



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 AM GMT

PDB ID : 3GTL  
Title : Backtracked RNA polymerase II complex with 13mer with G<>U mismatch  
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.  
Deposited on : 2009-03-27  
Resolution : 3.38 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

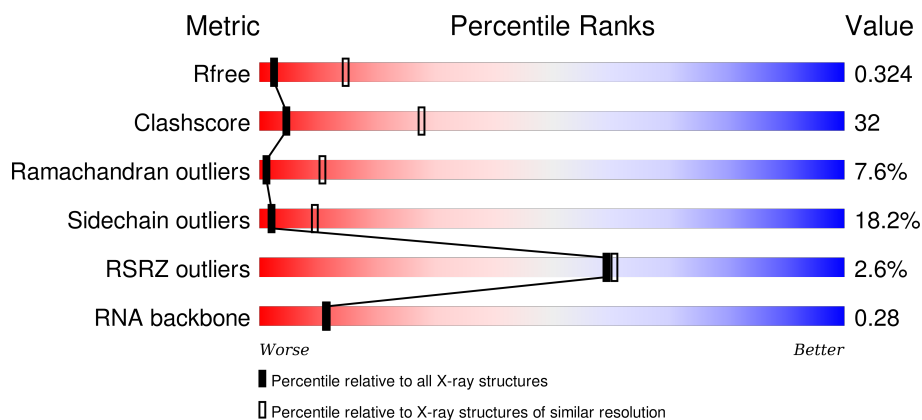
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)
RNA backbone	2183	1024 (3.96-2.80)

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	1733	
2	B	1224	
3	C	318	
4	E	215	

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	13	
12	T	28	
13	N	14	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			257	116	49	81	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 13 is a DNA chain called DNA (5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

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

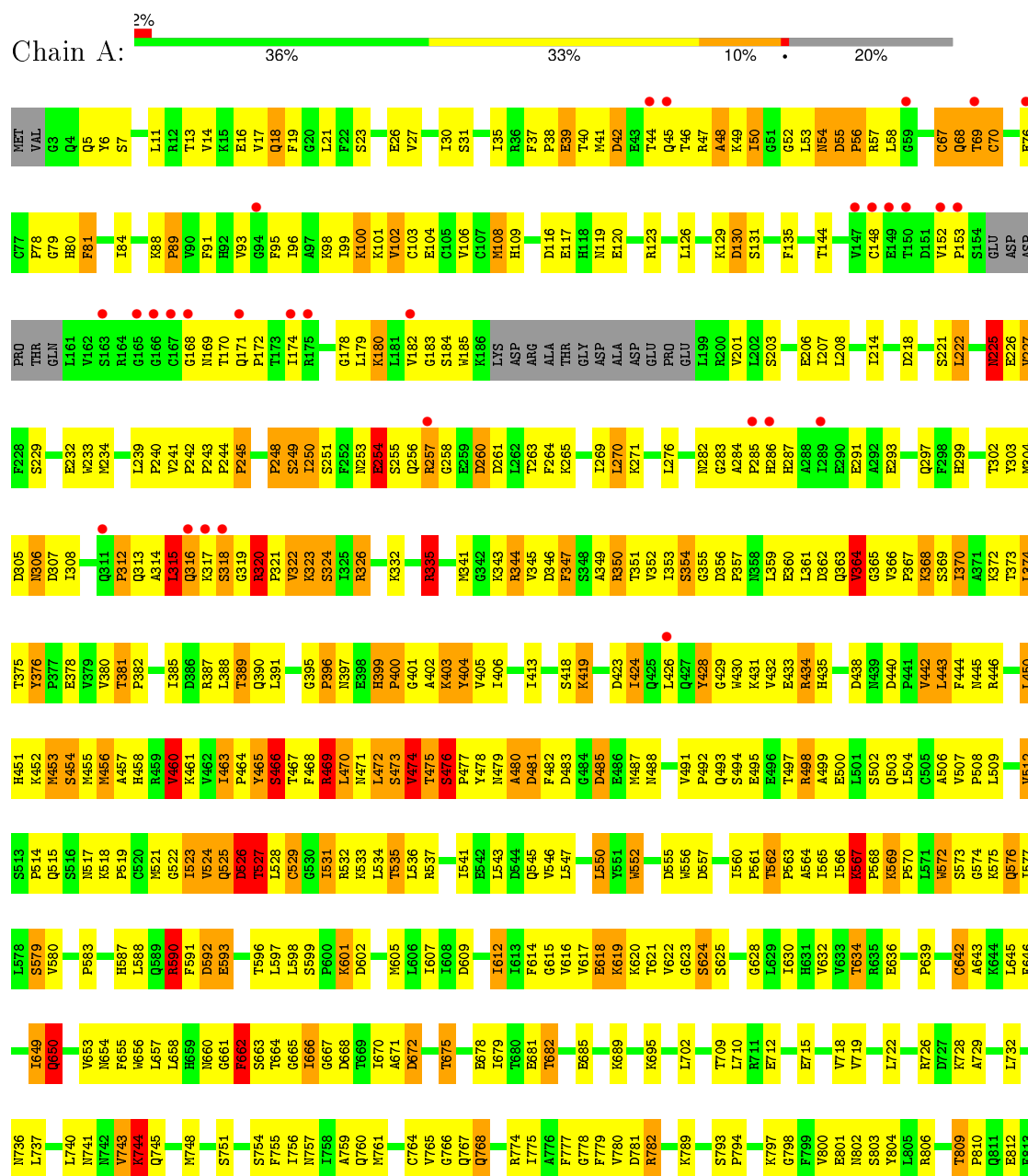
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 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 II subunit RPB1

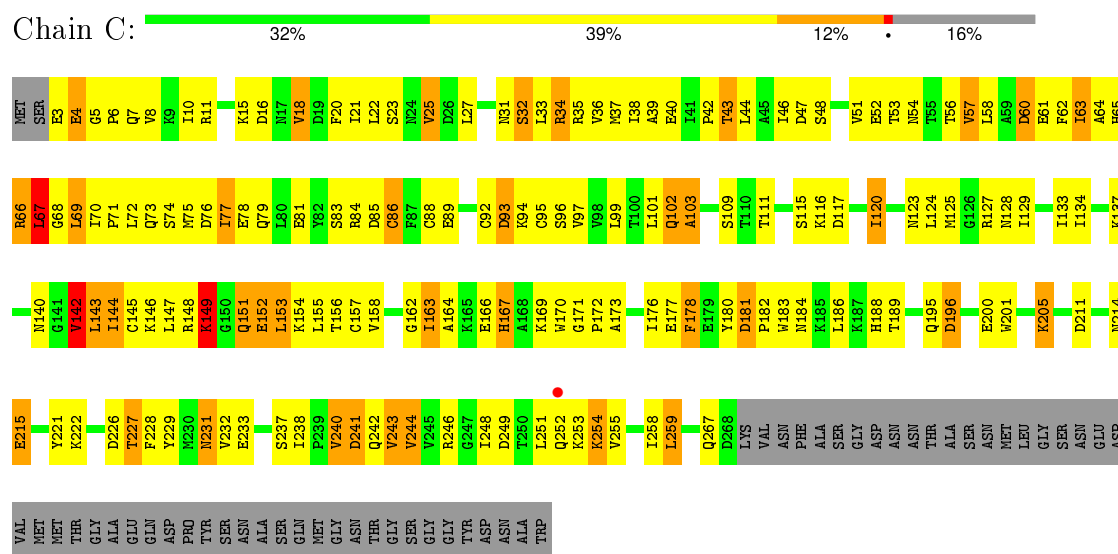




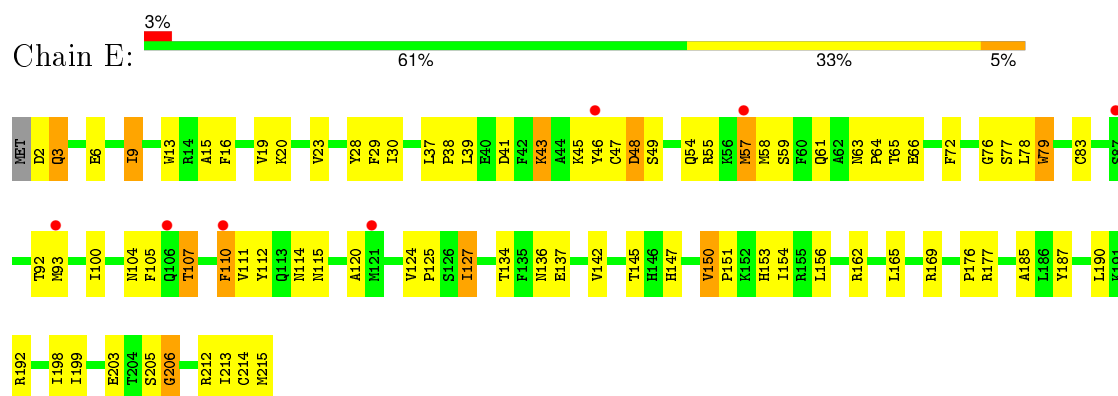




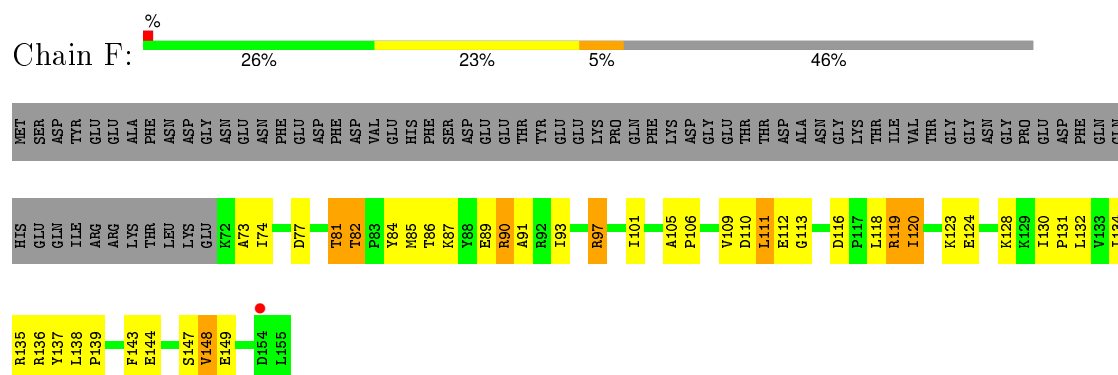
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

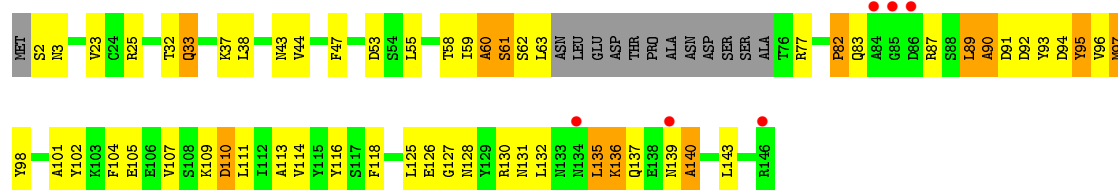


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

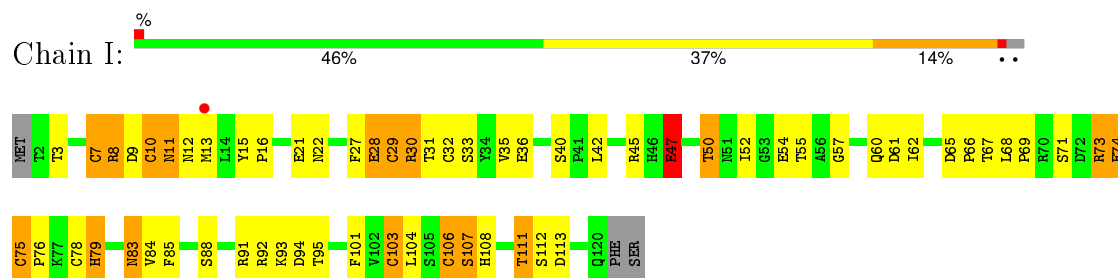


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

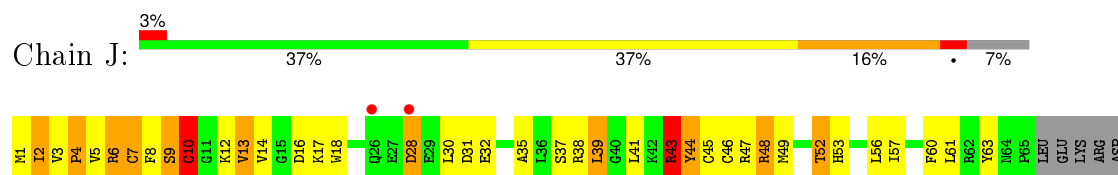




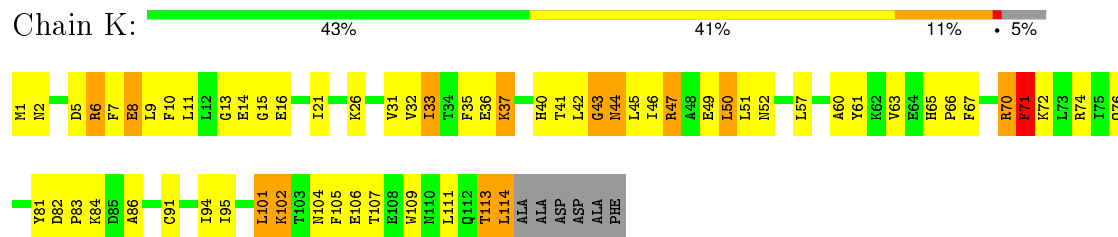
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



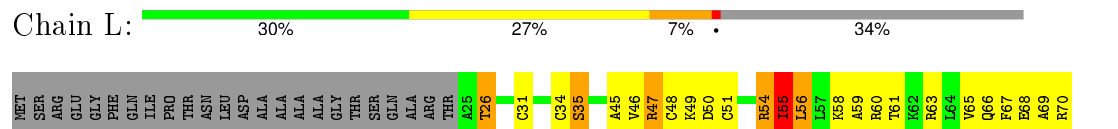
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



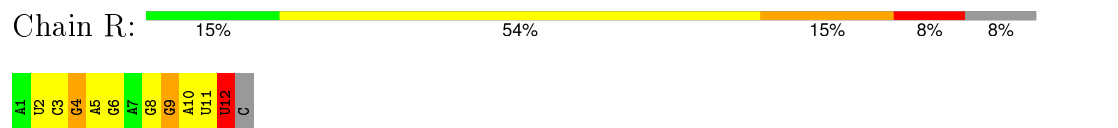
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*UP\*C)-3')

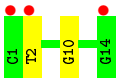
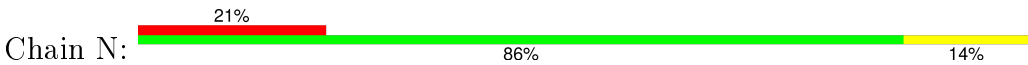


- Molecule 12: DNA (28-MER)





● Molecule 13: DNA (5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.53Å 222.28Å 194.81Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	50.00 – 3.38 41.75 – 3.38	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.38) 91.1 (41.75-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.270 , 0.322 0.277 , 0.324	Depositor DCC
$R_{free}$ test set	4514 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 80.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 90365 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	29256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	0.57	1/11163 (0.0%)	0.74	5/15091 (0.0%)
2	B	0.62	0/8963	0.79	4/12086 (0.0%)
3	C	0.65	0/2133	0.80	0/2891
4	E	0.46	0/1788	0.60	0/2406
5	F	0.47	0/691	0.71	0/933
6	H	0.45	0/1086	0.71	0/1470
7	I	0.48	0/989	0.66	0/1331
8	J	0.81	1/541 (0.2%)	0.96	1/727 (0.1%)
9	K	0.61	0/937	0.76	1/1265 (0.1%)
10	L	0.59	0/365	0.86	0/485
11	R	1.06	1/288 (0.3%)	1.71	4/448 (0.9%)
12	T	0.91	1/634 (0.2%)	1.69	17/975 (1.7%)
13	N	0.82	0/317	1.43	1/488 (0.2%)
All	All	0.60	4/29895 (0.0%)	0.82	33/40596 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	12	U	C1'-N1	5.54	1.57	1.48
12	T	21	DC	C3'-O3'	-5.29	1.37	1.44
8	J	9	SER	N-CA	5.02	1.56	1.46
1	A	360	GLU	CG-CD	5.01	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	27	DA	O4'-C4'-C3'	-12.07	98.75	106.00
12	T	16	DC	O4'-C4'-C3'	-9.86	100.08	106.00
2	B	535	LEU	CA-CB-CG	8.83	135.62	115.30
12	T	28	DT	O4'-C1'-N1	7.64	113.34	108.00
2	B	983	ARG	NE-CZ-NH1	7.48	124.04	120.30
12	T	6	DG	P-O3'-C3'	7.34	128.51	119.70
1	A	469	ARG	NE-CZ-NH1	7.21	123.91	120.30
13	N	10	DG	P-O3'-C3'	7.08	128.19	119.70
12	T	19	DT	O4'-C1'-N1	6.63	112.64	108.00
12	T	15	DA	P-O3'-C3'	6.47	127.47	119.70
8	J	10	CYS	CA-CB-SG	6.41	125.53	114.00
12	T	4	DC	O4'-C1'-N1	6.34	112.44	108.00
12	T	27	DA	O4'-C1'-N9	6.20	112.34	108.00
12	T	20	DC	O4'-C4'-C3'	-6.07	102.07	104.50
12	T	25	DC	O4'-C1'-N1	6.06	112.24	108.00
12	T	16	DC	O4'-C1'-N1	6.00	112.20	108.00
9	K	111	LEU	CA-CB-CG	5.73	128.48	115.30
12	T	15	DA	O4'-C1'-N9	5.72	112.00	108.00
12	T	22	DT	C4'-C3'-C2'	-5.64	98.02	103.10
1	A	1116	LEU	CA-CB-CG	5.59	128.16	115.30
12	T	10	DA	O4'-C1'-N9	5.50	111.85	108.00
12	T	22	DT	P-O3'-C3'	5.49	126.28	119.70
12	T	24	DT	N3-C4-O4	5.39	123.13	119.90
1	A	315	LEU	CA-CB-CG	5.32	127.53	115.30
2	B	535	LEU	CB-CG-CD1	-5.31	101.97	111.00
11	R	8	G	C4'-C3'-C2'	-5.31	97.29	102.60
1	A	460	VAL	CB-CA-C	-5.29	101.34	111.40
12	T	15	DA	C1'-O4'-C4'	-5.24	104.86	110.10
11	R	9	G	P-O3'-C3'	-5.20	113.46	119.70
1	A	590	ARG	NE-CZ-NH1	5.16	122.88	120.30
11	R	12	U	C2-N1-C1'	5.09	123.81	117.70
11	R	10	A	C5'-C4'-O4'	5.05	115.16	109.10
2	B	539	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	4	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11071	767	0
2	B	8792	0	8823	775	0
3	C	2095	0	2051	157	0
4	E	1752	0	1776	52	0
5	F	679	0	701	40	0
6	H	1068	0	1040	59	0
7	I	971	0	930	45	0
8	J	532	0	543	71	0
9	K	919	0	929	65	0
10	L	363	0	387	18	0
11	R	257	0	131	15	0
12	T	566	0	316	18	0
13	N	284	0	161	1	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29256	0	28859	1868	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 32.

All (1868) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:PRO:CB	2:B:637:LEU:HA	1.49	1.35
2:B:848:ARG:HD2	8:J:7:CYS:O	1.32	1.26
2:B:827:ILE:HG23	2:B:1012:ILE:CD1	1.68	1.24
2:B:1002:THR:CG2	2:B:1006:ILE:HG12	1.66	1.24
1:A:482:PHE:CD1	2:B:836:GLU:HB3	1.73	1.23
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.74	1.21
2:B:1096:ARG:CD	2:B:1097:HIS:H	1.55	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:CB	2:B:835:GLN:HG2	1.75	1.16
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.77	1.14
2:B:1002:THR:HG23	2:B:1006:ILE:HG12	1.23	1.13
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.28	1.12
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.13	1.12
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.27	1.12
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.19	1.11
2:B:1096:ARG:CG	2:B:1097:HIS:H	1.64	1.09
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.17	1.09
11:R:4:G:H2'	11:R:5:A:H8	1.14	1.09
2:B:636:PRO:CB	2:B:637:LEU:CA	2.30	1.09
1:A:482:PHE:CD1	2:B:836:GLU:CB	2.34	1.09
2:B:839:MET:HG2	2:B:989:THR:O	1.52	1.09
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.80	1.08
2:B:464:GLY:HA2	2:B:480:SER:HB2	1.11	1.07
2:B:1096:ARG:HD3	2:B:1097:HIS:N	1.69	1.07
2:B:759:PRO:HB3	2:B:767:ASN:HD21	1.18	1.07
2:B:464:GLY:HA2	2:B:480:SER:CB	1.85	1.06
1:A:1063:MET:SD	1:A:1436:ILE:HG12	1.95	1.06
1:A:351:THR:HG22	1:A:352:VAL:N	1.70	1.06
8:J:7:CYS:SG	8:J:10:CYS:N	2.26	1.06
2:B:465:ASN:HA	2:B:476:ARG:HB3	1.35	1.06
2:B:969:ARG:HD2	3:C:61:GLU:OE2	1.54	1.05
1:A:525:GLN:HB3	2:B:835:GLN:HG2	1.33	1.05
1:A:464:PRO:HG2	9:K:67:PHE:CD1	1.91	1.05
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.55	1.05
1:A:567:LYS:HB3	6:H:96:VAL:H	1.18	1.04
2:B:780:VAL:HG12	2:B:817:LEU:HG	1.40	1.03
2:B:827:ILE:HG23	2:B:1012:ILE:CG1	1.89	1.03
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.40	1.03
1:A:573:SER:H	1:A:576:GLN:HG3	1.22	1.03
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.38	1.03
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.39	1.02
2:B:992:ILE:HD11	9:K:67:PHE:CE2	1.95	1.01
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.38	1.01
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	1.76	1.01
2:B:1096:ARG:HD3	2:B:1097:HIS:H	1.17	1.00
1:A:480:ALA:HB1	1:A:485:ASP:OD2	1.62	1.00
2:B:836:GLU:OE1	2:B:836:GLU:HA	1.62	0.99
1:A:474:VAL:HG13	1:A:474:VAL:O	1.59	0.99
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.13	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HD21	1:A:487:MET:CE	1.92	0.99
1:A:364:VAL:HG12	1:A:460:VAL:HA	1.40	0.98
1:A:483:ASP:HB3	2:B:837:ASP:OD2	1.63	0.98
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.42	0.98
1:A:482:PHE:HD1	2:B:836:GLU:HB3	1.25	0.98
1:A:535:THR:HG21	1:A:617:VAL:H	1.28	0.98
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.94	0.97
2:B:764:SER:HB2	2:B:765:PRO:HD3	1.46	0.97
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.47	0.96
1:A:525:GLN:HB3	2:B:835:GLN:CG	1.94	0.96
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.47	0.96
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.95	0.96
11:R:4:G:H2'	11:R:5:A:C8	2.01	0.96
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.47	0.96
3:C:3:GLU:HG3	3:C:4:GLU:H	1.31	0.95
2:B:839:MET:HG3	2:B:990:ILE:HA	1.48	0.95
2:B:1002:THR:CG2	2:B:1006:ILE:CG1	2.44	0.95
1:A:892:ALA:HA	1:A:895:LYS:HE3	1.46	0.95
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	1.48	0.95
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.46	0.95
2:B:464:GLY:CA	2:B:480:SER:CB	2.44	0.95
2:B:1013:ASN:CG	2:B:1014:PRO:HD2	1.86	0.95
2:B:412:LEU:HD11	2:B:479:VAL:HG11	1.47	0.95
2:B:655:LYS:O	2:B:658:ILE:HG22	1.66	0.94
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.49	0.94
1:A:482:PHE:HD1	2:B:836:GLU:CB	1.77	0.94
3:C:167:HIS:HD2	3:C:169:LYS:H	1.17	0.93
2:B:464:GLY:CA	2:B:480:SER:HB2	1.96	0.93
8:J:3:VAL:HG22	8:J:53:HIS:CE1	2.03	0.93
1:A:376:TYR:HE1	1:A:498:ARG:HE	1.05	0.92
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.37	0.92
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.85	0.92
2:B:780:VAL:CG1	2:B:817:LEU:HG	1.98	0.92
2:B:1115:THR:HB	2:B:1117:GLN:HG3	1.49	0.92
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.35	0.91
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.35	0.91
8:J:8:PHE:H	8:J:49:MET:HE3	1.36	0.91
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.35	0.91
2:B:1151:LEU:O	2:B:1152:MET:HG2	1.71	0.91
2:B:1120:GLU:HG2	2:B:1121:GLY:H	1.34	0.90
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.51	0.90
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.53	0.90
2:B:1017:ILE:HD12	2:B:1026:LEU:HD21	1.52	0.90
1:A:99:ILE:HG12	1:A:234:MET:SD	2.13	0.89
8:J:1:MET:N	8:J:56:LEU:H	1.70	0.89
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.56	0.88
1:A:446:ARG:CZ	1:A:480:ALA:HB2	2.03	0.88
1:A:567:LYS:HB2	1:A:568:PRO:HD2	0.90	0.88
1:A:482:PHE:CE1	2:B:836:GLU:CB	2.57	0.88
2:B:827:ILE:CG2	2:B:1012:ILE:CD1	2.51	0.88
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.54	0.88
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.54	0.87
2:B:1007:VAL:HG12	2:B:1007:VAL:O	1.74	0.87
2:B:278:GLN:HG2	2:B:279:ASP:H	1.37	0.87
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.38	0.87
1:A:662:PHE:HD2	1:A:663:SER:H	1.17	0.87
1:A:662:PHE:HD2	1:A:663:SER:N	1.71	0.87
2:B:744:HIS:HD2	2:B:746:SER:OG	1.57	0.87
1:A:445:ASN:CB	1:A:455:MET:HG2	2.05	0.87
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.04	0.87
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.92	0.86
1:A:315:LEU:CB	1:A:316:GLN:HA	2.04	0.86
2:B:850:LEU:HD13	8:J:8:PHE:HD1	1.40	0.86
1:A:531:ILE:HG13	1:A:653:VAL:HG21	1.57	0.86
1:A:351:THR:CG2	2:B:1103:ILE:HD12	2.04	0.85
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.11	0.85
2:B:770:GLN:HG2	2:B:983:ARG:O	1.76	0.85
2:B:1096:ARG:CG	2:B:1097:HIS:N	2.37	0.85
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.59	0.85
1:A:376:TYR:HE1	1:A:498:ARG:NE	1.75	0.84
1:A:482:PHE:CE1	2:B:836:GLU:CG	2.59	0.84
1:A:1066:VAL:HG21	2:B:1139:ILE:HG21	1.59	0.84
7:I:10:CYS:HB3	7:I:31:THR:HG21	1.57	0.84
2:B:465:ASN:HA	2:B:476:ARG:CB	2.06	0.84
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.41	0.84
1:A:357:PRO:HG3	2:B:832:GLY:O	1.77	0.84
2:B:835:GLN:O	2:B:836:GLU:HB2	1.77	0.84
2:B:637:LEU:HD21	2:B:740:HIS:HB3	1.59	0.84
2:B:980:PHE:O	2:B:1095:LEU:HG	1.77	0.84
2:B:882:THR:HG21	2:B:935:ARG:HA	1.55	0.84
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:113:THR:O	9:K:114:LEU:HB2	1.77	0.83
2:B:803:LEU:H	2:B:822:ASN:HD21	1.26	0.83
2:B:1028:GLU:OE1	2:B:1090:THR:HG22	1.77	0.83
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.60	0.83
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.43	0.82
2:B:827:ILE:HG23	2:B:1012:ILE:HD11	1.61	0.82
2:B:759:PRO:HB3	2:B:767:ASN:ND2	1.94	0.82
2:B:711:GLU:H	2:B:712:PRO:HD3	1.44	0.82
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.79	0.82
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.62	0.82
1:A:899:VAL:HG12	1:A:899:VAL:O	1.78	0.82
1:A:18:GLN:HG2	1:A:1418:LEU:HD12	1.61	0.82
1:A:401:GLY:H	1:A:435:HIS:HD2	1.27	0.82
5:F:135:ARG:HG2	5:F:137:TYR:HE1	1.44	0.82
2:B:847:ASP:OD1	2:B:847:ASP:N	2.09	0.82
2:B:589:VAL:HG12	2:B:590:HIS:H	1.46	0.81
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.61	0.81
2:B:841:MET:HG3	2:B:1010:LEU:HB3	1.61	0.81
3:C:40:GLU:OE1	3:C:254:LYS:HE3	1.81	0.81
2:B:845:SER:O	2:B:848:ARG:HB2	1.79	0.81
1:A:440:ASP:HB2	1:A:460:VAL:HG21	1.62	0.81
7:I:78:CYS:O	7:I:79:HIS:HB2	1.80	0.81
2:B:412:LEU:CD1	2:B:479:VAL:HG11	2.10	0.81
1:A:343:LYS:HD2	2:B:1151:LEU:HG	1.63	0.80
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.10	0.80
2:B:708:GLU:HG3	2:B:709:ASP:H	1.47	0.80
1:A:351:THR:HG22	1:A:352:VAL:H	1.43	0.80
1:A:471:ASN:OD1	1:A:473:SER:HB2	1.81	0.80
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.15	0.80
10:L:55:ILE:O	10:L:56:LEU:HB2	1.82	0.80
2:B:803:LEU:N	2:B:822:ASN:HD21	1.80	0.79
2:B:1098:MET:HB3	2:B:1101:ASP:OD2	1.81	0.79
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.12	0.79
1:A:464:PRO:HG2	9:K:67:PHE:CE1	2.17	0.79
1:A:376:TYR:CE1	1:A:498:ARG:NE	2.50	0.79
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.18	0.79
7:I:29:CYS:SG	7:I:31:THR:N	2.55	0.79
2:B:978:ASP:OD1	2:B:1099:VAL:HG23	1.83	0.79
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.12	0.78
11:R:3:C:H42	12:T:26:DG:H1	1.30	0.78
2:B:1031:LEU:HD12	2:B:1031:LEU:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.18	0.78
3:C:142:VAL:HG13	3:C:143:LEU:N	1.98	0.78
3:C:178:PHE:C	3:C:178:PHE:HD2	1.87	0.78
3:C:73:GLN:NE2	3:C:75:MET:HB2	1.97	0.78
2:B:1004:GLU:HB3	2:B:1006:ILE:HD11	1.65	0.78
3:C:99:LEU:HD23	3:C:120:ILE:HA	1.65	0.78
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.64	0.78
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.95	0.78
1:A:1064:VAL:HG12	1:A:1064:VAL:O	1.82	0.77
3:C:242:GLN:OE1	3:C:242:GLN:HA	1.82	0.77
2:B:1028:GLU:HG3	2:B:1090:THR:CG2	2.14	0.77
3:C:66:ARG:NH2	8:J:4:PRO:HA	1.99	0.77
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.20	0.77
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.64	0.77
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.65	0.77
1:A:525:GLN:HB2	2:B:835:GLN:HG2	1.64	0.77
2:B:759:PRO:CB	2:B:767:ASN:HD21	1.95	0.77
1:A:335:ARG:HD2	2:B:1202:LEU:HD12	1.67	0.77
1:A:361:LEU:HD11	1:A:473:SER:HB3	1.64	0.77
2:B:541:LEU:HD12	2:B:747:MET:SD	2.23	0.77
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.14	0.77
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.67	0.77
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.20	0.77
3:C:16:ASP:O	3:C:233:GLU:HA	1.84	0.77
1:A:1364:ASN:C	1:A:1364:ASN:HD22	1.89	0.77
4:E:176:PRO:O	4:E:212:ARG:HA	1.85	0.77
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.67	0.77
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.65	0.76
9:K:21:ILE:HD12	9:K:33:ILE:HG12	1.66	0.76
1:A:901:LEU:H	1:A:926:GLN:NE2	1.81	0.76
1:A:351:THR:HG21	1:A:467:THR:HA	1.66	0.76
2:B:744:HIS:CD2	2:B:746:SER:OG	2.37	0.76
1:A:512:VAL:HA	1:A:519:PRO:HA	1.66	0.76
2:B:64:CYS:HA	2:B:67:SER:HB2	1.66	0.76
2:B:848:ARG:CD	8:J:7:CYS:O	2.25	0.76
2:B:827:ILE:HG23	2:B:1012:ILE:HD12	1.66	0.76
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.68	0.76
1:A:679:ILE:O	1:A:682:THR:HG22	1.86	0.76
1:A:622:VAL:O	1:A:630:ILE:HD11	1.85	0.76
3:C:167:HIS:HE1	10:L:70:ARG:O	1.67	0.76
3:C:178:PHE:C	3:C:178:PHE:CD2	2.56	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:CG2	1:A:352:VAL:N	2.43	0.76
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.65	0.76
2:B:60:GLN:O	2:B:63:ILE:HG22	1.85	0.76
2:B:1096:ARG:HG3	2:B:1097:HIS:H	1.48	0.76
1:A:446:ARG:NE	1:A:480:ALA:HB2	2.00	0.75
1:A:481:ASP:HB2	2:B:836:GLU:O	1.87	0.75
1:A:404:TYR:HA	1:A:413:ILE:O	1.86	0.75
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.21	0.75
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.67	0.75
2:B:821:GLN:OE1	2:B:851:PHE:N	2.20	0.75
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.69	0.75
1:A:779:PHE:CZ	2:B:517:THR:HA	2.22	0.75
1:A:456:MET:HG3	1:A:507:VAL:HG22	1.67	0.75
11:R:3:C:H2'	11:R:4:G:C8	2.22	0.75
2:B:764:SER:HB2	2:B:765:PRO:CD	2.15	0.75
1:A:182:VAL:HG12	1:A:183:GLY:H	1.52	0.75
9:K:70:ARG:O	9:K:71:PHE:HB3	1.84	0.75
2:B:764:SER:CB	2:B:765:PRO:HD3	2.15	0.75
7:I:10:CYS:O	7:I:11:ASN:CB	2.35	0.75
8:J:35:ALA:O	8:J:39:LEU:HD11	1.85	0.75
5:F:111:LEU:H	5:F:111:LEU:HD13	1.52	0.75
2:B:706:GLN:O	2:B:710:LEU:HB2	1.87	0.74
8:J:5:VAL:O	8:J:6:ARG:O	2.05	0.74
1:A:1066:VAL:HG21	2:B:1139:ILE:CG2	2.17	0.74
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.69	0.74
2:B:836:GLU:O	2:B:837:ASP:HB2	1.87	0.74
1:A:567:LYS:HB3	6:H:96:VAL:N	2.00	0.74
3:C:73:GLN:HE21	3:C:75:MET:HB2	1.50	0.74
8:J:7:CYS:HG	8:J:9:SER:HG	1.35	0.74
2:B:1017:ILE:CD1	2:B:1026:LEU:HD21	2.18	0.74
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.23	0.74
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.52	0.74
2:B:759:PRO:HD2	2:B:1046:PRO:HG3	1.69	0.74
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.68	0.74
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.75	0.74
5:F:128:LYS:HD3	5:F:149:GLU:HA	1.67	0.74
1:A:662:PHE:CD2	1:A:663:SER:N	2.52	0.73
1:A:55:ASP:H	1:A:56:PRO:HD2	1.53	0.73
3:C:166:GLU:O	3:C:167:HIS:HB2	1.89	0.73
1:A:672:ASP:H	1:A:736:ASN:HD21	1.33	0.73
1:A:1386:ARG:HD3	1:A:1403:GLU:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.23	0.73
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.89	0.73
1:A:525:GLN:CB	2:B:835:GLN:CG	2.57	0.73
6:H:109:LYS:HB3	6:H:110:ASP:C	2.09	0.73
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.21	0.73
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.70	0.73
1:A:476:SER:N	1:A:477:PRO:HD2	2.03	0.73
2:B:980:PHE:O	2:B:981:ALA:CB	2.36	0.73
2:B:980:PHE:O	2:B:981:ALA:HB3	1.87	0.73
1:A:573:SER:O	1:A:576:GLN:HB2	1.89	0.73
1:A:709:THR:HB	1:A:712:GLU:H	1.54	0.73
1:A:440:ASP:H	1:A:460:VAL:HG23	1.54	0.73
2:B:763:GLN:CG	2:B:765:PRO:HD2	2.15	0.73
1:A:474:VAL:CG1	1:A:474:VAL:O	2.31	0.73
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.70	0.73
2:B:346:GLU:HA	2:B:349:ILE:HD13	1.71	0.73
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.52	0.73
1:A:364:VAL:CG1	1:A:460:VAL:HA	2.19	0.72
1:A:482:PHE:HE1	2:B:836:GLU:CG	1.99	0.72
1:A:485:ASP:N	1:A:485:ASP:OD1	2.20	0.72
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.53	0.72
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.19	0.72
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.71	0.72
1:A:649:ILE:O	1:A:653:VAL:HG23	1.88	0.72
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.54	0.72
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.68	0.72
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.71	0.72
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.53	0.72
3:C:3:GLU:HG3	3:C:4:GLU:N	2.05	0.72
1:A:446:ARG:CZ	1:A:479:ASN:O	2.37	0.72
1:A:440:ASP:HB2	1:A:460:VAL:CG2	2.18	0.72
2:B:828:ALA:HB2	2:B:1085:ILE:CG2	2.16	0.72
2:B:839:MET:HG2	2:B:989:THR:C	2.09	0.72
2:B:464:GLY:CA	2:B:480:SER:HB3	2.20	0.72
1:A:318:SER:HA	12:T:28:DT:H2"	1.70	0.72
2:B:955:THR:HG22	2:B:956:THR:N	2.03	0.72
3:C:133:ILE:CD1	3:C:237:SER:HA	2.19	0.72
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.55	0.72
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.71	0.72
2:B:780:VAL:HG12	2:B:817:LEU:CG	2.19	0.72
2:B:850:LEU:HB2	8:J:8:PHE:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:VAL:HG12	10:L:47:ARG:H	1.55	0.72
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.24	0.71
2:B:1138:MET:CE	2:B:1138:MET:HA	2.16	0.71
2:B:363:HIS:O	2:B:364:ILE:HB	1.89	0.71
2:B:1103:ILE:HD13	2:B:1103:ILE:H	1.55	0.71
1:A:899:VAL:HG22	1:A:1029:ARG:HG3	1.71	0.71
8:J:1:MET:H1	8:J:56:LEU:H	1.34	0.71
3:C:66:ARG:HH22	8:J:4:PRO:HA	1.55	0.71
4:E:83:CYS:SG	4:E:110:PHE:HE1	2.12	0.71
2:B:486:TYR:CE2	2:B:777:ALA:O	2.44	0.71
1:A:479:ASN:O	1:A:480:ALA:HB2	1.90	0.71
2:B:827:ILE:HD12	2:B:1086:PHE:HB3	1.72	0.71
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.71	0.71
1:A:715:GLU:OE1	1:A:774:ARG:HD3	1.89	0.71
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.56	0.71
7:I:29:CYS:SG	7:I:30:ARG:N	2.64	0.71
2:B:982:SER:O	2:B:1093:GLN:HG2	1.89	0.71
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.73	0.70
1:A:525:GLN:O	1:A:526:ASP:C	2.29	0.70
7:I:10:CYS:O	7:I:11:ASN:HB2	1.91	0.70
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.73	0.70
2:B:977:GLY:O	2:B:989:THR:HB	1.91	0.70
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.90	0.70
1:A:129:LYS:O	1:A:130:ASP:HB2	1.90	0.70
2:B:842:ASN:HB3	2:B:845:SER:HB3	1.73	0.70
6:H:58:THR:HG22	6:H:59:ILE:N	2.06	0.70
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.72	0.70
1:A:821:ARG:O	1:A:825:ILE:HG12	1.91	0.70
2:B:1029:CYS:SG	2:B:1088:GLY:HA3	2.32	0.70
2:B:322:PHE:CZ	7:I:30:ARG:HD2	2.25	0.70
1:A:901:LEU:N	1:A:926:GLN:NE2	2.40	0.70
2:B:293:PRO:O	2:B:297:ILE:HG12	1.91	0.70
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.21	0.70
2:B:203:PHE:CE1	2:B:212:LEU:HD12	2.26	0.70
1:A:527:THR:O	1:A:653:VAL:HG11	1.91	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.70
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.73	0.70
2:B:635:ARG:HG2	2:B:635:ARG:O	1.91	0.70
2:B:789:MET:HE2	2:B:965:LYS:HD3	1.73	0.70
1:A:664:THR:HA	1:A:668:ASP:OD2	1.92	0.69
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:1:MET:N	8:J:56:LEU:N	2.40	0.69
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.75	0.69
1:A:1151:GLU:HG2	7:I:45:ARG:HG3	1.72	0.69
2:B:637:LEU:N	2:B:637:LEU:HD13	2.07	0.69
2:B:763:GLN:NE2	2:B:765:PRO:HG2	2.07	0.69
3:C:69:LEU:HB3	8:J:6:ARG:CD	2.23	0.69
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.58	0.69
3:C:18:VAL:O	3:C:20:PHE:HD2	1.75	0.69
1:A:754:SER:H	1:A:757:ASN:HD22	1.40	0.69
6:H:89:LEU:O	6:H:91:ASP:N	2.23	0.68
1:A:660:ASN:OD1	2:B:1082:MET:CB	2.40	0.68
1:A:855:THR:CG2	1:A:857:ARG:HE	2.06	0.68
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.28	0.68
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.76	0.68
1:A:365:GLY:O	1:A:468:PHE:HA	1.93	0.68
2:B:1028:GLU:HG3	2:B:1090:THR:HG23	1.75	0.68
2:B:955:THR:HG22	2:B:956:THR:H	1.57	0.68
2:B:900:ALA:HB3	10:L:61:THR:HG23	1.74	0.68
2:B:833:TYR:O	2:B:835:GLN:N	2.27	0.68
2:B:1151:LEU:O	2:B:1152:MET:CG	2.41	0.68
2:B:839:MET:CG	2:B:990:ILE:HA	2.23	0.68
2:B:850:LEU:HD13	8:J:8:PHE:CD1	2.27	0.68
1:A:464:PRO:CG	9:K:67:PHE:HD1	2.06	0.68
3:C:34:ARG:HG2	3:C:35:ARG:N	2.08	0.68
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.21	0.68
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.58	0.68
9:K:35:PHE:HB2	9:K:71:PHE:CE2	2.29	0.68
1:A:665:GLY:HA2	2:B:1086:PHE:CD1	2.28	0.68
12:T:26:DG:C2	12:T:27:DA:H1'	2.29	0.68
2:B:465:ASN:HA	2:B:476:ARG:HA	1.76	0.68
2:B:764:SER:CB	2:B:765:PRO:CD	2.65	0.68
1:A:1348:LEU:CD2	1:A:1372:VAL:HG22	2.20	0.68
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.75	0.68
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.74	0.68
2:B:1107:ALA:O	2:B:1108:ARG:HB3	1.92	0.67
1:A:660:ASN:OD1	2:B:1082:MET:HB3	1.94	0.67
1:A:845:LEU:O	1:A:848:ILE:HG12	1.94	0.67
1:A:385:ILE:HD11	1:A:428:TYR:CZ	2.30	0.67
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.08	0.67
2:B:796:LEU:HD23	2:B:821:GLN:NE2	2.09	0.67
2:B:864:LYS:HB3	2:B:872:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:LEU:O	1:A:931:GLU:HB3	1.94	0.67
7:I:8:ARG:O	7:I:9:ASP:HB2	1.94	0.67
1:A:476:SER:H	1:A:477:PRO:HD2	1.58	0.67
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.67
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.27	0.67
1:A:533:LYS:HD2	1:A:662:PHE:HD1	1.60	0.67
1:A:364:VAL:O	1:A:364:VAL:HG13	1.94	0.67
1:A:810:PRO:HD3	2:B:1047:PHE:CD2	2.30	0.67
2:B:955:THR:HG23	10:L:54:ARG:O	1.95	0.67
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.59	0.67
3:C:167:HIS:CD2	3:C:169:LYS:H	2.07	0.67
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.29	0.67
2:B:637:LEU:O	2:B:691:GLU:N	2.25	0.67
1:A:663:SER:OG	2:B:828:ALA:HB2	1.94	0.67
1:A:13:THR:HG22	1:A:14:VAL:H	1.60	0.67
1:A:1273:LEU:O	1:A:1274:ARG:HB3	1.94	0.67
1:A:575:LYS:HD3	1:A:612:ILE:HD11	1.77	0.67
2:B:1106:ARG:CZ	2:B:1109:GLY:H	2.09	0.66
1:A:472:LEU:O	1:A:475:THR:HB	1.95	0.66
3:C:69:LEU:HB3	8:J:6:ARG:HD2	1.75	0.66
2:B:345:LYS:O	2:B:348:ARG:HG2	1.94	0.66
2:B:956:THR:HA	2:B:961:LEU:O	1.95	0.66
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.77	0.66
2:B:128:LEU:HB2	2:B:167:ILE:O	1.95	0.66
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.10	0.66
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.25	0.66
1:A:354:SER:O	1:A:469:ARG:HA	1.96	0.66
1:A:751:SER:HB2	2:B:1015:HIS:HE1	1.60	0.66
4:E:29:PHE:O	4:E:30:ILE:HG13	1.94	0.66
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.78	0.66
2:B:836:GLU:O	2:B:837:ASP:CB	2.42	0.66
2:B:827:ILE:CG2	2:B:1012:ILE:HD12	2.25	0.66
2:B:322:PHE:CD1	2:B:322:PHE:O	2.48	0.66
1:A:955:PRO:O	1:A:956:LEU:HG	1.96	0.66
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.31	0.66
2:B:190:TYR:CZ	2:B:196:PRO:HG2	2.31	0.66
1:A:364:VAL:CG1	1:A:364:VAL:O	2.43	0.66
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.06	0.66
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.31	0.66
6:H:104:PHE:HD2	6:H:114:VAL:HG12	1.58	0.66
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.78	0.66
7:I:92:ARG:HG2	7:I:93:LYS:H	1.61	0.66
2:B:412:LEU:HD13	2:B:466:TRP:NE1	2.10	0.66
1:A:503:GLN:HB2	1:A:504:LEU:HD12	1.78	0.65
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.77	0.65
2:B:637:LEU:HD23	2:B:638:PHE:N	2.10	0.65
1:A:446:ARG:NE	1:A:480:ALA:CB	2.59	0.65
1:A:573:SER:N	1:A:576:GLN:HG3	2.05	0.65
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.60	0.65
2:B:1096:ARG:HG3	2:B:1097:HIS:N	2.08	0.65
1:A:661:GLY:O	1:A:662:PHE:HB2	1.96	0.65
1:A:929:LEU:HD23	1:A:983:ILE:CG2	2.26	0.65
3:C:73:GLN:HE21	3:C:75:MET:CB	2.09	0.65
1:A:344:ARG:HH11	1:A:344:ARG:CG	2.09	0.65
2:B:1153:GLU:CA	2:B:1153:GLU:OE2	2.44	0.65
1:A:526:ASP:O	1:A:527:THR:C	2.34	0.65
1:A:534:LEU:O	1:A:574:GLY:HA3	1.97	0.65
1:A:473:SER:HG	1:A:646:PHE:HD2	1.41	0.65
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.30	0.65
1:A:440:ASP:N	1:A:460:VAL:HG23	2.10	0.65
2:B:1096:ARG:O	2:B:1097:HIS:C	2.34	0.65
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.78	0.65
12:T:26:DG:N3	12:T:27:DA:H1'	2.12	0.65
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.79	0.65
3:C:3:GLU:CG	3:C:4:GLU:H	2.07	0.65
2:B:589:VAL:HG12	2:B:590:HIS:N	2.11	0.65
2:B:465:ASN:CA	2:B:476:ARG:HB3	2.18	0.65
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.77	0.65
1:A:401:GLY:N	1:A:435:HIS:HD2	1.93	0.64
1:A:900:ASP:HB3	1:A:906:HIS:O	1.97	0.64
1:A:369:SER:HB3	9:K:2:ASN:OD1	1.97	0.64
12:T:26:DG:N2	12:T:27:DA:H1'	2.13	0.64
3:C:31:ASN:O	3:C:33:LEU:N	2.30	0.64
1:A:588:LEU:CD1	1:A:632:VAL:HG21	2.27	0.64
2:B:638:PHE:CE1	2:B:743:ILE:HD13	2.32	0.64
8:J:3:VAL:HG21	8:J:18:TRP:CD1	2.32	0.64
8:J:35:ALA:O	8:J:39:LEU:CD1	2.44	0.64
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.80	0.64
2:B:833:TYR:OH	9:K:66:PRO:HG3	1.97	0.64
2:B:764:SER:O	2:B:765:PRO:C	2.36	0.64
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HA	1:A:463:ILE:HD12	1.80	0.64
11:R:3:C:H2'	11:R:4:G:H8	1.62	0.64
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.10	0.64
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.80	0.64
1:A:575:LYS:NZ	1:A:615:GLY:O	2.29	0.64
1:A:1127:ASP:O	1:A:1130:GLN:HB3	1.98	0.64
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.66	0.64
1:A:457:ALA:O	1:A:507:VAL:HG23	1.98	0.64
1:A:575:LYS:CG	1:A:612:ILE:HD11	2.28	0.64
2:B:516:ASN:H	2:B:516:ASN:HD22	1.45	0.64
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.79	0.64
2:B:1028:GLU:HG3	2:B:1029:CYS:N	2.13	0.64
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.10	0.64
2:B:465:ASN:HA	2:B:476:ARG:CA	2.27	0.64
1:A:391:LEU:HD23	1:A:400:PRO:O	1.98	0.64
2:B:45:SER:OG	2:B:46:GLN:N	2.26	0.64
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.80	0.64
1:A:344:ARG:HG3	1:A:344:ARG:NH1	2.11	0.64
3:C:47:ASP:HA	10:L:69:ALA:CB	2.27	0.64
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.80	0.64
1:A:1093:LYS:O	1:A:1094:VAL:HG13	1.97	0.64
2:B:567:GLU:CD	2:B:567:GLU:H	2.00	0.64
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.33	0.64
2:B:1028:GLU:CD	2:B:1090:THR:HG22	2.18	0.64
9:K:21:ILE:CD1	9:K:33:ILE:HG12	2.28	0.64
2:B:526:GLU:HG3	2:B:752:ALA:HB3	1.80	0.64
7:I:10:CYS:HB3	7:I:31:THR:CG2	2.28	0.63
2:B:986:GLN:C	2:B:986:GLN:NE2	2.51	0.63
2:B:637:LEU:CD2	2:B:638:PHE:N	2.61	0.63
2:B:1002:THR:HG21	2:B:1006:ILE:CG1	2.28	0.63
2:B:957:ASN:ND2	2:B:959:ASP:H	1.97	0.63
1:A:926:GLN:O	1:A:930:ASP:HB2	1.98	0.63
2:B:377:PHE:O	2:B:380:TYR:N	2.31	0.63
2:B:33:VAL:HG11	2:B:638:PHE:CZ	2.33	0.63
1:A:465:TYR:CB	2:B:976:ILE:HG21	2.28	0.63
3:C:176:ILE:HG22	3:C:176:ILE:O	1.97	0.63
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.80	0.63
1:A:257:ARG:HH22	1:A:317:LYS:HE2	1.61	0.63
1:A:660:ASN:OD1	2:B:1082:MET:HG3	1.99	0.63
2:B:31:TRP:CD2	2:B:807:ARG:HD2	2.33	0.63
2:B:1131:GLY:HA3	2:B:1134:GLU:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASP:OD2	3:C:128:ASN:HB3	1.98	0.63
2:B:464:GLY:O	2:B:476:ARG:HA	1.98	0.63
1:A:760:GLN:HA	1:A:764:CYS:O	1.99	0.63
3:C:229:TYR:N	3:C:229:TYR:CD1	2.67	0.63
2:B:552:MET:HA	2:B:555:ILE:HB	1.79	0.63
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.80	0.63
1:A:351:THR:CG2	1:A:352:VAL:H	2.09	0.63
1:A:526:ASP:HB3	1:A:657:LEU:HD22	1.80	0.63
2:B:1028:GLU:CG	2:B:1090:THR:CG2	2.77	0.63
2:B:964:VAL:HG12	2:B:965:LYS:N	2.13	0.63
5:F:109:VAL:HG12	5:F:110:ASP:H	1.63	0.63
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.99	0.63
2:B:1154:ALA:O	2:B:1155:SER:C	2.37	0.63
2:B:986:GLN:C	2:B:986:GLN:HE21	2.02	0.63
1:A:928:LEU:HB3	1:A:987:VAL:HG11	1.79	0.63
1:A:42:ASP:HA	1:A:46:THR:O	1.98	0.63
1:A:446:ARG:NH2	1:A:480:ALA:HB2	2.13	0.63
2:B:827:ILE:HD11	2:B:1086:PHE:HD2	1.62	0.62
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.31	0.62
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.64	0.62
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.81	0.62
8:J:7:CYS:SG	8:J:9:SER:OG	2.55	0.62
1:A:899:VAL:HG22	1:A:1029:ARG:CG	2.29	0.62
2:B:287:ARG:HA	2:B:291:ILE:O	1.99	0.62
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.32	0.62
1:A:848:ILE:HA	1:A:857:ARG:O	1.99	0.62
1:A:444:PHE:O	1:A:478:TYR:HE2	1.83	0.62
1:A:482:PHE:HE1	2:B:836:GLU:HG2	1.63	0.62
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.34	0.62
1:A:903:ASN:O	1:A:904:THR:C	2.36	0.62
2:B:451:LYS:HA	2:B:454:THR:HB	1.82	0.62
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.17	0.62
1:A:55:ASP:N	1:A:56:PRO:HD2	2.14	0.62
2:B:115:GLN:OE1	2:B:115:GLN:HA	1.99	0.62
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.62
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.14	0.62
2:B:390:LEU:HD13	2:B:392:ARG:HH12	1.63	0.62
2:B:458:LYS:O	2:B:462:ALA:HB2	1.99	0.62
2:B:1006:ILE:HD13	2:B:1006:ILE:N	2.13	0.62
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.80	0.62
1:A:663:SER:C	2:B:1014:PRO:HB3	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:SER:HA	2:B:476:ARG:NE	2.15	0.62
2:B:942:ARG:C	2:B:944:THR:H	2.02	0.62
2:B:834:ASN:HD22	2:B:834:ASN:N	1.97	0.62
4:E:46:TYR:CE2	4:E:58:MET:HA	2.35	0.62
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.81	0.61
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.82	0.61
1:A:357:PRO:HG3	2:B:832:GLY:C	2.19	0.61
2:B:215:GLN:O	2:B:406:LEU:HA	2.00	0.61
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.82	0.61
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.49	0.61
2:B:524:PRO:HD2	2:B:748:ILE:O	2.00	0.61
7:I:35:VAL:HG12	7:I:36:GLU:N	2.15	0.61
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.00	0.61
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.31	0.61
5:F:109:VAL:HG12	5:F:110:ASP:N	2.14	0.61
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.35	0.61
1:A:645:LEU:CD1	1:A:649:ILE:HD11	2.29	0.61
2:B:1084:GLN:C	2:B:1085:ILE:HG13	2.21	0.61
2:B:486:TYR:HE2	2:B:777:ALA:O	1.80	0.61
3:C:229:TYR:HD1	3:C:229:TYR:H	1.48	0.61
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.31	0.61
2:B:637:LEU:CD2	2:B:741:CYS:O	2.48	0.61
1:A:302:THR:HA	1:A:305:ASP:O	2.00	0.61
1:A:482:PHE:CE1	2:B:836:GLU:HG3	2.35	0.61
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.98	0.61
6:H:91:ASP:HA	6:H:93:TYR:HD1	1.66	0.61
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.81	0.61
1:A:1118:VAL:HG13	1:A:1327:ILE:HD11	1.83	0.61
8:J:1:MET:H1	8:J:56:LEU:N	1.99	0.61
3:C:66:ARG:O	3:C:68:GLY:N	2.34	0.61
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.83	0.61
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.65	0.61
1:A:814:PHE:O	1:A:817:ALA:HB3	2.00	0.61
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.33	0.61
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.31	0.61
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.33	0.61
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.81	0.60
1:A:900:ASP:O	1:A:907:THR:HA	2.01	0.60
2:B:986:GLN:NE2	2:B:986:GLN:O	2.30	0.60
2:B:904:ARG:CZ	2:B:948:ILE:HD11	2.30	0.60
1:A:1116:LEU:HD13	1:A:1329:THR:OG1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HG13	1:A:653:VAL:CG2	2.28	0.60
2:B:1096:ARG:HD3	2:B:1097:HIS:CA	2.30	0.60
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.83	0.60
12:T:18:DA:H2''	12:T:19:DT:H5'	1.82	0.60
1:A:504:LEU:HD11	5:F:91:ALA:HB1	1.82	0.60
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.00	0.60
1:A:380:VAL:HG11	1:A:428:TYR:H	1.66	0.60
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.48	0.60
2:B:33:VAL:HG11	2:B:638:PHE:CE2	2.36	0.60
2:B:315:LYS:N	2:B:316:PRO:HD2	2.16	0.60
1:A:353:ILE:HG12	1:A:487:MET:HE2	1.83	0.60
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.82	0.60
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.84	0.60
1:A:482:PHE:HD1	2:B:836:GLU:HB2	1.60	0.60
2:B:1004:GLU:HB3	2:B:1006:ILE:CD1	2.31	0.60
1:A:313:GLN:HG2	1:A:314:ALA:H	1.67	0.60
2:B:1028:GLU:OE1	2:B:1090:THR:CG2	2.48	0.60
2:B:1023:VAL:O	2:B:1026:LEU:HD12	2.01	0.60
1:A:765:VAL:HG13	1:A:802:ASN:O	2.00	0.60
1:A:670:ILE:HG22	1:A:671:ALA:H	1.66	0.60
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.17	0.60
6:H:135:LEU:HD13	6:H:137:GLN:HE22	1.66	0.60
2:B:733:HIS:O	2:B:735:ALA:N	2.34	0.60
1:A:483:ASP:CB	2:B:837:ASP:OD2	2.46	0.60
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.37	0.60
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.82	0.60
2:B:65:GLU:CD	2:B:66:ASP:H	2.04	0.60
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.66	0.60
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.32	0.60
4:E:83:CYS:HG	4:E:110:PHE:HE1	1.50	0.60
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.83	0.60
1:A:376:TYR:CD2	1:A:376:TYR:C	2.76	0.59
2:B:842:ASN:O	2:B:845:SER:N	2.27	0.59
1:A:757:ASN:O	1:A:761:MET:HG3	2.02	0.59
6:H:44:VAL:O	6:H:44:VAL:CG1	2.50	0.59
1:A:465:TYR:HB3	2:B:976:ILE:CG2	2.31	0.59
2:B:1028:GLU:CG	2:B:1090:THR:HG22	2.32	0.59
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.83	0.59
2:B:1013:ASN:ND2	2:B:1014:PRO:HD2	2.16	0.59
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.83	0.59
11:R:9:G:C2	12:T:21:DC:O2	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:ILE:HG22	1:A:1050:GLU:N	2.17	0.59
1:A:1121:GLU:OE2	1:A:1321:GLY:HA2	2.02	0.59
2:B:956:THR:HB	10:L:46:VAL:HG21	1.85	0.59
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.67	0.59
2:B:982:SER:OG	2:B:986:GLN:HB3	2.03	0.59
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.02	0.59
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.84	0.59
1:A:526:ASP:O	1:A:528:LEU:N	2.35	0.59
1:A:670:ILE:HG21	2:B:1067:ARG:HH21	1.67	0.59
11:R:9:G:C6	12:T:21:DC:N3	2.71	0.59
1:A:1384:VAL:HG12	1:A:1384:VAL:O	2.02	0.59
1:A:264:PHE:HZ	1:A:317:LYS:HB3	1.66	0.59
2:B:287:ARG:NH1	2:B:324:ILE:O	2.35	0.59
1:A:1261:LYS:C	1:A:1263:ILE:H	2.06	0.59
2:B:827:ILE:CG2	2:B:1012:ILE:HG13	2.27	0.59
2:B:765:PRO:O	2:B:767:ASN:N	2.35	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.03	0.59
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.85	0.59
4:E:6:GLU:O	4:E:9:ILE:HG22	2.03	0.59
2:B:791:THR:HA	2:B:858:SER:HB2	1.84	0.59
1:A:519:PRO:HG2	1:A:624:SER:O	2.03	0.58
9:K:102:LYS:O	9:K:106:GLU:HG2	2.02	0.58
3:C:148:ARG:O	3:C:151:GLN:HG3	2.03	0.58
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.42	0.58
2:B:637:LEU:HD13	2:B:637:LEU:H	1.66	0.58
2:B:1029:CYS:HB2	2:B:1090:THR:CG2	2.32	0.58
1:A:858:ASN:HD22	1:A:858:ASN:C	2.05	0.58
1:A:364:VAL:HG11	1:A:442:VAL:HG21	1.85	0.58
2:B:834:ASN:HB2	2:B:1013:ASN:HB2	1.85	0.58
7:I:103:CYS:SG	7:I:104:LEU:N	2.76	0.58
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.34	0.58
1:A:899:VAL:CG1	1:A:929:LEU:HD11	2.33	0.58
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.85	0.58
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.85	0.58
1:A:218:ASP:O	1:A:222:LEU:HG	2.03	0.58
2:B:825:VAL:HA	2:B:1010:LEU:O	2.03	0.58
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.68	0.58
2:B:1007:VAL:O	2:B:1007:VAL:CG1	2.48	0.58
3:C:254:LYS:HD3	9:K:42:LEU:HD12	1.86	0.58
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.86	0.58
1:A:527:THR:O	1:A:531:ILE:HB	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:LEU:O	2:B:799:PRO:HD3	2.03	0.58
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.68	0.58
6:H:58:THR:HG22	6:H:59:ILE:H	1.68	0.58
1:A:473:SER:OG	1:A:646:PHE:HD2	1.85	0.58
2:B:1151:LEU:O	2:B:1152:MET:CB	2.50	0.58
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.86	0.58
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.37	0.58
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.67	0.58
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.85	0.58
1:A:779:PHE:CE2	2:B:517:THR:HG22	2.39	0.58
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.34	0.58
7:I:111:THR:CG2	7:I:113:ASP:H	2.17	0.58
1:A:41:MET:HG3	1:A:49:LYS:HA	1.85	0.58
2:B:800:GLN:HB3	8:J:52:THR:HB	1.85	0.58
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.03	0.58
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.85	0.58
3:C:243:VAL:HG12	3:C:244:VAL:N	2.19	0.58
1:A:819:GLY:O	1:A:821:ARG:N	2.36	0.57
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.85	0.57
4:E:78:LEU:HD12	4:E:107:THR:HB	1.86	0.57
6:H:104:PHE:CZ	6:H:136:LYS:HA	2.39	0.57
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.04	0.57
8:J:28:ASP:OD1	8:J:28:ASP:N	2.34	0.57
2:B:803:LEU:N	2:B:822:ASN:ND2	2.51	0.57
2:B:1006:ILE:HG22	2:B:1007:VAL:H	1.69	0.57
2:B:759:PRO:CD	2:B:1046:PRO:HG3	2.34	0.57
10:L:60:ARG:HG3	10:L:61:THR:H	1.68	0.57
1:A:588:LEU:HD11	1:A:632:VAL:HG21	1.85	0.57
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.85	0.57
4:E:199:ILE:O	4:E:199:ILE:HG22	2.03	0.57
1:A:557:ASP:HA	9:K:26:LYS:CE	2.31	0.57
1:A:1021:LEU:O	1:A:1024:SER:N	2.37	0.57
1:A:341:MET:HB3	2:B:1132:GLU:HG3	1.85	0.57
2:B:773:MET:HA	2:B:776:GLN:HG3	1.85	0.57
2:B:1065:GLN:NE2	2:B:1069:PHE:H	2.02	0.57
1:A:481:ASP:CB	2:B:836:GLU:O	2.52	0.57
1:A:568:PRO:HD3	6:H:94:ASP:O	2.05	0.57
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.86	0.57
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.34	0.57
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.44	0.57
1:A:628:GLY:O	1:A:632:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:46:ILE:O	9:K:50:LEU:HB2	2.05	0.57
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.86	0.57
8:J:48:ARG:HH21	8:J:49:MET:CE	2.18	0.57
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.86	0.57
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.69	0.57
1:A:523:ILE:HG23	1:A:527:THR:HB	1.86	0.57
2:B:1029:CYS:HB2	2:B:1090:THR:HG21	1.86	0.57
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.86	0.57
5:F:105:ALA:HB1	5:F:106:PRO:CD	2.35	0.57
9:K:81:TYR:OH	9:K:86:ALA:HA	2.05	0.57
1:A:1000:LEU:HD23	1:A:1001:ARG:H	1.69	0.57
2:B:847:ASP:HB3	3:C:167:HIS:CE1	2.40	0.57
3:C:178:PHE:O	3:C:178:PHE:HD2	1.87	0.57
2:B:294:ASP:O	2:B:296:GLU:N	2.38	0.57
1:A:1116:LEU:HA	1:A:1329:THR:OG1	2.04	0.57
3:C:142:VAL:CG1	3:C:143:LEU:N	2.68	0.56
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.35	0.56
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.86	0.56
9:K:61:TYR:HA	9:K:72:LYS:O	2.05	0.56
1:A:203:SER:O	1:A:207:ILE:HD12	2.05	0.56
2:B:969:ARG:HH11	3:C:61:GLU:CD	2.09	0.56
1:A:350:ARG:HB2	1:A:487:MET:O	2.05	0.56
2:B:692:TYR:N	2:B:692:TYR:HD2	2.03	0.56
1:A:55:ASP:O	1:A:57:ARG:N	2.38	0.56
3:C:31:ASN:O	3:C:34:ARG:N	2.35	0.56
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.87	0.56
2:B:213:ILE:HD11	2:B:481:GLN:HG3	1.87	0.56
2:B:424:LEU:O	2:B:428:ILE:HG12	2.05	0.56
2:B:980:PHE:O	2:B:1095:LEU:CG	2.50	0.56
2:B:516:ASN:ND2	2:B:516:ASN:H	2.02	0.56
3:C:167:HIS:HD2	3:C:169:LYS:N	1.96	0.56
1:A:767:GLN:NE2	1:A:774:ARG:HE	2.03	0.56
2:B:650:GLU:HG3	2:B:651:LEU:N	2.21	0.56
1:A:494:SER:O	1:A:498:ARG:HG3	2.06	0.56
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.87	0.56
1:A:565:ILE:HG23	1:A:567:LYS:CG	2.34	0.56
8:J:44:TYR:C	8:J:44:TYR:CD1	2.79	0.56
3:C:176:ILE:HG12	3:C:232:VAL:HG13	1.88	0.56
1:A:543:LEU:CD1	1:A:547:LEU:HD11	2.36	0.56
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.88	0.56
1:A:479:ASN:O	1:A:480:ALA:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.86	0.56
2:B:711:GLU:H	2:B:712:PRO:CD	2.18	0.56
5:F:82:THR:HG22	5:F:84:TYR:HB2	1.86	0.56
1:A:623:GLY:C	1:A:625:SER:H	2.09	0.56
1:A:533:LYS:HD2	1:A:662:PHE:CD1	2.41	0.56
2:B:31:TRP:CH2	2:B:807:ARG:HB3	2.41	0.56
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.70	0.56
2:B:637:LEU:HD23	2:B:638:PHE:H	1.70	0.56
2:B:708:GLU:O	2:B:710:LEU:N	2.39	0.56
2:B:411:PRO:HA	2:B:414:ALA:HB3	1.88	0.56
1:A:352:VAL:HG12	1:A:353:ILE:N	2.22	0.55
3:C:143:LEU:C	3:C:143:LEU:HD12	2.27	0.55
6:H:135:LEU:HD13	6:H:137:GLN:NE2	2.21	0.55
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.87	0.55
2:B:636:PRO:O	2:B:691:GLU:O	2.23	0.55
1:A:741:ASN:HD22	1:A:744:LYS:H	1.54	0.55
2:B:824:ILE:HD13	2:B:1089:PRO:HA	1.87	0.55
1:A:793:SER:HB2	1:A:794:PRO:CD	2.37	0.55
1:A:318:SER:HA	12:T:28:DT:C2'	2.37	0.55
2:B:815:ARG:HB2	2:B:816:GLU:OE1	2.05	0.55
3:C:241:ASP:HB3	9:K:109:TRP:CH2	2.40	0.55
3:C:33:LEU:O	3:C:36:VAL:HG12	2.07	0.55
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.70	0.55
2:B:512:ARG:HH21	2:B:533:CYS:H	1.54	0.55
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.71	0.55
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.89	0.55
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.07	0.55
2:B:827:ILE:CG2	2:B:1012:ILE:HD11	2.28	0.55
2:B:473:MET:O	2:B:476:ARG:HG3	2.06	0.55
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.36	0.55
1:A:885:THR:O	1:A:940:ARG:HG3	2.06	0.55
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.72	0.55
1:A:1232:ASN:OD1	1:A:1232:ASN:N	2.40	0.55
10:L:55:ILE:O	10:L:56:LEU:CB	2.54	0.55
1:A:670:ILE:HG21	2:B:1067:ARG:NH2	2.22	0.55
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.40	0.55
1:A:982:THR:C	1:A:984:LYS:H	2.10	0.55
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.72	0.55
4:E:177:ARG:HD3	4:E:215:MET:SD	2.47	0.55
1:A:956:LEU:HD23	1:A:957:PRO:HD2	1.88	0.55
2:B:859:TYR:HB2	2:B:966:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:PHE:O	1:A:782:ARG:O	2.25	0.55
2:B:401:PHE:CD2	2:B:521:LEU:HD12	2.40	0.55
1:A:488:ASN:ND2	2:B:1128:LEU:HD22	2.22	0.55
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.33	0.54
8:J:57:ILE:HA	8:J:60:PHE:HD2	1.72	0.54
2:B:258:LEU:HD13	2:B:269:ILE:HG12	1.89	0.54
2:B:692:TYR:CD2	2:B:692:TYR:N	2.75	0.54
1:A:405:VAL:O	1:A:413:ILE:HB	2.07	0.54
3:C:66:ARG:HH22	8:J:4:PRO:CA	2.20	0.54
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.88	0.54
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.41	0.54
1:A:599:SER:HG	1:A:614:PHE:HD1	1.56	0.54
1:A:893:PHE:CD2	1:A:893:PHE:C	2.81	0.54
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.72	0.54
1:A:527:THR:HG21	1:A:650:GLN:HG3	1.90	0.54
1:A:567:LYS:CB	6:H:96:VAL:H	2.06	0.54
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.89	0.54
1:A:27:VAL:O	1:A:30:ILE:HG22	2.08	0.54
1:A:657:LEU:HD21	2:B:829:CYS:HB3	1.89	0.54
5:F:81:THR:OG1	5:F:144:GLU:OE1	2.24	0.54
2:B:901:PRO:HD3	2:B:952:VAL:HG23	1.89	0.54
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.07	0.54
1:A:535:THR:HG21	1:A:617:VAL:N	2.11	0.54
2:B:1017:ILE:HD12	2:B:1026:LEU:CD2	2.33	0.54
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.42	0.54
2:B:682:SER:O	2:B:686:ASN:ND2	2.40	0.54
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.71	0.54
2:B:860:MET:SD	2:B:861:ASP:N	2.81	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.71	0.54
1:A:663:SER:OG	2:B:828:ALA:CB	2.55	0.54
8:J:43:ARG:HH11	8:J:43:ARG:HB3	1.71	0.54
9:K:35:PHE:CB	9:K:71:PHE:CE2	2.91	0.54
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.08	0.54
1:A:349:ALA:HB1	1:A:370:ILE:HD13	1.90	0.54
3:C:78:GLU:OE1	3:C:246:ARG:HG2	2.07	0.54
2:B:1153:GLU:OE2	2:B:1153:GLU:HA	2.07	0.54
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.90	0.54
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.89	0.54
1:A:569:LYS:HE3	3:C:222:LYS:HA	1.90	0.54
2:B:637:LEU:O	2:B:690:VAL:HA	2.08	0.54
1:A:523:ILE:H	1:A:523:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE3	2:B:796:LEU:HD12	1.90	0.54
2:B:816:GLU:O	8:J:56:LEU:HD21	2.07	0.54
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.57	0.54
1:A:54:ASN:O	1:A:55:ASP:HB2	2.08	0.54
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.90	0.54
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.54
1:A:526:ASP:O	1:A:529:CYS:N	2.40	0.53
1:A:642:CYS:O	1:A:645:LEU:HB3	2.07	0.53
1:A:663:SER:O	2:B:1014:PRO:HB3	2.09	0.53
2:B:843:GLN:O	2:B:847:ASP:OD1	2.25	0.53
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.05	0.53
2:B:955:THR:CG2	2:B:956:THR:N	2.71	0.53
1:A:901:LEU:N	1:A:926:GLN:HE21	2.06	0.53
1:A:364:VAL:HG13	1:A:366:VAL:HG23	1.90	0.53
3:C:21:ILE:HG22	3:C:22:LEU:N	2.24	0.53
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.91	0.53
1:A:550:LEU:HG	1:A:556:TRP:CE2	2.44	0.53
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.89	0.53
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.89	0.53
2:B:955:THR:CG2	2:B:956:THR:H	2.22	0.53
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.08	0.53
1:A:376:TYR:HD2	1:A:376:TYR:C	2.10	0.53
10:L:46:VAL:HG12	10:L:47:ARG:N	2.22	0.53
1:A:31:SER:HB2	1:A:81:PHE:O	2.09	0.53
7:I:73:ARG:HG3	7:I:101:PHE:CE2	2.43	0.53
2:B:635:ARG:O	2:B:636:PRO:O	2.26	0.53
2:B:780:VAL:HG11	2:B:817:LEU:HG	1.89	0.53
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.74	0.53
1:A:399:HIS:O	1:A:401:GLY:N	2.41	0.53
1:A:396:PRO:C	1:A:397:ASN:OD1	2.47	0.53
2:B:635:ARG:O	2:B:636:PRO:C	2.45	0.53
1:A:512:VAL:CG1	1:A:512:VAL:O	2.57	0.53
1:A:344:ARG:NH1	1:A:344:ARG:CG	2.71	0.53
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.74	0.53
2:B:952:VAL:HG12	2:B:953:LEU:N	2.24	0.53
2:B:430:ARG:HG2	2:B:433:GLN:NE2	2.24	0.53
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.89	0.53
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.90	0.53
1:A:575:LYS:CD	1:A:612:ILE:HD11	2.38	0.53
3:C:248:ILE:HG12	9:K:101:LEU:HD13	1.89	0.53
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:ASP:HB3	10:L:67:PHE:CZ	2.43	0.53
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.91	0.53
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.30	0.53
7:I:78:CYS:O	7:I:79:HIS:CB	2.56	0.53
6:H:91:ASP:C	6:H:93:TYR:H	2.12	0.53
4:E:213:ILE:HG12	4:E:214:CYS:H	1.74	0.53
1:A:1427:ASN:H	1:A:1427:ASN:HD22	1.57	0.53
3:C:5:GLY:O	3:C:7:GLN:HG2	2.08	0.53
1:A:760:GLN:HE21	1:A:765:VAL:HA	1.74	0.53
1:A:401:GLY:H	1:A:435:HIS:CD2	2.17	0.53
2:B:286:PHE:HB3	2:B:297:ILE:CD1	2.39	0.53
1:A:858:ASN:ND2	1:A:862:ASN:H	2.07	0.53
1:A:880:LYS:HA	1:A:955:PRO:HA	1.91	0.53
1:A:491:VAL:O	1:A:493:GLN:NE2	2.42	0.53
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.91	0.53
1:A:49:LYS:O	1:A:50:ILE:HG12	2.09	0.53
1:A:514:PRO:O	1:A:515:GLN:C	2.45	0.53
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.91	0.53
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.89	0.53
2:B:917:PRO:HA	2:B:934:LYS:HA	1.89	0.53
9:K:35:PHE:HB2	9:K:71:PHE:CD2	2.43	0.52
1:A:904:THR:O	1:A:905:ASP:C	2.46	0.52
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.09	0.52
2:B:301:ILE:HG22	2:B:302:CYS:N	2.24	0.52
2:B:302:CYS:SG	2:B:304:ASP:O	2.66	0.52
2:B:842:ASN:HD22	2:B:845:SER:CB	2.20	0.52
2:B:842:ASN:O	2:B:843:GLN:C	2.46	0.52
11:R:5:A:C2	11:R:6:G:C5	2.98	0.52
1:A:1436:ILE:O	1:A:1437:GLY:C	2.47	0.52
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.91	0.52
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.44	0.52
1:A:982:THR:C	1:A:984:LYS:N	2.61	0.52
6:H:2:SER:O	6:H:3:ASN:HB2	2.10	0.52
1:A:446:ARG:NH1	1:A:479:ASN:O	2.42	0.52
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.40	0.52
2:B:1096:ARG:CD	2:B:1097:HIS:N	2.33	0.52
2:B:841:MET:HG2	2:B:1009:ASP:O	2.09	0.52
2:B:850:LEU:HB2	8:J:8:PHE:CB	2.38	0.52
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.44	0.52
2:B:708:GLU:O	2:B:712:PRO:HD3	2.09	0.52
2:B:750:GLY:O	2:B:752:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:111:THR:HG23	7:I:113:ASP:H	1.74	0.52
1:A:117:GLU:HG3	1:A:126:LEU:HD13	1.91	0.52
1:A:95:PHE:O	1:A:99:ILE:HG13	2.09	0.52
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.45	0.52
2:B:256:VAL:CG1	2:B:382:ILE:HD11	2.39	0.52
6:H:98:TYR:C	6:H:118:PHE:HD2	2.13	0.52
1:A:1407:GLU:HA	1:A:1410:PHE:HB2	1.90	0.52
2:B:215:GLN:NE2	2:B:499:ASN:HB3	2.25	0.52
8:J:44:TYR:CD1	8:J:45:CYS:N	2.78	0.52
2:B:486:TYR:CD2	2:B:777:ALA:O	2.62	0.52
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.28	0.52
2:B:205:ILE:O	2:B:206:ASN:HB2	2.09	0.52
2:B:830:TYR:N	2:B:834:ASN:OD1	2.34	0.52
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.10	0.52
7:I:29:CYS:SG	7:I:31:THR:HB	2.50	0.52
1:A:385:ILE:O	1:A:389:THR:HB	2.09	0.52
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.43	0.52
7:I:71:SER:HB3	7:I:85:PHE:CE2	2.45	0.52
9:K:57:LEU:HD12	9:K:76:GLN:HG2	1.90	0.52
2:B:637:LEU:HG	2:B:741:CYS:O	2.09	0.52
2:B:1084:GLN:O	2:B:1085:ILE:CG1	2.58	0.52
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.92	0.52
8:J:43:ARG:NH1	8:J:43:ARG:HB3	2.25	0.52
3:C:69:LEU:HD12	8:J:6:ARG:HB2	1.92	0.52
1:A:858:ASN:HD21	1:A:862:ASN:H	1.55	0.52
1:A:304:MET:SD	2:B:1210:MET:HG3	2.50	0.52
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.92	0.52
1:A:564:ALA:N	1:A:576:GLN:OE1	2.39	0.52
1:A:575:LYS:O	1:A:579:SER:OG	2.27	0.52
7:I:35:VAL:HG12	7:I:36:GLU:H	1.74	0.52
2:B:549:THR:HG22	2:B:550:ASP:H	1.75	0.52
2:B:1119:VAL:O	2:B:1126:GLY:HA2	2.09	0.52
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.42	0.52
1:A:660:ASN:OD1	2:B:1082:MET:CG	2.58	0.52
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.75	0.52
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.10	0.52
1:A:353:ILE:HG13	1:A:485:ASP:O	2.09	0.52
2:B:996:ARG:CG	2:B:1007:VAL:HG21	2.36	0.52
6:H:59:ILE:O	6:H:60:ALA:HB3	2.10	0.52
2:B:482:VAL:O	2:B:483:LEU:C	2.47	0.52
1:A:182:VAL:HG13	1:A:201:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:HG22	1:A:41:MET:SD	2.50	0.52
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.74	0.52
2:B:792:MET:CE	2:B:857:ARG:HG2	2.40	0.52
1:A:526:ASP:N	2:B:1015:HIS:NE2	2.59	0.51
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.91	0.51
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.10	0.51
9:K:43:GLY:CA	9:K:71:PHE:CE1	2.92	0.51
2:B:998:ASP:OD2	2:B:998:ASP:N	2.39	0.51
3:C:52:GLU:O	3:C:53:THR:HG23	2.10	0.51
4:E:127:ILE:HG12	4:E:127:ILE:O	2.09	0.51
2:B:942:ARG:C	2:B:944:THR:N	2.63	0.51
1:A:789:LYS:HB2	7:I:67:THR:O	2.10	0.51
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.56	0.51
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.74	0.51
1:A:1064:VAL:O	1:A:1064:VAL:CG1	2.55	0.51
1:A:1441:PHE:CE2	5:F:89:GLU:HG3	2.46	0.51
3:C:69:LEU:HB3	8:J:6:ARG:HD3	1.93	0.51
2:B:980:PHE:O	2:B:1095:LEU:CD1	2.58	0.51
2:B:1023:VAL:HG12	2:B:1027:ILE:CD1	2.41	0.51
7:I:8:ARG:O	7:I:9:ASP:CB	2.58	0.51
1:A:341:MET:HE2	1:A:1401:SER:HB2	1.92	0.51
2:B:386:LEU:C	2:B:388:CYS:H	2.14	0.51
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	1.92	0.51
1:A:1423:GLY:O	1:A:1425:SER:N	2.44	0.51
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.59	0.51
2:B:942:ARG:O	2:B:944:THR:N	2.44	0.51
8:J:17:LYS:HE2	8:J:39:LEU:O	2.11	0.51
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.91	0.51
2:B:302:CYS:HB2	2:B:310:MET:HG2	1.92	0.51
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.92	0.51
6:H:58:THR:CG2	6:H:59:ILE:N	2.72	0.51
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.93	0.51
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	2.11	0.51
2:B:900:ALA:O	2:B:902:GLY:N	2.43	0.51
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.91	0.51
10:L:34:CYS:O	10:L:35:SER:CB	2.59	0.51
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	1.91	0.51
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.10	0.51
1:A:565:ILE:HA	1:A:567:LYS:HE3	1.92	0.51
1:A:889:SER:HB2	1:A:892:ALA:H	1.76	0.51
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HD11	1:A:433:GLU:OE2	2.11	0.51
2:B:839:MET:HE3	2:B:1010:LEU:HD13	1.93	0.51
2:B:780:VAL:HG12	2:B:817:LEU:CD2	2.40	0.51
2:B:996:ARG:HB3	2:B:996:ARG:HH11	1.76	0.51
1:A:323:LYS:O	1:A:324:SER:CB	2.58	0.51
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.26	0.51
1:A:351:THR:HG21	1:A:466:SER:O	2.11	0.51
4:E:77:SER:CB	4:E:105:PHE:HA	2.41	0.51
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.93	0.51
2:B:776:GLN:NE2	11:R:9:G:OP1	2.40	0.51
5:F:97:ARG:HD2	5:F:101:ILE:HD11	1.92	0.51
2:B:1064:TYR:CD1	2:B:1064:TYR:N	2.79	0.51
2:B:458:LYS:O	2:B:462:ALA:CB	2.58	0.51
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.93	0.51
1:A:35:ILE:HG22	1:A:270:LEU:HD11	1.93	0.51
9:K:7:PHE:C	9:K:9:LEU:H	2.15	0.51
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.74	0.51
1:A:504:LEU:HD12	1:A:504:LEU:N	2.25	0.50
1:A:645:LEU:O	1:A:649:ILE:HG13	2.10	0.50
2:B:1152:MET:HE2	2:B:1196:ILE:HA	1.93	0.50
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.92	0.50
3:C:178:PHE:CD2	3:C:178:PHE:O	2.61	0.50
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.94	0.50
1:A:98:LYS:O	1:A:102:VAL:HG23	2.11	0.50
2:B:1007:VAL:O	2:B:1008:PRO:O	2.29	0.50
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.93	0.50
1:A:1271:ILE:HG22	1:A:1273:LEU:HD12	1.93	0.50
1:A:824:LEU:HB3	2:B:529:GLU:OE1	2.12	0.50
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.24	0.50
8:J:8:PHE:H	8:J:49:MET:CE	2.17	0.50
2:B:487:THR:CG2	2:B:488:TYR:N	2.75	0.50
1:A:399:HIS:HD2	1:A:400:PRO:HG3	1.75	0.50
1:A:276:LEU:HD21	1:A:293:GLU:HG2	1.92	0.50
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.92	0.50
2:B:474:SER:HA	2:B:476:ARG:CZ	2.40	0.50
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.45	0.50
1:A:471:ASN:O	1:A:474:VAL:N	2.43	0.50
3:C:145:CYS:SG	3:C:146:LYS:N	2.84	0.50
1:A:473:SER:OG	1:A:646:PHE:CD2	2.53	0.50
9:K:40:HIS:HE1	9:K:63:VAL:HG22	1.77	0.50
1:A:343:LYS:HB3	2:B:1155:SER:OG	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD12	3:C:157:CYS:CB	2.41	0.50
1:A:68:GLN:O	1:A:70:CYS:N	2.44	0.50
3:C:31:ASN:C	3:C:33:LEU:H	2.14	0.50
2:B:512:ARG:NH2	2:B:533:CYS:H	2.10	0.50
2:B:1029:CYS:CA	2:B:1090:THR:HG23	2.41	0.50
2:B:996:ARG:CB	2:B:996:ARG:HH11	2.24	0.50
6:H:95:TYR:CD2	6:H:95:TYR:C	2.85	0.50
2:B:407:ASP:HB3	2:B:412:LEU:CD2	2.42	0.50
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.26	0.50
1:A:1059:HIS:CE1	5:F:86:THR:HA	2.47	0.50
9:K:49:GLU:HA	9:K:52:ASN:HD22	1.77	0.50
2:B:329:THR:HA	2:B:332:ASP:HB3	1.94	0.50
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.46	0.50
2:B:763:GLN:O	2:B:764:SER:O	2.30	0.50
1:A:471:ASN:O	1:A:472:LEU:C	2.50	0.50
1:A:1021:LEU:CD1	1:A:1025:ARG:HE	2.23	0.50
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.47	0.50
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.76	0.50
2:B:278:GLN:CG	2:B:279:ASP:H	2.12	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
1:A:678:GLU:HA	1:A:681:GLU:CG	2.41	0.50
7:I:111:THR:HG23	7:I:112:SER:N	2.27	0.50
1:A:587:HIS:HA	1:A:607:ILE:O	2.12	0.50
12:T:15:DA:N3	12:T:15:DA:H2'	2.26	0.50
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.27	0.50
2:B:808:ALA:O	2:B:812:LEU:HG	2.11	0.50
3:C:249:ASP:O	3:C:253:LYS:HG3	2.11	0.50
2:B:636:PRO:C	2:B:691:GLU:O	2.50	0.50
1:A:522:GLY:O	1:A:523:ILE:O	2.30	0.50
2:B:765:PRO:O	2:B:766:ARG:C	2.50	0.50
3:C:34:ARG:O	3:C:37:MET:HB3	2.11	0.50
1:A:587:HIS:CE1	1:A:609:ASP:H	2.29	0.50
1:A:685:GLU:O	1:A:689:LYS:HB2	2.12	0.50
1:A:577:ILE:O	1:A:580:VAL:HB	2.12	0.50
2:B:249:ARG:HE	2:B:249:ARG:HA	1.76	0.50
1:A:524:VAL:O	1:A:525:GLN:O	2.30	0.49
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.11	0.49
2:B:465:ASN:O	2:B:467:GLY:N	2.45	0.49
1:A:855:THR:HG21	1:A:857:ARG:HE	1.77	0.49
2:B:519:TRP:C	2:B:519:TRP:CD1	2.85	0.49
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:57:ILE:O	8:J:61:LEU:HG	2.12	0.49
2:B:248:SER:H	2:B:418:LYS:HE3	1.77	0.49
1:A:599:SER:C	1:A:601:LYS:H	2.15	0.49
2:B:837:ASP:O	2:B:838:SER:O	2.30	0.49
2:B:843:GLN:HB3	2:B:995:ARG:HG3	1.95	0.49
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.47	0.49
2:B:1058:LEU:O	2:B:1062:HIS:HB2	2.12	0.49
1:A:562:THR:HB	6:H:98:TYR:CE2	2.48	0.49
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.32	0.49
2:B:176:SER:OG	2:B:177:LYS:N	2.44	0.49
2:B:654:ARG:H	2:B:657:HIS:HD2	1.60	0.49
2:B:1096:ARG:O	2:B:1097:HIS:O	2.30	0.49
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.27	0.49
11:R:2:U:H2'	11:R:3:C:C6	2.47	0.49
1:A:1434:ALA:O	1:A:1436:ILE:N	2.46	0.49
2:B:519:TRP:O	2:B:519:TRP:CD1	2.65	0.49
1:A:982:THR:O	1:A:984:LYS:N	2.45	0.49
11:R:4:G:C2'	11:R:5:A:H8	2.04	0.49
2:B:708:GLU:HG3	2:B:709:ASP:N	2.24	0.49
2:B:1031:LEU:HD12	2:B:1031:LEU:C	2.32	0.49
1:A:67:CYS:O	1:A:68:GLN:HG3	2.13	0.49
1:A:904:THR:HG22	1:A:905:ASP:N	2.27	0.49
9:K:36:GLU:O	9:K:37:LYS:C	2.50	0.49
4:E:2:ASP:O	4:E:3:GLN:HB3	2.13	0.49
12:T:26:DG:H21	12:T:27:DA:H1'	1.77	0.49
2:B:546:SER:OG	2:B:631:GLY:N	2.45	0.49
1:A:382:PRO:CD	1:A:428:TYR:CE2	2.95	0.49
1:A:1030:ARG:O	1:A:1031:VAL:C	2.50	0.49
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.94	0.49
1:A:79:GLY:O	1:A:243:PRO:HG3	2.12	0.49
4:E:93:MET:HG2	4:E:120:ALA:O	2.12	0.49
2:B:108:VAL:HG12	2:B:109:THR:H	1.76	0.49
7:I:15:TYR:CE1	7:I:30:ARG:HG3	2.48	0.49
1:A:1328:TYR:OH	1:A:1351:GLU:OE1	2.30	0.49
1:A:91:PHE:HB3	1:A:96:ILE:HD11	1.95	0.49
2:B:803:LEU:HD12	2:B:1089:PRO:HB2	1.94	0.49
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.95	0.49
7:I:28:GLU:OE2	7:I:29:CYS:O	2.30	0.49
2:B:493:SER:OG	2:B:775:LYS:HE3	2.13	0.49
3:C:76:ASP:O	3:C:79:GLN:HG2	2.13	0.49
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ASN:O	1:A:123:ARG:HG3	2.13	0.49
4:E:41:ASP:O	4:E:45:LYS:HB2	2.12	0.49
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.28	0.49
4:E:15:ALA:O	4:E:19:VAL:HG23	2.12	0.49
8:J:48:ARG:O	8:J:48:ARG:HD2	2.13	0.49
1:A:899:VAL:CG2	1:A:1029:ARG:HB2	2.43	0.49
3:C:99:LEU:CD2	3:C:120:ILE:HA	2.38	0.49
6:H:139:ASN:O	6:H:140:ALA:CB	2.61	0.49
1:A:1066:VAL:HG11	2:B:1136:ASP:O	2.13	0.49
1:A:1423:GLY:O	1:A:1424:VAL:C	2.51	0.49
8:J:41:LEU:O	8:J:47:ARG:HG3	2.13	0.49
1:A:929:LEU:CD2	1:A:983:ILE:CG2	2.90	0.49
8:J:1:MET:H3	8:J:56:LEU:H	1.59	0.49
1:A:403:LYS:HB2	1:A:404:TYR:CD1	2.48	0.49
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	2.28	0.49
1:A:382:PRO:N	1:A:428:TYR:HE2	2.11	0.49
1:A:1329:THR:HG22	1:A:1331:SER:H	1.77	0.49
4:E:19:VAL:O	4:E:23:VAL:HG23	2.13	0.49
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.52	0.49
2:B:1096:ARG:O	2:B:1098:MET:HE2	2.13	0.49
2:B:412:LEU:CD1	2:B:479:VAL:CG1	2.89	0.49
3:C:71:PRO:HG3	8:J:13:VAL:HG11	1.95	0.49
2:B:470:LYS:O	2:B:471:LYS:HG3	2.12	0.49
1:A:438:ASP:HA	1:A:460:VAL:O	2.13	0.48
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.48
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	2.96	0.48
1:A:314:ALA:HB1	1:A:315:LEU:HD22	1.94	0.48
12:T:27:DA:H2'	12:T:28:DT:H5'	1.94	0.48
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.41	0.48
2:B:329:THR:HA	2:B:332:ASP:CB	2.43	0.48
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.48	0.48
3:C:233:GLU:OE1	8:J:12:LYS:HE2	2.12	0.48
10:L:34:CYS:O	10:L:35:SER:HB2	2.12	0.48
3:C:102:GLN:O	3:C:103:ALA:HB2	2.13	0.48
2:B:814:PHE:O	2:B:816:GLU:N	2.46	0.48
1:A:396:PRO:O	1:A:397:ASN:OD1	2.31	0.48
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.96	0.48
2:B:1029:CYS:HA	2:B:1090:THR:HG23	1.95	0.48
1:A:361:LEU:CD1	1:A:473:SER:HB3	2.40	0.48
2:B:1017:ILE:CD1	2:B:1026:LEU:CD2	2.91	0.48
1:A:1292:PRO:HD3	1:A:1298:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:128:ASN:O	6:H:131:ASN:ND2	2.47	0.48
2:B:635:ARG:NH2	2:B:698:GLU:OE2	2.46	0.48
2:B:1098:MET:CB	2:B:1101:ASP:OD2	2.58	0.48
2:B:826:ALA:HB3	2:B:1011:ILE:HG23	1.94	0.48
1:A:777:PHE:HD2	1:A:782:ARG:C	2.17	0.48
2:B:283:VAL:HG12	2:B:297:ILE:HG21	1.94	0.48
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.93	0.48
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.86	0.48
1:A:443:LEU:HD12	2:B:1146:PHE:HZ	1.75	0.48
1:A:346:ASP:HB2	2:B:1154:ALA:HB1	1.94	0.48
2:B:708:GLU:CG	2:B:709:ASP:H	2.17	0.48
1:A:68:GLN:C	1:A:70:CYS:H	2.16	0.48
1:A:858:ASN:ND2	1:A:858:ASN:C	2.67	0.48
1:A:380:VAL:CG2	1:A:430:TRP:HB2	2.43	0.48
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.95	0.48
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.13	0.48
2:B:430:ARG:HG2	2:B:433:GLN:HE22	1.78	0.48
1:A:525:GLN:HB3	2:B:835:GLN:HG3	1.89	0.48
2:B:848:ARG:CB	8:J:8:PHE:HA	2.44	0.48
2:B:980:PHE:CE2	2:B:1094:ARG:CG	2.96	0.48
1:A:372:LYS:O	1:A:435:HIS:CE1	2.67	0.48
10:L:59:ALA:O	10:L:60:ARG:HB2	2.14	0.48
1:A:775:ILE:HG13	1:A:798:GLY:CA	2.43	0.48
6:H:113:ALA:HA	6:H:125:LEU:O	2.13	0.48
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.93	0.48
2:B:834:ASN:N	2:B:834:ASN:ND2	2.61	0.48
2:B:976:ILE:HD11	2:B:992:ILE:CD1	2.39	0.48
2:B:911:ILE:CD1	2:B:941:LEU:HD23	2.44	0.48
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	2.04	0.48
3:C:186:LEU:HD23	3:C:188:HIS:NE2	2.28	0.48
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.95	0.48
1:A:320:ARG:HB3	1:A:321:PRO:HA	1.96	0.48
2:B:1152:MET:O	2:B:1153:GLU:C	2.52	0.48
1:A:1339:LEU:HD11	4:E:147:HIS:CD2	2.49	0.48
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.48
2:B:637:LEU:HD23	2:B:741:CYS:O	2.14	0.48
1:A:463:ILE:HG22	1:A:464:PRO:HD2	1.96	0.48
1:A:464:PRO:HB2	1:A:465:TYR:CD1	2.48	0.48
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.47	0.48
1:A:315:LEU:CB	1:A:316:GLN:CA	2.83	0.48
12:T:27:DA:N3	12:T:27:DA:H2'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	1.94	0.48
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.49	0.48
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.43	0.48
1:A:741:ASN:ND2	1:A:744:LYS:H	2.12	0.47
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.14	0.47
2:B:827:ILE:HA	2:B:1012:ILE:HG13	1.96	0.47
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.96	0.47
1:A:361:LEU:O	1:A:363:GLN:N	2.46	0.47
2:B:1151:LEU:N	2:B:1151:LEU:HD12	2.29	0.47
6:H:63:LEU:CB	6:H:90:ALA:HB2	2.41	0.47
4:E:114:ASN:O	4:E:115:ASN:HB3	2.14	0.47
1:A:826:ASP:O	1:A:830:LYS:N	2.47	0.47
2:B:690:VAL:HG12	2:B:691:GLU:N	2.29	0.47
2:B:825:VAL:HG23	2:B:1010:LEU:O	2.14	0.47
9:K:82:ASP:OD2	9:K:84:LYS:HB2	2.14	0.47
3:C:56:THR:HG22	3:C:147:LEU:CD2	2.44	0.47
2:B:1013:ASN:OD1	2:B:1015:HIS:CD2	2.68	0.47
2:B:1023:VAL:HA	2:B:1026:LEU:CD1	2.43	0.47
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.96	0.47
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.79	0.47
1:A:901:LEU:HB2	1:A:926:GLN:CG	2.45	0.47
1:A:672:ASP:H	1:A:736:ASN:ND2	2.08	0.47
1:A:947:PHE:CD2	1:A:954:TRP:CE2	3.02	0.47
1:A:592:ASP:HB3	1:A:593:GLU:H	1.52	0.47
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.97	0.47
2:B:459:TYR:C	2:B:459:TYR:CD2	2.87	0.47
8:J:7:CYS:HB3	8:J:46:CYS:SG	2.54	0.47
2:B:216:GLU:HB2	2:B:499:ASN:O	2.13	0.47
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.79	0.47
2:B:899:ILE:CD1	2:B:966:VAL:HG11	2.44	0.47
2:B:545:ILE:HG23	2:B:631:GLY:HA2	1.95	0.47
3:C:133:ILE:HD11	3:C:237:SER:HA	1.97	0.47
1:A:380:VAL:CG1	1:A:428:TYR:HA	2.45	0.47
1:A:522:GLY:O	1:A:523:ILE:C	2.51	0.47
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.47
2:B:477:ALA:O	11:R:6:G:H5'	2.15	0.47
1:A:535:THR:CG2	1:A:616:VAL:HA	2.44	0.47
3:C:52:GLU:CD	3:C:154:LYS:HG2	2.35	0.47
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.95	0.47
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.97	0.47
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:7:CYS:SG	8:J:9:SER:N	2.88	0.47
6:H:61:SER:HB2	6:H:139:ASN:HB3	1.95	0.47
1:A:590:ARG:NH1	1:A:590:ARG:HG3	2.12	0.47
1:A:821:ARG:CZ	2:B:514:LEU:HB2	2.44	0.47
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.50	0.47
9:K:65:HIS:HA	9:K:66:PRO:HD2	1.63	0.47
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.96	0.47
2:B:803:LEU:H	2:B:822:ASN:ND2	2.01	0.47
2:B:464:GLY:N	2:B:480:SER:CB	2.78	0.47
1:A:475:THR:HG23	1:A:475:THR:O	2.13	0.47
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.45	0.47
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.97	0.47
4:E:78:LEU:HD12	4:E:107:THR:CB	2.44	0.47
1:A:264:PHE:CZ	1:A:317:LYS:HB3	2.48	0.47
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.15	0.47
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.30	0.47
2:B:1084:GLN:C	2:B:1085:ILE:CG1	2.83	0.47
1:A:346:ASP:O	1:A:347:PHE:C	2.52	0.47
4:E:77:SER:HB2	4:E:105:PHE:HA	1.94	0.47
2:B:44:VAL:HG11	2:B:495:LEU:CD1	2.44	0.47
2:B:411:PRO:HA	2:B:414:ALA:CB	2.44	0.47
2:B:530:GLY:O	2:B:531:GLN:C	2.53	0.47
2:B:37:PHE:O	2:B:38:PHE:HB2	2.15	0.47
2:B:467:GLY:O	2:B:468:GLU:CB	2.63	0.47
2:B:1076:HIS:ND1	9:K:40:HIS:NE2	2.62	0.47
9:K:63:VAL:HG23	9:K:63:VAL:O	2.15	0.47
3:C:63:ILE:O	3:C:66:ARG:N	2.48	0.47
1:A:57:ARG:HA	1:A:68:GLN:HB3	1.96	0.47
1:A:562:THR:HB	6:H:98:TYR:CD2	2.50	0.47
1:A:446:ARG:HE	1:A:480:ALA:CB	2.26	0.47
1:A:665:GLY:CA	2:B:1086:PHE:CD1	2.97	0.47
1:A:804:TYR:OH	2:B:763:GLN:HB2	2.15	0.47
2:B:493:SER:HA	2:B:751:VAL:HG11	1.96	0.47
4:E:136:ASN:OD1	4:E:137:GLU:N	2.48	0.47
2:B:175:ARG:CG	2:B:175:ARG:O	2.63	0.47
2:B:384:ARG:HD2	2:B:384:ARG:HA	1.60	0.47
2:B:1013:ASN:CG	2:B:1014:PRO:CD	2.74	0.46
5:F:147:SER:C	5:F:149:GLU:H	2.19	0.46
3:C:31:ASN:C	3:C:33:LEU:N	2.68	0.46
2:B:175:ARG:HG3	2:B:175:ARG:O	2.16	0.46
3:C:93:ASP:O	3:C:127:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:O	1:A:104:GLU:HG3	2.14	0.46
8:J:48:ARG:HH21	8:J:49:MET:HE2	1.80	0.46
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.80	0.46
5:F:128:LYS:CD	5:F:149:GLU:HA	2.39	0.46
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.97	0.46
2:B:228:LYS:HD3	2:B:234:ILE:HB	1.96	0.46
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.55	0.46
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.98	0.46
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.79	0.46
1:A:744:LYS:O	1:A:748:MET:HG3	2.14	0.46
2:B:1102:LYS:O	2:B:1104:HIS:N	2.48	0.46
2:B:590:HIS:CD2	2:B:591:ARG:O	2.69	0.46
2:B:998:ASP:N	3:C:35:ARG:HH21	2.14	0.46
1:A:382:PRO:CD	1:A:428:TYR:HE2	2.28	0.46
3:C:152:GLU:O	3:C:153:LEU:HB2	2.15	0.46
2:B:277:LYS:HE3	2:B:335:GLY:O	2.15	0.46
2:B:628:THR:O	2:B:628:THR:HG22	2.15	0.46
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.46
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.81	0.46
1:A:374:LEU:HD22	1:A:491:VAL:HG23	1.98	0.46
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.97	0.46
1:A:1343:ALA:O	1:A:1344:GLY:C	2.53	0.46
1:A:1079:MET:HG2	1:A:1359:ASP:OD1	2.15	0.46
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.16	0.46
2:B:325:GLN:O	2:B:325:GLN:HG3	2.15	0.46
2:B:850:LEU:CD1	8:J:8:PHE:CD1	2.97	0.46
1:A:899:VAL:O	1:A:899:VAL:CG1	2.51	0.46
1:A:983:ILE:HG22	1:A:983:ILE:O	2.14	0.46
2:B:692:TYR:H	2:B:692:TYR:HD2	1.61	0.46
2:B:483:LEU:O	2:B:484:ASN:HB2	2.16	0.46
2:B:487:THR:HG22	2:B:489:SER:N	2.30	0.46
1:A:632:VAL:O	1:A:636:GLU:HB2	2.15	0.46
3:C:226:ASP:O	3:C:227:THR:O	2.33	0.46
1:A:19:PHE:CE1	1:A:1396:ALA:HB3	2.50	0.46
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.84	0.46
9:K:91:CYS:O	9:K:94:ILE:HB	2.15	0.46
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.96	0.46
6:H:58:THR:CG2	6:H:59:ILE:H	2.28	0.46
6:H:109:LYS:CB	6:H:110:ASP:C	2.84	0.46
1:A:1261:LYS:C	1:A:1263:ILE:N	2.68	0.46
1:A:526:ASP:HB3	1:A:657:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.98	0.46
2:B:476:ARG:O	2:B:477:ALA:C	2.53	0.46
2:B:1037:LEU:HB3	2:B:1062:HIS:CE1	2.50	0.46
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.98	0.46
2:B:363:HIS:O	2:B:364:ILE:CB	2.62	0.46
1:A:767:GLN:HE22	1:A:774:ARG:HE	1.62	0.46
2:B:986:GLN:NE2	2:B:986:GLN:CA	2.78	0.46
1:A:855:THR:O	1:A:855:THR:CG2	2.63	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.18	0.46
6:H:82:PRO:O	6:H:83:GLN:HB3	2.16	0.46
1:A:849:MET:O	1:A:850:VAL:C	2.54	0.46
1:A:458:HIS:CD2	1:A:478:TYR:HH	2.27	0.46
2:B:1007:VAL:O	2:B:1008:PRO:C	2.54	0.46
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.49	0.46
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.16	0.46
1:A:709:THR:HG23	7:I:94:ASP:HA	1.97	0.46
2:B:964:VAL:CG1	2:B:965:LYS:N	2.79	0.46
2:B:58:THR:O	2:B:62:ILE:HG12	2.16	0.46
5:F:81:THR:O	5:F:82:THR:C	2.55	0.46
1:A:917:SER:C	1:A:919:ILE:H	2.18	0.46
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.67	0.46
2:B:1016:ALA:HA	2:B:1020:ARG:NH2	2.30	0.46
1:A:108:MET:SD	1:A:108:MET:N	2.89	0.46
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.60	0.46
2:B:850:LEU:CD1	8:J:8:PHE:HD1	2.20	0.46
1:A:315:LEU:HD13	1:A:319:GLY:O	2.14	0.46
1:A:401:GLY:O	1:A:435:HIS:CD2	2.69	0.46
2:B:45:SER:O	2:B:46:GLN:C	2.54	0.46
1:A:630:ILE:HD12	1:A:630:ILE:H	1.81	0.46
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.98	0.46
1:A:492:PRO:C	1:A:493:GLN:HE21	2.19	0.46
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.64	0.46
1:A:1377:THR:O	1:A:1379:GLY:N	2.49	0.46
2:B:762:ASN:HD21	2:B:1023:VAL:N	2.13	0.45
2:B:770:GLN:OE1	2:B:770:GLN:HA	2.15	0.45
3:C:46:ILE:HD11	3:C:99:LEU:HD12	1.99	0.45
1:A:819:GLY:O	1:A:820:GLY:C	2.55	0.45
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.30	0.45
1:A:829:VAL:C	1:A:831:THR:H	2.20	0.45
1:A:909:ASP:OD2	1:A:910:PRO:HD2	2.16	0.45
2:B:537:LYS:HG3	2:B:537:LYS:HZ3	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:106:CYS:O	7:I:107:SER:C	2.54	0.45
1:A:366:VAL:HG22	1:A:468:PHE:HE2	1.81	0.45
2:B:1006:ILE:O	2:B:1007:VAL:HG23	2.16	0.45
6:H:58:THR:HB	6:H:143:LEU:HB2	1.97	0.45
6:H:60:ALA:O	6:H:61:SER:HB3	2.16	0.45
2:B:322:PHE:CE2	7:I:30:ARG:HD2	2.51	0.45
8:J:16:ASP:OD1	8:J:17:LYS:CG	2.64	0.45
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.50	0.45
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.16	0.45
2:B:377:PHE:C	2:B:379:GLY:N	2.68	0.45
2:B:395:GLN:HG2	2:B:396:ASP:H	1.81	0.45
1:A:254:GLU:HA	1:A:255:SER:HA	1.61	0.45
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.56	0.45
2:B:968:VAL:HG12	2:B:969:ARG:N	2.32	0.45
1:A:361:LEU:HD22	1:A:646:PHE:CG	2.51	0.45
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.76	0.45
2:B:346:GLU:HA	2:B:349:ILE:CD1	2.43	0.45
1:A:818:MET:HG2	2:B:514:LEU:O	2.16	0.45
12:T:15:DA:H2''	12:T:16:DC:O5'	2.16	0.45
1:A:5:GLN:H	2:B:1159:ARG:NH2	2.15	0.45
2:B:238:ALA:HB2	2:B:385:LEU:HD13	1.99	0.45
2:B:1080:LYS:HB2	3:C:180:TYR:CZ	2.52	0.45
1:A:666:ILE:HD11	2:B:1030:LEU:HB2	1.98	0.45
2:B:990:ILE:HG22	2:B:991:GLY:N	2.30	0.45
3:C:3:GLU:HB3	9:K:104:ASN:HD21	1.81	0.45
3:C:56:THR:HG22	3:C:147:LEU:HD23	1.98	0.45
1:A:593:GLU:OE1	1:A:593:GLU:HA	2.16	0.45
1:A:11:LEU:HA	2:B:1193:GLN:O	2.17	0.45
3:C:10:ILE:HG22	3:C:11:ARG:N	2.32	0.45
5:F:73:ALA:O	5:F:74:ILE:HG12	2.17	0.45
1:A:942:PHE:C	1:A:942:PHE:CD2	2.89	0.45
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.99	0.45
2:B:478:GLY:O	2:B:479:VAL:C	2.55	0.45
8:J:44:TYR:C	8:J:44:TYR:HD1	2.18	0.45
2:B:1148:LYS:O	2:B:1151:LEU:O	2.35	0.45
5:F:135:ARG:CZ	5:F:143:PHE:CE1	2.99	0.45
1:A:53:LEU:O	1:A:56:PRO:HD2	2.16	0.45
1:A:1025:ARG:HG3	1:A:1030:ARG:HH12	1.80	0.45
1:A:1427:ASN:N	1:A:1427:ASN:ND2	2.64	0.45
1:A:423:ASP:O	1:A:424:ILE:HD12	2.16	0.45
1:A:464:PRO:HB2	1:A:465:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.99	0.45
2:B:798:TYR:CZ	3:C:62:PHE:CZ	3.04	0.45
3:C:62:PHE:O	3:C:65:HIS:N	2.50	0.45
1:A:53:LEU:HB3	1:A:54:ASN:H	1.57	0.45
6:H:109:LYS:HD2	6:H:111:LEU:HG	1.97	0.45
1:A:569:LYS:CD	3:C:221:TYR:HB2	2.46	0.45
2:B:227:LYS:N	2:B:395:GLN:OE1	2.50	0.45
1:A:537:ARG:HD2	6:H:23:VAL:HG11	1.97	0.45
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.81	0.45
2:B:56:ASP:C	2:B:57:TYR:HD1	2.19	0.45
1:A:1441:PHE:HZ	5:F:89:GLU:HA	1.76	0.45
2:B:524:PRO:CD	2:B:748:ILE:O	2.65	0.45
9:K:44:ASN:HB2	9:K:61:TYR:OH	2.16	0.45
1:A:120:GLU:HA	1:A:123:ARG:HD3	1.98	0.45
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.47	0.45
1:A:378:GLU:O	1:A:431:LYS:HA	2.17	0.45
9:K:14:GLU:C	9:K:16:GLU:H	2.20	0.45
1:A:419:LYS:NZ	1:A:419:LYS:HB3	2.32	0.45
2:B:978:ASP:OD1	2:B:1099:VAL:CG2	2.61	0.45
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.47	0.45
2:B:762:ASN:ND2	2:B:1023:VAL:H	2.15	0.45
4:E:29:PHE:C	4:E:30:ILE:HG13	2.37	0.45
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.98	0.45
3:C:184:ASN:HD21	3:C:189:THR:H	1.65	0.45
6:H:37:LYS:HB3	6:H:37:LYS:HE2	1.78	0.45
2:B:841:MET:HG2	2:B:842:ASN:H	1.82	0.45
1:A:399:HIS:CD2	1:A:400:PRO:HG3	2.52	0.45
2:B:545:ILE:HG13	2:B:633:VAL:HG22	1.98	0.45
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.37	0.45
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.17	0.45
1:A:499:ALA:O	1:A:503:GLN:HG2	2.17	0.45
1:A:523:ILE:CG2	1:A:527:THR:HB	2.47	0.45
6:H:109:LYS:HD3	6:H:110:ASP:OD2	2.16	0.45
1:A:13:THR:HG22	1:A:14:VAL:N	2.30	0.45
2:B:213:ILE:CD1	2:B:481:GLN:OE1	2.65	0.45
1:A:341:MET:CE	1:A:843:LYS:NZ	2.80	0.45
1:A:1399:ARG:NH2	1:A:1417:GLU:OE1	2.49	0.45
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.17	0.45
3:C:96:SER:HB2	3:C:158:VAL:HG12	1.98	0.45
11:R:12:U:H2'	11:R:12:U:O2	2.16	0.45
1:A:743:VAL:C	1:A:745:GLN:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:O	2:B:363:HIS:O	2.34	0.44
1:A:344:ARG:HB3	2:B:1118:PRO:HB2	1.98	0.44
3:C:79:GLN:O	3:C:79:GLN:HG3	2.17	0.44
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.99	0.44
7:I:101:PHE:N	7:I:101:PHE:CD1	2.83	0.44
2:B:792:MET:O	2:B:793:ALA:HB2	2.17	0.44
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.99	0.44
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.32	0.44
2:B:546:SER:HB2	2:B:632:ARG:HH21	1.82	0.44
1:A:380:VAL:HB	1:A:429:GLY:H	1.82	0.44
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.99	0.44
4:E:111:VAL:HG12	4:E:137:GLU:HG2	2.00	0.44
1:A:248:PRO:HB2	1:A:249:SER:H	1.60	0.44
1:A:572:TRP:N	1:A:572:TRP:CE3	2.85	0.44
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.98	0.44
2:B:778:MET:HE3	2:B:796:LEU:CD1	2.47	0.44
2:B:975:GLN:HG2	2:B:976:ILE:N	2.31	0.44
2:B:991:GLY:O	2:B:992:ILE:HD12	2.18	0.44
2:B:992:ILE:HD11	9:K:67:PHE:CZ	2.48	0.44
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.99	0.44
1:A:672:ASP:HB3	1:A:675:THR:OG1	2.17	0.44
12:T:18:DA:H2''	12:T:19:DT:C5'	2.47	0.44
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.44
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.82	0.44
1:A:527:THR:CG2	1:A:650:GLN:HG3	2.47	0.44
2:B:839:MET:O	2:B:839:MET:HG3	2.17	0.44
2:B:478:GLY:O	2:B:480:SER:N	2.51	0.44
2:B:899:ILE:HD13	2:B:966:VAL:HG11	1.98	0.44
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.53	0.44
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.16	0.44
1:A:257:ARG:NH2	1:A:317:LYS:HE2	2.31	0.44
2:B:45:SER:O	2:B:48:LEU:N	2.51	0.44
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.77	0.44
2:B:650:GLU:HG3	2:B:651:LEU:H	1.83	0.44
1:A:599:SER:HB3	1:A:614:PHE:HE1	1.82	0.44
1:A:1407:GLU:H	1:A:1407:GLU:CD	2.19	0.44
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	1.99	0.44
2:B:1158:PHE:HE2	2:B:1201:LYS:HE3	1.82	0.44
1:A:440:ASP:OD1	1:A:498:ARG:NH2	2.49	0.44
1:A:442:VAL:O	1:A:457:ALA:HA	2.17	0.44
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.52	0.44
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.53	0.44
9:K:101:LEU:O	9:K:102:LYS:C	2.55	0.44
9:K:6:ARG:O	9:K:8:GLU:N	2.51	0.44
2:B:905:VAL:HG13	2:B:909:ASP:OD2	2.18	0.44
1:A:478:TYR:O	1:A:479:ASN:HB3	2.18	0.44
1:A:498:ARG:O	1:A:499:ALA:C	2.56	0.44
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.99	0.44
3:C:173:ALA:O	3:C:233:GLU:O	2.36	0.44
1:A:546:VAL:O	1:A:550:LEU:HB2	2.18	0.44
3:C:148:ARG:HG2	3:C:149:LYS:H	1.83	0.44
1:A:826:ASP:N	1:A:826:ASP:OD2	2.51	0.44
2:B:906:SER:O	2:B:909:ASP:CG	2.56	0.44
1:A:503:GLN:HB2	1:A:504:LEU:CD1	2.47	0.44
2:B:981:ALA:CB	2:B:987:LYS:HA	2.48	0.44
2:B:765:PRO:HB2	2:B:766:ARG:H	1.61	0.44
1:A:894:GLU:C	1:A:896:ARG:H	2.21	0.44
3:C:18:VAL:O	3:C:20:PHE:CD2	2.62	0.44
2:B:864:LYS:HD3	2:B:871:THR:HG23	2.00	0.44
6:H:38:LEU:HD13	6:H:125:LEU:HD13	2.00	0.44
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.47	0.44
1:A:658:LEU:HD13	2:B:831:SER:H	1.82	0.44
1:A:634:THR:HG23	1:A:639:PRO:HA	2.00	0.44
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.18	0.44
2:B:824:ILE:CG1	8:J:48:ARG:HH12	2.27	0.44
2:B:590:HIS:NE2	2:B:592:ASN:O	2.46	0.44
1:A:782:ARG:HG2	1:A:789:LYS:HG3	2.00	0.44
3:C:144:ILE:HG22	3:C:145:CYS:HB3	2.00	0.44
2:B:485:ARG:HG2	2:B:491:THR:OG1	2.18	0.44
1:A:569:LYS:HD3	3:C:221:TYR:HB2	1.99	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.88	0.44
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.95	0.44
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.17	0.44
2:B:839:MET:CG	2:B:990:ILE:CA	2.94	0.43
3:C:3:GLU:CG	3:C:4:GLU:N	2.75	0.43
7:I:32:CYS:SG	7:I:33:SER:N	2.91	0.43
3:C:62:PHE:O	3:C:63:ILE:C	2.55	0.43
1:A:1349:TYR:O	1:A:1350:LYS:C	2.56	0.43
2:B:1159:ARG:HG3	2:B:1193:GLN:HE21	1.83	0.43
2:B:261:ARG:N	2:B:264:SER:HB3	2.33	0.43
3:C:42:PRO:HA	3:C:163:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:153:HIS:O	4:E:154:ILE:HD13	2.17	0.43
1:A:476:SER:O	1:A:477:PRO:C	2.56	0.43
1:A:353:ILE:CG1	1:A:487:MET:HE2	2.48	0.43
2:B:467:GLY:O	2:B:468:GLU:HB2	2.17	0.43
3:C:120:ILE:HG21	3:C:124:LEU:HD21	2.00	0.43
9:K:35:PHE:CG	9:K:71:PHE:CE2	3.06	0.43
7:I:7:CYS:SG	7:I:8:ARG:O	2.64	0.43
12:T:18:DA:C2	12:T:19:DT:N3	2.86	0.43
1:A:44:THR:O	1:A:45:GLN:HB2	2.18	0.43
1:A:756:ILE:HD12	1:A:759:ALA:HB3	2.00	0.43
1:A:16:GLU:HB2	2:B:1217:TYR:HB2	2.00	0.43
2:B:637:LEU:N	2:B:637:LEU:CD1	2.79	0.43
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.99	0.43
2:B:711:GLU:N	2:B:712:PRO:HD3	2.23	0.43
2:B:577:ALA:HB1	2:B:589:VAL:HG12	1.97	0.43
3:C:69:LEU:H	3:C:69:LEU:HD23	1.82	0.43
1:A:1017:LEU:HB2	4:E:205:SER:HA	2.00	0.43
7:I:73:ARG:HB2	7:I:83:ASN:OD1	2.19	0.43
2:B:420:LEU:HD22	2:B:453:ILE:HA	1.99	0.43
1:A:525:GLN:CG	2:B:835:GLN:HG2	2.43	0.43
1:A:302:THR:HG23	1:A:306:ASN:HB3	2.00	0.43
1:A:450:LEU:O	1:A:1070:GLN:HB3	2.19	0.43
5:F:135:ARG:CZ	5:F:143:PHE:HE1	2.32	0.43
1:A:55:ASP:O	1:A:58:LEU:N	2.52	0.43
2:B:44:VAL:O	2:B:45:SER:C	2.56	0.43
3:C:43:THR:HG23	3:C:74:SER:OG	2.18	0.43
1:A:781:ASP:OD1	7:I:91:ARG:NH2	2.51	0.43
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.53	0.43
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.48	0.43
1:A:476:SER:CB	1:A:477:PRO:CD	2.95	0.43
1:A:464:PRO:HG3	9:K:67:PHE:CD1	2.48	0.43
1:A:361:LEU:HD11	1:A:473:SER:CB	2.43	0.43
2:B:193:LYS:HD3	2:B:787:VAL:CG1	2.45	0.43
2:B:879:ARG:HB2	2:B:880:THR:H	1.56	0.43
2:B:648:HIS:HD2	2:B:649:LYS:O	2.02	0.43
1:A:639:PRO:O	1:A:642:CYS:HB3	2.19	0.43
2:B:1110:PRO:HG2	2:B:1119:VAL:HG21	1.99	0.43
2:B:859:TYR:CZ	2:B:941:LEU:HD22	2.53	0.43
3:C:63:ILE:O	3:C:66:ARG:HB2	2.19	0.43
4:E:83:CYS:SG	4:E:110:PHE:CE1	3.01	0.43
1:A:857:ARG:HB2	1:A:858:ASN:H	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:640:VAL:HG13	2:B:651:LEU:HA	2.01	0.43
1:A:849:MET:O	1:A:849:MET:HG3	2.19	0.43
1:A:423:ASP:O	1:A:424:ILE:O	2.37	0.43
12:T:13:DA:H61	13:N:2:DT:C7	2.32	0.43
2:B:240:ILE:O	2:B:240:ILE:HG23	2.18	0.43
1:A:367:PRO:HD3	1:A:467:THR:O	2.19	0.43
2:B:821:GLN:HG2	8:J:8:PHE:HE1	1.83	0.43
1:A:451:HIS:HB2	1:A:454:SER:H	1.83	0.43
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.49	0.43
1:A:836:TYR:O	1:A:837:ILE:C	2.57	0.43
2:B:797:TYR:HB3	2:B:798:TYR:CE1	2.54	0.43
2:B:115:GLN:O	2:B:119:LEU:HD12	2.18	0.43
1:A:1116:LEU:H	1:A:1308:THR:HB	1.84	0.43
2:B:680:THR:N	2:B:683:SER:OG	2.51	0.43
2:B:1207:LEU:HA	2:B:1207:LEU:HD23	1.88	0.43
7:I:50:THR:HG22	7:I:52:ILE:HG22	2.01	0.43
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.34	0.43
1:A:523:ILE:CG2	1:A:524:VAL:N	2.82	0.43
1:A:661:GLY:O	1:A:662:PHE:CB	2.65	0.43
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.27	0.43
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.99	0.43
1:A:886:ILE:HD11	1:A:943:LEU:HB2	1.95	0.43
1:A:265:LYS:HZ1	1:A:322:VAL:HB	1.83	0.43
1:A:344:ARG:NH1	2:B:1129:ARG:H	2.17	0.43
1:A:562:THR:HG22	1:A:563:PRO:HD2	2.00	0.43
1:A:103:CYS:O	1:A:174:ILE:HD12	2.19	0.43
5:F:85:MET:SD	5:F:90:ARG:HB2	2.59	0.43
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.87	0.43
2:B:589:VAL:CG1	2:B:590:HIS:N	2.81	0.43
1:A:240:PRO:HG2	2:B:1209:ALA:HA	2.01	0.43
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.43
7:I:73:ARG:HB3	7:I:74:GLU:H	1.42	0.43
1:A:152:VAL:HA	1:A:153:PRO:HD3	1.93	0.43
2:B:806:THR:H	2:B:809:MET:HG3	1.84	0.43
1:A:477:PRO:HG2	1:A:478:TYR:H	1.84	0.43
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.43
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.54	0.43
2:B:34:ILE:HD13	2:B:542:MET:HE1	2.00	0.43
3:C:181:ASP:HA	3:C:182:PRO:HD2	1.74	0.43
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.19	0.43
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:THR:O	2:B:736:THR:HG22	2.19	0.43
1:A:482:PHE:H	2:B:837:ASP:HB2	1.83	0.42
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.34	0.42
6:H:109:LYS:HB2	6:H:111:LEU:HB2	2.01	0.42
1:A:129:LYS:O	1:A:130:ASP:CB	2.62	0.42
4:E:112:TYR:O	4:E:137:GLU:HG3	2.18	0.42
3:C:92:CYS:O	3:C:95:CYS:N	2.46	0.42
1:A:376:TYR:OH	1:A:498:ARG:HD2	2.19	0.42
1:A:662:PHE:O	2:B:829:CYS:N	2.48	0.42
2:B:975:GLN:O	2:B:977:GLY:N	2.51	0.42
2:B:487:THR:HG22	2:B:490:SER:H	1.84	0.42
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.18	0.42
1:A:1325:THR:HA	4:E:147:HIS:HA	1.99	0.42
4:E:145:THR:HG21	4:E:187:TYR:CE2	2.54	0.42
1:A:172:PRO:HA	1:A:184:SER:O	2.18	0.42
9:K:32:VAL:O	9:K:32:VAL:HG13	2.18	0.42
1:A:523:ILE:O	1:A:524:VAL:HG13	2.19	0.42
2:B:1099:VAL:C	2:B:1101:ASP:H	2.23	0.42
11:R:4:G:C4	11:R:5:A:N7	2.87	0.42
2:B:211:VAL:CG2	2:B:483:LEU:HG	2.49	0.42
1:A:860:LEU:HB2	1:A:862:ASN:OD1	2.19	0.42
2:B:998:ASP:CA	3:C:35:ARG:HH21	2.32	0.42
2:B:213:ILE:HD11	2:B:481:GLN:CG	2.48	0.42
1:A:48:ALA:C	1:A:49:LYS:HG2	2.40	0.42
1:A:98:LYS:O	1:A:101:LYS:N	2.52	0.42
1:A:269:ILE:HG13	1:A:299:HIS:HB3	2.01	0.42
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.49	0.42
2:B:778:MET:O	2:B:819:ALA:HB1	2.18	0.42
1:A:368:LYS:O	1:A:372:LYS:N	2.52	0.42
1:A:56:PRO:O	1:A:57:ARG:HB2	2.20	0.42
2:B:751:VAL:HG13	2:B:752:ALA:N	2.34	0.42
2:B:519:TRP:O	2:B:519:TRP:HD1	2.03	0.42
4:E:43:LYS:O	4:E:47:CYS:HB2	2.19	0.42
1:A:179:LEU:HB2	1:A:180:LYS:HD2	2.00	0.42
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.61	0.42
2:B:188:ASP:O	2:B:192:LEU:HD12	2.19	0.42
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.82	0.42
2:B:978:ASP:O	2:B:980:PHE:CD1	2.73	0.42
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.47	0.42
2:B:757:PRO:HG3	2:B:983:ARG:NH2	2.33	0.42
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:98:TYR:C	6:H:118:PHE:CD2	2.93	0.42
2:B:753:ALA:C	2:B:755:ILE:H	2.21	0.42
2:B:905:VAL:HG13	2:B:909:ASP:CB	2.49	0.42
1:A:171:GLN:HA	1:A:172:PRO:HD3	1.91	0.42
8:J:38:ARG:O	8:J:38:ARG:HG3	2.19	0.42
2:B:1006:ILE:HG22	2:B:1007:VAL:N	2.35	0.42
1:A:929:LEU:HD21	1:A:1028:THR:HG21	2.01	0.42
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.49	0.42
2:B:224:GLN:O	2:B:238:ALA:HA	2.19	0.42
1:A:868:TYR:O	1:A:872:GLY:N	2.51	0.42
6:H:95:TYR:HD2	6:H:95:TYR:C	2.21	0.42
1:A:760:GLN:HE21	1:A:765:VAL:CA	2.31	0.42
1:A:401:GLY:C	1:A:435:HIS:CD2	2.93	0.42
1:A:372:LYS:O	1:A:435:HIS:HE1	2.02	0.42
2:B:589:VAL:CG1	2:B:590:HIS:H	2.25	0.42
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.48	0.42
1:A:874:ASP:OD1	1:A:875:ALA:N	2.52	0.42
3:C:47:ASP:CG	3:C:47:ASP:O	2.58	0.42
3:C:8:VAL:HG21	9:K:105:PHE:HB2	2.00	0.42
1:A:655:PHE:O	1:A:656:TRP:C	2.58	0.42
7:I:75:CYS:SG	7:I:108:HIS:HD2	2.43	0.42
1:A:560:ILE:HG12	1:A:560:ILE:H	1.67	0.42
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.78	0.42
2:B:999:MET:CE	2:B:1011:ILE:HD11	2.50	0.42
8:J:7:CYS:SG	8:J:9:SER:CA	3.08	0.42
2:B:1002:THR:HG21	2:B:1006:ILE:HG12	1.74	0.42
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.20	0.42
1:A:361:LEU:C	1:A:363:GLN:H	2.23	0.42
2:B:203:PHE:HE1	2:B:212:LEU:CD1	2.24	0.42
2:B:745:PRO:C	2:B:747:MET:H	2.21	0.42
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.00	0.42
1:A:135:PHE:HD1	1:A:222:LEU:O	2.03	0.42
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.19	0.42
6:H:126:GLU:C	6:H:130:ARG:NH1	2.72	0.42
1:A:913:LEU:HG	1:A:914:GLU:H	1.85	0.42
1:A:225:ASN:O	1:A:227:VAL:N	2.53	0.42
2:B:1084:GLN:O	2:B:1085:ILE:HG12	2.20	0.42
2:B:826:ALA:O	2:B:1011:ILE:HA	2.19	0.42
2:B:763:GLN:HE21	2:B:765:PRO:HG2	1.83	0.42
9:K:40:HIS:CE1	9:K:63:VAL:CG2	3.02	0.42
1:A:345:VAL:HG12	2:B:1155:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:ILE:O	1:A:1065:GLY:N	2.52	0.42
1:A:855:THR:OG1	1:A:866:PHE:HA	2.19	0.42
2:B:382:ILE:HD13	2:B:382:ILE:HA	1.87	0.42
7:I:111:THR:CG2	7:I:112:SER:N	2.82	0.42
3:C:84:ARG:CZ	9:K:11:LEU:HD11	2.50	0.42
2:B:274:PRO:O	2:B:275:TYR:HB2	2.20	0.42
2:B:637:LEU:O	2:B:690:VAL:CA	2.68	0.42
1:A:476:SER:O	1:A:479:ASN:N	2.53	0.42
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.85	0.42
2:B:1029:CYS:HB2	2:B:1090:THR:OG1	2.19	0.42
2:B:1017:ILE:N	2:B:1018:PRO:HD3	2.34	0.42
2:B:762:ASN:HD21	2:B:1022:THR:CA	2.33	0.42
1:A:852:TYR:CZ	5:F:136:ARG:HG2	2.54	0.42
1:A:265:LYS:HZ3	1:A:323:LYS:HE2	1.85	0.42
2:B:515:HIS:CD2	2:B:517:THR:H	2.37	0.42
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.40	0.42
1:A:1427:ASN:ND2	1:A:1427:ASN:H	2.18	0.42
2:B:808:ALA:C	2:B:810:GLU:N	2.73	0.42
2:B:1029:CYS:SG	2:B:1086:PHE:CE2	3.10	0.41
1:A:567:LYS:HB2	6:H:95:TYR:HA	2.01	0.41
3:C:258:ILE:CD1	9:K:42:LEU:HD21	2.51	0.41
4:E:213:ILE:HG12	4:E:214:CYS:N	2.35	0.41
2:B:792:MET:HE2	2:B:792:MET:CA	2.50	0.41
9:K:31:VAL:O	9:K:74:ARG:HA	2.19	0.41
4:E:55:ARG:O	4:E:57:MET:N	2.53	0.41
1:A:284:ALA:HA	1:A:285:PRO:HD3	1.84	0.41
1:A:726:ARG:HD3	1:A:766:GLY:HA3	2.02	0.41
1:A:483:ASP:HB2	2:B:987:LYS:HD2	2.01	0.41
2:B:1084:GLN:O	2:B:1085:ILE:HG13	2.19	0.41
8:J:37:SER:OG	8:J:47:ARG:NH2	2.53	0.41
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.02	0.41
6:H:44:VAL:O	6:H:44:VAL:HG13	2.20	0.41
1:A:1104:ILE:HD11	1:A:1351:GLU:HB3	2.01	0.41
1:A:355:GLY:HA2	1:A:470:LEU:O	2.20	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
1:A:453:MET:O	1:A:477:PRO:HB2	2.20	0.41
2:B:978:ASP:O	2:B:979:LYS:C	2.57	0.41
2:B:992:ILE:HG21	2:B:994:TYR:CE2	2.56	0.41
2:B:1029:CYS:SG	2:B:1086:PHE:HE2	2.43	0.41
2:B:590:HIS:NE2	2:B:591:ARG:O	2.53	0.41
2:B:373:ARG:HA	2:B:566:LEU:CD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HA	1:A:1329:THR:HG1	1.86	0.41
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.54	0.41
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	2.02	0.41
2:B:487:THR:HG23	2:B:488:TYR:N	2.35	0.41
1:A:182:VAL:HG12	1:A:183:GLY:N	2.29	0.41
3:C:72:LEU:O	3:C:237:SER:HB2	2.21	0.41
2:B:293:PRO:HG2	2:B:296:GLU:HB3	2.02	0.41
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.86	0.41
1:A:48:ALA:O	1:A:49:LYS:HG2	2.21	0.41
1:A:1368:MET:O	1:A:1369:ALA:C	2.58	0.41
8:J:32:GLU:CD	8:J:32:GLU:H	2.23	0.41
1:A:1046:LEU:O	1:A:1047:SER:C	2.59	0.41
1:A:366:VAL:HG22	1:A:468:PHE:CE2	2.54	0.41
1:A:444:PHE:O	1:A:478:TYR:CE2	2.69	0.41
2:B:780:VAL:HG23	2:B:799:PRO:HG3	2.01	0.41
3:C:164:ALA:HB2	3:C:171:GLY:CA	2.50	0.41
3:C:167:HIS:CE1	10:L:70:ARG:O	2.58	0.41
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.32	0.41
1:A:315:LEU:HD12	1:A:318:SER:O	2.21	0.41
3:C:238:ILE:HG23	3:C:242:GLN:CB	2.48	0.41
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.44	0.41
2:B:982:SER:O	2:B:1093:GLN:CG	2.63	0.41
1:A:264:PHE:CZ	1:A:317:LYS:CB	3.03	0.41
4:E:150:VAL:HA	4:E:151:PRO:HD3	1.86	0.41
1:A:577:ILE:H	1:A:577:ILE:HG13	1.72	0.41
1:A:248:PRO:HD2	1:A:260:ASP:OD2	2.21	0.41
2:B:47:GLN:HB3	2:B:173:MET:HE1	2.02	0.41
2:B:894:ASP:N	2:B:894:ASP:OD1	2.53	0.41
1:A:1205:LYS:HG2	1:A:1205:LYS:H	1.63	0.41
1:A:353:ILE:HA	1:A:468:PHE:O	2.20	0.41
2:B:976:ILE:CD1	2:B:992:ILE:HD12	2.43	0.41
1:A:443:LEU:HD21	1:A:455:MET:HB3	2.02	0.41
1:A:346:ASP:O	1:A:347:PHE:O	2.39	0.41
2:B:484:ASN:ND2	2:B:490:SER:OG	2.53	0.41
1:A:405:VAL:HG22	1:A:432:VAL:HG22	2.02	0.41
1:A:754:SER:OG	1:A:755:PHE:N	2.52	0.41
7:I:35:VAL:CG1	7:I:36:GLU:N	2.82	0.41
2:B:256:VAL:HG11	2:B:382:ILE:HD11	1.97	0.41
1:A:718:VAL:O	1:A:719:VAL:C	2.59	0.41
2:B:619:ILE:HD12	7:I:61:ASP:HB3	2.01	0.41
1:A:356:ASP:HB3	1:A:359:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HA	2:B:412:LEU:HD22	1.77	0.41
1:A:765:VAL:HG22	1:A:800:VAL:CB	2.39	0.41
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.51	0.41
1:A:619:LYS:O	1:A:623:GLY:N	2.42	0.41
1:A:395:GLY:HA2	1:A:396:PRO:HD3	1.90	0.41
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.85	0.41
2:B:56:ASP:C	2:B:57:TYR:CD1	2.94	0.41
5:F:132:LEU:O	5:F:148:VAL:HG23	2.20	0.41
5:F:138:LEU:HB3	5:F:139:PRO:HD2	2.02	0.41
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.54	0.41
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.40	0.41
3:C:20:PHE:HD1	3:C:21:ILE:O	2.04	0.41
2:B:552:MET:N	2:B:553:PRO:CD	2.84	0.41
4:E:147:HIS:HB3	4:E:150:VAL:CG2	2.48	0.41
5:F:105:ALA:HB1	5:F:106:PRO:HD3	2.00	0.41
7:I:68:LEU:HA	7:I:69:PRO:HD2	1.63	0.41
2:B:637:LEU:CG	2:B:741:CYS:O	2.69	0.41
1:A:662:PHE:O	2:B:828:ALA:HA	2.21	0.41
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.85	0.41
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	2.03	0.41
2:B:1002:THR:HG22	2:B:1006:ILE:CB	2.49	0.41
1:A:312:PRO:HB2	1:A:313:GLN:H	1.71	0.41
9:K:40:HIS:CE1	9:K:63:VAL:HG22	2.55	0.41
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.36	0.41
2:B:203:PHE:CE1	2:B:212:LEU:CD1	3.01	0.41
3:C:66:ARG:C	3:C:68:GLY:N	2.75	0.41
2:B:1209:ALA:C	2:B:1211:ASN:H	2.23	0.41
1:A:381:THR:O	1:A:382:PRO:C	2.59	0.41
2:B:190:TYR:CZ	2:B:196:PRO:CG	3.03	0.41
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.84	0.41
2:B:485:ARG:NE	2:B:788:ARG:NH2	2.68	0.41
2:B:234:ILE:HG23	2:B:258:LEU:H	1.85	0.41
2:B:855:PHE:N	2:B:970:THR:O	2.46	0.41
2:B:27:ALA:O	2:B:28:GLU:C	2.59	0.41
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.74	0.41
2:B:435:THR:O	2:B:437:GLU:N	2.35	0.41
1:A:915:SER:O	1:A:918:GLU:N	2.54	0.41
7:I:16:PRO:HA	7:I:27:PHE:HA	2.03	0.41
2:B:1102:LYS:O	2:B:1103:ILE:C	2.59	0.41
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.86	0.41
1:A:1364:ASN:ND2	1:A:1366:ARG:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.20	0.41
2:B:297:ILE:HD13	2:B:297:ILE:HA	1.86	0.41
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.60	0.41
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.95	0.41
1:A:618:GLU:OE2	1:A:620:LYS:N	2.54	0.41
2:B:638:PHE:HA	2:B:690:VAL:HA	2.03	0.40
2:B:997:GLU:HG2	3:C:39:ALA:HB2	2.02	0.40
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.86	0.40
3:C:258:ILE:O	3:C:259:LEU:C	2.59	0.40
1:A:947:PHE:CD2	1:A:954:TRP:NE1	2.90	0.40
2:B:865:LYS:HG2	2:B:866:TYR:N	2.36	0.40
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.56	0.40
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	2.04	0.40
1:A:1004:ASN:OD1	1:A:1004:ASN:C	2.59	0.40
1:A:495:GLU:O	1:A:498:ARG:HB2	2.21	0.40
1:A:662:PHE:O	2:B:828:ALA:HB1	2.21	0.40
6:H:95:TYR:HE2	6:H:97:MET:SD	2.44	0.40
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.97	0.40
2:B:912:ILE:HD11	2:B:966:VAL:HG23	2.03	0.40
8:J:12:LYS:HD2	8:J:43:ARG:HD2	2.02	0.40
1:A:901:LEU:O	1:A:920:LEU:HD23	2.21	0.40
2:B:293:PRO:C	2:B:294:ASP:O	2.56	0.40
11:R:9:G:C2	12:T:21:DC:C2	3.09	0.40
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.37	0.40
1:A:826:ASP:O	1:A:829:VAL:N	2.54	0.40
2:B:435:THR:C	2:B:437:GLU:H	2.21	0.40
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.87	0.40
10:L:48:CYS:SG	10:L:49:LYS:N	2.94	0.40
6:H:33:GLN:HE21	6:H:33:GLN:HB3	1.62	0.40
2:B:289:LEU:HA	2:B:289:LEU:HD23	1.77	0.40
1:A:355:GLY:O	1:A:357:PRO:CD	2.69	0.40
2:B:203:PHE:C	2:B:204:ILE:HD12	2.42	0.40
2:B:211:VAL:HG12	2:B:212:LEU:O	2.21	0.40
1:A:777:PHE:CE2	1:A:782:ARG:HA	2.57	0.40
1:A:492:PRO:CB	1:A:497:THR:HG22	2.47	0.40
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.40
2:B:213:ILE:HD11	2:B:481:GLN:CD	2.40	0.40
2:B:392:ARG:O	2:B:393:LYS:HD2	2.21	0.40
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.36	0.40
2:B:788:ARG:O	2:B:967:ARG:NH1	2.54	0.40
2:B:453:ILE:HG23	2:B:457:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:HA	1:A:504:LEU:HD13	2.03	0.40
1:A:567:LYS:HE2	6:H:97:MET:HG2	2.03	0.40
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.20	0.40
5:F:134:ILE:HD13	5:F:134:ILE:HA	1.90	0.40
3:C:74:SER:O	3:C:77:ILE:HB	2.22	0.40
3:C:196:ASP:O	3:C:200:GLU:HB2	2.22	0.40
3:C:116:LYS:HE2	3:C:117:ASP:OD1	2.22	0.40
2:B:839:MET:CE	2:B:1010:LEU:HD13	2.52	0.40
2:B:1002:THR:HG22	2:B:1006:ILE:CG1	2.45	0.40
1:A:323:LYS:O	1:A:324:SER:OG	2.30	0.40
1:A:1390:ASN:ND2	1:A:1402:PHE:HB3	2.37	0.40
1:A:670:ILE:HG22	1:A:671:ALA:N	2.35	0.40
1:A:857:ARG:HA	1:A:864:ILE:HG12	2.03	0.40
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.51	0.40
3:C:85:ASP:O	3:C:86:CYS:C	2.59	0.40
1:A:1053:PHE:C	1:A:1053:PHE:CD2	2.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1021 (74%)	249 (18%)	113 (8%)	1	9
2	B	1088/1224 (89%)	820 (75%)	186 (17%)	82 (8%)	1	11
3	C	264/318 (83%)	192 (73%)	48 (18%)	24 (9%)	1	7
4	E	212/215 (99%)	177 (84%)	28 (13%)	7 (3%)	5	34
5	F	82/155 (53%)	58 (71%)	20 (24%)	4 (5%)	3	22
6	H	129/146 (88%)	101 (78%)	19 (15%)	9 (7%)	1	12
7	I	117/122 (96%)	84 (72%)	22 (19%)	11 (9%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	50 (79%)	10 (16%)	3 (5%)	3	23
9	K	112/120 (93%)	88 (79%)	18 (16%)	6 (5%)	2	19
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0	1
All	All	3494/4173 (84%)	2616 (75%)	612 (18%)	266 (8%)	1	11

All (266) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	130	ASP
1	A	226	GLU
1	A	248	PRO
1	A	250	ILE
1	A	258	GLY
1	A	312	PRO
1	A	315	LEU
1	A	322	VAL
1	A	335	ARG
1	A	362	ASP
1	A	399	HIS
1	A	404	TYR
1	A	424	ILE
1	A	465	TYR
1	A	466	SER
1	A	480	ALA
1	A	523	ILE
1	A	526	ASP
1	A	527	THR
1	A	567	LYS
1	A	583	PRO
1	A	904	THR
1	A	972	HIS
1	A	1036	ARG
1	A	1274	ARG
1	A	1341	ILE
1	A	1379	GLY
1	A	1393	ASN
1	A	1424	VAL
2	B	67	SER
2	B	436	VAL

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Mol	Chain	Res	Type
2	B	466	TRP
2	B	468	GLU
2	B	477	ALA
2	B	484	ASN
2	B	531	GLN
2	B	619	ILE
2	B	636	PRO
2	B	709	ASP
2	B	711	GLU
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	764	SER
2	B	765	PRO
2	B	766	ARG
2	B	780	VAL
2	B	815	ARG
2	B	823	ALA
2	B	831	SER
2	B	834	ASN
2	B	837	ASP
2	B	838	SER
2	B	879	ARG
2	B	901	PRO
2	B	981	ALA
2	B	1046	PRO
2	B	1096	ARG
2	B	1097	HIS
2	B	1103	ILE
2	B	1152	MET
2	B	1223	ASP
3	C	67	LEU
3	C	103	ALA
3	C	153	LEU
3	C	227	THR
3	C	240	VAL
3	C	267	GLN
4	E	3	GLN
4	E	49	SER
6	H	61	SER
6	H	82	PRO
6	H	140	ALA

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Mol	Chain	Res	Type
7	I	11	ASN
7	I	54	GLU
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
10	L	26	THR
10	L	35	SER
10	L	45	ALA
10	L	55	ILE
1	A	42	ASP
1	A	48	ALA
1	A	56	PRO
1	A	68	GLN
1	A	69	THR
1	A	178	GLY
1	A	225	ASN
1	A	253	ASN
1	A	257	ARG
1	A	324	SER
1	A	347	PHE
1	A	525	GLN
1	A	662	PHE
1	A	820	GLY
1	A	916	GLY
1	A	922	ASP
1	A	998	LEU
1	A	1054	LEU
1	A	1221	LYS
1	A	1261	LYS
1	A	1378	GLN
1	A	1435	PRO
2	B	21	GLU
2	B	100	PRO
2	B	294	ASP
2	B	410	GLY
2	B	480	SER
2	B	483	LEU
2	B	728	ARG
2	B	891	ASP
2	B	943	SER
2	B	976	ILE
2	B	1008	PRO

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Mol	Chain	Res	Type
2	B	1047	PHE
2	B	1100	ASP
2	B	1126	GLY
2	B	1155	SER
3	C	6	PRO
3	C	63	ILE
3	C	86	CYS
3	C	142	VAL
3	C	152	GLU
3	C	167	HIS
4	E	59	SER
4	E	206	GLY
5	F	81	THR
6	H	32	THR
6	H	60	ALA
6	H	90	ALA
7	I	107	SER
8	J	43	ARG
10	L	54	ARG
10	L	56	LEU
1	A	54	ASN
1	A	76	GLU
1	A	89	PRO
1	A	249	SER
1	A	251	SER
1	A	286	HIS
1	A	418	SER
1	A	428	TYR
1	A	498	ARG
1	A	509	LEU
1	A	570	PRO
1	A	593	GLU
1	A	819	GLY
1	A	830	LYS
1	A	871	ASP
1	A	969	GLN
1	A	983	ILE
1	A	1062	GLU
1	A	1365	TYR
1	A	1389	PHE
1	A	1437	GLY
2	B	38	PHE

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Mol	Chain	Res	Type
2	B	467	GLY
2	B	516	ASN
2	B	631	GLY
2	B	793	ALA
2	B	866	TYR
2	B	1108	ARG
3	C	32	SER
3	C	215	GLU
3	C	243	VAL
6	H	43	ASN
6	H	77	ARG
7	I	47	GLU
7	I	73	ARG
7	I	74	GLU
7	I	79	HIS
9	K	44	ASN
10	L	47	ARG
1	A	39	GLU
1	A	109	HIS
1	A	332	LYS
1	A	387	ARG
1	A	426	LEU
1	A	476	SER
1	A	517	ASN
1	A	597	LEU
1	A	744	LYS
1	A	827	THR
1	A	846	GLU
1	A	895	LYS
1	A	1270	ASN
1	A	1410	PHE
2	B	387	LEU
2	B	411	PRO
2	B	642	ASP
2	B	792	MET
2	B	979	LYS
2	B	1060	ARG
2	B	1165	ILE
2	B	1181	GLU
2	B	1190	ASP
3	C	48	SER
3	C	66	ARG

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Mol	Chain	Res	Type
3	C	172	PRO
3	C	205	LYS
4	E	192	ARG
5	F	113	GLY
7	I	3	THR
7	I	57	GLY
7	I	88	SER
1	A	254	GLU
1	A	474	VAL
1	A	536	LEU
1	A	591	PHE
1	A	624	SER
1	A	850	VAL
1	A	958	VAL
1	A	1047	SER
1	A	1204	ASP
2	B	251	ILE
2	B	364	ILE
2	B	451	LYS
2	B	501	PRO
2	B	864	LYS
2	B	1001	PHE
2	B	1071	VAL
2	B	1153	GLU
3	C	149	LYS
3	C	214	ASN
5	F	148	VAL
6	H	62	SER
9	K	15	GLY
1	A	131	SER
1	A	320	ARG
1	A	400	PRO
1	A	472	LEU
1	A	650	GLN
1	A	780	VAL
1	A	986	ILE
2	B	307	ASP
2	B	978	ASP
2	B	986	GLN
2	B	991	GLY
2	B	1016	ALA
2	B	1178	ASN

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Mol	Chain	Res	Type
3	C	60	ASP
9	K	8	GLU
1	A	364	VAL
1	A	1064	VAL
1	A	1066	VAL
3	C	38	ILE
2	B	832	GLY
2	B	1118	PRO
7	I	76	PRO
9	K	13	GLY
9	K	43	GLY
1	A	283	GLY
1	A	396	PRO
1	A	743	VAL
2	B	295	GLY
4	E	76	GLY
5	F	82	THR
2	B	743	ILE
3	C	181	ASP
1	A	245	PRO
1	A	948	VAL
1	A	1107	VAL
4	E	38	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	984 (81%)	234 (19%)	2	7
2	B	960/1061 (90%)	779 (81%)	181 (19%)	2	8
3	C	234/274 (85%)	186 (80%)	48 (20%)	1	6
4	E	196/197 (100%)	176 (90%)	20 (10%)	9	35
5	F	74/137 (54%)	65 (88%)	9 (12%)	6	25
6	H	117/128 (91%)	103 (88%)	14 (12%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	113/116 (97%)	90 (80%)	23 (20%)	1	6
8	J	60/65 (92%)	47 (78%)	13 (22%)	1	5
9	K	99/102 (97%)	83 (84%)	16 (16%)	3	14
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	4
All	All	3111/3657 (85%)	2544 (82%)	567 (18%)	2	9

All (567) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	18	GLN
1	A	23	SER
1	A	26	GLU
1	A	39	GLU
1	A	47	ARG
1	A	67	CYS
1	A	69	THR
1	A	70	CYS
1	A	80	HIS
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	100	LYS
1	A	102	VAL
1	A	108	MET
1	A	116	ASP
1	A	144	THR
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	185	TRP
1	A	206	GLU
1	A	208	LEU
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	227	VAL
1	A	250	ILE
1	A	254	GLU
1	A	260	ASP
1	A	263	THR

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	271	LYS
1	A	282	ASN
1	A	287	HIS
1	A	291	GLU
1	A	297	GLN
1	A	303	TYR
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	315	LEU
1	A	316	GLN
1	A	318	SER
1	A	320	ARG
1	A	323	LYS
1	A	326	ARG
1	A	335	ARG
1	A	344	ARG
1	A	350	ARG
1	A	354	SER
1	A	364	VAL
1	A	368	LYS
1	A	370	ILE
1	A	373	THR
1	A	374	LEU
1	A	376	TYR
1	A	381	THR
1	A	389	THR
1	A	390	GLN
1	A	403	LYS
1	A	419	LYS
1	A	434	ARG
1	A	442	VAL
1	A	443	LEU
1	A	450	LEU
1	A	452	LYS
1	A	453	MET
1	A	454	SER
1	A	456	MET
1	A	460	VAL
1	A	463	ILE
1	A	466	SER

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Mol	Chain	Res	Type
1	A	469	ARG
1	A	470	LEU
1	A	473	SER
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	502	SER
1	A	512	VAL
1	A	518	LYS
1	A	521	MET
1	A	524	VAL
1	A	526	ASP
1	A	527	THR
1	A	529	CYS
1	A	531	ILE
1	A	532	ARG
1	A	535	THR
1	A	545	GLN
1	A	550	LEU
1	A	552	TRP
1	A	555	ASP
1	A	562	THR
1	A	566	ILE
1	A	567	LYS
1	A	569	LYS
1	A	572	TRP
1	A	576	GLN
1	A	579	SER
1	A	590	ARG
1	A	592	ASP
1	A	601	LYS
1	A	602	ASP
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	619	LYS
1	A	621	THR
1	A	634	THR
1	A	642	CYS
1	A	649	ILE

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Mol	Chain	Res	Type
1	A	650	GLN
1	A	654	ASN
1	A	662	PHE
1	A	666	ILE
1	A	672	ASP
1	A	675	THR
1	A	682	THR
1	A	695	LYS
1	A	702	LEU
1	A	710	LEU
1	A	728	LYS
1	A	732	LEU
1	A	740	LEU
1	A	744	LYS
1	A	768	GLN
1	A	782	ARG
1	A	797	LYS
1	A	801	GLU
1	A	803	SER
1	A	806	ARG
1	A	809	THR
1	A	826	ASP
1	A	837	ILE
1	A	855	THR
1	A	857	ARG
1	A	858	ASN
1	A	864	ILE
1	A	867	ILE
1	A	879	GLU
1	A	885	THR
1	A	889	SER
1	A	890	ASP
1	A	893	PHE
1	A	895	LYS
1	A	896	ARG
1	A	900	ASP
1	A	902	LEU
1	A	908	LEU
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
1	A	929	LEU

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Mol	Chain	Res	Type
1	A	949	ASP
1	A	953	ASN
1	A	958	VAL
1	A	969	GLN
1	A	982	THR
1	A	988	LEU
1	A	994	GLN
1	A	996	ASN
1	A	997	LEU
1	A	1000	LEU
1	A	1006	ILE
1	A	1025	ARG
1	A	1029	ARG
1	A	1030	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1054	LEU
1	A	1058	VAL
1	A	1067	LEU
1	A	1077	THR
1	A	1093	LYS
1	A	1094	VAL
1	A	1095	THR
1	A	1110	ASN
1	A	1116	LEU
1	A	1146	VAL
1	A	1147	THR
1	A	1161	THR
1	A	1172	LEU
1	A	1187	GLN
1	A	1193	LEU
1	A	1195	LEU
1	A	1205	LYS
1	A	1215	ARG
1	A	1221	LYS
1	A	1222	ASN
1	A	1229	SER
1	A	1231	ASP
1	A	1232	ASN
1	A	1235	LYS

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Mol	Chain	Res	Type
1	A	1240	CYS
1	A	1264	GLU
1	A	1270	ASN
1	A	1273	LEU
1	A	1274	ARG
1	A	1280	GLU
1	A	1291	VAL
1	A	1299	VAL
1	A	1300	LYS
1	A	1314	SER
1	A	1322	ILE
1	A	1333	ILE
1	A	1336	MET
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1370	LEU
1	A	1376	THR
1	A	1382	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1406	VAL
1	A	1407	GLU
1	A	1418	LEU
1	A	1427	ASN
1	A	1430	LEU
1	A	1444	MET
1	A	1445	ILE
2	B	26	THR
2	B	28	GLU
2	B	34	ILE
2	B	35	SER
2	B	40	GLU
2	B	44	VAL
2	B	46	GLN
2	B	55	VAL

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Mol	Chain	Res	Type
2	B	63	ILE
2	B	65	GLU
2	B	66	ASP
2	B	94	LYS
2	B	98	THR
2	B	104	GLU
2	B	108	VAL
2	B	110	HIS
2	B	120	ARG
2	B	187	SER
2	B	188	ASP
2	B	199	MET
2	B	202	TYR
2	B	213	ILE
2	B	217	ARG
2	B	218	SER
2	B	232	SER
2	B	237	VAL
2	B	244	LEU
2	B	245	GLU
2	B	246	LYS
2	B	249	ARG
2	B	253	THR
2	B	261	ARG
2	B	262	GLU
2	B	268	THR
2	B	276	ILE
2	B	283	VAL
2	B	286	PHE
2	B	304	ASP
2	B	313	MET
2	B	315	LYS
2	B	322	PHE
2	B	324	ILE
2	B	347	LYS
2	B	348	ARG
2	B	355	ILE
2	B	371	GLU
2	B	384	ARG
2	B	392	ARG
2	B	393	LYS
2	B	398	ARG

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Mol	Chain	Res	Type
2	B	401	PHE
2	B	404	LYS
2	B	412	LEU
2	B	415	GLN
2	B	416	LEU
2	B	420	LEU
2	B	424	LEU
2	B	425	THR
2	B	427	ASP
2	B	459	TYR
2	B	461	LEU
2	B	471	LYS
2	B	473	MET
2	B	475	SER
2	B	476	ARG
2	B	479	VAL
2	B	480	SER
2	B	481	GLN
2	B	483	LEU
2	B	487	THR
2	B	527	THR
2	B	533	CYS
2	B	540	SER
2	B	544	CYS
2	B	549	THR
2	B	552	MET
2	B	560	GLU
2	B	570	VAL
2	B	582	VAL
2	B	600	LEU
2	B	604	ARG
2	B	612	GLU
2	B	613	VAL
2	B	614	SER
2	B	624	LEU
2	B	625	LYS
2	B	635	ARG
2	B	637	LEU
2	B	639	ILE
2	B	641	GLU
2	B	645	SER
2	B	664	THR

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Mol	Chain	Res	Type
2	B	666	TYR
2	B	668	ASP
2	B	680	THR
2	B	682	SER
2	B	692	TYR
2	B	694	ASP
2	B	705	MET
2	B	737	THR
2	B	762	ASN
2	B	770	GLN
2	B	782	LEU
2	B	788	ARG
2	B	790	ASP
2	B	792	MET
2	B	796	LEU
2	B	801	LYS
2	B	805	THR
2	B	807	ARG
2	B	821	GLN
2	B	827	ILE
2	B	834	ASN
2	B	835	GLN
2	B	836	GLU
2	B	838	SER
2	B	843	GLN
2	B	845	SER
2	B	847	ASP
2	B	857	ARG
2	B	873	THR
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	894	ASP
2	B	899	ILE
2	B	906	SER
2	B	916	THR
2	B	939	THR
2	B	942	ARG
2	B	963	PHE
2	B	967	ARG

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Mol	Chain	Res	Type
2	B	970	THR
2	B	973	ILE
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1011	ILE
2	B	1019	SER
2	B	1022	THR
2	B	1026	LEU
2	B	1028	GLU
2	B	1031	LEU
2	B	1051	THR
2	B	1062	HIS
2	B	1067	ARG
2	B	1071	VAL
2	B	1081	LEU
2	B	1082	MET
2	B	1090	THR
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1100	ASP
2	B	1103	ILE
2	B	1112	GLN
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1138	MET
2	B	1147	LEU
2	B	1149	GLU
2	B	1150	ARG
2	B	1153	GLU
2	B	1156	ASP
2	B	1166	CYS
2	B	1175	LEU
2	B	1185	CYS

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Mol	Chain	Res	Type
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1223	ASP
3	C	4	GLU
3	C	15	LYS
3	C	18	VAL
3	C	25	VAL
3	C	32	SER
3	C	34	ARG
3	C	43	THR
3	C	54	ASN
3	C	57	VAL
3	C	58	LEU
3	C	67	LEU
3	C	69	LEU
3	C	77	ILE
3	C	81	GLU
3	C	83	SER
3	C	88	CYS
3	C	89	GLU
3	C	93	ASP
3	C	97	VAL
3	C	101	LEU
3	C	102	GLN
3	C	109	SER
3	C	111	THR
3	C	120	ILE
3	C	129	ILE
3	C	134	ILE
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	143	LEU
3	C	144	ILE
3	C	149	LYS
3	C	151	GLN
3	C	156	THR
3	C	163	ILE
3	C	178	PHE
3	C	183	TRP

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Mol	Chain	Res	Type
3	C	195	GLN
3	C	196	ASP
3	C	205	LYS
3	C	211	ASP
3	C	215	GLU
3	C	231	ASN
3	C	240	VAL
3	C	241	ASP
3	C	244	VAL
3	C	254	LYS
3	C	259	LEU
4	E	9	ILE
4	E	37	LEU
4	E	43	LYS
4	E	48	ASP
4	E	57	MET
4	E	65	THR
4	E	66	GLU
4	E	72	PHE
4	E	79	TRP
4	E	92	THR
4	E	104	ASN
4	E	107	THR
4	E	110	PHE
4	E	127	ILE
4	E	134	THR
4	E	150	VAL
4	E	156	LEU
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
5	F	77	ASP
5	F	90	ARG
5	F	97	ARG
5	F	111	LEU
5	F	112	GLU
5	F	118	LEU
5	F	119	ARG
5	F	120	ILE
5	F	123	LYS
6	H	33	GLN
6	H	53	ASP

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Mol	Chain	Res	Type
6	H	55	LEU
6	H	87	ARG
6	H	89	LEU
6	H	92	ASP
6	H	95	TYR
6	H	97	MET
6	H	102	TYR
6	H	107	VAL
6	H	110	ASP
6	H	132	LEU
6	H	135	LEU
6	H	136	LYS
7	I	7	CYS
7	I	8	ARG
7	I	10	CYS
7	I	12	ASN
7	I	13	MET
7	I	21	GLU
7	I	22	ASN
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	40	SER
7	I	42	LEU
7	I	47	GLU
7	I	50	THR
7	I	55	THR
7	I	60	GLN
7	I	62	ILE
7	I	75	CYS
7	I	83	ASN
7	I	95	THR
7	I	103	CYS
7	I	106	CYS
7	I	111	THR
8	J	2	ILE
8	J	7	CYS
8	J	10	CYS
8	J	13	VAL
8	J	14	VAL
8	J	28	ASP
8	J	30	LEU

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Mol	Chain	Res	Type
8	J	31	ASP
8	J	39	LEU
8	J	43	ARG
8	J	44	TYR
8	J	48	ARG
8	J	52	THR
9	K	1	MET
9	K	5	ASP
9	K	6	ARG
9	K	33	ILE
9	K	37	LYS
9	K	45	LEU
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	70	ARG
9	K	71	PHE
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	26	THR
10	L	31	CYS
10	L	50	ASP
10	L	51	CYS
10	L	55	ILE
10	L	63	ARG
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	306	ASN
1	A	313	GLN
1	A	399	HIS
1	A	435	HIS
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	503	GLN
1	A	517	ASN
1	A	545	GLN
1	A	654	ASN
1	A	736	ASN
1	A	741	ASN
1	A	757	ASN
1	A	760	GLN
1	A	851	HIS
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	1171	GLN
1	A	1203	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	433	GLN
2	B	494	HIS
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	587	HIS
2	B	657	HIS
2	B	686	ASN
2	B	744	HIS
2	B	762	ASN
2	B	767	ASN
2	B	822	ASN
2	B	842	ASN
2	B	878	GLN
2	B	957	ASN
2	B	1065	GLN
2	B	1161	HIS
2	B	1193	GLN
2	B	1195	HIS

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Mol	Chain	Res	Type
2	B	1211	ASN
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	184	ASN
3	C	203	GLN
3	C	231	ASN
4	E	32	GLN
4	E	61	GLN
4	E	101	GLN
4	E	143	ASN
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	131	ASN
6	H	137	GLN
7	I	60	GLN
7	I	108	HIS
7	I	116	ASN
8	J	53	HIS
9	K	40	HIS
9	K	52	ASN
9	K	65	HIS
10	L	66	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/13 (84%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	11	U
11	R	12	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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	1395/1733 (80%)	-0.02	38 (2%) 58 59	13, 87, 161, 194	0
2	B	1106/1224 (90%)	0.01	28 (2%) 61 62	16, 81, 127, 148	0
3	C	266/318 (83%)	-0.27	1 (0%) 93 94	45, 75, 113, 128	0
4	E	214/215 (99%)	0.03	7 (3%) 50 51	72, 122, 161, 166	0
5	F	84/155 (54%)	-0.10	1 (1%) 81 82	67, 91, 112, 121	0
6	H	133/146 (91%)	0.12	6 (4%) 37 38	97, 117, 137, 140	0
7	I	119/122 (97%)	-0.06	1 (0%) 87 89	79, 104, 123, 134	0
8	J	65/70 (92%)	-0.25	2 (3%) 52 55	24, 67, 95, 101	0
9	K	114/120 (95%)	-0.18	0 100 100	60, 82, 96, 97	0
10	L	46/70 (65%)	-0.01	0 100 100	86, 138, 153, 154	0
11	R	12/13 (92%)	-0.47	0 100 100	53, 77, 140, 150	0
12	T	28/28 (100%)	1.18	8 (28%) 1 1	52, 198, 323, 324	0
13	N	14/14 (100%)	1.22	3 (21%) 1 1	287, 311, 319, 321	0
All	All	3596/4228 (85%)	-0.02	95 (2%) 59 61	13, 86, 153, 324	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	8.9
13	N	1	DC	7.3
1	A	1176	LEU	5.6
1	A	44	THR	5.6
12	T	2	DT	5.5
1	A	168	GLY	5.2
1	A	153	PRO	5.0
12	T	3	DA	4.8
6	H	84	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	882	THR	4.2
13	N	14	DG	4.2
2	B	883	LEU	4.2
12	T	4	DC	4.2
2	B	869	SER	4.1
1	A	286	HIS	4.1
1	A	150	THR	4.0
1	A	316	GLN	4.0
1	A	69	THR	3.9
12	T	10	DA	3.8
2	B	1222	ARG	3.7
12	T	1	DC	3.7
2	B	474	SER	3.6
2	B	868	MET	3.6
1	A	1126	ALA	3.5
2	B	715	ALA	3.4
12	T	11	DG	3.3
2	B	1224	PHE	3.3
2	B	1221	SER	3.2
2	B	870	ILE	3.2
1	A	426	LEU	3.2
2	B	689	LEU	3.2
1	A	175	ARG	3.1
2	B	709	ASP	3.1
4	E	110	PHE	2.9
1	A	94	GLY	2.8
2	B	646	LEU	2.8
2	B	1223	ASP	2.8
1	A	1125	ALA	2.8
4	E	121	MET	2.8
2	B	90	ILE	2.8
1	A	1256	GLU	2.8
13	N	2	DT	2.7
1	A	163	SER	2.7
2	B	866	TYR	2.7
1	A	59	GLY	2.7
1	A	1225	PHE	2.7
1	A	152	VAL	2.6
2	B	92	PHE	2.6
2	B	250	PHE	2.6
1	A	166	GLY	2.6
4	E	93	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	76	GLU	2.6
8	J	26	GLN	2.6
12	T	5	DC	2.6
7	I	13	MET	2.6
2	B	257	LYS	2.5
4	E	106	GLN	2.5
1	A	311	GLN	2.5
2	B	645	SER	2.5
12	T	9	DA	2.5
6	H	134	ASN	2.4
1	A	147	VAL	2.4
1	A	148	CYS	2.4
6	H	146	ARG	2.4
1	A	1234	GLU	2.3
1	A	45	GLN	2.3
6	H	86	ASP	2.3
2	B	643	ASP	2.3
3	C	252	GLN	2.3
2	B	1191	ILE	2.3
1	A	182	VAL	2.2
6	H	85	GLY	2.2
6	H	139	ASN	2.2
4	E	57	MET	2.2
4	E	46	TYR	2.2
4	E	87	SER	2.1
1	A	171	GLN	2.1
2	B	1183	LYS	2.1
2	B	746	SER	2.1
1	A	289	ILE	2.1
1	A	1439	GLY	2.1
1	A	257	ARG	2.1
1	A	318	SER	2.1
2	B	1172	ILE	2.1
2	B	666	TYR	2.1
2	B	714	GLU	2.1
1	A	285	PRO	2.0
1	A	165	GLY	2.0
1	A	317	LYS	2.0
1	A	167	CYS	2.0
1	A	174	ILE	2.0
1	A	1156	PRO	2.0
5	F	154	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
8	J	28	ASP	2.0
2	B	69	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	ZN	A	1734	1/1	0.93	0.13	-0.95	150,150,150,150	0
14	ZN	I	203	1/1	0.94	0.13	-1.00	98,98,98,98	0
15	MG	A	1736	1/1	0.93	0.12	-1.35	61,61,61,61	0
14	ZN	C	319	1/1	0.99	0.05	-1.41	59,59,59,59	0
14	ZN	A	1735	1/1	0.98	0.08	-1.63	148,148,148,148	0
14	ZN	I	204	1/1	0.99	0.04	-1.71	101,101,101,101	0
14	ZN	B	1307	1/1	0.96	0.03	-2.25	112,112,112,112	0
14	ZN	J	101	1/1	0.99	0.09	-3.10	66,66,66,66	0
14	ZN	L	105	1/1	0.99	0.08	-	135,135,135,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.