



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:40 PM GMT

PDB ID : 4XLS  
Title : Crystal structure of T. aquaticus transcription initiation complex with CarD containing upstream fork promoter.  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.01 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

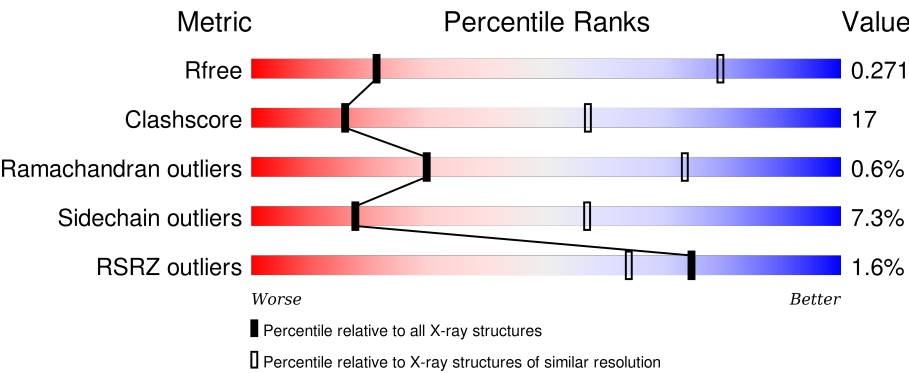
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.01 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	1015 (4.48-3.56)
Clashscore	102246	1054 (4.44-3.60)
Ramachandran outliers	100387	1006 (4.42-3.60)
Sidechain outliers	100360	1016 (4.46-3.58)
RSRZ outliers	91569	1018 (4.48-3.56)

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	314	<div><div></div><div>41%30%•28%</div></div>
1	B	314	<div><div></div><div>43%27%•28%</div></div>
1	G	314	<div><div>4%</div><div>42%29%•28%</div></div>
1	H	314	<div><div></div><div>38%32%•28%</div></div>
2	C	1119	<div><div>2%</div><div>58%38%••</div></div>

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Mol	Chain	Length	Quality of chain
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	30	
7	R	30	
8	P	24	
8	S	24	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 58966 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	162	Total	C	N	O	S	0	0	0
			1274	807	234	231	2			
6	N	162	Total	C	N	O	S	0	0	0
			1274	807	234	231	2			

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
7	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 8 is a DNA chain called DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*TP\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	24	Total	C	N	O	P	0	0	0
			489	235	86	144	24			
8	S	24	Total	C	N	O	P	0	0	0
			489	235	86	144	24			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	2	Total	Zn	0	0
			2	2		
9	D	2	Total	Zn	0	0
			2	2		

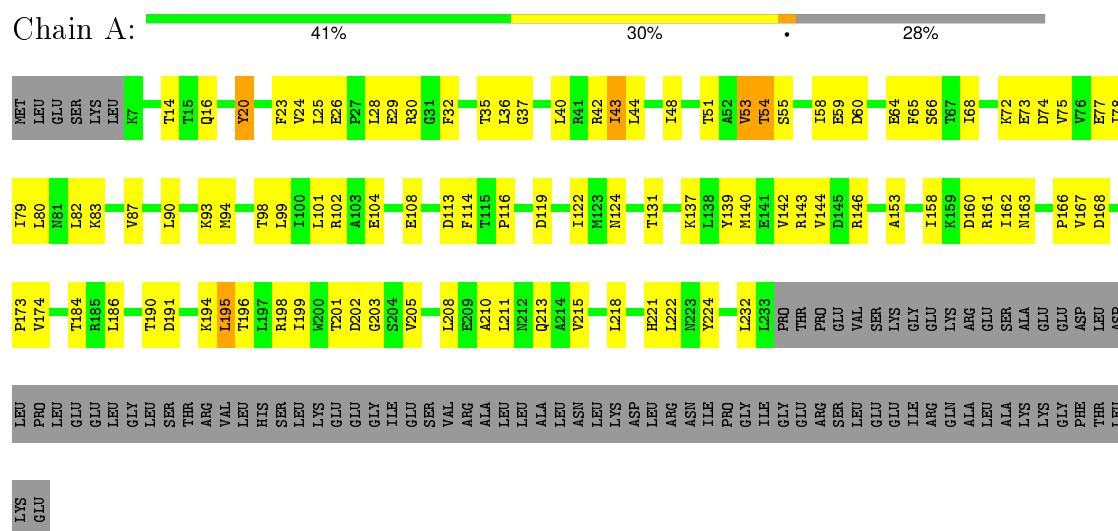
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	J	1	Total 1	Mg 1	0	0
10	D	1	Total 1	Mg 1	0	0

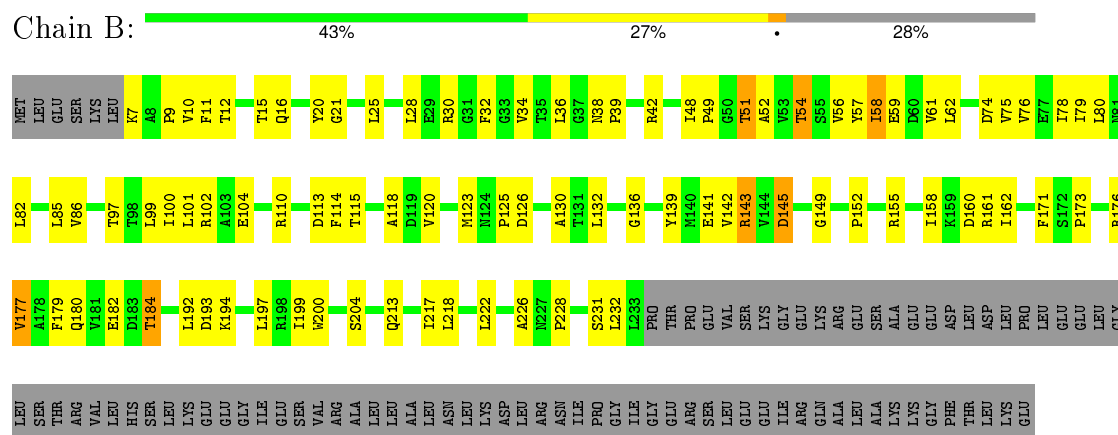
### 3 Residue-property plots

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

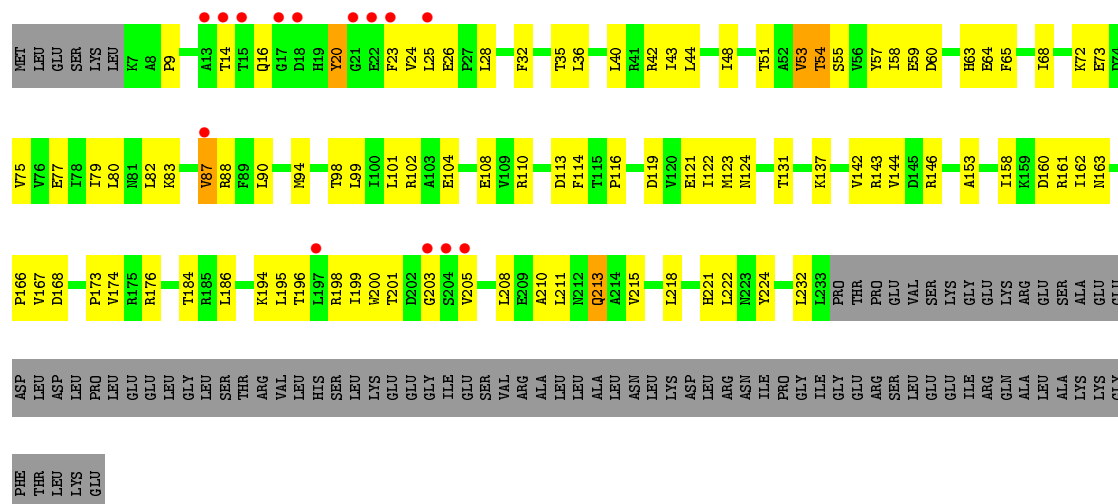


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

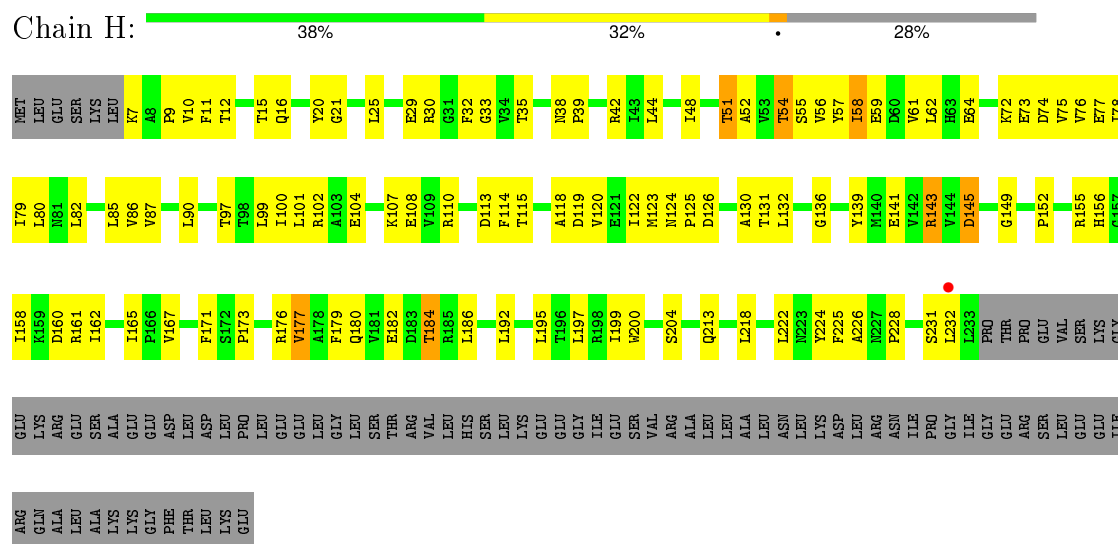


#### • Molecule 1: DNA-directed RNA polymerase subunit alpha

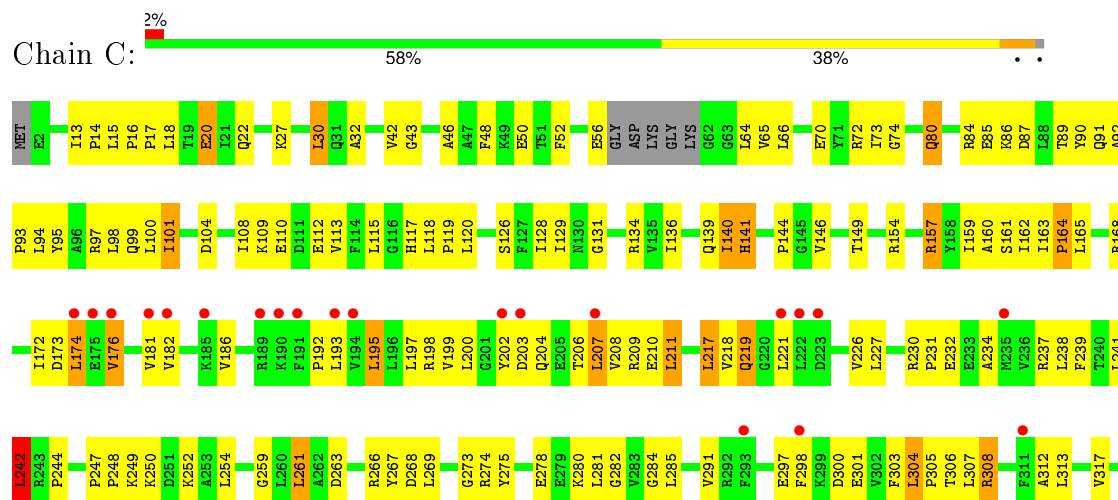




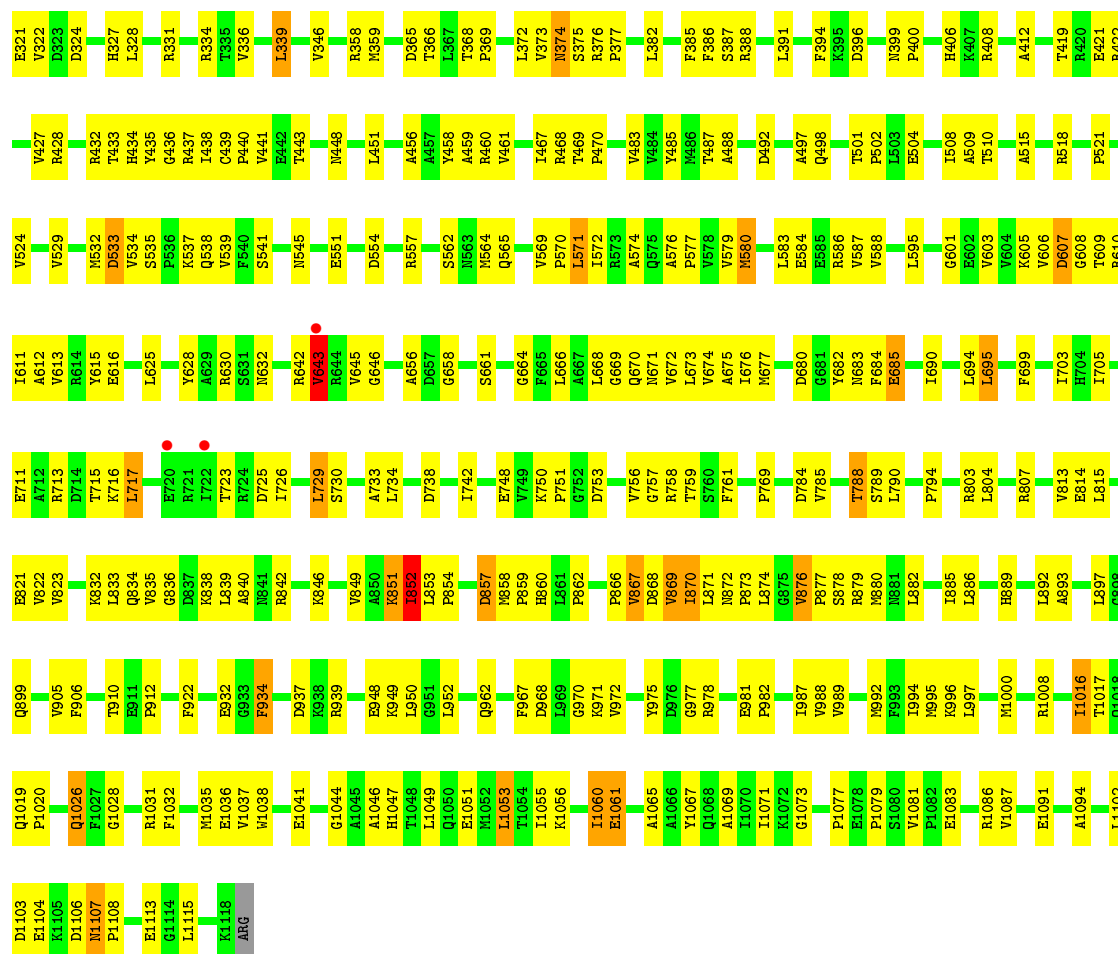
• Molecule 1: DNA-directed RNA polymerase subunit alpha



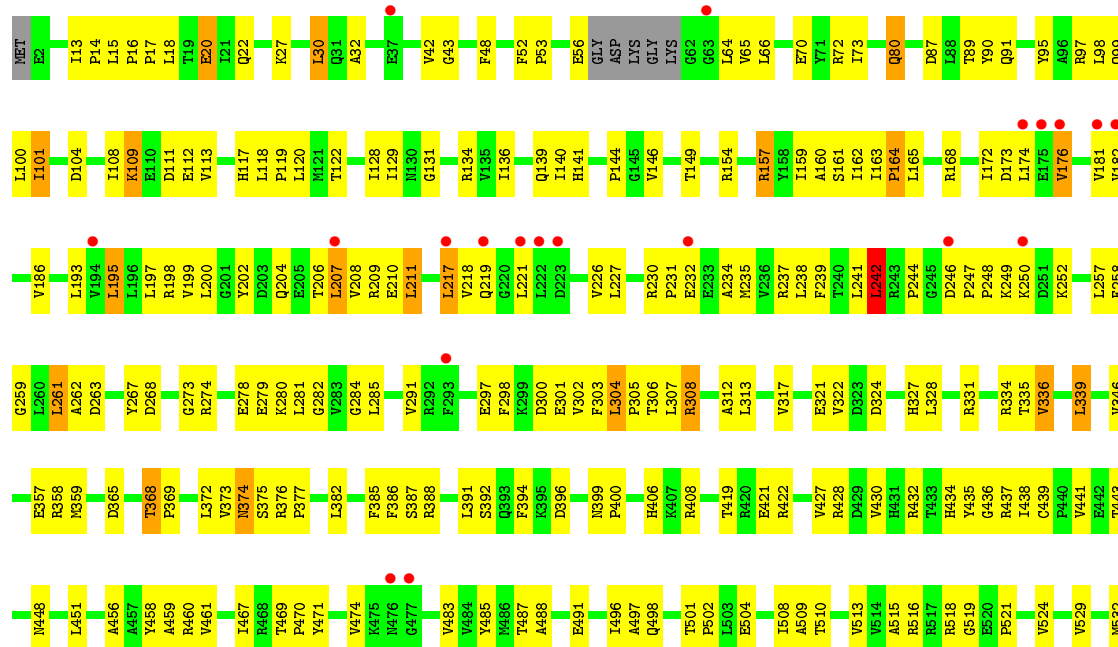
• Molecule 2: DNA-directed RNA polymerase subunit beta

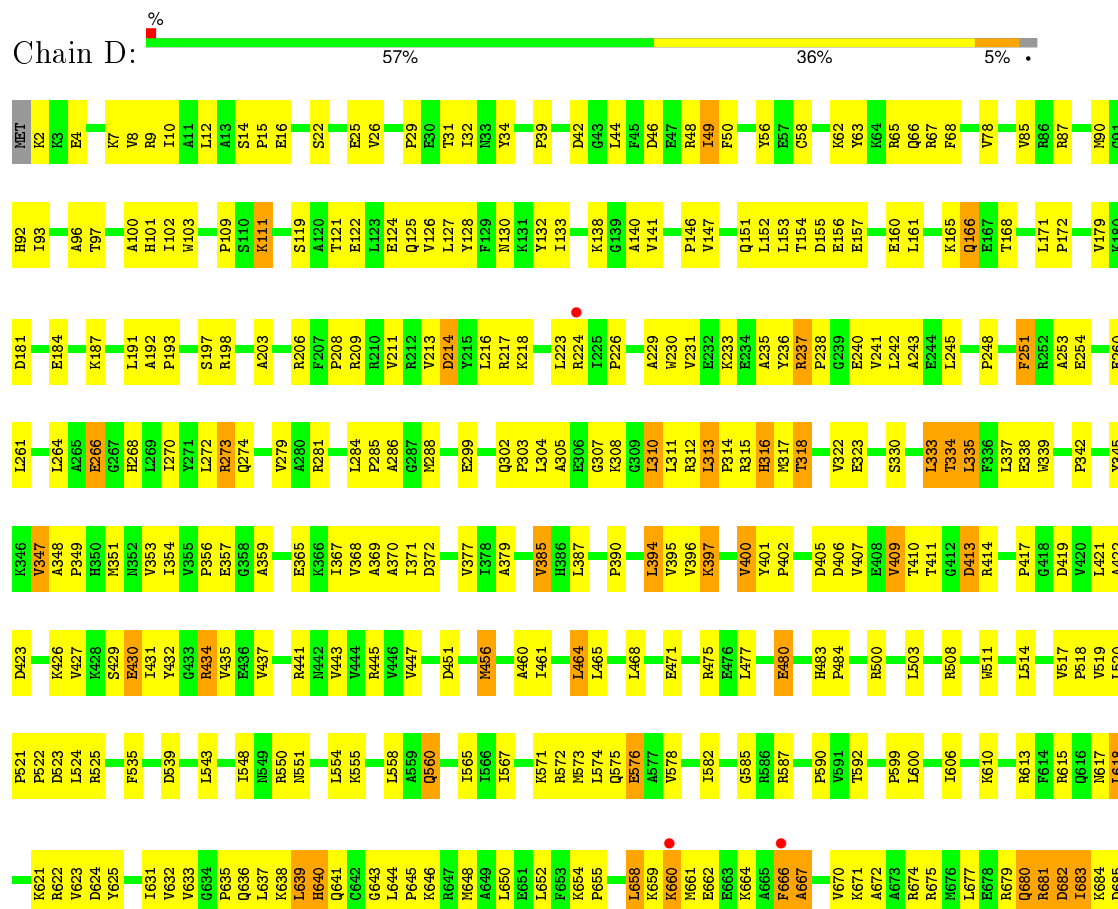


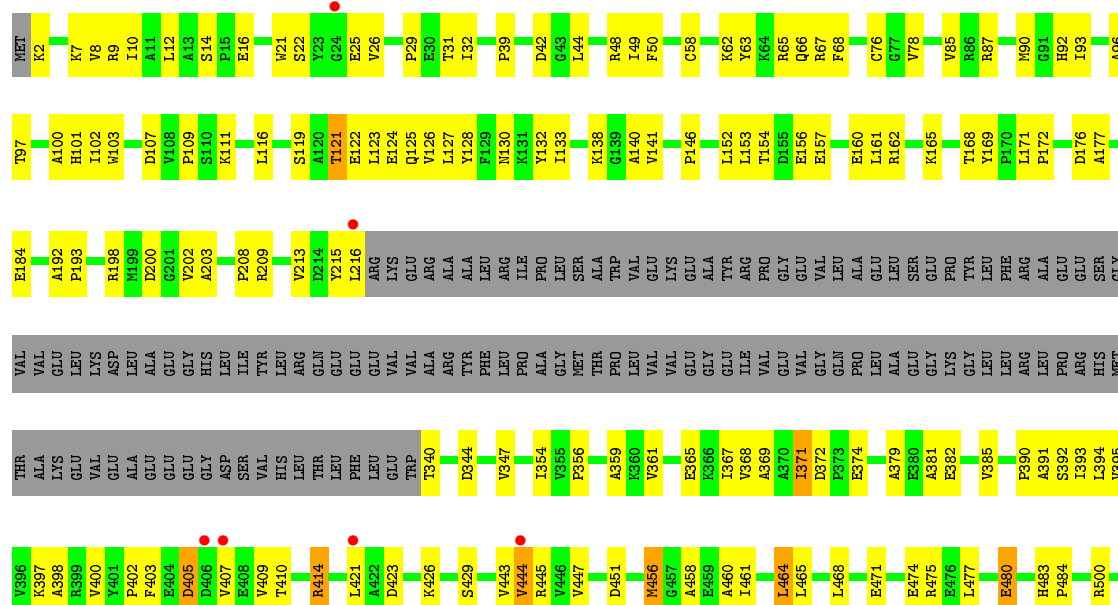


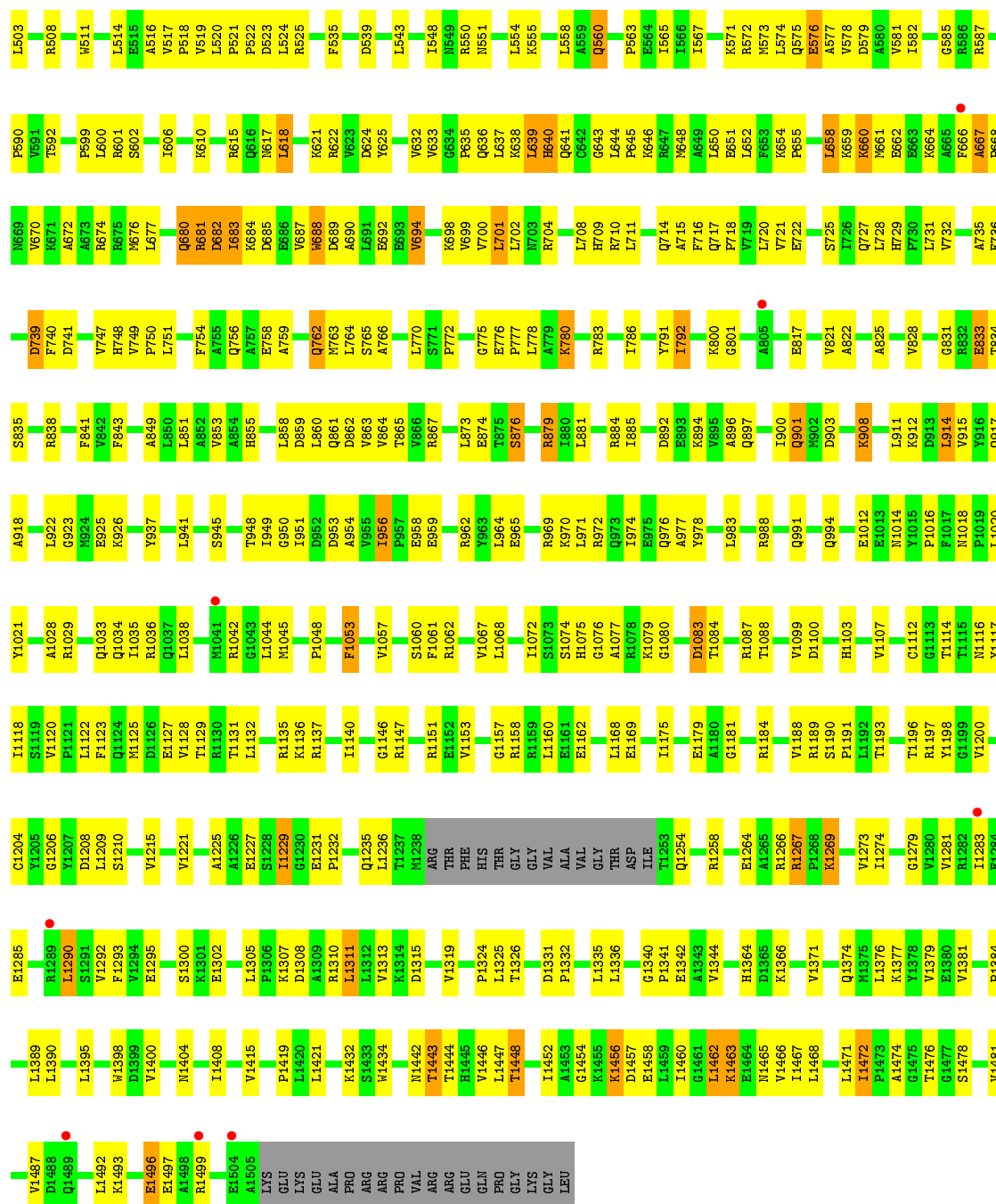


● Molecule 2: DNA-directed RNA polymerase subunit beta



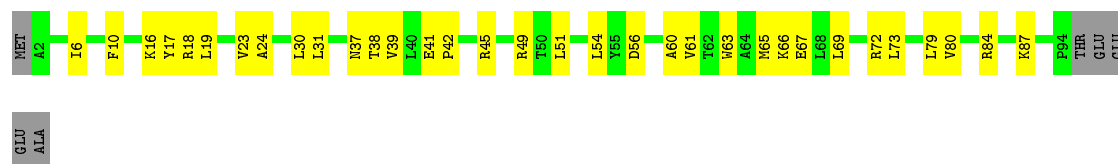




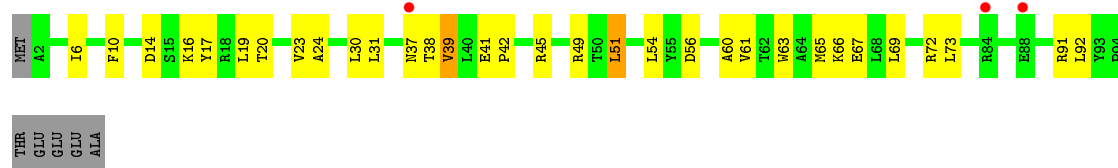


- Molecule 4: DNA-directed RNA polymerase subunit omega

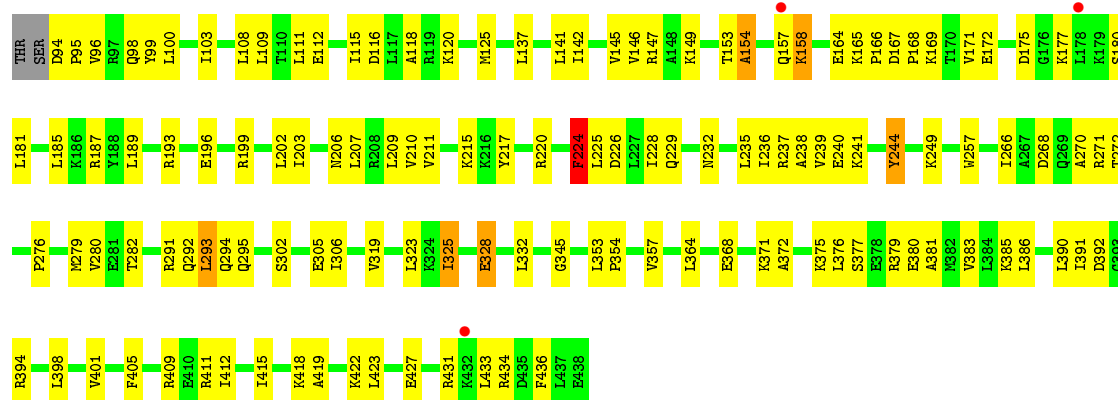
Chain E:



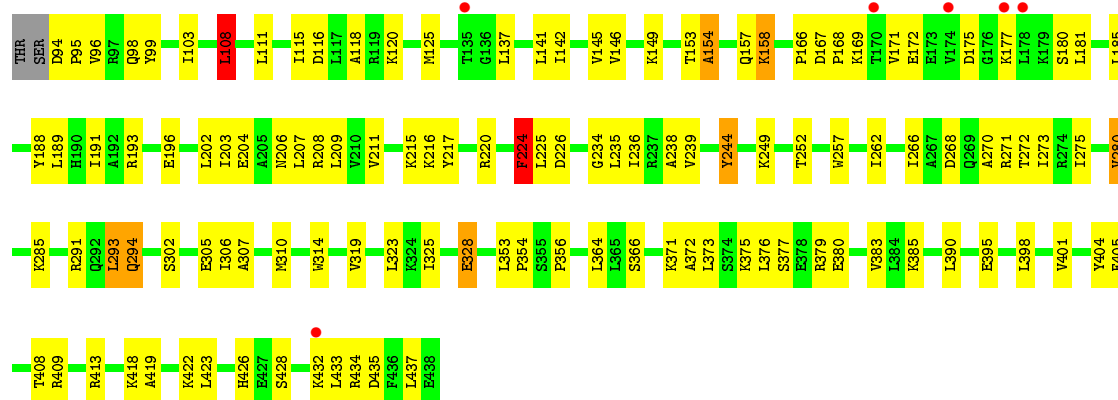
- Molecule 4: DNA-directed RNA polymerase subunit omega



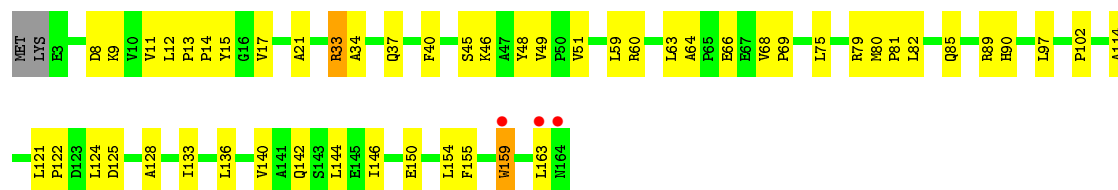
- Molecule 5: RNA polymerase sigma factor SigA



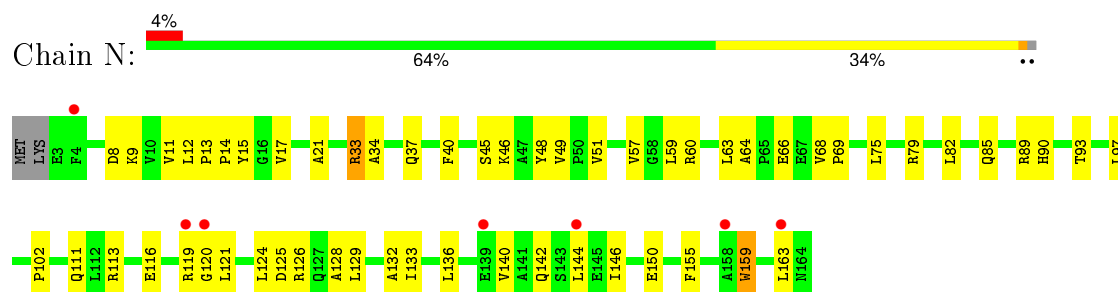
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: CarD-like transcriptional regulator



- Molecule 6: CarD-like transcriptional regulator



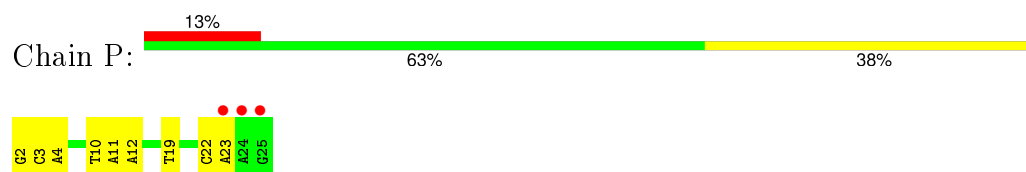
- Molecule 7: DNA (30-MER)



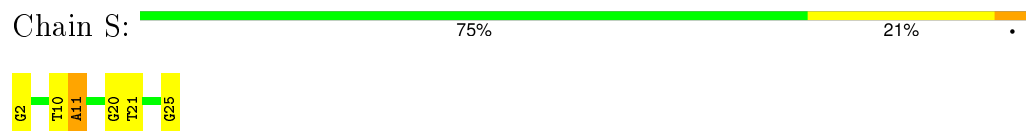
- Molecule 7: DNA (30-MER)



- Molecule 8: DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*T  
P\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3')



- Molecule 8: DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*T  
P\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	293.15Å 293.15Å 539.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 4.01 49.86 – 4.01	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.79-4.01) 75.7 (49.86-4.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1839)	Depositor
R, $R_{free}$	0.232 , 0.272 0.228 , 0.271	Depositor DCC
$R_{free}$ test set	7465 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	146.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 191.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	1 of 148260 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	58966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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, 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	0.27	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.54	0/2455
1	G	0.27	0/1804	0.52	0/2455
1	H	0.28	0/1804	0.55	0/2455
2	C	0.26	0/8905	0.53	1/12040 (0.0%)
2	I	0.26	0/8905	0.53	1/12040 (0.0%)
3	D	0.27	0/11963	0.52	0/16165
3	J	0.27	0/10959	0.51	0/14802
4	E	0.25	0/783	0.52	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.52	0/3804
5	L	0.27	0/2829	0.53	0/3804
6	M	0.26	0/1302	0.51	0/1765
6	N	0.26	0/1302	0.49	0/1765
7	O	0.46	0/687	1.08	0/1059
7	R	0.46	0/687	1.11	1/1059 (0.1%)
8	P	0.45	0/547	1.13	3/841 (0.4%)
8	S	0.48	0/547	1.18	2/841 (0.2%)
All	All	0.28	0/60244	0.56	8/81913 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	25	DG	P-O5'-C5'	-6.14	111.08	120.90
2	I	242	LEU	CA-CB-CG	5.95	128.99	115.30
2	C	242	LEU	CA-CB-CG	5.89	128.85	115.30
7	R	28	DA	O4'-C1'-N9	5.80	112.06	108.00
8	P	19	DT	C5-C4-O4	-5.26	121.22	124.90
8	S	11	DA	O4'-C1'-N9	5.26	111.68	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	19	DT	O4'-C1'-N1	5.05	111.54	108.00
8	P	19	DT	N3-C4-O4	5.05	122.93	119.90

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	1770	0	1799	75	0
1	B	1770	0	1799	61	0
1	G	1770	0	1799	78	0
1	H	1770	0	1799	74	0
2	C	8739	0	8841	357	0
2	I	8739	0	8841	363	0
3	D	11761	0	11976	449	0
3	J	10779	0	10993	397	0
4	E	768	0	784	27	0
4	K	768	0	784	27	0
5	F	2787	0	2866	86	0
5	L	2787	0	2866	79	0
6	M	1274	0	1288	34	0
6	N	1274	0	1288	39	0
7	O	613	0	343	14	0
7	R	613	0	343	9	0
8	P	489	0	273	7	0
8	S	489	0	273	5	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58966	0	58955	2002	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 17.

All (2002) 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)
5:F:149:LYS:HB3	5:F:193:ARG:HH12	1.35	0.91
2:I:204:GLN:HB2	2:I:227:LEU:HD21	1.54	0.90
5:L:149:LYS:HB3	5:L:193:ARG:HH12	1.37	0.88
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.38	0.88
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.55	0.88
2:C:204:GLN:HB2	2:C:227:LEU:HD21	1.57	0.86
2:I:374:ASN:HD21	5:L:291:ARG:HD2	1.40	0.86
2:I:502:PRO:HG3	2:I:510:THR:HG22	1.56	0.86
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.40	0.85
2:I:199:VAL:HA	2:I:231:PRO:HB3	1.58	0.85
2:C:234:ALA:HA	2:C:237:ARG:HB2	1.58	0.85
1:G:42:ARG:HH12	2:I:857:ASP:HB3	1.43	0.84
2:I:211:LEU:HD11	2:I:221:LEU:HB3	1.60	0.84
2:I:428:ARG:HE	2:I:451:LEU:HD21	1.43	0.84
2:I:324:ASP:HB3	2:I:327:HIS:HB2	1.60	0.83
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.60	0.83
2:C:211:LEU:HD11	2:C:221:LEU:HB3	1.61	0.83
2:I:313:LEU:HD13	2:I:321:GLU:HA	1.62	0.81
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.63	0.81
2:I:683:ASN:HB2	2:I:872:ASN:HB2	1.62	0.81
2:C:674:VAL:HA	2:C:869:VAL:HG13	1.63	0.81
4:K:39:VAL:HB	4:K:72:ARG:HD2	1.62	0.80
3:J:800:LYS:HB3	3:J:822:ALA:HB2	1.63	0.80
3:D:166:GLN:HB3	3:D:396:VAL:HG22	1.62	0.80
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.62	0.80
2:I:328:LEU:HD23	2:I:437:ARG:HD2	1.63	0.80
2:I:751:PRO:HB3	2:I:794:PRO:HA	1.62	0.80
2:I:1102:LEU:HB2	3:J:7:LYS:HB2	1.62	0.80
3:D:700:VAL:HG22	3:D:718:PRO:HG3	1.63	0.79
2:C:428:ARG:HE	2:C:451:LEU:HD21	1.48	0.79
2:I:32:ALA:HB1	2:I:73:ILE:HD13	1.63	0.79
3:D:974:ILE:HG12	3:D:991:GLN:HE21	1.48	0.79
2:C:313:LEU:HD13	2:C:321:GLU:HA	1.63	0.79
2:I:658:GLY:H	2:I:661:SER:HB3	1.47	0.78
4:E:39:VAL:HB	4:E:72:ARG:HD2	1.66	0.78
3:D:660:LYS:HD2	3:D:694:VAL:HG13	1.65	0.78
3:D:226:PRO:HA	3:D:330:SER:HA	1.63	0.78
3:D:1122:LEU:HD23	3:D:1140:ILE:HD13	1.64	0.78
3:J:1147:ARG:HH12	3:J:1191:PRO:HD3	1.50	0.77
2:C:328:LEU:HD23	2:C:437:ARG:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.67	0.77
3:J:1122:LEU:HD23	3:J:1140:ILE:HD13	1.66	0.76
3:J:184:GLU:HG2	3:J:202:VAL:HG22	1.65	0.76
3:D:977:ALA:HB2	3:J:831:GLY:HA3	1.66	0.76
1:A:53:VAL:HG22	1:A:54:THR:H	1.49	0.76
5:L:271:ARG:HG2	5:L:328:GLU:HB3	1.67	0.76
5:F:431:ARG:HG3	5:F:434:ARG:HE	1.49	0.76
2:C:32:ALA:HB1	2:C:73:ILE:HD13	1.67	0.76
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.51	0.75
2:C:374:ASN:HD22	2:C:375:SER:H	1.34	0.75
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.68	0.75
2:I:584:GLU:HB3	2:I:666:LEU:H	1.52	0.75
4:K:30:LEU:HD23	4:K:63:TRP:HB3	1.69	0.74
3:D:400:VAL:HG23	3:D:443:VAL:HG21	1.68	0.74
3:D:349:PRO:HB3	5:F:112:GLU:HG2	1.70	0.74
2:C:537:LYS:HZ3	2:C:905:VAL:H	1.35	0.74
2:C:373:VAL:HG12	2:C:374:ASN:H	1.53	0.74
2:I:1060:ILE:HD12	2:I:1061:GLU:H	1.52	0.74
2:I:432:ARG:HH12	2:I:518:ARG:HH21	1.35	0.74
2:C:197:LEU:HD23	2:C:200:LEU:HD23	1.70	0.73
2:I:515:ALA:HB3	2:I:524:VAL:HG21	1.68	0.73
3:D:1267:ARG:H	3:D:1267:ARG:HE	1.34	0.73
2:C:684:PHE:HE1	3:D:783:ARG:HB2	1.52	0.73
3:J:974:ILE:HG12	3:J:991:GLN:HE21	1.54	0.73
2:C:836:GLY:H	2:C:849:VAL:HB	1.54	0.73
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.69	0.73
2:C:14:PRO:HB3	2:C:586:ARG:HH22	1.52	0.73
3:D:1103:HIS:HB2	3:D:1462:LEU:HD11	1.69	0.73
2:C:584:GLU:HB3	2:C:666:LEU:H	1.54	0.73
2:I:197:LEU:HD23	2:I:200:LEU:HD23	1.71	0.73
2:I:684:PHE:HE1	3:J:783:ARG:HB2	1.52	0.73
2:I:373:VAL:HG12	2:I:374:ASN:H	1.54	0.73
4:K:67:GLU:HB3	4:K:73:LEU:HD11	1.69	0.72
3:D:1147:ARG:HH12	3:D:1191:PRO:HD3	1.52	0.72
2:I:278:GLU:HG3	2:I:284:GLY:HA2	1.70	0.72
4:K:31:LEU:HG	4:K:60:ALA:HB2	1.71	0.72
1:G:53:VAL:HG22	1:G:54:THR:H	1.54	0.72
2:C:146:VAL:HG23	2:C:280:LYS:HD2	1.71	0.72
2:I:537:LYS:HZ3	2:I:905:VAL:H	1.35	0.72
2:C:1046:ALA:HB1	3:D:1471:LEU:HD11	1.72	0.72
2:C:165:LEU:HB2	2:C:168:ARG:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:742:ILE:HG22	2:C:756:VAL:HG12	1.72	0.71
2:I:674:VAL:HA	2:I:869:VAL:HG13	1.70	0.71
1:H:52:ALA:HB2	1:H:171:PHE:HA	1.71	0.71
3:D:646:LYS:HE3	3:D:688:TRP:HZ2	1.56	0.71
1:A:158:ILE:HG22	1:A:160:ASP:H	1.56	0.71
1:B:161:ARG:HG3	1:B:162:ILE:H	1.55	0.71
1:H:51:THR:HG21	1:H:86:VAL:HG23	1.71	0.71
3:J:1267:ARG:HE	3:J:1267:ARG:H	1.37	0.71
2:I:144:PRO:HB3	2:I:164:PRO:O	1.90	0.71
2:I:139:GLN:HB3	2:I:334:ARG:HB2	1.73	0.70
4:K:49:ARG:HA	4:K:54:LEU:HG	1.71	0.70
2:C:261:LEU:HB2	2:C:291:VAL:HG22	1.71	0.70
2:C:690:ILE:HG13	2:C:852:ILE:HG23	1.73	0.70
2:C:374:ASN:HD21	5:F:291:ARG:HD2	1.56	0.70
1:G:55:SER:HB3	1:G:143:ARG:HB2	1.73	0.70
2:C:432:ARG:HH12	2:C:518:ARG:HH21	1.39	0.70
1:B:52:ALA:HB2	1:B:171:PHE:HA	1.74	0.70
5:L:203:ILE:HG12	5:L:239:VAL:HG21	1.73	0.70
2:C:278:GLU:HG3	2:C:284:GLY:HA2	1.73	0.70
1:H:78:ILE:HD12	1:H:130:ALA:HB2	1.72	0.70
2:I:261:LEU:HB2	2:I:291:VAL:HG22	1.72	0.70
2:I:234:ALA:HA	2:I:237:ARG:HB2	1.74	0.70
6:N:85:GLN:HE21	7:R:25:DT:H4'	1.56	0.69
2:C:1008:ARG:HD3	2:C:1028:GLY:HA2	1.74	0.69
2:I:876:VAL:HG11	2:I:885:ILE:HD11	1.72	0.69
1:H:161:ARG:HG3	1:H:162:ILE:H	1.56	0.69
2:C:515:ALA:HB3	2:C:524:VAL:HG21	1.73	0.69
2:C:1094:ALA:HB2	3:D:520:LEU:HD13	1.74	0.69
4:E:30:LEU:HD23	4:E:63:TRP:HB3	1.75	0.69
2:C:144:PRO:HB3	2:C:164:PRO:O	1.92	0.69
3:D:550:ARG:HH21	5:F:226:ASP:HB2	1.56	0.69
5:F:411:ARG:HD3	7:O:1:DC:H2'	1.74	0.69
3:J:1264:GLU:HB3	3:J:1266:ARG:HG3	1.75	0.69
1:G:218:LEU:HG	1:H:222:LEU:HD11	1.74	0.69
5:L:428:SER:HA	5:L:434:ARG:HH21	1.55	0.69
3:J:543:LEU:HG	3:J:600:LEU:HD23	1.74	0.69
3:D:44:LEU:HB3	3:D:525:ARG:HH22	1.58	0.69
3:J:700:VAL:HG22	3:J:718:PRO:HG3	1.74	0.69
1:B:51:THR:HG21	1:B:86:VAL:HG23	1.74	0.69
2:I:502:PRO:HB2	2:I:509:ALA:HB3	1.74	0.68
3:D:213:VAL:HG22	3:D:385:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:HB1	1:A:166:PRO:HB2	1.74	0.68
3:J:44:LEU:HB3	3:J:525:ARG:HH22	1.57	0.68
2:I:157:ARG:HA	2:I:157:ARG:HH11	1.58	0.68
2:C:853:LEU:HD12	2:C:854:PRO:HD2	1.75	0.68
1:B:78:ILE:HD12	1:B:130:ALA:HB2	1.74	0.68
2:I:1094:ALA:HB2	3:J:520:LEU:HD13	1.75	0.68
5:F:376:LEU:HD21	5:F:423:LEU:HG	1.74	0.68
2:I:165:LEU:HB2	2:I:168:ARG:HB2	1.76	0.68
5:F:157:GLN:HE22	5:F:171:VAL:HG21	1.59	0.68
2:C:971:LYS:HG2	2:C:988:VAL:HG12	1.74	0.68
2:C:572:ILE:HD11	2:C:703:ILE:HD11	1.75	0.68
2:I:154:ARG:HD2	2:I:157:ARG:HB2	1.75	0.68
5:L:376:LEU:HD21	5:L:423:LEU:HG	1.74	0.68
3:D:354:ILE:HD11	3:D:369:ALA:HB2	1.75	0.68
3:J:900:ILE:HG12	3:J:914:LEU:HD21	1.75	0.68
2:C:607:ASP:O	2:C:609:THR:N	2.26	0.68
5:L:137:LEU:HD11	5:L:177:LYS:HE3	1.76	0.68
3:D:1264:GLU:HB3	3:D:1266:ARG:HG3	1.75	0.68
2:C:658:GLY:H	2:C:661:SER:HB3	1.60	0.67
2:I:571:LEU:HB2	2:I:574:ALA:HB2	1.76	0.67
6:N:49:VAL:HG11	6:N:59:LEU:HD22	1.76	0.67
2:I:193:LEU:HD22	2:I:221:LEU:HD11	1.76	0.67
3:J:96:ALA:HB2	3:J:555:LYS:HG2	1.76	0.67
3:J:192:ALA:HB1	3:J:193:PRO:HD2	1.76	0.67
3:J:100:ALA:H	3:J:575:GLN:HE22	1.42	0.67
6:M:155:PHE:HB2	6:M:163:LEU:HD11	1.77	0.67
3:J:203:ALA:HA	3:J:395:VAL:HA	1.76	0.67
3:D:1042:ARG:HB3	3:D:1057:VAL:HG21	1.77	0.67
1:A:184:THR:HB	1:A:194:LYS:HB3	1.77	0.67
1:H:184:THR:HG23	1:H:192:LEU:HB2	1.75	0.67
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.77	0.67
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.76	0.67
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.77	0.67
2:I:603:VAL:HA	2:I:613:VAL:HG12	1.77	0.67
1:G:174:VAL:HA	1:G:201:THR:HG22	1.76	0.67
2:I:853:LEU:HD12	2:I:854:PRO:HD2	1.76	0.67
2:C:157:ARG:HA	2:C:157:ARG:HH11	1.59	0.67
2:C:376:ARG:HG3	2:C:377:PRO:HD3	1.77	0.67
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.76	0.67
4:E:49:ARG:HA	4:E:54:LEU:HG	1.77	0.67
3:D:560:GLN:HE22	5:F:236:ILE:HG21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.77	0.66
2:I:108:ILE:HB	6:N:48:TYR:HB2	1.76	0.66
2:I:874:LEU:HD13	3:J:783:ARG:HB3	1.76	0.66
1:G:153:ALA:HB1	1:G:166:PRO:HB2	1.76	0.66
3:D:860:LEU:HD12	3:D:860:LEU:H	1.60	0.66
1:A:222:LEU:HD21	1:B:218:LEU:HB3	1.77	0.66
2:C:139:GLN:HB3	2:C:334:ARG:HB2	1.75	0.66
2:I:113:VAL:HG21	2:I:373:VAL:HG21	1.77	0.66
2:I:1046:ALA:HB1	3:J:1471:LEU:HD11	1.78	0.66
3:J:1254:GLN:HB3	3:J:1258:ARG:HB2	1.78	0.66
3:D:166:GLN:HB2	3:D:394:LEU:HD21	1.77	0.66
3:J:97:THR:HG21	3:J:571:LYS:HG3	1.78	0.66
2:I:91:GLN:HA	2:I:119:PRO:HA	1.76	0.66
3:D:1493:LYS:HA	3:D:1496:GLU:HB2	1.78	0.66
7:O:24:DC:H42	8:P:2:DG:H1	1.44	0.66
3:J:400:VAL:HG12	3:J:445:ARG:HG2	1.78	0.66
1:G:184:THR:HB	1:G:194:LYS:HB3	1.78	0.66
2:I:282:GLY:HA3	2:I:308:ARG:HH21	1.59	0.66
3:D:1462:LEU:HD12	3:D:1463:LYS:H	1.58	0.65
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.31	0.65
3:D:96:ALA:HB2	3:D:555:LYS:HG2	1.78	0.65
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.77	0.65
2:C:172:ILE:HA	2:C:186:VAL:HG22	1.79	0.65
3:D:1131:THR:HG22	3:J:1179:GLU:HB3	1.78	0.65
1:A:55:SER:HB3	1:A:143:ARG:HB2	1.77	0.65
2:I:304:LEU:HB3	2:I:305:PRO:HD3	1.78	0.65
2:I:1008:ARG:HD3	2:I:1028:GLY:HA2	1.77	0.65
2:I:759:THR:HB	2:I:785:VAL:HG21	1.77	0.65
3:J:8:VAL:HG21	3:J:1468:LEU:HD21	1.77	0.65
4:E:31:LEU:HG	4:E:60:ALA:HB2	1.77	0.65
2:C:163:ILE:HD12	2:C:164:PRO:HD2	1.79	0.65
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.78	0.65
2:C:101:ILE:HD12	2:C:108:ILE:HG23	1.79	0.65
3:D:203:ALA:HA	3:D:395:VAL:HA	1.77	0.65
3:J:1042:ARG:HB3	3:J:1057:VAL:HG21	1.76	0.65
6:N:155:PHE:HB2	6:N:163:LEU:HD11	1.78	0.65
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.78	0.65
3:J:560:GLN:HE22	5:L:236:ILE:HG21	1.62	0.65
2:I:577:PRO:HG2	2:I:580:MET:HG2	1.77	0.65
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.79	0.65
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HB2	1:A:119:ASP:HA	1.77	0.65
3:D:670:VAL:HB	5:F:364:LEU:HD11	1.77	0.65
2:C:97:ARG:HE	2:C:112:GLU:HB2	1.61	0.65
3:J:698:LYS:HG2	3:J:756:GLN:HG2	1.79	0.65
2:I:607:ASP:O	2:I:609:THR:N	2.29	0.65
2:I:172:ILE:HA	2:I:186:VAL:HG22	1.79	0.64
3:J:367:ILE:HG22	3:J:368:VAL:HG23	1.79	0.64
2:C:742:ILE:HD13	2:C:803:ARG:HD2	1.79	0.64
3:D:650:LEU:HD12	3:D:688:TRP:HZ3	1.63	0.64
2:C:579:VAL:HG13	2:C:842:ARG:HH22	1.63	0.64
3:D:241:VAL:HG22	3:D:312:ARG:HD3	1.80	0.64
2:I:711:GLU:HG2	2:I:822:VAL:HG12	1.80	0.64
1:G:14:THR:HG1	1:H:231:SER:HG	1.43	0.64
3:J:670:VAL:HB	5:L:364:LEU:HD11	1.78	0.64
3:D:500:ARG:HD3	3:D:503:LEU:HD12	1.77	0.64
3:D:266:GLU:HG3	3:D:286:ALA:HB2	1.79	0.64
2:C:282:GLY:HA3	2:C:308:ARG:HH21	1.61	0.64
2:C:154:ARG:HD2	2:C:157:ARG:HB2	1.79	0.64
2:I:470:PRO:HG3	2:I:485:TYR:CZ	2.33	0.64
2:C:759:THR:HB	2:C:785:VAL:HG21	1.79	0.64
5:F:271:ARG:HG2	5:F:328:GLU:HB3	1.78	0.64
4:E:79:LEU:HG	4:E:80:VAL:HG13	1.80	0.64
3:D:407:VAL:HG22	3:D:409:VAL:H	1.62	0.64
3:D:132:TYR:HA	3:D:456:MET:HB3	1.79	0.64
1:A:108:GLU:HG2	1:A:131:THR:HG23	1.79	0.64
3:J:1395:LEU:HD11	3:J:1400:VAL:HB	1.79	0.64
2:I:742:ILE:HD13	2:I:803:ARG:HD2	1.80	0.64
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.79	0.64
2:I:181:VAL:HG22	2:I:182:VAL:H	1.63	0.64
3:J:661:MET:HG2	3:J:666:PHE:CZ	2.33	0.64
2:C:886:LEU:HD21	3:D:951:ILE:HD13	1.80	0.64
1:G:158:ILE:HG22	1:G:160:ASP:H	1.63	0.63
3:D:543:LEU:HG	3:D:600:LEU:HD23	1.80	0.63
2:C:91:GLN:HA	2:C:119:PRO:HA	1.79	0.63
1:A:174:VAL:HA	1:A:201:THR:HG22	1.79	0.63
3:D:97:THR:HG21	3:D:571:LYS:HG3	1.80	0.63
3:J:822:ALA:HB3	3:J:825:ALA:HB2	1.80	0.63
5:L:157:GLN:HE22	5:L:171:VAL:HG21	1.63	0.63
3:J:1379:VAL:HG12	3:J:1419:PRO:HA	1.80	0.63
3:J:132:TYR:HA	3:J:456:MET:HB3	1.80	0.63
3:D:831:GLY:HA3	3:J:977:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:ILE:HD12	2:I:108:ILE:HG23	1.80	0.63
3:J:520:LEU:HB3	3:J:525:ARG:HD3	1.79	0.63
3:J:677:LEU:HD21	3:J:687:VAL:HG11	1.80	0.63
3:J:860:LEU:H	3:J:860:LEU:HD12	1.63	0.63
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.80	0.63
1:A:26:GLU:HG3	1:A:186:LEU:HD12	1.80	0.63
3:J:1099:VAL:O	3:J:1103:HIS:HB3	1.99	0.63
2:I:742:ILE:HG22	2:I:756:VAL:HG12	1.81	0.63
1:G:198:ARG:HH22	2:I:932:GLU:HB3	1.64	0.63
5:L:293:LEU:HD11	5:L:306:ILE:HD13	1.81	0.63
1:G:90:LEU:HB2	1:G:119:ASP:HA	1.81	0.63
2:C:108:ILE:HB	6:M:48:TYR:HB2	1.81	0.62
3:J:550:ARG:HH21	5:L:226:ASP:HB2	1.63	0.62
3:J:1462:LEU:HD12	3:J:1463:LYS:H	1.64	0.62
1:H:87:VAL:HG12	1:H:122:ILE:HG12	1.80	0.62
3:J:215:TYR:HB3	3:J:381:ALA:HB3	1.80	0.62
2:I:1019:GLN:HE21	3:J:617:ASN:HB3	1.64	0.62
2:I:682:TYR:HA	3:J:633:VAL:HG11	1.80	0.62
2:C:181:VAL:HG22	2:C:182:VAL:H	1.63	0.62
2:C:470:PRO:HG3	2:C:485:TYR:CZ	2.34	0.62
3:D:211:VAL:HG13	3:D:345:TYR:HB2	1.81	0.62
1:G:23:PHE:HE2	1:G:199:ILE:HD12	1.64	0.62
1:B:184:THR:HG23	1:B:192:LEU:HB2	1.81	0.62
1:H:58:ILE:HD13	1:H:61:VAL:HB	1.81	0.62
3:D:353:VAL:HG21	3:D:387:LEU:HD21	1.81	0.62
2:I:97:ARG:HE	2:I:112:GLU:HB2	1.64	0.62
1:G:25:LEU:HD23	1:G:28:LEU:HD11	1.81	0.62
1:G:26:GLU:HG3	1:G:186:LEU:HD12	1.80	0.62
3:D:313:LEU:HG	3:D:314:PRO:HD2	1.81	0.62
2:C:239:PHE:HA	2:C:242:LEU:HD12	1.81	0.62
3:D:900:ILE:HG12	3:D:914:LEU:HD21	1.82	0.62
2:I:14:PRO:HB3	2:I:586:ARG:HH22	1.64	0.62
2:I:163:ILE:HD12	2:I:164:PRO:HD2	1.82	0.62
3:J:1197:ARG:HE	3:J:1398:TRP:HB3	1.65	0.62
1:B:152:PRO:HD2	1:B:155:ARG:HG3	1.82	0.62
2:C:498:GLN:HG3	3:D:1068:LEU:HD11	1.80	0.62
1:G:222:LEU:HD21	1:H:218:LEU:HB3	1.81	0.61
2:I:249:LYS:HB2	2:I:252:LYS:HE3	1.82	0.61
1:B:101:LEU:HD22	1:B:102:ARG:H	1.65	0.61
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.82	0.61
3:J:792:ILE:HG21	3:J:941:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1103:HIS:HB2	3:J:1462:LEU:HD11	1.82	0.61
3:J:176:ASP:OD1	3:J:177:ALA:N	2.33	0.61
2:I:339:LEU:HD13	2:I:385:PHE:CZ	2.35	0.61
2:C:676:ILE:HG22	2:C:873:PRO:HB3	1.83	0.61
1:B:177:VAL:HG12	1:B:199:ILE:HG12	1.82	0.61
3:J:1197:ARG:NE	3:J:1398:TRP:HB3	2.15	0.61
2:I:64:LEU:HD21	2:I:66:LEU:HG	1.82	0.61
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.01	0.61
1:A:218:LEU:HG	1:B:222:LEU:HD11	1.81	0.61
3:D:636:GLN:HG2	3:D:637:LEU:HD12	1.83	0.61
3:J:365:GLU:H	3:J:379:ALA:HB3	1.65	0.61
3:D:314:PRO:HG2	3:D:317:MET:HB3	1.83	0.61
6:N:119:ARG:HG3	6:N:120:GLY:H	1.65	0.61
2:I:376:ARG:HG3	2:I:377:PRO:HD3	1.83	0.61
3:D:1197:ARG:NE	3:D:1398:TRP:HB3	2.15	0.61
3:D:698:LYS:HG2	3:D:756:GLN:HG2	1.83	0.61
2:I:1037:VAL:HG13	2:I:1049:LEU:HD11	1.82	0.61
1:A:23:PHE:HE2	1:A:199:ILE:HD12	1.65	0.61
3:J:650:LEU:HD12	3:J:688:TRP:HZ3	1.66	0.61
1:A:53:VAL:HG23	1:A:144:VAL:HG22	1.82	0.61
2:I:1019:GLN:HG3	3:J:617:ASN:HD22	1.65	0.61
3:J:644:LEU:HD12	3:J:645:PRO:HD2	1.83	0.61
3:D:1132:LEU:HD12	3:J:1181:GLY:HA3	1.83	0.61
2:I:694:LEU:HD11	2:I:868:ASP:HB3	1.82	0.60
4:E:38:THR:OG1	4:E:39:VAL:N	2.34	0.60
3:D:371:ILE:HG23	3:D:372:ASP:H	1.66	0.60
2:I:886:LEU:HD21	3:J:951:ILE:HD13	1.83	0.60
1:H:101:LEU:HD22	1:H:102:ARG:H	1.65	0.60
3:D:224:ARG:NH2	3:D:254:GLU:OE2	2.34	0.60
3:J:354:ILE:HD11	3:J:369:ALA:HB2	1.83	0.60
2:I:369:PRO:O	2:I:373:VAL:HG23	2.01	0.60
2:I:756:VAL:HG11	2:I:823:VAL:HG11	1.84	0.60
3:J:169:TYR:O	3:J:392:SER:HB2	2.01	0.60
1:B:58:ILE:HD13	1:B:61:VAL:HB	1.84	0.60
2:I:971:LYS:HG2	2:I:988:VAL:HG12	1.82	0.60
3:J:1125:MET:HG3	3:J:1132:LEU:HG	1.84	0.60
2:I:146:VAL:HG23	2:I:280:LYS:HD2	1.83	0.60
2:C:711:GLU:HG2	2:C:822:VAL:HG12	1.84	0.60
5:F:293:LEU:HD11	5:F:306:ILE:HD13	1.83	0.60
1:G:72:LYS:HG3	2:I:606:VAL:HG11	1.83	0.60
3:D:521:PRO:HD2	3:D:524:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:181:LEU:HD23	5:L:185:LEU:HB2	1.83	0.59
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.84	0.59
1:B:28:LEU:HB3	1:B:193:ASP:HB2	1.83	0.59
2:C:603:VAL:HA	2:C:613:VAL:HG12	1.84	0.59
3:J:660:LYS:HD2	3:J:694:VAL:HG13	1.83	0.59
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.83	0.59
5:F:180:SER:O	5:F:181:LEU:HD12	2.01	0.59
2:I:239:PHE:HA	2:I:242:LEU:HD12	1.84	0.59
2:C:369:PRO:O	2:C:373:VAL:HG23	2.01	0.59
2:C:905:VAL:HG12	2:C:906:PHE:HD2	1.66	0.59
6:N:82:LEU:HB3	6:N:89:ARG:HG3	1.84	0.59
1:G:104:GLU:HG3	1:G:137:LYS:HG2	1.85	0.59
3:D:1197:ARG:HE	3:D:1398:TRP:HB3	1.67	0.59
2:I:939:ARG:HB3	2:I:982:PRO:HG3	1.83	0.59
3:D:792:ILE:HG21	3:D:941:LEU:HD13	1.85	0.59
3:J:681:ARG:O	3:J:683:ILE:HG12	2.02	0.59
3:J:1123:PHE:HB3	3:J:1132:LEU:HD22	1.84	0.59
3:J:917:GLN:HE22	3:J:1168:LEU:HD11	1.67	0.59
5:F:412:ILE:HD13	5:F:415:ILE:HD12	1.84	0.59
2:C:1060:ILE:HD12	2:C:1061:GLU:H	1.67	0.59
2:I:439:CYS:HB2	2:I:541:SER:HB3	1.84	0.59
3:D:310:LEU:H	3:D:310:LEU:HD12	1.67	0.59
3:D:286:ALA:O	3:D:311:LEU:HA	2.03	0.59
2:I:160:ALA:HB3	2:I:174:LEU:HD13	1.85	0.59
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.85	0.59
3:D:1198:TYR:HE2	3:D:1432:LYS:HE2	1.68	0.59
5:F:137:LEU:HD11	5:F:177:LYS:HE3	1.85	0.59
2:C:458:TYR:HB3	2:C:470:PRO:HG2	1.84	0.58
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.85	0.58
1:G:35:THR:HG23	1:H:39:PRO:HA	1.85	0.58
2:I:357:GLU:HG2	5:L:216:LYS:HE2	1.85	0.58
2:I:557:ARG:HD3	2:I:879:ARG:HB3	1.84	0.58
3:J:48:ARG:HA	3:J:78:VAL:HG22	1.85	0.58
3:D:48:ARG:HA	3:D:78:VAL:HG22	1.83	0.58
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.84	0.58
3:J:636:GLN:HG2	3:J:637:LEU:HD12	1.85	0.58
4:K:38:THR:OG1	4:K:39:VAL:N	2.36	0.58
3:D:8:VAL:HG21	3:D:1468:LEU:HD21	1.84	0.58
2:C:64:LEU:HD21	2:C:66:LEU:HG	1.85	0.58
3:J:402:PRO:HA	3:J:443:VAL:HA	1.85	0.58
3:J:141:VAL:HA	3:J:146:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ALA:HB3	2:C:174:LEU:HD13	1.84	0.58
2:I:690:ILE:HG13	2:I:852:ILE:HG23	1.86	0.58
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.84	0.58
6:N:124:LEU:HD21	8:S:2:DG:H5"	1.85	0.58
2:I:836:GLY:H	2:I:849:VAL:HB	1.68	0.58
5:F:96:VAL:HA	5:F:225:LEU:HD11	1.86	0.58
2:I:285:LEU:HD11	2:I:301:GLU:HB3	1.85	0.58
2:C:729:LEU:HD12	2:C:734:LEU:HD13	1.84	0.58
3:J:715:ALA:HB3	3:J:764:LEU:HA	1.86	0.58
2:C:756:VAL:HG11	2:C:823:VAL:HG11	1.85	0.58
2:C:876:VAL:HG11	2:C:885:ILE:HD11	1.85	0.58
1:G:44:LEU:O	1:G:174:VAL:HG11	2.03	0.58
2:C:682:TYR:HA	3:D:633:VAL:HG11	1.84	0.58
3:J:1198:TYR:HE2	3:J:1432:LYS:HE2	1.69	0.58
2:I:65:VAL:HG13	2:I:101:ILE:HB	1.86	0.58
1:H:177:VAL:HG12	1:H:199:ILE:HG12	1.85	0.58
3:D:44:LEU:HD23	3:D:525:ARG:HH12	1.69	0.58
3:J:853:VAL:HG22	3:J:858:LEU:HD23	1.85	0.58
5:F:319:VAL:O	5:F:323:LEU:HB2	2.04	0.58
5:F:203:ILE:HG12	5:F:239:VAL:HG21	1.86	0.58
1:A:94:MET:O	1:A:146:ARG:HD3	2.03	0.58
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.86	0.58
2:I:729:LEU:HD12	2:I:734:LEU:HD13	1.86	0.58
2:I:905:VAL:HG12	2:I:906:PHE:HD2	1.69	0.57
3:J:216:LEU:N	3:J:382:GLU:O	2.37	0.57
5:F:372:ALA:HA	5:F:375:LYS:HE3	1.86	0.57
2:C:605:LYS:HG2	2:C:612:ALA:HB3	1.85	0.57
3:D:793:THR:O	3:D:879:ARG:NH1	2.34	0.57
3:J:1042:ARG:HD3	3:J:1045:MET:HE3	1.86	0.57
2:I:339:LEU:HD13	2:I:385:PHE:HZ	1.68	0.57
3:J:521:PRO:HD2	3:J:524:LEU:HD12	1.86	0.57
1:A:53:VAL:HA	1:A:144:VAL:HG13	1.86	0.57
3:D:692:GLU:HG2	3:D:720:LEU:HD12	1.85	0.57
2:I:195:LEU:O	2:I:198:ARG:HG3	2.04	0.57
3:J:471:GLU:O	3:J:475:ARG:HG2	2.04	0.57
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.86	0.57
3:J:680:GLN:C	3:J:682:ASP:H	2.06	0.57
2:C:675:ALA:HB3	2:C:870:ILE:HA	1.86	0.57
2:C:321:GLU:HG2	2:C:322:VAL:N	2.20	0.57
5:L:428:SER:HA	5:L:434:ARG:NH2	2.19	0.57
3:J:1208:ASP:HB2	3:J:1215:VAL:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:569:VAL:O	2:C:995:MET:HE1	2.04	0.57
2:I:498:GLN:HG3	3:J:1068:LEU:HD11	1.86	0.57
3:J:125:GLN:HB2	3:J:130:ASN:HB3	1.87	0.57
3:J:772:PRO:HG3	3:J:1210:SER:HB3	1.85	0.57
3:J:801:GLY:HA2	3:J:821:VAL:HA	1.86	0.57
3:J:896:ALA:O	3:J:900:ILE:HG13	2.05	0.57
5:F:167:ASP:HB3	5:F:168:PRO:HD3	1.87	0.57
2:C:461:VAL:HG22	2:C:467:ILE:HG12	1.86	0.57
3:D:770:LEU:HB2	3:D:1210:SER:O	2.05	0.57
3:J:1048:PRO:HD3	3:J:1075:HIS:HB3	1.85	0.57
2:I:207:LEU:O	2:I:211:LEU:HD12	2.05	0.57
1:A:54:THR:O	1:A:167:VAL:HG22	2.04	0.57
2:C:113:VAL:HG21	2:C:373:VAL:HG21	1.85	0.57
1:G:53:VAL:HG23	1:G:144:VAL:HG22	1.86	0.57
1:A:44:LEU:O	1:A:174:VAL:HG11	2.04	0.57
3:D:772:PRO:HG3	3:D:1210:SER:HB3	1.87	0.57
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.86	0.57
6:N:124:LEU:HD11	8:S:2:DG:H4'	1.85	0.57
3:D:65:ARG:HD3	3:D:66:GLN:H	1.68	0.57
3:J:881:LEU:O	3:J:885:ILE:HG13	2.05	0.57
2:C:234:ALA:CA	2:C:237:ARG:HB2	2.34	0.57
2:I:576:ALA:HB1	2:I:580:MET:HE3	1.87	0.57
3:D:896:ALA:O	3:D:900:ILE:HG13	2.05	0.57
2:C:193:LEU:HD22	2:C:221:LEU:HD11	1.86	0.57
3:D:261:LEU:HD21	3:D:268:HIS:HD2	1.70	0.57
2:I:676:ILE:HG22	2:I:873:PRO:HB3	1.86	0.57
3:D:323:GLU:HB3	3:D:334:THR:H	1.69	0.56
5:L:408:THR:HG21	7:R:2:DT:H2'	1.87	0.56
3:J:661:MET:SD	3:J:677:LEU:HD11	2.45	0.56
3:J:660:LYS:HE3	3:J:660:LYS:HA	1.87	0.56
2:C:209:ARG:HG3	2:C:210:GLU:HG2	1.86	0.56
2:C:1065:ALA:HB1	2:C:1077:PRO:HG2	1.86	0.56
2:C:437:ARG:HB2	2:C:438:ILE:HD12	1.87	0.56
1:G:232:LEU:HD23	1:H:16:GLN:HA	1.87	0.56
3:J:643:GLY:H	3:J:727:GLN:HB2	1.70	0.56
3:D:881:LEU:O	3:D:885:ILE:HG13	2.06	0.56
2:C:321:GLU:HG2	2:C:322:VAL:H	1.70	0.56
2:C:281:LEU:O	2:C:308:ARG:NH2	2.38	0.56
2:I:757:GLY:HA2	2:I:789:SER:HB3	1.87	0.56
5:L:353:LEU:HD12	5:L:354:PRO:HD2	1.88	0.56
3:J:87:ARG:HG2	3:J:523:ASP:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HG23	1:A:124:ASN:H	1.70	0.56
2:I:857:ASP:HB2	2:I:978:ARG:HG2	1.88	0.56
2:I:458:TYR:HB3	2:I:470:PRO:HG2	1.87	0.56
6:N:90:HIS:CD2	6:N:124:LEU:HB3	2.40	0.56
3:J:759:ALA:HA	3:J:763:MET:HB3	1.88	0.56
3:J:1487:VAL:HG21	3:J:1492:LEU:HD23	1.87	0.56
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.88	0.56
3:J:664:LYS:NZ	3:J:690:ALA:HB2	2.21	0.56
3:D:1269:LYS:H	3:D:1269:LYS:HD3	1.71	0.56
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.88	0.56
2:I:672:VAL:HG22	2:I:994:ILE:HD13	1.88	0.56
3:J:1458:GLU:HB2	3:J:1460:ILE:HG23	1.87	0.56
3:J:1472:ILE:HD11	3:J:1474:ALA:HB3	1.88	0.56
2:C:588:VAL:HG21	2:C:664:GLY:HA2	1.88	0.56
3:J:1493:LYS:HA	3:J:1496:GLU:HB2	1.86	0.56
1:A:232:LEU:HD23	1:B:16:GLN:HA	1.88	0.56
5:L:385:LYS:HB3	5:L:390:LEU:HD12	1.87	0.56
2:I:605:LYS:HG2	2:I:612:ALA:HB3	1.86	0.56
1:A:35:THR:HG23	1:B:39:PRO:HA	1.88	0.56
2:C:694:LEU:HD11	2:C:868:ASP:HB3	1.86	0.56
1:G:94:MET:O	1:G:146:ARG:HD3	2.05	0.56
3:J:640:HIS:CD2	3:J:641:GLN:HG3	2.41	0.56
3:D:762:GLN:HB3	4:E:16:LYS:HE2	1.87	0.56
2:C:285:LEU:HD11	2:C:301:GLU:HB3	1.87	0.56
3:D:514:LEU:HD21	3:D:518:PRO:HD3	1.88	0.56
2:C:195:LEU:O	2:C:198:ARG:HG3	2.05	0.56
5:L:376:LEU:HD11	5:L:423:LEU:HD11	1.88	0.56
3:D:477:LEU:HA	3:D:480:GLU:HB2	1.87	0.56
3:D:1042:ARG:HD3	3:D:1045:MET:HE3	1.88	0.55
5:L:180:SER:O	5:L:181:LEU:HD12	2.06	0.55
2:C:835:VAL:HG13	2:C:851:LYS:H	1.71	0.55
3:D:573:MET:HA	3:D:576:GLU:HG2	1.88	0.55
3:D:1487:VAL:HG21	3:D:1492:LEU:HD23	1.87	0.55
5:L:203:ILE:HG23	5:L:235:LEU:HD23	1.87	0.55
3:D:1123:PHE:HB3	3:D:1132:LEU:HD22	1.88	0.55
5:F:203:ILE:HG23	5:F:235:LEU:HD23	1.87	0.55
3:J:721:VAL:HG21	3:J:727:GLN:NE2	2.22	0.55
3:D:853:VAL:HG22	3:D:858:LEU:HB3	1.89	0.55
3:D:233:LYS:HG3	3:D:235:ALA:H	1.70	0.55
5:F:99:TYR:OH	5:F:207:LEU:HD21	2.06	0.55
3:D:12:LEU:HD21	3:D:1452:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:288:MET:HA	3:D:307:GLY:HA2	1.89	0.55
3:D:413:ASP:O	3:D:435:VAL:HG12	2.06	0.55
2:I:374:ASN:HD22	2:I:375:SER:H	1.53	0.55
3:D:660:LYS:HA	3:D:660:LYS:HE3	1.88	0.55
5:F:376:LEU:HD11	5:F:423:LEU:HD11	1.89	0.55
3:D:1125:MET:HG3	3:D:1132:LEU:HG	1.87	0.55
5:F:385:LYS:HB3	5:F:390:LEU:HD12	1.88	0.55
2:I:259:GLY:HA2	2:I:263:ASP:HB2	1.89	0.55
6:M:64:ALA:HB3	6:M:66:GLU:HG2	1.89	0.55
2:C:328:LEU:HD21	2:C:434:HIS:HA	1.88	0.55
3:J:1472:ILE:HG13	3:J:1474:ALA:H	1.70	0.55
3:J:168:THR:HA	3:J:394:LEU:HD13	1.88	0.55
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.89	0.55
2:C:554:ASP:HB2	3:D:1061:PHE:HE1	1.70	0.55
2:I:675:ALA:HB3	2:I:870:ILE:HA	1.88	0.55
2:I:15:LEU:H	2:I:586:ARG:HH12	1.54	0.55
6:M:49:VAL:HG11	6:M:59:LEU:HD22	1.89	0.55
3:D:133:ILE:HG22	3:D:152:LEU:HG	1.89	0.55
2:I:456:ALA:HB3	2:I:459:ALA:HB2	1.89	0.55
5:F:237:ARG:NH2	7:O:24:DC:OP2	2.40	0.55
2:I:15:LEU:N	2:I:586:ARG:HH12	2.05	0.55
3:D:759:ALA:HA	3:D:763:MET:HB3	1.88	0.55
2:C:230:ARG:HB3	2:C:231:PRO:HD2	1.88	0.55
5:F:418:LYS:O	5:F:422:LYS:HB2	2.06	0.55
3:D:471:GLU:O	3:D:475:ARG:HG2	2.07	0.55
3:J:775:GLY:HA2	3:J:1209:LEU:HB3	1.87	0.55
2:C:339:LEU:HD13	2:C:385:PHE:CZ	2.42	0.55
2:C:897:LEU:HB2	2:C:899:GLN:HG2	1.88	0.55
1:H:179:PHE:HB3	1:H:197:LEU:HD13	1.89	0.55
3:D:1130:ARG:HH21	3:J:1179:GLU:HB2	1.71	0.55
2:I:595:LEU:HD23	2:I:656:ALA:HB3	1.89	0.55
5:F:249:LYS:HG2	7:O:29:DC:OP2	2.07	0.55
3:J:786:ILE:HD13	3:J:908:LYS:HG2	1.89	0.55
1:H:56:VAL:HG21	1:H:82:LEU:HD13	1.89	0.55
2:C:1044:GLY:HA3	4:E:17:TYR:CE1	2.41	0.54
3:J:668:PRO:HB2	5:L:432:LYS:HD3	1.89	0.54
3:D:680:GLN:HG3	3:D:682:ASP:HB3	1.89	0.54
6:N:64:ALA:HB3	6:N:66:GLU:HG2	1.89	0.54
3:D:141:VAL:HA	3:D:146:PRO:HA	1.89	0.54
2:I:328:LEU:HD21	2:I:434:HIS:HA	1.89	0.54
3:D:1472:ILE:HD11	3:D:1474:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:87:ASP:HA	2:I:131:GLY:HA3	1.89	0.54
3:D:1499:ARG:HE	3:D:1500:LYS:HG3	1.71	0.54
2:C:18:LEU:HB3	2:C:408:ARG:HD2	1.90	0.54
3:J:1080:GLY:HA2	3:J:1083:ASP:HB2	1.90	0.54
2:I:437:ARG:HB2	2:I:438:ILE:HD12	1.89	0.54
3:D:721:VAL:HG21	3:D:727:GLN:NE2	2.23	0.54
2:I:572:ILE:HD11	2:I:703:ILE:HD11	1.88	0.54
3:D:1273:VAL:HG23	3:D:1325:LEU:HB2	1.89	0.54
2:I:17:PRO:O	2:I:20:GLU:HG3	2.07	0.54
2:I:230:ARG:HB3	2:I:231:PRO:HD2	1.88	0.54
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.89	0.54
3:J:209:ARG:HH21	3:J:391:ALA:HB1	1.71	0.54
1:A:79:ILE:HD13	1:A:167:VAL:HG12	1.90	0.54
3:J:1123:PHE:HE2	3:J:1184:ARG:HA	1.73	0.54
3:J:216:LEU:HD22	3:J:382:GLU:HB3	1.90	0.54
3:J:911:LEU:O	3:J:915:VAL:HG23	2.08	0.54
6:N:17:VAL:HB	6:N:142:GLN:HG3	1.90	0.54
5:L:372:ALA:HA	5:L:375:LYS:HE3	1.88	0.54
3:J:103:TRP:HE3	3:J:1448:THR:HG23	1.71	0.54
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.89	0.54
2:I:1101:THR:HG22	3:J:8:VAL:HG22	1.90	0.54
2:I:668:LEU:HB3	2:I:995:MET:SD	2.47	0.54
3:D:1080:GLY:HA2	3:D:1083:ASP:HB2	1.89	0.54
3:J:477:LEU:HA	3:J:480:GLU:HB2	1.89	0.54
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.90	0.54
4:E:42:PRO:HA	4:E:45:ARG:HG3	1.88	0.54
2:I:154:ARG:HH12	2:I:176:VAL:HG23	1.72	0.54
3:D:592:THR:HG22	3:D:599:PRO:HA	1.90	0.54
5:L:167:ASP:HB3	5:L:168:PRO:HD3	1.89	0.54
3:D:1472:ILE:HG13	3:D:1474:ALA:H	1.72	0.54
3:J:735:ALA:HB2	3:J:778:LEU:HD11	1.89	0.54
2:I:461:VAL:HG22	2:I:467:ILE:HG12	1.90	0.54
1:H:97:THR:HG21	1:H:120:VAL:HG21	1.88	0.54
1:A:198:ARG:HD2	2:C:934:PHE:HE1	1.73	0.54
3:D:223:LEU:HB3	3:D:333:LEU:HG	1.90	0.54
3:D:917:GLN:HE22	3:D:1168:LEU:HD11	1.72	0.54
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.90	0.54
3:J:680:GLN:HG3	3:J:682:ASP:HB3	1.89	0.54
3:J:140:ALA:HB1	3:J:161:LEU:HD23	1.89	0.54
3:D:645:PRO:HB2	3:D:648:MET:HB3	1.89	0.54
3:D:1484:THR:OG1	4:E:18:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:646:LYS:HE3	3:J:688:TRP:HZ2	1.73	0.53
2:I:669:GLY:HA3	2:I:994:ILE:O	2.08	0.53
2:I:1103:ASP:OD1	2:I:1103:ASP:N	2.41	0.53
1:A:161:ARG:HD2	1:A:162:ILE:HG22	1.89	0.53
3:D:671:LYS:HG3	5:F:436:PHE:CE2	2.42	0.53
6:N:63:LEU:HD21	6:N:102:PRO:HG3	1.89	0.53
3:J:565:ILE:H	3:J:565:ILE:HD12	1.72	0.53
3:J:1336:LEU:HD22	3:J:1421:LEU:HB3	1.90	0.53
8:P:10:DT:H2"	8:P:11:DA:C8	2.42	0.53
2:C:207:LEU:O	2:C:211:LEU:HD12	2.08	0.53
2:I:321:GLU:HG2	2:I:322:VAL:H	1.73	0.53
2:I:321:GLU:HG2	2:I:322:VAL:N	2.23	0.53
2:I:168:ARG:HD3	2:I:268:ASP:HB3	1.90	0.53
3:D:434:ARG:HH11	3:D:447:VAL:HG21	1.73	0.53
6:M:9:LYS:HD3	6:M:142:GLN:HE22	1.73	0.53
5:F:368:GLU:HB3	5:F:433:LEU:HD21	1.90	0.53
2:C:249:LYS:HD3	2:C:250:LYS:H	1.74	0.53
2:I:1019:GLN:HG3	3:J:617:ASN:ND2	2.24	0.53
3:J:1364:HIS:CD2	3:J:1366:LYS:HE2	2.44	0.53
3:D:911:LEU:O	3:D:915:VAL:HG23	2.08	0.53
3:J:714:GLN:HB3	3:J:765:SER:HB3	1.89	0.53
3:D:859:ASP:HB2	3:D:862:ASP:OD2	2.09	0.53
1:G:79:ILE:HD13	1:G:167:VAL:HG12	1.90	0.53
7:O:24:DC:N4	8:P:2:DG:H1	2.06	0.53
3:D:658:LEU:HD11	3:D:674:ARG:HG2	1.91	0.53
1:H:44:LEU:HD13	1:H:177:VAL:HG11	1.89	0.53
3:D:214:ASP:HA	3:D:342:PRO:HA	1.91	0.53
3:D:218:LYS:HD3	3:D:338:GLU:HB3	1.89	0.53
3:J:514:LEU:HD21	3:J:517:VAL:HA	1.90	0.53
5:L:103:ILE:HD13	5:L:211:VAL:HG21	1.90	0.53
2:C:468:ARG:HG2	2:C:487:THR:HA	1.91	0.53
2:C:65:VAL:HG13	2:C:101:ILE:HB	1.90	0.53
2:I:129:ILE:HG12	2:I:386:PHE:HB3	1.90	0.53
8:S:10:DT:H2"	8:S:11:DA:C8	2.44	0.53
2:I:42:VAL:HG12	2:I:43:GLY:H	1.73	0.53
2:C:675:ALA:HA	2:C:989:VAL:HG12	1.90	0.53
3:D:702:LEU:HG	3:D:747:VAL:HG22	1.91	0.53
3:D:103:TRP:HE3	3:D:1448:THR:HG23	1.73	0.53
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.90	0.53
5:F:149:LYS:HD3	5:F:193:ARG:HH22	1.73	0.53
1:B:101:LEU:HD22	1:B:102:ARG:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:367:ILE:HB	3:D:377:VAL:HB	1.90	0.53
5:L:319:VAL:O	5:L:323:LEU:HB2	2.08	0.53
3:D:125:GLN:HB2	3:D:130:ASN:HB3	1.91	0.53
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.89	0.53
3:J:93:ILE:HD13	3:J:548:ILE:HG12	1.89	0.53
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	1.91	0.53
2:I:1019:GLN:HE22	3:J:621:LYS:HD3	1.73	0.53
2:C:358:ARG:HB2	2:C:372:LEU:HD12	1.89	0.53
3:D:675:ARG:HH21	3:D:679:ARG:HH12	1.55	0.53
5:L:379:ARG:HG3	5:L:405:PHE:CE2	2.44	0.53
1:B:180:GLN:NE2	1:B:182:GLU:OE1	2.39	0.53
1:G:53:VAL:HA	1:G:144:VAL:HG13	1.91	0.53
2:C:1103:ASP:OD1	2:C:1103:ASP:N	2.41	0.53
2:I:685:GLU:HG2	3:J:739:ASP:HB3	1.90	0.53
2:C:42:VAL:HG12	2:C:43:GLY:H	1.73	0.53
5:F:189:LEU:HD21	5:F:193:ARG:HE	1.74	0.52
3:D:974:ILE:HG22	3:D:988:ARG:HG3	1.90	0.52
1:B:110:ARG:HH12	1:B:126:ASP:HA	1.75	0.52
3:D:87:ARG:HG2	3:D:523:ASP:HB2	1.91	0.52
2:I:874:LEU:HD22	3:J:1029:ARG:HB2	1.92	0.52
3:D:592:THR:HA	3:D:600:LEU:HD13	1.91	0.52
3:D:618:LEU:HG	3:D:1467:ILE:HA	1.91	0.52
3:D:1179:GLU:HB3	3:J:1131:THR:HG22	1.91	0.52
2:I:1031:ARG:HA	3:J:622:ARG:HA	1.91	0.52
3:J:421:LEU:HB3	3:J:444:VAL:HG21	1.91	0.52
3:J:122:GLU:O	3:J:126:VAL:HG23	2.09	0.52
6:M:85:GLN:NE2	7:O:25:DT:O2	2.43	0.52
2:C:683:ASN:OD1	2:C:872:ASN:ND2	2.42	0.52
2:C:607:ASP:C	2:C:609:THR:H	2.11	0.52
2:I:607:ASP:C	2:I:609:THR:H	2.13	0.52
3:J:770:LEU:HD23	3:J:777:PRO:HA	1.91	0.52
2:I:1016:ILE:O	3:J:87:ARG:NH2	2.42	0.52
3:J:405:ASP:N	3:J:405:ASP:OD1	2.42	0.52
3:J:689:ASP:O	3:J:692:GLU:HB2	2.09	0.52
3:D:154:THR:HG22	3:D:157:GLU:HG2	1.90	0.52
5:F:217:TYR:O	5:F:220:ARG:HG2	2.09	0.52
3:D:714:GLN:HB3	3:D:765:SER:HB3	1.90	0.52
2:I:198:ARG:NE	2:I:234:ALA:O	2.41	0.52
5:L:249:LYS:HG2	7:R:29:DC:OP2	2.09	0.52
3:J:729:HIS:HE1	3:J:731:LEU:HG	1.75	0.52
2:C:1017:THR:HG21	3:D:617:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:LYS:HG2	3:D:639:LEU:N	2.25	0.52
3:D:735:ALA:HB2	3:D:778:LEU:HD11	1.92	0.52
2:I:118:LEU:HD13	2:I:382:LEU:HD23	1.92	0.52
2:C:339:LEU:HD13	2:C:385:PHE:HZ	1.73	0.52
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.45	0.52
1:G:205:VAL:HG11	1:G:213:GLN:HE22	1.74	0.52
3:D:208:PRO:HA	3:D:390:PRO:HA	1.91	0.52
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	1.91	0.52
2:I:922:PHE:HB2	2:I:967:PHE:CD2	2.44	0.52
4:K:42:PRO:HA	4:K:45:ARG:HG3	1.92	0.52
2:C:241:LEU:O	2:C:244:PRO:HD3	2.10	0.52
2:C:154:ARG:HH12	2:C:176:VAL:HG23	1.74	0.52
3:D:1130:ARG:NH2	3:J:1179:GLU:HB2	2.24	0.52
2:I:569:VAL:O	2:I:995:MET:HE1	2.10	0.52
6:N:60:ARG:CZ	6:N:102:PRO:HD3	2.40	0.52
3:D:127:LEU:HG	3:D:461:ILE:HG13	1.91	0.52
2:C:195:LEU:HB3	2:C:238:LEU:HD11	1.90	0.52
2:C:149:THR:HA	2:C:322:VAL:HG13	1.90	0.52
2:C:1019:GLN:HE22	3:D:621:LYS:HD3	1.74	0.52
1:A:224:TYR:CD1	1:B:9:PRO:HG2	2.44	0.52
2:C:939:ARG:HB3	2:C:982:PRO:HG3	1.90	0.52
3:D:299:GLU:N	3:D:302:GLN:OE1	2.43	0.52
3:D:585:GLY:HA2	3:D:590:PRO:HG3	1.91	0.52
3:J:1274:ILE:HG22	3:J:1324:PRO:HA	1.92	0.52
2:C:601:GLY:HA2	2:C:615:TYR:HA	1.91	0.52
1:H:161:ARG:HG3	1:H:162:ILE:N	2.25	0.52
5:F:103:ILE:HD13	5:F:211:VAL:HG21	1.91	0.52
5:F:353:LEU:HD12	5:F:354:PRO:HD2	1.91	0.52
3:J:500:ARG:HD3	3:J:503:LEU:HD12	1.91	0.52
1:A:14:THR:OG1	1:B:231:SER:OG	2.20	0.52
3:J:407:VAL:HG22	3:J:409:VAL:H	1.74	0.52
2:C:1069:ALA:O	2:C:1073:GLY:N	2.42	0.52
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.91	0.52
2:I:852:ILE:HG22	2:I:853:LEU:H	1.75	0.52
3:D:229:ALA:HB2	3:D:245:LEU:HA	1.92	0.52
2:C:672:VAL:HG22	2:C:994:ILE:HD13	1.91	0.52
2:C:695:LEU:HD21	2:C:832:LYS:HD3	1.92	0.52
5:L:377:SER:HB3	5:L:380:GLU:HG2	1.92	0.52
3:J:508:ARG:HB2	3:J:511:TRP:CE2	2.45	0.52
3:J:974:ILE:HG22	3:J:988:ARG:HG3	1.92	0.52
2:C:146:VAL:HG21	2:C:281:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:9:LYS:HD3	6:N:142:GLN:HE22	1.75	0.52
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.92	0.52
3:J:65:ARG:HD3	3:J:66:GLN:H	1.74	0.52
3:J:127:LEU:HG	3:J:461:ILE:HG13	1.92	0.52
3:J:1273:VAL:HG23	3:J:1325:LEU:HB2	1.92	0.52
4:K:45:ARG:HD2	4:K:63:TRP:HH2	1.76	0.51
3:J:978:TYR:HB2	3:J:988:ARG:HD3	1.91	0.51
3:D:521:PRO:HB2	3:D:524:LEU:HG	1.92	0.51
3:J:770:LEU:HB2	3:J:1210:SER:O	2.09	0.51
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.92	0.51
3:J:1281:VAL:HG21	3:J:1313:VAL:HG11	1.91	0.51
2:I:897:LEU:HB2	2:I:899:GLN:HG2	1.93	0.51
2:C:374:ASN:HD22	2:C:375:SER:N	2.05	0.51
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.92	0.51
1:B:102:ARG:HB2	1:B:139:TYR:HD1	1.75	0.51
6:N:144:LEU:HB2	6:N:146:ILE:HG12	1.91	0.51
3:D:1048:PRO:HD3	3:D:1075:HIS:HB3	1.92	0.51
5:F:431:ARG:HG3	5:F:434:ARG:NE	2.22	0.51
2:I:584:GLU:HB3	2:I:666:LEU:N	2.24	0.51
5:L:373:LEU:HD12	5:L:376:LEU:HD12	1.91	0.51
3:D:49:ILE:HG13	3:D:50:PHE:N	2.25	0.51
2:C:669:GLY:HA3	2:C:994:ILE:O	2.10	0.51
3:J:1269:LYS:H	3:J:1269:LYS:HD3	1.75	0.51
3:D:1292:VAL:HG21	3:D:1311:LEU:HD13	1.92	0.51
3:D:119:SER:HB3	3:D:122:GLU:HG2	1.91	0.51
3:D:801:GLY:HA2	3:D:821:VAL:HA	1.92	0.51
3:D:1476:THR:HG22	4:E:17:TYR:HB3	1.91	0.51
6:M:133:ILE:HA	6:M:136:LEU:HD12	1.92	0.51
6:N:133:ILE:HA	6:N:136:LEU:HD12	1.91	0.51
2:I:714:ASP:HA	2:I:719:PRO:HA	1.91	0.51
2:I:554:ASP:HB2	3:J:1061:PHE:HE1	1.75	0.51
3:J:356:PRO:HG2	3:J:359:ALA:HB2	1.93	0.51
2:I:606:VAL:HG23	2:I:645:VAL:HA	1.92	0.51
2:C:668:LEU:HB3	2:C:995:MET:SD	2.51	0.51
3:J:1060:SER:OG	3:J:1061:PHE:N	2.43	0.51
3:J:465:LEU:HA	3:J:468:LEU:HD12	1.92	0.51
3:D:100:ALA:H	3:D:575:GLN:HE22	1.57	0.51
2:C:606:VAL:HG23	2:C:645:VAL:HA	1.93	0.51
3:D:1181:GLY:HA3	3:J:1132:LEU:HD12	1.92	0.51
3:D:9:ARG:HA	3:D:1456:LYS:HA	1.93	0.51
5:L:108:LEU:HD23	5:L:208:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:154:THR:HG22	3:J:157:GLU:HG2	1.92	0.51
5:L:189:LEU:HD21	5:L:193:ARG:HE	1.76	0.51
1:G:54:THR:O	1:G:167:VAL:HG22	2.11	0.51
2:I:1044:GLY:HA3	4:K:17:TYR:CE1	2.46	0.51
3:J:1476:THR:HA	4:K:17:TYR:HB3	1.93	0.51
6:M:34:ALA:HB3	6:M:51:VAL:HG21	1.92	0.51
2:C:611:ILE:HG13	2:C:625:LEU:HD11	1.93	0.51
5:L:383:VAL:HG13	5:L:401:VAL:HG11	1.93	0.51
2:I:587:VAL:HG11	2:I:666:LEU:HD22	1.92	0.51
3:D:701:LEU:HD23	3:D:763:MET:HG2	1.93	0.51
3:J:680:GLN:O	3:J:682:ASP:N	2.34	0.51
1:A:53:VAL:HG13	1:A:167:VAL:HG21	1.93	0.51
2:C:857:ASP:N	2:C:857:ASP:OD1	2.41	0.51
3:D:783:ARG:NH1	3:D:1029:ARG:HD2	2.26	0.51
2:C:101:ILE:HG23	2:C:108:ILE:HA	1.91	0.51
3:J:12:LEU:HD11	3:J:1452:ILE:HA	1.93	0.51
5:L:99:TYR:OH	5:L:207:LEU:HD21	2.10	0.51
3:D:639:LEU:HD22	3:D:766:ALA:HA	1.92	0.51
3:J:754:PHE:HA	4:K:24:ALA:HB1	1.93	0.51
1:H:186:LEU:HD12	4:K:51:LEU:HD13	1.92	0.51
3:J:423:ASP:HB3	3:J:426:LYS:HE3	1.93	0.51
3:D:508:ARG:HB2	3:D:511:TRP:CE2	2.45	0.51
5:F:199:ARG:HD2	5:F:240:GLU:HG2	1.93	0.51
1:H:48:ILE:HG13	1:H:213:GLN:HE21	1.76	0.51
5:F:383:VAL:HG13	5:F:401:VAL:HG11	1.91	0.51
2:I:545:ASN:HB3	2:I:583:LEU:HD22	1.93	0.51
3:D:539:ASP:HB3	3:D:600:LEU:HG	1.92	0.51
3:D:680:GLN:C	3:D:682:ASP:H	2.13	0.51
3:J:101:HIS:ND1	3:J:103:TRP:HB2	2.26	0.51
1:H:15:THR:HA	1:H:21:GLY:HA2	1.94	0.51
2:I:584:GLU:H	2:I:584:GLU:CD	2.14	0.50
2:C:584:GLU:CD	2:C:584:GLU:H	2.14	0.50
3:J:119:SER:HB3	3:J:122:GLU:HG2	1.92	0.50
3:D:681:ARG:O	3:D:683:ILE:HG12	2.10	0.50
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.11	0.50
3:D:643:GLY:H	3:D:727:GLN:HB2	1.76	0.50
3:J:962:ARG:O	3:J:965:GLU:HG2	2.11	0.50
2:I:1069:ALA:O	2:I:1073:GLY:N	2.43	0.50
2:C:723:THR:HG23	2:C:725:ASP:H	1.75	0.50
3:J:783:ARG:HD3	3:J:1028:ALA:O	2.11	0.50
2:I:675:ALA:HB2	2:I:867:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:654:LYS:HB3	3:J:655:PRO:HD3	1.94	0.50
3:D:923:GLY:O	3:D:926:LYS:HB2	2.12	0.50
5:F:377:SER:HB3	5:F:380:GLU:HG2	1.92	0.50
3:D:786:ILE:HD13	3:D:908:LYS:HG2	1.92	0.50
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.93	0.50
3:D:1331:ASP:HB3	3:D:1334:GLN:HB2	1.94	0.50
2:C:713:ARG:HH12	2:C:716:LYS:HZ1	1.59	0.50
4:E:45:ARG:HD2	4:E:63:TRP:HH2	1.76	0.50
2:C:584:GLU:HB3	2:C:666:LEU:N	2.24	0.50
1:G:53:VAL:HA	1:G:144:VAL:HA	1.94	0.50
2:C:164:PRO:HG2	2:C:165:LEU:H	1.77	0.50
2:I:673:LEU:HB3	2:I:867:VAL:HG12	1.92	0.50
3:J:122:GLU:HB2	3:J:152:LEU:HD21	1.94	0.50
3:D:729:HIS:HE1	3:D:731:LEU:HG	1.76	0.50
3:D:191:LEU:CD1	3:D:197:SER:HB2	2.42	0.50
3:D:918:ALA:HA	3:D:922:LEU:HD23	1.94	0.50
2:C:1067:TYR:O	2:C:1071:ILE:HB	2.12	0.50
6:M:82:LEU:HB3	6:M:89:ARG:HG3	1.92	0.50
3:J:1120:VAL:HG12	3:J:1135:ARG:HH12	1.76	0.50
3:D:977:ALA:HB2	3:J:831:GLY:CA	2.40	0.50
2:I:164:PRO:HG2	2:I:165:LEU:H	1.77	0.50
3:D:132:TYR:CE1	3:D:456:MET:HG2	2.47	0.50
1:A:72:LYS:HG3	2:C:606:VAL:HG11	1.93	0.50
3:J:585:GLY:HA2	3:J:590:PRO:HG3	1.94	0.50
5:L:206:ASN:O	5:L:209:LEU:HB3	2.11	0.50
1:G:64:GLU:HG3	1:G:79:ILE:HD12	1.93	0.50
2:I:18:LEU:HB3	2:I:408:ARG:HD2	1.93	0.50
1:G:43:ILE:HD11	1:H:35:THR:HG21	1.94	0.50
3:D:365:GLU:H	3:D:379:ALA:HB3	1.77	0.50
5:L:238:ALA:HB2	5:L:257:TRP:HB2	1.94	0.50
1:G:198:ARG:HD2	2:I:934:PHE:HE1	1.77	0.50
2:I:995:MET:HE3	2:I:996:LYS:H	1.77	0.50
3:D:32:ILE:HG22	3:D:39:PRO:HA	1.93	0.50
3:D:1448:THR:O	3:D:1452:ILE:HG12	2.11	0.50
7:O:3:DT:H5'	7:O:3:DT:H6	1.76	0.50
6:N:33:ARG:HD2	6:N:33:ARG:H	1.77	0.50
3:J:859:ASP:HB2	3:J:862:ASP:OD2	2.12	0.50
3:J:1290:LEU:HB2	3:J:1307:LYS:HD2	1.93	0.50
2:I:1065:ALA:HB1	2:I:1077:PRO:HG2	1.94	0.50
2:I:1081:VAL:HG21	2:I:1086:ARG:CZ	2.42	0.50
2:I:249:LYS:HD3	2:I:250:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:881:ASN:OD1	2:I:884:GLN:NE2	2.45	0.50
2:I:1115:LEU:HD23	3:J:85:VAL:HG12	1.93	0.50
3:D:1117:TYR:HB2	3:D:1188:VAL:O	2.12	0.50
3:D:402:PRO:HA	3:D:443:VAL:HA	1.93	0.49
1:B:149:GLY:O	1:B:171:PHE:HB2	2.12	0.49
3:J:638:LYS:HG2	3:J:639:LEU:N	2.27	0.49
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.77	0.49
2:I:1008:ARG:NH2	2:I:1020:PRO:HB3	2.27	0.49
3:D:658:LEU:HD22	3:D:670:VAL:HG13	1.94	0.49
1:A:43:ILE:HD11	1:A:218:LEU:HD13	1.94	0.49
3:D:14:SER:HB3	3:D:511:TRP:CD2	2.47	0.49
2:C:72:ARG:HG3	2:C:95:TYR:HB2	1.94	0.49
3:D:578:VAL:O	3:D:582:ILE:HG12	2.12	0.49
1:H:143:ARG:HG3	1:H:160:ASP:OD2	2.11	0.49
3:D:253:ALA:HB2	3:D:304:LEU:HG	1.93	0.49
2:I:999:HIS:CD2	2:I:1004:LYS:HE3	2.47	0.49
4:K:38:THR:HG21	4:K:63:TRP:CZ3	2.47	0.49
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.47	0.49
3:J:645:PRO:HB2	3:J:648:MET:HB3	1.94	0.49
2:I:146:VAL:HG21	2:I:281:LEU:HG	1.93	0.49
5:F:211:VAL:HG13	5:F:228:ILE:HD13	1.95	0.49
3:D:1458:GLU:HB2	3:D:1460:ILE:HG23	1.93	0.49
3:J:1107:VAL:HG22	3:J:1200:VAL:HG23	1.94	0.49
1:A:16:GLN:HB3	1:A:20:TYR:HB3	1.94	0.49
2:C:1047:HIS:O	2:C:1051:GLU:HG2	2.12	0.49
1:A:114:PHE:O	1:A:116:PRO:HD3	2.12	0.49
2:I:211:LEU:HB3	2:I:218:VAL:HG13	1.95	0.49
3:D:1048:PRO:HD3	3:D:1075:HIS:CG	2.47	0.49
2:I:399:ASN:HB2	2:I:400:PRO:HD2	1.93	0.49
3:J:851:LEU:O	3:J:855:HIS:HB2	2.12	0.49
5:L:149:LYS:HD3	5:L:193:ARG:HH22	1.77	0.49
5:F:181:LEU:HD23	5:F:185:LEU:HB2	1.94	0.49
2:I:209:ARG:HG3	2:I:210:GLU:HG2	1.95	0.49
3:D:754:PHE:HA	4:E:24:ALA:HB1	1.94	0.49
1:B:99:LEU:HB2	1:B:142:VAL:HG22	1.94	0.49
3:J:838:ARG:HE	3:J:863:VAL:HG11	1.78	0.49
5:L:217:TYR:O	5:L:220:ARG:HG2	2.13	0.49
3:J:398:ALA:HB2	3:J:447:VAL:HG12	1.94	0.49
2:C:209:ARG:HG3	2:C:210:GLU:N	2.27	0.49
5:F:103:ILE:HG22	5:F:207:LEU:HD13	1.92	0.49
3:D:12:LEU:HD11	3:D:1452:ILE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH22	2:C:932:GLU:HB3	1.77	0.49
1:G:122:ILE:HG23	1:G:124:ASN:H	1.77	0.49
2:I:858:MET:H	2:I:977:GLY:HA3	1.77	0.49
2:C:858:MET:SD	2:C:859:PRO:HD2	2.52	0.49
3:D:853:VAL:HG22	3:D:858:LEU:HD23	1.95	0.49
3:D:950:GLY:H	3:D:953:ASP:CG	2.14	0.49
2:C:838:LYS:HG2	2:C:997:LEU:HD22	1.94	0.49
3:J:44:LEU:HD23	3:J:525:ARG:HH12	1.77	0.49
5:L:419:ALA:O	5:L:423:LEU:HD12	2.13	0.49
3:D:264:LEU:HD21	3:D:339:TRP:CE2	2.47	0.49
5:F:103:ILE:HG21	5:F:207:LEU:HD22	1.94	0.49
1:H:226:ALA:O	1:H:228:PRO:HD3	2.13	0.49
7:R:23:DG:H1'	7:R:24:DC:H5'	1.94	0.49
3:D:851:LEU:O	3:D:855:HIS:HB2	2.13	0.49
1:G:16:GLN:HB3	1:G:20:TYR:HB3	1.94	0.49
3:D:664:LYS:NZ	3:D:690:ALA:HB2	2.27	0.49
1:A:210:ALA:HA	1:A:213:GLN:HE21	1.77	0.49
2:C:306:THR:HG23	2:C:307:LEU:HD12	1.94	0.49
3:J:1147:ARG:HB3	3:J:1188:VAL:HG11	1.95	0.49
5:F:157:GLN:NE2	5:F:171:VAL:HG21	2.26	0.49
1:G:40:LEU:O	1:G:44:LEU:HB2	2.13	0.49
3:J:633:VAL:HG22	3:J:635:PRO:HD3	1.93	0.49
2:C:833:LEU:HD21	2:C:839:LEU:HD11	1.94	0.49
5:F:427:GLU:OE1	5:F:433:LEU:HB2	2.13	0.49
3:D:710:ARG:HG3	3:D:711:LEU:HD22	1.95	0.49
1:H:173:PRO:HB3	1:H:204:SER:HB2	1.94	0.49
3:D:273:ARG:HA	3:D:279:VAL:HG23	1.94	0.49
2:C:750:LYS:N	2:C:753:ASP:OD2	2.34	0.49
3:J:667:ALA:HB1	3:J:672:ALA:HB3	1.95	0.49
3:D:1336:LEU:HD22	3:D:1421:LEU:HB3	1.94	0.49
3:D:335:LEU:HD13	3:D:337:LEU:HD11	1.94	0.49
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.95	0.49
2:C:535:SER:O	2:C:538:GLN:HG2	2.13	0.49
2:C:874:LEU:O	2:C:877:PRO:HD2	2.12	0.49
1:G:210:ALA:HA	1:G:213:GLN:HE21	1.77	0.49
3:J:213:VAL:HG13	3:J:385:VAL:HG22	1.95	0.49
1:B:226:ALA:O	1:B:228:PRO:HD3	2.13	0.49
1:B:11:PHE:HB2	1:B:25:LEU:HD13	1.95	0.49
3:J:601:ARG:HH21	3:J:606:ILE:HA	1.78	0.49
5:L:215:LYS:HA	5:L:224:PHE:HE2	1.77	0.49
2:C:198:ARG:HG2	2:C:234:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:237:ARG:NH2	2:C:241:LEU:HD11	2.28	0.49
3:D:783:ARG:HD3	3:D:1028:ALA:O	2.13	0.49
1:G:53:VAL:HG13	1:G:167:VAL:HG21	1.95	0.49
2:I:1067:TYR:O	2:I:1071:ILE:HB	2.13	0.49
1:H:152:PRO:HD2	1:H:155:ARG:HG3	1.94	0.49
1:H:10:VAL:O	1:H:12:THR:HG23	2.13	0.49
5:F:386:LEU:HD22	5:F:391:ILE:HG13	1.95	0.49
1:G:58:ILE:HG21	1:G:68:ILE:HD13	1.94	0.49
8:P:22:DC:H2"	8:P:23:DA:C8	2.48	0.49
2:C:168:ARG:HH21	2:C:346:VAL:HG22	1.78	0.48
3:J:132:TYR:CE1	3:J:456:MET:HG2	2.48	0.48
3:J:758:GLU:O	3:J:762:GLN:HG2	2.13	0.48
3:D:316:HIS:H	3:D:316:HIS:HD1	1.59	0.48
3:D:667:ALA:HB1	3:D:672:ALA:HB3	1.95	0.48
6:M:63:LEU:HD21	6:M:102:PRO:HG3	1.95	0.48
2:I:432:ARG:NH1	2:I:518:ARG:HH21	2.06	0.48
3:J:699:VAL:HA	3:J:718:PRO:HD3	1.94	0.48
3:J:169:TYR:OH	3:J:198:ARG:N	2.45	0.48
3:J:421:LEU:HD11	3:J:429:SER:HB2	1.94	0.48
1:G:161:ARG:HD2	1:G:162:ILE:HG22	1.94	0.48
2:C:419:THR:HG22	2:C:422:ARG:HG2	1.95	0.48
6:N:68:VAL:HB	6:N:69:PRO:HD3	1.95	0.48
6:N:34:ALA:HB3	6:N:51:VAL:HG21	1.95	0.48
2:C:48:PHE:O	2:C:52:PHE:HB2	2.12	0.48
2:I:195:LEU:HB3	2:I:238:LEU:HD11	1.94	0.48
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.28	0.48
1:G:43:ILE:HD11	1:G:218:LEU:HD13	1.95	0.48
3:D:238:PRO:HB3	3:D:315:ARG:O	2.13	0.48
6:M:17:VAL:HB	6:M:142:GLN:HG3	1.95	0.48
2:I:893:ALA:O	2:I:897:LEU:HG	2.14	0.48
2:C:366:THR:HG23	6:M:14:PRO:HD3	1.96	0.48
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.95	0.48
2:C:259:GLY:HA2	2:C:263:ASP:HB2	1.95	0.48
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.95	0.48
1:G:108:GLU:HB2	1:G:110:ARG:HH11	1.78	0.48
3:D:140:ALA:HB1	3:D:161:LEU:HD23	1.95	0.48
1:G:114:PHE:O	1:G:116:PRO:HD3	2.14	0.48
1:G:53:VAL:H	1:G:144:VAL:HG13	1.78	0.48
2:I:241:LEU:O	2:I:244:PRO:HD3	2.12	0.48
3:J:65:ARG:HG3	3:J:67:ARG:H	1.79	0.48
2:I:209:ARG:HG3	2:I:210:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:858:MET:SD	2:I:859:PRO:HD2	2.53	0.48
3:J:50:PHE:CD2	3:J:522:PRO:HD3	2.49	0.48
3:J:918:ALA:HA	3:J:922:LEU:HD23	1.94	0.48
3:J:483:HIS:ND1	3:J:484:PRO:HD2	2.29	0.48
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.95	0.48
3:J:1112:CYS:HB3	3:J:1196:THR:OG1	2.14	0.48
3:J:1116:ASN:HB2	3:J:1193:THR:HB	1.95	0.48
3:J:162:ARG:HG2	3:J:414:ARG:HH21	1.77	0.48
3:J:969:ARG:HG3	3:J:972:ARG:HH21	1.78	0.48
2:C:448:ASN:C	2:C:451:LEU:HD23	2.34	0.48
3:D:1060:SER:OG	3:D:1061:PHE:N	2.46	0.48
3:J:103:TRP:CE2	3:J:1444:THR:HG23	2.48	0.48
2:I:882:LEU:HD21	3:J:1038:LEU:HD22	1.94	0.48
2:I:880:MET:HG2	3:J:1038:LEU:HD11	1.96	0.48
3:J:658:LEU:HD11	3:J:674:ARG:HG2	1.96	0.48
2:I:750:LYS:HD3	3:J:681:ARG:HG3	1.95	0.48
5:F:202:LEU:HD22	5:F:239:VAL:HG22	1.95	0.48
2:C:94:LEU:O	2:C:115:LEU:HB2	2.14	0.48
2:I:1047:HIS:O	2:I:1051:GLU:HG2	2.14	0.48
1:B:15:THR:HA	1:B:21:GLY:HA2	1.96	0.48
3:D:423:ASP:HB3	3:D:426:LYS:HB3	1.95	0.48
2:I:99:GLN:HB2	2:I:101:ILE:HD11	1.96	0.48
5:L:202:LEU:HD22	5:L:239:VAL:HG22	1.95	0.48
3:J:567:ILE:HG22	3:J:571:LYS:NZ	2.29	0.48
3:J:658:LEU:HD22	3:J:670:VAL:HG13	1.95	0.48
1:H:101:LEU:HD22	1:H:102:ARG:N	2.27	0.48
3:D:1273:VAL:HG22	3:D:1326:THR:HG23	1.95	0.48
3:D:122:GLU:O	3:D:126:VAL:HG23	2.13	0.48
3:J:49:ILE:HG13	3:J:50:PHE:N	2.29	0.48
1:H:59:GLU:HG3	1:H:139:TYR:HD2	1.79	0.48
5:F:266:ILE:O	5:F:270:ALA:HB2	2.13	0.48
1:G:48:ILE:HG22	1:G:173:PRO:HD2	1.94	0.48
2:I:72:ARG:HG3	2:I:95:TYR:HB2	1.96	0.48
2:C:508:ILE:HD11	2:C:529:VAL:HG11	1.96	0.48
2:C:1081:VAL:HG21	2:C:1086:ARG:CZ	2.44	0.48
2:C:537:LYS:HZ3	2:C:905:VAL:N	2.07	0.48
2:I:734:LEU:HA	2:I:737:LEU:HD13	1.96	0.48
2:C:46:ALA:O	2:C:50:GLU:HB2	2.13	0.48
3:J:1292:VAL:HG21	3:J:1311:LEU:HD13	1.96	0.48
6:M:146:ILE:HB	6:M:150:GLU:HB2	1.94	0.48
2:I:860:HIS:HA	2:I:866:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1127:GLU:C	3:J:1129:THR:H	2.16	0.48
3:D:1127:GLU:C	3:D:1129:THR:H	2.17	0.48
3:D:1283:ILE:HD12	3:D:1315:ASP:HB2	1.96	0.48
4:E:30:LEU:CD2	4:E:63:TRP:HB3	2.44	0.48
2:I:193:LEU:HD21	2:I:307:LEU:HD21	1.94	0.48
2:I:874:LEU:O	2:I:877:PRO:HD2	2.14	0.48
2:C:206:THR:HG23	2:C:209:ARG:CZ	2.43	0.48
3:J:1313:VAL:HG21	3:J:1325:LEU:HD13	1.96	0.48
2:I:206:THR:HG23	2:I:209:ARG:CZ	2.43	0.48
3:J:1283:ILE:HD12	3:J:1315:ASP:HB2	1.96	0.48
3:D:128:TYR:O	3:D:572:ARG:NH1	2.46	0.48
1:A:79:ILE:HA	1:A:82:LEU:HB2	1.95	0.48
1:G:79:ILE:HA	1:G:82:LEU:HB2	1.96	0.48
3:J:1434:TRP:CD1	3:J:1457:ASP:HB2	2.48	0.48
5:L:157:GLN:NE2	5:L:171:VAL:HG21	2.28	0.48
3:J:701:LEU:HD23	3:J:763:MET:HG2	1.96	0.48
3:D:675:ARG:HH21	3:D:679:ARG:NH1	2.12	0.48
1:H:72:LYS:HG3	1:H:131:THR:HB	1.94	0.48
3:D:483:HIS:ND1	3:D:484:PRO:HD2	2.29	0.48
2:C:399:ASN:HB2	2:C:400:PRO:HD2	1.95	0.48
3:J:702:LEU:HG	3:J:747:VAL:HG22	1.95	0.48
5:F:379:ARG:HG3	5:F:405:PHE:CE2	2.48	0.48
2:I:198:ARG:HG2	2:I:234:ALA:HB1	1.96	0.47
1:G:215:VAL:HG13	1:H:222:LEU:HD22	1.95	0.47
3:J:592:THR:HG22	3:J:599:PRO:HA	1.95	0.47
2:I:570:PRO:O	2:I:571:LEU:HD13	2.14	0.47
2:I:1053:LEU:HA	3:J:621:LYS:HE3	1.95	0.47
3:J:858:LEU:HD21	3:J:864:VAL:HG11	1.96	0.47
3:D:1313:VAL:HG21	3:D:1325:LEU:HD13	1.95	0.47
1:B:132:LEU:HD12	1:B:136:GLY:HA3	1.96	0.47
6:M:21:ALA:HB3	6:M:37:GLN:HG2	1.96	0.47
1:B:42:ARG:NH1	2:C:981:GLU:OE2	2.46	0.47
2:I:984:GLU:HG3	3:J:945:SER:HA	1.94	0.47
3:J:90:MET:HB3	3:J:519:VAL:O	2.14	0.47
3:D:699:VAL:HA	3:D:718:PRO:HD3	1.96	0.47
3:D:310:LEU:H	3:D:310:LEU:CD1	2.27	0.47
2:C:769:PRO:HD3	3:D:65:ARG:HH22	1.79	0.47
3:J:731:LEU:HD22	3:J:780:LYS:O	2.14	0.47
3:D:179:VAL:HG11	3:D:191:LEU:HG	1.95	0.47
5:L:418:LYS:O	5:L:422:LYS:HB2	2.14	0.47
2:I:13:ILE:HD13	2:I:483:VAL:HG11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:LEU:HB2	1:G:142:VAL:HG23	1.97	0.47
2:C:1031:ARG:HA	3:D:622:ARG:HA	1.96	0.47
3:J:1118:ILE:HG12	3:J:1190:SER:HB3	1.95	0.47
3:D:954:ALA:HB2	3:D:1020:LEU:HD22	1.97	0.47
5:F:108:LEU:HB2	5:F:109:LEU:H	1.48	0.47
2:I:27:LYS:HA	2:I:30:LEU:HD22	1.96	0.47
6:M:68:VAL:HB	6:M:69:PRO:HD3	1.95	0.47
2:I:306:THR:HG23	2:I:307:LEU:HD12	1.96	0.47
2:I:146:VAL:HG12	2:I:162:ILE:HG13	1.94	0.47
2:C:726:ILE:HB	2:C:729:LEU:HB2	1.96	0.47
3:D:916:TYR:CE2	3:D:1168:LEU:HD13	2.49	0.47
3:J:702:LEU:HD22	3:J:728:LEU:HD13	1.96	0.47
1:B:123:MET:C	1:B:125:PRO:HD3	2.34	0.47
5:F:95:PRO:O	5:F:98:GLN:HB3	2.13	0.47
4:E:66:LYS:HA	4:E:69:LEU:HD12	1.96	0.47
5:L:285:LYS:HG2	5:L:310:MET:HE1	1.95	0.47
2:I:1056:LYS:O	3:J:624:ASP:N	2.48	0.47
2:I:274:ARG:O	2:I:278:GLU:HB2	2.15	0.47
1:B:85:LEU:HD12	1:B:86:VAL:H	1.78	0.47
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.96	0.47
2:I:713:ARG:HH12	2:I:716:LYS:HZ1	1.61	0.47
3:D:400:VAL:HG22	3:D:402:PRO:HD3	1.96	0.47
2:I:159:ILE:HG13	2:I:174:LEU:O	2.14	0.47
1:A:59:GLU:HG3	1:A:60:ASP:H	1.79	0.47
3:D:1478:SER:HB3	3:D:1481:VAL:HG22	1.96	0.47
1:G:32:PHE:O	1:G:36:LEU:HG	2.15	0.47
6:M:45:SER:OG	6:M:46:LYS:N	2.47	0.47
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.50	0.47
1:A:53:VAL:HG22	1:A:54:THR:N	2.25	0.47
3:D:241:VAL:HG13	3:D:312:ARG:HG2	1.95	0.47
5:F:302:SER:H	5:F:305:GLU:CG	2.28	0.47
2:C:726:ILE:HD12	2:C:729:LEU:HG	1.96	0.47
3:D:272:LEU:O	3:D:279:VAL:N	2.45	0.47
7:R:15:DT:H6	7:R:15:DT:H5'	1.80	0.47
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.48	0.47
1:B:10:VAL:O	1:B:12:THR:HG23	2.15	0.47
1:B:161:ARG:HG3	1:B:162:ILE:N	2.24	0.47
2:I:168:ARG:HH21	2:I:346:VAL:HG22	1.79	0.47
3:J:639:LEU:HD22	3:J:766:ALA:HA	1.95	0.47
3:J:648:MET:O	3:J:652:LEU:HB2	2.14	0.47
3:D:49:ILE:HD11	3:D:50:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:853:VAL:HG22	3:J:858:LEU:HB3	1.97	0.47
2:I:726:ILE:HB	2:I:729:LEU:HB2	1.97	0.47
2:I:726:ILE:HD12	2:I:729:LEU:HG	1.96	0.47
3:D:858:LEU:HD21	3:D:864:VAL:HG11	1.97	0.47
1:A:162:ILE:HG23	1:A:163:ASN:H	1.79	0.47
2:C:858:MET:H	2:C:977:GLY:HA3	1.80	0.47
2:C:685:GLU:HG2	3:D:739:ASP:HB3	1.96	0.47
2:I:579:VAL:HG13	2:I:842:ARG:HH22	1.80	0.47
3:J:841:PHE:HB3	3:J:843:PHE:CE1	2.50	0.47
2:C:126:SER:HB3	2:C:134:ARG:O	2.14	0.47
3:D:109:PRO:HG2	3:D:111:LYS:NZ	2.29	0.47
3:J:710:ARG:HG3	3:J:711:LEU:HD22	1.97	0.47
2:C:521:PRO:HG2	3:D:1072:ILE:HD11	1.95	0.47
2:I:601:GLY:HA2	2:I:615:TYR:HA	1.97	0.47
1:H:29:GLU:HB3	1:H:32:PHE:CD1	2.49	0.47
3:D:22:SER:HB2	3:D:92:HIS:HB3	1.95	0.47
1:G:218:LEU:HD23	1:H:222:LEU:HD21	1.96	0.47
2:C:118:LEU:HD13	2:C:382:LEU:HD23	1.96	0.47
3:J:977:ALA:HB3	3:J:983:LEU:HD12	1.96	0.47
3:J:1168:LEU:HD23	3:J:1169:GLU:H	1.79	0.47
3:J:521:PRO:HB2	3:J:524:LEU:HG	1.97	0.47
3:D:682:ASP:C	3:D:684:LYS:H	2.18	0.47
2:I:1032:PHE:CZ	2:I:1036:GLU:HB3	2.50	0.47
1:G:162:ILE:HG23	1:G:163:ASN:H	1.77	0.47
4:K:41:GLU:HB3	4:K:42:PRO:HD2	1.96	0.47
2:I:149:THR:HA	2:I:322:VAL:HG13	1.96	0.47
3:D:717:GLN:HA	3:D:718:PRO:HD3	1.76	0.47
1:G:153:ALA:HB2	1:G:167:VAL:C	2.35	0.47
2:C:274:ARG:O	2:C:278:GLU:HB2	2.15	0.47
2:I:154:ARG:NH1	2:I:176:VAL:HG23	2.29	0.47
2:I:1038:TRP:CE2	3:J:1099:VAL:HG11	2.50	0.47
3:D:217:ARG:HB2	3:D:339:TRP:CE2	2.50	0.47
3:D:1476:THR:HA	4:E:17:TYR:HB3	1.97	0.47
3:D:1443:THR:HG22	3:D:1447:LEU:HD13	1.97	0.47
6:M:12:LEU:HD13	6:M:59:LEU:HD13	1.97	0.47
1:A:221:HIS:HA	1:A:224:TYR:CD1	2.50	0.47
2:I:1086:ARG:HD2	2:I:1112:PHE:CE2	2.49	0.47
3:J:828:VAL:HG22	3:J:833:GLU:HB2	1.96	0.47
3:J:1381:VAL:HG21	3:J:1389:LEU:HD23	1.96	0.47
2:I:1063:ARG:HG3	5:L:356:PRO:HG3	1.96	0.47
2:I:497:ALA:HB1	2:I:501:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1225:ALA:O	3:D:1229:ILE:HG12	2.15	0.47
5:F:206:ASN:O	5:F:209:LEU:HB3	2.14	0.47
2:I:1097:LEU:HD22	3:J:10:ILE:HD11	1.96	0.47
2:C:807:ARG:HB3	2:C:821:GLU:HB3	1.96	0.47
1:G:123:MET:HG3	1:G:203:GLY:HA3	1.95	0.47
1:H:149:GLY:O	1:H:171:PHE:HB2	2.15	0.47
2:I:198:ARG:HG2	2:I:234:ALA:CB	2.45	0.47
2:I:146:VAL:HG11	2:I:281:LEU:HD11	1.96	0.47
2:I:893:ALA:HB2	2:I:918:LEU:HD22	1.96	0.47
2:C:1067:TYR:CZ	5:F:357:VAL:HG12	2.49	0.47
2:C:56:GLU:HB3	2:C:359:MET:HE2	1.96	0.47
3:D:401:TYR:HB3	3:D:427:VAL:HG21	1.97	0.47
2:I:336:VAL:HA	2:I:339:LEU:HD11	1.97	0.46
3:J:500:ARG:NH1	3:J:1390:LEU:HD21	2.30	0.46
3:D:731:LEU:HB3	3:D:779:ALA:HB1	1.98	0.46
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.50	0.46
3:D:610:LYS:HD3	3:D:615:ARG:NH1	2.31	0.46
1:B:48:ILE:HG13	1:B:213:GLN:HE21	1.78	0.46
2:C:86:LYS:HE2	2:C:814:GLU:H	1.79	0.46
5:L:96:VAL:HA	5:L:225:LEU:HD11	1.96	0.46
1:A:53:VAL:HA	1:A:144:VAL:HA	1.96	0.46
3:J:638:LYS:HD3	3:J:640:HIS:CD2	2.49	0.46
3:D:49:ILE:HG13	3:D:50:PHE:H	1.81	0.46
2:I:300:ASP:OD1	2:I:301:GLU:N	2.49	0.46
2:C:300:ASP:OD1	2:C:301:GLU:N	2.48	0.46
3:J:12:LEU:HD21	3:J:1452:ILE:HD13	1.97	0.46
6:M:144:LEU:HB2	6:M:146:ILE:HG12	1.97	0.46
3:D:1142:SER:O	3:D:1364:HIS:ND1	2.48	0.46
3:J:710:ARG:HB3	3:J:1227:GLU:OE1	2.15	0.46
3:D:460:ALA:O	3:D:464:LEU:HG	2.15	0.46
3:J:577:ALA:O	3:J:581:VAL:HG23	2.15	0.46
5:F:229:GLN:HA	5:F:232:ASN:HD22	1.80	0.46
2:C:742:ILE:CD1	2:C:803:ARG:HD2	2.45	0.46
2:I:688:ILE:HG12	2:I:871:LEU:HD21	1.98	0.46
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.97	0.46
2:C:838:LYS:HB3	2:C:997:LEU:HB2	1.98	0.46
1:H:76:VAL:HA	1:H:79:ILE:HD12	1.98	0.46
3:D:26:VAL:HG13	3:D:42:ASP:O	2.15	0.46
5:L:302:SER:H	5:L:305:GLU:CG	2.29	0.46
2:C:305:PRO:O	2:C:308:ARG:HG2	2.16	0.46
3:J:539:ASP:HB3	3:J:600:LEU:HG	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:75:LEU:HG	6:N:159:TRP:CZ3	2.51	0.46
2:C:89:THR:HG23	2:C:129:ILE:HA	1.96	0.46
3:D:633:VAL:HG22	3:D:635:PRO:HD3	1.96	0.46
2:I:98:LEU:HD23	2:I:98:LEU:H	1.80	0.46
3:D:441:ARG:HH11	3:D:445:ARG:HH12	1.64	0.46
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.97	0.46
2:I:508:ILE:HD11	2:I:529:VAL:HG11	1.97	0.46
2:C:889:HIS:CE1	2:C:970:GLY:HA3	2.50	0.46
1:A:58:ILE:HG21	1:A:68:ILE:HD13	1.97	0.46
2:C:1107:ASN:HA	2:C:1107:ASN:HD22	1.59	0.46
1:H:74:ASP:O	1:H:78:ILE:HG12	2.15	0.46
5:F:419:ALA:O	5:F:423:LEU:HD12	2.16	0.46
3:J:100:ALA:N	3:J:575:GLN:HE22	2.11	0.46
7:O:23:DG:H1'	7:O:24:DC:H5'	1.97	0.46
5:F:181:LEU:HD23	5:F:185:LEU:CB	2.46	0.46
6:M:11:VAL:O	6:M:59:LEU:HD12	2.16	0.46
3:D:1020:LEU:HG	3:D:1035:ILE:HD12	1.97	0.46
3:J:950:GLY:H	3:J:953:ASP:CG	2.18	0.46
2:I:671:ASN:HA	2:I:992:MET:O	2.14	0.46
3:J:1151:ARG:HA	3:J:1162:GLU:HG3	1.97	0.46
1:G:73:GLU:HB3	1:G:77:GLU:HB3	1.97	0.46
2:C:988:VAL:HG22	3:D:948:THR:OG1	2.15	0.46
1:H:76:VAL:O	1:H:80:LEU:HD13	2.15	0.46
2:C:98:LEU:HD23	2:C:98:LEU:H	1.81	0.46
5:F:238:ALA:HB2	5:F:257:TRP:HB2	1.97	0.46
2:C:950:LEU:HD11	2:C:952:LEU:HB2	1.98	0.46
2:C:860:HIS:HA	2:C:866:PRO:HA	1.97	0.46
5:L:275:ILE:HG22	5:L:280:VAL:HG12	1.98	0.46
2:I:940:GLU:HG2	2:I:973:VAL:HG21	1.98	0.46
1:B:32:PHE:O	1:B:36:LEU:HG	2.16	0.46
2:I:56:GLU:HB3	2:I:359:MET:HE2	1.98	0.46
1:H:54:THR:HG23	1:H:55:SER:H	1.80	0.46
3:D:187:LYS:HG2	3:D:198:ARG:C	2.36	0.46
1:H:123:MET:C	1:H:125:PRO:HD3	2.36	0.46
5:L:166:PRO:HG2	5:L:169:LYS:HE3	1.98	0.46
3:D:834:THR:OG1	3:D:838:ARG:HB2	2.16	0.46
1:A:32:PHE:O	1:A:36:LEU:HG	2.16	0.46
2:C:85:GLU:HB2	2:C:804:LEU:HD21	1.98	0.46
3:J:160:GLU:HG3	3:J:165:LYS:HD3	1.98	0.46
6:N:12:LEU:HD13	6:N:59:LEU:HD13	1.98	0.46
3:D:677:LEU:HD21	3:D:687:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:672:VAL:HB	2:C:868:ASP:HB2	1.97	0.46
3:D:216:LEU:HB3	3:D:218:LYS:HZ3	1.81	0.46
5:F:206:ASN:HA	7:O:30:DT:O2	2.15	0.46
3:J:10:ILE:O	3:J:1454:GLY:HA2	2.16	0.46
5:L:294:GLN:HE21	5:L:294:GLN:HB3	1.57	0.46
1:G:83:LYS:HE3	1:G:168:ASP:HB2	1.97	0.46
5:F:154:ALA:HB1	5:F:158:LYS:NZ	2.31	0.46
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.15	0.46
3:J:1384:PRO:HA	3:J:1415:VAL:HG13	1.98	0.46
1:H:176:ARG:HB3	1:H:200:TRP:CE3	2.51	0.46
3:D:229:ALA:CB	3:D:245:LEU:H	2.29	0.46
3:D:841:PHE:CZ	3:D:858:LEU:HD13	2.50	0.46
5:L:234:GLY:O	5:L:257:TRP:HB3	2.16	0.46
1:G:108:GLU:HG2	1:G:131:THR:HG23	1.97	0.46
3:D:954:ALA:O	3:D:1062:ARG:NE	2.49	0.46
5:L:154:ALA:HB1	5:L:158:LYS:NZ	2.31	0.46
3:D:209:ARG:HA	3:D:347:VAL:HG12	1.96	0.46
3:J:901:GLN:H	3:J:901:GLN:HG2	1.53	0.46
2:I:66:LEU:HA	2:I:99:GLN:O	2.15	0.46
2:I:679:PHE:H	2:I:683:ASN:HD21	1.64	0.46
6:M:124:LEU:HD11	8:P:2:DG:H4'	1.98	0.46
3:D:661:MET:SD	3:D:677:LEU:HD11	2.56	0.46
3:J:834:THR:OG1	3:J:838:ARG:HB2	2.16	0.46
2:I:758:ARG:HE	2:I:788:THR:HB	1.80	0.46
4:K:66:LYS:HA	4:K:69:LEU:HD12	1.98	0.46
2:I:521:PRO:HG2	3:J:1072:ILE:HD11	1.97	0.46
2:I:101:ILE:HG23	2:I:108:ILE:HA	1.97	0.45
2:C:675:ALA:HB2	2:C:867:VAL:HG21	1.98	0.45
1:G:54:THR:HG23	1:G:143:ARG:O	2.15	0.45
1:B:57:TYR:HB3	1:B:141:GLU:HG3	1.97	0.45
2:I:835:VAL:HG13	2:I:851:LYS:H	1.80	0.45
2:C:729:LEU:HD11	2:C:733:ALA:HB3	1.98	0.45
3:D:758:GLU:HA	3:D:762:GLN:NE2	2.32	0.45
3:D:682:ASP:O	3:D:684:LYS:N	2.45	0.45
1:G:205:VAL:HG11	1:G:213:GLN:NE2	2.31	0.45
1:B:76:VAL:O	1:B:80:LEU:HD13	2.16	0.45
3:D:1293:PHE:HA	3:D:1302:GLU:HA	1.98	0.45
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.72	0.45
2:C:435:TYR:HB3	2:C:436:GLY:H	1.56	0.45
3:J:1074:SER:HA	3:J:1077:ALA:HB3	1.98	0.45
2:I:358:ARG:HB2	2:I:372:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:646:LYS:HE3	3:D:688:TRP:CZ2	2.44	0.45
2:C:154:ARG:NH1	2:C:176:VAL:HG23	2.30	0.45
2:I:305:PRO:O	2:I:308:ARG:HG2	2.16	0.45
3:J:838:ARG:HB3	3:J:865:THR:HG23	1.99	0.45
2:C:534:VAL:H	2:C:538:GLN:HE22	1.64	0.45
1:B:48:ILE:HA	1:B:49:PRO:HD2	1.80	0.45
3:D:441:ARG:NH1	3:D:445:ARG:HH12	2.14	0.45
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	1.98	0.45
3:D:34:TYR:HD1	5:F:325:ILE:HG21	1.80	0.45
3:D:90:MET:HB3	3:D:519:VAL:O	2.16	0.45
2:I:838:LYS:HB3	2:I:997:LEU:HB2	1.98	0.45
5:L:307:ALA:HB1	5:L:314:TRP:HB3	1.98	0.45
1:G:64:GLU:O	1:G:75:VAL:HB	2.16	0.45
3:D:689:ASP:O	3:D:692:GLU:HB2	2.16	0.45
3:J:717:GLN:HA	3:J:718:PRO:HD3	1.75	0.45
2:C:671:ASN:HA	2:C:992:MET:O	2.16	0.45
3:J:750:PRO:HG2	3:J:756:GLN:NE2	2.31	0.45
2:I:835:VAL:O	3:J:725:SER:OG	2.34	0.45
2:C:1083:GLU:OE2	3:D:87:ARG:NH1	2.49	0.45
2:I:1086:ARG:HD2	2:I:1112:PHE:CD2	2.51	0.45
2:C:840:ALA:HB3	2:C:997:LEU:HD11	1.98	0.45
6:M:33:ARG:HD2	6:M:33:ARG:H	1.81	0.45
2:C:882:LEU:HD21	3:D:1038:LEU:HD22	1.98	0.45
1:G:63:HIS:NE2	2:I:801:VAL:HG13	2.31	0.45
2:I:691:SER:HB3	2:I:868:ASP:HA	1.97	0.45
2:C:66:LEU:HD23	2:C:100:LEU:HA	1.98	0.45
2:I:729:LEU:HD13	2:I:730:SER:O	2.17	0.45
2:I:676:ILE:CG2	2:I:873:PRO:HB3	2.47	0.45
3:D:103:TRP:CE2	3:D:1444:THR:HG23	2.51	0.45
3:J:1448:THR:O	3:J:1452:ILE:HG12	2.16	0.45
1:H:156:HIS:NE2	1:H:167:VAL:O	2.49	0.45
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.98	0.45
2:C:16:PRO:HB2	2:C:460:ARG:NH2	2.30	0.45
7:R:5:DA:H1'	7:R:6:DC:H5''	1.98	0.45
3:D:1341:PRO:O	3:D:1344:VAL:HB	2.17	0.45
3:D:165:LYS:H	3:D:397:LYS:HE3	1.81	0.45
4:K:30:LEU:CD2	4:K:63:TRP:HB3	2.44	0.45
2:I:66:LEU:HD23	2:I:100:LEU:HA	1.98	0.45
2:I:200:LEU:HD21	2:I:303:PHE:HB2	1.98	0.45
3:J:560:GLN:HB2	3:J:560:GLN:HE21	1.58	0.45
2:C:995:MET:HE2	2:C:996:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLN:NE2	1:B:182:GLU:HB3	2.31	0.45
4:K:19:LEU:O	4:K:23:VAL:HG23	2.16	0.45
3:J:923:GLY:O	3:J:926:LYS:HB2	2.17	0.45
2:C:583:LEU:O	2:C:587:VAL:HG23	2.16	0.45
3:D:62:LYS:HE2	3:D:62:LYS:HB2	1.78	0.45
3:J:1044:LEU:HD23	3:J:1053:PHE:O	2.17	0.45
3:D:791:TYR:CE2	3:D:945:SER:HB3	2.51	0.45
5:F:141:LEU:O	5:F:145:VAL:HG23	2.17	0.45
1:G:59:GLU:HG3	1:G:60:ASP:H	1.81	0.45
1:A:53:VAL:H	1:A:144:VAL:HG13	1.82	0.45
2:C:200:LEU:HD21	2:C:303:PHE:HB2	1.99	0.45
7:O:22:DT:H2"	7:O:23:DG:C8	2.52	0.45
5:L:217:TYR:CD2	5:L:262:ILE:HG21	2.51	0.45
3:J:618:LEU:HG	3:J:1467:ILE:HG23	1.97	0.45
3:J:1012:GLU:HG2	3:J:1021:TYR:OH	2.17	0.45
7:O:10:DA:H1'	7:O:11:DG:H5"	1.99	0.45
2:C:1056:LYS:O	3:D:624:ASP:N	2.49	0.45
3:D:699:VAL:HB	3:D:716:PHE:O	2.17	0.45
3:J:592:THR:HA	3:J:600:LEU:HD13	1.99	0.45
2:C:118:LEU:HD12	2:C:119:PRO:HD2	1.99	0.45
3:J:849:ALA:O	3:J:853:VAL:HG23	2.17	0.45
2:I:677:MET:SD	2:I:987:ILE:HD13	2.56	0.45
5:F:111:LEU:O	5:F:115:ILE:HG12	2.16	0.45
2:C:869:VAL:HG21	2:C:871:LEU:HG	1.99	0.45
6:N:13:PRO:HA	6:N:14:PRO:HA	1.70	0.45
3:D:31:THR:HG21	5:F:272:THR:HG22	1.98	0.45
2:I:1086:ARG:HB3	2:I:1112:PHE:HE2	1.82	0.45
3:J:1293:PHE:HA	3:J:1302:GLU:HA	1.99	0.45
2:C:312:ALA:O	2:C:317:VAL:HG12	2.17	0.45
3:J:1295:GLU:HG2	3:J:1300:SER:OG	2.16	0.45
6:N:79:ARG:HB3	6:N:111:GLN:HB2	1.98	0.45
3:J:1443:THR:HG22	3:J:1447:LEU:HD13	1.98	0.45
2:C:971:LYS:HA	2:C:988:VAL:HA	1.97	0.45
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.98	0.45
3:D:65:ARG:HG3	3:D:67:ARG:H	1.82	0.45
2:C:249:LYS:HB2	2:C:252:LYS:HE3	1.99	0.45
4:K:65:MET:O	4:K:69:LEU:HG	2.17	0.45
3:D:565:ILE:H	3:D:565:ILE:HD12	1.81	0.45
3:J:573:MET:HA	3:J:576:GLU:HG2	1.97	0.45
1:G:176:ARG:HG3	1:G:200:TRP:CE3	2.51	0.45
7:O:14:DT:H3	8:P:12:DA:H61	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:95:PRO:O	5:L:98:GLN:HB3	2.17	0.45
2:C:545:ASN:HA	2:C:905:VAL:HG21	1.99	0.45
2:I:144:PRO:HG2	2:I:273:GLY:N	2.32	0.45
2:C:1053:LEU:HA	3:D:621:LYS:HE3	1.99	0.45
2:I:834:GLN:HG2	2:I:835:VAL:H	1.82	0.45
3:D:681:ARG:C	3:D:683:ILE:H	2.20	0.45
1:B:11:PHE:HB2	1:B:25:LEU:CD1	2.47	0.45
3:J:1374:GLN:HA	3:J:1377:LYS:HD2	1.99	0.45
1:A:73:GLU:HB3	1:A:77:GLU:HB3	1.99	0.45
5:F:166:PRO:HG2	5:F:169:LYS:HE3	1.98	0.45
2:C:17:PRO:O	2:C:20:GLU:HG3	2.16	0.45
2:C:532:MET:HG2	2:C:533:ASP:N	2.32	0.45
2:I:578:VAL:HG12	2:I:900:ARG:HA	1.98	0.45
2:I:535:SER:O	2:I:538:GLN:HG2	2.16	0.44
2:I:22:GLN:O	2:I:336:VAL:HG21	2.17	0.44
3:J:565:ILE:HD13	5:L:204:GLU:HG2	2.00	0.44
3:J:692:GLU:HG2	3:J:720:LEU:HD12	1.99	0.44
1:H:156:HIS:ND1	1:H:158:ILE:HG22	2.31	0.44
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.17	0.44
2:I:642:ARG:O	2:I:643:VAL:HG13	2.17	0.44
5:F:332:LEU:HD22	5:F:345:GLY:HA2	1.98	0.44
6:N:97:LEU:HD21	6:N:132:ALA:HB2	1.98	0.44
3:J:109:PRO:HG2	3:J:111:LYS:NZ	2.33	0.44
2:I:16:PRO:HB2	2:I:460:ARG:NH2	2.32	0.44
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.99	0.44
2:C:192:PRO:HB2	2:C:195:LEU:HB2	1.99	0.44
2:I:428:ARG:NE	2:I:451:LEU:HD21	2.22	0.44
2:I:683:ASN:OD1	2:I:872:ASN:ND2	2.50	0.44
1:B:74:ASP:O	1:B:78:ILE:HG12	2.17	0.44
5:L:181:LEU:HD23	5:L:185:LEU:CB	2.47	0.44
3:D:849:ALA:O	3:D:853:VAL:HG23	2.18	0.44
3:J:371:ILE:HG23	3:J:372:ASP:H	1.81	0.44
2:I:394:PHE:CE2	2:I:632:ASN:HB3	2.52	0.44
3:J:1442:ASN:O	3:J:1446:VAL:HG23	2.18	0.44
2:I:448:ASN:HA	2:I:451:LEU:HD23	2.00	0.44
6:N:11:VAL:O	6:N:59:LEU:HD12	2.17	0.44
3:D:554:LEU:O	3:D:558:LEU:HG	2.17	0.44
1:G:14:THR:OG1	1:H:231:SER:OG	2.20	0.44
3:D:264:LEU:HD21	3:D:339:TRP:CD1	2.52	0.44
2:I:335:THR:O	2:I:339:LEU:HG	2.18	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:133:ILE:HG22	3:J:152:LEU:HG	1.99	0.44
3:D:302:GLN:HG2	3:D:303:PRO:HD2	1.99	0.44
3:J:762:GLN:HB3	4:K:16:LYS:HE2	1.99	0.44
2:C:217:LEU:HD23	2:C:217:LEU:H	1.82	0.44
2:C:595:LEU:HD23	2:C:656:ALA:HB3	2.00	0.44
1:B:143:ARG:HG3	1:B:160:ASP:OD2	2.16	0.44
3:D:977:ALA:HB3	3:D:983:LEU:HD12	2.00	0.44
1:H:57:TYR:HB3	1:H:141:GLU:HG3	1.98	0.44
1:A:40:LEU:HD21	1:A:215:VAL:HG22	2.00	0.44
2:C:834:GLN:HG2	2:C:835:VAL:H	1.82	0.44
2:C:1087:VAL:HG12	2:C:1091:GLU:OE1	2.18	0.44
2:C:713:ARG:HH22	2:C:716:LYS:NZ	2.16	0.44
2:I:950:LEU:HD11	2:I:952:LEU:HB2	1.99	0.44
1:B:54:THR:OG1	1:B:158:ILE:HG21	2.17	0.44
3:J:92:HIS:HD2	3:J:516:ALA:HB1	1.82	0.44
3:D:1232:PRO:HB2	3:D:1356:TYR:HE2	1.82	0.44
1:B:176:ARG:HD2	3:D:884:ARG:HH22	1.82	0.44
2:C:539:VAL:HG21	3:D:1067:VAL:HG11	1.99	0.44
2:I:327:HIS:O	2:I:331:ARG:HG3	2.17	0.44
2:C:673:LEU:HB3	2:C:867:VAL:HG12	1.99	0.44
2:C:428:ARG:NE	2:C:451:LEU:HD21	2.24	0.44
1:G:53:VAL:HG22	1:G:54:THR:N	2.28	0.44
2:C:690:ILE:CG1	2:C:852:ILE:HG23	2.45	0.44
2:C:99:GLN:HB3	2:C:110:GLU:HG3	1.98	0.44
3:D:264:LEU:HD21	3:D:339:TRP:CD2	2.52	0.44
3:D:317:MET:HG3	3:D:339:TRP:HB3	1.99	0.44
3:J:153:LEU:HB3	3:J:157:GLU:HG3	2.00	0.44
1:H:48:ILE:HG22	1:H:173:PRO:HD2	1.98	0.44
3:J:49:ILE:HD11	3:J:50:PHE:CZ	2.52	0.44
4:E:65:MET:O	4:E:69:LEU:HG	2.17	0.44
5:L:266:ILE:O	5:L:270:ALA:HB2	2.18	0.44
2:I:630:ARG:HA	2:I:705:ILE:HD13	2.00	0.44
2:I:441:VAL:O	2:I:443:THR:HG22	2.17	0.44
2:C:853:LEU:HA	2:C:854:PRO:HD3	1.83	0.44
6:N:49:VAL:HG13	6:N:57:VAL:HG21	1.99	0.44
5:F:237:ARG:NH2	5:F:241:LYS:HD2	2.33	0.44
5:F:302:SER:O	5:F:306:ILE:HG22	2.17	0.44
2:C:839:LEU:HD23	2:C:995:MET:O	2.18	0.44
3:D:261:LEU:HD21	3:D:268:HIS:CD2	2.50	0.44
3:J:123:LEU:HG	3:J:127:LEU:HD12	1.99	0.44
3:D:206:ARG:HH11	3:D:206:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:TYR:CD1	1:H:9:PRO:HG2	2.53	0.44
2:I:936:VAL:HB	2:I:941:LYS:HE2	1.99	0.44
2:I:564:MET:SD	2:I:846:LYS:HG2	2.58	0.44
8:P:3:DC:H2"	8:P:4:DA:C8	2.52	0.44
3:D:417:PRO:HA	3:D:430:GLU:HA	1.99	0.44
4:E:41:GLU:HB3	4:E:42:PRO:HD2	1.99	0.44
2:C:198:ARG:CZ	2:C:238:LEU:HB2	2.47	0.44
2:I:164:PRO:HG3	2:I:267:TYR:CE1	2.53	0.44
2:C:91:GLN:HG3	2:C:117:HIS:HB3	1.98	0.44
3:J:683:ILE:HD12	3:J:688:TRP:CZ2	2.53	0.44
3:J:682:ASP:C	3:J:684:LYS:H	2.21	0.44
3:D:1281:VAL:HG21	3:D:1313:VAL:HG11	1.99	0.44
5:L:103:ILE:HG21	5:L:207:LEU:HD22	1.99	0.44
2:C:937:ASP:OD2	2:C:939:ARG:NE	2.51	0.44
6:N:136:LEU:O	6:N:140:VAL:HG23	2.17	0.44
3:J:1476:THR:HG22	4:K:17:TYR:HB3	2.00	0.44
1:H:54:THR:OG1	1:H:158:ILE:HG21	2.18	0.44
1:H:176:ARG:HD3	1:H:200:TRP:HZ3	1.83	0.44
2:I:588:VAL:HG21	2:I:664:GLY:HA2	2.00	0.44
2:C:1035:MET:HB2	3:D:707:THR:HB	1.99	0.44
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.52	0.44
2:I:839:LEU:HD23	2:I:995:MET:O	2.18	0.44
3:D:268:HIS:HB2	3:D:284:LEU:HD22	2.00	0.44
3:D:573:MET:HA	3:D:576:GLU:CG	2.48	0.44
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.99	0.44
4:E:19:LEU:O	4:E:23:VAL:HG23	2.18	0.44
1:A:99:LEU:HB2	1:A:142:VAL:HG23	2.00	0.44
1:G:9:PRO:HG3	1:H:224:TYR:CG	2.53	0.44
2:I:743:VAL:HG21	2:I:800:VAL:HG21	1.99	0.44
6:N:45:SER:OG	6:N:46:LYS:N	2.48	0.44
1:H:51:THR:HG23	1:H:52:ALA:H	1.83	0.44
3:D:646:LYS:HA	3:D:720:LEU:HD22	1.99	0.44
2:I:934:PHE:HD2	2:I:934:PHE:HA	1.74	0.44
6:N:129:LEU:O	6:N:133:ILE:HG12	2.18	0.44
3:J:758:GLU:HG2	3:J:1476:THR:HG21	1.99	0.44
4:E:6:ILE:HD11	4:E:10:PHE:CZ	2.53	0.44
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.75	0.44
3:J:1020:LEU:HG	3:J:1035:ILE:HD12	2.00	0.44
2:I:396:ASP:HB2	2:I:406:HIS:ND1	2.32	0.44
5:L:188:TYR:HA	5:L:191:ILE:HD12	2.00	0.44
3:J:970:LYS:O	3:J:974:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:852:ILE:HG22	2:C:853:LEU:H	1.83	0.43
3:J:664:LYS:HZ1	3:J:690:ALA:HB2	1.82	0.43
3:D:15:PRO:HG3	3:D:514:LEU:HD12	2.00	0.43
3:J:160:GLU:HG2	3:J:165:LYS:HB2	2.00	0.43
2:I:111:ASP:OD1	2:I:368:THR:OG1	2.32	0.43
2:I:312:ALA:O	2:I:317:VAL:HG12	2.18	0.43
3:D:231:VAL:H	3:D:243:ALA:H	1.66	0.43
1:A:101:LEU:HD12	1:A:102:ARG:H	1.82	0.43
3:D:1074:SER:HA	3:D:1077:ALA:HB3	2.00	0.43
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.53	0.43
6:M:90:HIS:CD2	6:M:124:LEU:HB3	2.53	0.43
2:I:557:ARG:HG3	2:I:881:ASN:HD22	1.83	0.43
2:C:42:VAL:HA	2:C:46:ALA:HB2	2.00	0.43
2:I:1031:ARG:HG2	2:I:1032:PHE:N	2.32	0.43
3:J:956:ILE:HD11	3:J:1062:ARG:HH11	1.83	0.43
3:D:124:GLU:OE1	3:D:587:ARG:NH2	2.52	0.43
3:J:876:SER:O	3:J:879:ARG:HB3	2.17	0.43
1:H:11:PHE:HB2	1:H:25:LEU:CD1	2.48	0.43
2:I:435:TYR:HB3	2:I:436:GLY:H	1.54	0.43
2:I:583:LEU:O	2:I:587:VAL:HG23	2.17	0.43
2:I:545:ASN:HA	2:I:905:VAL:HG21	2.00	0.43
2:I:874:LEU:O	3:J:1029:ARG:HG2	2.18	0.43
3:D:648:MET:O	3:D:652:LEU:HB2	2.17	0.43
3:J:116:LEU:HD21	3:J:465:LEU:HG	2.00	0.43
3:J:554:LEU:O	3:J:558:LEU:HG	2.17	0.43
2:C:677:MET:SD	2:C:987:ILE:HD13	2.58	0.43
5:L:111:LEU:O	5:L:115:ILE:HG12	2.18	0.43
2:C:717:LEU:HD23	2:C:761:PHE:HB2	2.01	0.43
3:D:156:GLU:O	3:D:160:GLU:HB2	2.18	0.43
2:I:915:LYS:HG2	2:I:968:ASP:OD2	2.18	0.43
1:A:211:LEU:O	1:A:215:VAL:HG23	2.17	0.43
3:D:1123:PHE:HE2	3:D:1184:ARG:HA	1.84	0.43
2:C:159:ILE:HG13	2:C:174:LEU:O	2.18	0.43
2:C:569:VAL:HG22	2:C:996:LYS:O	2.18	0.43
2:C:22:GLN:O	2:C:336:VAL:HG21	2.18	0.43
5:F:94:ASP:HA	5:F:95:PRO:HD2	1.89	0.43
2:C:880:MET:SD	3:D:1034:GLN:HG2	2.58	0.43
2:C:90:TYR:HB3	2:C:128:ILE:HB	2.00	0.43
3:D:1033:GLN:O	3:D:1036:ARG:HB3	2.17	0.43
4:E:41:GLU:O	4:E:45:ARG:HG2	2.19	0.43
2:C:164:PRO:HG3	2:C:267:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:THR:HA	2:C:470:PRO:HD3	1.85	0.43
1:B:184:THR:HB	1:B:194:LYS:HB2	2.01	0.43
3:D:632:VAL:O	3:D:727:GLN:HA	2.19	0.43
2:C:934:PHE:HA	2:C:934:PHE:HD2	1.70	0.43
3:J:14:SER:HB3	3:J:511:TRP:CD2	2.54	0.43
3:D:1048:PRO:HD3	3:D:1075:HIS:CB	2.49	0.43
3:J:585:GLY:CA	3:J:590:PRO:HG3	2.48	0.43
1:G:57:TYR:HD1	1:G:163:ASN:O	2.02	0.43
3:J:1279:GLY:H	3:J:1319:VAL:HG23	1.83	0.43
2:C:136:ILE:HA	2:C:391:LEU:O	2.18	0.43
3:J:610:LYS:HD3	3:J:615:ARG:NH1	2.33	0.43
2:C:198:ARG:HG2	2:C:234:ALA:HB3	2.01	0.43
2:C:869:VAL:HG22	2:C:870:ILE:N	2.33	0.43
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.00	0.43
2:C:261:LEU:HD13	2:C:291:VAL:HG21	2.00	0.43
1:H:57:TYR:CE1	1:H:161:ARG:HG2	2.52	0.43
3:J:563:PRO:O	3:J:567:ILE:HG12	2.19	0.43
1:H:87:VAL:HG11	1:H:99:LEU:HD21	2.01	0.43
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.53	0.43
2:C:336:VAL:HA	2:C:339:LEU:HD11	2.01	0.43
3:J:103:TRP:CE3	3:J:1448:THR:HG23	2.52	0.43
3:D:1168:LEU:HD23	3:D:1169:GLU:H	1.82	0.43
2:I:217:LEU:HD23	2:I:217:LEU:H	1.83	0.43
2:I:562:SER:O	2:I:565:GLN:HB2	2.18	0.43
3:J:460:ALA:O	3:J:464:LEU:HG	2.18	0.43
2:C:92:ALA:HA	2:C:93:PRO:HD3	1.89	0.43
5:L:141:LEU:O	5:L:145:VAL:HG23	2.18	0.43
2:C:140:ILE:HG12	2:C:141:HIS:N	2.33	0.43
3:J:138:LYS:HD2	3:J:451:ASP:O	2.18	0.43
3:D:147:VAL:HG21	3:D:153:LEU:HD21	2.00	0.43
1:A:158:ILE:HD11	1:A:166:PRO:HA	2.00	0.43
2:I:673:LEU:HA	2:I:990:GLY:O	2.19	0.43
2:I:262:ALA:HB2	2:I:291:VAL:HG23	2.01	0.43
2:C:570:PRO:O	2:C:571:LEU:HD13	2.19	0.43
2:C:1067:TYR:CE2	5:F:357:VAL:HA	2.54	0.43
3:J:865:THR:HG22	3:J:874:GLU:HG2	2.00	0.43
1:A:104:GLU:HG3	1:A:137:LYS:HG2	1.99	0.43
6:N:21:ALA:HB3	6:N:37:GLN:HG2	2.01	0.43
3:D:236:TYR:CZ	3:D:242:LEU:HD13	2.53	0.43
1:H:180:GLN:NE2	1:H:182:GLU:HB3	2.33	0.43
2:I:532:MET:HG2	2:I:533:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:970:LYS:O	3:D:974:ILE:HG13	2.18	0.43
2:I:537:LYS:HZ3	2:I:905:VAL:N	2.09	0.43
2:C:327:HIS:O	2:C:331:ARG:HG3	2.18	0.43
3:D:322:VAL:HG22	3:D:323:GLU:H	1.83	0.43
3:D:103:TRP:HZ3	3:D:1447:LEU:HB2	1.84	0.43
3:D:638:LYS:HG2	3:D:639:LEU:H	1.84	0.43
1:H:176:ARG:HD2	3:J:884:ARG:HH22	1.84	0.43
2:I:838:LYS:HG2	2:I:997:LEU:HD22	2.01	0.43
2:C:880:MET:HG2	3:D:1038:LEU:HD11	2.00	0.43
1:H:110:ARG:HH12	1:H:126:ASP:HA	1.84	0.43
3:J:1225:ALA:O	3:J:1229:ILE:HG12	2.18	0.43
3:J:1229:ILE:H	3:J:1229:ILE:HG12	1.65	0.43
3:J:1146:GLY:O	3:J:1206:GLY:HA3	2.18	0.43
5:L:116:ASP:O	5:L:120:LYS:HG2	2.18	0.43
3:D:245:LEU:HD12	3:D:311:LEU:HD21	2.01	0.43
3:D:46:ASP:OD2	3:D:48:ARG:HB2	2.19	0.43
3:D:876:SER:O	3:D:879:ARG:HB3	2.19	0.43
3:D:56:TYR:CD1	3:D:66:GLN:HG2	2.54	0.43
2:C:897:LEU:HB3	2:C:899:GLN:HE21	1.82	0.43
2:C:893:ALA:O	2:C:897:LEU:HG	2.19	0.43
3:D:714:GLN:HE22	3:D:732:VAL:HB	1.83	0.43
1:B:99:LEU:HB2	1:B:142:VAL:CG2	2.49	0.43
3:D:260:GLU:O	3:D:270:ILE:HA	2.18	0.43
2:I:136:ILE:HA	2:I:391:LEU:O	2.18	0.43
1:H:90:LEU:HB2	1:H:119:ASP:HB3	2.01	0.43
3:J:32:ILE:HG22	3:J:39:PRO:HA	2.01	0.43
5:L:142:ILE:O	5:L:146:VAL:HG23	2.19	0.43
3:D:971:LEU:HD21	3:D:992:VAL:HG13	2.01	0.43
5:F:142:ILE:O	5:F:146:VAL:HG23	2.19	0.43
5:L:398:LEU:HD23	5:L:409:ARG:O	2.19	0.43
2:I:807:ARG:HB3	2:I:821:GLU:HB3	2.01	0.43
2:C:1102:LEU:HD12	2:C:1107:ASN:N	2.34	0.43
2:I:437:ARG:NH2	2:I:491:GLU:OE1	2.52	0.43
3:J:645:PRO:HG3	3:J:725:SER:O	2.18	0.43
3:D:251:PHE:HB3	3:D:305:ALA:H	1.84	0.43
3:J:29:PRO:HB3	3:J:548:ILE:HB	2.00	0.43
6:N:146:ILE:HB	6:N:150:GLU:HB2	2.00	0.43
2:I:880:MET:SD	3:J:1034:GLN:HG2	2.59	0.43
2:C:219:GLN:HG3	2:C:219:GLN:H	1.56	0.43
3:D:1118:ILE:O	3:D:1118:ILE:HG13	2.19	0.43
4:K:91:ARG:HH21	4:K:92:LEU:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1340:GLY:O	3:J:1344:VAL:HG23	2.19	0.43
2:I:701:THR:HG23	2:I:831:ARG:O	2.18	0.43
2:I:674:VAL:HA	2:I:869:VAL:CG1	2.44	0.42
2:I:164:PRO:HD3	2:I:267:TYR:OH	2.19	0.42
2:I:195:LEU:HD21	2:I:226:VAL:HG21	2.01	0.42
2:I:14:PRO:HB3	2:I:586:ARG:NH2	2.32	0.42
2:I:146:VAL:HA	2:I:161:SER:O	2.19	0.42
3:D:1465:ASN:O	3:D:1468:LEU:N	2.52	0.42
2:I:430:VAL:HB	3:J:1075:HIS:ND1	2.34	0.42
2:I:89:THR:HG23	2:I:129:ILE:HA	2.00	0.42
2:I:713:ARG:CZ	2:I:715:THR:HG22	2.49	0.42
7:R:6:DC:H2"	7:R:7:DA:C8	2.54	0.42
3:J:31:THR:OG1	3:J:32:ILE:N	2.52	0.42
2:C:642:ARG:O	2:C:643:VAL:HG13	2.18	0.42
3:D:1295:GLU:HG2	3:D:1300:SER:OG	2.19	0.42
1:G:65:PHE:HB3	2:I:628:TYR:CD2	2.54	0.42
1:G:101:LEU:HD12	1:G:102:ARG:H	1.83	0.42
2:I:658:GLY:N	2:I:661:SER:HB3	2.26	0.42
1:A:153:ALA:HB2	1:A:167:VAL:C	2.39	0.42
1:A:158:ILE:HG13	1:A:166:PRO:HG3	2.01	0.42
2:C:537:LYS:NZ	2:C:905:VAL:H	2.12	0.42
2:I:869:VAL:HG21	2:I:871:LEU:HG	2.01	0.42
3:J:640:HIS:O	3:J:717:GLN:HB2	2.19	0.42
3:J:721:VAL:HG21	3:J:727:GLN:HE22	1.82	0.42
3:D:680:GLN:O	3:D:682:ASP:N	2.44	0.42
6:M:136:LEU:O	6:M:140:VAL:HG23	2.19	0.42
6:M:13:PRO:HA	6:M:14:PRO:HA	1.73	0.42
1:G:73:GLU:HG2	1:G:77:GLU:HG2	2.00	0.42
5:L:154:ALA:HB1	5:L:158:LYS:HZ3	1.84	0.42
2:I:387:SER:HB2	2:I:388:ARG:HD2	2.00	0.42
3:J:62:LYS:HG3	3:J:63:TYR:N	2.34	0.42
2:I:419:THR:HG22	2:I:422:ARG:HG2	2.01	0.42
2:C:1055:ILE:HD11	2:C:1079:PRO:HD3	2.01	0.42
2:C:195:LEU:HD21	2:C:226:VAL:HG21	2.01	0.42
2:C:15:LEU:N	2:C:586:ARG:HH12	2.16	0.42
1:H:85:LEU:HD12	1:H:86:VAL:H	1.83	0.42
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.01	0.42
6:N:113:ARG:HB2	6:N:159:TRP:CZ2	2.54	0.42
5:L:157:GLN:HE22	5:L:171:VAL:HG11	1.83	0.42
2:C:676:ILE:CG2	2:C:873:PRO:HB3	2.48	0.42
3:D:879:ARG:HA	3:D:879:ARG:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:284:LEU:HA	3:D:285:PRO:HD2	1.91	0.42
3:J:87:ARG:HG2	3:J:523:ASP:CB	2.49	0.42
3:D:841:PHE:HB3	3:D:843:PHE:CE1	2.54	0.42
3:J:171:LEU:HB3	3:J:391:ALA:O	2.19	0.42
2:I:1044:GLY:HA3	4:K:17:TYR:HE1	1.83	0.42
3:D:956:ILE:HD11	3:D:1062:ARG:HH11	1.83	0.42
3:J:22:SER:HB2	3:J:92:HIS:HB3	2.00	0.42
1:G:9:PRO:HG3	1:H:224:TYR:CD2	2.53	0.42
1:H:11:PHE:HB2	1:H:25:LEU:HD13	2.01	0.42
3:J:1341:PRO:O	3:J:1344:VAL:HB	2.19	0.42
2:C:562:SER:O	2:C:565:GLN:HB2	2.18	0.42
2:I:772:ARG:HD3	5:L:395:GLU:OE1	2.19	0.42
3:D:1146:GLY:O	3:D:1206:GLY:HA3	2.19	0.42
3:J:124:GLU:OE1	3:J:587:ARG:NH2	2.52	0.42
2:I:889:HIS:CE1	2:I:970:GLY:HA3	2.54	0.42
1:B:59:GLU:C	1:B:61:VAL:H	2.23	0.42
3:D:567:ILE:HG22	3:D:571:LYS:NZ	2.35	0.42
2:I:672:VAL:HB	2:I:868:ASP:HB2	2.01	0.42
3:J:403:PHE:HD2	3:J:444:VAL:HG22	1.84	0.42
1:A:59:GLU:HG2	1:A:139:TYR:HB3	2.02	0.42
1:A:58:ILE:HG12	1:A:140:MET:HG3	2.01	0.42
2:I:1026:GLN:HE21	2:I:1026:GLN:HB2	1.55	0.42
1:H:73:GLU:HB3	1:H:77:GLU:HB3	2.01	0.42
6:M:125:ASP:HA	6:M:128:ALA:HB3	2.01	0.42
2:C:497:ALA:HB1	2:C:501:THR:HG21	2.02	0.42
3:D:138:LYS:HD2	3:D:451:ASP:O	2.18	0.42
2:I:258:PHE:HA	2:I:298:PHE:HE2	1.83	0.42
3:D:1434:TRP:CD1	3:D:1457:ASP:HB2	2.54	0.42
2:I:100:LEU:N	2:I:109:LYS:O	2.52	0.42
3:J:1117:TYR:HB2	3:J:1188:VAL:O	2.19	0.42
3:D:1267:ARG:H	3:D:1267:ARG:NE	2.09	0.42
3:D:658:LEU:CD2	3:D:670:VAL:HG13	2.50	0.42
3:D:701:LEU:HD11	3:D:750:PRO:HD3	2.01	0.42
2:C:603:VAL:HB	2:C:646:GLY:HA2	2.01	0.42
2:C:439:CYS:HA	2:C:440:PRO:HD2	1.92	0.42
5:L:244:TYR:HD2	5:L:244:TYR:H	1.68	0.42
3:J:1478:SER:HB3	3:J:1481:VAL:HG22	2.01	0.42
2:C:80:GLN:O	2:C:84:ARG:HG3	2.20	0.42
2:I:516:ARG:HD2	2:I:519:GLY:HA2	2.01	0.42
2:C:1041:GLU:OE1	3:D:1462:LEU:HD13	2.19	0.42
2:I:302:VAL:O	2:I:305:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1071:ILE:HD12	3:J:655:PRO:O	2.19	0.42
3:J:49:ILE:HG13	3:J:50:PHE:H	1.83	0.42
3:J:791:TYR:CE2	3:J:945:SER:HB3	2.54	0.42
5:L:409:ARG:NH2	8:S:20:DG:O6	2.52	0.42
2:C:670:GLN:HE22	2:C:699:PHE:HA	1.83	0.42
1:A:65:PHE:HB3	2:C:628:TYR:CD2	2.55	0.42
2:C:910:THR:OG1	2:C:912:PRO:HD2	2.20	0.42
2:I:448:ASN:C	2:I:451:LEU:HD23	2.39	0.42
2:C:674:VAL:O	2:C:989:VAL:HA	2.20	0.42
1:H:57:TYR:CD1	1:H:161:ARG:HG2	2.55	0.42
3:J:937:TYR:O	3:J:941:LEU:HG	2.19	0.42
2:I:376:ARG:H	2:I:376:ARG:HG2	1.65	0.42
2:I:988:VAL:HG22	3:J:948:THR:OG1	2.20	0.42
2:C:994:ILE:HG22	2:C:995:MET:N	2.35	0.42
3:D:268:HIS:HB2	3:D:284:LEU:HB2	2.02	0.42
6:M:11:VAL:HB	6:M:60:ARG:HG3	2.01	0.42
2:C:1083:GLU:O	2:C:1087:VAL:HG23	2.19	0.42
5:F:147:ARG:HH21	5:F:199:ARG:HH12	1.68	0.42
3:D:780:LYS:HE3	3:D:908:LYS:HE2	2.01	0.42
2:I:840:ALA:HB3	2:I:997:LEU:HD11	2.02	0.42
2:C:80:GLN:H	2:C:80:GLN:HG2	1.60	0.42
3:D:93:ILE:HD13	3:D:548:ILE:HG12	2.00	0.42
2:I:48:PHE:O	2:I:52:PHE:HB2	2.19	0.42
3:J:704:ARG:HB3	3:J:736:PHE:HB3	2.01	0.42
1:A:202:ASP:OD1	1:A:203:GLY:N	2.53	0.42
2:C:230:ARG:CB	2:C:231:PRO:HD2	2.50	0.42
2:C:211:LEU:HD13	2:C:218:VAL:HA	2.01	0.42
3:J:699:VAL:HB	3:J:716:PHE:O	2.20	0.42
3:J:551:ASN:O	3:J:555:LYS:HG3	2.20	0.42
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.87	0.42
3:D:1040:GLY:O	3:D:1060:SER:HB2	2.19	0.42
3:D:916:TYR:HE2	3:D:1168:LEU:HD13	1.85	0.42
2:C:1031:ARG:HG2	2:C:1032:PHE:N	2.34	0.42
3:J:397:LYS:HB3	3:J:397:LYS:HE3	1.90	0.42
2:I:471:TYR:CZ	2:I:496:ILE:HD13	2.55	0.42
3:J:208:PRO:HA	3:J:390:PRO:HA	2.02	0.42
3:J:1404:ASN:O	3:J:1408:ILE:HG12	2.18	0.42
1:G:24:VAL:HG22	1:G:196:THR:HG23	2.01	0.42
3:D:1044:LEU:HD23	3:D:1053:PHE:O	2.19	0.42
3:J:892:ASP:HB2	3:J:894:LYS:HG2	2.02	0.42
3:D:1153:VAL:HB	3:D:1160:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:198:ARG:NH2	2:C:238:LEU:HB2	2.34	0.42
2:I:674:VAL:O	2:I:989:VAL:HA	2.20	0.42
2:I:237:ARG:NH2	2:I:241:LEU:HD11	2.35	0.42
3:D:645:PRO:HG3	3:D:725:SER:O	2.19	0.42
3:J:750:PRO:HG2	3:J:756:GLN:HE22	1.84	0.42
1:H:38:ASN:HB2	1:H:39:PRO:HD3	2.01	0.42
3:J:777:PRO:HB2	3:J:912:LYS:HE2	2.02	0.42
2:C:202:TYR:HD1	2:C:206:THR:HG21	1.85	0.42
3:J:514:LEU:HD21	3:J:518:PRO:HD3	2.00	0.42
2:I:897:LEU:HB3	2:I:899:GLN:HE21	1.85	0.42
3:D:1232:PRO:O	3:D:1235:GLN:HG2	2.20	0.42
2:C:74:GLY:O	2:C:92:ALA:HB1	2.20	0.42
3:D:465:LEU:HA	3:D:468:LEU:HD12	2.01	0.42
2:I:602:GLU:HA	2:I:648:ARG:HA	2.02	0.42
1:H:42:ARG:NH1	2:I:981:GLU:OE2	2.53	0.42
3:J:1232:PRO:O	3:J:1235:GLN:HG2	2.19	0.42
5:F:398:LEU:HD23	5:F:409:ARG:O	2.20	0.42
2:I:53:PRO:HB3	2:I:66:LEU:O	2.19	0.42
3:J:1114:THR:HG22	3:J:1189:ARG:HH22	1.85	0.42
3:J:783:ARG:NH1	3:J:1029:ARG:HD2	2.35	0.42
2:I:580:MET:O	2:I:903:SER:N	2.50	0.42
3:J:681:ARG:C	3:J:683:ILE:H	2.22	0.42
3:D:31:THR:OG1	3:D:32:ILE:N	2.52	0.42
2:C:100:LEU:HD12	2:C:372:LEU:HD22	2.01	0.42
2:C:994:ILE:HG22	2:C:995:MET:H	1.84	0.42
3:J:1048:PRO:HD3	3:J:1075:HIS:CG	2.55	0.42
3:D:731:LEU:HD22	3:D:780:LYS:O	2.19	0.42
3:D:1331:ASP:HA	3:D:1332:PRO:HD3	1.90	0.42
2:I:1068:GLN:NE2	2:I:1072:LYS:HD2	2.35	0.42
4:E:61:VAL:O	4:E:65:MET:HG2	2.20	0.42
3:D:401:TYR:HB3	3:D:427:VAL:CG2	2.50	0.42
5:L:154:ALA:O	5:L:158:LYS:HB2	2.20	0.42
3:J:26:VAL:HG13	3:J:42:ASP:O	2.19	0.42
3:D:1003:VAL:HG21	3:D:1041:MET:HB3	2.01	0.42
1:H:132:LEU:HD12	1:H:136:GLY:HA3	2.02	0.42
3:D:1120:VAL:HG12	3:D:1135:ARG:HH12	1.84	0.42
1:H:64:GLU:HG3	1:H:165:ILE:HG21	2.02	0.42
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.34	0.41
6:N:12:LEU:O	6:N:15:TYR:HB2	2.19	0.41
3:D:551:ASN:O	3:D:555:LYS:HG3	2.20	0.41
3:D:654:LYS:NZ	3:D:674:ARG:HH21	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:177:ALA:HB2	3:J:393:ILE:HD11	2.01	0.41
3:D:585:GLY:CA	3:D:590:PRO:HG3	2.50	0.41
3:J:758:GLU:HG3	4:K:20:THR:HG21	2.02	0.41
1:A:205:VAL:HG11	1:A:213:GLN:HE22	1.84	0.41
2:I:992:MET:HG2	2:I:993:PHE:N	2.35	0.41
3:D:102:ILE:HD11	3:D:587:ARG:HG3	2.02	0.41
3:J:121:THR:O	3:J:124:GLU:HB3	2.21	0.41
2:I:770:GLU:HG2	5:L:366:SER:HA	2.00	0.41
5:F:276:PRO:O	5:F:280:VAL:HG23	2.19	0.41
3:J:1087:ARG:HH22	3:J:1236:LEU:H	1.67	0.41
5:F:292:GLN:O	5:F:295:GLN:HB3	2.20	0.41
1:A:30:ARG:HD3	1:A:191:ASP:OD2	2.20	0.41
3:D:237:ARG:HG2	3:D:240:GLU:HB2	2.02	0.41
3:D:431:ILE:HG13	3:D:432:TYR:N	2.35	0.41
6:M:79:ARG:NH1	6:M:114:ALA:HB2	2.34	0.41
2:C:1107:ASN:HA	2:C:1108:PRO:HD3	1.86	0.41
1:H:51:THR:O	1:H:145:ASP:O	2.39	0.41
3:D:750:PRO:HG2	3:D:756:GLN:NE2	2.35	0.41
2:C:263:ASP:HB3	2:C:266:ARG:HB2	2.02	0.41
1:B:176:ARG:HB3	1:B:200:TRP:CE3	2.55	0.41
2:I:258:PHE:HA	2:I:298:PHE:CE2	2.55	0.41
3:D:29:PRO:HB3	3:D:548:ILE:HB	2.02	0.41
2:I:279:GLU:HG2	2:I:279:GLU:H	1.69	0.41
7:O:5:DA:H1'	7:O:6:DC:H5''	2.02	0.41
3:J:659:LYS:HZ2	3:J:662:GLU:HG2	1.86	0.41
3:J:102:ILE:HB	3:J:579:ASP:CG	2.40	0.41
2:I:954:SER:HA	2:I:955:PRO:HD3	1.88	0.41
2:I:90:TYR:HB3	2:I:128:ILE:HB	2.02	0.41
1:G:88:ARG:HD3	1:G:121:GLU:OE1	2.20	0.41
3:D:947:ILE:HG22	3:D:1019:PRO:HB3	2.02	0.41
1:A:37:GLY:N	1:A:195:LEU:HD11	2.35	0.41
1:H:33:GLY:O	1:H:195:LEU:HD22	2.19	0.41
3:J:625:TYR:CE1	3:J:751:LEU:HD11	2.56	0.41
2:I:695:LEU:HD21	2:I:832:LYS:HD3	2.01	0.41
3:J:1084:THR:O	3:J:1088:THR:HG23	2.20	0.41
2:C:161:SER:C	2:C:162:ILE:HD12	2.40	0.41
1:H:85:LEU:HD12	1:H:124:ASN:HB3	2.01	0.41
1:G:43:ILE:H	1:G:43:ILE:HG13	1.58	0.41
6:M:155:PHE:O	6:M:159:TRP:HB2	2.20	0.41
2:I:458:TYR:HB2	2:I:538:GLN:HB3	2.03	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:PRO:HB3	3:D:46:ASP:HA	2.02	0.41
2:C:729:LEU:HD13	2:C:730:SER:O	2.20	0.41
3:D:101:HIS:ND1	3:D:103:TRP:HB2	2.35	0.41
3:J:500:ARG:HA	3:J:503:LEU:HD12	2.02	0.41
5:L:401:VAL:O	5:L:404:TYR:HB3	2.20	0.41
7:O:3:DT:H5'	7:O:3:DT:C6	2.53	0.41
3:D:1188:VAL:HG12	3:D:1189:ARG:N	2.35	0.41
6:M:121:LEU:HA	6:M:122:PRO:HD3	1.88	0.41
2:C:396:ASP:HB2	2:C:406:HIS:ND1	2.35	0.41
2:I:1050:GLN:O	2:I:1054:THR:N	2.53	0.41
2:I:247:PRO:HA	2:I:248:PRO:HD3	1.74	0.41
3:D:704:ARG:HB3	3:D:736:PHE:HB3	2.01	0.41
3:J:9:ARG:HA	3:J:1456:LYS:HA	2.02	0.41
5:F:412:ILE:HA	5:F:415:ILE:HD12	2.02	0.41
3:D:758:GLU:O	3:D:762:GLN:HG2	2.20	0.41
2:C:1044:GLY:HA3	4:E:17:TYR:HE1	1.82	0.41
3:D:103:TRP:HH2	3:D:1447:LEU:HD22	1.86	0.41
3:D:907:GLU:O	3:D:911:LEU:HG	2.21	0.41
3:D:272:LEU:HD12	3:D:272:LEU:HA	1.91	0.41
4:K:61:VAL:O	4:K:65:MET:HG2	2.20	0.41
3:J:925:GLU:H	3:J:925:GLU:HG3	1.60	0.41
2:I:847:GLY:HA2	3:J:741:ASP:HA	2.02	0.41
3:D:1290:LEU:O	3:D:1305:LEU:HB2	2.20	0.41
3:J:1033:GLN:O	3:J:1036:ARG:HB3	2.20	0.41
2:C:27:LYS:HA	2:C:30:LEU:HD22	2.01	0.41
1:G:211:LEU:O	1:G:215:VAL:HG23	2.20	0.41
2:C:66:LEU:HD11	2:C:372:LEU:HD23	2.02	0.41
5:F:235:LEU:O	5:F:239:VAL:HG23	2.21	0.41
3:D:758:GLU:HG2	3:D:1476:THR:HG21	2.02	0.41
1:G:99:LEU:N	1:G:142:VAL:O	2.51	0.41
1:H:54:THR:O	1:H:167:VAL:HB	2.20	0.41
3:D:835:SER:OG	3:D:838:ARG:HG3	2.19	0.41
1:B:76:VAL:HA	1:B:79:ILE:HD12	2.03	0.41
3:D:62:LYS:HG3	3:D:63:TYR:N	2.36	0.41
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	2.01	0.41
5:L:118:ALA:HB3	5:L:244:TYR:HB3	2.03	0.41
3:D:1290:LEU:HB2	3:D:1307:LYS:HD2	2.03	0.41
1:H:107:LYS:HG3	1:H:108:GLU:N	2.34	0.41
1:A:66:SER:O	1:A:75:VAL:HG23	2.20	0.41
3:J:128:TYR:O	3:J:572:ARG:NH1	2.53	0.41
3:D:892:ASP:HB2	3:D:894:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:VAL:O	2:C:443:THR:HG22	2.19	0.41
3:D:623:VAL:HG21	3:D:748:HIS:CD2	2.56	0.41
2:C:146:VAL:HG12	2:C:162:ILE:HG13	2.02	0.41
1:B:57:TYR:CD1	1:B:161:ARG:HG2	2.55	0.41
3:J:749:VAL:HA	3:J:750:PRO:HD2	1.93	0.41
2:I:469:THR:HA	2:I:470:PRO:HD3	1.83	0.41
3:D:409:VAL:HG22	3:D:421:LEU:O	2.21	0.41
3:D:224:ARG:HB3	3:D:251:PHE:CE1	2.55	0.41
3:D:1459:LEU:HD21	3:D:1468:LEU:HG	2.03	0.41
3:J:471:GLU:O	3:J:474:GLU:HB3	2.19	0.41
2:C:285:LEU:CD1	2:C:301:GLU:HB3	2.49	0.41
3:D:606:ILE:HG22	3:D:613:ARG:HB2	2.01	0.41
3:D:711:LEU:HG	3:D:778:LEU:HD22	2.02	0.41
3:J:127:LEU:HD23	3:J:458:ALA:HA	2.02	0.41
2:I:1065:ALA:HA	2:I:1068:GLN:HB3	2.01	0.41
3:D:274:GLN:HG3	3:D:279:VAL:HG21	2.01	0.41
3:J:1118:ILE:HG13	3:J:1118:ILE:O	2.20	0.41
2:C:86:LYS:HE2	2:C:814:GLU:N	2.36	0.41
1:G:221:HIS:HA	1:G:224:TYR:CD1	2.56	0.41
6:N:126:ARG:HB2	6:N:126:ARG:HH11	1.85	0.41
6:N:116:GLU:HG3	6:N:121:LEU:HD22	2.01	0.41
6:N:125:ASP:HA	6:N:128:ALA:HB3	2.02	0.41
2:I:487:THR:HG22	2:I:488:ALA:H	1.86	0.41
1:A:74:ASP:O	1:A:78:ILE:HG13	2.21	0.41
5:L:413:ARG:HE	8:S:21:DT:H2'	1.86	0.41
2:I:679:PHE:N	2:I:683:ASN:HD21	2.18	0.41
2:C:892:LEU:HD13	2:C:989:VAL:O	2.21	0.41
1:B:34:VAL:HG11	2:C:978:ARG:HB3	2.03	0.41
2:C:14:PRO:HB3	2:C:586:ARG:NH2	2.30	0.41
3:D:1462:LEU:HG	3:D:1462:LEU:H	1.66	0.41
2:C:267:TYR:HE2	2:C:269:LEU:HD12	1.86	0.41
2:C:275:TYR:O	2:C:278:GLU:HB3	2.21	0.41
1:G:215:VAL:HG21	1:H:225:PHE:HD1	1.86	0.41
3:D:860:LEU:CD1	3:D:860:LEU:H	2.31	0.41
2:I:118:LEU:HD12	2:I:119:PRO:HD2	2.02	0.41
2:I:994:ILE:HG22	2:I:995:MET:H	1.86	0.41
3:D:632:VAL:N	3:D:726:ILE:O	2.51	0.41
2:I:202:TYR:HD1	2:I:206:THR:HG21	1.84	0.41
3:J:602:SER:O	3:J:606:ILE:HG13	2.20	0.41
1:B:213:GLN:O	1:B:217:ILE:HG13	2.21	0.41
2:I:610:ARG:HG2	2:I:610:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:659:LYS:HZ2	3:D:662:GLU:HG2	1.86	0.41
2:C:862:PRO:HG3	2:C:975:TYR:HE2	1.85	0.41
3:J:1331:ASP:HA	3:J:1332:PRO:HD3	1.87	0.41
2:I:539:VAL:HG21	3:J:1067:VAL:HG11	2.01	0.41
4:K:6:ILE:HD11	4:K:10:PHE:CZ	2.56	0.41
2:I:100:LEU:CB	2:I:369:PRO:HD3	2.50	0.41
2:I:100:LEU:HD12	2:I:372:LEU:HD22	2.03	0.41
2:I:100:LEU:HB3	2:I:369:PRO:HD3	2.03	0.41
3:J:1122:LEU:HA	3:J:1135:ARG:HD3	2.03	0.41
3:J:783:ARG:NH1	3:J:1029:ARG:HA	2.36	0.41
2:C:492:ASP:OD2	2:C:518:ARG:HG2	2.20	0.41
2:C:432:ARG:NH1	2:C:518:ARG:HH21	2.13	0.41
6:M:75:LEU:HG	6:M:159:TRP:CZ3	2.55	0.41
2:C:99:GLN:HB2	2:C:101:ILE:HD11	2.01	0.41
1:A:40:LEU:O	1:A:44:LEU:HB2	2.20	0.41
2:I:285:LEU:CD1	2:I:301:GLU:HB3	2.48	0.41
3:D:233:LYS:HE3	3:D:235:ALA:H	1.84	0.41
3:J:103:TRP:O	3:J:107:ASP:HB2	2.21	0.41
2:C:949:LYS:NZ	3:D:859:ASP:OD2	2.54	0.41
6:M:140:VAL:HG11	6:M:154:LEU:HD22	2.03	0.41
1:H:80:LEU:HB3	3:J:867:ARG:HH11	1.86	0.41
3:J:156:GLU:O	3:J:160:GLU:HB2	2.21	0.41
3:J:954:ALA:HB2	3:J:1020:LEU:HD22	2.02	0.41
3:J:1231:GLU:HB3	3:J:1232:PRO:HD3	2.03	0.41
2:C:1026:GLN:HB2	2:C:1026:GLN:HE21	1.64	0.41
2:I:1009:SER:HB3	3:J:651:GLU:O	2.19	0.41
2:C:232:GLU:H	2:C:232:GLU:CD	2.24	0.41
3:D:1365:ASP:O	3:D:1369:GLU:HG3	2.20	0.41
2:I:670:GLN:HE22	2:I:699:PHE:HA	1.85	0.41
2:I:80:GLN:HE22	2:I:122:THR:HG22	1.85	0.41
4:K:41:GLU:O	4:K:45:ARG:HG2	2.20	0.41
3:J:1188:VAL:HG12	3:J:1189:ARG:N	2.36	0.41
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.36	0.41
3:D:348:ALA:HB1	3:D:349:PRO:HD2	2.02	0.41
2:C:877:PRO:HD3	3:D:949:ILE:CD1	2.50	0.41
2:C:144:PRO:HG2	2:C:273:GLY:N	2.35	0.41
2:I:675:ALA:HA	2:I:989:VAL:HG12	2.02	0.41
2:I:238:LEU:HD23	2:I:241:LEU:HD12	2.02	0.41
1:B:51:THR:O	1:B:145:ASP:O	2.38	0.41
3:J:1462:LEU:O	3:J:1466:VAL:HG23	2.20	0.41
2:I:1041:GLU:OE1	3:J:1462:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1103:HIS:HB2	3:J:1462:LEU:CD1	2.48	0.41
3:D:317:MET:HG2	3:D:318:THR:N	2.35	0.41
3:D:701:LEU:O	3:D:747:VAL:HA	2.21	0.41
3:J:632:VAL:O	3:J:727:GLN:HA	2.21	0.41
5:F:381:ALA:O	5:F:385:LYS:HG2	2.21	0.41
3:D:1275:SER:HB2	3:D:1325:LEU:HD21	2.03	0.41
3:J:672:ALA:O	3:J:676:MET:HB2	2.21	0.41
1:B:173:PRO:HB3	1:B:204:SER:HB2	2.01	0.41
1:A:29:GLU:HB3	1:A:32:PHE:CD1	2.56	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
6:M:97:LEU:HA	6:M:97:LEU:HD23	1.87	0.41
2:C:387:SER:HB2	2:C:388:ARG:HD2	2.02	0.41
2:C:254:LEU:HD12	2:C:298:PHE:HE1	1.86	0.41
3:J:1153:VAL:HB	3:J:1160:LEU:HB2	2.03	0.41
1:A:93:LYS:HB3	1:A:93:LYS:NZ	2.35	0.41
2:I:232:GLU:H	2:I:232:GLU:CD	2.24	0.41
3:D:1279:GLY:H	3:D:1319:VAL:HG23	1.86	0.41
2:C:948:GLU:OE2	2:C:962:GLN:NE2	2.50	0.41
5:F:116:ASP:O	5:F:120:LYS:HG2	2.21	0.41
1:A:158:ILE:HG22	1:A:160:ASP:N	2.31	0.41
1:A:53:VAL:CG2	1:A:54:THR:H	2.27	0.41
1:A:54:THR:HG23	1:A:143:ARG:O	2.19	0.41
2:C:874:LEU:HD23	2:C:874:LEU:HA	1.92	0.41
3:J:1175:ILE:O	3:J:1179:GLU:HG3	2.21	0.41
3:D:841:PHE:CD1	3:D:858:LEU:HD22	2.55	0.41
3:D:841:PHE:CE2	3:D:858:LEU:HD13	2.55	0.41
3:D:410:THR:HB	3:D:413:ASP:OD2	2.21	0.41
2:C:1091:GLU:OE2	3:D:606:ILE:HG21	2.21	0.41
5:F:353:LEU:HA	5:F:354:PRO:HD3	1.94	0.41
3:J:835:SER:OG	3:J:838:ARG:HG3	2.21	0.41
3:D:1290:LEU:HD12	3:D:1307:LYS:HG3	2.02	0.41
2:I:699:PHE:HB3	2:I:700:TYR:HD1	1.85	0.41
3:J:1014:ASN:C	3:J:1016:PRO:HD3	2.41	0.41
2:C:758:ARG:HE	2:C:788:THR:HB	1.86	0.41
2:I:1093:GLN:O	3:J:21:TRP:HZ3	2.04	0.41
4:E:84:ARG:HA	4:E:87:LYS:HB3	2.03	0.41
5:F:118:ALA:HB3	5:F:244:TYR:HB3	2.03	0.41
2:I:91:GLN:HG3	2:I:117:HIS:HB3	2.02	0.40
6:N:155:PHE:O	6:N:159:TRP:HB2	2.21	0.40
3:D:264:LEU:HD21	3:D:339:TRP:CG	2.56	0.40
3:J:650:LEU:HD12	3:J:688:TRP:CZ3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:12:LEU:O	6:M:15:TYR:HB2	2.21	0.40
3:D:684:LYS:HG2	3:D:685:ASP:N	2.36	0.40
3:J:171:LEU:HD23	3:J:172:PRO:O	2.21	0.40
2:C:456:ALA:HB1	2:C:538:GLN:O	2.21	0.40
2:C:535:SER:H	2:C:538:GLN:HE21	1.69	0.40
3:J:1311:LEU:HA	3:J:1326:THR:HA	2.02	0.40
3:D:760:ARG:HH21	4:E:61:VAL:HG12	1.87	0.40
2:C:86:LYS:HE2	2:C:813:VAL:HG23	2.02	0.40
5:F:210:VAL:HG11	5:F:232:ASN:HA	2.03	0.40
5:F:153:THR:HG22	5:F:154:ALA:H	1.86	0.40
6:N:93:THR:O	6:N:97:LEU:HG	2.21	0.40
2:C:140:ILE:HG23	2:C:412:ALA:HA	2.03	0.40
3:D:147:VAL:HG23	3:D:151:GLN:CD	2.42	0.40
1:A:190:THR:OG1	1:A:191:ASP:N	2.52	0.40
3:J:659:LYS:O	3:J:659:LYS:HD3	2.20	0.40
3:D:181:ASP:HB3	3:D:357:GLU:HG2	2.03	0.40
3:D:631:ILE:HG13	3:D:740:PHE:HD2	1.86	0.40
3:D:1404:ASN:O	3:D:1408:ILE:HG12	2.21	0.40
5:F:392:ASP:OD2	5:F:394:ARG:HB2	2.21	0.40
3:D:1151:ARG:HA	3:D:1162:GLU:HG3	2.03	0.40
3:J:1076:GLY:HA2	3:J:1079:LYS:HB3	2.03	0.40
3:D:722:GLU:H	3:D:722:GLU:HG2	1.52	0.40
3:D:266:GLU:CD	3:D:315:ARG:H	2.25	0.40
5:L:167:ASP:O	5:L:171:VAL:HB	2.21	0.40
5:F:302:SER:H	5:F:305:GLU:HG2	1.85	0.40
3:D:633:VAL:HG13	3:D:635:PRO:HD3	2.03	0.40
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.54	0.40
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.21	0.40
1:G:161:ARG:HG2	1:G:162:ILE:H	1.86	0.40
2:I:474:VAL:HG11	2:I:529:VAL:HG22	2.03	0.40
6:M:80:MET:HA	6:M:81:PRO:HD3	1.88	0.40
3:D:1318:TYR:HB2	3:J:1157:GLY:O	2.22	0.40
2:I:877:PRO:HD3	3:J:949:ILE:CD1	2.52	0.40
2:I:690:ILE:HA	2:I:869:VAL:HA	2.03	0.40
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.95	0.40
3:J:8:VAL:HG12	3:J:1434:TRP:HZ2	1.84	0.40
5:L:252:THR:HA	7:R:29:DC:H5	1.86	0.40
2:I:718:GLY:HA2	2:I:719:PRO:HD3	1.84	0.40
3:D:918:ALA:O	3:D:922:LEU:HB2	2.20	0.40
3:J:1290:LEU:O	3:J:1305:LEU:HB2	2.21	0.40
1:B:49:PRO:HD2	1:B:213:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:94:ASP:HA	5:L:95:PRO:HD2	1.87	0.40
2:C:564:MET:SD	2:C:846:LYS:HG2	2.61	0.40
2:I:134:ARG:HH12	2:I:392:SER:C	2.25	0.40
3:D:1076:GLY:HA2	3:D:1079:LYS:HB3	2.03	0.40
2:I:502:PRO:HD2	2:I:513:VAL:HG13	2.04	0.40
3:J:1189:ARG:NH2	3:J:1204:CYS:SG	2.94	0.40
1:G:87:VAL:CG1	1:G:144:VAL:HG11	2.51	0.40
1:B:57:TYR:CG	1:B:58:ILE:N	2.89	0.40
6:N:11:VAL:HG12	6:N:13:PRO:HD3	2.03	0.40
2:C:576:ALA:HB1	2:C:580:MET:HE3	2.03	0.40
3:J:361:VAL:CG2	3:J:367:ILE:HD11	2.51	0.40
3:J:1048:PRO:HD3	3:J:1075:HIS:CB	2.48	0.40
1:G:161:ARG:HB3	1:G:161:ARG:NH1	2.36	0.40
2:C:86:LYS:CE	2:C:814:GLU:H	2.35	0.40
3:J:953:ASP:O	3:J:1018:ASN:ND2	2.37	0.40
3:D:171:LEU:HA	3:D:172:PRO:HD2	1.95	0.40
2:I:856:GLU:HG3	2:I:856:GLU:H	1.69	0.40
3:J:578:VAL:O	3:J:582:ILE:HG12	2.21	0.40
2:I:235:MET:HE2	2:I:257:LEU:HD12	2.03	0.40
5:F:215:LYS:HA	5:F:224:PHE:HE2	1.85	0.40
3:J:991:GLN:HA	3:J:994:GLN:HG2	2.04	0.40
3:J:654:LYS:NZ	3:J:674:ARG:HH21	2.20	0.40
3:D:39:PRO:CB	3:D:46:ASP:HA	2.52	0.40
3:D:514:LEU:HD21	3:D:517:VAL:HA	2.03	0.40
1:A:161:ARG:HG2	1:A:162:ILE:H	1.86	0.40
2:C:713:ARG:CZ	2:C:715:THR:HG22	2.52	0.40
2:I:408:ARG:NH1	2:I:408:ARG:HB3	2.36	0.40
2:I:878:SER:HA	3:J:1034:GLN:OE1	2.20	0.40
2:I:643:VAL:HG12	2:I:647:GLN:OE1	2.22	0.40
3:J:31:THR:HG21	5:L:272:THR:HG22	2.04	0.40
3:D:1363:LEU:HD11	3:D:1368:ILE:HD11	2.04	0.40
7:R:10:DA:H1'	7:R:11:DG:H5''	2.02	0.40
5:F:164:GLU:OE1	5:F:165:LYS:HG2	2.21	0.40
3:D:625:TYR:CE1	3:D:751:LEU:HD11	2.56	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	225/314 (72%)	198 (88%)	26 (12%)	1 (0%)	39	79
1	B	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	39	79
1	G	225/314 (72%)	200 (89%)	24 (11%)	1 (0%)	39	79
1	H	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	39	79
2	C	1108/1119 (99%)	980 (88%)	119 (11%)	9 (1%)	24	69
2	I	1108/1119 (99%)	977 (88%)	123 (11%)	8 (1%)	26	71
3	D	1486/1524 (98%)	1333 (90%)	143 (10%)	10 (1%)	26	71
3	J	1361/1524 (89%)	1227 (90%)	126 (9%)	8 (1%)	30	73
4	E	91/99 (92%)	79 (87%)	12 (13%)	0	100	100
4	K	91/99 (92%)	80 (88%)	11 (12%)	0	100	100
5	F	343/347 (99%)	309 (90%)	32 (9%)	2 (1%)	30	73
5	L	343/347 (99%)	309 (90%)	31 (9%)	3 (1%)	21	67
6	M	160/164 (98%)	142 (89%)	18 (11%)	0	100	100
6	N	160/164 (98%)	141 (88%)	19 (12%)	0	100	100
All	All	7151/7762 (92%)	6373 (89%)	734 (10%)	44 (1%)	30	73

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	683	ILE
3	D	1128	VAL
1	G	53	VAL
3	J	681	ARG
3	J	683	ILE
3	J	1128	VAL
2	C	164	PRO
2	C	608	GLY

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Mol	Chain	Res	Type
2	C	852	ILE
3	D	666	PHE
3	D	681	ARG
2	I	164	PRO
2	I	608	GLY
2	I	851	LYS
2	I	852	ILE
3	J	682	ASP
1	B	118	ALA
2	C	607	ASP
2	C	851	LYS
3	D	230	TRP
3	D	682	ASP
1	H	118	ALA
2	I	607	ASP
2	C	1106	ASP
3	D	680	GLN
5	F	224	PHE
2	I	1106	ASP
5	F	154	ALA
3	J	680	GLN
3	J	685	ASP
5	L	224	PHE
3	D	1130	ARG
3	D	1221	VAL
3	J	1221	VAL
5	L	108	LEU
5	L	154	ALA
3	D	667	ALA
2	C	870	ILE
2	C	1016	ILE
2	I	870	ILE
2	I	1016	ILE
2	C	643	VAL
3	J	667	ALA

### 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	194/270 (72%)	184 (95%)	10 (5%)	29	68
1	B	194/270 (72%)	176 (91%)	18 (9%)	11	46
1	G	194/270 (72%)	184 (95%)	10 (5%)	29	68
1	H	194/270 (72%)	176 (91%)	18 (9%)	11	46
2	C	931/936 (100%)	864 (93%)	67 (7%)	18	57
2	I	931/936 (100%)	863 (93%)	68 (7%)	17	57
3	D	1252/1281 (98%)	1139 (91%)	113 (9%)	12	47
3	J	1150/1281 (90%)	1062 (92%)	88 (8%)	16	55
4	E	83/88 (94%)	81 (98%)	2 (2%)	57	82
4	K	83/88 (94%)	79 (95%)	4 (5%)	31	69
5	F	296/299 (99%)	279 (94%)	17 (6%)	25	65
5	L	296/299 (99%)	275 (93%)	21 (7%)	18	58
6	M	131/133 (98%)	127 (97%)	4 (3%)	47	78
6	N	131/133 (98%)	127 (97%)	4 (3%)	47	78
All	All	6060/6554 (92%)	5616 (93%)	444 (7%)	17	57

All (444) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	43	ILE
1	A	51	THR
1	A	54	THR
1	A	80	LEU
1	A	87	VAL
1	A	98	THR
1	A	113	ASP
1	A	195	LEU
1	A	208	LEU
1	B	7	LYS
1	B	20	TYR
1	B	30	ARG
1	B	51	THR
1	B	54	THR
1	B	58	ILE
1	B	62	LEU

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Mol	Chain	Res	Type
1	B	75	VAL
1	B	100	ILE
1	B	104	GLU
1	B	113	ASP
1	B	114	PHE
1	B	115	THR
1	B	143	ARG
1	B	145	ASP
1	B	177	VAL
1	B	184	THR
1	B	232	LEU
2	C	20	GLU
2	C	30	LEU
2	C	70	GLU
2	C	80	GLN
2	C	101	ILE
2	C	104	ASP
2	C	109	LYS
2	C	120	LEU
2	C	140	ILE
2	C	141	HIS
2	C	157	ARG
2	C	173	ASP
2	C	174	LEU
2	C	176	VAL
2	C	195	LEU
2	C	203	ASP
2	C	207	LEU
2	C	208	VAL
2	C	211	LEU
2	C	217	LEU
2	C	219	GLN
2	C	242	LEU
2	C	261	LEU
2	C	297	GLU
2	C	304	LEU
2	C	308	ARG
2	C	339	LEU
2	C	365	ASP
2	C	368	THR
2	C	374	ASN
2	C	421	GLU

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Mol	Chain	Res	Type
2	C	427	VAL
2	C	504	GLU
2	C	533	ASP
2	C	551	GLU
2	C	571	LEU
2	C	580	MET
2	C	610	ARG
2	C	616	GLU
2	C	643	VAL
2	C	680	ASP
2	C	685	GLU
2	C	695	LEU
2	C	717	LEU
2	C	729	LEU
2	C	738	ASP
2	C	748	GLU
2	C	784	ASP
2	C	788	THR
2	C	790	LEU
2	C	815	LEU
2	C	852	ILE
2	C	857	ASP
2	C	867	VAL
2	C	869	VAL
2	C	876	VAL
2	C	934	PHE
2	C	968	ASP
2	C	972	VAL
2	C	1000	MET
2	C	1026	GLN
2	C	1053	LEU
2	C	1060	ILE
2	C	1061	GLU
2	C	1104	GLU
2	C	1107	ASN
2	C	1113	GLU
3	D	2	LYS
3	D	4	GLU
3	D	16	GLU
3	D	25	GLU
3	D	49	ILE
3	D	58	CYS

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Mol	Chain	Res	Type
3	D	68	PHE
3	D	111	LYS
3	D	121	THR
3	D	155	ASP
3	D	166	GLN
3	D	168	THR
3	D	184	GLU
3	D	214	ASP
3	D	237	ARG
3	D	251	PHE
3	D	266	GLU
3	D	273	ARG
3	D	281	ARG
3	D	310	LEU
3	D	313	LEU
3	D	316	HIS
3	D	318	THR
3	D	333	LEU
3	D	334	THR
3	D	335	LEU
3	D	347	VAL
3	D	385	VAL
3	D	394	LEU
3	D	397	LYS
3	D	400	VAL
3	D	405	ASP
3	D	406	ASP
3	D	409	VAL
3	D	411	THR
3	D	413	ASP
3	D	414	ARG
3	D	419	ASP
3	D	430	GLU
3	D	434	ARG
3	D	437	VAL
3	D	456	MET
3	D	464	LEU
3	D	480	GLU
3	D	535	PHE
3	D	560	GLN
3	D	574	LEU
3	D	576	GLU

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Mol	Chain	Res	Type
3	D	618	LEU
3	D	639	LEU
3	D	640	HIS
3	D	658	LEU
3	D	660	LYS
3	D	688	TRP
3	D	694	VAL
3	D	701	LEU
3	D	708	LEU
3	D	709	HIS
3	D	722	GLU
3	D	732	VAL
3	D	739	ASP
3	D	740	PHE
3	D	762	GLN
3	D	776	GLU
3	D	780	LYS
3	D	792	ILE
3	D	817	GLU
3	D	833	GLU
3	D	834	THR
3	D	861	GLN
3	D	863	VAL
3	D	873	LEU
3	D	879	ARG
3	D	897	GLN
3	D	901	GLN
3	D	903	ASP
3	D	908	LYS
3	D	914	LEU
3	D	956	ILE
3	D	958	GLU
3	D	959	GLU
3	D	964	LEU
3	D	971	LEU
3	D	976	GLN
3	D	987	GLU
3	D	1053	PHE
3	D	1100	ASP
3	D	1136	LYS
3	D	1137	ARG
3	D	1158	ARG

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Mol	Chain	Res	Type
3	D	1170	ASP
3	D	1229	ILE
3	D	1267	ARG
3	D	1269	LYS
3	D	1285	GLU
3	D	1290	LEU
3	D	1308	ASP
3	D	1310	ARG
3	D	1311	LEU
3	D	1335	LEU
3	D	1342	GLU
3	D	1371	VAL
3	D	1376	LEU
3	D	1443	THR
3	D	1448	THR
3	D	1456	LYS
3	D	1462	LEU
3	D	1463	LYS
3	D	1465	ASN
3	D	1472	ILE
3	D	1496	GLU
3	D	1497	GLU
3	D	1499	ARG
4	E	51	LEU
4	E	56	ASP
5	F	100	LEU
5	F	125	MET
5	F	158	LYS
5	F	172	GLU
5	F	175	ASP
5	F	187	ARG
5	F	196	GLU
5	F	224	PHE
5	F	244	TYR
5	F	268	ASP
5	F	279	MET
5	F	282	THR
5	F	293	LEU
5	F	294	GLN
5	F	325	ILE
5	F	328	GLU
5	F	371	LYS

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Mol	Chain	Res	Type
1	G	20	TYR
1	G	51	THR
1	G	54	THR
1	G	80	LEU
1	G	87	VAL
1	G	98	THR
1	G	113	ASP
1	G	195	LEU
1	G	208	LEU
1	G	213	GLN
1	H	7	LYS
1	H	20	TYR
1	H	30	ARG
1	H	51	THR
1	H	54	THR
1	H	58	ILE
1	H	62	LEU
1	H	75	VAL
1	H	100	ILE
1	H	104	GLU
1	H	113	ASP
1	H	114	PHE
1	H	115	THR
1	H	143	ARG
1	H	145	ASP
1	H	177	VAL
1	H	184	THR
1	H	232	LEU
2	I	20	GLU
2	I	30	LEU
2	I	70	GLU
2	I	80	GLN
2	I	101	ILE
2	I	104	ASP
2	I	109	LYS
2	I	120	LEU
2	I	140	ILE
2	I	141	HIS
2	I	157	ARG
2	I	173	ASP
2	I	176	VAL
2	I	195	LEU

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Mol	Chain	Res	Type
2	I	207	LEU
2	I	208	VAL
2	I	211	LEU
2	I	217	LEU
2	I	219	GLN
2	I	242	LEU
2	I	246	ASP
2	I	261	LEU
2	I	297	GLU
2	I	304	LEU
2	I	308	ARG
2	I	336	VAL
2	I	339	LEU
2	I	365	ASP
2	I	368	THR
2	I	374	ASN
2	I	421	GLU
2	I	427	VAL
2	I	504	GLU
2	I	533	ASP
2	I	551	GLU
2	I	571	LEU
2	I	580	MET
2	I	610	ARG
2	I	616	GLU
2	I	643	VAL
2	I	680	ASP
2	I	685	GLU
2	I	695	LEU
2	I	717	LEU
2	I	729	LEU
2	I	738	ASP
2	I	748	GLU
2	I	784	ASP
2	I	788	THR
2	I	790	LEU
2	I	815	LEU
2	I	852	ILE
2	I	857	ASP
2	I	867	VAL
2	I	869	VAL
2	I	876	VAL

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Mol	Chain	Res	Type
2	I	934	PHE
2	I	968	ASP
2	I	969	LEU
2	I	972	VAL
2	I	1000	MET
2	I	1026	GLN
2	I	1053	LEU
2	I	1060	ILE
2	I	1061	GLU
2	I	1104	GLU
2	I	1107	ASN
2	I	1113	GLU
3	J	2	LYS
3	J	16	GLU
3	J	25	GLU
3	J	58	CYS
3	J	68	PHE
3	J	76	CYS
3	J	121	THR
3	J	200	ASP
3	J	340	THR
3	J	344	ASP
3	J	347	VAL
3	J	371	ILE
3	J	374	GLU
3	J	405	ASP
3	J	410	THR
3	J	414	ARG
3	J	444	VAL
3	J	456	MET
3	J	464	LEU
3	J	480	GLU
3	J	535	PHE
3	J	560	GLN
3	J	574	LEU
3	J	576	GLU
3	J	618	LEU
3	J	639	LEU
3	J	640	HIS
3	J	658	LEU
3	J	660	LYS
3	J	688	TRP

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Mol	Chain	Res	Type
3	J	694	VAL
3	J	701	LEU
3	J	708	LEU
3	J	709	HIS
3	J	722	GLU
3	J	732	VAL
3	J	739	ASP
3	J	740	PHE
3	J	748	HIS
3	J	762	GLN
3	J	776	GLU
3	J	780	LYS
3	J	792	ILE
3	J	817	GLU
3	J	833	GLU
3	J	861	GLN
3	J	873	LEU
3	J	876	SER
3	J	879	ARG
3	J	897	GLN
3	J	901	GLN
3	J	903	ASP
3	J	908	LYS
3	J	914	LEU
3	J	956	ILE
3	J	958	GLU
3	J	959	GLU
3	J	964	LEU
3	J	971	LEU
3	J	976	GLN
3	J	1053	PHE
3	J	1083	ASP
3	J	1100	ASP
3	J	1136	LYS
3	J	1137	ARG
3	J	1158	ARG
3	J	1229	ILE
3	J	1267	ARG
3	J	1269	LYS
3	J	1285	GLU
3	J	1290	LEU
3	J	1308	ASP

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Mol	Chain	Res	Type
3	J	1310	ARG
3	J	1311	LEU
3	J	1335	LEU
3	J	1342	GLU
3	J	1371	VAL
3	J	1376	LEU
3	J	1443	THR
3	J	1448	THR
3	J	1456	LYS
3	J	1462	LEU
3	J	1463	LYS
3	J	1465	ASN
3	J	1472	ILE
3	J	1496	GLU
3	J	1497	GLU
3	J	1499	ARG
4	K	14	ASP
4	K	39	VAL
4	K	51	LEU
4	K	56	ASP
5	L	108	LEU
5	L	125	MET
5	L	153	THR
5	L	158	LYS
5	L	172	GLU
5	L	175	ASP
5	L	196	GLU
5	L	224	PHE
5	L	244	TYR
5	L	268	ASP
5	L	273	ILE
5	L	280	VAL
5	L	293	LEU
5	L	294	GLN
5	L	325	ILE
5	L	328	GLU
5	L	371	LYS
5	L	426	HIS
5	L	433	LEU
5	L	435	ASP
5	L	437	LEU
6	M	8	ASP

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Mol	Chain	Res	Type
6	M	33	ARG
6	M	40	PHE
6	M	159	TRP
6	N	8	ASP
6	N	33	ARG
6	N	40	PHE
6	N	159	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	163	ASN
1	A	212	ASN
1	A	213	GLN
1	B	19	HIS
1	B	38	ASN
1	B	63	HIS
1	B	213	GLN
2	C	80	GLN
2	C	374	ASN
2	C	448	ASN
2	C	538	GLN
2	C	671	ASN
2	C	765	GLN
2	C	829	GLN
2	C	881	ASN
2	C	884	GLN
2	C	899	GLN
2	C	930	GLN
2	C	1026	GLN
2	C	1050	GLN
2	C	1068	GLN
2	C	1100	GLN
2	C	1107	ASN
3	D	125	GLN
3	D	268	HIS
3	D	274	GLN
3	D	549	ASN
3	D	560	GLN
3	D	575	GLN
3	D	617	ASN

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Mol	Chain	Res	Type
3	D	640	HIS
3	D	680	GLN
3	D	727	GLN
3	D	756	GLN
3	D	762	GLN
3	D	897	GLN
3	D	917	GLN
3	D	991	GLN
3	D	1014	ASN
3	D	1359	GLN
4	E	37	ASN
4	E	59	ASN
5	F	157	GLN
5	F	190	HIS
5	F	200	GLN
5	F	232	ASN
5	F	233	GLN
5	F	263	ASN
5	F	269	GLN
5	F	294	GLN
5	F	352	ASN
5	F	417	ASN
1	G	38	ASN
1	G	163	ASN
1	G	180	GLN
1	G	212	ASN
1	G	213	GLN
1	H	19	HIS
1	H	38	ASN
1	H	63	HIS
1	H	213	GLN
2	I	80	GLN
2	I	374	ASN
2	I	448	ASN
2	I	538	GLN
2	I	671	ASN
2	I	704	HIS
2	I	765	GLN
2	I	829	GLN
2	I	843	HIS
2	I	899	GLN
2	I	930	GLN

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Mol	Chain	Res	Type
2	I	999	HIS
2	I	1019	GLN
2	I	1026	GLN
2	I	1050	GLN
2	I	1068	GLN
2	I	1107	ASN
3	J	350	HIS
3	J	507	ASN
3	J	549	ASN
3	J	560	GLN
3	J	575	GLN
3	J	617	ASN
3	J	640	HIS
3	J	680	GLN
3	J	727	GLN
3	J	756	GLN
3	J	762	GLN
3	J	897	GLN
3	J	917	GLN
3	J	991	GLN
3	J	994	GLN
3	J	1014	ASN
3	J	1353	GLN
4	K	37	ASN
5	L	157	GLN
5	L	200	GLN
5	L	263	ASN
5	L	269	GLN
5	L	294	GLN
5	L	352	ASN
6	M	85	GLN
6	M	134	HIS
6	N	37	GLN
6	N	85	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	227/314 (72%)	-0.15	0 100 100	120, 182, 228, 247	0
1	B	227/314 (72%)	-0.29	0 100 100	83, 155, 210, 239	0
1	G	227/314 (72%)	0.33	14 (6%) 24 16	127, 193, 236, 261	0
1	H	227/314 (72%)	-0.14	1 (0%) 93 90	93, 165, 210, 245	0
2	C	1112/1119 (99%)	-0.09	24 (2%) 65 54	70, 174, 245, 303	0
2	I	1112/1119 (99%)	-0.04	25 (2%) 65 54	82, 182, 250, 314	0
3	D	1490/1524 (97%)	-0.17	8 (0%) 91 88	66, 147, 206, 277	0
3	J	1367/1524 (89%)	-0.15	14 (1%) 84 77	70, 153, 211, 274	0
4	E	93/99 (93%)	-0.12	0 100 100	93, 158, 217, 254	0
4	K	93/99 (93%)	0.06	3 (3%) 51 39	106, 166, 222, 247	0
5	F	345/347 (99%)	-0.10	3 (0%) 85 80	108, 179, 259, 323	0
5	L	345/347 (99%)	-0.21	6 (1%) 73 62	119, 184, 260, 323	0
6	M	162/164 (98%)	0.15	3 (1%) 70 59	154, 223, 269, 295	0
6	N	162/164 (98%)	0.47	7 (4%) 39 29	161, 228, 271, 302	0
7	O	30/30 (100%)	0.15	3 (10%) 9 7	139, 200, 269, 277	0
7	R	30/30 (100%)	-0.35	0 100 100	156, 209, 257, 267	0
8	P	24/24 (100%)	0.23	3 (12%) 5 5	162, 229, 257, 280	0
8	S	24/24 (100%)	-0.47	0 100 100	173, 222, 252, 265	0
All	All	7297/7870 (92%)	-0.09	114 (1%) 74 64	66, 168, 242, 323	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	221	LEU	5.8
2	I	182	VAL	5.0
1	G	13	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	175	GLU	4.6
6	N	119	ARG	4.3
2	C	223	ASP	4.2
2	I	222	LEU	4.2
1	G	204	SER	4.1
2	C	190	LYS	4.1
2	I	207	LEU	4.1
3	D	1238	MET	4.0
2	I	175	GLU	4.0
2	C	176	VAL	3.9
3	J	216	LEU	3.8
1	G	14	THR	3.7
1	G	18	ASP	3.5
1	G	203	GLY	3.5
2	C	189	ARG	3.4
3	J	1499	ARG	3.4
6	N	139	GLU	3.4
2	C	194	VAL	3.4
3	J	406	ASP	3.4
6	M	159	TRP	3.3
2	I	176	VAL	3.3
1	G	87	VAL	3.3
2	C	174	LEU	3.3
2	I	219	GLN	3.2
1	G	15	THR	3.2
2	C	207	LEU	3.2
8	P	24	DA	3.2
2	I	63	GLY	3.1
1	G	22	GLU	3.1
3	D	1499	ARG	3.1
1	H	232	LEU	3.0
3	J	24	GLY	3.0
6	N	4	PHE	3.0
5	L	135	THR	3.0
2	I	648	ARG	3.0
3	J	1041	MET	2.9
2	C	203	ASP	2.9
1	G	25	LEU	2.8
2	C	221	LEU	2.8
2	I	232	GLU	2.8
3	D	224	ARG	2.8
2	I	476	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	23	PHE	2.8
2	I	805	ARG	2.7
2	I	181	VAL	2.7
5	L	177	LYS	2.7
3	J	1504	GLU	2.7
3	J	1283	ILE	2.7
6	M	163	LEU	2.7
2	C	185	LYS	2.7
2	C	222	LEU	2.7
6	N	158	ALA	2.7
2	C	182	VAL	2.6
5	F	432	LYS	2.6
2	C	298	PHE	2.6
7	O	2	DT	2.6
8	P	23	DA	2.6
6	M	164	ASN	2.6
2	C	193	LEU	2.6
7	O	3	DT	2.5
2	C	181	VAL	2.5
2	I	755	LEU	2.5
5	L	432	LYS	2.5
2	I	217	LEU	2.5
2	C	720	GLU	2.4
3	D	666	PHE	2.4
5	F	157	GLN	2.4
2	I	477	GLY	2.4
2	I	223	ASP	2.4
2	I	37	GLU	2.4
3	D	1253	THR	2.3
8	P	25	DG	2.3
2	I	174	LEU	2.3
2	C	643	VAL	2.3
6	N	120	GLY	2.3
1	G	17	GLY	2.3
1	G	205	VAL	2.3
6	N	163	LEU	2.2
2	C	235	MET	2.2
2	I	643	VAL	2.2
3	J	444	VAL	2.2
3	J	666	PHE	2.2
2	I	293	PHE	2.2
1	G	197	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	J	1489	GLN	2.2
7	O	5	DA	2.2
3	J	1289	ARG	2.2
5	F	178	LEU	2.2
5	L	170	THR	2.2
2	I	649	VAL	2.2
6	N	144	LEU	2.2
1	G	21	GLY	2.1
2	C	311	PHE	2.1
3	D	1237	THR	2.1
2	C	202	TYR	2.1
3	D	660	LYS	2.1
4	K	88	GLU	2.1
2	C	191	PHE	2.1
2	C	293	PHE	2.1
3	D	1289	ARG	2.1
2	C	722	ILE	2.1
4	K	84	ARG	2.1
3	J	421	LEU	2.1
2	I	246	ASP	2.0
5	L	178	LEU	2.0
3	J	407	VAL	2.0
2	I	250	LYS	2.0
2	I	194	VAL	2.0
3	J	805	ALA	2.0
5	L	174	VAL	2.0
4	K	37	ASN	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( $\text{\AA}^2$ )	Q<0.9
9	ZN	J	2001	1/1	0.93	0.20	-0.25	200,200,200,200	0
9	ZN	D	2001	1/1	0.97	0.13	-1.10	96,96,96,96	0
9	ZN	D	2002	1/1	0.94	0.14	-1.11	203,203,203,203	0
9	ZN	J	2002	1/1	0.97	0.06	-1.76	242,242,242,242	0
10	MG	D	2003	1/1	0.95	0.27	-	198,198,198,198	0
10	MG	J	2003	1/1	0.88	0.29	-	219,219,219,219	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.