



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 AM GMT

PDB ID : 2WB1  
Title : The complete structure of the archaeal 13-subunit DNA-directed RNA Polymerase  
Authors : Korkhin, Y.; Unligil, U.M.; Littlefield, O.; Nelson, P.J.; Stuart, D.I.; Sigler, P.B.; Bell, S.D.; Abrescia, N.G.A.  
Deposited on : 2009-02-19  
Resolution : 3.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

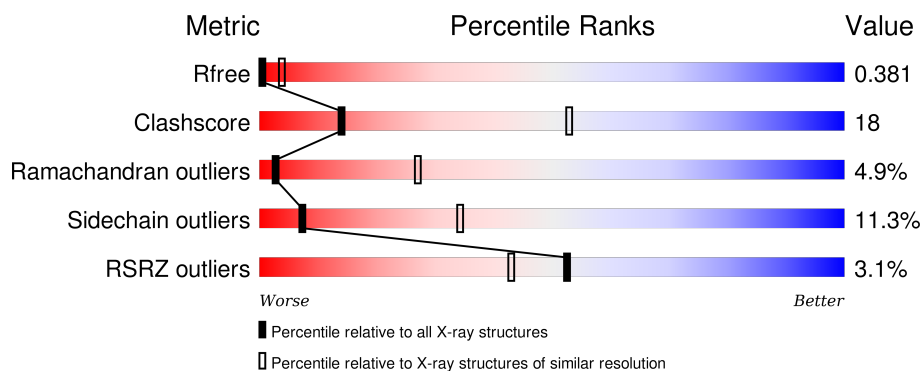
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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))
$R_{free}$	91344	1089 (3.64-3.40)
Clashscore	102246	1197 (3.64-3.40)
Ramachandran outliers	100387	1159 (3.64-3.40)
Sidechain outliers	100360	1160 (3.64-3.40)
RSRZ outliers	91569	1096 (3.64-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	880	<div> <div>2%</div> <div>52% 36% 7% .</div> </div>
1	W	880	<div> <div>2%</div> <div>51% 37% 7% . .</div> </div>
2	B	1131	<div> <div>2%</div> <div>52% 37% 7% . .</div> </div>
2	R	1131	<div> <div>2%</div> <div>51% 37% 7% . .</div> </div>
3	C	395	<div> <div>4%</div> <div>47% 39% 6% . 7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	395	
4	D	265	
4	S	265	
5	E	180	
5	T	180	
6	F	113	
6	U	113	
7	G	132	
7	V	132	
8	H	84	
8	Z	84	
9	I	95	
9	K	95	
10	J	104	
10	Q	104	
11	L	92	
11	M	92	
12	N	66	
12	O	66	
13	P	48	
13	X	48	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 52739 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 RPO1N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			
1	W	841	Total	C	N	O	S	0	0	0
			6691	4256	1183	1226	26			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			
2	R	1090	Total	C	N	O	S	0	0	0
			8652	5484	1534	1605	29			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			
3	Y	367	Total	C	N	O	S	0	0	0
			2833	1797	481	547	8			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			
4	S	260	Total	C	N	O	S	0	0	0
			2071	1332	334	392	13			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			
5	T	174	Total	C	N	O	S	0	0	0
			1384	893	232	255	4			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	0	1
			702	439	115	145	3			
6	U	91	Total	C	N	O	S	0	0	1
			702	439	115	145	3			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			
7	V	113	Total	C	N	O	S	0	0	0
			901	572	152	173	4			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O		0	0	0
			609	396	108	105				
8	Z	74	Total	C	N	O		0	0	0
			609	396	108	105				

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	35	Total	C	N	O		0	0	0
			301	186	53	62				

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	Q	33	Total	C	N	O	S	0	0	1
			274	172	45	56	1			

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	92	Total	C	N	O	S	0	0	1
			708	454	115	137	2			
11	M	92	Total	C	N	O	S	0	0	1
			708	454	115	137	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			
12	O	64	Total	C	N	O	S	0	0	0
			514	327	93	87	7			

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
13	X	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	P	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	W	2	Total	Zn	0	0
			2	2		
14	A	2	Total	Zn	0	0
			2	2		
14	N	1	Total	Zn	0	0
			1	1		
14	X	1	Total	Zn	0	0
			1	1		

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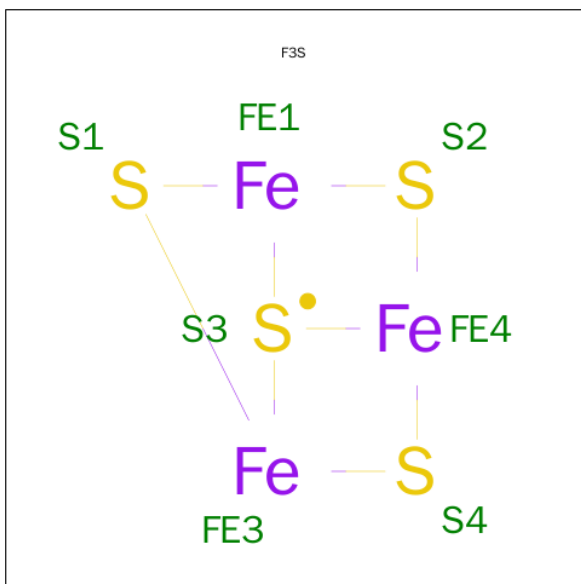
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	O	1	Total	Zn	0	0
			1	1		
14	R	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	W	1	Total	Mg	0	0
			1	1		
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).

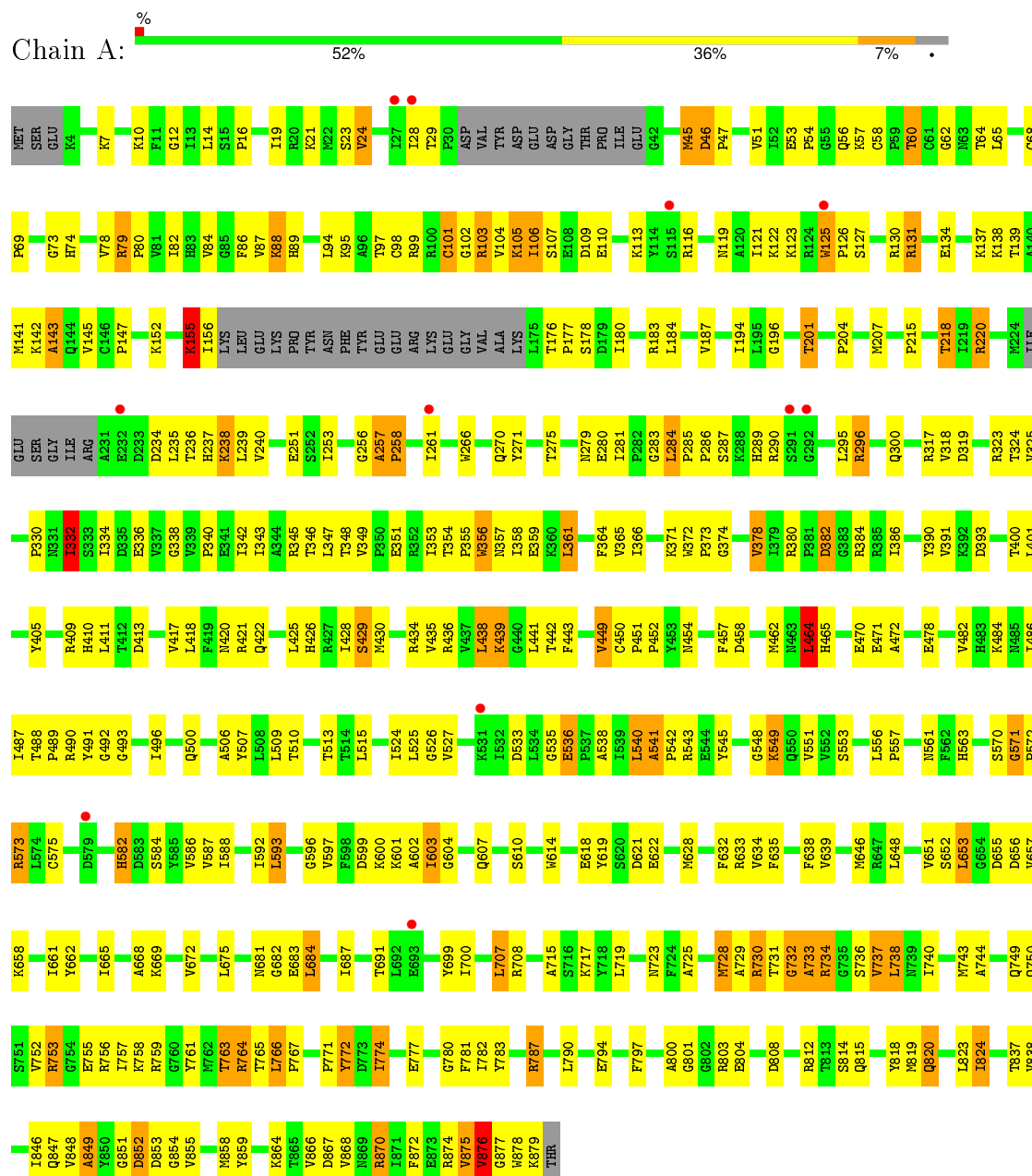


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			7	3	4		
16	S	1	Total	Fe	S	0	0
			7	3	4		

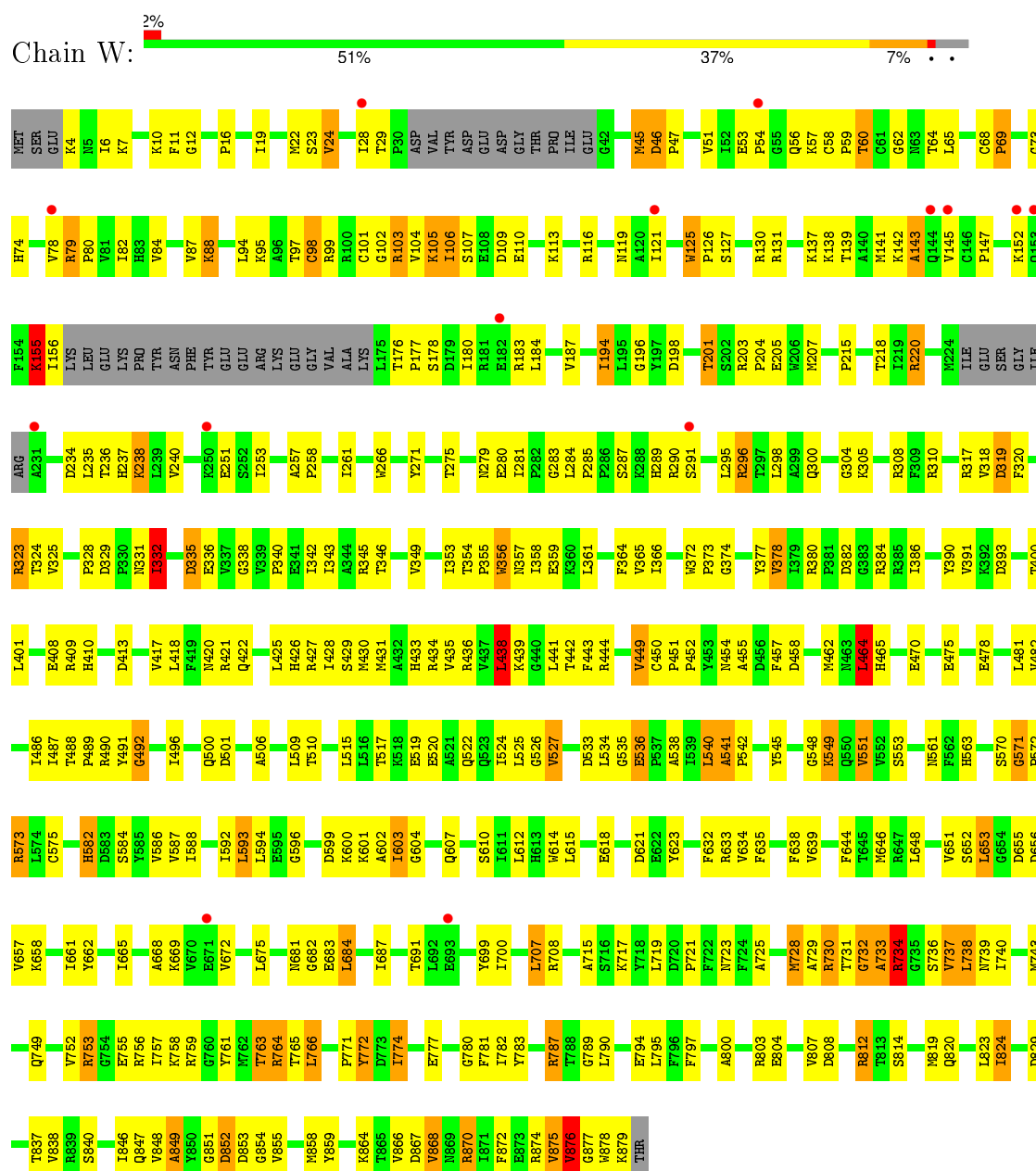
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

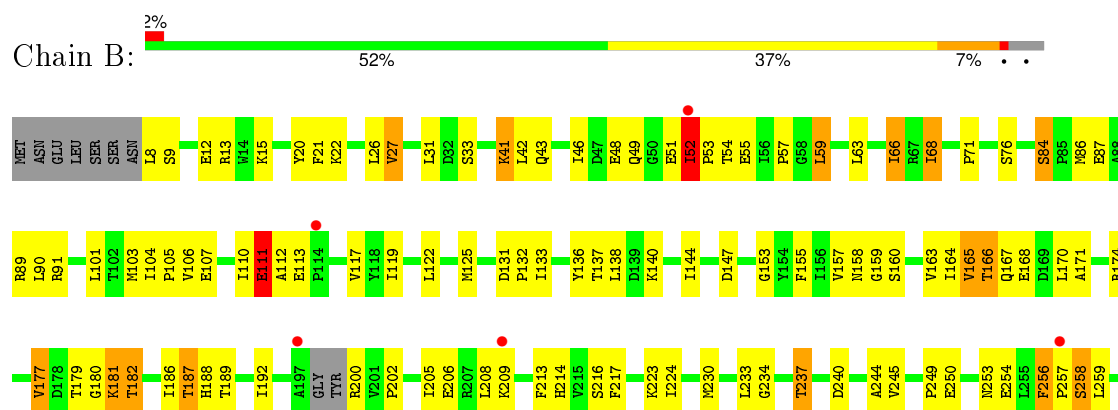
#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE RPO1N SUBUNIT





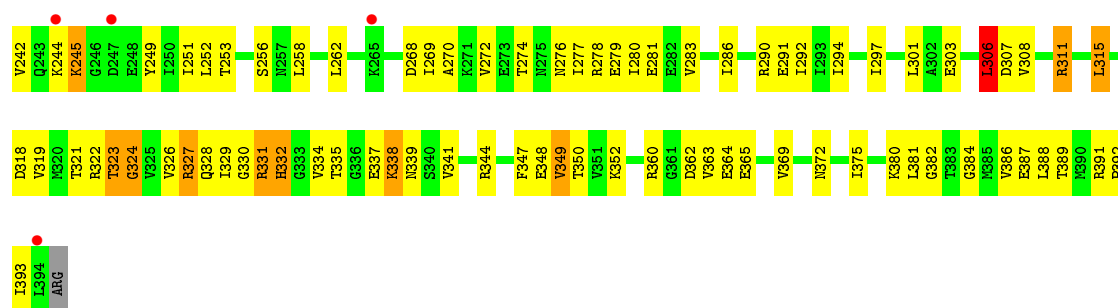


• Molecule 2: DNA-DIRECTED RNA POLYMERASE RPO2 SUBUNIT

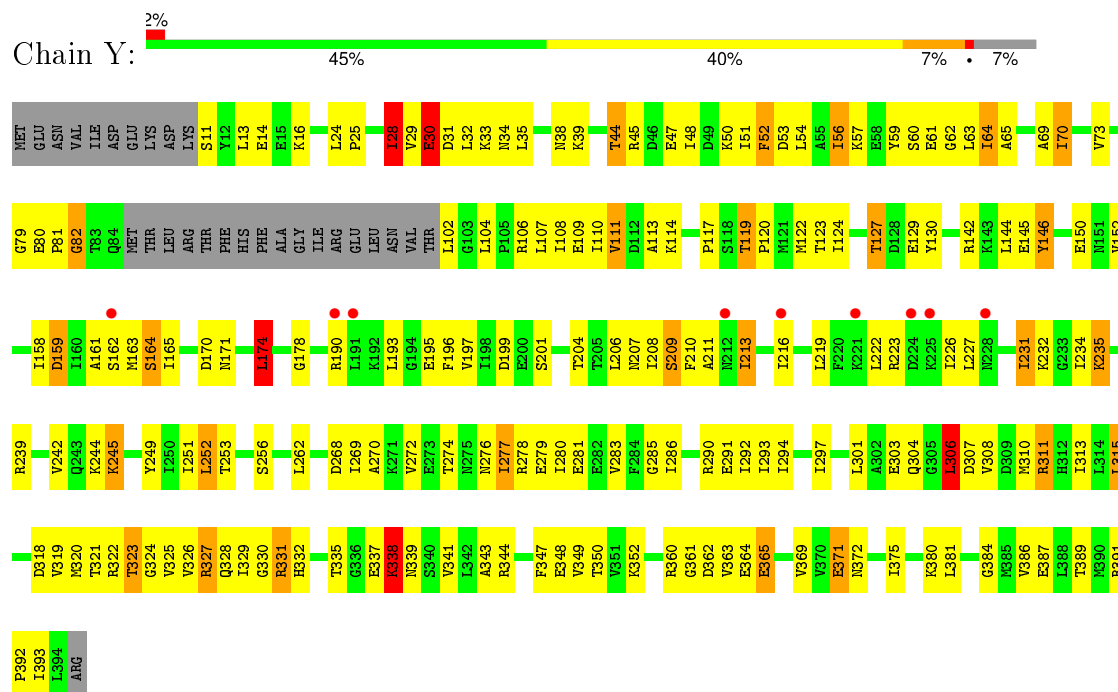




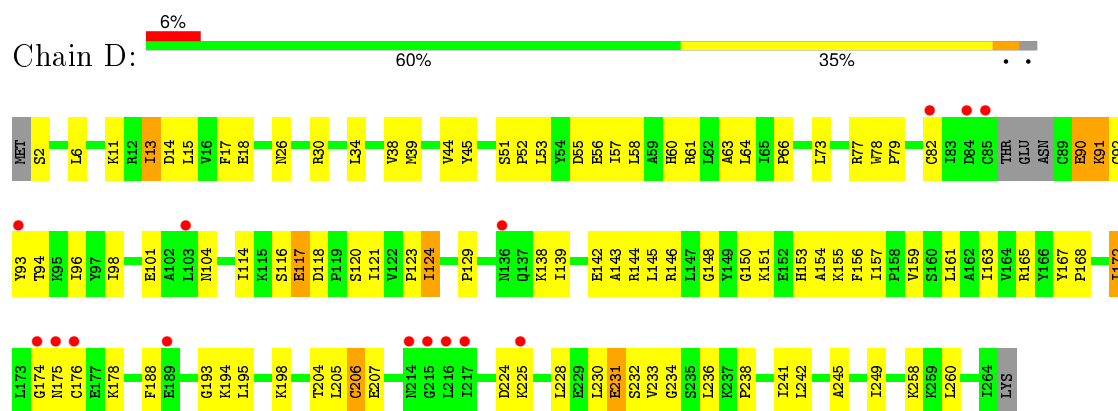




• Molecule 3: DNA-DIRECTED RNA POLYMERASE RPO1C SUBUNIT

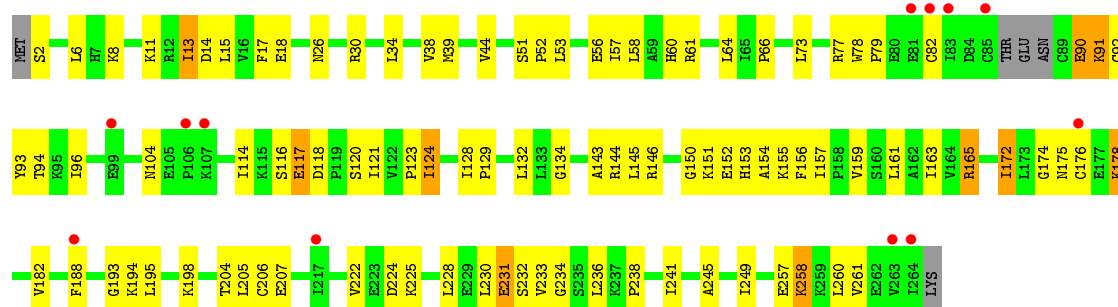


• Molecule 4: DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT

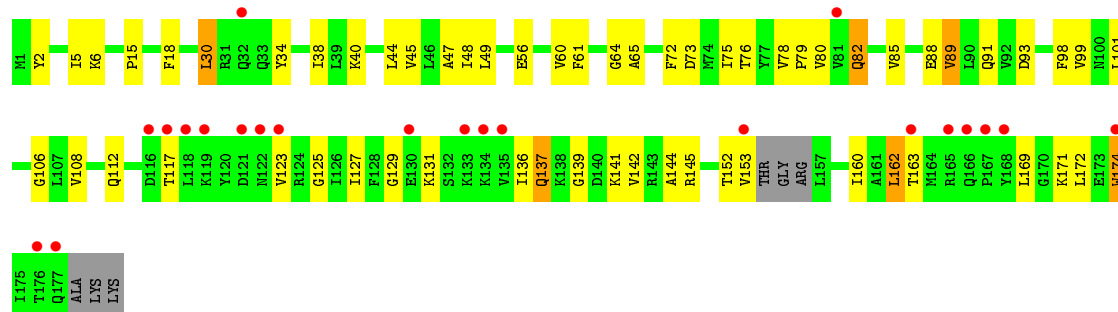


• Molecule 4: DNA-DIRECTED RNA POLYMERASERPO3 SUBUNIT

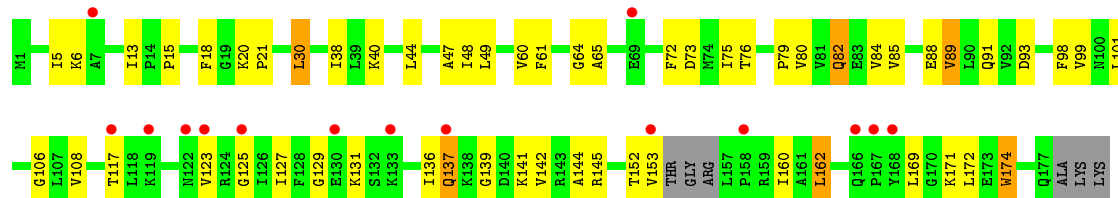




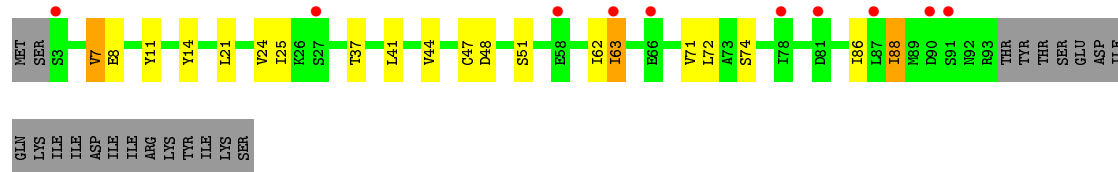
• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT



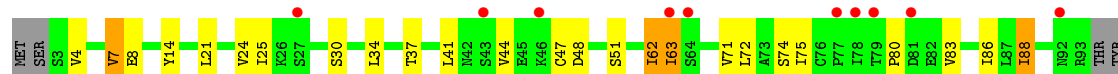
• Molecule 5: DNA-DIRECTED RNA POLYMERASE RPO7 SUBUNIT



• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



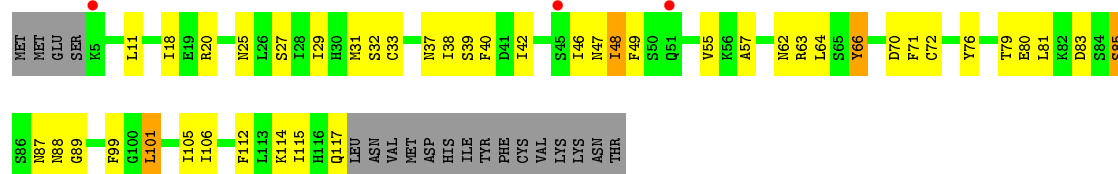
• Molecule 6: DNA-DIRECTED RNA POLYMERASE RPO4 SUBUNIT



THR  
SER  
GLU  
ASP  
ILE  
GLN  
LYS  
ILE  
ASP  
ILE  
ILE  
ARG  
LYS  
TYR  
ILE  
LYS  
SER

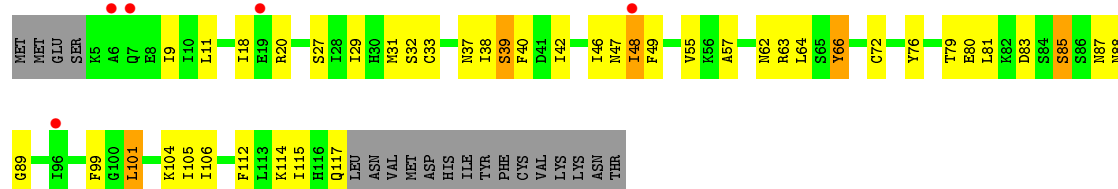
• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT

Chain G:  2% 52% 30% 14%



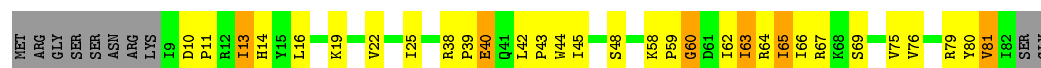
• Molecule 7: DNA-DIRECTED RNA POLYMERASE RPO8 SUBUNIT

Chain V:  4% 53% 29% 14%



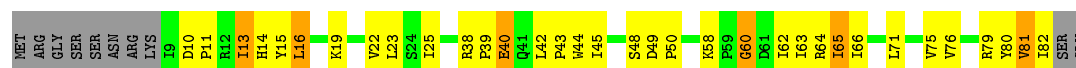
• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT

Chain H:  51% 30% 7% 12%



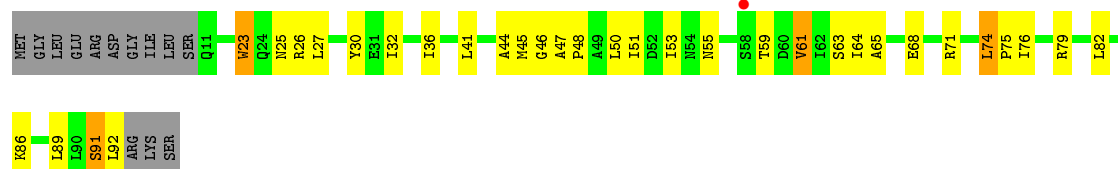
• Molecule 8: DNA-DIRECTED RNA POLYMERASE RPO5 SUBUNIT

Chain Z:  48% 33% 7% 12%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

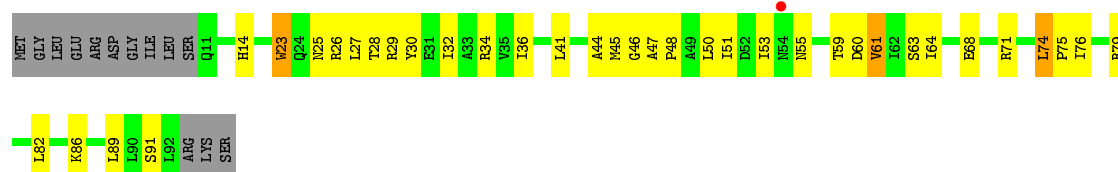
Chain I:  % 52% 31% 14%



• Molecule 9: DNA-DIRECTED RNA POLYMERASE RPO6 SUBUNIT

Chain K:  % 48% 35% 14%

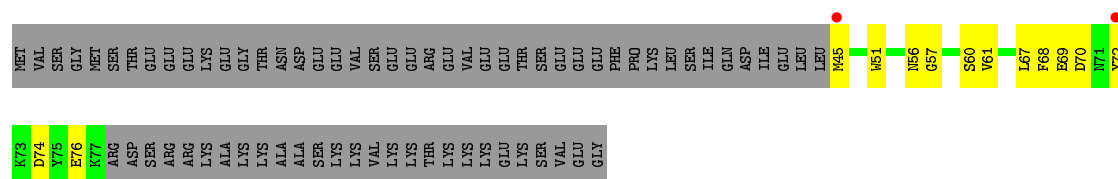




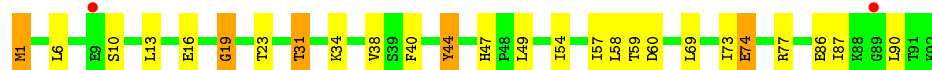
• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



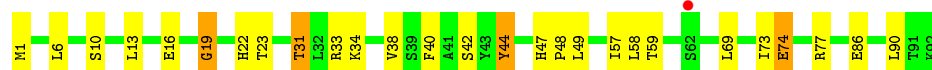
• Molecule 10: DNA-DIRECTED RNA POLYMERASE RPO13 SUBUNIT



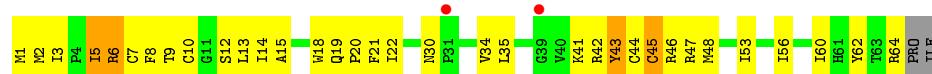
• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



• Molecule 11: DNA-DIRECTED RNA POLYMERASE RPO11 SUBUNIT



• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT

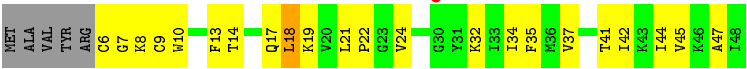


• Molecule 12: DNA-DIRECTED RNA POLYMERASE RPO10 SUBUNIT

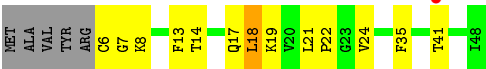




● Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT



● Molecule 13: DNA-DIRECTED RNA POLYMERASE RPO12 SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.09Å 211.87Å 238.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.20 – 3.52 30.21 – 3.52	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.20-3.52) 92.4 (30.21-3.52)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 3.56Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.333 , 0.384 0.332 , 0.381	Depositor DCC
$R_{free}$ test set	5721 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	10 of 113894 reflections (0.009%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	52739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.85 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4742e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, F3S, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.44	0/6834	0.61	1/9247 (0.0%)
1	W	0.44	0/6834	0.63	2/9247 (0.0%)
2	B	0.45	0/8816	0.64	0/11926
2	R	0.45	0/8816	0.63	0/11926
3	C	0.44	0/2857	0.62	1/3847 (0.0%)
3	Y	0.47	0/2857	0.64	1/3847 (0.0%)
4	D	0.40	0/2106	0.57	0/2845
4	S	0.39	0/2106	0.57	1/2845 (0.0%)
5	E	0.40	0/1405	0.55	0/1899
5	T	0.42	0/1405	0.56	0/1899
6	F	0.40	0/710	0.51	0/963
6	U	0.40	0/710	0.51	0/963
7	G	0.47	0/913	0.57	0/1224
7	V	0.47	0/913	0.58	0/1224
8	H	0.43	0/623	0.62	0/845
8	Z	0.45	0/623	0.64	0/845
9	I	0.46	0/667	0.66	0/903
9	K	0.45	0/667	0.64	0/903
10	J	0.50	0/305	0.62	0/408
10	Q	0.51	0/278	0.58	0/373
11	L	0.43	0/718	0.56	0/970
11	M	0.43	0/718	0.55	0/970
12	N	0.44	0/524	0.58	0/706
12	O	0.45	0/524	0.57	0/706
13	P	0.52	0/354	0.66	0/475
13	X	0.48	0/354	0.65	0/475
All	All	0.44	0/53637	0.61	6/72481 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	174	LEU	CA-CB-CG	6.97	131.33	115.30
3	C	174	LEU	CA-CB-CG	6.75	130.82	115.30
1	W	464	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	464	LEU	CA-CB-CG	6.38	129.98	115.30
1	W	438	LEU	CA-CB-CG	5.22	127.30	115.30
4	S	132	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6691	0	6756	296	0
1	W	6691	0	6760	327	0
2	B	8652	0	8795	352	0
2	R	8652	0	8796	376	0
3	C	2833	0	2992	132	0
3	Y	2833	0	2992	157	0
4	D	2071	0	2116	78	0
4	S	2071	0	2116	76	0
5	E	1384	0	1444	40	0
5	T	1384	0	1444	35	0
6	F	702	0	708	16	0
6	U	702	0	708	19	0
7	G	901	0	912	35	0
7	V	901	0	912	33	0
8	H	609	0	640	26	0
8	Z	609	0	640	33	0
9	I	658	0	692	25	0
9	K	658	0	692	31	0
10	J	301	0	284	8	0
10	Q	274	0	258	9	0
11	L	708	0	739	16	0
11	M	708	0	739	23	0
12	N	514	0	528	30	0
12	O	514	0	529	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	346	0	376	21	0
13	X	346	0	374	8	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	N	1	0	0	0	0
14	O	1	0	0	0	0
14	P	1	0	0	0	0
14	R	1	0	0	0	0
14	W	2	0	0	0	0
14	X	1	0	0	0	0
15	A	1	0	0	0	0
15	W	1	0	0	0	0
16	D	7	0	0	0	0
16	S	7	0	0	0	0
All	All	52739	0	53942	1946	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 18.

All (1946) 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:R:816:LYS:H	2:R:839:SER:HB3	1.13	1.12
2:B:856:THR:HG22	2:B:857:GLU:H	1.14	1.11
2:R:893:MET:HE2	2:R:894:LEU:H	1.10	1.10
2:R:856:THR:HG22	2:R:857:GLU:H	1.17	1.08
3:Y:244:LYS:HA	3:Y:245:LYS:HB3	1.33	1.07
3:C:244:LYS:HA	3:C:245:LYS:HB3	1.32	1.07
2:B:981:LYS:HE2	4:D:205:LEU:HD13	1.37	1.06
2:R:110:ILE:HA	2:R:111:GLU:CB	1.84	1.05
2:B:400:ALA:HA	2:B:403:THR:HG22	1.38	1.05
2:B:110:ILE:HA	2:B:111:GLU:HB2	1.10	1.05
2:B:110:ILE:HA	2:B:111:GLU:CB	1.87	1.04
3:C:62:GLY:O	3:C:63:LEU:HG	1.59	1.02
3:Y:62:GLY:O	3:Y:63:LEU:HG	1.59	1.02
2:B:461:THR:HG21	2:B:468:GLY:H	1.24	1.01
2:R:110:ILE:HA	2:R:111:GLU:HB2	1.04	1.01
2:R:898:VAL:HG21	4:S:34:LEU:HD21	1.38	1.01
2:B:816:LYS:H	2:B:839:SER:HB3	1.22	1.00
6:U:14:TYR:HD2	6:U:74:SER:HG	1.10	0.98
2:R:110:ILE:CA	2:R:111:GLU:HB2	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:573:ARG:HH11	1:W:573:ARG:HG3	1.28	0.96
2:B:665:GLN:HG2	2:B:667:PRO:HD2	1.48	0.94
2:B:110:ILE:CA	2:B:111:GLU:HB2	1.97	0.94
2:R:400:ALA:HA	2:R:403:THR:HG22	1.47	0.94
1:A:573:ARG:HH11	1:A:573:ARG:HG3	1.33	0.93
2:R:953:ILE:HD13	2:R:953:ILE:H	1.34	0.93
2:R:461:THR:HG21	2:R:468:GLY:H	1.29	0.92
6:F:14:TYR:HD2	6:F:74:SER:HG	1.11	0.92
2:B:884:ARG:NH1	2:B:992:TYR:HB3	1.84	0.91
2:R:736:ASN:HD22	2:R:736:ASN:H	1.19	0.90
2:R:1074:ASP:HB3	2:R:1075:LYS:HB3	1.53	0.90
3:Y:70:ILE:HA	3:Y:73:VAL:HG22	1.51	0.89
2:B:430:ARG:HD3	2:B:653:ILE:HG12	1.52	0.89
2:R:31:LEU:HA	2:R:125:MET:HE1	1.55	0.89
1:W:235:LEU:HA	1:W:238:LYS:HE3	1.54	0.89
2:B:736:ASN:H	2:B:736:ASN:HD22	1.17	0.89
3:C:13:LEU:HD13	3:C:48:ILE:HG12	1.55	0.88
3:C:163:MET:HB2	3:C:164:SER:HA	1.55	0.88
1:A:235:LEU:HA	1:A:238:LYS:HE3	1.53	0.88
2:B:1074:ASP:HB3	2:B:1075:LYS:HB3	1.51	0.88
2:B:953:ILE:H	2:B:953:ILE:HD13	1.38	0.87
3:C:70:ILE:HA	3:C:73:VAL:HG22	1.57	0.87
2:R:884:ARG:NH1	2:R:992:TYR:HB3	1.89	0.87
1:A:486:ILE:HA	1:A:496:ILE:HD12	1.56	0.87
2:R:816:LYS:N	2:R:839:SER:HB3	1.88	0.86
1:A:23:SER:HB2	1:A:74:HIS:NE2	1.90	0.86
2:R:665:GLN:HG2	2:R:667:PRO:HD2	1.55	0.86
11:M:69:LEU:HD23	4:S:260:LEU:HD11	1.57	0.86
2:R:430:ARG:HD3	2:R:653:ILE:HG12	1.57	0.86
3:Y:315:LEU:O	3:Y:319:VAL:HG23	1.74	0.86
2:B:31:LEU:HA	2:B:125:MET:HE1	1.58	0.85
2:R:245:VAL:HG21	2:R:256:PHE:CE2	2.10	0.85
3:Y:163:MET:HB2	3:Y:164:SER:HA	1.55	0.85
2:B:703:ARG:O	2:B:724:ASN:ND2	2.10	0.85
2:B:106:VAL:HG22	2:B:110:ILE:HG23	1.57	0.84
1:A:573:ARG:HH11	1:A:573:ARG:CG	1.90	0.83
1:A:69:PRO:HG2	2:B:1101:LYS:HE3	1.61	0.83
1:W:23:SER:HB2	1:W:74:HIS:NE2	1.93	0.83
1:W:573:ARG:HH11	1:W:573:ARG:CG	1.92	0.82
1:W:867:ASP:HA	1:W:870:ARG:NH2	1.94	0.82
2:R:106:VAL:HG22	2:R:110:ILE:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:13:LEU:HD13	3:Y:48:ILE:HG12	1.62	0.82
2:R:703:ARG:O	2:R:724:ASN:ND2	2.12	0.81
3:Y:152:VAL:HG22	3:Y:174:LEU:HD12	1.61	0.81
2:B:245:VAL:HG21	2:B:256:PHE:CE2	2.15	0.81
3:C:327:ARG:HH22	3:C:337:GLU:HB3	1.45	0.81
3:C:16:LYS:HD2	3:C:52:PHE:CE1	2.15	0.81
2:B:419:ARG:HH12	2:B:690:ARG:HH12	1.25	0.81
3:C:152:VAL:HG22	3:C:174:LEU:HD12	1.63	0.81
3:C:163:MET:CB	3:C:164:SER:HA	2.11	0.81
3:Y:327:ARG:HH22	3:Y:337:GLU:HB3	1.46	0.81
9:K:79:ARG:HG2	9:K:89:LEU:HD23	1.63	0.80
2:B:816:LYS:N	2:B:839:SER:HB3	1.97	0.80
1:W:600:LYS:O	1:W:601:LYS:HB2	1.81	0.80
10:J:51:TRP:HE3	8:Z:25:ILE:HG12	1.47	0.80
9:I:79:ARG:HG2	9:I:89:LEU:HD23	1.64	0.79
2:R:856:THR:HG22	2:R:857:GLU:N	1.98	0.79
1:A:106:ILE:HG22	1:A:107:SER:H	1.46	0.79
2:R:9:SER:HB3	2:R:12:GLU:OE1	1.83	0.79
1:A:324:THR:HG21	1:A:441:LEU:O	1.83	0.79
2:B:480:ALA:HB2	2:B:579:ARG:HD2	1.63	0.79
2:B:367:ASP:O	2:B:371:GLN:HB2	1.82	0.79
2:R:480:ALA:HB2	2:R:579:ARG:HD2	1.63	0.79
2:R:31:LEU:HA	2:R:125:MET:CE	2.13	0.79
3:Y:163:MET:CB	3:Y:164:SER:HA	2.11	0.79
1:W:614:TRP:O	1:W:618:GLU:HG2	1.84	0.78
4:S:66:PRO:HG2	4:S:124:ILE:HG12	1.63	0.78
2:B:400:ALA:HA	2:B:403:THR:CG2	2.13	0.77
2:B:31:LEU:HA	2:B:125:MET:CE	2.14	0.77
3:C:315:LEU:O	3:C:319:VAL:HG23	1.84	0.77
3:Y:16:LYS:HD2	3:Y:52:PHE:CE1	2.18	0.77
1:A:603:ILE:HG21	1:A:632:PHE:HE1	1.49	0.77
1:W:486:ILE:HA	1:W:496:ILE:HD12	1.64	0.77
1:A:600:LYS:O	1:A:601:LYS:HB2	1.84	0.77
3:Y:348:GLU:OE1	3:Y:350:THR:HB	1.86	0.76
2:R:893:MET:HE2	2:R:894:LEU:N	1.95	0.76
2:R:367:ASP:O	2:R:371:GLN:HB2	1.86	0.76
4:D:66:PRO:HG2	4:D:124:ILE:HG12	1.66	0.76
2:B:545:GLU:O	2:B:549:LYS:HG2	1.86	0.76
8:H:25:ILE:HG12	10:Q:51:TRP:HE3	1.50	0.76
2:B:856:THR:HG22	2:B:857:GLU:N	1.96	0.76
1:A:652:SER:HB3	1:A:787:ARG:HE	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:106:ILE:HG22	1:W:107:SER:H	1.51	0.76
3:Y:329:ILE:O	3:Y:335:THR:HG22	1.85	0.75
1:A:870:ARG:HD2	3:C:57:LYS:CB	2.16	0.75
2:R:594:ARG:NH1	2:R:615:LYS:HB2	2.00	0.75
1:W:324:THR:HG21	1:W:441:LEU:O	1.87	0.75
2:R:545:GLU:O	2:R:549:LYS:HG2	1.86	0.75
5:E:30:LEU:HD22	5:E:72:PHE:CE1	2.22	0.75
2:R:627:ALA:HB1	2:R:642:HIS:HD2	1.51	0.75
4:D:73:LEU:HD11	4:D:236:LEU:HD21	1.66	0.75
5:T:30:LEU:HD22	5:T:72:PHE:CE1	2.22	0.75
2:R:563:THR:HG22	2:R:564:ASP:H	1.52	0.74
2:B:594:ARG:NH1	2:B:615:LYS:HB2	2.02	0.74
2:B:1065:ASP:HB3	2:B:1089:SER:HB2	1.69	0.74
2:R:245:VAL:HG21	2:R:256:PHE:HE2	1.47	0.74
1:W:864:LYS:NZ	3:Y:29:VAL:O	2.18	0.74
3:C:339:ASN:HB2	3:C:344:ARG:HD3	1.68	0.74
8:H:45:ILE:O	8:H:81:VAL:HA	1.87	0.74
12:N:6:ARG:HA	12:N:12:SER:O	1.87	0.74
2:R:1065:ASP:HB3	2:R:1089:SER:HB2	1.68	0.74
1:A:859:TYR:OH	9:K:29:ARG:HD2	1.87	0.74
2:R:539:LEU:HD12	2:R:569:VAL:HG11	1.69	0.74
2:R:918:LEU:HD13	1:W:646:MET:HG2	1.68	0.74
1:W:652:SER:HB3	1:W:787:ARG:HE	1.51	0.73
5:T:6:LYS:HA	5:T:72:PHE:O	1.88	0.73
1:W:603:ILE:HG21	1:W:632:PHE:HE1	1.52	0.73
2:B:245:VAL:HG21	2:B:256:PHE:HE2	1.52	0.73
2:B:106:VAL:HG22	2:B:110:ILE:CG2	2.18	0.73
1:A:870:ARG:HD2	3:C:57:LYS:HB3	1.71	0.73
2:B:857:GLU:HG3	13:P:24:VAL:HG11	1.71	0.73
2:B:256:PHE:HB2	2:B:257:PRO:HD3	1.71	0.73
4:S:73:LEU:HD11	4:S:236:LEU:HD21	1.68	0.73
3:C:348:GLU:OE1	3:C:350:THR:HB	1.89	0.73
3:Y:127:THR:H	3:Y:268:ASP:HB2	1.54	0.73
1:A:271:TYR:HE1	1:A:285:PRO:HB3	1.54	0.72
8:Z:45:ILE:O	8:Z:81:VAL:HA	1.88	0.72
2:R:783:VAL:HG12	2:R:784:ARG:HB2	1.70	0.72
2:R:749:GLU:O	4:S:60:HIS:HE1	1.72	0.72
2:B:627:ALA:HB1	2:B:642:HIS:HD2	1.55	0.72
2:R:898:VAL:CG2	4:S:34:LEU:HD21	2.18	0.72
2:R:256:PHE:HB2	2:R:257:PRO:HD3	1.72	0.72
5:E:6:LYS:HA	5:E:72:PHE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:419:ARG:HH12	2:R:690:ARG:HH12	1.38	0.72
2:R:703:ARG:HD2	2:R:717:THR:HG22	1.71	0.71
1:A:867:ASP:HA	1:A:870:ARG:NH2	2.05	0.71
2:B:733:THR:HG23	2:B:735:TYR:HB2	1.73	0.71
11:M:22:HIS:CG	2:R:977:ARG:HB2	2.26	0.71
2:B:563:THR:HG22	2:B:564:ASP:H	1.55	0.71
2:B:856:THR:CG2	2:B:857:GLU:H	1.98	0.71
2:B:405:ASN:HB2	2:B:413:VAL:HB	1.73	0.71
1:A:614:TRP:O	1:A:618:GLU:HG2	1.90	0.71
3:C:127:THR:H	3:C:268:ASP:HB2	1.56	0.71
1:A:603:ILE:HG21	1:A:632:PHE:CE1	2.26	0.71
1:W:603:ILE:HG21	1:W:632:PHE:CE1	2.26	0.71
3:C:331:ARG:H	3:C:331:ARG:HD3	1.56	0.71
3:Y:244:LYS:HA	3:Y:245:LYS:CB	2.15	0.71
2:B:1010:GLY:HA3	2:B:1027:GLY:HA2	1.71	0.71
2:R:405:ASN:HB2	2:R:413:VAL:HB	1.73	0.71
2:R:856:THR:CG2	2:R:857:GLU:H	2.01	0.70
9:I:82:LEU:HD12	9:I:86:LYS:HB3	1.72	0.70
7:V:88:ASN:HD22	1:W:538:ALA:HB2	1.55	0.70
2:R:31:LEU:HD23	2:R:125:MET:HE3	1.73	0.70
2:B:711:LEU:HD13	2:B:716:TYR:HB3	1.74	0.70
9:I:26:ARG:HG2	9:I:27:LEU:H	1.56	0.70
1:A:184:LEU:HB3	1:A:204:PRO:HB2	1.73	0.70
1:W:105:LYS:HE2	1:W:105:LYS:HA	1.71	0.70
3:Y:30:GLU:O	3:Y:33:LYS:HG2	1.92	0.70
2:R:711:LEU:HD13	2:R:716:TYR:HB3	1.74	0.70
1:A:471:GLU:HG3	9:K:41:LEU:HD13	1.73	0.70
2:B:333:ARG:O	2:B:334:GLU:HB3	1.92	0.70
2:B:981:LYS:CE	4:D:205:LEU:HD13	2.20	0.69
2:B:703:ARG:HD2	2:B:717:THR:HG22	1.72	0.69
5:E:5:ILE:HA	6:F:8:GLU:O	1.91	0.69
3:C:158:ILE:HG13	3:C:223:ARG:HH21	1.57	0.69
1:W:876:VAL:C	1:W:878:TRP:H	1.93	0.69
2:R:904:VAL:O	4:S:163:ILE:HG12	1.92	0.69
1:A:549:LYS:HE2	7:G:89:GLY:HA2	1.73	0.69
2:R:893:MET:CE	2:R:894:LEU:H	1.97	0.69
1:W:599:ASP:H	1:W:602:ALA:HB3	1.57	0.69
1:A:540:LEU:HB3	7:G:66:TYR:CE2	2.28	0.69
3:Y:339:ASN:HB2	3:Y:344:ARG:HD3	1.74	0.69
3:Y:331:ARG:HD3	3:Y:331:ARG:H	1.56	0.69
1:A:575:CYS:SG	1:A:584:SER:HB3	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:184:LEU:HB3	1:W:204:PRO:HB2	1.73	0.69
1:W:651:VAL:HG11	1:W:743:MET:HB3	1.75	0.69
2:R:694:ARG:HA	2:R:758:PHE:O	1.92	0.69
2:R:106:VAL:HG22	2:R:110:ILE:CG2	2.23	0.69
1:W:725:ALA:HA	1:W:728:MET:HE2	1.73	0.69
3:C:329:ILE:O	3:C:335:THR:HG22	1.93	0.69
8:H:44:TRP:O	8:H:79:ARG:HD2	1.93	0.69
1:W:99:ARG:HG2	1:W:183:ARG:HH22	1.58	0.68
3:C:144:LEU:O	3:C:235:LYS:HG3	1.93	0.68
2:R:333:ARG:O	2:R:334:GLU:HB3	1.92	0.68
2:B:419:ARG:NH1	2:B:690:ARG:HH12	1.89	0.68
1:W:58:CYS:SG	1:W:60:THR:HG23	2.33	0.68
2:R:400:ALA:HA	2:R:403:THR:CG2	2.20	0.68
2:R:419:ARG:NH1	2:R:690:ARG:HH12	1.91	0.68
1:W:271:TYR:HE1	1:W:285:PRO:HB3	1.58	0.68
1:A:803:ARG:HG2	2:B:447:ASP:HA	1.76	0.68
3:C:30:GLU:O	3:C:33:LYS:HG2	1.93	0.68
3:Y:222:LEU:O	3:Y:226:ILE:HG13	1.93	0.68
1:A:573:ARG:NH1	1:A:573:ARG:HG3	2.07	0.68
1:W:488:THR:HG22	1:W:490:ARG:H	1.59	0.68
4:D:233:VAL:HG21	12:N:6:ARG:NH2	2.09	0.68
1:A:876:VAL:C	1:A:878:TRP:H	1.97	0.68
1:A:97:THR:HG22	1:A:99:ARG:H	1.57	0.68
1:A:99:ARG:HG2	1:A:183:ARG:HH22	1.58	0.68
2:B:543:ILE:HD13	2:B:558:VAL:HG21	1.75	0.68
2:B:133:ILE:HA	2:B:136:TYR:CD1	2.29	0.68
9:I:41:LEU:HD12	1:W:470:GLU:HG3	1.76	0.68
2:R:733:THR:HG23	2:R:735:TYR:HB2	1.76	0.68
2:R:560:HIS:HB3	2:R:626:ASN:HD21	1.59	0.68
1:A:64:THR:HG22	1:A:65:LEU:HG	1.75	0.68
1:A:105:LYS:HE2	1:A:105:LYS:HA	1.75	0.68
1:W:729:ALA:O	1:W:730:ARG:HB2	1.94	0.67
2:B:893:MET:CE	2:B:894:LEU:H	2.06	0.67
4:D:260:LEU:HD11	11:L:69:LEU:HD23	1.74	0.67
6:F:72:LEU:HD11	6:F:86:ILE:HG12	1.77	0.67
2:B:783:VAL:HG12	2:B:784:ARG:HB2	1.74	0.67
1:W:95:LYS:HB3	1:W:138:LYS:HG2	1.75	0.67
1:A:651:VAL:HG11	1:A:743:MET:HB3	1.76	0.67
2:R:905:LYS:H	2:R:905:LYS:HE2	1.58	0.67
9:K:26:ARG:HG2	9:K:27:LEU:H	1.59	0.67
3:Y:158:ILE:HG13	3:Y:223:ARG:HH21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:982:ILE:HD12	2:B:984:SER:H	1.60	0.67
1:A:866:VAL:C	1:A:870:ARG:HH22	1.97	0.67
2:B:598:GLU:HA	2:B:602:SER:CB	2.25	0.67
2:B:668:ARG:NH1	2:B:921:ARG:HD2	2.10	0.67
10:J:51:TRP:CE3	8:Z:25:ILE:HG12	2.30	0.67
1:W:575:CYS:SG	1:W:584:SER:HB3	2.34	0.67
2:B:461:THR:CG2	2:B:468:GLY:H	2.06	0.66
2:R:974:TYR:CE2	2:R:981:LYS:HB3	2.30	0.66
2:B:560:HIS:HB3	2:B:626:ASN:HD21	1.58	0.66
3:Y:226:ILE:HB	3:Y:227:LEU:HD12	1.76	0.66
1:A:95:LYS:HB3	1:A:138:LYS:HG2	1.77	0.66
12:O:13:LEU:HD11	4:S:66:PRO:HG3	1.76	0.66
3:C:146:TYR:HD1	3:C:235:LYS:H	1.44	0.66
6:U:72:LEU:HD11	6:U:86:ILE:HG12	1.76	0.66
2:B:539:LEU:HD12	2:B:569:VAL:HG11	1.76	0.66
2:B:972:VAL:HG11	4:D:204:THR:HB	1.78	0.66
1:A:729:ALA:O	1:A:730:ARG:HB2	1.94	0.66
5:E:145:ARG:HD3	6:F:88:ILE:HG21	1.78	0.66
3:Y:64:ILE:HG22	3:Y:65:ALA:H	1.60	0.66
3:Y:146:TYR:HD1	3:Y:235:LYS:H	1.42	0.66
2:B:694:ARG:HA	2:B:758:PHE:O	1.95	0.66
5:T:15:PRO:HD3	5:T:65:ALA:HB2	1.78	0.66
2:B:897:GLN:HG3	2:B:908:VAL:HG21	1.78	0.66
9:K:68:GLU:O	9:K:74:LEU:HG	1.95	0.66
2:R:133:ILE:HA	2:R:136:TYR:CD1	2.30	0.66
10:J:51:TRP:HE3	8:Z:25:ILE:CG1	2.09	0.66
1:W:421:ARG:HG3	1:W:462:MET:HG2	1.78	0.66
1:W:838:VAL:HB	1:W:847:GLN:HB2	1.77	0.65
4:S:17:PHE:O	4:S:225:LYS:HA	1.96	0.65
8:H:42:LEU:O	8:H:44:TRP:CD1	2.49	0.65
1:W:97:THR:HG22	1:W:99:ARG:H	1.60	0.65
3:C:64:ILE:HG22	3:C:65:ALA:H	1.60	0.65
1:A:538:ALA:HB2	7:G:88:ASN:HD22	1.62	0.65
1:A:599:ASP:H	1:A:602:ALA:HB3	1.61	0.65
8:Z:43:PRO:HB2	8:Z:79:ARG:HD3	1.79	0.65
2:R:897:GLN:HG3	2:R:908:VAL:HG21	1.79	0.65
2:B:975:ASP:OD2	2:B:977:ARG:HD3	1.96	0.65
4:D:17:PHE:O	4:D:225:LYS:HA	1.97	0.65
9:K:23:TRP:HA	9:K:23:TRP:CE3	2.32	0.65
1:A:130:ARG:HH11	1:A:196:GLY:HA2	1.62	0.65
2:R:972:VAL:HG11	4:S:204:THR:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:347:PHE:O	3:Y:348:GLU:HB3	1.97	0.64
2:R:975:ASP:OD2	2:R:977:ARG:HD3	1.97	0.64
2:B:768:TYR:HD1	2:B:819:PRO:HG2	1.62	0.64
5:E:15:PRO:HD3	5:E:65:ALA:HB2	1.78	0.64
2:R:446:ARG:HH22	2:R:465:PRO:HA	1.62	0.64
3:Y:53:ASP:HA	3:Y:56:ILE:HG12	1.79	0.64
1:W:868:VAL:HG22	3:Y:39:LYS:NZ	2.12	0.64
2:B:974:TYR:CE2	2:B:981:LYS:HB3	2.31	0.64
3:C:341:VAL:HG12	3:C:344:ARG:HH22	1.61	0.64
4:D:66:PRO:HG3	12:N:13:LEU:HD11	1.80	0.64
2:R:922:MET:HG2	1:W:743:MET:HG3	1.80	0.64
9:I:68:GLU:O	9:I:74:LEU:HG	1.97	0.64
2:R:709:ARG:HG3	2:R:944:ASP:OD2	1.97	0.64
3:Y:341:VAL:HG12	3:Y:344:ARG:HH22	1.62	0.64
12:O:6:ARG:HA	12:O:12:SER:O	1.97	0.64
3:Y:150:GLU:HG3	3:Y:227:LEU:HB3	1.80	0.64
1:W:365:VAL:HG11	1:W:401:LEU:HD11	1.78	0.64
5:T:141:LYS:HB3	5:T:172:LEU:HD13	1.78	0.64
5:E:108:VAL:HB	5:E:162:LEU:HB2	1.80	0.64
2:B:502:GLU:O	2:B:506:ARG:HB2	1.97	0.64
2:B:168:GLU:O	2:B:435:SER:HB2	1.98	0.64
2:R:359:VAL:HG11	2:R:407:VAL:HG13	1.80	0.64
5:T:40:LYS:HG3	5:T:153:VAL:HB	1.80	0.64
3:Y:69:ALA:HB2	3:Y:381:LEU:HD13	1.80	0.64
3:Y:274:THR:HG22	3:Y:276:ASN:H	1.63	0.64
3:C:69:ALA:HB2	3:C:381:LEU:HD13	1.80	0.63
2:R:380:ARG:HD3	2:R:381:LYS:HE3	1.80	0.63
2:B:1005:HIS:NE2	2:B:1007:ARG:HD2	2.13	0.63
2:B:736:ASN:ND2	2:B:736:ASN:H	1.91	0.63
1:W:866:VAL:C	1:W:870:ARG:HH22	2.02	0.63
3:C:53:ASP:HA	3:C:56:ILE:HG12	1.80	0.63
5:E:141:LYS:HB3	5:E:172:LEU:HD13	1.80	0.63
2:B:91:ARG:HD3	2:B:856:THR:HG21	1.78	0.63
2:R:590:PRO:O	2:R:615:LYS:HD2	1.99	0.63
1:W:99:ARG:HG2	1:W:183:ARG:NH2	2.13	0.63
1:A:99:ARG:HG2	1:A:183:ARG:NH2	2.13	0.63
1:A:777:GLU:HG3	1:A:783:TYR:HE2	1.63	0.63
2:B:905:LYS:H	2:B:905:LYS:HE2	1.62	0.63
3:C:150:GLU:HG3	3:C:227:LEU:HB3	1.80	0.63
2:B:1074:ASP:HB3	2:B:1075:LYS:CB	2.28	0.63
2:R:543:ILE:HD13	2:R:558:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:761:TYR:HE2	2:R:843:ARG:HG2	1.64	0.63
1:A:852:ASP:CG	8:H:75:VAL:HG21	2.19	0.63
4:S:155:LYS:HE3	4:S:156:PHE:CE1	2.34	0.63
1:W:78:VAL:O	1:W:79:ARG:HB2	1.99	0.63
2:B:446:ARG:HH22	2:B:465:PRO:HA	1.63	0.63
3:C:244:LYS:HA	3:C:245:LYS:CB	2.14	0.62
2:B:786:TYR:CE2	2:B:788:GLY:HA2	2.34	0.62
1:W:380:ARG:HH11	1:W:384:ARG:HE	1.47	0.62
2:B:52:ILE:N	2:B:53:PRO:HD3	2.14	0.62
2:B:759:ARG:NH1	2:B:846:GLU:OE2	2.31	0.62
2:B:31:LEU:HD23	2:B:125:MET:HE3	1.80	0.62
12:O:6:ARG:NH2	4:S:233:VAL:HG21	2.14	0.62
7:V:88:ASN:HD22	1:W:538:ALA:CB	2.12	0.62
2:R:446:ARG:HH11	1:W:807:VAL:HG13	1.64	0.62
2:R:786:TYR:CE2	2:R:788:GLY:HA2	2.34	0.62
2:B:380:ARG:HD3	2:B:381:LYS:HE3	1.81	0.62
2:R:1111:ILE:HG22	2:R:1111:ILE:O	1.99	0.62
1:W:573:ARG:NH1	1:W:573:ARG:HG3	2.05	0.62
2:R:51:GLU:HB2	2:R:53:PRO:HD3	1.81	0.62
4:D:34:LEU:HA	4:D:150:GLY:HA3	1.81	0.62
1:W:553:SER:OG	1:W:592:ILE:HA	2.00	0.62
9:I:47:ALA:HB1	9:I:48:PRO:CD	2.30	0.62
2:R:52:ILE:N	2:R:53:PRO:HD3	2.15	0.62
2:R:1074:ASP:HB3	2:R:1075:LYS:CB	2.28	0.62
1:A:600:LYS:HB2	1:A:732:GLY:CA	2.29	0.62
3:C:226:ILE:HB	3:C:227:LEU:HD12	1.81	0.62
1:A:78:VAL:O	1:A:79:ARG:HB2	2.00	0.62
2:B:709:ARG:HG3	2:B:944:ASP:OD2	1.99	0.62
2:R:708:THR:O	2:R:711:LEU:HB2	2.00	0.62
1:W:130:ARG:HH11	1:W:196:GLY:HA2	1.63	0.62
2:B:430:ARG:HD3	2:B:653:ILE:CG1	2.28	0.62
2:R:982:ILE:HD12	2:R:984:SER:H	1.65	0.62
5:E:47:ALA:HB3	5:E:75:ILE:HD12	1.81	0.62
5:E:40:LYS:HG3	5:E:153:VAL:HB	1.82	0.62
2:R:502:GLU:O	2:R:506:ARG:HB2	1.99	0.61
2:R:563:THR:HG22	2:R:564:ASP:N	2.15	0.61
3:C:222:LEU:O	3:C:226:ILE:HG13	1.99	0.61
1:A:761:TYR:HB3	2:B:625:GLU:OE1	2.00	0.61
2:B:43:GLN:HA	2:B:66:ILE:HD11	1.82	0.61
5:T:47:ALA:HB3	5:T:75:ILE:HD12	1.82	0.61
5:T:108:VAL:HB	5:T:162:LEU:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:LYS:HB2	6:F:8:GLU:HB2	1.81	0.61
1:A:127:SER:HA	1:A:130:ARG:HD2	1.81	0.61
3:Y:276:ASN:ND2	3:Y:279:GLU:OE2	2.31	0.61
1:W:109:ASP:HB3	1:W:113:LYS:HE3	1.81	0.61
1:W:867:ASP:HA	1:W:870:ARG:HH21	1.65	0.61
2:B:584:ILE:HD11	2:B:617:GLU:HB2	1.82	0.61
1:A:380:ARG:HH11	1:A:384:ARG:HE	1.46	0.61
1:A:549:LYS:HD2	1:A:593:LEU:HD22	1.81	0.61
8:Z:42:LEU:O	8:Z:44:TRP:CD1	2.54	0.61
1:W:541:ALA:HB3	1:W:542:PRO:CD	2.30	0.61
1:W:64:THR:HG22	1:W:65:LEU:HG	1.81	0.61
3:Y:286:ILE:HG12	8:Z:49:ASP:CG	2.21	0.61
3:C:270:ALA:HA	8:H:14:HIS:HB3	1.81	0.61
1:A:109:ASP:HB3	1:A:113:LYS:HE3	1.81	0.61
2:R:168:GLU:O	2:R:435:SER:HB2	2.00	0.61
2:B:870:ARG:NH1	4:D:56:GLU:OE2	2.32	0.61
1:A:488:THR:HG22	1:A:490:ARG:H	1.65	0.61
2:R:91:ARG:HD3	2:R:856:THR:HG21	1.82	0.61
2:R:433:ILE:HG12	2:R:470:VAL:HB	1.81	0.61
1:A:365:VAL:HG11	1:A:401:LEU:HD11	1.83	0.61
2:B:857:GLU:HA	2:B:862:ASN:O	2.01	0.61
12:O:47:ARG:HD2	2:R:724:ASN:O	2.00	0.61
2:R:984:SER:O	2:R:985:ARG:HB2	2.01	0.61
4:D:2:SER:HB2	4:D:18:GLU:HB3	1.83	0.61
7:V:79:THR:HG22	7:V:80:GLU:N	2.16	0.61
2:B:9:SER:HB3	2:B:12:GLU:OE1	2.00	0.61
2:R:930:GLY:HA2	2:R:990:VAL:O	2.01	0.61
3:Y:144:LEU:O	3:Y:235:LYS:HG3	2.00	0.61
1:A:854:GLY:O	3:C:64:ILE:CG2	2.49	0.61
7:V:72:CYS:HB3	7:V:114:LYS:HG2	1.82	0.61
1:A:449:VAL:HG12	1:A:452:PRO:HG2	1.82	0.61
3:C:372:ASN:HA	3:C:375:ILE:HG22	1.82	0.61
9:K:47:ALA:HB1	9:K:48:PRO:CD	2.31	0.60
1:W:755:GLU:HB3	1:W:758:LYS:NZ	2.15	0.60
2:R:1005:HIS:NE2	2:R:1007:ARG:HD2	2.16	0.60
2:R:736:ASN:ND2	2:R:736:ASN:H	1.93	0.60
12:N:64:ARG:HH22	13:P:37:VAL:HG23	1.66	0.60
5:T:6:LYS:HB2	6:U:8:GLU:HB2	1.82	0.60
4:S:188:PHE:HB3	4:S:195:LEU:HD22	1.84	0.60
1:W:876:VAL:C	1:W:878:TRP:N	2.55	0.60
1:W:879:LYS:NZ	3:Y:44:THR:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:PHE:HB3	4:D:195:LEU:HD22	1.84	0.60
2:R:110:ILE:CA	2:R:111:GLU:CB	2.68	0.60
3:Y:328:GLN:HG2	3:Y:330:GLY:H	1.66	0.60
7:V:80:GLU:HG3	7:V:81:LEU:H	1.66	0.60
7:G:79:THR:HG22	7:G:80:GLU:H	1.67	0.60
7:G:18:ILE:HD12	7:G:29:ILE:HG12	1.83	0.60
3:C:122:MET:HG2	3:C:274:THR:HG23	1.84	0.60
1:A:545:TYR:CD2	7:G:46:ILE:HD11	2.37	0.60
2:B:984:SER:O	2:B:985:ARG:HB2	2.01	0.60
2:B:1042:PHE:O	9:K:30:TYR:HE2	1.85	0.60
2:R:759:ARG:NH1	2:R:846:GLU:OE2	2.33	0.60
1:A:848:VAL:O	1:A:849:ALA:HB3	2.00	0.60
2:B:708:THR:O	2:B:711:LEU:HB2	2.02	0.60
7:G:79:THR:HG22	7:G:80:GLU:N	2.16	0.60
2:R:768:TYR:HD1	2:R:819:PRO:HG2	1.66	0.60
3:C:328:GLN:HG2	3:C:330:GLY:H	1.66	0.60
12:O:35:LEU:HD13	12:O:46:ARG:HG3	1.83	0.60
3:C:281:GLU:OE1	3:C:326:VAL:HG12	2.02	0.60
1:W:127:SER:HA	1:W:130:ARG:HD2	1.84	0.59
1:W:109:ASP:O	1:W:113:LYS:HG3	2.01	0.59
4:D:38:VAL:CG1	4:D:39:MET:N	2.65	0.59
2:B:91:ARG:CD	2:B:856:THR:HG21	2.33	0.59
1:W:601:LYS:O	1:W:610:SER:HB2	2.02	0.59
4:S:38:VAL:CG1	4:S:39:MET:N	2.65	0.59
1:W:325:VAL:O	1:W:442:THR:HB	2.01	0.59
2:B:563:THR:HG22	2:B:564:ASP:N	2.18	0.59
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.83	0.59
2:B:684:ALA:O	2:B:687:TYR:HB3	2.01	0.59
1:A:734:ARG:NH1	2:B:916:HIS:O	2.33	0.59
11:M:33:ARG:HD2	1:W:519:GLU:HG2	1.82	0.59
4:S:34:LEU:HA	4:S:150:GLY:HA3	1.83	0.59
2:B:371:GLN:O	2:B:375:SER:HB2	2.01	0.59
1:A:109:ASP:O	1:A:113:LYS:HG3	2.02	0.59
7:G:80:GLU:HG3	7:G:81:LEU:H	1.67	0.59
2:B:406:TRP:CG	2:B:407:VAL:N	2.70	0.59
3:Y:262:LEU:HD11	3:Y:283:VAL:HG11	1.84	0.59
4:S:2:SER:HB2	4:S:18:GLU:HB3	1.83	0.59
4:S:153:HIS:HB3	4:S:155:LYS:HG2	1.83	0.59
3:Y:281:GLU:OE1	3:Y:326:VAL:HG12	2.03	0.59
2:R:584:ILE:HD11	2:R:617:GLU:HB2	1.84	0.59
2:B:585:VAL:HG21	2:B:636:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:44:TRP:HA	8:Z:80:TYR:H	1.68	0.59
1:W:734:ARG:HH11	1:W:734:ARG:HB3	1.66	0.59
1:W:753:ARG:HG3	1:W:804:GLU:OE1	2.03	0.59
2:R:43:GLN:HA	2:R:66:ILE:HD11	1.85	0.59
5:T:5:ILE:HA	6:U:8:GLU:O	2.01	0.59
3:C:347:PHE:C	3:C:349:VAL:H	2.05	0.59
1:A:875:VAL:O	1:A:877:GLY:N	2.32	0.59
2:R:1117:ILE:HD11	1:W:10:LYS:HG3	1.83	0.59
5:E:6:LYS:O	6:F:7:VAL:HG12	2.03	0.59
4:D:38:VAL:HG12	4:D:39:MET:N	2.18	0.59
2:B:1050:ASP:HA	2:B:1054:ASP:HB2	1.84	0.59
1:W:777:GLU:HG3	1:W:783:TYR:HE2	1.67	0.59
8:H:44:TRP:HA	8:H:80:TYR:H	1.66	0.59
7:G:72:CYS:HB3	7:G:114:LYS:HG2	1.85	0.59
2:B:1069:TYR:CB	2:B:1070:ILE:HB	2.33	0.59
1:A:646:MET:HG2	2:B:918:LEU:HD13	1.83	0.59
1:W:324:THR:HG22	1:W:325:VAL:H	1.68	0.58
1:W:281:ILE:HG21	3:Y:352:LYS:NZ	2.18	0.58
2:R:598:GLU:HA	2:R:602:SER:CB	2.33	0.58
2:R:916:HIS:O	1:W:734:ARG:NH1	2.33	0.58
11:L:31:THR:HA	11:L:34:LYS:HD2	1.85	0.58
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.85	0.58
5:E:123:VAL:HG22	5:E:125:GLY:H	1.68	0.58
1:A:853:ASP:HB3	1:A:855:VAL:H	1.68	0.58
1:A:58:CYS:SG	1:A:60:THR:HG23	2.43	0.58
12:N:14:ILE:HG13	12:N:48:MET:HG3	1.85	0.58
2:R:417:LEU:HD21	2:R:425:MET:HG3	1.85	0.58
1:A:851:GLY:O	1:A:853:ASP:N	2.35	0.58
2:R:953:ILE:HG13	1:W:787:ARG:HH12	1.68	0.58
8:H:25:ILE:HG12	10:Q:51:TRP:CE3	2.37	0.58
5:T:6:LYS:O	6:U:7:VAL:HG12	2.04	0.58
7:V:79:THR:HG22	7:V:80:GLU:H	1.68	0.58
4:S:38:VAL:HG12	4:S:39:MET:N	2.18	0.58
1:W:715:ALA:O	1:W:719:LEU:HB3	2.03	0.58
1:A:715:ALA:O	1:A:719:LEU:HB3	2.04	0.58
9:K:82:LEU:HD12	9:K:86:LYS:HB3	1.84	0.58
2:R:1047:LEU:HD21	1:W:418:LEU:HD21	1.84	0.58
2:R:658:ILE:O	2:R:661:PRO:HG3	2.04	0.58
2:R:430:ARG:HD3	2:R:653:ILE:CG1	2.30	0.58
3:C:219:LEU:HA	3:C:222:LEU:HD13	1.86	0.58
5:T:123:VAL:HG22	5:T:125:GLY:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:347:PHE:C	3:Y:349:VAL:H	2.07	0.58
11:M:48:PRO:HG2	2:R:735:TYR:CE2	2.38	0.58
8:Z:44:TRP:O	8:Z:79:ARG:HD2	2.04	0.58
13:X:7:GLY:HA2	13:X:35:PHE:O	2.03	0.58
1:W:874:ARG:HB2	3:Y:54:LEU:HD21	1.85	0.58
1:W:870:ARG:HD2	3:Y:57:LYS:CB	2.34	0.58
2:B:598:GLU:HA	2:B:602:SER:HB2	1.85	0.58
1:A:542:PRO:HG2	7:G:46:ILE:HD12	1.86	0.58
2:R:41:LYS:O	2:R:43:GLN:N	2.37	0.58
1:W:812:ARG:HH22	3:Y:304:GLN:HE22	1.52	0.58
2:B:41:LYS:O	2:B:43:GLN:N	2.37	0.58
3:C:199:ASP:HB2	3:C:206:LEU:HB2	1.86	0.58
2:R:731:SER:OG	1:W:644:PHE:HB3	2.04	0.58
4:D:155:LYS:HE3	4:D:156:PHE:CE1	2.38	0.58
12:N:7:CYS:SG	12:N:45:CYS:HA	2.44	0.58
2:R:668:ARG:NH1	2:R:921:ARG:HD2	2.19	0.57
4:D:63:ALA:HB2	13:P:47:ALA:HB1	1.86	0.57
3:Y:47:GLU:HG3	3:Y:51:ILE:HG12	1.86	0.57
3:C:64:ILE:O	9:K:23:TRP:HZ2	1.87	0.57
9:I:23:TRP:CE3	9:I:23:TRP:HA	2.39	0.57
13:P:6:CYS:SG	13:P:18:LEU:HG	2.44	0.57
8:Z:65:ILE:HD11	8:Z:79:ARG:HG2	1.86	0.57
2:B:761:TYR:HE2	2:B:843:ARG:HG2	1.68	0.57
3:C:244:LYS:CA	3:C:245:LYS:HB3	2.22	0.57
3:Y:341:VAL:H	3:Y:364:GLU:HG2	1.69	0.57
2:B:13:ARG:HH12	2:B:647:SER:H	1.51	0.57
2:R:393:VAL:O	2:R:397:ILE:HB	2.04	0.57
2:R:371:GLN:O	2:R:375:SER:HB2	2.04	0.57
1:W:819:MET:SD	3:Y:107:LEU:HD22	2.45	0.57
2:B:590:PRO:O	2:B:615:LYS:HD2	2.05	0.57
4:S:161:LEU:HG	4:S:163:ILE:HD13	1.86	0.57
1:A:317:ARG:HA	2:B:1030:ARG:HA	1.86	0.57
1:A:177:PRO:HD2	1:A:266:TRP:HZ2	1.69	0.57
2:R:1104:ILE:HA	2:R:1107:LEU:HD12	1.85	0.57
2:R:684:ALA:O	2:R:687:TYR:HB3	2.05	0.57
2:R:688:GLN:O	2:R:868:ARG:NH2	2.37	0.57
1:W:177:PRO:HD2	1:W:266:TRP:HZ2	1.70	0.57
6:F:7:VAL:HG13	6:F:8:GLU:HG2	1.86	0.57
6:U:7:VAL:HG13	6:U:8:GLU:HG2	1.87	0.57
1:A:876:VAL:C	1:A:878:TRP:N	2.58	0.57
7:V:38:ILE:HG22	7:V:39:SER:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:ASN:O	3:C:174:LEU:HD22	2.05	0.57
3:C:347:PHE:O	3:C:348:GLU:HB3	2.05	0.57
2:B:136:TYR:HD2	2:B:140:LYS:HB3	1.70	0.57
4:S:245:ALA:O	4:S:249:ILE:HG12	2.05	0.57
1:A:289:HIS:HB2	1:A:295:LEU:HD21	1.85	0.57
2:R:973:THR:HG21	2:R:988:PHE:CE1	2.39	0.57
2:R:857:GLU:HA	2:R:862:ASN:O	2.05	0.56
8:H:39:PRO:HG3	10:Q:67:LEU:HD11	1.85	0.56
1:A:854:GLY:O	3:C:64:ILE:HG12	2.05	0.56
2:B:973:THR:HG21	2:B:988:PHE:CE1	2.40	0.56
3:Y:199:ASP:HB2	3:Y:206:LEU:HB2	1.87	0.56
4:D:245:ALA:O	4:D:249:ILE:HG12	2.05	0.56
2:B:953:ILE:CD1	2:B:953:ILE:H	2.11	0.56
6:F:71:VAL:HG13	6:F:72:LEU:HD12	1.87	0.56
2:R:761:TYR:CE2	2:R:843:ARG:HG2	2.40	0.56
7:V:46:ILE:HD12	1:W:542:PRO:HG2	1.87	0.56
7:V:18:ILE:HD12	7:V:29:ILE:HG12	1.87	0.56
2:R:1069:TYR:CB	2:R:1070:ILE:HB	2.35	0.56
2:B:1104:ILE:HA	2:B:1107:LEU:HD12	1.85	0.56
1:A:220:ARG:HG2	1:A:235:LEU:HB3	1.88	0.56
1:A:549:LYS:CE	7:G:89:GLY:HA2	2.35	0.56
2:R:981:LYS:HE2	4:S:205:LEU:HD13	1.87	0.56
1:W:510:THR:O	1:W:549:LYS:HD3	2.04	0.56
13:P:7:GLY:HA2	13:P:35:PHE:O	2.04	0.56
4:S:53:LEU:HD22	4:S:57:ILE:HG21	1.88	0.56
1:W:324:THR:HG22	1:W:325:VAL:N	2.20	0.56
3:Y:29:VAL:HG12	3:Y:61:GLU:HG3	1.87	0.56
2:B:1007:ARG:HH22	2:B:1022:GLY:N	2.04	0.56
2:R:870:ARG:NH1	4:S:56:GLU:OE2	2.38	0.56
2:B:21:PHE:HZ	2:B:475:LEU:HB3	1.71	0.56
2:B:186:ILE:HD12	2:B:209:LYS:HB3	1.87	0.56
11:M:42:SER:HB3	1:W:522:GLN:O	2.05	0.56
3:C:291:GLU:HA	3:C:294:ILE:HD12	1.88	0.56
1:A:417:VAL:HG13	1:A:465:HIS:O	2.06	0.56
11:L:6:LEU:HD11	11:L:16:GLU:HB2	1.88	0.56
2:B:157:VAL:O	2:B:159:GLY:N	2.38	0.56
11:M:31:THR:HA	11:M:34:LYS:HD2	1.88	0.56
1:A:82:ILE:HD12	1:A:156:ILE:HG13	1.86	0.56
3:Y:291:GLU:HA	3:Y:294:ILE:HD12	1.87	0.56
2:R:978:THR:O	4:S:26:ASN:ND2	2.38	0.56
3:Y:372:ASN:HA	3:Y:375:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:7:CYS:SG	12:O:45:CYS:HA	2.45	0.56
4:D:53:LEU:HD22	4:D:57:ILE:HG21	1.86	0.56
2:B:522:LYS:HG2	2:B:532:TYR:CE2	2.41	0.56
2:B:930:GLY:HA2	2:B:990:VAL:O	2.06	0.56
3:C:301:LEU:HD22	3:C:308:VAL:HG12	1.87	0.56
13:P:24:VAL:HG13	13:P:24:VAL:O	2.06	0.56
3:Y:70:ILE:HA	3:Y:73:VAL:CG2	2.32	0.56
8:H:43:PRO:HB2	8:H:79:ARG:HD3	1.88	0.56
2:B:600:LEU:O	2:B:601:ASP:HB2	2.05	0.56
2:B:393:VAL:O	2:B:397:ILE:HB	2.06	0.56
3:Y:219:LEU:HA	3:Y:222:LEU:HD13	1.88	0.56
10:J:67:LEU:HD11	8:Z:39:PRO:HG3	1.88	0.56
9:I:30:TYR:HE2	2:R:1042:PHE:O	1.89	0.56
3:Y:337:GLU:HG3	3:Y:339:ASN:OD1	2.06	0.55
2:R:583:ILE:HD12	2:R:591:LEU:HD21	1.89	0.55
2:B:583:ILE:HD12	2:B:591:LEU:HD21	1.86	0.55
2:B:110:ILE:CA	2:B:111:GLU:CB	2.71	0.55
1:A:323:ARG:HH21	1:A:422:GLN:HE21	1.54	0.55
2:B:1111:ILE:HG22	2:B:1111:ILE:O	2.06	0.55
2:R:1010:GLY:HA3	2:R:1027:GLY:HA2	1.86	0.55
4:S:51:SER:HB2	4:S:52:PRO:HD2	1.88	0.55
3:Y:171:ASN:O	3:Y:174:LEU:HD22	2.05	0.55
7:V:88:ASN:ND2	1:W:538:ALA:HB2	2.22	0.55
1:A:854:GLY:O	3:C:64:ILE:HG21	2.05	0.55
3:C:276:ASN:ND2	3:C:279:GLU:OE2	2.37	0.55
1:W:281:ILE:HG21	3:Y:352:LYS:HZ1	1.72	0.55
1:A:421:ARG:HB2	1:A:462:MET:HE3	1.88	0.55
2:R:68:ILE:H	2:R:68:ILE:HD12	1.71	0.55
2:B:763:THR:HG21	2:B:816:LYS:HD3	1.87	0.55
1:A:652:SER:HB3	1:A:787:ARG:NE	2.19	0.55
2:R:783:VAL:CG1	2:R:784:ARG:HB2	2.34	0.55
7:G:66:TYR:CD1	7:G:66:TYR:N	2.74	0.55
7:G:38:ILE:HG22	7:G:39:SER:N	2.22	0.55
7:V:11:LEU:HB2	7:V:57:ALA:HB3	1.88	0.55
2:R:46:ILE:HG13	2:R:66:ILE:HG12	1.88	0.55
11:L:6:LEU:CD1	11:L:16:GLU:HB2	2.36	0.55
1:W:142:LYS:O	1:W:143:ALA:HB3	2.06	0.55
3:C:262:LEU:HD11	3:C:283:VAL:HG11	1.89	0.55
4:D:13:ILE:HG22	4:D:230:LEU:HB2	1.88	0.55
1:W:652:SER:HB3	1:W:787:ARG:NE	2.19	0.55
1:A:553:SER:OG	1:A:592:ILE:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:VAL:HG11	2:B:407:VAL:HG13	1.89	0.55
1:W:737:VAL:HG23	1:W:738:LEU:H	1.72	0.55
5:T:38:ILE:HG12	5:T:44:LEU:HD11	1.88	0.55
4:D:154:ALA:HA	4:D:157:ILE:HG13	1.89	0.55
1:A:867:ASP:HA	1:A:870:ARG:HH21	1.72	0.55
3:C:328:GLN:HB3	3:C:332:HIS:ND1	2.22	0.55
3:C:29:VAL:HB	3:C:32:LEU:HD12	1.88	0.55
4:S:57:ILE:O	4:S:61:ARG:HG3	2.07	0.55
3:C:25:PRO:HA	3:C:28:ILE:HA	1.89	0.55
1:A:668:ALA:HB2	1:A:707:LEU:HD22	1.89	0.55
2:B:665:GLN:CG	2:B:667:PRO:HD2	2.31	0.55
1:A:866:VAL:O	1:A:870:ARG:NH2	2.38	0.55
1:A:864:LYS:NZ	3:C:29:VAL:O	2.34	0.55
12:O:43:TYR:HB3	2:R:938:LEU:HD23	1.89	0.55
2:R:447:ASP:HA	1:W:803:ARG:HG2	1.88	0.55
1:A:330:PRO:HG3	2:B:734:GLY:CA	2.36	0.55
2:B:724:ASN:O	12:N:47:ARG:HD2	2.07	0.55
1:W:600:LYS:HB2	1:W:732:GLY:CA	2.37	0.55
9:I:41:LEU:HD23	5:T:64:GLY:N	2.22	0.55
5:T:18:PHE:HD2	3:Y:392:PRO:HB3	1.72	0.55
7:V:55:VAL:HG23	7:V:117:GLN:HA	1.89	0.55
3:Y:29:VAL:HB	3:Y:32:LEU:HD12	1.89	0.54
3:C:47:GLU:HG3	3:C:51:ILE:HG12	1.89	0.54
1:W:421:ARG:HB2	1:W:462:MET:HE3	1.89	0.54
3:C:274:THR:HG22	3:C:276:ASN:H	1.73	0.54
1:W:10:LYS:HG2	3:Y:363:VAL:HG13	1.89	0.54
7:V:66:TYR:CD1	7:V:66:TYR:N	2.75	0.54
3:C:341:VAL:H	3:C:364:GLU:HG2	1.72	0.54
2:B:51:GLU:HB2	2:B:53:PRO:HD3	1.88	0.54
2:R:1007:ARG:HH22	2:R:1022:GLY:N	2.05	0.54
2:B:583:ILE:HB	2:B:643:LEU:HB3	1.90	0.54
1:A:354:THR:O	1:A:356:TRP:N	2.41	0.54
4:S:159:VAL:HG23	4:S:231:GLU:H	1.72	0.54
1:W:417:VAL:HG13	1:W:465:HIS:O	2.07	0.54
11:M:6:LEU:HD11	11:M:16:GLU:HB2	1.88	0.54
1:A:655:ASP:O	1:A:657:VAL:N	2.41	0.54
1:A:838:VAL:HB	1:A:847:GLN:HB2	1.89	0.54
1:A:421:ARG:HG3	1:A:462:MET:HG2	1.89	0.54
2:R:585:VAL:HG21	2:R:636:LEU:HD11	1.89	0.54
2:R:186:ILE:HD12	2:R:209:LYS:HB3	1.88	0.54
2:R:872:LEU:HD22	2:R:874:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:875:VAL:O	1:W:877:GLY:N	2.36	0.54
2:B:783:VAL:CG1	2:B:784:ARG:HB2	2.38	0.54
1:W:509:LEU:O	1:W:548:GLY:HA3	2.07	0.54
1:A:737:VAL:HG23	1:A:738:LEU:H	1.73	0.54
3:Y:244:LYS:CA	3:Y:245:LYS:HB3	2.23	0.54
2:R:768:TYR:HB2	2:R:773:GLU:H	1.72	0.54
5:T:38:ILE:HG12	5:T:44:LEU:CD1	2.37	0.54
5:E:64:GLY:N	9:K:41:LEU:HD23	2.23	0.54
9:K:26:ARG:CG	9:K:27:LEU:H	2.19	0.54
2:B:768:TYR:HB2	2:B:773:GLU:H	1.73	0.54
1:A:155:LYS:CB	1:A:156:ILE:HA	2.38	0.54
5:E:38:ILE:HG12	5:E:44:LEU:HD11	1.90	0.54
4:D:120:SER:OG	4:D:121:ILE:HD12	2.08	0.54
1:A:509:LEU:O	1:A:548:GLY:HA3	2.07	0.54
1:W:82:ILE:HD12	1:W:156:ILE:HG13	1.89	0.54
3:C:29:VAL:O	3:C:30:GLU:HB2	2.08	0.54
2:R:136:TYR:HD2	2:R:140:LYS:HB3	1.72	0.54
4:D:161:LEU:HG	4:D:163:ILE:HD13	1.90	0.54
2:R:286:GLU:OE1	2:R:286:GLU:N	2.41	0.54
2:R:406:TRP:CG	2:R:407:VAL:N	2.74	0.54
1:A:318:VAL:HG11	2:B:1051:ARG:O	2.07	0.54
2:R:520:TRP:O	2:R:521:SER:CB	2.56	0.54
4:S:154:ALA:HA	4:S:157:ILE:HG13	1.90	0.54
1:W:125:TRP:N	1:W:126:PRO:CD	2.71	0.54
2:B:26:LEU:HG	2:B:27:VAL:HG23	1.90	0.54
1:W:763:THR:HB	1:W:764:ARG:HD2	1.90	0.54
2:R:1102:LEU:HD13	1:W:308:ARG:NH2	2.23	0.54
2:R:774:ASP:HB3	2:R:817:VAL:O	2.08	0.54
13:X:24:VAL:HG13	13:X:24:VAL:O	2.08	0.54
1:A:600:LYS:HB2	1:A:732:GLY:HA3	1.90	0.54
2:R:985:ARG:HG3	4:S:205:LEU:HD23	1.89	0.54
5:T:89:VAL:HG13	5:T:139:GLY:HA2	1.90	0.54
1:W:848:VAL:O	1:W:849:ALA:HB3	2.07	0.54
3:C:106:ARG:O	3:C:110:ILE:HG22	2.07	0.53
2:R:491:THR:HG21	2:R:552:ILE:HD13	1.89	0.53
2:R:233:LEU:HD13	2:R:315:ALA:HA	1.89	0.53
2:R:662:GLU:O	1:W:789:GLY:HA2	2.09	0.53
1:A:763:THR:HB	1:A:764:ARG:HD2	1.89	0.53
2:B:884:ARG:HH11	2:B:992:TYR:HB3	1.69	0.53
1:A:470:GLU:HG3	9:K:41:LEU:HD12	1.89	0.53
4:S:13:ILE:HG22	4:S:230:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:GLY:H	5:E:137:GLN:HB3	1.73	0.53
1:W:58:CYS:SG	1:W:60:THR:CG2	2.97	0.53
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.38	0.53
4:S:96:ILE:HG12	4:S:145:LEU:HD11	1.90	0.53
2:R:249:PRO:HG2	2:R:253:ASN:OD1	2.09	0.53
1:W:829:ASP:O	1:W:840:SER:HA	2.09	0.53
3:Y:25:PRO:HA	3:Y:28:ILE:HA	1.91	0.53
1:W:563:HIS:CE1	1:W:587:VAL:HG13	2.43	0.53
3:Y:122:MET:HG2	3:Y:274:THR:HG23	1.91	0.53
1:A:848:VAL:O	1:A:849:ALA:CB	2.56	0.53
4:S:96:ILE:HG22	4:S:116:SER:HA	1.91	0.53
1:W:853:ASP:HB3	1:W:855:VAL:H	1.73	0.53
1:A:378:VAL:HG13	1:A:386:ILE:HB	1.90	0.53
2:R:493:TYR:OH	2:R:530:VAL:HG13	2.08	0.53
2:R:1050:ASP:HA	2:R:1054:ASP:HB2	1.89	0.53
1:W:490:ARG:HH22	3:Y:306:LEU:HD11	1.73	0.53
1:W:879:LYS:HZ3	3:Y:44:THR:HB	1.74	0.53
7:G:29:ILE:O	7:G:39:SER:HA	2.09	0.53
2:B:973:THR:HG21	2:B:988:PHE:HE1	1.74	0.53
1:W:125:TRP:N	1:W:126:PRO:HD2	2.23	0.53
2:R:625:GLU:OE1	1:W:761:TYR:HB3	2.09	0.53
7:G:11:LEU:HB2	7:G:57:ALA:HB3	1.91	0.53
3:C:11:SER:HB2	3:C:14:GLU:HB2	1.89	0.53
11:M:40:PHE:HB3	11:M:58:LEU:HD23	1.89	0.53
2:B:665:GLN:HG2	2:B:667:PRO:CD	2.32	0.53
2:R:627:ALA:HB1	2:R:642:HIS:CD2	2.38	0.53
2:B:233:LEU:HD13	2:B:315:ALA:HA	1.91	0.53
2:R:927:ILE:HG23	2:R:987:TYR:CE2	2.44	0.53
2:R:600:LEU:O	2:R:601:ASP:HB2	2.07	0.53
3:Y:197:VAL:HB	3:Y:208:ILE:HB	1.91	0.53
1:W:868:VAL:HG22	3:Y:39:LYS:HZ3	1.72	0.53
4:D:242:LEU:HB3	11:L:87:ILE:HD13	1.90	0.53
3:C:337:GLU:HG3	3:C:339:ASN:OD1	2.08	0.53
2:B:59:LEU:HD23	2:B:107:GLU:HG2	1.91	0.53
13:X:17:GLN:C	13:X:19:LYS:H	2.12	0.53
1:W:289:HIS:HB2	1:W:295:LEU:HD21	1.91	0.53
1:A:755:GLU:HB3	1:A:758:LYS:NZ	2.24	0.53
1:W:323:ARG:HH21	1:W:422:GLN:HE21	1.55	0.53
11:M:44:TYR:CD1	1:W:527:VAL:HA	2.44	0.53
3:Y:331:ARG:H	3:Y:331:ARG:CD	2.22	0.53
3:Y:328:GLN:HB3	3:Y:332:HIS:ND1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:SER:HB3	2:B:866:LYS:HG2	1.91	0.53
12:N:35:LEU:HD13	12:N:46:ARG:HG3	1.91	0.53
1:W:413:ASP:OD2	1:W:436:ARG:HA	2.08	0.53
5:T:98:PHE:HA	5:T:106:GLY:O	2.09	0.53
2:B:627:ALA:HB1	2:B:642:HIS:CD2	2.41	0.53
2:R:916:HIS:CD2	1:W:733:ALA:HB1	2.44	0.53
11:M:6:LEU:CD1	11:M:16:GLU:HB2	2.39	0.53
2:B:15:LYS:NZ	2:B:599:LYS:HE3	2.24	0.53
2:R:459:PHE:HZ	1:W:795:LEU:HD11	1.74	0.53
8:Z:38:ARG:HB3	8:Z:40:GLU:OE1	2.09	0.53
2:B:286:GLU:OE1	2:B:286:GLU:N	2.42	0.53
6:U:71:VAL:HG13	6:U:72:LEU:HD12	1.91	0.52
2:R:973:THR:HG21	2:R:988:PHE:HE1	1.74	0.52
2:R:26:LEU:HG	2:R:27:VAL:HG23	1.89	0.52
1:W:604:GLY:O	1:W:607:GLN:HB2	2.09	0.52
2:B:658:ILE:O	2:B:661:PRO:HG3	2.10	0.52
4:D:38:VAL:CG1	4:D:39:MET:H	2.23	0.52
5:E:38:ILE:HG12	5:E:44:LEU:CD1	2.40	0.52
1:W:870:ARG:HD2	3:Y:57:LYS:HB3	1.91	0.52
1:A:542:PRO:HD3	7:G:70:ASP:O	2.08	0.52
2:B:345:ARG:HG3	2:B:576:GLY:HA3	1.92	0.52
1:A:457:PHE:CD1	2:B:738:GLU:HB2	2.44	0.52
1:A:220:ARG:HG2	1:A:235:LEU:HD22	1.91	0.52
4:S:38:VAL:CG1	4:S:39:MET:H	2.22	0.52
2:R:921:ARG:HH21	1:W:734:ARG:NH2	2.07	0.52
2:B:1069:TYR:CA	2:B:1070:ILE:HB	2.40	0.52
4:D:57:ILE:O	4:D:61:ARG:HG3	2.10	0.52
10:J:78:ARG:CZ	8:Z:82:ILE:HG22	2.39	0.52
2:B:855:ILE:O	13:P:34:ILE:HG23	2.09	0.52
2:B:493:TYR:OH	2:B:530:VAL:HG13	2.10	0.52
5:T:145:ARG:HD3	6:U:88:ILE:HG21	1.91	0.52
1:W:378:VAL:HG13	1:W:386:ILE:HB	1.90	0.52
1:A:258:PRO:HG2	1:A:261:ILE:HD12	1.90	0.52
2:R:284:LYS:HB3	2:R:287:ASN:HD22	1.75	0.52
6:F:48:ASP:HB3	6:F:51:SER:HB2	1.91	0.52
13:X:6:CYS:SG	13:X:18:LEU:HG	2.49	0.52
1:W:340:PRO:HD2	1:W:343:ILE:HG13	1.91	0.52
2:B:189:THR:HA	2:B:208:LEU:O	2.09	0.52
9:I:26:ARG:CG	9:I:27:LEU:H	2.20	0.52
1:W:78:VAL:HG21	1:W:253:ILE:HD11	1.92	0.52
1:A:734:ARG:HH22	2:B:917:ALA:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:8:LYS:HD3	13:X:13:PHE:HD2	1.73	0.52
1:W:535:GLY:O	1:W:536:GLU:HB2	2.08	0.52
2:B:459:PHE:O	2:B:670:THR:HG23	2.08	0.52
1:A:271:TYR:CE1	1:A:285:PRO:HB3	2.40	0.52
1:A:78:VAL:HG21	1:A:253:ILE:HD11	1.92	0.52
2:B:761:TYR:CE2	2:B:843:ARG:HG2	2.44	0.52
1:W:572:PRO:HG2	1:W:717:LYS:HE2	1.91	0.52
1:A:731:THR:O	1:A:733:ALA:N	2.42	0.52
2:R:928:MET:HG2	1:W:648:LEU:HD11	1.91	0.52
1:A:524:ILE:HD11	1:A:638:PHE:HD1	1.75	0.52
7:V:29:ILE:O	7:V:39:SER:HA	2.10	0.52
1:W:6:ILE:HD13	3:Y:375:ILE:HD11	1.90	0.52
1:W:428:ILE:HG22	1:W:452:PRO:HB3	1.92	0.52
1:W:449:VAL:HG12	1:W:452:PRO:HG2	1.91	0.52
1:A:345:ARG:HA	1:A:410:HIS:CD2	2.44	0.52
2:R:91:ARG:CD	2:R:856:THR:HG21	2.39	0.52
2:R:105:PRO:O	2:R:111:GLU:HB3	2.09	0.52
1:A:542:PRO:HG3	7:G:46:ILE:HG23	1.92	0.52
5:T:129:GLY:H	5:T:137:GLN:HB3	1.74	0.52
2:R:17:ILE:HG13	2:R:476:MET:SD	2.50	0.52
13:P:8:LYS:HD3	13:P:13:PHE:HD2	1.74	0.52
7:G:55:VAL:HG23	7:G:117:GLN:HA	1.91	0.52
2:B:742:ILE:HG23	2:B:912:ILE:HB	1.92	0.52
1:W:867:ASP:CA	1:W:870:ARG:HH22	2.23	0.52
1:W:864:LYS:HG3	1:W:864:LYS:O	2.08	0.52
7:G:87:ASN:O	7:G:88:ASN:C	2.47	0.52
3:Y:286:ILE:HG12	8:Z:49:ASP:OD2	2.09	0.52
1:W:855:VAL:O	3:Y:311:ARG:NH1	2.42	0.52
4:D:96:ILE:HG22	4:D:116:SER:HA	1.92	0.52
1:A:372:TRP:O	1:A:374:GLY:N	2.42	0.52
13:P:9:CYS:SG	13:P:10:TRP:N	2.82	0.52
2:B:46:ILE:HG13	2:B:66:ILE:HG12	1.91	0.51
1:A:125:TRP:N	1:A:126:PRO:CD	2.73	0.51
5:E:98:PHE:HA	5:E:106:GLY:O	2.10	0.51
1:W:681:ASN:HB2	1:W:683:GLU:HG2	1.91	0.51
2:B:807:VAL:HG11	2:B:813:LEU:HD21	1.92	0.51
2:R:213:PHE:HB3	2:R:214:HIS:ND1	2.24	0.51
1:W:867:ASP:CA	1:W:870:ARG:NH2	2.69	0.51
1:A:324:THR:HG22	1:A:325:VAL:N	2.25	0.51
4:S:66:PRO:HG2	4:S:124:ILE:CG1	2.36	0.51
3:Y:29:VAL:O	3:Y:30:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PRO:HA	5:E:18:PHE:CE1	2.45	0.51
2:R:1069:TYR:CA	2:R:1070:ILE:HB	2.40	0.51
2:B:688:GLN:O	2:B:868:ARG:NH2	2.43	0.51
2:R:187:THR:HB	2:R:188:HIS:CD2	2.45	0.51
4:S:26:ASN:O	4:S:30:ARG:HG3	2.11	0.51
1:W:155:LYS:CB	1:W:156:ILE:HA	2.41	0.51
10:J:78:ARG:NH1	8:Z:82:ILE:HG22	2.26	0.51
1:W:450:CYS:N	1:W:451:PRO:CD	2.73	0.51
2:B:320:TYR:CD2	2:B:529:LEU:HD12	2.45	0.51
7:G:76:TYR:O	7:G:85:SER:HB2	2.10	0.51
2:B:371:GLN:O	2:B:375:SER:CB	2.59	0.51
1:W:876:VAL:HA	1:W:879:LYS:HB2	1.92	0.51
2:B:380:ARG:HH11	2:B:381:LYS:HE3	1.76	0.51
1:A:672:VAL:HG13	1:A:700:ILE:HG12	1.93	0.51
1:W:852:ASP:CG	8:Z:75:VAL:HG21	2.30	0.51
2:B:730:ILE:HG12	2:B:986:ILE:HG21	1.92	0.51
2:B:597:ILE:HD13	2:B:597:ILE:H	1.75	0.51
1:A:851:GLY:HA3	3:C:311:ARG:HG3	1.92	0.51
3:Y:122:MET:SD	3:Y:256:SER:HA	2.50	0.51
1:W:323:ARG:NH2	1:W:422:GLN:HE21	2.09	0.51
1:W:449:VAL:HG11	1:W:482:VAL:HG11	1.93	0.51
2:R:522:LYS:HG2	2:R:532:TYR:CE2	2.45	0.51
3:C:290:ARG:HA	3:C:321:THR:HG21	1.92	0.51
1:A:725:ALA:HA	1:A:728:MET:HE2	1.91	0.51
1:A:450:CYS:HB2	1:A:451:PRO:HD3	1.93	0.51
2:B:284:LYS:HB3	2:B:287:ASN:HD22	1.75	0.51
1:A:572:PRO:HG2	1:A:717:LYS:HE2	1.92	0.51
2:B:898:VAL:HG21	4:D:34:LEU:HD21	1.93	0.51
4:D:78:TRP:HB3	4:D:79:PRO:HD2	1.91	0.51
1:A:68:CYS:N	1:A:69:PRO:HD3	2.26	0.51
1:A:515:LEU:HB3	1:A:545:TYR:CD1	2.46	0.51
8:H:40:GLU:CD	8:H:40:GLU:H	2.13	0.51
12:O:15:ALA:HB1	4:S:129:PRO:HD2	1.93	0.51
4:D:153:HIS:HB3	4:D:155:LYS:HG2	1.92	0.51
4:D:175:ASN:HD21	4:D:194:LYS:HA	1.75	0.51
3:Y:290:ARG:HA	3:Y:321:THR:HG21	1.92	0.51
1:A:53:GLU:HB3	1:A:54:PRO:HD2	1.93	0.51
1:W:668:ALA:HB2	1:W:707:LEU:HD22	1.92	0.51
1:W:427:ARG:NH1	3:Y:73:VAL:HG11	2.25	0.51
9:I:47:ALA:HB1	9:I:48:PRO:HD2	1.92	0.51
1:W:734:ARG:HH11	1:W:734:ARG:CB	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:ASP:OD2	2:B:132:PRO:HD2	2.10	0.51
1:A:604:GLY:O	1:A:607:GLN:HB2	2.11	0.51
3:C:29:VAL:HG12	3:C:61:GLU:HG3	1.93	0.51
2:B:668:ARG:HH12	2:B:921:ARG:HD2	1.75	0.51
2:B:433:ILE:HG12	2:B:470:VAL:HB	1.91	0.51
3:Y:11:SER:O	3:Y:45:ARG:NH2	2.44	0.51
5:E:89:VAL:HG13	5:E:139:GLY:HA2	1.92	0.51
12:N:42:ARG:C	12:N:44:CYS:H	2.13	0.50
1:W:428:ILE:HD11	1:W:489:PRO:HD3	1.92	0.50
4:D:45:TYR:HB3	13:P:42:ILE:HD11	1.93	0.50
2:B:872:LEU:HD22	2:B:874:ILE:HG13	1.92	0.50
2:B:1080:TYR:HB3	2:B:1091:LEU:HD12	1.92	0.50
2:B:594:ARG:HH11	2:B:610:LEU:HD23	1.76	0.50
12:O:15:ALA:HB3	4:S:128:ILE:HG23	1.92	0.50
9:I:44:ALA:C	9:I:46:GLY:H	2.15	0.50
2:R:1009:ARG:HA	1:W:319:ASP:OD2	2.11	0.50
9:I:79:ARG:HB2	3:Y:387:GLU:HG3	1.93	0.50
1:A:122:LYS:HZ2	8:H:40:GLU:HG2	1.76	0.50
4:S:93:TYR:CD2	4:S:146:ARG:HB3	2.46	0.50
1:W:524:ILE:HD11	1:W:638:PHE:HD1	1.75	0.50
1:W:662:TYR:HA	1:W:665:ILE:HG12	1.93	0.50
1:A:681:ASN:HB2	1:A:683:GLU:HG2	1.94	0.50
5:E:79:PRO:HB2	5:E:160:ILE:HD11	1.94	0.50
6:U:41:LEU:HA	6:U:44:VAL:HG12	1.92	0.50
2:B:774:ASP:HB3	2:B:817:VAL:O	2.12	0.50
1:W:541:ALA:CB	1:W:542:PRO:CD	2.89	0.50
1:A:487:ILE:HD12	1:A:858:MET:O	2.11	0.50
1:W:125:TRP:CZ3	8:Z:82:ILE:HG21	2.47	0.50
5:T:144:ALA:HA	5:T:169:LEU:HD23	1.93	0.50
1:A:342:ILE:HD13	1:A:345:ARG:HH22	1.77	0.50
1:A:125:TRP:N	1:A:126:PRO:HD2	2.26	0.50
1:A:563:HIS:CE1	1:A:587:VAL:HG13	2.46	0.50
2:R:1080:TYR:HB3	2:R:1091:LEU:HD12	1.93	0.50
2:R:742:ILE:HG23	2:R:912:ILE:HB	1.93	0.50
4:D:93:TYR:CD2	4:D:146:ARG:HB3	2.47	0.50
3:Y:106:ARG:O	3:Y:110:ILE:HG22	2.11	0.50
1:A:662:TYR:HA	1:A:665:ILE:HG12	1.93	0.50
2:R:672:GLN:OE1	2:R:884:ARG:HA	2.11	0.50
3:C:341:VAL:HG12	3:C:344:ARG:NH2	2.27	0.50
1:W:600:LYS:HB2	1:W:732:GLY:HA3	1.93	0.50
1:A:258:PRO:HD2	1:A:261:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:341:TYR:CE1	2:R:452:GLN:HG2	2.46	0.50
1:A:102:GLY:O	1:A:103:ARG:HG2	2.11	0.50
2:R:1031:PHE:HE1	1:W:430:MET:CE	2.25	0.50
1:W:490:ARG:HH12	3:Y:306:LEU:HG	1.76	0.50
1:W:489:PRO:HA	1:W:858:MET:HB2	1.93	0.50
2:B:155:PHE:CD2	2:B:155:PHE:N	2.79	0.50
1:W:651:VAL:CG1	1:W:743:MET:HB3	2.42	0.50
1:W:549:LYS:HD2	1:W:593:LEU:HD22	1.93	0.50
1:A:281:ILE:HG21	3:C:352:LYS:NZ	2.26	0.50
1:W:332:ILE:O	1:W:332:ILE:HG13	2.11	0.50
2:R:371:GLN:HE22	2:R:389:ARG:NE	2.10	0.50
2:R:598:GLU:HA	2:R:602:SER:HB2	1.94	0.50
2:R:774:ASP:HB2	2:R:818:SER:HA	1.94	0.50
2:B:462:PRO:HG2	2:B:470:VAL:HG13	1.93	0.50
1:A:24:VAL:O	1:A:73:GLY:HA2	2.12	0.50
9:I:61:VAL:O	9:I:63:SER:N	2.45	0.50
1:W:354:THR:O	1:W:356:TRP:N	2.45	0.50
2:R:13:ARG:HH12	2:R:647:SER:H	1.59	0.50
7:V:76:TYR:O	7:V:85:SER:HB2	2.11	0.50
2:R:345:ARG:HG3	2:R:576:GLY:HA3	1.94	0.50
12:O:14:ILE:HG13	12:O:48:MET:HG3	1.93	0.50
2:B:491:THR:HG21	2:B:552:ILE:HD13	1.94	0.50
2:B:927:ILE:HG23	2:B:987:TYR:CE2	2.47	0.50
2:B:736:ASN:N	2:B:736:ASN:HD22	1.97	0.50
4:D:124:ILE:HD13	4:D:234:GLY:HA3	1.94	0.50
2:R:1092:PHE:CD2	1:W:4:LYS:HD2	2.47	0.50
1:A:753:ARG:HG3	1:A:804:GLU:OE1	2.11	0.50
2:R:605:ILE:HG23	2:R:606:THR:H	1.77	0.50
2:R:939:SER:HA	2:R:963:TYR:CE2	2.47	0.50
2:B:205:ILE:HD12	2:B:205:ILE:H	1.76	0.50
2:R:763:THR:HG21	2:R:816:LYS:HD3	1.94	0.49
4:S:161:LEU:O	4:S:230:LEU:HA	2.12	0.49
1:W:846:ILE:HG22	1:W:847:GLN:HG3	1.93	0.49
4:D:161:LEU:O	4:D:230:LEU:HA	2.12	0.49
2:R:1119:GLU:OE2	1:W:7:LYS:HE2	2.11	0.49
12:O:1:MET:HB2	2:R:699:HIS:O	2.11	0.49
2:R:1101:LYS:HE3	1:W:69:PRO:HG2	1.94	0.49
1:A:324:THR:HG22	1:A:325:VAL:H	1.77	0.49
3:C:392:PRO:HB3	5:E:18:PHE:HD2	1.76	0.49
2:R:320:TYR:CD2	2:R:529:LEU:HD12	2.47	0.49
2:B:873:ARG:HB3	2:B:999:MET:CE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ILE:HD11	1:A:699:TYR:CE2	2.47	0.49
2:B:483:ILE:HD12	2:B:555:GLU:HB2	1.93	0.49
2:R:703:ARG:NH2	2:R:942:ILE:HG21	2.27	0.49
2:B:794:LEU:HD22	2:B:805:VAL:HG11	1.93	0.49
1:W:220:ARG:HG2	1:W:235:LEU:HB3	1.95	0.49
1:W:58:CYS:H	1:W:62:GLY:HA2	1.76	0.49
3:Y:146:TYR:HD1	3:Y:235:LYS:N	2.10	0.49
1:W:851:GLY:O	1:W:853:ASP:N	2.45	0.49
1:W:852:ASP:CB	8:Z:75:VAL:HG21	2.42	0.49
1:A:450:CYS:N	1:A:451:PRO:CD	2.75	0.49
2:R:272:LEU:O	2:R:276:GLY:N	2.35	0.49
3:C:197:VAL:HB	3:C:208:ILE:HB	1.94	0.49
1:W:755:GLU:HB3	1:W:758:LYS:HZ1	1.78	0.49
2:B:760:LEU:HD12	2:B:868:ARG:HB3	1.94	0.49
3:Y:242:VAL:HG22	3:Y:251:ILE:HG12	1.95	0.49
9:K:32:ILE:O	9:K:36:ILE:HG12	2.12	0.49
2:R:1051:ARG:NE	2:R:1051:ARG:HA	2.27	0.49
2:R:597:ILE:H	2:R:597:ILE:HD13	1.76	0.49
7:V:87:ASN:O	7:V:88:ASN:C	2.50	0.49
12:O:42:ARG:C	12:O:44:CYS:H	2.16	0.49
2:B:633:PRO:HD3	2:B:643:LEU:HD11	1.93	0.49
2:B:417:LEU:HD21	2:B:425:MET:HG3	1.93	0.49
1:A:94:LEU:HD21	1:A:180:ILE:HG23	1.94	0.49
2:B:701:PRO:HB2	2:B:720:PRO:HG2	1.95	0.49
1:A:734:ARG:HB3	1:A:734:ARG:HH11	1.78	0.49
7:G:20:ARG:HA	7:G:27:SER:HA	1.94	0.49
2:R:884:ARG:HH11	2:R:992:TYR:HB3	1.76	0.49
3:Y:301:LEU:HD22	3:Y:308:VAL:HG12	1.95	0.49
2:R:766:VAL:HG23	2:R:773:GLU:HG3	1.94	0.49
4:D:96:ILE:HG12	4:D:145:LEU:HD11	1.95	0.49
5:E:89:VAL:HA	5:E:99:VAL:HA	1.93	0.49
1:A:665:ILE:O	1:A:669:LYS:HG3	2.13	0.49
2:R:1092:PHE:CE2	1:W:4:LYS:HD2	2.48	0.49
2:B:939:SER:HA	2:B:963:TYR:CE2	2.48	0.49
2:R:21:PHE:HZ	2:R:475:LEU:HB3	1.77	0.49
12:N:18:TRP:CE2	12:N:22:ILE:HG12	2.47	0.49
2:B:1081:VAL:HG22	2:B:1085:HIS:HA	1.94	0.49
9:I:32:ILE:O	9:I:36:ILE:HG12	2.13	0.49
11:M:48:PRO:HG2	2:R:735:TYR:HE2	1.77	0.49
2:R:27:VAL:HG12	2:R:429:LEU:HB2	1.94	0.49
3:Y:11:SER:HB2	3:Y:14:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:68:CYS:N	1:W:69:PRO:HD3	2.28	0.49
4:D:66:PRO:HG2	4:D:124:ILE:CG1	2.40	0.49
4:S:205:LEU:O	4:S:207:GLU:N	2.46	0.49
2:B:975:ASP:HB3	2:B:978:THR:CG2	2.43	0.49
2:B:768:TYR:C	2:B:770:GLY:H	2.15	0.49
3:C:122:MET:SD	3:C:256:SER:HA	2.53	0.49
2:B:1069:TYR:HB2	2:B:1070:ILE:HB	1.94	0.49
8:H:13:ILE:HG21	8:H:19:LYS:NZ	2.28	0.49
11:L:40:PHE:HB3	11:L:58:LEU:HD23	1.95	0.49
7:V:20:ARG:HA	7:V:27:SER:HA	1.93	0.49
1:W:490:ARG:HD2	1:W:491:TYR:HD1	1.78	0.48
8:H:25:ILE:HG13	10:Q:51:TRP:HB3	1.94	0.48
4:D:233:VAL:HG21	12:N:6:ARG:HH21	1.77	0.48
1:A:113:LYS:HG2	1:A:116:ARG:CZ	2.43	0.48
1:A:764:ARG:H	1:A:764:ARG:HD3	1.78	0.48
2:B:284:LYS:HB3	2:B:287:ASN:HB2	1.95	0.48
2:R:1081:VAL:HG22	2:R:1085:HIS:HA	1.95	0.48
1:A:413:ASP:OD2	1:A:436:ARG:HA	2.13	0.48
3:Y:35:LEU:HD23	3:Y:38:ASN:HD22	1.77	0.48
9:K:61:VAL:O	9:K:63:SER:N	2.45	0.48
1:W:80:PRO:HD2	1:W:178:SER:HB3	1.95	0.48
11:M:13:LEU:HD23	11:M:57:ILE:HD13	1.95	0.48
13:P:17:GLN:C	13:P:19:LYS:H	2.16	0.48
1:W:24:VAL:O	1:W:73:GLY:HA2	2.13	0.48
2:R:736:ASN:HD22	2:R:736:ASN:N	2.00	0.48
4:S:124:ILE:HD13	4:S:234:GLY:HA3	1.94	0.48
1:A:541:ALA:HB3	7:G:72:CYS:H	1.77	0.48
2:B:680:LEU:HD21	2:B:997:HIS:HB3	1.95	0.48
4:S:44:VAL:HA	4:S:143:ALA:HA	1.94	0.48
1:A:506:ALA:O	1:A:510:THR:OG1	2.29	0.48
3:Y:330:GLY:HA3	3:Y:331:ARG:HH11	1.79	0.48
1:A:490:ARG:HD2	1:A:491:TYR:HD1	1.78	0.48
1:W:731:THR:O	1:W:733:ALA:N	2.46	0.48
1:W:420:ASN:HB2	1:W:430:MET:HG3	1.96	0.48
2:R:345:ARG:HA	2:R:576:GLY:O	2.14	0.48
1:A:535:GLY:O	1:A:536:GLU:HB2	2.13	0.48
2:B:749:GLU:O	4:D:60:HIS:HE1	1.96	0.48
1:W:220:ARG:HG2	1:W:235:LEU:HD22	1.95	0.48
4:S:13:ILE:HB	4:S:238:PRO:HB2	1.96	0.48
1:A:864:LYS:O	1:A:864:LYS:HG3	2.13	0.48
2:B:543:ILE:CD1	2:B:558:VAL:HG21	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:281:ILE:HD13	3:Y:352:LYS:HZ1	1.77	0.48
2:B:13:ARG:NH1	2:B:647:SER:H	2.11	0.48
2:R:852:LEU:HB3	2:R:868:ARG:HG2	1.95	0.48
5:T:89:VAL:HA	5:T:99:VAL:HA	1.95	0.48
1:A:142:LYS:O	1:A:143:ALA:HB3	2.13	0.48
12:O:18:TRP:CE2	12:O:22:ILE:HG12	2.48	0.48
1:W:234:ASP:OD1	1:W:296:ARG:NH1	2.47	0.48
3:C:244:LYS:HG3	3:C:249:TYR:HE2	1.79	0.48
2:B:105:PRO:O	2:B:111:GLU:HB3	2.13	0.48
2:R:371:GLN:O	2:R:375:SER:CB	2.61	0.48
1:A:651:VAL:CG1	1:A:743:MET:HB3	2.42	0.48
2:R:1094:VAL:HG11	1:W:6:ILE:HG13	1.95	0.48
11:M:86:GLU:O	11:M:90:LEU:HB2	2.14	0.48
2:R:59:LEU:HD23	2:R:107:GLU:HG2	1.95	0.48
3:C:242:VAL:HG22	3:C:251:ILE:HG12	1.95	0.48
2:B:904:VAL:HG21	4:D:204:THR:CG2	2.44	0.48
2:B:893:MET:HE2	2:B:894:LEU:H	1.76	0.48
2:R:974:TYR:CE2	4:S:165:ARG:HA	2.48	0.48
2:R:772:GLN:O	2:R:773:GLU:HB3	2.13	0.48
2:R:119:ILE:HG22	2:R:393:VAL:HG21	1.94	0.48
3:C:297:ILE:O	3:C:301:LEU:HD12	2.13	0.48
7:G:31:MET:HE2	7:G:55:VAL:HG11	1.96	0.48
1:A:801:GLY:O	1:A:804:GLU:HG2	2.14	0.48
1:A:364:PHE:CD1	1:A:409:ARG:HD2	2.49	0.48
1:A:340:PRO:HD2	1:A:343:ILE:HG13	1.94	0.48
2:B:520:TRP:O	2:B:521:SER:CB	2.61	0.48
2:R:404:GLY:HA2	2:R:414:SER:H	1.78	0.48
2:B:856:THR:HG23	13:P:32:LYS:O	2.13	0.48
2:R:256:PHE:C	2:R:258:SER:H	2.17	0.48
12:O:7:CYS:HB3	12:O:10:CYS:SG	2.53	0.48
2:B:1103:LEU:O	2:B:1107:LEU:HG	2.13	0.48
1:W:764:ARG:N	1:W:764:ARG:HD3	2.29	0.48
1:A:764:ARG:HD3	1:A:764:ARG:N	2.28	0.48
1:W:635:PHE:O	1:W:639:VAL:HG23	2.14	0.48
1:W:749:GLN:HA	1:W:781:PHE:HA	1.95	0.48
1:A:439:LYS:HB3	11:L:49:LEU:HD22	1.95	0.48
2:R:648:PRO:HB3	2:R:947:PRO:HG2	1.95	0.48
6:U:48:ASP:HB3	6:U:51:SER:HB2	1.95	0.48
2:B:672:GLN:OE1	2:B:884:ARG:HA	2.13	0.48
12:O:6:ARG:HB2	4:S:64:LEU:HD22	1.94	0.48
1:A:449:VAL:HG11	1:A:482:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:VAL:HA	4:D:143:ALA:HA	1.95	0.48
2:R:189:THR:HA	2:R:208:LEU:O	2.14	0.48
2:R:72:ARG:HG2	2:R:82:GLU:HG2	1.95	0.48
1:A:510:THR:O	1:A:549:LYS:HD3	2.13	0.48
5:E:82:GLN:HB3	6:F:88:ILE:HB	1.95	0.48
2:B:774:ASP:HB2	2:B:818:SER:HA	1.95	0.48
4:D:13:ILE:HB	4:D:238:PRO:HB2	1.96	0.48
4:S:116:SER:O	4:S:118:ASP:N	2.47	0.48
2:R:459:PHE:O	2:R:670:THR:HG23	2.14	0.48
2:B:187:THR:HB	2:B:188:HIS:CD2	2.49	0.48
2:R:633:PRO:HD3	2:R:643:LEU:HD11	1.95	0.48
2:B:1051:ARG:HA	2:B:1051:ARG:NE	2.29	0.48
1:W:764:ARG:HD3	1:W:764:ARG:H	1.78	0.48
1:W:487:ILE:HD12	1:W:858:MET:O	2.14	0.48
1:A:10:LYS:HG2	3:C:363:VAL:HG13	1.95	0.48
1:W:672:VAL:HG13	1:W:700:ILE:HG12	1.94	0.48
3:C:11:SER:O	3:C:45:ARG:NH2	2.47	0.47
2:R:284:LYS:HB3	2:R:287:ASN:HB2	1.96	0.47
1:W:94:LEU:HD21	1:W:180:ILE:HG23	1.94	0.47
3:C:391:ARG:HD2	9:K:75:PRO:HB2	1.96	0.47
1:W:102:GLY:O	1:W:103:ARG:HG2	2.13	0.47
2:R:66:ILE:HG23	2:R:101:LEU:HB2	1.96	0.47
2:B:679:ALA:CB	2:B:721:ALA:HB1	2.44	0.47
13:X:21:LEU:HD22	13:X:22:PRO:HA	1.96	0.47
1:W:782:ILE:HG23	1:W:794:GLU:CD	2.34	0.47
12:N:30:ASN:O	12:N:34:VAL:HG23	2.14	0.47
2:R:953:ILE:CD1	2:R:953:ILE:H	2.06	0.47
2:B:772:GLN:O	2:B:773:GLU:HB3	2.14	0.47
2:R:768:TYR:CD1	2:R:819:PRO:HG2	2.47	0.47
2:R:605:ILE:HG12	2:R:606:THR:H	1.78	0.47
2:B:893:MET:HE3	2:B:894:LEU:H	1.78	0.47
1:A:457:PHE:HD1	2:B:738:GLU:HB2	1.78	0.47
1:W:198:ASP:HB2	3:Y:361:GLY:HA3	1.96	0.47
3:Y:108:ILE:O	3:Y:111:VAL:HG12	2.13	0.47
6:U:47:CYS:SG	6:U:74:SER:HA	2.55	0.47
2:R:679:ALA:HB3	2:R:721:ALA:HB1	1.97	0.47
3:C:46:ASP:N	3:C:47:GLU:OE1	2.43	0.47
7:G:72:CYS:HA	7:G:114:LYS:HA	1.95	0.47
1:W:258:PRO:HG2	1:W:261:ILE:HD12	1.95	0.47
2:B:301:LEU:N	2:B:302:PRO:HD3	2.29	0.47
1:A:635:PHE:O	1:A:639:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLY:C	1:A:684:LEU:H	2.18	0.47
2:R:737:MET:H	2:R:740:SER:HB3	1.79	0.47
1:W:236:THR:O	1:W:240:VAL:HG23	2.15	0.47
4:D:159:VAL:HG23	4:D:231:GLU:H	1.78	0.47
1:W:525:LEU:HD11	1:W:551:VAL:HG23	1.96	0.47
2:B:658:ILE:HG12	2:B:672:GLN:HG2	1.96	0.47
1:W:271:TYR:CE1	1:W:285:PRO:HB3	2.43	0.47
1:W:553:SER:HB2	1:W:593:LEU:H	1.78	0.47
12:N:43:TYR:HA	12:N:46:ARG:HB3	1.96	0.47
1:W:296:ARG:HD2	1:W:296:ARG:H	1.79	0.47
6:F:41:LEU:HA	6:F:44:VAL:HG12	1.95	0.47
3:Y:33:LYS:HG3	3:Y:34:ASN:N	2.30	0.47
1:W:421:ARG:HG3	1:W:462:MET:CG	2.45	0.47
1:W:421:ARG:HD3	1:W:455:ALA:HB2	1.97	0.47
1:A:127:SER:HB2	3:C:360:ARG:HH12	1.80	0.47
2:R:446:ARG:NH1	1:W:807:VAL:HG13	2.29	0.47
7:V:72:CYS:HA	7:V:114:LYS:HA	1.97	0.47
2:R:493:TYR:HD2	2:R:497:VAL:O	1.97	0.47
10:J:66:ARG:NH1	8:Z:40:GLU:OE1	2.48	0.47
2:R:532:TYR:O	2:R:533:TYR:HB3	2.15	0.47
2:R:1063:VAL:O	2:R:1091:LEU:HA	2.15	0.47
2:B:1043:GLY:HA3	3:C:382:GLY:HA3	1.95	0.47
2:B:84:SER:HB2	2:B:144:ILE:HD12	1.97	0.47
7:V:32:SER:HA	7:V:37:ASN:OD1	2.15	0.47
1:W:12:GLY:HA3	1:W:201:THR:HG22	1.97	0.47
7:G:42:ILE:HG21	7:G:48:ILE:HG23	1.97	0.47
1:W:345:ARG:HA	1:W:410:HIS:CD2	2.49	0.47
2:B:747:SER:HB3	12:N:8:PHE:HB3	1.97	0.47
1:A:80:PRO:HD2	1:A:178:SER:HB3	1.96	0.47
2:R:555:GLU:HA	2:R:579:ARG:HH22	1.79	0.47
3:Y:285:GLY:HA2	8:Z:50:PRO:HG2	1.96	0.47
2:B:852:LEU:HB3	2:B:868:ARG:HG2	1.96	0.47
1:A:281:ILE:HG21	3:C:352:LYS:HZ3	1.77	0.47
1:A:749:GLN:HA	1:A:781:PHE:HA	1.96	0.47
12:O:30:ASN:O	12:O:34:VAL:HG23	2.14	0.47
1:W:357:ASN:OD1	1:W:357:ASN:C	2.53	0.47
2:R:975:ASP:HB3	2:R:978:THR:CG2	2.45	0.47
7:V:72:CYS:HB2	1:W:541:ALA:HB2	1.96	0.47
12:O:43:TYR:HA	12:O:46:ARG:HB3	1.96	0.47
11:M:38:VAL:HA	11:M:59:THR:HA	1.97	0.47
1:W:771:PRO:O	1:W:772:TYR:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:461:THR:CG2	2:R:468:GLY:H	2.15	0.47
9:K:23:TRP:HA	9:K:23:TRP:HE3	1.76	0.47
2:B:742:ILE:CG2	2:B:912:ILE:HB	2.44	0.47
2:R:888:LYS:HB3	1:W:458:ASP:HB2	1.96	0.47
2:R:807:VAL:HG11	2:R:813:LEU:HD21	1.96	0.47
3:C:117:PRO:HG2	3:C:120:PRO:HB3	1.97	0.47
2:R:376:LYS:C	2:R:378:ARG:H	2.18	0.47
3:Y:117:PRO:HG2	3:Y:120:PRO:HB3	1.97	0.47
2:R:374:LYS:HA	2:R:374:LYS:HD2	1.74	0.47
4:D:26:ASN:O	4:D:30:ARG:HG3	2.15	0.47
1:W:854:GLY:O	3:Y:64:ILE:HG12	2.15	0.46
9:K:23:TRP:C	9:K:25:ASN:H	2.18	0.46
2:R:380:ARG:HH11	2:R:381:LYS:HE3	1.79	0.46
7:V:89:GLY:HA2	1:W:549:LYS:NZ	2.31	0.46
12:N:44:CYS:SG	12:N:45:CYS:SG	3.13	0.46
3:C:25:PRO:O	3:C:28:ILE:HG12	2.15	0.46
1:A:846:ILE:HG22	1:A:847:GLN:HG3	1.97	0.46
1:W:258:PRO:HD2	1:W:261:ILE:HD12	1.96	0.46
3:C:142:ARG:HD2	3:C:178:GLY:HA3	1.97	0.46
1:W:490:ARG:HG2	3:Y:308:VAL:HG23	1.98	0.46
2:R:966:LEU:HD22	2:R:985:ARG:NH2	2.30	0.46
2:B:788:GLY:O	2:B:791:TYR:HB2	2.16	0.46
2:R:1069:TYR:HB2	2:R:1070:ILE:HB	1.97	0.46
1:A:417:VAL:HG11	1:A:464:LEU:CD1	2.45	0.46
2:R:624:GLU:OE1	1:W:761:TYR:OH	2.33	0.46
2:R:1031:PHE:HE1	1:W:430:MET:HE1	1.80	0.46
3:C:213:ILE:HA	3:C:216:ILE:HD11	1.97	0.46
5:T:79:PRO:HB2	5:T:160:ILE:HD11	1.97	0.46
2:B:171:ALA:HB1	2:B:174:ARG:HD2	1.97	0.46
2:R:716:TYR:OH	2:R:721:ALA:HB3	2.15	0.46
1:A:330:PRO:HG3	2:B:734:GLY:HA2	1.96	0.46
2:R:970:THR:HG22	2:R:987:TYR:HA	1.96	0.46
5:T:84:VAL:HG22	6:U:75:ILE:HD13	1.96	0.46
3:Y:142:ARG:HD2	3:Y:178:GLY:HA3	1.96	0.46
1:A:601:LYS:O	1:A:610:SER:HB2	2.15	0.46
3:Y:348:GLU:CD	3:Y:350:THR:HB	2.35	0.46
1:A:553:SER:HB2	1:A:593:LEU:H	1.81	0.46
5:E:144:ALA:HA	5:E:169:LEU:HD23	1.97	0.46
1:W:837:THR:HG22	1:W:838:VAL:N	2.31	0.46
2:R:46:ILE:HG13	2:R:66:ILE:CG1	2.45	0.46
4:S:232:SER:HB3	4:S:241:ILE:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:701:PRO:HB2	2:R:720:PRO:HG2	1.98	0.46
8:Z:13:ILE:HG21	8:Z:19:LYS:NZ	2.30	0.46
2:B:249:PRO:HG2	2:B:253:ASN:OD1	2.15	0.46
2:B:112:ALA:O	2:B:113:GLU:HB2	2.16	0.46
1:A:851:GLY:O	3:C:311:ARG:HD2	2.15	0.46
11:M:69:LEU:O	11:M:73:ILE:HG12	2.15	0.46
1:A:69:PRO:HB3	1:A:218:THR:HG21	1.96	0.46
2:B:961:LEU:HA	2:B:965:TYR:O	2.14	0.46
1:A:541:ALA:HB3	7:G:71:PHE:HA	1.98	0.46
1:W:561:ASN:HA	1:W:588:ILE:O	2.16	0.46
2:R:605:ILE:HG12	2:R:606:THR:N	2.31	0.46
11:L:13:LEU:HD23	11:L:57:ILE:HD13	1.97	0.46
3:C:389:THR:O	9:K:76:ILE:HA	2.15	0.46
3:Y:213:ILE:HA	3:Y:216:ILE:HD11	1.97	0.46
2:B:903:THR:HG22	2:B:904:VAL:H	1.80	0.46
11:M:73:ILE:HG21	4:S:257:GLU:HB2	1.98	0.46
2:B:371:GLN:HE22	2:B:389:ARG:NE	2.13	0.46
2:R:594:ARG:HH11	2:R:610:LEU:HD23	1.81	0.46
4:D:94:THR:HG23	4:D:145:LEU:HB2	1.97	0.46
11:L:74:GLU:HG2	11:L:77:ARG:HH21	1.81	0.46
8:H:64:ARG:O	8:H:64:ARG:HG2	2.15	0.46
3:Y:327:ARG:NH2	3:Y:337:GLU:HB3	2.23	0.46
3:C:331:ARG:HD3	3:C:331:ARG:N	2.28	0.46
5:T:88:GLU:HG2	5:T:141:LYS:HA	1.97	0.46
2:B:213:PHE:HB3	2:B:214:HIS:ND1	2.30	0.46
1:A:296:ARG:H	1:A:296:ARG:HD2	1.81	0.46
2:B:748:VAL:HG22	2:B:875:PRO:HG2	1.98	0.46
2:B:605:ILE:HG23	2:B:606:THR:H	1.80	0.46
1:A:332:ILE:HG13	1:A:332:ILE:O	2.15	0.46
9:I:53:ILE:HG23	9:I:55:ASN:HD22	1.80	0.46
4:D:205:LEU:O	4:D:207:GLU:N	2.49	0.46
1:W:864:LYS:HE2	8:Z:71:LEU:O	2.16	0.46
1:A:123:LYS:C	1:A:126:PRO:HD2	2.35	0.46
8:H:38:ARG:HB3	8:H:40:GLU:OE1	2.15	0.46
3:C:201:SER:HB2	3:C:204:THR:HB	1.97	0.46
2:R:322:ILE:O	2:R:326:ILE:HG12	2.15	0.46
1:W:655:ASP:O	1:W:657:VAL:N	2.48	0.46
2:B:648:PRO:HB3	2:B:947:PRO:HG2	1.98	0.46
3:C:35:LEU:HD23	3:C:38:ASN:HD22	1.81	0.46
3:Y:244:LYS:HG3	3:Y:249:TYR:HE2	1.80	0.46
1:W:69:PRO:HB3	1:W:218:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:170:ASP:O	3:Y:174:LEU:HD21	2.15	0.46
1:A:325:VAL:O	1:A:442:THR:HB	2.15	0.46
3:Y:276:ASN:O	3:Y:280:ILE:HG12	2.16	0.46
2:B:646:TRP:CZ3	2:B:648:PRO:HB2	2.51	0.46
4:S:175:ASN:HD21	4:S:194:LYS:HA	1.81	0.46
1:W:687:ILE:HD11	1:W:699:TYR:CE2	2.51	0.46
2:R:968:ASP:O	2:R:969:ALA:HB3	2.16	0.46
2:B:374:LYS:HA	2:B:374:LYS:HD2	1.73	0.46
3:Y:30:GLU:HB3	3:Y:31:ASP:H	1.49	0.46
3:C:33:LYS:HG3	3:C:34:ASN:N	2.30	0.46
1:A:874:ARG:HG3	3:C:53:ASP:OD2	2.16	0.46
1:W:308:ARG:HA	1:W:308:ARG:HD3	1.70	0.46
1:W:665:ILE:O	1:W:669:LYS:HG3	2.16	0.46
3:Y:106:ARG:O	3:Y:106:ARG:HG3	2.15	0.46
1:W:655:ASP:H	1:W:658:LYS:HD2	1.80	0.46
2:R:794:LEU:HD22	2:R:805:VAL:HG11	1.97	0.46
1:A:771:PRO:O	1:A:772:TYR:HB2	2.16	0.46
2:R:668:ARG:HH11	2:R:921:ARG:HB3	1.80	0.45
1:A:58:CYS:SG	1:A:60:THR:CG2	3.03	0.45
2:B:119:ILE:HG22	2:B:393:VAL:HG21	1.98	0.45
7:V:31:MET:HE2	7:V:55:VAL:HG11	1.98	0.45
1:A:837:THR:HG22	1:A:838:VAL:N	2.32	0.45
1:W:572:PRO:CG	1:W:717:LYS:HE2	2.46	0.45
4:S:77:ARG:HD2	4:S:92:CYS:SG	2.56	0.45
2:R:15:LYS:NZ	2:R:599:LYS:HE3	2.31	0.45
2:R:776:ILE:HG23	2:R:815:GLY:O	2.16	0.45
7:G:32:SER:HA	7:G:37:ASN:OD1	2.17	0.45
11:L:1:MET:HA	11:L:19:GLY:HA3	1.97	0.45
4:D:15:LEU:HD12	4:D:228:LEU:HD22	1.98	0.45
3:Y:338:LYS:HE2	3:Y:338:LYS:H	1.81	0.45
1:A:549:LYS:NZ	7:G:89:GLY:HA2	2.31	0.45
3:C:276:ASN:O	3:C:280:ILE:HG12	2.16	0.45
7:V:66:TYR:CE2	1:W:540:LEU:HB3	2.51	0.45
2:R:874:ILE:HD12	2:R:874:ILE:H	1.80	0.45
2:B:27:VAL:HG12	2:B:429:LEU:HB2	1.97	0.45
4:S:114:ILE:HD12	4:S:123:PRO:HG3	1.98	0.45
3:Y:28:ILE:HG13	3:Y:28:ILE:H	1.51	0.45
1:W:563:HIS:HB2	1:W:872:PHE:HE2	1.81	0.45
1:A:372:TRP:HB3	1:A:373:PRO:HD3	1.98	0.45
9:I:61:VAL:N	9:I:64:ILE:HG13	2.31	0.45
3:Y:104:LEU:O	3:Y:108:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:42:ILE:HG21	7:V:48:ILE:HG23	1.98	0.45
1:W:16:PRO:HA	1:W:19:ILE:HD12	1.98	0.45
5:T:131:LYS:HD2	5:T:136:ILE:HD13	1.99	0.45
2:R:322:ILE:HA	2:R:322:ILE:HD13	1.88	0.45
7:V:40:PHE:HZ	7:V:115:ILE:HG12	1.81	0.45
1:W:372:TRP:O	1:W:374:GLY:N	2.50	0.45
1:W:364:PHE:CD1	1:W:409:ARG:HD2	2.51	0.45
12:N:64:ARG:HH22	13:P:37:VAL:CG2	2.28	0.45
1:A:58:CYS:H	1:A:62:GLY:HA2	1.81	0.45
2:B:345:ARG:HA	2:B:576:GLY:O	2.16	0.45
5:T:145:ARG:HG3	5:T:169:LEU:HD21	1.99	0.45
3:C:231:ILE:HG22	3:C:232:LYS:H	1.80	0.45
9:I:76:ILE:HA	3:Y:389:THR:O	2.17	0.45
2:B:453:TRP:HZ3	2:B:644:GLU:CD	2.20	0.45
6:F:47:CYS:SG	6:F:74:SER:HA	2.56	0.45
3:C:331:ARG:CD	3:C:331:ARG:H	2.22	0.45
2:R:920:SER:HA	1:W:739:ASN:HD21	1.82	0.45
7:V:89:GLY:HA2	1:W:549:LYS:HZ1	1.82	0.45
1:W:113:LYS:HG2	1:W:116:ARG:CZ	2.46	0.45
1:W:541:ALA:HB3	1:W:542:PRO:HD3	1.97	0.45
1:A:491:TYR:O	1:A:493:GLY:N	2.50	0.45
1:A:489:PRO:HA	1:A:858:MET:HB2	1.99	0.45
1:A:428:ILE:HD11	1:A:489:PRO:HD3	1.97	0.45
2:R:921:ARG:NH2	1:W:734:ARG:NH2	2.64	0.45
2:B:776:ILE:HG23	2:B:815:GLY:O	2.16	0.45
1:A:280:GLU:HB2	1:A:300:GLN:NE2	2.31	0.45
3:C:145:GLU:HG2	3:C:239:ARG:HA	1.98	0.45
2:B:256:PHE:C	2:B:258:SER:H	2.20	0.45
3:Y:327:ARG:HH22	3:Y:337:GLU:CB	2.23	0.45
1:W:421:ARG:NH2	1:W:454:ASN:O	2.50	0.45
1:W:848:VAL:O	1:W:849:ALA:CB	2.64	0.45
1:A:561:ASN:HA	1:A:588:ILE:O	2.17	0.45
2:R:67:ARG:HG3	2:R:100:TRP:HB2	1.97	0.45
3:C:387:GLU:HG3	9:K:79:ARG:HB2	1.99	0.45
2:R:961:LEU:HA	2:R:965:TYR:O	2.16	0.45
2:R:981:LYS:O	2:R:981:LYS:HG3	2.16	0.45
2:B:766:VAL:H	2:B:767:LYS:HE3	1.82	0.45
5:E:88:GLU:HG2	5:E:141:LYS:HA	1.98	0.45
1:W:755:GLU:HB3	1:W:758:LYS:HZ2	1.80	0.45
5:E:91:GLN:O	5:E:98:PHE:HB2	2.17	0.45
2:B:970:THR:HG22	2:B:987:TYR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:CG2	1:A:358:ILE:HD13	2.47	0.45
3:Y:145:GLU:HG2	3:Y:239:ARG:HA	1.98	0.45
1:W:275:THR:HG23	1:W:279:ASN:ND2	2.31	0.45
2:R:1077:LYS:N	2:R:1078:ASN:HA	2.31	0.45
5:E:2:TYR:O	6:F:11:TYR:HA	2.17	0.45
2:R:294:GLN:HA	2:R:297:ASP:HB2	1.98	0.45
1:W:682:GLY:C	1:W:684:LEU:H	2.20	0.45
1:W:780:GLY:HA2	1:W:797:PHE:CG	2.52	0.45
2:B:904:VAL:HG21	4:D:204:THR:HG21	1.97	0.45
2:R:658:ILE:HG12	2:R:672:GLN:HG2	1.97	0.45
1:A:490:ARG:HH22	3:C:306:LEU:HD11	1.82	0.45
2:R:768:TYR:C	2:R:770:GLY:H	2.20	0.45
4:D:45:TYR:HB2	4:D:142:GLU:HB3	1.99	0.45
3:Y:106:ARG:HH22	3:Y:277:ILE:HD11	1.81	0.45
4:D:11:LYS:O	4:D:231:GLU:HA	2.16	0.45
1:W:820:GLN:O	1:W:824:ILE:HB	2.16	0.45
6:U:80:PRO:O	6:U:83:VAL:HG12	2.17	0.45
4:D:77:ARG:HD2	4:D:92:CYS:SG	2.57	0.45
2:R:748:VAL:HG22	2:R:875:PRO:HG2	1.98	0.45
11:L:86:GLU:O	11:L:90:LEU:HB2	2.16	0.45
2:R:730:ILE:HG12	2:R:986:ILE:HG21	1.98	0.45
4:S:78:TRP:HB3	4:S:79:PRO:HD2	1.99	0.45
8:H:58:LYS:O	8:H:60:GLY:N	2.48	0.45
3:C:327:ARG:NH2	3:C:337:GLU:HB3	2.24	0.45
3:Y:341:VAL:HG12	3:Y:344:ARG:NH2	2.29	0.45
2:R:1065:ASP:CB	2:R:1089:SER:HB2	2.43	0.45
2:B:766:VAL:HG23	2:B:773:GLU:HG3	1.98	0.45
1:W:736:SER:O	1:W:738:LEU:N	2.50	0.45
4:D:116:SER:O	4:D:118:ASP:N	2.50	0.45
1:W:102:GLY:HA3	1:W:187:VAL:HG12	1.97	0.45
1:A:622:GLU:OE1	1:A:622:GLU:HA	2.17	0.45
1:A:382:ASP:OD1	1:A:382:ASP:N	2.49	0.45
3:Y:159:ASP:HB2	3:Y:163:MET:HB2	1.99	0.45
2:R:632:GLU:CD	2:R:633:PRO:HD2	2.36	0.45
2:R:543:ILE:CD1	2:R:558:VAL:HG21	2.45	0.45
11:M:22:HIS:ND1	2:R:977:ARG:HB2	2.32	0.45
1:W:875:VAL:HG12	1:W:876:VAL:H	1.82	0.45
8:Z:39:PRO:HB2	8:Z:80:TYR:CD2	2.52	0.45
1:A:176:THR:HA	1:A:177:PRO:HD2	1.84	0.45
2:B:552:ILE:HG13	2:B:553:SER:H	1.82	0.45
3:Y:231:ILE:HG22	3:Y:232:LYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:83:ASP:HB2	7:V:101:LEU:HG	1.99	0.45
1:W:353:ILE:CG2	1:W:358:ILE:HD13	2.47	0.45
2:B:376:LYS:C	2:B:378:ARG:H	2.19	0.45
1:W:194:ILE:H	1:W:194:ILE:HG13	1.56	0.45
3:Y:348:GLU:OE1	3:Y:350:THR:CB	2.62	0.44
2:R:903:THR:HG22	2:R:904:VAL:H	1.82	0.44
1:W:110:GLU:HA	1:W:113:LYS:HD2	1.99	0.44
2:R:68:ILE:N	2:R:68:ILE:HD12	2.33	0.44
4:D:96:ILE:HD13	4:D:114:ILE:HG23	1.98	0.44
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.81	0.44
3:C:66:PRO:HD2	9:K:28:THR:HG22	1.99	0.44
2:B:857:GLU:CG	13:P:24:VAL:HG11	2.43	0.44
1:A:853:ASP:HB2	3:C:311:ARG:NH1	2.32	0.44
2:R:1000:VAL:HG21	1:W:442:THR:HG22	2.00	0.44
2:R:161:GLU:OE1	2:R:419:ARG:NH1	2.51	0.44
2:R:679:ALA:CB	2:R:721:ALA:HB1	2.47	0.44
3:Y:165:ILE:HG13	3:Y:219:LEU:HD23	2.00	0.44
3:C:384:GLY:HA2	5:E:61:PHE:CZ	2.52	0.44
5:E:60:VAL:HG22	5:E:61:PHE:H	1.81	0.44
1:W:600:LYS:O	1:W:601:LYS:CB	2.57	0.44
1:A:204:PRO:O	1:A:207:MET:HB2	2.17	0.44
12:O:1:MET:O	12:O:2:MET:HB2	2.16	0.44
1:A:438:LEU:HD12	11:L:47:HIS:CE1	2.53	0.44
2:B:166:THR:HG23	2:B:431:ARG:O	2.18	0.44
2:B:117:VAL:HG11	2:B:388:VAL:HG21	2.00	0.44
4:S:120:SER:OG	4:S:121:ILE:HD12	2.17	0.44
2:B:68:ILE:HD12	2:B:68:ILE:H	1.82	0.44
8:Z:64:ARG:O	8:Z:64:ARG:HG2	2.17	0.44
2:B:461:THR:HG21	2:B:468:GLY:N	2.09	0.44
2:R:28:ARG:HA	2:R:31:LEU:HD12	1.99	0.44
1:W:215:PRO:O	1:W:220:ARG:NH1	2.51	0.44
2:R:430:ARG:HH11	2:R:653:ILE:HG13	1.83	0.44
1:W:491:TYR:O	1:W:491:TYR:CG	2.70	0.44
3:Y:293:ILE:O	3:Y:297:ILE:HG12	2.18	0.44
8:H:63:ILE:CG2	8:H:65:ILE:HG13	2.48	0.44
7:V:112:PHE:HD2	7:V:114:LYS:HE3	1.81	0.44
1:A:655:ASP:H	1:A:658:LYS:HD2	1.81	0.44
1:W:782:ILE:HG12	1:W:794:GLU:HG2	2.00	0.44
1:A:236:THR:O	1:A:240:VAL:HG23	2.16	0.44
1:A:513:THR:HG21	7:G:25:ASN:HB2	1.98	0.44
11:L:38:VAL:HA	11:L:59:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:91:SER:O	9:I:92:LEU:HB2	2.17	0.44
4:D:129:PRO:HD2	12:N:15:ALA:HB1	1.99	0.44
7:G:40:PHE:HZ	7:G:115:ILE:HG12	1.83	0.44
8:Z:66:ILE:HG12	8:Z:76:VAL:HG22	1.99	0.44
4:S:144:ARG:HE	4:S:144:ARG:HB3	1.61	0.44
3:Y:320:MET:O	3:Y:327:ARG:HG2	2.17	0.44
8:Z:43:PRO:HB3	8:Z:79:ARG:HH11	1.82	0.44
2:R:1069:TYR:OH	2:R:1115:ARG:NH1	2.50	0.44
1:A:102:GLY:HA3	1:A:187:VAL:HG12	1.98	0.44
1:W:820:GLN:NE2	3:Y:79:GLY:HA3	2.32	0.44
1:W:515:LEU:HB3	1:W:545:TYR:CD1	2.52	0.44
3:C:269:ILE:HA	3:C:272:VAL:HG23	2.00	0.44
11:M:74:GLU:HG2	11:M:77:ARG:HH21	1.81	0.44
2:B:857:GLU:CD	13:P:24:VAL:CG1	2.86	0.44
1:A:867:ASP:CA	1:A:870:ARG:NH2	2.79	0.44
2:B:905:LYS:H	2:B:905:LYS:CE	2.30	0.44
2:B:380:ARG:HH11	2:B:381:LYS:CE	2.31	0.44
2:R:1102:LEU:HD22	1:W:308:ARG:HH21	1.83	0.44
2:B:284:LYS:HD3	2:B:287:ASN:ND2	2.33	0.44
2:R:742:ILE:CG2	2:R:912:ILE:HB	2.48	0.44
1:A:436:ARG:O	1:A:438:LEU:HD22	2.18	0.44
2:B:681:GLY:HA2	2:B:698:LEU:HB3	1.99	0.44
11:M:1:MET:HA	11:M:19:GLY:HA3	2.00	0.44
6:U:21:LEU:O	6:U:24:VAL:HG12	2.18	0.44
1:W:582:HIS:CD2	1:W:582:HIS:N	2.85	0.44
1:A:215:PRO:HB3	2:B:1109:SER:HB3	1.99	0.44
1:A:470:GLU:CG	9:K:41:LEU:HD12	2.48	0.44
2:B:766:VAL:N	2:B:767:LYS:HE3	2.33	0.44
7:G:112:PHE:HD2	7:G:114:LYS:HE3	1.83	0.44
12:N:42:ARG:O	12:N:44:CYS:N	2.50	0.44
2:B:606:THR:HB	2:B:609:ASP:OD1	2.17	0.44
1:A:7:LYS:HE2	2:B:1119:GLU:OE2	2.18	0.44
11:M:47:HIS:HE1	11:M:49:LEU:HD12	1.83	0.44
1:A:556:LEU:HA	1:A:557:PRO:HD3	1.88	0.44
2:B:432:VAL:HG21	2:B:456:MET:CE	2.47	0.44
3:Y:201:SER:HB2	3:Y:204:THR:HB	1.99	0.44
2:R:240:ASP:O	2:R:244:ALA:HB2	2.17	0.44
1:W:517:THR:H	1:W:520:GLU:HB2	1.83	0.44
2:R:892:GLY:HA2	1:W:328:PRO:HD2	1.98	0.44
3:Y:328:GLN:CB	3:Y:332:HIS:ND1	2.81	0.44
2:B:768:TYR:CD1	2:B:819:PRO:HG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:127:SER:HB2	3:Y:360:ARG:HH12	1.83	0.44
12:N:64:ARG:NH2	13:P:37:VAL:HG23	2.32	0.44
3:Y:47:GLU:HB3	3:Y:50:LYS:HB2	2.00	0.44
2:R:686:ASN:O	2:R:688:GLN:N	2.50	0.44
2:B:801:VAL:HG21	2:B:813:LEU:HD23	2.00	0.44
2:R:224:ILE:HD11	2:R:278:ARG:HD2	1.99	0.44
2:B:33:SER:HB2	2:B:348:LEU:HD13	2.00	0.44
1:A:582:HIS:CD2	1:A:582:HIS:N	2.86	0.44
6:F:14:TYR:HD2	6:F:74:SER:OG	1.86	0.44
1:W:204:PRO:O	1:W:207:MET:HB2	2.17	0.44
3:Y:226:ILE:HG13	3:Y:226:ILE:H	1.68	0.44
2:B:1007:ARG:HE	2:B:1026:GLU:C	2.20	0.44
3:C:28:ILE:HG13	3:C:28:ILE:H	1.59	0.44
2:B:900:MET:SD	2:B:912:ILE:HD11	2.58	0.44
4:D:98:ILE:HD11	4:D:114:ILE:HG12	2.00	0.44
4:D:78:TRP:CB	4:D:79:PRO:HD2	2.46	0.44
4:S:90:GLU:HB3	4:S:91:LYS:H	1.54	0.44
5:E:131:LYS:HD2	5:E:136:ILE:HD13	2.00	0.44
2:R:1057:ASP:N	2:R:1057:ASP:OD2	2.51	0.44
6:U:4:VAL:O	6:U:4:VAL:HG13	2.18	0.44
3:C:327:ARG:HG3	3:C:334:VAL:HG23	2.00	0.43
3:Y:308:VAL:HG13	3:Y:313:ILE:HD11	2.00	0.43
1:W:304:GLY:O	3:Y:349:VAL:HG21	2.18	0.43
1:A:653:LEU:HD21	1:A:744:ALA:O	2.18	0.43
12:N:42:ARG:C	12:N:44:CYS:N	2.72	0.43
5:T:91:GLN:O	5:T:98:PHE:HB2	2.18	0.43
2:R:1119:GLU:HB2	1:W:7:LYS:HB2	1.99	0.43
2:B:84:SER:HB3	2:B:87:GLU:OE2	2.18	0.43
2:B:322:ILE:HA	2:B:322:ILE:HD13	1.85	0.43
4:S:178:LYS:O	4:S:182:VAL:HG22	2.18	0.43
2:R:460:GLU:HG2	2:R:673:SER:HB3	2.00	0.43
1:W:427:ARG:HH11	3:Y:73:VAL:HG11	1.83	0.43
1:A:215:PRO:O	1:A:220:ARG:NH1	2.51	0.43
1:W:867:ASP:HB2	3:Y:39:LYS:HZ3	1.82	0.43
4:D:64:LEU:HD22	12:N:6:ARG:HB2	2.00	0.43
3:C:330:GLY:HA3	3:C:331:ARG:HH11	1.83	0.43
1:W:506:ALA:O	1:W:510:THR:OG1	2.34	0.43
9:K:61:VAL:N	9:K:64:ILE:HG13	2.32	0.43
3:Y:323:THR:O	3:Y:325:VAL:N	2.51	0.43
1:W:53:GLU:HB3	1:W:54:PRO:HD2	1.99	0.43
1:W:56:GLN:HB3	1:W:57:LYS:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:338:GLY:O	1:W:443:PHE:HA	2.18	0.43
2:R:1029:LEU:HB3	2:R:1030:ARG:H	1.59	0.43
1:A:766:LEU:HB3	1:A:767:PRO:HD2	1.99	0.43
2:B:1065:ASP:CB	2:B:1089:SER:HB2	2.46	0.43
3:Y:330:GLY:HA3	3:Y:331:ARG:NH1	2.34	0.43
2:B:907:VAL:HG21	12:N:43:TYR:CE2	2.53	0.43
1:A:752:VAL:O	1:A:753:ARG:C	2.55	0.43
4:D:167:TYR:HA	4:D:168:PRO:HD3	1.85	0.43
2:R:463:GLU:OE1	2:R:463:GLU:N	2.47	0.43
1:A:855:VAL:HG13	3:C:63:LEU:O	2.19	0.43
2:B:31:LEU:HA	2:B:125:MET:HE3	1.97	0.43
2:B:641:THR:HB	2:B:642:HIS:CD2	2.53	0.43
12:O:42:ARG:O	12:O:44:CYS:N	2.51	0.43
11:M:48:PRO:HD3	1:W:331:ASN:ND2	2.34	0.43
1:A:101:CYS:HB2	1:A:102:GLY:H	1.54	0.43
1:A:343:ILE:HG22	1:A:347:LEU:HD12	2.00	0.43
12:O:60:ILE:HD11	4:S:134:GLY:N	2.32	0.43
2:R:157:VAL:O	2:R:159:GLY:N	2.51	0.43
8:Z:58:LYS:O	8:Z:60:GLY:N	2.46	0.43
1:A:215:PRO:HG2	1:A:220:ARG:HD2	2.01	0.43
2:R:583:ILE:HB	2:R:643:LEU:HB3	2.00	0.43
1:A:471:GLU:CG	9:K:41:LEU:HD13	2.44	0.43
12:O:44:CYS:SG	12:O:45:CYS:N	2.91	0.43
4:S:8:LYS:HB2	4:S:13:ILE:HG12	1.99	0.43
5:T:15:PRO:HA	5:T:18:PHE:CE1	2.54	0.43
1:A:777:GLU:HG3	1:A:783:TYR:CE2	2.49	0.43
8:H:69:SER:HB2	8:H:75:VAL:HG23	1.98	0.43
8:Z:49:ASP:HA	8:Z:50:PRO:HD2	1.81	0.43
1:A:482:VAL:C	1:A:484:LYS:H	2.22	0.43
1:A:541:ALA:HB3	1:A:542:PRO:HD3	1.99	0.43
1:A:258:PRO:CD	1:A:261:ILE:HD12	2.47	0.43
1:A:561:ASN:HB2	1:A:872:PHE:O	2.18	0.43
2:R:13:ARG:NH1	2:R:647:SER:H	2.16	0.43
2:R:524:ILE:HG13	2:R:529:LEU:HA	1.99	0.43
7:V:48:ILE:HG22	7:V:49:PHE:H	1.83	0.43
4:D:90:GLU:HB3	4:D:91:LYS:H	1.55	0.43
1:A:557:PRO:HG2	1:A:619:TYR:CE1	2.54	0.43
2:B:460:GLU:HG2	2:B:673:SER:HB3	2.00	0.43
1:A:418:LEU:HD11	2:B:1047:LEU:HD21	2.01	0.43
1:A:780:GLY:HA2	1:A:797:PHE:CG	2.53	0.43
2:R:179:THR:HG22	2:R:181:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:177:VAL:HG23	2:R:336:ASP:OD1	2.18	0.43
2:B:972:VAL:HG21	4:D:205:LEU:HB3	2.00	0.43
1:A:875:VAL:HG12	1:A:876:VAL:H	1.83	0.43
9:K:47:ALA:HB1	9:K:48:PRO:HD2	2.00	0.43
1:A:237:HIS:HE1	1:A:289:HIS:CD2	2.36	0.43
2:R:1078:ASN:HD22	2:R:1079:LYS:HG2	1.82	0.43
2:R:166:THR:HG23	2:R:431:ARG:O	2.17	0.43
1:A:420:ASN:HB2	1:A:430:MET:HG3	2.00	0.43
2:B:179:THR:HG22	2:B:181:LYS:HB2	2.01	0.43
2:R:131:ASP:OD2	2:R:132:PRO:HD2	2.18	0.43
5:E:85:VAL:HG23	6:F:14:TYR:OH	2.19	0.43
1:A:323:ARG:NH2	1:A:422:GLN:HE21	2.15	0.43
2:R:662:GLU:H	2:R:662:GLU:HG3	1.53	0.43
8:Z:40:GLU:CD	8:Z:40:GLU:H	2.21	0.43
1:A:572:PRO:CG	1:A:717:LYS:HE2	2.48	0.43
1:A:472:ALA:HB1	2:B:1047:LEU:HD12	2.00	0.43
1:W:280:GLU:HB2	1:W:300:GLN:NE2	2.33	0.43
1:A:338:GLY:O	1:A:443:PHE:HA	2.18	0.43
3:C:126:LEU:HB2	3:C:131:LYS:HG3	2.01	0.43
1:A:16:PRO:HA	1:A:19:ILE:HD12	2.01	0.43
1:W:586:VAL:HA	1:W:596:GLY:HA3	1.99	0.43
3:Y:371:GLU:N	3:Y:371:GLU:OE2	2.39	0.43
1:W:615:LEU:HD22	1:W:623:TYR:OH	2.19	0.43
7:G:83:ASP:HB2	7:G:101:LEU:HG	1.99	0.43
2:R:777:VAL:HG12	2:R:778:MET:H	1.84	0.43
2:B:279:VAL:HB	2:B:280:ALA:H	1.68	0.43
2:B:904:VAL:HG11	4:D:204:THR:HG22	2.01	0.43
3:Y:165:ILE:HG22	3:Y:207:ASN:HD22	1.84	0.43
2:B:985:ARG:HD2	4:D:206:CYS:HA	2.00	0.43
2:B:765:GLU:HA	2:B:767:LYS:HZ1	1.84	0.43
1:W:561:ASN:HB2	1:W:872:PHE:O	2.18	0.43
4:D:114:ILE:HD12	4:D:123:PRO:HG3	2.01	0.43
2:R:605:ILE:HG23	2:R:606:THR:N	2.34	0.43
2:R:1072:TRP:C	2:R:1073:TYR:HD2	2.22	0.43
1:A:782:ILE:HG23	1:A:794:GLU:CD	2.38	0.43
4:S:258:LYS:O	4:S:261:VAL:HG22	2.19	0.43
2:B:163:VAL:O	2:B:414:SER:HA	2.19	0.43
2:B:1077:LYS:N	2:B:1078:ASN:HA	2.32	0.43
4:D:232:SER:HB3	4:D:241:ILE:CD1	2.48	0.43
1:W:335:ASP:O	1:W:433:HIS:HA	2.19	0.43
2:B:1057:ASP:OD2	2:B:1057:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:ASP:O	3:C:174:LEU:HD21	2.19	0.43
9:I:41:LEU:HD12	1:W:470:GLU:CG	2.45	0.43
2:R:51:GLU:C	2:R:53:PRO:HD3	2.39	0.43
3:C:81:PRO:HB3	3:C:306:LEU:HD21	2.00	0.43
12:N:7:CYS:HB3	12:N:10:CYS:SG	2.59	0.43
9:I:64:ILE:CD1	1:W:356:TRP:CE2	3.02	0.43
2:B:86:MET:HE2	2:B:89:ARG:HH21	1.84	0.43
4:S:15:LEU:HD12	4:S:228:LEU:HD22	2.01	0.43
1:W:570:SER:O	1:W:571:GLY:C	2.56	0.43
2:B:240:ASP:O	2:B:244:ALA:HB2	2.18	0.43
2:B:180:GLY:O	2:B:182:THR:N	2.52	0.43
12:N:1:MET:O	12:N:2:MET:HB2	2.19	0.43
1:A:586:VAL:HA	1:A:596:GLY:HA3	2.01	0.43
2:B:953:ILE:O	2:B:957:GLN:HG3	2.17	0.43
2:B:668:ARG:HH11	2:B:921:ARG:HB3	1.84	0.43
2:R:14:TRP:CD1	2:R:709:ARG:NH1	2.87	0.43
12:O:5:ILE:HG12	4:S:64:LEU:HB3	2.00	0.43
2:B:1005:HIS:CE1	2:B:1007:ARG:HD2	2.54	0.43
2:B:781:PRO:HA	2:B:786:TYR:CZ	2.53	0.43
2:B:913:LEU:HD22	2:B:914:ASN:H	1.84	0.43
1:W:417:VAL:HG11	1:W:464:LEU:CD1	2.49	0.43
2:R:284:LYS:HD3	2:R:287:ASN:ND2	2.34	0.43
1:W:524:ILE:CG2	1:W:634:VAL:HG13	2.49	0.43
2:R:913:LEU:HD22	2:R:914:ASN:H	1.83	0.43
2:R:914:ASN:HA	2:R:915:PRO:HD2	1.82	0.43
2:R:1078:ASN:ND2	2:R:1079:LYS:HG2	2.33	0.43
2:B:689:LEU:CD1	12:N:62:TYR:HB3	2.49	0.43
5:E:112:GLN:HB3	5:E:163:THR:HG23	2.01	0.43
1:A:104:VAL:HG12	1:A:104:VAL:O	2.19	0.43
3:C:159:ASP:HB2	3:C:163:MET:HB2	2.01	0.42
2:R:52:ILE:N	2:R:53:PRO:CD	2.81	0.42
2:B:46:ILE:HG13	2:B:66:ILE:CG1	2.49	0.42
12:O:4:PRO:HA	4:S:61:ARG:HH12	1.84	0.42
4:S:11:LYS:O	4:S:231:GLU:HA	2.19	0.42
2:R:914:ASN:HD21	1:W:501:ASP:CG	2.23	0.42
1:W:372:TRP:HB3	1:W:373:PRO:HD3	2.01	0.42
1:A:765:THR:HG22	1:A:766:LEU:HD22	2.00	0.42
1:W:765:THR:HG22	1:W:766:LEU:HD22	2.02	0.42
2:R:1021:GLU:HG2	1:W:317:ARG:NH2	2.34	0.42
2:R:1046:MET:HB2	1:W:475:GLU:OE2	2.19	0.42
2:R:483:ILE:HD12	2:R:555:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:VAL:C	2:B:159:GLY:N	2.72	0.42
2:B:532:TYR:O	2:B:533:TYR:HB3	2.19	0.42
1:A:736:SER:O	1:A:738:LEU:N	2.52	0.42
10:J:78:ARG:NH2	8:Z:82:ILE:HG22	2.33	0.42
1:W:524:ILE:C	1:W:526:GLY:H	2.21	0.42
3:Y:232:LYS:HE3	3:Y:232:LYS:HB2	1.90	0.42
2:R:796:GLU:O	2:R:797:ASP:C	2.58	0.42
12:O:8:PHE:HB3	2:R:747:SER:HB3	2.00	0.42
3:C:165:ILE:HG22	3:C:207:ASN:HD22	1.83	0.42
2:B:659:PRO:O	2:B:660:TYR:C	2.57	0.42
2:R:205:ILE:H	2:R:205:ILE:HD12	1.83	0.42
4:D:144:ARG:HB3	4:D:144:ARG:HE	1.63	0.42
5:E:30:LEU:HD22	5:E:72:PHE:HE1	1.82	0.42
12:O:6:ARG:HH21	4:S:233:VAL:HG21	1.85	0.42
1:W:176:THR:HA	1:W:177:PRO:HD2	1.83	0.42
2:R:552:ILE:HG13	2:R:553:SER:H	1.85	0.42
4:D:96:ILE:HD13	4:D:114:ILE:CG2	2.49	0.42
1:W:342:ILE:HD13	1:W:345:ARG:HH22	1.84	0.42
3:Y:119:THR:N	3:Y:120:PRO:HD3	2.34	0.42
1:A:782:ILE:HG12	1:A:794:GLU:HG2	2.00	0.42
2:R:122:LEU:HD11	2:R:353:PHE:CE2	2.54	0.42
1:W:481:LEU:HD23	1:W:481:LEU:HA	1.90	0.42
2:B:466:ASN:HD22	2:B:466:ASN:HA	1.59	0.42
2:B:981:LYS:HG3	2:B:981:LYS:O	2.18	0.42
1:A:573:ARG:NH1	1:A:573:ARG:CG	2.61	0.42
2:B:703:ARG:CD	2:B:717:THR:HG22	2.47	0.42
1:W:870:ARG:CZ	1:W:870:ARG:HB2	2.44	0.42
11:M:23:THR:HG23	4:S:30:ARG:HB2	2.00	0.42
3:C:112:ASP:OD1	3:C:329:ILE:HG22	2.19	0.42
8:H:39:PRO:HB2	8:H:80:TYR:CD2	2.54	0.42
3:C:146:TYR:HD1	3:C:235:LYS:N	2.14	0.42
2:R:462:PRO:HG2	2:R:470:VAL:HG13	2.01	0.42
12:O:46:ARG:HD2	2:R:937:ALA:O	2.19	0.42
2:B:233:LEU:HD22	2:B:311:ARG:O	2.19	0.42
1:W:289:HIS:O	1:W:291:SER:N	2.49	0.42
1:W:413:ASP:HA	1:W:435:VAL:O	2.19	0.42
2:R:1051:ARG:O	1:W:318:VAL:HG11	2.18	0.42
4:D:30:ARG:HB2	11:L:23:THR:HG23	2.02	0.42
2:R:364:PHE:HE1	2:R:388:VAL:HG13	1.84	0.42
4:S:172:ILE:HG22	4:S:174:GLY:O	2.19	0.42
2:R:951:THR:HA	2:R:952:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:123:THR:HG22	3:Y:252:LEU:HD22	2.00	0.42
2:R:814:ILE:O	2:R:839:SER:HB2	2.19	0.42
2:R:539:LEU:O	2:R:543:ILE:HG13	2.20	0.42
1:W:729:ALA:O	1:W:730:ARG:CB	2.67	0.42
2:B:52:ILE:N	2:B:53:PRO:CD	2.82	0.42
1:A:490:ARG:HD2	1:A:491:TYR:CD1	2.54	0.42
1:W:653:LEU:HB3	1:W:719:LEU:HD12	2.02	0.42
2:R:1103:LEU:O	2:R:1107:LEU:HG	2.19	0.42
2:R:180:GLY:O	2:R:182:THR:N	2.50	0.42
2:B:1072:TRP:HB3	2:B:1073:TYR:H	1.44	0.42
1:A:275:THR:HG23	1:A:279:ASN:ND2	2.34	0.42
2:R:301:LEU:N	2:R:302:PRO:HD3	2.34	0.42
1:W:438:LEU:HG	1:W:444:ARG:NH1	2.34	0.42
13:P:21:LEU:HD22	13:P:22:PRO:HA	2.00	0.42
1:A:86:PHE:HA	1:A:89:HIS:HD2	1.83	0.42
2:B:125:MET:SD	2:B:153:GLY:HA2	2.60	0.42
1:W:490:ARG:HD2	1:W:491:TYR:CD1	2.55	0.42
2:R:632:GLU:OE1	2:R:633:PRO:HD2	2.20	0.42
9:I:65:ALA:HA	9:I:68:GLU:HG2	2.02	0.42
3:Y:122:MET:HE2	3:Y:124:ILE:HD11	2.02	0.42
2:R:668:ARG:HH12	2:R:921:ARG:HD2	1.85	0.42
13:X:17:GLN:C	13:X:19:LYS:N	2.72	0.42
5:E:79:PRO:CB	5:E:160:ILE:HD11	2.50	0.42
2:B:679:ALA:HB3	2:B:721:ALA:HB1	2.01	0.42
2:B:605:ILE:HG12	2:B:606:THR:H	1.85	0.42
4:D:90:GLU:O	4:D:92:CYS:N	2.53	0.42
1:W:756:ARG:NH2	1:W:774:ILE:HG22	2.34	0.42
2:B:43:GLN:HA	2:B:66:ILE:CD1	2.48	0.42
1:A:542:PRO:HD3	7:G:71:PHE:HA	2.02	0.42
2:B:600:LEU:O	2:B:601:ASP:CB	2.67	0.42
1:W:517:THR:N	1:W:520:GLU:HB2	2.35	0.42
2:B:237:THR:HB	2:B:240:ASP:HB2	2.02	0.42
2:R:1113:SER:O	1:W:11:PHE:HA	2.19	0.42
3:C:108:ILE:O	3:C:111:VAL:HG12	2.20	0.42
10:Q:45:MET:HB3	10:Q:68:PHE:HE1	1.84	0.42
3:C:286:ILE:HG23	3:C:324:GLY:O	2.20	0.42
3:C:162:SER:HB2	3:C:210:PHE:CZ	2.55	0.42
3:C:210:PHE:HB3	3:C:211:ALA:H	1.53	0.42
3:C:322:ARG:O	3:C:323:THR:HB	2.19	0.42
1:A:458:ASP:HB2	2:B:888:LYS:HB3	2.01	0.42
1:A:507:TYR:CD1	1:A:597:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:85:VAL:HG23	6:U:14:TYR:OH	2.19	0.42
2:B:430:ARG:NH1	2:B:653:ILE:HG13	2.35	0.42
1:W:106:ILE:HG22	1:W:107:SER:N	2.28	0.42
3:C:226:ILE:HG13	3:C:226:ILE:H	1.69	0.42
9:I:23:TRP:C	9:I:25:ASN:H	2.22	0.42
4:S:96:ILE:HD13	4:S:114:ILE:HG23	2.01	0.42
3:Y:239:ARG:O	3:Y:253:THR:HA	2.19	0.42
3:Y:80:GLU:OE1	3:Y:81:PRO:HD3	2.19	0.42
3:C:109:GLU:OE2	3:C:118:SER:OG	2.33	0.42
5:E:34:TYR:O	5:E:45:VAL:HG13	2.20	0.42
1:W:104:VAL:O	1:W:137:LYS:HG2	2.20	0.42
2:B:1005:HIS:CE1	2:B:1007:ARG:NH1	2.87	0.42
1:W:592:ILE:O	1:W:594:LEU:HD22	2.19	0.42
1:A:421:ARG:NH2	1:A:454:ASN:O	2.53	0.42
1:A:524:ILE:C	1:A:526:GLY:H	2.23	0.42
9:K:60:ASP:O	9:K:61:VAL:O	2.37	0.42
2:B:122:LEU:HD11	2:B:353:PHE:CE2	2.55	0.42
4:S:6:LEU:HB3	4:S:14:ASP:HB3	2.02	0.42
2:R:1074:ASP:HB3	2:R:1075:LYS:CA	2.50	0.42
1:A:648:LEU:HD21	1:A:787:ARG:HD3	2.02	0.42
3:Y:13:LEU:HD21	3:Y:48:ILE:HG23	2.01	0.42
12:O:47:ARG:NH1	2:R:726:ILE:HD12	2.34	0.42
8:H:25:ILE:CG1	10:Q:51:TRP:HE3	2.24	0.42
1:A:284:LEU:HD23	1:A:286:PRO:HG3	2.02	0.42
2:R:905:LYS:HE3	2:R:965:TYR:HE2	1.85	0.42
2:R:905:LYS:CE	2:R:905:LYS:H	2.27	0.42
2:R:906:GLY:H	4:S:163:ILE:HD11	1.84	0.42
1:W:740:ILE:HA	1:W:743:MET:HE3	2.02	0.42
1:W:58:CYS:HA	1:W:59:PRO:HD3	1.83	0.42
1:A:113:LYS:HA	1:A:116:ARG:HB3	2.02	0.42
1:A:541:ALA:CB	1:A:542:PRO:CD	2.98	0.42
1:A:156:ILE:HG21	1:A:270:GLN:O	2.19	0.42
1:A:14:LEU:HB3	2:B:1111:ILE:HG23	2.02	0.42
1:W:258:PRO:CD	1:W:261:ILE:HD12	2.50	0.42
1:W:353:ILE:HG21	1:W:358:ILE:HD13	2.01	0.42
3:Y:322:ARG:O	3:Y:323:THR:HB	2.20	0.42
3:C:388:LEU:HD11	9:K:34:ARG:HG3	2.02	0.42
4:D:101:GLU:HB3	4:D:138:LYS:HG3	2.01	0.42
10:Q:57:GLY:C	10:Q:61:VAL:HB	2.41	0.42
11:L:44:TYR:CE2	11:L:54:ILE:HB	2.55	0.42
1:W:573:ARG:NH2	1:W:721:PRO:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:868:VAL:HG13	3:Y:39:LYS:HE2	2.01	0.41
2:R:591:LEU:HB2	2:R:594:ARG:HD2	2.02	0.41
2:R:922:MET:SD	1:W:739:ASN:HB2	2.60	0.41
1:W:196:GLY:O	3:Y:360:ARG:HD3	2.20	0.41
1:W:752:VAL:O	1:W:753:ARG:C	2.59	0.41
2:B:762:SER:HB3	2:B:866:LYS:HA	2.02	0.41
5:T:82:GLN:HB3	6:U:88:ILE:HG13	2.01	0.41
2:R:606:THR:HB	2:R:609:ASP:OD1	2.20	0.41
2:B:873:ARG:HB3	2:B:999:MET:HE3	2.01	0.41
3:C:102:LEU:HD21	3:C:119:THR:OG1	2.20	0.41
1:A:353:ILE:HD13	1:A:405:TYR:HB2	2.02	0.41
2:B:322:ILE:O	2:B:326:ILE:HG12	2.19	0.41
6:F:21:LEU:O	6:F:24:VAL:HG12	2.19	0.41
1:A:819:MET:SD	3:C:107:LEU:HD22	2.60	0.41
12:O:19:GLN:HB2	12:O:20:PRO:HD3	2.01	0.41
1:A:653:LEU:HB3	1:A:719:LEU:HD12	2.02	0.41
2:R:686:ASN:C	2:R:688:GLN:N	2.74	0.41
1:W:142:LYS:O	1:W:143:ALA:CB	2.68	0.41
1:W:851:GLY:HA3	3:Y:311:ARG:HG3	2.02	0.41
2:R:600:LEU:O	2:R:601:ASP:CB	2.69	0.41
2:R:646:TRP:CZ3	2:R:648:PRO:HB2	2.55	0.41
1:W:46:ASP:H	1:W:47:PRO:CD	2.33	0.41
1:A:256:GLY:O	1:A:257:ALA:HB3	2.20	0.41
2:R:196:THR:OG1	2:R:200:ARG:O	2.38	0.41
1:A:56:GLN:HB3	1:A:57:LYS:H	1.66	0.41
2:R:440:GLN:OE1	2:R:440:GLN:HA	2.20	0.41
2:R:703:ARG:HH22	2:R:942:ILE:HG21	1.85	0.41
1:W:491:TYR:O	1:W:492:GLY:C	2.58	0.41
3:Y:297:ILE:O	3:Y:301:LEU:HD12	2.20	0.41
5:E:145:ARG:HG3	5:E:169:LEU:HD21	2.02	0.41
2:B:765:GLU:HA	2:B:767:LYS:NZ	2.35	0.41
2:B:1007:ARG:NH2	2:B:1026:GLU:O	2.39	0.41
2:B:905:LYS:HE3	2:B:965:TYR:HE2	1.86	0.41
4:S:38:VAL:HG13	4:S:39:MET:H	1.85	0.41
2:R:1047:LEU:HD11	1:W:418:LEU:HD11	2.02	0.41
1:A:156:ILE:HD13	1:A:270:GLN:O	2.20	0.41
7:G:48:ILE:HG22	7:G:49:PHE:H	1.84	0.41
2:R:84:SER:HB2	2:R:144:ILE:HD12	2.01	0.41
2:R:453:TRP:HZ3	2:R:644:GLU:CD	2.23	0.41
1:A:815:GLN:O	1:A:818:TYR:HB3	2.20	0.41
2:B:165:VAL:O	2:B:167:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:HB3	1:A:361:LEU:HD21	2.02	0.41
1:W:859:TYR:HB3	3:Y:63:LEU:HB3	2.03	0.41
2:B:1074:ASP:HB3	2:B:1075:LYS:CA	2.51	0.41
1:W:864:LYS:HD2	3:Y:32:LEU:HD11	2.03	0.41
2:R:380:ARG:HH11	2:R:381:LYS:CE	2.33	0.41
2:R:766:VAL:N	2:R:767:LYS:HE3	2.34	0.41
2:R:921:ARG:H	2:R:921:ARG:HG2	1.74	0.41
2:B:157:VAL:C	2:B:159:GLY:H	2.24	0.41
4:S:90:GLU:O	4:S:92:CYS:N	2.53	0.41
2:B:627:ALA:CB	2:B:642:HIS:HD2	2.30	0.41
12:O:42:ARG:NH1	4:S:161:LEU:HD13	2.35	0.41
1:A:879:LYS:NZ	3:C:46:ASP:HB2	2.35	0.41
2:B:914:ASN:C	2:B:916:HIS:H	2.22	0.41
11:M:33:ARG:HE	1:W:522:GLN:HB2	1.85	0.41
2:B:1069:TYR:OH	2:B:1115:ARG:NH1	2.53	0.41
13:X:19:LYS:HA	13:X:19:LYS:HD3	1.83	0.41
2:B:855:ILE:O	13:P:34:ILE:CG2	2.68	0.41
1:A:371:LYS:CD	1:A:373:PRO:HD2	2.50	0.41
3:Y:102:LEU:HD21	3:Y:119:THR:OG1	2.19	0.41
2:B:404:GLY:HA2	2:B:414:SER:H	1.84	0.41
3:C:323:THR:O	3:C:323:THR:HG22	2.20	0.41
1:A:820:GLN:O	1:A:824:ILE:HB	2.20	0.41
2:R:762:SER:HB3	2:R:866:LYS:HG2	2.02	0.41
12:O:50:LEU:CD2	2:R:940:GLY:HA2	2.50	0.41
2:R:873:ARG:HB3	2:R:999:MET:CE	2.50	0.41
1:W:98:CYS:SG	1:W:98:CYS:O	2.78	0.41
2:B:1098:TYR:CE1	2:B:1101:LYS:HD3	2.54	0.41
2:R:641:THR:HB	2:R:642:HIS:CD2	2.55	0.41
12:O:42:ARG:C	12:O:44:CYS:N	2.74	0.41
1:A:876:VAL:HA	1:A:879:LYS:HB2	2.03	0.41
2:R:766:VAL:H	2:R:767:LYS:HE3	1.85	0.41
1:W:431:MET:HE1	1:W:482:VAL:HG13	2.02	0.41
2:R:740:SER:HB2	1:W:457:PHE:HB2	2.02	0.41
2:R:322:ILE:C	2:R:324:LYS:H	2.23	0.41
2:R:743:MET:HE1	2:R:875:PRO:HB2	2.03	0.41
12:N:2:MET:HG2	12:N:56:ILE:HD13	2.03	0.41
2:R:167:GLN:HG2	2:R:352:LEU:HD21	2.03	0.41
1:A:411:LEU:HD23	1:A:435:VAL:HG21	2.03	0.41
7:V:9:ILE:CD1	7:V:104:LYS:HD2	2.51	0.41
9:K:44:ALA:C	9:K:46:GLY:H	2.23	0.41
3:Y:270:ALA:HA	8:Z:14:HIS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:727:LEU:HD12	2:B:911:VAL:HB	2.03	0.41
2:B:224:ILE:HD11	2:B:278:ARG:HD2	2.02	0.41
2:R:155:PHE:N	2:R:155:PHE:CD2	2.87	0.41
2:R:466:ASN:HD22	2:R:466:ASN:HA	1.59	0.41
2:B:440:GLN:OE1	2:B:440:GLN:HA	2.20	0.41
2:B:972:VAL:CG2	4:D:205:LEU:HB3	2.51	0.41
3:Y:337:GLU:O	3:Y:339:ASN:N	2.52	0.41
11:L:69:LEU:O	11:L:73:ILE:HG12	2.21	0.41
2:R:380:ARG:HD3	2:R:381:LYS:CE	2.48	0.41
2:R:781:PRO:HA	2:R:786:TYR:CZ	2.55	0.41
9:I:23:TRP:HE3	9:I:23:TRP:HA	1.85	0.41
3:C:258:LEU:O	3:C:262:LEU:HG	2.21	0.41
2:R:1102:LEU:HB3	1:W:308:ARG:HH21	1.86	0.41
3:C:239:ARG:O	3:C:253:THR:HA	2.20	0.41
1:A:750:GLN:CG	1:A:782:ILE:HD12	2.51	0.41
3:C:104:LEU:HB3	3:C:105:PRO:HD3	2.03	0.41
1:W:757:ILE:HD13	1:W:800:ALA:HB3	2.03	0.41
3:Y:269:ILE:HA	3:Y:272:VAL:HG23	2.01	0.41
12:N:19:GLN:HB2	12:N:20:PRO:HD3	2.02	0.41
2:B:423:LEU:HD21	2:B:654:THR:HG23	2.02	0.41
8:Z:23:LEU:HD12	8:Z:62:ILE:HG13	2.03	0.41
1:W:235:LEU:HD11	1:W:298:LEU:HG	2.02	0.41
1:A:740:ILE:HD13	1:A:743:MET:HE3	2.03	0.41
1:A:134:GLU:HA	1:A:137:LYS:HD2	2.02	0.41
1:A:543:ARG:HB2	1:A:545:TYR:CE2	2.56	0.41
2:R:1069:TYR:HA	2:R:1070:ILE:HB	2.03	0.41
2:B:394:THR:O	2:B:397:ILE:HG22	2.21	0.41
2:R:1072:TRP:HB3	2:R:1073:TYR:H	1.43	0.41
1:W:104:VAL:O	1:W:104:VAL:HG12	2.20	0.41
2:R:432:VAL:HG21	2:R:456:MET:CE	2.51	0.41
1:W:203:ARG:HE	1:W:205:GLU:CD	2.24	0.41
1:A:756:ARG:NH2	1:A:774:ILE:HG22	2.36	0.41
2:B:737:MET:H	2:B:740:SER:HB3	1.84	0.41
1:W:336:GLU:HA	1:W:434:ARG:H	1.86	0.41
1:A:357:ASN:C	1:A:357:ASN:OD1	2.58	0.41
1:A:648:LEU:HD11	2:B:928:MET:HG2	2.03	0.41
1:A:285:PRO:HB2	1:A:286:PRO:HA	2.01	0.41
8:H:62:ILE:HG22	8:H:80:TYR:HD2	1.86	0.41
3:Y:219:LEU:HG	3:Y:222:LEU:HD22	2.01	0.41
1:A:134:GLU:HB3	1:A:138:LYS:HE3	2.03	0.41
1:A:131:ARG:NH2	3:C:360:ARG:HH21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:767:LYS:NZ	2:B:774:ASP:O	2.54	0.41
2:B:1007:ARG:HH22	2:B:1022:GLY:H	1.68	0.41
1:W:812:ARG:NH2	3:Y:304:GLN:HE22	2.18	0.41
4:D:148:GLY:HA3	4:D:156:PHE:CE1	2.56	0.41
7:V:31:MET:CE	7:V:55:VAL:HG11	2.51	0.41
2:B:15:LYS:HZ3	2:B:599:LYS:HE3	1.86	0.41
7:G:31:MET:CE	7:G:55:VAL:HG11	2.51	0.41
1:W:319:ASP:O	1:W:320:PHE:C	2.59	0.41
5:E:78:VAL:HA	5:E:79:PRO:HD3	1.87	0.41
4:D:44:VAL:HG13	4:D:143:ALA:HB2	2.02	0.41
2:R:737:MET:SD	1:W:501:ASP:HB2	2.61	0.41
3:C:119:THR:N	3:C:120:PRO:HD3	2.36	0.41
3:Y:81:PRO:O	3:Y:82:GLY:C	2.60	0.41
2:B:167:GLN:HG2	2:B:352:LEU:HD21	2.03	0.41
1:A:757:ILE:HD13	1:A:800:ALA:HB3	2.03	0.41
1:A:46:ASP:H	1:A:47:PRO:CD	2.34	0.41
3:Y:162:SER:HB2	3:Y:210:PHE:CZ	2.56	0.41
1:A:525:LEU:HD11	1:A:551:VAL:HG23	2.03	0.41
2:B:608:ASP:O	2:B:612:ARG:HG3	2.21	0.41
3:Y:195:GLU:HB3	3:Y:209:SER:HA	2.02	0.41
6:U:30:SER:HB2	6:U:34:LEU:HD13	2.03	0.41
2:B:294:GLN:HA	2:B:297:ASP:HB2	2.02	0.41
2:R:1039:LEU:HA	2:R:1039:LEU:HD23	1.84	0.41
3:Y:293:ILE:HD12	3:Y:320:MET:CE	2.51	0.41
12:O:5:ILE:HD12	4:S:128:ILE:HG21	2.02	0.41
1:A:110:GLU:HA	1:A:113:LYS:HD2	2.03	0.41
4:S:94:THR:HG23	4:S:145:LEU:HB2	2.02	0.41
8:H:13:ILE:HG21	8:H:19:LYS:HZ1	1.86	0.41
2:R:177:VAL:HG13	2:R:325:VAL:HG22	2.01	0.41
12:N:56:ILE:O	12:N:60:ILE:HB	2.21	0.41
2:B:122:LEU:HD11	2:B:353:PHE:HE2	1.86	0.41
1:W:377:TYR:HB2	1:W:408:GLU:HB2	2.03	0.41
2:B:177:VAL:HG23	2:B:336:ASP:OD1	2.21	0.41
3:C:195:GLU:HB3	3:C:209:SER:HA	2.03	0.41
2:B:63:LEU:HD23	2:B:103:MET:HG2	2.03	0.41
2:R:90:LEU:HD22	2:R:854:LEU:CD1	2.51	0.41
9:I:75:PRO:HB2	3:Y:391:ARG:HD2	2.02	0.41
2:B:192:ILE:HB	2:B:206:GLU:HB2	2.01	0.41
10:Q:76:GLU:OE1	10:Q:76:GLU:N	2.54	0.41
2:B:857:GLU:CD	13:P:24:VAL:HG12	2.41	0.40
2:R:430:ARG:NH1	2:R:653:ILE:HG13	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:SER:C	2:B:377:VAL:H	2.25	0.40
3:C:30:GLU:HB3	3:C:31:ASP:H	1.51	0.40
5:E:18:PHE:HB2	9:K:48:PRO:HD3	2.03	0.40
5:T:171:LYS:HB2	5:T:174:TRP:HB2	2.03	0.40
5:T:20:LYS:O	5:T:21:PRO:C	2.60	0.40
1:A:12:GLY:HA3	1:A:201:THR:HG22	2.03	0.40
1:W:88:LYS:H	1:W:88:LYS:HD3	1.86	0.40
1:A:215:PRO:HD2	1:A:239:LEU:HD11	2.04	0.40
1:A:787:ARG:HH12	2:B:953:ILE:HG13	1.86	0.40
4:D:64:LEU:HB3	12:N:5:ILE:HG12	2.02	0.40
12:O:42:ARG:HD2	2:R:905:LYS:O	2.21	0.40
3:Y:53:ASP:HA	3:Y:56:ILE:CG1	2.50	0.40
1:A:428:ILE:HG22	1:A:452:PRO:HB3	2.02	0.40
3:C:28:ILE:HG21	9:K:14:HIS:NE2	2.36	0.40
7:V:66:TYR:HD1	7:V:66:TYR:N	2.18	0.40
1:W:764:ARG:N	1:W:764:ARG:CD	2.84	0.40
1:A:764:ARG:N	1:A:764:ARG:CD	2.84	0.40
1:A:122:LYS:HZ3	10:Q:70:ASP:CG	2.24	0.40
2:R:163:VAL:O	2:R:414:SER:HA	2.21	0.40
2:R:646:TRP:CD2	2:R:648:PRO:HD2	2.57	0.40
2:B:605:ILE:HG12	2:B:606:THR:N	2.35	0.40
4:D:172:ILE:HG22	4:D:174:GLY:O	2.21	0.40
1:W:305:LYS:HB3	1:W:310:ARG:NH1	2.35	0.40
5:T:60:VAL:HG22	5:T:61:PHE:H	1.87	0.40
2:R:954:GLU:HA	2:R:957:GLN:HB2	2.02	0.40
4:D:6:LEU:HB3	4:D:14:ASP:HB3	2.02	0.40
2:R:681:GLY:HA2	2:R:698:LEU:HB3	2.03	0.40
1:A:88:LYS:H	1:A:88:LYS:HD3	1.85	0.40
2:R:703:ARG:CD	2:R:717:THR:HG22	2.47	0.40
1:A:106:ILE:HG22	1:A:107:SER:N	2.24	0.40
2:B:627:ALA:CB	2:B:642:HIS:CD2	3.04	0.40
1:W:777:GLU:HG3	1:W:783:TYR:CE2	2.53	0.40
1:A:421:ARG:HB2	1:A:462:MET:CE	2.51	0.40
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.51	0.40
1:A:348:THR:HG22	1:A:410:HIS:HA	2.03	0.40
2:R:900:MET:SD	2:R:912:ILE:HD11	2.61	0.40
13:P:19:LYS:HA	13:P:19:LYS:HD3	1.85	0.40
3:C:389:THR:HG21	5:E:56:GLU:HB3	2.03	0.40
1:A:234:ASP:OD1	1:A:296:ARG:NH1	2.54	0.40
2:B:775:LYS:HB3	2:B:776:ILE:H	1.75	0.40
2:R:680:LEU:HD21	2:R:997:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:SER:O	1:A:571:GLY:C	2.59	0.40
2:R:696:HIS:CE1	2:R:757:PHE:HD1	2.39	0.40
6:U:62:ILE:H	6:U:62:ILE:HG13	1.77	0.40
2:R:91:ARG:O	2:R:92:ASN:HB2	2.22	0.40
1:W:734:ARG:NH1	1:W:734:ARG:CB	2.84	0.40
1:W:237:HIS:HE1	1:W:289:HIS:CD2	2.38	0.40
2:B:907:VAL:HG21	12:N:43:TYR:HE2	1.86	0.40
2:R:775:LYS:HB3	2:R:776:ILE:H	1.79	0.40
2:R:157:VAL:HG21	2:R:162:ARG:HD3	2.03	0.40
3:Y:343:ALA:HB2	3:Y:371:GLU:HG3	2.03	0.40
2:B:177:VAL:HG13	2:B:325:VAL:HG22	2.03	0.40
2:B:90:LEU:HD22	2:B:854:LEU:CD1	2.51	0.40
2:B:147:ASP:HB3	2:B:685:ALA:HB3	2.04	0.40
2:R:171:ALA:HB1	2:R:174:ARG:HD2	2.04	0.40
2:B:753:TYR:CD1	2:B:881:PHE:HE2	2.40	0.40
1:A:336:GLU:HA	1:A:434:ARG:H	1.85	0.40
9:K:53:ILE:HG23	9:K:55:ASN:HD22	1.86	0.40
1:A:334:ILE:HD11	1:A:628:MET:HB3	2.03	0.40
8:Z:15:TYR:CD2	8:Z:16:LEU:HG	2.56	0.40
2:B:272:LEU:O	2:B:276:GLY:N	2.34	0.40
2:B:20:TYR:OH	2:B:478:GLN:HG3	2.22	0.40
2:B:164:ILE:HG22	2:B:164:ILE:O	2.21	0.40
1:W:648:LEU:HD21	1:W:787:ARG:HD3	2.02	0.40
12:O:13:LEU:CD1	4:S:66:PRO:HG3	2.48	0.40
1:W:603:ILE:HG22	1:W:612:LEU:HD22	2.03	0.40
5:T:13:ILE:O	5:T:65:ALA:HB1	2.21	0.40
4:S:222:VAL:HB	4:S:225:LYS:HB2	2.03	0.40
2:R:788:GLY:H	2:R:792:TYR:HE1	1.68	0.40
1:A:491:TYR:CG	1:A:491:TYR:O	2.74	0.40
7:V:79:THR:CG2	7:V:80:GLU:N	2.84	0.40
4:D:51:SER:HB3	4:D:139:ILE:HD11	2.02	0.40
2:R:520:TRP:O	2:R:521:SER:HB2	2.21	0.40
3:C:290:ARG:NH2	8:H:67:ARG:HE	2.19	0.40
2:B:322:ILE:C	2:B:324:LYS:H	2.25	0.40
1:A:418:LEU:HD21	2:B:1047:LEU:HD21	2.03	0.40
2:R:122:LEU:HD11	2:R:353:PHE:HE2	1.86	0.40
5:T:61:PHE:CZ	3:Y:384:GLY:HA2	2.57	0.40
8:H:66:ILE:HG12	8:H:76:VAL:HG22	2.03	0.40
5:E:171:LYS:HB2	5:E:174:TRP:HB2	2.03	0.40
2:B:956:LEU:O	2:B:960:ILE:HG23	2.21	0.40
4:D:55:ASP:HB3	13:P:45:VAL:HG21	2.03	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	833/880 (95%)	664 (80%)	130 (16%)	39 (5%)	3	28
1	W	833/880 (95%)	666 (80%)	127 (15%)	40 (5%)	3	28
2	B	1082/1131 (96%)	853 (79%)	164 (15%)	65 (6%)	2	21
2	R	1082/1131 (96%)	852 (79%)	160 (15%)	70 (6%)	1	20
3	C	363/395 (92%)	277 (76%)	66 (18%)	20 (6%)	2	24
3	Y	363/395 (92%)	276 (76%)	64 (18%)	23 (6%)	2	20
4	D	256/265 (97%)	226 (88%)	23 (9%)	7 (3%)	6	44
4	S	256/265 (97%)	226 (88%)	22 (9%)	8 (3%)	5	41
5	E	170/180 (94%)	148 (87%)	20 (12%)	2 (1%)	16	61
5	T	170/180 (94%)	148 (87%)	20 (12%)	2 (1%)	16	61
6	F	89/113 (79%)	78 (88%)	10 (11%)	1 (1%)	17	63
6	U	89/113 (79%)	79 (89%)	9 (10%)	1 (1%)	17	63
7	G	111/132 (84%)	92 (83%)	15 (14%)	4 (4%)	4	37
7	V	111/132 (84%)	92 (83%)	15 (14%)	4 (4%)	4	37
8	H	72/84 (86%)	60 (83%)	6 (8%)	6 (8%)	1	13
8	Z	72/84 (86%)	60 (83%)	7 (10%)	5 (7%)	1	18
9	I	80/95 (84%)	61 (76%)	15 (19%)	4 (5%)	3	26
9	K	80/95 (84%)	61 (76%)	15 (19%)	4 (5%)	3	26
10	J	33/104 (32%)	28 (85%)	5 (15%)	0	100	100
10	Q	31/104 (30%)	27 (87%)	4 (13%)	0	100	100
11	L	90/92 (98%)	80 (89%)	8 (9%)	2 (2%)	8	48
11	M	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	N	62/66 (94%)	42 (68%)	15 (24%)	5 (8%)	1	13
12	O	62/66 (94%)	42 (68%)	16 (26%)	4 (6%)	1	20
13	P	41/48 (85%)	34 (83%)	6 (15%)	1 (2%)	7	47
13	X	41/48 (85%)	35 (85%)	5 (12%)	1 (2%)	7	47
All	All	6562/7170 (92%)	5288 (81%)	954 (14%)	320 (5%)	3	27

All (320) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	A	287	SER
1	A	378	VAL
1	A	732	GLY
1	A	734	ARG
1	A	737	VAL
1	A	876	VAL
2	B	111	GLU
2	B	158	ASN
2	B	521	SER
2	B	590	PRO
2	B	601	ASP
2	B	605	ILE
2	B	797	ASP
2	B	1044	THR
2	B	1070	ILE
2	B	1072	TRP
3	C	28	ILE
3	C	30	GLU
4	D	117	GLU
4	D	206	CYS
7	G	105	ILE
8	H	13	ILE
9	I	61	VAL
9	K	61	VAL
9	K	91	SER
2	R	111	GLU
2	R	158	ASN
2	R	181	LYS
2	R	521	SER
2	R	590	PRO
2	R	601	ASP

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Mol	Chain	Res	Type
2	R	605	ILE
2	R	797	ASP
2	R	1029	LEU
2	R	1070	ILE
2	R	1072	TRP
4	S	91	LYS
4	S	117	GLU
4	S	206	CYS
7	V	105	ILE
1	W	287	SER
1	W	378	VAL
1	W	732	GLY
1	W	734	ARG
1	W	737	VAL
3	Y	28	ILE
3	Y	114	LYS
8	Z	13	ILE
1	A	143	ALA
1	A	332	ILE
1	A	355	PRO
1	A	492	GLY
1	A	753	ARG
1	A	849	ALA
2	B	22	LYS
2	B	42	LEU
2	B	71	PRO
2	B	181	LYS
2	B	250	GLU
2	B	279	VAL
2	B	382	LEU
2	B	453	TRP
2	B	535	ASP
2	B	603	GLY
2	B	606	THR
2	B	735	TYR
2	B	793	ARG
2	B	809	GLY
2	B	1029	LEU
3	C	114	LYS
3	C	245	LYS
3	C	324	GLY
3	C	362	ASP

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Mol	Chain	Res	Type
3	C	393	ILE
4	D	91	LYS
4	D	231	GLU
6	F	63	ILE
9	I	91	SER
2	R	22	LYS
2	R	42	LEU
2	R	49	GLN
2	R	71	PRO
2	R	250	GLU
2	R	279	VAL
2	R	382	LEU
2	R	453	TRP
2	R	535	ASP
2	R	606	THR
2	R	735	TYR
2	R	793	ARG
2	R	809	GLY
2	R	1026	GLU
2	R	1044	THR
6	U	63	ILE
1	W	45	MET
1	W	143	ALA
1	W	145	VAL
1	W	155	LYS
1	W	290	ARG
1	W	332	ILE
1	W	355	PRO
1	W	541	ALA
1	W	812	ARG
1	W	876	VAL
13	X	18	LEU
3	Y	30	GLU
3	Y	82	GLY
3	Y	245	LYS
3	Y	324	GLY
3	Y	362	ASP
3	Y	393	ILE
1	A	45	MET
1	A	103	ARG
1	A	155	LYS
1	A	290	ARG

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Mol	Chain	Res	Type
1	A	393	ASP
1	A	541	ALA
1	A	656	ASP
1	A	730	ARG
1	A	733	ALA
1	A	812	ARG
1	A	852	ASP
1	A	875	VAL
2	B	41	LYS
2	B	49	GLN
2	B	202	PRO
2	B	256	PHE
2	B	281	ILE
2	B	375	SER
2	B	406	TRP
2	B	437	ALA
2	B	592	VAL
2	B	633	PRO
2	B	949	TYR
2	B	950	LYS
2	B	951	THR
2	B	1026	GLU
2	B	1111	ILE
3	C	113	ALA
3	C	306	LEU
3	C	323	THR
3	C	338	LYS
7	G	63	ARG
7	G	99	PHE
8	H	11	PRO
8	H	81	VAL
11	L	10	SER
11	M	10	SER
12	N	6	ARG
12	N	41	LYS
12	N	43	TYR
12	O	6	ARG
12	O	41	LYS
12	O	43	TYR
13	P	18	LEU
2	R	202	PRO
2	R	256	PHE

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Mol	Chain	Res	Type
2	R	281	ILE
2	R	375	SER
2	R	406	TRP
2	R	603	GLY
2	R	638	PRO
2	R	687	TYR
2	R	949	TYR
2	R	950	LYS
2	R	951	THR
2	R	1111	ILE
4	S	231	GLU
7	V	99	PHE
1	W	103	ARG
1	W	393	ASP
1	W	429	SER
1	W	730	ARG
1	W	733	ALA
1	W	753	ARG
1	W	849	ALA
1	W	852	ASP
1	W	875	VAL
3	Y	113	ALA
3	Y	161	ALA
3	Y	235	LYS
3	Y	306	LEU
3	Y	310	MET
3	Y	323	THR
3	Y	338	LYS
8	Z	11	PRO
8	Z	81	VAL
1	A	79	ARG
1	A	257	ALA
1	A	429	SER
1	A	536	GLU
2	B	57	PRO
2	B	334	GLU
2	B	383	ALA
2	B	563	THR
2	B	587	ASN
2	B	638	PRO
2	B	739	ASP
2	B	773	GLU

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Mol	Chain	Res	Type
2	B	918	LEU
2	B	948	PHE
3	C	127	THR
3	C	161	ALA
3	C	196	PHE
3	C	235	LYS
5	E	82	GLN
8	H	60	GLY
9	I	45	MET
12	O	9	THR
2	R	41	LYS
2	R	57	PRO
2	R	334	GLU
2	R	437	ALA
2	R	563	THR
2	R	587	ASN
2	R	633	PRO
2	R	734	GLY
2	R	739	ASP
2	R	773	GLU
2	R	918	LEU
5	T	82	GLN
7	V	63	ARG
1	W	79	ARG
1	W	257	ALA
1	W	283	GLY
1	W	492	GLY
1	W	536	GLU
1	W	656	ASP
3	Y	127	THR
3	Y	196	PHE
1	A	283	GLY
1	A	772	TYR
2	B	52	ILE
2	B	223	LYS
2	B	734	GLY
2	B	907	VAL
2	B	943	VAL
2	B	1073	TYR
2	B	1114	PRO
3	C	211	ALA
4	D	90	GLU

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Mol	Chain	Res	Type
4	D	104	ASN
7	G	64	LEU
8	H	10	ASP
9	K	51	ILE
12	N	9	THR
12	N	21	PHE
2	R	52	ILE
2	R	196	THR
2	R	383	ALA
2	R	460	GLU
2	R	592	VAL
2	R	907	VAL
2	R	943	VAL
2	R	948	PHE
2	R	1073	TYR
2	R	1114	PRO
4	S	90	GLU
4	S	104	ASN
4	S	152	GLU
7	V	64	LEU
1	W	22	MET
1	W	106	ILE
1	W	772	TYR
3	Y	109	GLU
3	Y	211	ALA
8	Z	10	ASP
1	A	46	ASP
1	A	106	ILE
2	B	653	ILE
2	B	706	VAL
3	C	82	GLY
9	K	45	MET
2	R	223	LYS
2	R	653	ILE
2	R	706	VAL
1	W	46	ASP
3	Y	146	TYR
3	Y	365	GLU
8	Z	60	GLY
1	A	147	PRO
2	B	597	ILE
3	C	234	ILE

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Mol	Chain	Res	Type
4	D	193	GLY
2	R	407	VAL
2	R	783	VAL
1	A	571	GLY
2	B	234	GLY
2	B	377	VAL
2	B	766	VAL
2	B	769	PRO
9	I	51	ILE
2	R	377	VAL
2	R	597	ILE
2	R	766	VAL
2	R	769	PRO
3	Y	234	ILE
1	A	29	THR
1	A	121	ILE
1	A	125	TRP
2	B	407	VAL
1	W	29	THR
1	W	69	PRO
1	W	121	ILE
1	W	125	TRP
1	W	147	PRO
1	W	571	GLY
8	H	59	PRO
11	L	19	GLY
2	R	234	GLY
4	S	193	GLY
5	T	127	ILE
1	A	258	PRO
3	C	56	ILE
3	C	349	VAL
5	E	127	ILE
11	M	19	GLY
2	R	183	GLY
3	Y	56	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/766 (95%)	647 (89%)	82 (11%)	7	35
1	W	729/766 (95%)	645 (88%)	84 (12%)	7	33
2	B	941/975 (96%)	805 (86%)	136 (14%)	4	23
2	R	941/975 (96%)	806 (86%)	135 (14%)	4	24
3	C	315/341 (92%)	274 (87%)	41 (13%)	5	28
3	Y	315/341 (92%)	276 (88%)	39 (12%)	6	29
4	D	233/238 (98%)	220 (94%)	13 (6%)	26	66
4	S	233/238 (98%)	220 (94%)	13 (6%)	26	66
5	E	154/158 (98%)	139 (90%)	15 (10%)	10	42
5	T	154/158 (98%)	139 (90%)	15 (10%)	10	42
6	F	84/107 (78%)	78 (93%)	6 (7%)	18	58
6	U	84/107 (78%)	78 (93%)	6 (7%)	18	58
7	G	106/125 (85%)	98 (92%)	8 (8%)	17	56
7	V	106/125 (85%)	97 (92%)	9 (8%)	13	49
8	H	67/75 (89%)	61 (91%)	6 (9%)	12	47
8	Z	67/75 (89%)	61 (91%)	6 (9%)	12	47
9	I	72/83 (87%)	67 (93%)	5 (7%)	19	59
9	K	72/83 (87%)	67 (93%)	5 (7%)	19	59
10	J	33/96 (34%)	26 (79%)	7 (21%)	1	8
10	Q	30/96 (31%)	25 (83%)	5 (17%)	3	16
11	L	79/80 (99%)	74 (94%)	5 (6%)	22	63
11	M	79/80 (99%)	76 (96%)	3 (4%)	40	76
12	N	58/60 (97%)	54 (93%)	4 (7%)	19	59
12	O	58/60 (97%)	53 (91%)	5 (9%)	13	49
13	P	39/43 (91%)	36 (92%)	3 (8%)	16	54
13	X	39/43 (91%)	37 (95%)	2 (5%)	29	69
All	All	5817/6294 (92%)	5159 (89%)	658 (11%)	7	34

All (658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	24	VAL
1	A	28	ILE
1	A	45	MET
1	A	51	VAL
1	A	60	THR
1	A	84	VAL
1	A	87	VAL
1	A	88	LYS
1	A	98	CYS
1	A	101	CYS
1	A	105	LYS
1	A	119	ASN
1	A	131	ARG
1	A	139	THR
1	A	141	MET
1	A	152	LYS
1	A	155	LYS
1	A	194	ILE
1	A	201	THR
1	A	218	THR
1	A	220	ARG
1	A	238	LYS
1	A	251	GLU
1	A	284	LEU
1	A	296	ARG
1	A	319	ASP
1	A	332	ILE
1	A	346	THR
1	A	349	VAL
1	A	356	TRP
1	A	359	GLU
1	A	361	LEU
1	A	366	ILE
1	A	382	ASP
1	A	390	TYR
1	A	391	VAL
1	A	400	THR
1	A	425	LEU
1	A	426	HIS
1	A	429	SER
1	A	438	LEU
1	A	439	LYS

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	464	LEU
1	A	478	GLU
1	A	500	GLN
1	A	527	VAL
1	A	533	ASP
1	A	540	LEU
1	A	549	LYS
1	A	573	ARG
1	A	582	HIS
1	A	593	LEU
1	A	603	ILE
1	A	621	ASP
1	A	633	ARG
1	A	653	LEU
1	A	661	ILE
1	A	675	LEU
1	A	684	LEU
1	A	691	THR
1	A	707	LEU
1	A	708	ARG
1	A	723	ASN
1	A	728	MET
1	A	738	LEU
1	A	759	ARG
1	A	763	THR
1	A	764	ARG
1	A	766	LEU
1	A	774	ILE
1	A	787	ARG
1	A	790	LEU
1	A	808	ASP
1	A	814	SER
1	A	820	GLN
1	A	823	LEU
1	A	824	ILE
1	A	868	VAL
1	A	870	ARG
1	A	876	VAL
2	B	8	LEU
2	B	27	VAL
2	B	48	GLU

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Mol	Chain	Res	Type
2	B	52	ILE
2	B	54	THR
2	B	55	GLU
2	B	59	LEU
2	B	66	ILE
2	B	68	ILE
2	B	76	SER
2	B	84	SER
2	B	101	LEU
2	B	104	ILE
2	B	111	GLU
2	B	137	THR
2	B	138	LEU
2	B	160	SER
2	B	165	VAL
2	B	166	THR
2	B	170	LEU
2	B	177	VAL
2	B	182	THR
2	B	187	THR
2	B	200	ARG
2	B	216	SER
2	B	217	PHE
2	B	230	MET
2	B	237	THR
2	B	254	GLU
2	B	258	SER
2	B	259	LEU
2	B	263	SER
2	B	306	THR
2	B	307	SER
2	B	312	ARG
2	B	318	LEU
2	B	330	LEU
2	B	333	ARG
2	B	344	LYS
2	B	345	ARG
2	B	374	LYS
2	B	375	SER
2	B	397	ILE
2	B	405	ASN
2	B	418	ASP

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Mol	Chain	Res	Type
2	B	419	ARG
2	B	421	ASN
2	B	426	LEU
2	B	448	LEU
2	B	456	MET
2	B	457	CYS
2	B	466	ASN
2	B	467	SER
2	B	470	VAL
2	B	471	LYS
2	B	489	GLU
2	B	503	VAL
2	B	505	ARG
2	B	525	LEU
2	B	529	LEU
2	B	539	LEU
2	B	554	ASP
2	B	575	SER
2	B	591	LEU
2	B	595	GLU
2	B	596	ASP
2	B	597	ILE
2	B	604	SER
2	B	610	LEU
2	B	613	GLN
2	B	637	THR
2	B	641	THR
2	B	646	TRP
2	B	650	ILE
2	B	653	ILE
2	B	662	GLU
2	B	675	MET
2	B	688	GLN
2	B	711	LEU
2	B	717	THR
2	B	730	ILE
2	B	735	TYR
2	B	736	ASN
2	B	741	ILE
2	B	742	ILE
2	B	763	THR
2	B	764	GLU

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Mol	Chain	Res	Type
2	B	767	LYS
2	B	777	VAL
2	B	783	VAL
2	B	797	ASP
2	B	802	SER
2	B	838	THR
2	B	839	SER
2	B	843	ARG
2	B	873	ARG
2	B	874	ILE
2	B	884	ARG
2	B	898	VAL
2	B	899	ASP
2	B	905	LYS
2	B	907	VAL
2	B	913	LEU
2	B	921	ARG
2	B	923	THR
2	B	924	LEU
2	B	941	ASN
2	B	944	ASP
2	B	950	LYS
2	B	953	ILE
2	B	961	LEU
2	B	972	VAL
2	B	973	THR
2	B	977	ARG
2	B	982	ILE
2	B	984	SER
2	B	993	TYR
2	B	1017	ARG
2	B	1023	ARG
2	B	1033	GLU
2	B	1038	CYS
2	B	1048	LEU
2	B	1052	LEU
2	B	1056	SER
2	B	1059	THR
2	B	1060	THR
2	B	1061	ILE
2	B	1070	ILE
2	B	1072	TRP

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Mol	Chain	Res	Type
2	B	1081	VAL
2	B	1104	ILE
2	B	1115	ARG
2	B	1118	LEU
2	B	1120	ASP
2	B	1121	ARG
2	B	1122	VAL
3	C	24	LEU
3	C	28	ILE
3	C	30	GLU
3	C	44	THR
3	C	47	GLU
3	C	52	PHE
3	C	59	TYR
3	C	64	ILE
3	C	70	ILE
3	C	80	GLU
3	C	111	VAL
3	C	119	THR
3	C	129	GLU
3	C	130	TYR
3	C	159	ASP
3	C	164	SER
3	C	173	MET
3	C	174	LEU
3	C	190	ARG
3	C	193	LEU
3	C	209	SER
3	C	213	ILE
3	C	231	ILE
3	C	252	LEU
3	C	277	ILE
3	C	278	ARG
3	C	292	ILE
3	C	303	GLU
3	C	306	LEU
3	C	307	ASP
3	C	311	ARG
3	C	315	LEU
3	C	318	ASP
3	C	327	ARG
3	C	331	ARG

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Mol	Chain	Res	Type
3	C	332	HIS
3	C	338	LYS
3	C	365	GLU
3	C	369	VAL
3	C	380	LYS
3	C	386	VAL
4	D	13	ILE
4	D	58	LEU
4	D	82	CYS
4	D	117	GLU
4	D	124	ILE
4	D	151	LYS
4	D	165	ARG
4	D	172	ILE
4	D	176	CYS
4	D	178	LYS
4	D	198	LYS
4	D	224	ASP
4	D	258	LYS
5	E	30	LEU
5	E	48	ILE
5	E	49	LEU
5	E	73	ASP
5	E	76	THR
5	E	80	VAL
5	E	89	VAL
5	E	93	ASP
5	E	101	LEU
5	E	117	THR
5	E	137	GLN
5	E	142	VAL
5	E	152	THR
5	E	162	LEU
5	E	174	TRP
6	F	7	VAL
6	F	25	ILE
6	F	37	THR
6	F	62	ILE
6	F	63	ILE
6	F	88	ILE
7	G	33	CYS
7	G	47	ASN

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Mol	Chain	Res	Type
7	G	48	ILE
7	G	62	ASN
7	G	66	TYR
7	G	85	SER
7	G	101	LEU
7	G	106	ILE
8	H	16	LEU
8	H	22	VAL
8	H	40	GLU
8	H	48	SER
8	H	63	ILE
8	H	65	ILE
9	I	23	TRP
9	I	50	LEU
9	I	59	THR
9	I	71	ARG
9	I	74	LEU
10	J	56	ASN
10	J	60	SER
10	J	69	GLU
10	J	72	TYR
10	J	74	ASP
10	J	77	LYS
10	J	79	ASP
9	K	23	TRP
9	K	50	LEU
9	K	59	THR
9	K	71	ARG
9	K	74	LEU
11	L	1	MET
11	L	31	THR
11	L	44	TYR
11	L	60	ASP
11	L	74	GLU
11	M	31	THR
11	M	44	TYR
11	M	74	GLU
12	N	3	ILE
12	N	5	ILE
12	N	45	CYS
12	N	53	ILE
12	O	3	ILE

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Mol	Chain	Res	Type
12	O	5	ILE
12	O	45	CYS
12	O	53	ILE
12	O	63	THR
13	P	14	THR
13	P	41	THR
13	P	44	ILE
10	Q	56	ASN
10	Q	60	SER
10	Q	69	GLU
10	Q	72	TYR
10	Q	74	ASP
2	R	8	LEU
2	R	27	VAL
2	R	33	SER
2	R	48	GLU
2	R	52	ILE
2	R	54	THR
2	R	55	GLU
2	R	59	LEU
2	R	66	ILE
2	R	68	ILE
2	R	76	SER
2	R	84	SER
2	R	101	LEU
2	R	104	ILE
2	R	111	GLU
2	R	121	ASP
2	R	137	THR
2	R	138	LEU
2	R	160	SER
2	R	165	VAL
2	R	166	THR
2	R	170	LEU
2	R	177	VAL
2	R	182	THR
2	R	187	THR
2	R	200	ARG
2	R	216	SER
2	R	217	PHE
2	R	230	MET
2	R	254	GLU

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Mol	Chain	Res	Type
2	R	258	SER
2	R	259	LEU
2	R	263	SER
2	R	306	THR
2	R	307	SER
2	R	312	ARG
2	R	318	LEU
2	R	330	LEU
2	R	333	ARG
2	R	344	LYS
2	R	345	ARG
2	R	374	LYS
2	R	375	SER
2	R	397	ILE
2	R	405	ASN
2	R	419	ARG
2	R	421	ASN
2	R	426	LEU
2	R	448	LEU
2	R	456	MET
2	R	457	CYS
2	R	466	ASN
2	R	467	SER
2	R	470	VAL
2	R	471	LYS
2	R	489	GLU
2	R	503	VAL
2	R	505	ARG
2	R	525	LEU
2	R	539	LEU
2	R	554	ASP
2	R	575	SER
2	R	595	GLU
2	R	596	ASP
2	R	597	ILE
2	R	604	SER
2	R	610	LEU
2	R	613	GLN
2	R	637	THR
2	R	641	THR
2	R	646	TRP
2	R	650	ILE

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Mol	Chain	Res	Type
2	R	653	ILE
2	R	662	GLU
2	R	668	ARG
2	R	675	MET
2	R	688	GLN
2	R	711	LEU
2	R	717	THR
2	R	730	ILE
2	R	735	TYR
2	R	736	ASN
2	R	741	ILE
2	R	742	ILE
2	R	763	THR
2	R	764	GLU
2	R	767	LYS
2	R	777	VAL
2	R	783	VAL
2	R	797	ASP
2	R	802	SER
2	R	838	THR
2	R	839	SER
2	R	843	ARG
2	R	873	ARG
2	R	874	ILE
2	R	884	ARG
2	R	898	VAL
2	R	899	ASP
2	R	905	LYS
2	R	907	VAL
2	R	913	LEU
2	R	921	ARG
2	R	923	THR
2	R	924	LEU
2	R	941	ASN
2	R	944	ASP
2	R	950	LYS
2	R	953	ILE
2	R	961	LEU
2	R	972	VAL
2	R	973	THR
2	R	977	ARG
2	R	982	ILE

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Mol	Chain	Res	Type
2	R	984	SER
2	R	988	PHE
2	R	993	TYR
2	R	1017	ARG
2	R	1023	ARG
2	R	1033	GLU
2	R	1048	LEU
2	R	1052	LEU
2	R	1056	SER
2	R	1059	THR
2	R	1060	THR
2	R	1061	ILE
2	R	1070	ILE
2	R	1072	TRP
2	R	1081	VAL
2	R	1104	ILE
2	R	1115	ARG
2	R	1118	LEU
2	R	1120	ASP
2	R	1121	ARG
2	R	1122	VAL
4	S	13	ILE
4	S	58	LEU
4	S	82	CYS
4	S	117	GLU
4	S	124	ILE
4	S	151	LYS
4	S	165	ARG
4	S	172	ILE
4	S	176	CYS
4	S	178	LYS
4	S	198	LYS
4	S	224	ASP
4	S	258	LYS
5	T	30	LEU
5	T	48	ILE
5	T	49	LEU
5	T	73	ASP
5	T	76	THR
5	T	80	VAL
5	T	89	VAL
5	T	93	ASP

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Mol	Chain	Res	Type
5	T	101	LEU
5	T	117	THR
5	T	137	GLN
5	T	142	VAL
5	T	152	THR
5	T	162	LEU
5	T	174	TRP
6	U	7	VAL
6	U	25	ILE
6	U	37	THR
6	U	62	ILE
6	U	63	ILE
6	U	88	ILE
7	V	33	CYS
7	V	39	SER
7	V	47	ASN
7	V	48	ILE
7	V	62	ASN
7	V	66	TYR
7	V	85	SER
7	V	101	LEU
7	V	106	ILE
1	W	24	VAL
1	W	28	ILE
1	W	45	MET
1	W	51	VAL
1	W	60	THR
1	W	84	VAL
1	W	87	VAL
1	W	88	LYS
1	W	98	CYS
1	W	101	CYS
1	W	105	LYS
1	W	119	ASN
1	W	131	ARG
1	W	139	THR
1	W	141	MET
1	W	152	LYS
1	W	155	LYS
1	W	194	ILE
1	W	201	THR
1	W	220	ARG

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Mol	Chain	Res	Type
1	W	238	LYS
1	W	251	GLU
1	W	284	LEU
1	W	296	ARG
1	W	319	ASP
1	W	323	ARG
1	W	329	ASP
1	W	332	ILE
1	W	335	ASP
1	W	346	THR
1	W	349	VAL
1	W	356	TRP
1	W	359	GLU
1	W	361	LEU
1	W	366	ILE
1	W	382	ASP
1	W	390	TYR
1	W	391	VAL
1	W	400	THR
1	W	425	LEU
1	W	426	HIS
1	W	438	LEU
1	W	439	LYS
1	W	449	VAL
1	W	464	LEU
1	W	478	GLU
1	W	500	GLN
1	W	527	VAL
1	W	533	ASP
1	W	534	LEU
1	W	540	LEU
1	W	549	LYS
1	W	551	VAL
1	W	573	ARG
1	W	582	HIS
1	W	593	LEU
1	W	603	ILE
1	W	621	ASP
1	W	633	ARG
1	W	653	LEU
1	W	661	ILE
1	W	675	LEU

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Mol	Chain	Res	Type
1	W	684	LEU
1	W	691	THR
1	W	707	LEU
1	W	708	ARG
1	W	723	ASN
1	W	728	MET
1	W	734	ARG
1	W	738	LEU
1	W	759	ARG
1	W	763	THR
1	W	764	ARG
1	W	766	LEU
1	W	774	ILE
1	W	787	ARG
1	W	790	LEU
1	W	808	ASP
1	W	814	SER
1	W	823	LEU
1	W	824	ILE
1	W	868	VAL
1	W	870	ARG
1	W	876	VAL
13	X	14	THR
13	X	41	THR
3	Y	24	LEU
3	Y	28	ILE
3	Y	30	GLU
3	Y	44	THR
3	Y	52	PHE
3	Y	59	TYR
3	Y	60	SER
3	Y	64	ILE
3	Y	70	ILE
3	Y	111	VAL
3	Y	119	THR
3	Y	129	GLU
3	Y	130	TYR
3	Y	159	ASP
3	Y	164	SER
3	Y	174	LEU
3	Y	190	ARG
3	Y	193	LEU

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Mol	Chain	Res	Type
3	Y	209	SER
3	Y	213	ILE
3	Y	231	ILE
3	Y	252	LEU
3	Y	277	ILE
3	Y	278	ARG
3	Y	292	ILE
3	Y	303	GLU
3	Y	306	LEU
3	Y	307	ASP
3	Y	311	ARG
3	Y	315	LEU
3	Y	318	ASP
3	Y	327	ARG
3	Y	331	ARG
3	Y	338	LYS
3	Y	365	GLU
3	Y	369	VAL
3	Y	371	GLU
3	Y	380	LYS
3	Y	386	VAL
8	Z	16	LEU
8	Z	22	VAL
8	Z	40	GLU
8	Z	48	SER
8	Z	63	ILE
8	Z	65	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	89	HIS
1	A	237	HIS
1	A	272	HIS
1	A	279	ASN
1	A	422	GLN
1	A	500	GLN
1	A	567	ASN
1	A	582	HIS
1	A	820	GLN
2	B	188	HIS

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Mol	Chain	Res	Type
2	B	252	GLN
2	B	287	ASN
2	B	371	GLN
2	B	415	GLN
2	B	466	ASN
2	B	560	HIS
2	B	626	ASN
2	B	642	HIS
2	B	688	GLN
2	B	696	HIS
2	B	723	ASN
2	B	736	ASN
2	B	994	GLN
2	B	1078	ASN
3	C	207	ASN
3	C	304	GLN
4	D	136	ASN
4	D	199	ASN
7	G	16	ASN
7	G	62	ASN
7	G	88	ASN
9	I	55	ASN
9	K	55	ASN
12	N	61	HIS
12	O	61	HIS
2	R	188	HIS
2	R	252	GLN
2	R	287	ASN
2	R	371	GLN
2	R	442	ASN
2	R	466	ASN
2	R	478	GLN
2	R	560	HIS
2	R	626	ASN
2	R	642	HIS
2	R	688	GLN
2	R	696	HIS
2	R	723	ASN
2	R	736	ASN
2	R	994	GLN
2	R	1078	ASN
4	S	60	HIS

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Mol	Chain	Res	Type
4	S	136	ASN
4	S	199	ASN
7	V	16	ASN
7	V	47	ASN
7	V	62	ASN
7	V	88	ASN
1	W	83	HIS
1	W	272	HIS
1	W	289	HIS
1	W	331	ASN
1	W	422	GLN
1	W	500	GLN
1	W	567	ASN
1	W	739	ASN
1	W	820	GLN
3	Y	38	ASN
3	Y	207	ASN
3	Y	304	GLN

### 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 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
16	F3S	D	1265	4	0,9,9	0.00	-	0,15,15	0.00	-
16	F3S	S	1265	4	0,9,9	0.00	-	0,15,15	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	F3S	D	1265	4	-	0/0/24/24	0/0/3/3
16	F3S	S	1265	4	-	0/0/24/24	0/0/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	841/880 (95%)	0.04	11 (1%) 79 70	65, 91, 152, 185	0
1	W	841/880 (95%)	0.00	14 (1%) 73 64	61, 87, 141, 171	0
2	B	1090/1131 (96%)	0.06	25 (2%) 64 54	64, 87, 129, 155	0
2	R	1090/1131 (96%)	0.07	22 (2%) 68 59	64, 89, 120, 137	0
3	C	367/395 (92%)	0.22	16 (4%) 38 29	82, 106, 147, 155	0
3	Y	367/395 (92%)	0.03	9 (2%) 61 50	62, 89, 145, 160	0
4	D	260/265 (98%)	0.32	15 (5%) 26 21	90, 110, 127, 142	0
4	S	260/265 (98%)	0.28	12 (4%) 36 28	88, 106, 126, 140	0
5	E	174/180 (96%)	0.68	22 (12%) 5 6	98, 132, 196, 214	0
5	T	174/180 (96%)	0.56	15 (8%) 13 12	92, 125, 174, 189	0
6	F	91/113 (80%)	0.76	10 (10%) 7 7	135, 163, 191, 204	0
6	U	91/113 (80%)	0.86	10 (10%) 7 7	131, 160, 202, 216	0
7	G	113/132 (85%)	0.48	3 (2%) 58 47	87, 114, 138, 155	0
7	V	113/132 (85%)	0.40	5 (4%) 38 29	81, 112, 136, 149	0
8	H	74/84 (88%)	-0.06	0 100 100	75, 96, 118, 145	0
8	Z	74/84 (88%)	0.04	0 100 100	72, 95, 114, 144	0
9	I	82/95 (86%)	0.03	1 (1%) 81 73	61, 79, 103, 126	0
9	K	82/95 (86%)	0.04	1 (1%) 81 73	64, 82, 103, 121	0
10	J	35/104 (33%)	0.45	5 (14%) 4 4	112, 126, 147, 153	0
10	Q	33/104 (31%)	0.65	2 (6%) 25 19	129, 166, 225, 285	0
11	L	92/92 (100%)	0.09	2 (2%) 65 55	75, 97, 136, 181	0
11	M	92/92 (100%)	0.08	1 (1%) 82 74	68, 91, 141, 184	0
12	N	64/66 (96%)	0.22	2 (3%) 52 43	79, 96, 119, 136	0
12	O	64/66 (96%)	-0.08	0 100 100	74, 89, 103, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	P	43/48 (89%)	0.35	1 (2%) 64 54	80, 105, 127, 141	0
13	X	43/48 (89%)	0.33	1 (2%) 64 54	90, 106, 121, 125	0
All	All	6650/7170 (92%)	0.15	205 (3%) 52 43	61, 96, 153, 285	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	117	THR	6.3
5	E	116	ASP	6.0
11	L	9	GLU	4.9
6	U	78	ILE	4.9
3	C	212	ASN	4.9
1	A	232	GLU	4.7
5	T	7	ALA	4.5
6	U	64	SER	4.4
3	C	214	ASP	4.3
5	E	130	GLU	4.2
4	D	189	GLU	4.1
2	B	382	LEU	4.1
2	B	286	GLU	4.0
6	U	27	SER	3.9
6	U	79	THR	3.9
5	T	133	LYS	3.9
2	R	508	THR	3.9
2	B	114	PRO	3.9
5	E	119	LYS	3.9
1	A	261	ILE	3.9
5	T	119	LYS	3.8
6	F	66	GLU	3.7
10	J	77	LYS	3.7
13	P	30	GLY	3.6
2	R	601	ASP	3.6
5	E	176	THR	3.6
10	Q	72	TYR	3.6
3	C	190	ARG	3.6
6	U	77	PRO	3.5
6	F	27	SER	3.5
3	C	215	SER	3.5
2	B	378	ARG	3.5
4	D	176	CYS	3.4
5	E	134	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
5	T	117	THR	3.4
1	W	671	GLU	3.4
3	C	394	LEU	3.4
3	C	26	GLN	3.3
9	I	58	SER	3.3
2	R	251	ILE	3.2
4	D	93	TYR	3.2
5	T	137	GLN	3.2
5	T	153	VAL	3.2
4	S	263	VAL	3.2
5	E	123	VAL	3.2
3	C	216	ILE	3.2
7	G	51	GLN	3.2
5	E	153	VAL	3.2
7	G	5	LYS	3.2
2	B	1078	ASN	3.1
2	B	309	ASP	3.1
6	U	46	LYS	3.1
3	Y	224	ASP	3.1
4	D	136	ASN	3.1
2	B	1075	LYS	3.0
3	C	191	LEU	3.0
3	Y	221	LYS	3.0
4	D	217	ILE	3.0
1	A	28	ILE	3.0
1	A	125	TRP	3.0
3	C	27	LYS	3.0
5	E	118	LEU	3.0
3	Y	212	ASN	3.0
2	R	113	GLU	3.0
1	W	144	GLN	2.9
1	A	27	ILE	2.9
5	E	133	LYS	2.9
1	A	291	SER	2.9
4	D	103	LEU	2.9
3	C	213	ILE	2.9
10	Q	45	MET	2.9
6	U	92	ASN	2.9
2	R	84	SER	2.9
5	T	69	GLU	2.8
3	Y	191	LEU	2.8
6	F	91	SER	2.8

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Mol	Chain	Res	Type	RSRZ
5	T	123	VAL	2.8
2	B	769	PRO	2.8
5	E	122	ASN	2.7
5	T	125	GLY	2.7
6	F	63	ILE	2.7
4	D	174	GLY	2.7
4	D	214	ASN	2.7
2	R	110	ILE	2.7
6	F	3	SER	2.7
5	E	166	GLN	2.7
5	E	168	TYR	2.7
1	W	231	ALA	2.7
5	E	165	ARG	2.7
3	C	128	ASP	2.6
2	R	373	GLU	2.6
4	S	83	ILE	2.6
5	E	167	PRO	2.6
1	A	115	SER	2.6
4	S	99	GLU	2.6
3	Y	228	ASN	2.6
7	V	7	GLN	2.6
2	B	1072	TRP	2.6
5	T	122	ASN	2.6
1	W	121	ILE	2.6
12	N	39	GLY	2.6
1	W	78	VAL	2.6
2	B	52	ILE	2.6
1	W	152	LYS	2.6
7	V	6	ALA	2.6
4	S	82	CYS	2.5
4	S	106	PRO	2.5
2	R	768	TYR	2.5
2	R	820	PRO	2.5
4	D	82	CYS	2.5
2	B	768	TYR	2.5
4	S	176	CYS	2.5
5	T	130	GLU	2.5
4	D	215	GLY	2.5
2	B	197	ALA	2.5
4	D	175	ASN	2.5
5	E	121	ASP	2.5
1	W	28	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	693	GLU	2.5
2	B	294	GLN	2.5
2	R	1072	TRP	2.5
6	F	58	GLU	2.5
2	R	379	GLY	2.4
3	Y	190	ARG	2.4
10	J	79	ASP	2.4
13	X	41	THR	2.4
4	D	84	ASP	2.4
2	B	599	LYS	2.4
2	R	264	SER	2.4
3	C	265	LYS	2.4
4	D	216	LEU	2.4
4	S	264	ILE	2.3
1	W	153	GLN	2.3
1	W	693	GLU	2.3
3	C	247	ASP	2.3
5	E	135	VAL	2.3
4	D	225	LYS	2.3
7	G	45	SER	2.3
4	S	217	ILE	2.3
5	E	177	GLN	2.3
2	R	378	ARG	2.3
3	Y	216	ILE	2.3
4	S	85	CYS	2.3
10	J	48	THR	2.3
2	R	52	ILE	2.3
2	B	601	ASP	2.3
5	T	168	TYR	2.3
11	M	62	SER	2.2
2	B	299	TYR	2.2
6	F	87	LEU	2.2
1	W	291	SER	2.2
9	K	54	ASN	2.2
1	A	531	LYS	2.2
2	B	1118	LEU	2.2
2	B	379	GLY	2.2
2	B	1076	ASN	2.2
1	W	182	GLU	2.2
2	R	310	ASP	2.2
2	R	774	ASP	2.2
4	S	107	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	163	THR	2.2
6	F	78	ILE	2.2
4	D	85	CYS	2.2
1	A	579	ASP	2.2
6	F	81	ASP	2.2
6	U	43	SER	2.2
6	F	90	ASP	2.2
2	B	600	LEU	2.1
10	J	55	LEU	2.1
5	T	158	PRO	2.1
7	V	19	GLU	2.1
5	E	32	GLN	2.1
2	R	75	GLU	2.1
2	R	769	PRO	2.1
4	S	81	GLU	2.1
3	C	232	LYS	2.1
5	E	81	VAL	2.1
1	W	145	VAL	2.1
10	J	78	ARG	2.1
2	R	382	LEU	2.1
2	B	774	ASP	2.1
5	E	174	TRP	2.1
11	L	89	GLY	2.1
6	U	63	ILE	2.1
3	C	244	LYS	2.1
2	B	308	ALA	2.1
7	V	96	ILE	2.1
3	C	132	HIS	2.1
2	B	257	PRO	2.1
2	R	83	ILE	2.1
1	W	250	LYS	2.1
12	N	31	PRO	2.1
4	S	188	PHE	2.0
5	T	167	PRO	2.0
2	R	114	PRO	2.0
5	T	166	GLN	2.0
3	Y	162	SER	2.0
2	B	587	ASN	2.0
1	W	54	PRO	2.0
6	U	81	ASP	2.0
7	V	48	ILE	2.0
1	A	292	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	209	LYS	2.0
2	R	55	GLU	2.0
3	Y	225	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
16	F3S	D	1265	7/7	0.98	0.15	-1.36	88,88,88,88	0
16	F3S	S	1265	7/7	0.97	0.13	-1.41	86,86,86,86	0
14	ZN	W	1881	1/1	0.92	0.07	-1.51	81,81,81,81	0
14	ZN	X	1049	1/1	0.96	0.07	-1.58	91,91,91,91	0
14	ZN	N	1065	1/1	0.99	0.11	-1.83	83,83,83,83	0
14	ZN	P	1049	1/1	0.98	0.07	-1.94	87,87,87,87	0
14	ZN	O	1065	1/1	0.99	0.07	-2.25	81,81,81,81	0
14	ZN	W	1880	1/1	0.94	0.06	-2.60	81,81,81,81	0
14	ZN	A	1880	1/1	0.96	0.06	-2.62	79,79,79,79	0
14	ZN	R	2123	1/1	0.97	0.04	-2.77	76,76,76,76	0
14	ZN	B	2123	1/1	0.97	0.06	-2.83	75,75,75,75	0
14	ZN	A	1881	1/1	0.98	0.04	-2.96	79,79,79,79	0
15	MG	A	1882	1/1	0.94	0.43	-	79,79,79,79	0
15	MG	W	1882	1/1	0.93	0.22	-	81,81,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.