I	120	GLN	3.2
1	A	190	ALA	3.2
2	B	917	PRO	3.2
1	A	41	MET	3.2
2	B	868	MET	3.2
2	B	132	VAL	3.2
2	B	888	GLY	3.2
1	A	6	TYR	3.2
1	A	68	GLN	3.2
2	B	884	ARG	3.1
1	A	1391	ARG	3.1
2	B	70	ILE	3.1
2	B	437	GLU	3.1
5	F	72	LYS	3.1
1	A	2	VAL	3.0
1	A	256	GLN	3.0
1	A	313	GLN	3.0
2	B	1107	ALA	3.0
2	B	1178	ASN	3.0
2	B	1179	GLN	3.0
4	E	57	MET	3.0
1	A	54	ASN	3.0
1	A	278	THR	3.0
1	A	1394	THR	3.0
1	A	1216	ILE	3.0
2	B	723	VAL	3.0
1	A	46	THR	3.0
6	H	110	ASP	2.9
2	B	1171	VAL	2.9
6	H	136	LYS	2.9
3	C	216	GLY	2.9
4	E	2	ASP	2.9
1	A	1393	ASN	2.9
2	B	939	THR	2.9
1	A	311	GLN	2.9
2	B	869	SER	2.9
2	B	1128	LEU	2.9
1	A	413	ILE	2.8
1	A	247	ARG	2.8
1	A	258	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	187	LYS	2.8
6	H	84	ALA	2.8
1	A	1271	ILE	2.8
2	B	875	GLU	2.8
2	B	1108	ARG	2.8
1	A	47	ARG	2.7
1	A	257	ARG	2.7
2	B	1175	LEU	2.7
1	A	48	ALA	2.7
6	H	59	ILE	2.7
4	E	54	GLN	2.7
2	B	1219	ASP	2.7
1	A	66	LYS	2.7
3	C	215	GLU	2.7
6	H	146	ARG	2.7
2	B	643	ASP	2.7
2	B	1173	ALA	2.7
2	B	887	HIS	2.7
7	I	119	THR	2.6
1	A	1401	SER	2.6
6	H	128	ASN	2.6
4	E	50	MET	2.6
2	B	68	THR	2.6
7	I	93	LYS	2.6
2	B	728	ARG	2.6
1	A	1392	SER	2.6
2	B	96	TYR	2.6
1	A	115	LEU	2.6
7	I	1	MET	2.6
1	A	259	GLU	2.5
2	B	943	SER	2.5
2	B	129	PHE	2.5
2	B	429	PHE	2.5
7	I	83	ASN	2.5
9	K	79	GLU	2.5
5	F	108	PHE	2.5
1	A	1395	GLY	2.5
1	A	424	ILE	2.5
2	B	730	ARG	2.5
1	A	158	PRO	2.5
2	B	531	GLN	2.5
2	B	465	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
4	E	53	PRO	2.5
1	A	1301	GLU	2.5
1	A	1398	MET	2.5
2	B	25	ILE	2.5
2	B	1172	ILE	2.5
1	A	57	ARG	2.4
6	H	108	SER	2.4
1	A	1080	THR	2.4
4	E	90	VAL	2.4
1	A	1450	LEU	2.4
7	I	53	GLY	2.4
2	B	1181	GLU	2.4
9	K	80	GLY	2.4
1	A	199	LEU	2.4
1	A	37	PHE	2.4
1	A	43	GLU	2.4
2	B	245	GLU	2.4
1	A	114	LEU	2.4
4	E	94	LYS	2.4
6	H	140	ALA	2.4
1	A	260	ASP	2.4
6	H	60	ALA	2.4
1	A	71	GLN	2.4
1	A	405	VAL	2.3
1	A	1242	VAL	2.3
3	C	106	GLU	2.3
1	A	4	GLN	2.3
1	A	1396	ALA	2.3
2	B	178	ASN	2.3
6	H	6	PHE	2.3
1	A	161	LEU	2.3
1	A	426	LEU	2.3
7	I	56	ALA	2.3
2	B	908	GLU	2.3
3	C	108	GLU	2.3
1	A	65	LEU	2.3
2	B	135	ARG	2.3
1	A	392	VAL	2.2
1	A	149	GLU	2.2
1	A	421	ALA	2.2
1	A	834	THR	2.2
7	I	75	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
9	K	57	LEU	2.2
10	L	33	GLU	2.2
1	A	320	ARG	2.2
7	I	109	ILE	2.2
1	A	72	GLU	2.2
1	A	200	ARG	2.2
1	A	317	LYS	2.2
6	H	113	ALA	2.2
1	A	7	SER	2.2
1	A	202	LEU	2.2
6	H	82	PRO	2.1
1	A	192	GLY	2.1
5	F	111	LEU	2.1
6	H	58	THR	2.1
7	I	79	HIS	2.1
2	B	648	HIS	2.1
7	I	85	PHE	2.1
3	C	79	GLN	2.1
7	I	72	ASP	2.1
2	B	425	THR	2.1
1	A	157	ASP	2.1
1	A	1257	ASP	2.1
1	A	328	ARG	2.1
1	A	305	ASP	2.1
2	B	679	TYR	2.1
5	F	107	VAL	2.1
2	B	188	ASP	2.1
6	H	130	ARG	2.1
6	H	85	GLY	2.1
6	H	104	PHE	2.0
2	B	1190	ASP	2.0
2	B	138	GLU	2.0
6	H	88	SER	2.0
1	A	282	ASN	2.0
1	A	1219	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	ZN	L	3005	1/1	0.92	0.06	-1.29	128,128,128,128	0
11	ZN	I	3003	1/1	0.99	0.08	-1.44	97,97,97,97	0
11	ZN	A	3008	1/1	0.97	0.07	-1.67	143,143,143,143	0
11	ZN	J	3001	1/1	1.00	0.13	-1.79	68,68,68,68	0
11	ZN	C	3002	1/1	0.99	0.04	-1.82	79,79,79,79	0
11	ZN	B	3007	1/1	0.97	0.04	-1.99	87,87,87,87	0
11	ZN	I	3004	1/1	0.99	0.12	-2.10	117,117,117,117	0
11	ZN	A	3006	1/1	0.98	0.04	-3.03	95,95,95,95	0
12	MN	A	3010	1/1	0.83	0.11	-	50,50,50,50	0
12	MN	A	3009	1/1	0.95	0.15	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.