



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:43 am BST

PDB ID : 3GTQ
Title : Backtracked RNA polymerase II complex induced by damage
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

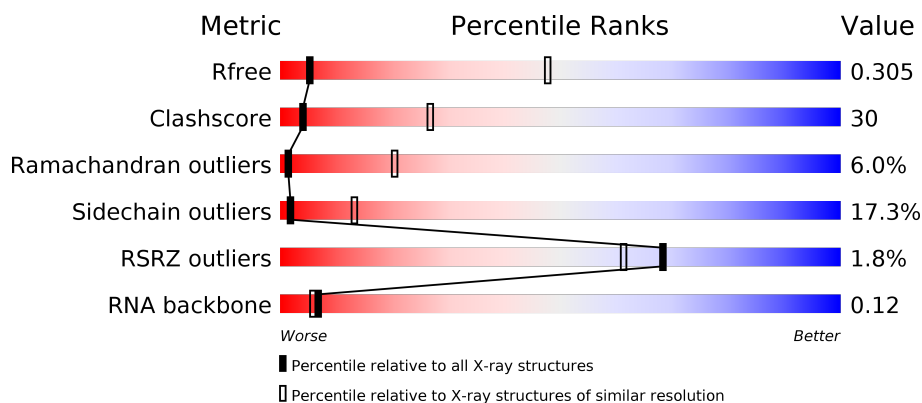
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>2%</div> <div>37% 33% 9% 20%</div> </div>
2	B	1224	<div> <div>%</div> <div>38% 42% 10% 10%</div> </div>
3	C	318	<div> <div>%</div> <div>35% 41% 7% 16%</div> </div>
4	E	215	<div> <div>3%</div> <div>55% 36% 8%</div> </div>

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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	12	
12	T	29	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28625 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(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*A P*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	11	Total	C	N	O	P	0	0	0
			243	108	50	74	11			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP *CP*CP*AP*CP*AP*GP*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	12	Total	C	N	O	P	0	0	0
			234	113	34	75	12			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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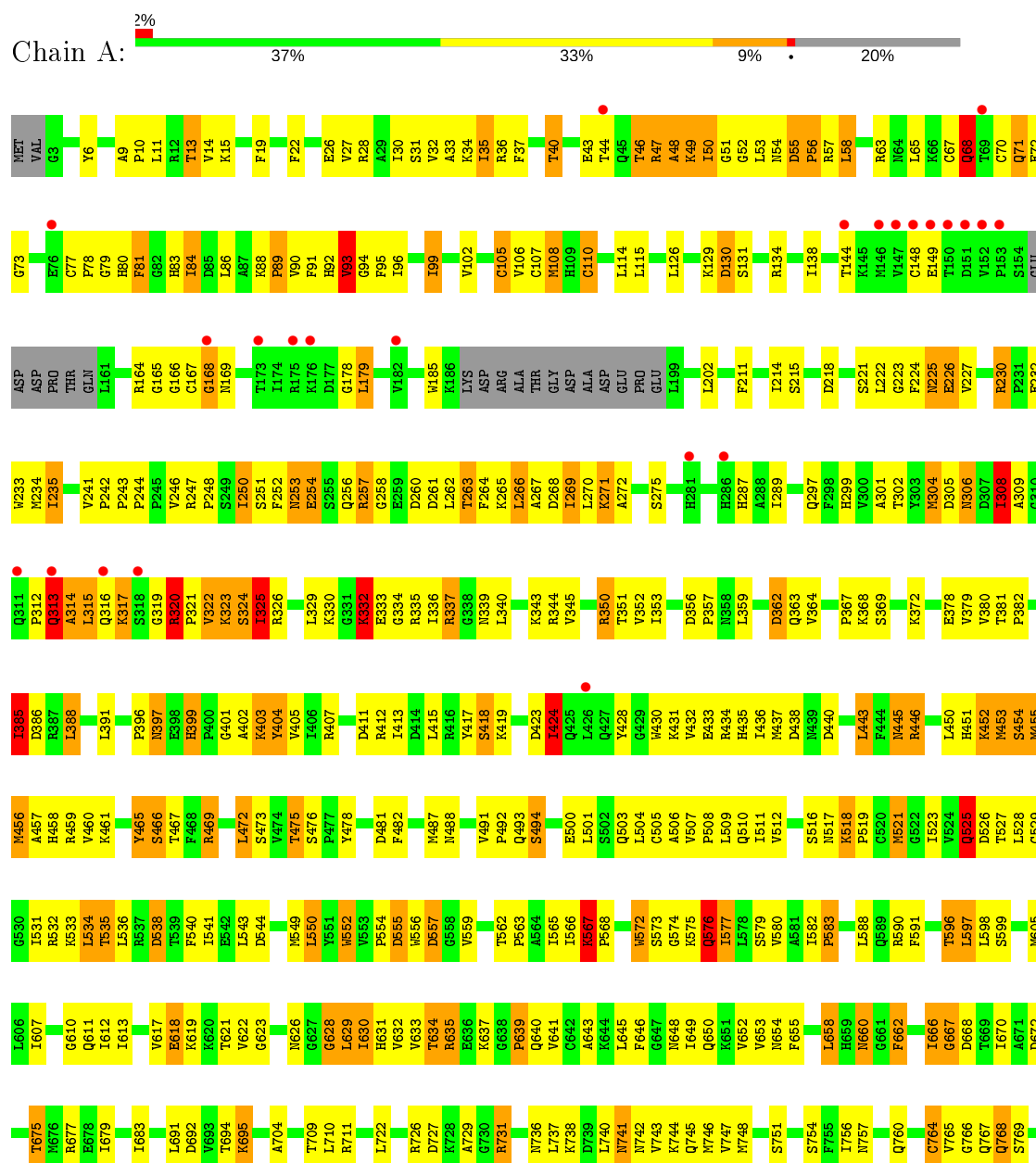
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	C	1	Total 1	Zn 1	0	0
13	A	2	Total 2	Zn 2	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

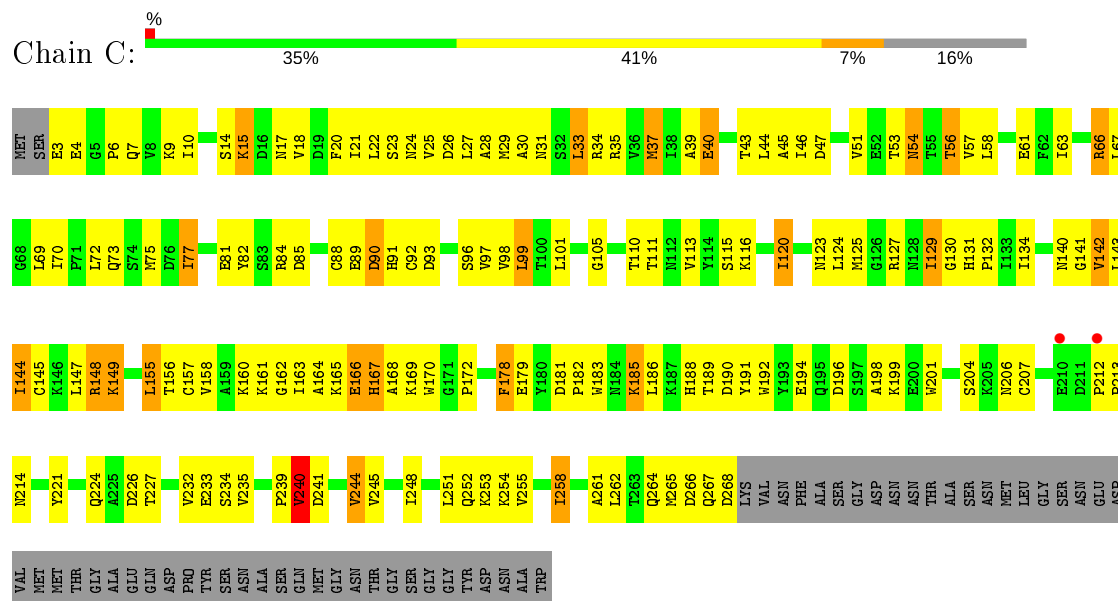




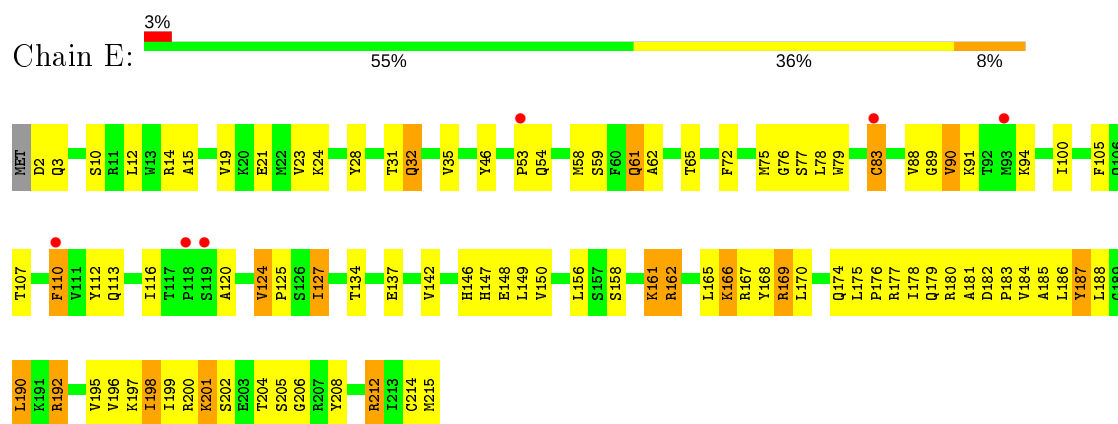




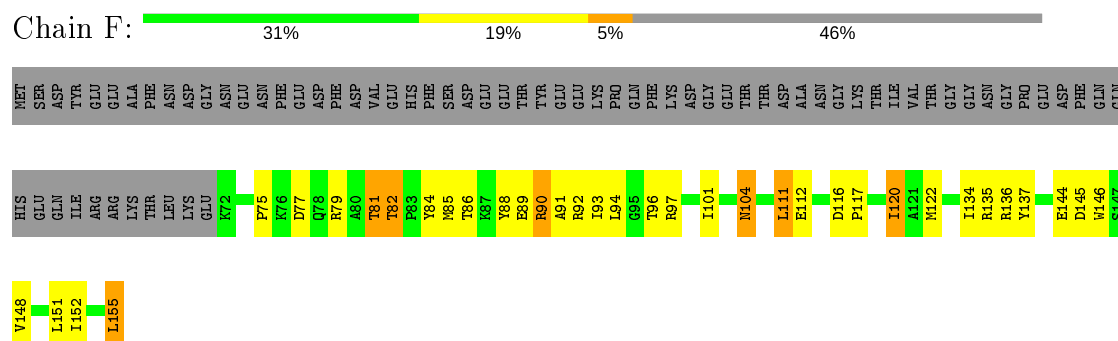
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



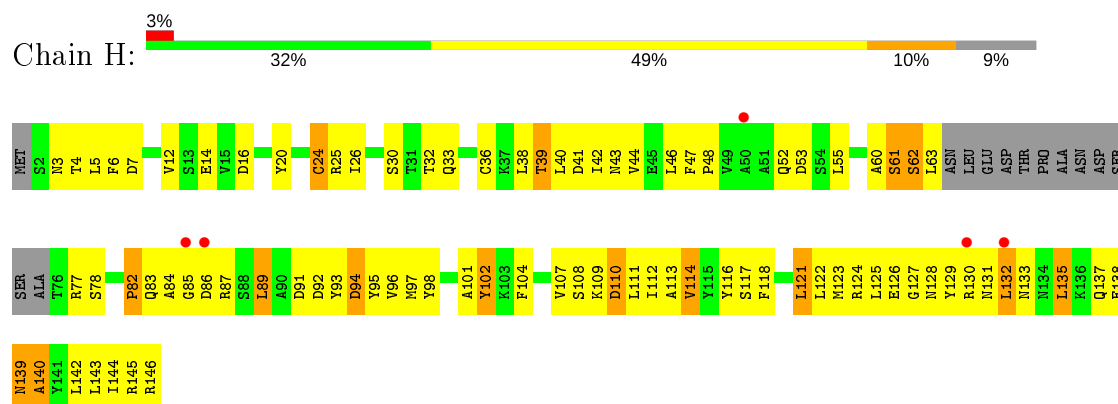
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



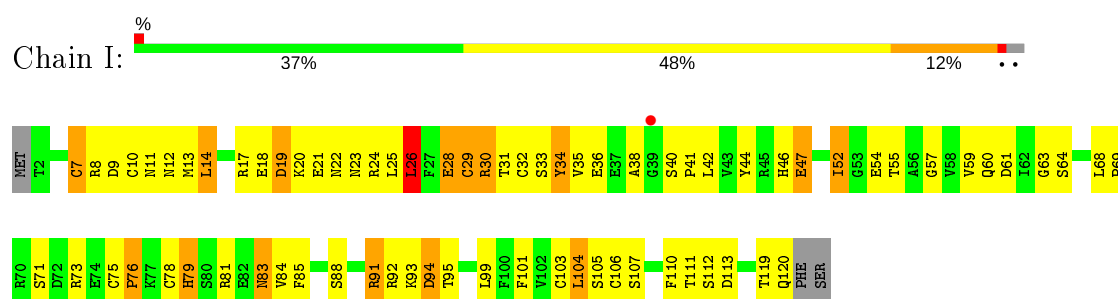
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



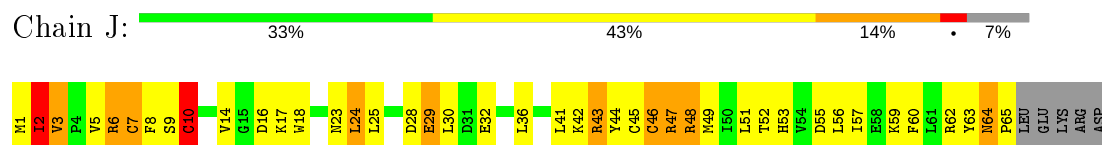
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



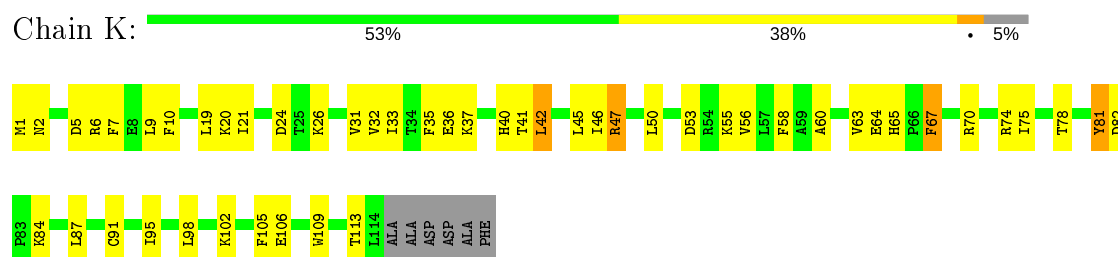
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



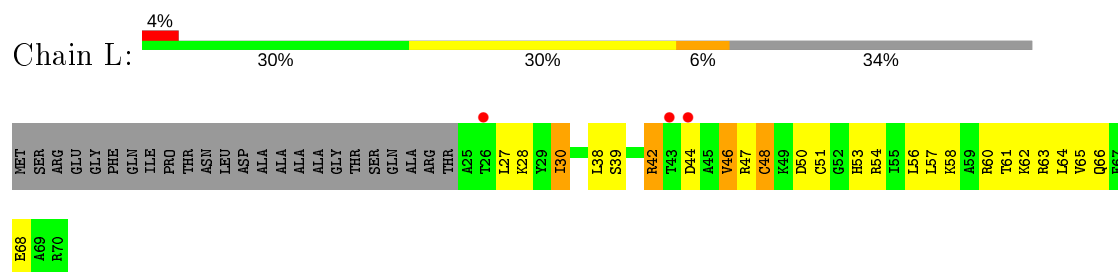
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



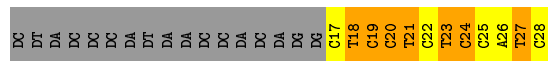
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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



- Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP*CP*CP*AP*CP*AP*GP*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.19Å 221.58Å 192.80Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 45.33 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-3.80) 95.5 (45.33-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.335 0.253 , 0.305	Depositor DCC
R_{free} test set	3287 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	98.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28625	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/11163	0.73	1/15091 (0.0%)
2	B	0.59	0/8963	0.74	1/12086 (0.0%)
3	C	0.55	0/2133	0.71	0/2891
4	E	0.50	0/1788	0.68	2/2406 (0.1%)
5	F	0.52	0/691	0.70	0/933
6	H	0.48	0/1086	0.76	1/1470 (0.1%)
7	I	0.57	0/989	0.75	1/1331 (0.1%)
8	J	0.59	0/541	0.86	2/727 (0.3%)
9	K	0.55	0/937	0.68	0/1265
10	L	0.57	0/365	0.80	0/485
11	R	1.00	0/273	1.71	3/425 (0.7%)
12	T	1.09	0/258	2.33	23/393 (5.9%)
All	All	0.57	0/29187	0.78	34/39503 (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
1	A	0	2
2	B	0	1
All	All	0	3

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	DT	O4'-C4'-C3'	-10.41	99.76	106.00
12	T	20	DC	OP2-P-O3'	-8.94	85.53	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	20	DC	OP1-P-O3'	-8.71	86.03	105.20
12	T	20	DC	O4'-C1'-N1	8.67	114.07	108.00
12	T	19	DC	N3-C2-O2	-8.28	116.11	121.90
12	T	25	DC	O4'-C1'-N1	8.26	113.78	108.00
12	T	20	DC	O3'-P-O5'	-7.82	89.14	104.00
12	T	20	DC	C4'-C3'-C2'	-7.69	96.18	103.10
4	E	161	LYS	N-CA-C	7.47	131.18	111.00
12	T	23	DT	O4'-C4'-C3'	-7.37	101.55	104.50
12	T	19	DC	O4'-C1'-N1	6.76	112.74	108.00
12	T	21	DT	OP1-P-OP2	6.74	129.72	119.60
12	T	23	DT	O4'-C1'-N1	6.46	112.52	108.00
4	E	162	ARG	N-CA-CB	-6.46	98.97	110.60
2	B	637	LEU	CA-CB-CG	6.43	130.09	115.30
12	T	20	DC	P-O3'-C3'	6.39	127.37	119.70
12	T	18	DT	C4-C5-C7	6.36	122.81	119.00
12	T	27	DT	C4'-C3'-C2'	-6.11	97.61	103.10
12	T	19	DC	N1-C2-O2	6.10	122.56	118.90
8	J	46	CYS	CA-CB-SG	-5.89	103.39	114.00
8	J	10	CYS	CA-CB-SG	5.87	124.56	114.00
12	T	21	DT	O5'-P-OP1	5.68	117.52	110.70
12	T	22	DC	C4'-C3'-C2'	-5.67	98.00	103.10
1	A	691	LEU	CA-CB-CG	5.64	128.28	115.30
12	T	27	DT	O4'-C1'-N1	5.57	111.90	108.00
6	H	132	LEU	CA-CB-CG	5.40	127.72	115.30
11	R	3	C	C6-N1-C2	-5.35	118.16	120.30
12	T	19	DC	C2-N3-C4	-5.28	117.26	119.90
11	R	9	G	C4-C5-N7	5.26	112.91	110.80
11	R	9	G	C5-N7-C8	-5.26	101.67	104.30
12	T	24	DC	O4'-C1'-N1	5.21	111.65	108.00
12	T	18	DT	C6-C5-C7	-5.07	119.86	122.90
12	T	27	DT	P-O3'-C3'	5.03	125.74	119.70
7	I	26	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1172	LEU	Peptide
1	A	320	ARG	Peptide
2	B	473	MET	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	11070	714	0
2	B	8792	0	8823	656	0
3	C	2095	0	2052	142	0
4	E	1752	0	1776	82	0
5	F	679	0	701	31	0
6	H	1068	0	1040	74	0
7	I	971	0	930	57	0
8	J	532	0	544	61	0
9	K	919	0	929	47	0
10	L	363	0	387	19	0
11	R	243	0	121	26	0
12	T	234	0	137	19	0
13	A	2	0	0	1	0
13	B	1	0	0	1	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0
All	All	28625	0	28510	1712	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 30.

All (1712) 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:704:ALA:HB1	2:B:710:LEU:CD1	1.55	1.34
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.51	1.28
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.52	1.27
2:B:879:ARG:CB	2:B:880:THR:HA	1.68	1.22
7:I:75:CYS:SG	7:I:78:CYS:HB2	1.82	1.19
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.04	1.14
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.26	1.14
2:B:879:ARG:HB2	2:B:880:THR:HA	1.20	1.14
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:43:ARG:HG3	8:J:46:CYS:HB2	1.32	1.11
2:B:222:ILE:HA	2:B:223:VAL:HB	1.17	1.11
2:B:464:GLY:HA3	2:B:478:GLY:HA2	1.32	1.10
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.53	1.09
1:A:899:VAL:CG1	1:A:929:LEU:HD13	1.84	1.08
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.13	1.08
2:B:778:MET:HE3	2:B:1094:ARG:HH11	0.99	1.07
1:A:809:THR:HB	1:A:810:PRO:CD	1.84	1.07
1:A:630:ILE:HD12	1:A:630:ILE:H	1.20	1.06
2:B:955:THR:HG22	2:B:956:THR:H	1.15	1.06
1:A:899:VAL:HG13	1:A:929:LEU:HD13	1.09	1.06
2:B:704:ALA:CB	2:B:710:LEU:HD12	1.85	1.06
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.18	1.05
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.08	1.04
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.33	1.04
1:A:1323:ASP:OD2	1:A:1326:ARG:HG3	1.56	1.03
2:B:549:THR:HG22	2:B:550:ASP:H	1.24	1.03
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.89	1.03
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.39	1.02
2:B:704:ALA:CB	2:B:710:LEU:CD1	2.37	1.01
2:B:778:MET:CE	2:B:1094:ARG:HH11	1.73	1.00
1:A:308:ILE:HG22	1:A:309:ALA:H	1.23	1.00
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.90	1.00
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.42	1.00
1:A:567:LYS:HB3	6:H:96:VAL:H	1.26	1.00
1:A:264:PHE:HE1	1:A:317:LYS:HB2	1.23	0.99
2:B:879:ARG:HB2	2:B:880:THR:CA	1.93	0.98
2:B:635:ARG:HB2	2:B:636:PRO:CD	1.95	0.97
2:B:902:GLY:O	2:B:903:VAL:O	1.83	0.97
2:B:635:ARG:CB	2:B:636:PRO:HD2	1.93	0.96
1:A:1284:MET:HB3	1:A:1306:LEU:HD23	1.44	0.96
1:A:827:THR:HG21	11:R:11:G:C4	1.99	0.95
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.06	0.95
2:B:778:MET:HE3	2:B:1094:ARG:NH1	1.80	0.95
2:B:636:PRO:CB	2:B:637:LEU:HA	1.96	0.95
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.96	0.94
1:A:1407:GLU:H	1:A:1407:GLU:CD	1.65	0.94
2:B:550:ASP:OD1	2:B:551:PRO:HD2	1.67	0.93
2:B:203:PHE:CE1	2:B:212:LEU:HD12	2.04	0.93
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.98	0.92
4:E:46:TYR:HE2	4:E:58:MET:HA	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.52	0.92
3:C:97:VAL:HG21	3:C:129:ILE:HG21	1.51	0.92
8:J:8:PHE:H	8:J:49:MET:HE3	1.34	0.92
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.52	0.92
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.52	0.91
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.00	0.91
7:I:10:CYS:HB2	7:I:31:THR:OG1	1.70	0.91
2:B:222:ILE:CA	2:B:223:VAL:HB	2.01	0.90
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.51	0.90
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.52	0.89
2:B:704:ALA:HB1	2:B:710:LEU:HD12	0.90	0.89
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.88	0.89
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.52	0.88
5:F:146:TRP:HB3	5:F:151:LEU:HD11	1.53	0.88
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	1.81	0.88
4:E:46:TYR:CE2	4:E:58:MET:HA	2.08	0.88
8:J:45:CYS:SG	8:J:46:CYS:N	2.46	0.88
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.38	0.87
12:T:27:DT:H2'	12:T:28:DC:H5''	1.54	0.87
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.75	0.87
2:B:567:GLU:CD	2:B:567:GLU:H	1.77	0.86
2:B:464:GLY:HA3	2:B:478:GLY:CA	2.06	0.86
1:A:648:ASN:O	1:A:652:VAL:HG23	1.75	0.86
2:B:169:ARG:HH11	2:B:169:ARG:CG	1.88	0.86
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.54	0.86
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.06	0.86
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.56	0.86
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.40	0.86
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.58	0.86
1:A:809:THR:HB	1:A:810:PRO:HD3	1.57	0.85
2:B:778:MET:CE	2:B:1094:ARG:NH1	2.35	0.85
2:B:879:ARG:HB3	2:B:880:THR:HA	1.58	0.84
1:A:351:THR:HG22	1:A:352:VAL:N	1.91	0.84
7:I:73:ARG:O	7:I:81:ARG:HG2	1.77	0.84
1:A:535:THR:HG21	1:A:617:VAL:H	1.42	0.84
2:B:955:THR:HG22	2:B:956:THR:N	1.91	0.84
2:B:248:SER:H	2:B:418:LYS:HZ2	1.21	0.84
2:B:706:GLN:O	2:B:710:LEU:HB2	1.77	0.84
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.60	0.84
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.93	0.83
1:A:315:LEU:CB	1:A:316:GLN:HA	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:CE1	1:A:317:LYS:HB2	2.13	0.83
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.13	0.83
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.42	0.83
2:B:986:GLN:NE2	2:B:1022:THR:HG21	1.93	0.83
2:B:1163:CYS:HB3	2:B:1167:GLY:H	1.44	0.83
1:A:780:VAL:HG22	2:B:699:GLU:OE2	1.79	0.82
1:A:14:VAL:HG11	1:A:1430:LEU:HD13	1.60	0.82
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.08	0.82
2:B:473:MET:HA	2:B:474:SER:CB	2.08	0.82
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.80	0.82
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.62	0.82
1:A:304:MET:HG2	2:B:1210:MET:HG3	1.62	0.81
3:C:167:HIS:CD2	3:C:169:LYS:H	1.98	0.81
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.63	0.81
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.61	0.81
2:B:169:ARG:HH11	2:B:169:ARG:HG3	1.44	0.80
4:E:198:ILE:HD11	4:E:212:ARG:HG2	1.62	0.80
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.63	0.80
1:A:573:SER:O	1:A:576:GLN:HB2	1.81	0.80
2:B:955:THR:CG2	2:B:956:THR:H	1.95	0.80
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.80
2:B:707:PRO:HB3	2:B:741:CYS:SG	2.22	0.80
1:A:445:ASN:HB2	1:A:454:SER:O	1.80	0.79
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.64	0.79
10:L:46:VAL:HG22	10:L:47:ARG:H	1.47	0.79
11:R:2:U:H2'	11:R:3:C:H6	1.47	0.79
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.65	0.79
1:A:518:LYS:HG2	1:A:519:PRO:HD2	1.64	0.79
1:A:827:THR:HB	11:R:11:G:N3	1.97	0.79
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.63	0.78
2:B:37:PHE:O	2:B:38:PHE:HB2	1.83	0.78
2:B:796:LEU:CB	2:B:799:PRO:HG3	2.13	0.78
1:A:43:GLU:HG3	1:A:46:THR:HB	1.65	0.78
1:A:820:GLY:O	1:A:821:ARG:HB3	1.83	0.78
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.66	0.78
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.41	0.78
3:C:123:ASN:HD22	3:C:125:MET:CG	1.96	0.78
1:A:1004:ASN:OD1	1:A:1006:ILE:HD13	1.84	0.78
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.19	0.78
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.64	0.78
2:B:34:ILE:HG12	2:B:542:MET:HE3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:104:PHE:HD2	6:H:114:VAL:HG12	1.49	0.78
2:B:223:VAL:O	2:B:223:VAL:HG12	1.83	0.77
2:B:1072:MET:HE2	2:B:1085:ILE:HD13	1.65	0.77
7:I:10:CYS:CB	7:I:31:THR:OG1	2.31	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.32	0.77
1:A:1256:GLU:C	1:A:1258:HIS:H	1.88	0.77
1:A:853:ASP:OD2	1:A:855:THR:HG22	1.85	0.77
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.49	0.77
2:B:222:ILE:HA	2:B:223:VAL:CB	2.09	0.77
1:A:164:ARG:HG3	1:A:165:GLY:H	1.50	0.77
1:A:56:PRO:O	1:A:57:ARG:HG3	1.86	0.76
1:A:351:THR:CG2	1:A:352:VAL:N	2.47	0.76
2:B:464:GLY:CA	2:B:478:GLY:HA2	2.13	0.76
4:E:198:ILE:HD11	4:E:212:ARG:CG	2.15	0.76
1:A:1029:ARG:HE	1:A:1033:GLN:HE22	1.32	0.76
2:B:956:THR:HA	2:B:961:LEU:O	1.84	0.76
3:C:123:ASN:ND2	3:C:125:MET:CG	2.48	0.76
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.66	0.76
1:A:809:THR:HG21	2:B:730:ARG:HG3	1.66	0.76
1:A:630:ILE:H	1:A:630:ILE:CD1	1.96	0.76
1:A:503:GLN:O	1:A:509:LEU:HD11	1.87	0.75
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.68	0.75
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.68	0.75
2:B:995:ARG:HG2	2:B:997:GLU:OE2	1.87	0.75
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.51	0.75
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.27	0.75
2:B:541:LEU:HD21	2:B:812:LEU:HD21	1.67	0.75
1:A:451:HIS:HB2	1:A:453:MET:H	1.50	0.75
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.69	0.75
11:R:2:U:H2'	11:R:3:C:C6	2.21	0.75
1:A:403:LYS:O	1:A:404:TYR:HB2	1.87	0.75
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.17	0.75
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.65	0.74
2:B:515:HIS:H	2:B:518:HIS:HD2	1.34	0.74
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.69	0.74
1:A:809:THR:HB	1:A:810:PRO:HD2	1.66	0.74
2:B:211:VAL:O	2:B:480:SER:HA	1.87	0.74
3:C:20:PHE:HD1	3:C:21:ILE:O	1.69	0.74
1:A:821:ARG:O	1:A:825:ILE:HG12	1.88	0.74
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.51	0.74
2:B:901:PRO:HG2	10:L:58:LYS:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:MET:HA	2:B:474:SER:HB3	1.69	0.73
1:A:870:GLU:HB3	4:E:204:THR:CG2	2.18	0.73
1:A:402:ALA:HB1	1:A:433:GLU:O	1.88	0.73
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.14	0.73
2:B:179:CYS:SG	2:B:181:LEU:HD13	2.27	0.73
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.70	0.73
2:B:481:GLN:HB2	2:B:494:HIS:HE1	1.54	0.73
1:A:829:VAL:C	1:A:831:THR:H	1.90	0.73
2:B:223:VAL:O	2:B:223:VAL:CG1	2.37	0.73
1:A:99:ILE:HD13	1:A:235:ILE:HG23	1.69	0.73
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.71	0.73
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.71	0.73
2:B:474:SER:O	2:B:476:ARG:N	2.21	0.72
3:C:23:SER:O	3:C:25:VAL:HG23	1.89	0.72
6:H:24:CYS:HB2	6:H:44:VAL:HG23	1.69	0.72
2:B:957:ASN:HB3	2:B:961:LEU:HD12	1.71	0.72
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.24	0.72
2:B:169:ARG:NH1	2:B:169:ARG:HG3	2.03	0.72
8:J:43:ARG:HG3	8:J:46:CYS:CB	2.16	0.72
1:A:455:MET:HE3	2:B:1134:GLU:HB3	1.71	0.72
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.54	0.72
1:A:34:LYS:HD3	1:A:36:ARG:HH22	1.55	0.72
9:K:63:VAL:HG23	9:K:63:VAL:O	1.89	0.72
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.72	0.72
2:B:125:SER:HA	2:B:171:PRO:HA	1.72	0.72
3:C:51:VAL:HA	3:C:155:LEU:HB3	1.72	0.71
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.90	0.71
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.72	0.71
2:B:879:ARG:CB	2:B:880:THR:CA	2.54	0.71
2:B:1051:THR:HB	2:B:1054:GLY:H	1.56	0.71
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.26	0.71
2:B:610:ASN:O	2:B:613:VAL:HG23	1.90	0.71
3:C:142:VAL:H	8:J:16:ASP:HB3	1.56	0.71
1:A:827:THR:HG21	11:R:11:G:N9	2.06	0.71
2:B:1056:SER:HB3	2:B:1066:SER:O	1.91	0.70
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.26	0.70
2:B:875:GLU:O	2:B:877:PRO:HD3	1.91	0.70
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.71	0.70
6:H:84:ALA:C	6:H:86:ASP:H	1.91	0.70
2:B:983:ARG:CD	2:B:1091:TYR:HB3	2.20	0.70
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.55	0.70
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.71	0.70
1:A:1025:ARG:CG	1:A:1025:ARG:HH11	1.95	0.70
1:A:820:GLY:O	1:A:821:ARG:CB	2.40	0.70
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.73	0.70
2:B:46:GLN:NE2	2:B:496:ARG:HG2	2.06	0.70
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.27	0.70
1:A:55:ASP:O	1:A:58:LEU:N	2.25	0.70
2:B:203:PHE:CE1	2:B:212:LEU:CD1	2.73	0.70
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.23	0.70
1:A:858:ASN:HD22	1:A:860:LEU:H	1.40	0.70
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.73	0.69
2:B:549:THR:HG22	2:B:550:ASP:N	2.04	0.69
8:J:41:LEU:HD22	8:J:46:CYS:O	1.92	0.69
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.21	0.69
7:I:75:CYS:SG	7:I:78:CYS:CB	2.74	0.69
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.73	0.69
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.56	0.69
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.74	0.69
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.90	0.69
1:A:304:MET:CG	2:B:1210:MET:HG3	2.22	0.69
2:B:476:ARG:C	2:B:478:GLY:H	1.96	0.69
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.75	0.69
8:J:43:ARG:CG	8:J:46:CYS:HB2	2.16	0.69
1:A:834:THR:HG21	1:A:1077:THR:HA	1.74	0.69
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.57	0.69
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.74	0.69
2:B:704:ALA:HB2	2:B:738:PHE:CE2	2.27	0.69
1:A:453:MET:C	1:A:455:MET:H	1.96	0.69
1:A:868:TYR:CE2	1:A:1366:ARG:HD3	2.28	0.69
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.21	0.68
1:A:401:GLY:C	1:A:435:HIS:CD2	2.67	0.68
1:A:511:ILE:HD13	1:A:646:PHE:HE1	1.59	0.68
1:A:77:CYS:SG	13:A:1735:ZN:ZN	1.83	0.68
2:B:487:THR:O	2:B:488:TYR:C	2.31	0.68
1:A:858:ASN:HD22	1:A:858:ASN:C	1.96	0.68
2:B:744:HIS:HD2	2:B:746:SER:H	1.41	0.68
1:A:308:ILE:HG22	1:A:309:ALA:N	2.03	0.68
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.75	0.68
3:C:35:ARG:HD3	9:K:41:THR:HA	1.75	0.68
4:E:199:ILE:O	4:E:199:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASN:OD1	1:A:397:ASN:N	2.27	0.68
1:A:265:LYS:NZ	1:A:322:VAL:HG12	2.09	0.68
1:A:324:SER:O	1:A:325:ILE:HB	1.92	0.68
6:H:109:LYS:HD2	6:H:111:LEU:HD12	1.75	0.68
2:B:493:SER:HB3	2:B:497:ARG:HH21	1.57	0.68
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.76	0.68
3:C:54:ASN:C	3:C:54:ASN:HD22	1.97	0.67
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.24	0.67
8:J:57:ILE:HA	8:J:60:PHE:HD2	1.58	0.67
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.94	0.67
3:C:54:ASN:ND2	3:C:56:THR:OG1	2.27	0.67
10:L:61:THR:CG2	10:L:62:LYS:N	2.56	0.67
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.30	0.67
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.60	0.67
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.30	0.67
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.75	0.67
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.76	0.67
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.25	0.67
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.77	0.67
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.60	0.67
3:C:58:LEU:CD2	3:C:145:CYS:HB2	2.25	0.67
2:B:957:ASN:O	2:B:959:ASP:N	2.28	0.67
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.75	0.67
3:C:77:ILE:HD12	3:C:161:LYS:HE2	1.77	0.67
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.94	0.66
2:B:359:GLU:HA	2:B:362:PRO:HG3	1.77	0.66
1:A:886:ILE:HG22	1:A:887:GLY:N	2.09	0.66
4:E:156:LEU:HD11	4:E:195:VAL:HB	1.76	0.66
2:B:212:LEU:HD23	2:B:479:VAL:O	1.96	0.66
2:B:751:VAL:HG13	2:B:812:LEU:CD1	2.25	0.66
1:A:946:VAL:HG22	4:E:201:LYS:HG3	1.78	0.66
2:B:1129:ARG:HE	2:B:1131:GLY:HA3	1.61	0.66
8:J:5:VAL:O	8:J:6:ARG:O	2.13	0.66
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.61	0.66
1:A:567:LYS:HZ1	6:H:97:MET:HB3	1.59	0.66
1:A:855:THR:HG21	1:A:857:ARG:HE	1.59	0.66
3:C:58:LEU:HD23	3:C:145:CYS:HB2	1.78	0.66
2:B:552:MET:HA	2:B:555:ILE:HB	1.78	0.65
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.78	0.65
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.60	0.65
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:42:LEU:O	9:K:42:LEU:HG	1.95	0.65
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.78	0.65
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.27	0.65
2:B:110:HIS:CE1	10:L:53:HIS:HE1	2.15	0.65
2:B:21:GLU:HA	2:B:656:GLY:CA	2.26	0.65
3:C:120:ILE:HG21	3:C:124:LEU:CD2	2.27	0.65
6:H:91:ASP:C	6:H:93:TYR:H	2.00	0.65
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.78	0.65
2:B:805:THR:HG21	2:B:815:ARG:HH21	1.62	0.65
1:A:93:VAL:O	1:A:96:ILE:HG22	1.97	0.65
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.37	0.65
1:A:13:THR:HG22	1:A:1432:GLN:NE2	2.12	0.65
1:A:809:THR:CB	1:A:810:PRO:HD3	2.27	0.65
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.79	0.65
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.79	0.65
6:H:82:PRO:C	6:H:84:ALA:H	2.00	0.65
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.62	0.65
1:A:827:THR:CB	11:R:11:G:N3	2.59	0.65
1:A:1004:ASN:ND2	4:E:167:ARG:HD3	2.12	0.65
1:A:554:PRO:HG2	1:A:555:ASP:OD1	1.97	0.65
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.79	0.65
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.79	0.64
2:B:476:ARG:O	2:B:478:GLY:N	2.30	0.64
3:C:255:VAL:O	3:C:258:ILE:HG22	1.97	0.64
11:R:9:G:H1	12:T:19:DC:H42	1.45	0.64
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.62	0.64
1:A:369:SER:CB	9:K:2:ASN:HD21	2.10	0.64
2:B:1072:MET:HB2	2:B:1085:ILE:HD12	1.78	0.64
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.32	0.64
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.13	0.64
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.77	0.64
6:H:14:GLU:O	6:H:26:ILE:HD12	1.97	0.64
9:K:21:ILE:HD12	9:K:33:ILE:HG12	1.78	0.64
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.78	0.64
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.32	0.64
2:B:64:CYS:HA	2:B:67:SER:HB2	1.80	0.64
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.62	0.64
2:B:803:LEU:H	2:B:822:ASN:HD21	1.44	0.64
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.62	0.64
1:A:899:VAL:HG13	1:A:929:LEU:CD1	2.04	0.64
2:B:1166:CYS:SG	13:B:1307:ZN:ZN	1.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:HD3	1:A:413:ILE:CD1	2.27	0.64
2:B:698:GLU:O	2:B:701:ILE:HD13	1.98	0.64
1:A:253:ASN:CG	1:A:254:GLU:H	2.01	0.64
1:A:381:THR:HG22	1:A:382:PRO:HD2	1.80	0.64
1:A:853:ASP:OD2	1:A:855:THR:CG2	2.46	0.64
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.19	0.64
2:B:20:ASP:N	2:B:655:LYS:HZ3	1.96	0.63
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.79	0.63
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.66	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.13	0.63
2:B:797:TYR:CE1	2:B:854:LEU:HD23	2.33	0.63
5:F:111:LEU:H	5:F:111:LEU:HD13	1.64	0.63
1:A:709:THR:HG23	7:I:94:ASP:HA	1.80	0.63
1:A:964:ILE:HD11	1:A:1037:LEU:HD21	1.81	0.63
1:A:630:ILE:O	1:A:634:THR:OG1	2.16	0.63
2:B:751:VAL:HG13	2:B:812:LEU:HD11	1.79	0.63
3:C:167:HIS:HD2	3:C:168:ALA:N	1.96	0.63
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.45	0.63
1:A:452:LYS:O	2:B:1141:HIS:CE1	2.51	0.63
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.81	0.63
4:E:15:ALA:O	4:E:19:VAL:HG23	1.98	0.63
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.34	0.63
2:B:706:GLN:O	2:B:710:LEU:CB	2.46	0.63
4:E:185:ALA:HB1	4:E:190:LEU:HG	1.80	0.63
7:I:17:ARG:HG2	7:I:18:GLU:H	1.64	0.63
2:B:476:ARG:C	2:B:478:GLY:N	2.53	0.63
2:B:902:GLY:O	2:B:903:VAL:C	2.37	0.63
3:C:261:ALA:HA	3:C:264:GLN:HG3	1.81	0.63
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.38	0.62
2:B:481:GLN:HB2	2:B:494:HIS:CE1	2.33	0.62
2:B:977:GLY:HA3	2:B:1099:VAL:CG1	2.29	0.62
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.82	0.62
1:A:630:ILE:HD12	1:A:630:ILE:N	2.03	0.62
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.81	0.62
1:A:402:ALA:CB	1:A:434:ARG:HA	2.29	0.62
1:A:613:ILE:HG23	6:H:117:SER:HB2	1.80	0.62
2:B:1065:GLN:O	2:B:1067:ARG:N	2.32	0.62
2:B:110:HIS:CE1	10:L:53:HIS:CE1	2.88	0.62
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.29	0.62
2:B:815:ARG:HG3	2:B:816:GLU:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:HIS:CD2	3:C:168:ALA:N	2.67	0.62
8:J:10:CYS:SG	8:J:43:ARG:CD	2.86	0.62
1:A:1332:PHE:CD1	1:A:1348:LEU:HD13	2.35	0.62
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.81	0.62
1:A:267:ALA:O	1:A:271:LYS:HB2	2.00	0.62
2:B:1034:VAL:HG22	2:B:1059:LEU:HB3	1.80	0.62
2:B:1066:SER:O	2:B:1067:ARG:HD2	2.00	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.35	0.62
2:B:345:LYS:N	2:B:348:ARG:HE	1.96	0.62
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.35	0.62
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.82	0.62
8:J:8:PHE:N	8:J:49:MET:HE3	2.09	0.62
10:L:61:THR:HG22	10:L:62:LYS:N	2.15	0.62
2:B:21:GLU:HA	2:B:656:GLY:HA3	1.81	0.62
2:B:478:GLY:O	2:B:480:SER:N	2.30	0.62
2:B:978:ASP:HB2	2:B:980:PHE:CE1	2.35	0.62
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.80	0.62
1:A:827:THR:CG2	11:R:11:G:C4	2.79	0.62
2:B:100:PRO:HA	2:B:126:SER:HA	1.81	0.61
2:B:468:GLU:HG3	2:B:469:GLN:H	1.65	0.61
2:B:248:SER:O	2:B:249:ARG:HB2	2.00	0.61
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.81	0.61
1:A:500:GLU:OE1	2:B:1144:ALA:N	2.32	0.61
1:A:577:ILE:O	1:A:580:VAL:HB	2.01	0.61
6:H:5:LEU:HD22	6:H:133:ASN:O	2.00	0.61
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.82	0.61
2:B:843:GLN:N	2:B:994:TYR:O	2.31	0.61
6:H:128:ASN:O	6:H:130:ARG:N	2.33	0.61
7:I:34:TYR:HE2	7:I:36:GLU:HG3	1.66	0.61
3:C:235:VAL:HG21	8:J:6:ARG:NH2	2.15	0.61
2:B:808:ALA:O	2:B:810:GLU:N	2.32	0.61
6:H:128:ASN:C	6:H:130:ARG:H	2.04	0.61
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.66	0.61
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.13	0.61
2:B:175:ARG:HG3	2:B:175:ARG:HH11	1.66	0.61
6:H:61:SER:HB2	6:H:139:ASN:HB3	1.83	0.61
1:A:265:LYS:C	1:A:267:ALA:H	2.04	0.61
1:A:956:LEU:HD21	1:A:1017:LEU:HD22	1.81	0.61
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.48	0.61
2:B:542:MET:HG3	2:B:747:MET:CE	2.30	0.61
1:A:889:SER:HB2	1:A:892:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:O	2:B:297:ILE:HG12	2.00	0.61
2:B:459:TYR:O	2:B:459:TYR:CD2	2.54	0.61
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.66	0.61
3:C:54:ASN:HD22	3:C:56:THR:H	1.48	0.61
7:I:7:CYS:SG	7:I:9:ASP:N	2.74	0.61
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.83	0.60
1:A:77:CYS:SG	1:A:80:HIS:CE1	2.94	0.60
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.01	0.60
2:B:492:LEU:HB3	2:B:751:VAL:HG11	1.82	0.60
5:F:111:LEU:H	5:F:111:LEU:CD1	2.13	0.60
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.84	0.60
3:C:18:VAL:HG23	3:C:240:VAL:HG22	1.83	0.60
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.83	0.60
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.83	0.60
1:A:979:SER:OG	1:A:980:ASP:N	2.34	0.60
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.83	0.60
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.83	0.60
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.82	0.60
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.83	0.60
6:H:40:LEU:HG	6:H:42:ILE:CD1	2.31	0.60
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.66	0.60
8:J:46:CYS:SG	13:J:101:ZN:ZN	1.89	0.60
1:A:1039:LYS:O	1:A:1043:ASP:HB2	2.01	0.60
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.00	0.60
2:B:315:LYS:O	2:B:319:GLU:HG2	2.02	0.60
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.34	0.60
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.50	0.60
2:B:613:VAL:HG13	2:B:628:THR:HB	1.84	0.60
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.37	0.60
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.36	0.60
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.31	0.60
2:B:999:MET:CG	2:B:1008:PRO:HD2	2.32	0.60
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.36	0.60
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.37	0.60
1:A:754:SER:N	1:A:757:ASN:HD22	2.00	0.60
2:B:449:ASN:O	2:B:451:LYS:N	2.35	0.60
2:B:451:LYS:HA	2:B:454:THR:HB	1.83	0.60
6:H:4:THR:HA	6:H:60:ALA:HA	1.84	0.60
2:B:952:VAL:HG12	2:B:953:LEU:N	2.16	0.59
3:C:145:CYS:HA	8:J:2:ILE:HD13	1.84	0.59
3:C:69:LEU:O	8:J:6:ARG:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.36	0.59
12:T:26:DA:H2"	12:T:27:DT:H5"	1.84	0.59
1:A:261:ASP:HB3	1:A:323:LYS:HG3	1.83	0.59
2:B:708:GLU:C	2:B:710:LEU:H	2.05	0.59
2:B:803:LEU:N	2:B:822:ASN:HD21	1.99	0.59
1:A:518:LYS:HG2	1:A:519:PRO:CD	2.31	0.59
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.83	0.59
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.83	0.59
2:B:470:LYS:O	2:B:471:LYS:HG3	2.02	0.59
3:C:77:ILE:CD1	3:C:161:LYS:HE2	2.32	0.59
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.66	0.59
2:B:901:PRO:CG	10:L:58:LYS:O	2.50	0.59
2:B:901:PRO:HB2	10:L:60:ARG:HA	1.84	0.59
1:A:868:TYR:HE2	1:A:1366:ARG:HD3	1.66	0.59
2:B:484:ASN:ND2	2:B:490:SER:HB2	2.17	0.59
1:A:1005:GLU:HG3	1:A:1009:ASN:ND2	2.18	0.59
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.49	0.59
2:B:638:PHE:O	2:B:740:HIS:HB2	2.03	0.59
3:C:98:VAL:HG12	3:C:99:LEU:N	2.18	0.59
7:I:94:ASP:N	7:I:94:ASP:OD2	2.34	0.59
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.42	0.59
1:A:350:ARG:HD3	1:A:488:ASN:OD1	2.02	0.59
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.67	0.59
1:A:848:ILE:HG13	1:A:858:ASN:HB3	1.83	0.59
1:A:1100:ARG:HH12	1:A:1111:MET:HE2	1.68	0.59
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.84	0.59
2:B:684:LEU:HD22	2:B:689:LEU:HD12	1.85	0.59
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.37	0.59
1:A:576:GLN:HA	1:A:576:GLN:HE21	1.68	0.58
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.83	0.58
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.32	0.58
2:B:130:VAL:HG12	2:B:131:ASP:N	2.18	0.58
4:E:168:TYR:O	4:E:169:ARG:HG2	2.03	0.58
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.03	0.58
2:B:230:ALA:HA	2:B:261:ARG:NH1	2.18	0.58
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.36	0.58
2:B:860:MET:SD	2:B:861:ASP:N	2.77	0.58
1:A:1155:ASP:OD1	1:A:1161:THR:HA	2.03	0.58
1:A:1256:GLU:C	1:A:1258:HIS:N	2.57	0.58
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.68	0.58
2:B:977:GLY:HA3	2:B:1099:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ALA:C	1:A:49:LYS:HG2	2.23	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.35	0.58
2:B:640:VAL:HG13	2:B:650:GLU:O	2.04	0.58
1:A:658:LEU:HD22	2:B:831:SER:HA	1.85	0.58
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.86	0.58
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.86	0.58
2:B:516:ASN:H	2:B:516:ASN:HD22	1.50	0.58
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.33	0.58
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.38	0.58
1:A:782:ARG:HB3	1:A:788:SER:O	2.04	0.58
2:B:34:ILE:HG12	2:B:542:MET:CE	2.34	0.58
9:K:82:ASP:OD2	9:K:84:LYS:HB2	2.03	0.58
1:A:1386:ARG:HG2	1:A:1403:GLU:OE1	2.04	0.57
1:A:827:THR:HB	11:R:11:G:C2	2.39	0.57
2:B:1187:ASN:HD21	2:B:1190:ASP:H	1.52	0.57
6:H:36:CYS:HB2	6:H:130:ARG:HH22	1.67	0.57
2:B:808:ALA:C	2:B:810:GLU:H	2.07	0.57
2:B:898:LEU:HB2	10:L:58:LYS:HE3	1.86	0.57
2:B:861:ASP:OD1	2:B:914:LYS:HE2	2.04	0.57
4:E:170:LEU:HD13	4:E:175:LEU:HD22	1.85	0.57
6:H:89:LEU:HB2	6:H:91:ASP:HB3	1.84	0.57
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.04	0.57
1:A:14:VAL:CG1	1:A:1430:LEU:HD13	2.32	0.57
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.86	0.57
4:E:90:VAL:H	4:E:120:ALA:HB2	1.68	0.57
1:A:540:PHE:HZ	6:H:121:LEU:HD21	1.69	0.57
1:A:870:GLU:HB3	4:E:204:THR:HG21	1.85	0.57
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.04	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
6:H:109:LYS:CD	6:H:111:LEU:HD12	2.34	0.57
1:A:211:PHE:HA	1:A:214:ILE:HG12	1.87	0.57
1:A:518:LYS:CG	1:A:519:PRO:HD2	2.35	0.57
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.40	0.57
1:A:802:ASN:ND2	2:B:729:ILE:H	2.02	0.57
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.84	0.57
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.19	0.57
6:H:139:ASN:O	6:H:140:ALA:HB2	2.05	0.57
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.84	0.57
1:A:738:LYS:HE2	3:C:194:GLU:HA	1.85	0.57
3:C:261:ALA:HA	3:C:264:GLN:CG	2.35	0.57
1:A:224:PHE:HZ	1:A:234:MET:CE	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:CB	1:A:316:GLN:CA	2.83	0.57
1:A:399:HIS:O	1:A:401:GLY:N	2.34	0.57
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.40	0.57
2:B:169:ARG:CG	2:B:169:ARG:NH1	2.56	0.57
1:A:559:VAL:HG23	1:A:559:VAL:O	2.05	0.57
1:A:802:ASN:HD21	2:B:729:ILE:N	2.03	0.57
5:F:146:TRP:HB3	5:F:151:LEU:CD1	2.32	0.57
6:H:96:VAL:HA	6:H:142:LEU:O	2.05	0.57
9:K:21:ILE:CD1	9:K:33:ILE:HG12	2.34	0.57
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.18	0.56
1:A:1301:GLU:HG3	1:A:1301:GLU:O	2.05	0.56
1:A:261:ASP:HB3	1:A:323:LYS:CG	2.35	0.56
1:A:579:SER:HB3	1:A:611:GLN:HA	1.86	0.56
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.87	0.56
1:A:455:MET:CE	2:B:1134:GLU:HB3	2.34	0.56
2:B:821:GLN:HE22	2:B:851:PHE:H	1.53	0.56
6:H:82:PRO:O	6:H:83:GLN:HB2	2.04	0.56
1:A:1404:GLU:HB3	1:A:1407:GLU:HG2	1.86	0.56
1:A:335:ARG:O	1:A:339:ASN:HB2	2.05	0.56
8:J:45:CYS:O	8:J:48:ARG:HG3	2.05	0.56
1:A:265:LYS:HZ1	1:A:322:VAL:HG12	1.71	0.56
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.87	0.56
1:A:775:ILE:O	1:A:797:LYS:HE2	2.05	0.56
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.88	0.56
1:A:457:ALA:HB2	1:A:505:CYS:HB2	1.86	0.56
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.06	0.56
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.56
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.05	0.56
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.87	0.56
3:C:91:HIS:HB3	3:C:96:SER:OG	2.04	0.56
1:A:1116:LEU:HB2	1:A:1308:THR:HG21	1.87	0.56
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.87	0.56
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.70	0.56
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.70	0.56
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.38	0.56
2:B:474:SER:C	2:B:476:ARG:N	2.59	0.56
1:A:567:LYS:NZ	6:H:97:MET:HB3	2.20	0.56
2:B:857:ARG:NH2	12:T:24:DC:OP1	2.38	0.56
1:A:1436:ILE:O	1:A:1439:GLY:N	2.38	0.56
1:A:596:THR:C	1:A:598:LEU:H	2.09	0.56
1:A:1428:VAL:HG22	2:B:1147:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.69	0.56
2:B:803:LEU:HD11	2:B:1036:ALA:HB2	1.88	0.56
1:A:1325:THR:O	4:E:148:GLU:HG3	2.06	0.56
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.86	0.56
1:A:1436:ILE:O	1:A:1437:GLY:C	2.44	0.56
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.38	0.56
1:A:658:LEU:CD2	2:B:831:SER:HA	2.36	0.56
1:A:466:SER:O	2:B:1103:ILE:HD12	2.04	0.56
3:C:134:ILE:HG23	3:C:141:GLY:H	1.71	0.56
3:C:91:HIS:CE1	3:C:158:VAL:HG11	2.40	0.56
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.31	0.56
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.88	0.56
1:A:1239:ARG:HB3	1:A:1239:ARG:HH11	1.70	0.56
1:A:662:PHE:HZ	1:A:746:MET:SD	2.28	0.56
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.05	0.56
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.36	0.56
1:A:855:THR:HG21	1:A:857:ARG:NE	2.21	0.56
2:B:1084:GLN:CD	2:B:1084:GLN:H	2.09	0.56
3:C:22:LEU:HD21	3:C:25:VAL:HG21	1.88	0.56
1:A:469:ARG:NH2	2:B:991:GLY:O	2.39	0.56
1:A:50:ILE:HG22	1:A:52:GLY:N	2.21	0.56
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.41	0.56
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.87	0.55
2:B:369:GLY:O	2:B:370:PHE:CD1	2.59	0.55
2:B:549:THR:CG2	2:B:550:ASP:H	2.07	0.55
1:A:1284:MET:HB3	1:A:1306:LEU:CD2	2.27	0.55
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.87	0.55
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.72	0.55
1:A:983:ILE:HG22	1:A:983:ILE:O	2.07	0.55
2:B:1138:MET:HE2	2:B:1138:MET:HA	1.88	0.55
3:C:129:ILE:HG23	3:C:130:GLY:N	2.22	0.55
10:L:60:ARG:HG3	10:L:61:THR:N	2.21	0.55
1:A:34:LYS:HD3	1:A:36:ARG:NH2	2.19	0.55
1:A:534:LEU:O	1:A:574:GLY:HA3	2.07	0.55
2:B:1034:VAL:CG2	2:B:1059:LEU:HB3	2.36	0.55
4:E:179:GLN:O	4:E:182:ASP:HB2	2.06	0.55
1:A:1378:GLN:NE2	1:A:1392:SER:HB2	2.21	0.55
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.42	0.55
4:E:202:SER:HB3	4:E:205:SER:O	2.06	0.55
1:A:827:THR:HG21	11:R:11:G:O4'	2.06	0.55
2:B:199:MET:N	2:B:199:MET:SD	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ARG:N	2:B:264:SER:HB3	2.21	0.55
2:B:805:THR:OG1	2:B:815:ARG:NH2	2.40	0.55
2:B:37:PHE:O	2:B:38:PHE:CB	2.54	0.55
2:B:256:VAL:CG1	2:B:382:ILE:HD13	2.32	0.55
2:B:638:PHE:O	2:B:740:HIS:CB	2.55	0.55
2:B:803:LEU:HD21	8:J:51:LEU:HD23	1.89	0.55
2:B:900:ALA:O	2:B:901:PRO:C	2.44	0.55
7:I:119:THR:O	7:I:120:GLN:HB2	2.05	0.55
1:A:351:THR:HG21	1:A:466:SER:O	2.06	0.55
7:I:92:ARG:HG2	7:I:93:LYS:H	1.72	0.55
1:A:1407:GLU:CD	1:A:1407:GLU:N	2.47	0.55
2:B:711:GLU:N	2:B:712:PRO:HD3	2.22	0.55
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.89	0.55
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.22	0.55
1:A:504:LEU:N	1:A:504:LEU:HD12	2.22	0.55
2:B:481:GLN:OE1	2:B:494:HIS:NE2	2.39	0.55
2:B:704:ALA:CB	2:B:710:LEU:HD13	2.33	0.55
1:A:364:VAL:O	1:A:364:VAL:HG13	2.07	0.54
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.55	0.54
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.88	0.54
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.88	0.54
1:A:999:VAL:HG23	1:A:1053:PHE:HE2	1.72	0.54
2:B:459:TYR:C	2:B:459:TYR:CD2	2.81	0.54
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.72	0.54
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.46	0.54
4:E:113:GLN:HA	4:E:137:GLU:HG3	1.88	0.54
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.54
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.89	0.54
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.54
2:B:1059:LEU:O	2:B:1059:LEU:HG	2.07	0.54
2:B:1154:ALA:O	2:B:1155:SER:HB3	2.07	0.54
2:B:801:LYS:O	8:J:52:THR:CG2	2.55	0.54
3:C:54:ASN:ND2	3:C:56:THR:H	2.05	0.54
6:H:128:ASN:C	6:H:130:ARG:N	2.61	0.54
7:I:111:THR:HG22	7:I:113:ASP:H	1.73	0.54
1:A:832:ALA:HB2	12:T:18:DT:H72	1.89	0.54
1:A:572:TRP:N	1:A:572:TRP:CE3	2.75	0.54
1:A:890:ASP:HB2	1:A:1295:THR:O	2.08	0.54
2:B:487:THR:CG2	2:B:819:ALA:HB2	2.37	0.54
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.89	0.54
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.20	0.54
1:A:869:GLY:O	4:E:204:THR:HG21	2.08	0.54
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.88	0.54
2:B:1077:THR:CG2	2:B:1079:LYS:HB2	2.37	0.54
1:A:852:TYR:CE2	5:F:136:ARG:HG2	2.42	0.54
5:F:92:ARG:HG2	5:F:92:ARG:O	2.08	0.54
1:A:1005:GLU:HG3	1:A:1009:ASN:HD21	1.73	0.54
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.43	0.54
2:B:1024:ALA:O	2:B:1027:ILE:N	2.41	0.54
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.90	0.54
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.88	0.54
1:A:566:ILE:O	1:A:566:ILE:HG22	2.08	0.54
2:B:240:ILE:HG21	2:B:381:MET:CE	2.37	0.54
1:A:675:THR:HG21	1:A:736:ASN:HB2	1.90	0.54
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.90	0.54
1:A:974:ASP:OD1	1:A:977:LYS:HB2	2.07	0.54
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.43	0.54
3:C:98:VAL:CG1	3:C:99:LEU:N	2.71	0.54
7:I:63:GLY:CA	7:I:104:LEU:HD11	2.37	0.54
1:A:1406:VAL:N	1:A:1407:GLU:OE2	2.40	0.54
2:B:1072:MET:HE1	2:B:1085:ILE:HG21	1.89	0.54
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.54
2:B:210:LYS:HB3	2:B:480:SER:OG	2.08	0.54
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.42	0.54
2:B:911:ILE:HG21	2:B:966:VAL:HG11	1.87	0.54
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.90	0.53
1:A:1436:ILE:CG2	1:A:1437:GLY:N	2.71	0.53
1:A:883:LEU:HB2	1:A:952:ALA:HB1	1.90	0.53
2:B:1076:HIS:HB3	9:K:40:HIS:CD2	2.43	0.53
2:B:581:PHE:HA	2:B:585:VAL:O	2.08	0.53
7:I:19:ASP:O	7:I:23:ASN:HA	2.08	0.53
1:A:827:THR:CG2	11:R:11:G:O4'	2.56	0.53
1:A:529:CYS:O	1:A:533:LYS:HG3	2.07	0.53
1:A:527:THR:HG23	1:A:653:VAL:HG21	1.89	0.53
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.89	0.53
1:A:993:LEU:HD21	1:A:1022:LEU:HD11	1.89	0.53
2:B:550:ASP:OD1	2:B:551:PRO:CD	2.49	0.53
1:A:482:PHE:HD1	2:B:835:GLN:O	1.91	0.53
2:B:240:ILE:HG21	2:B:381:MET:HE2	1.90	0.53
2:B:542:MET:HG3	2:B:747:MET:HE2	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.89	0.53
2:B:34:ILE:HG13	2:B:542:MET:HE1	1.90	0.53
4:E:32:GLN:HA	4:E:35:VAL:HG12	1.90	0.53
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.21	0.53
2:B:46:GLN:HE21	2:B:496:ARG:HG2	1.74	0.53
2:B:696:GLU:O	2:B:699:GLU:HB2	2.08	0.53
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.72	0.53
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.88	0.53
11:R:8:G:H2'	11:R:9:G:C8	2.43	0.53
1:A:14:VAL:HG11	1:A:1430:LEU:CD1	2.36	0.53
1:A:265:LYS:O	1:A:267:ALA:N	2.42	0.53
2:B:1129:ARG:HE	2:B:1131:GLY:CA	2.20	0.53
2:B:369:GLY:O	2:B:370:PHE:HD1	1.91	0.53
2:B:701:ILE:HG21	2:B:740:HIS:HE1	1.73	0.53
1:A:565:ILE:CG2	1:A:567:LYS:HE3	2.22	0.53
2:B:808:ALA:O	2:B:812:LEU:HD23	2.09	0.53
3:C:43:THR:HG22	3:C:44:LEU:H	1.73	0.53
8:J:9:SER:OG	8:J:48:ARG:NH2	2.41	0.53
9:K:58:PHE:HE2	9:K:74:ARG:HE	1.57	0.53
1:A:650:GLN:O	1:A:654:ASN:HB2	2.08	0.53
2:B:174:LEU:CD2	2:B:204:ILE:HD11	2.39	0.53
2:B:546:SER:HB3	2:B:632:ARG:H	1.74	0.53
3:C:248:ILE:O	3:C:252:GLN:HB2	2.08	0.53
9:K:65:HIS:C	9:K:67:PHE:H	2.11	0.53
1:A:1352:VAL:O	1:A:1355:VAL:CG1	2.53	0.53
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.06	0.53
4:E:10:SER:O	4:E:14:ARG:HG3	2.08	0.53
1:A:827:THR:CG2	11:R:11:G:N3	2.72	0.53
1:A:858:ASN:ND2	1:A:860:LEU:H	2.07	0.53
1:A:873:MET:CE	1:A:957:PRO:HG2	2.39	0.53
2:B:708:GLU:O	2:B:710:LEU:N	2.42	0.53
2:B:722:ASP:OD2	2:B:723:VAL:HG23	2.09	0.53
3:C:123:ASN:HD21	3:C:125:MET:HG2	1.71	0.53
7:I:59:VAL:HG12	7:I:60:GLN:H	1.73	0.53
1:A:226:GLU:HG3	1:A:230:ARG:HH21	1.74	0.52
1:A:434:ARG:HE	1:A:437:MET:HG3	1.73	0.52
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.44	0.52
2:B:634:TYR:HD1	2:B:692:TYR:HB3	1.74	0.52
7:I:25:LEU:HG	7:I:38:ALA:HB3	1.91	0.52
1:A:573:SER:H	1:A:576:GLN:HG3	1.75	0.52
2:B:175:ARG:HG3	2:B:175:ARG:NH1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:VAL:CG2	3:C:240:VAL:HG22	2.39	0.52
2:B:880:THR:O	2:B:881:ASN:HB2	2.08	0.52
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.44	0.52
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.45	0.52
1:A:1427:ASN:HB2	1:A:1434:ALA:HB2	1.92	0.52
1:A:247:ARG:HG3	1:A:262:LEU:HB2	1.91	0.52
2:B:1138:MET:CE	2:B:1138:MET:HA	2.40	0.52
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.92	0.52
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.45	0.52
1:A:795:GLU:HB3	2:B:731:VAL:HG11	1.92	0.52
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.45	0.52
2:B:490:SER:OG	2:B:491:THR:N	2.43	0.52
4:E:177:ARG:HD3	4:E:215:MET:SD	2.50	0.52
1:A:451:HIS:HB2	1:A:453:MET:N	2.23	0.52
1:A:899:VAL:O	1:A:899:VAL:HG13	2.09	0.52
2:B:306:ASN:O	2:B:308:TRP:N	2.43	0.52
2:B:474:SER:O	2:B:475:SER:OG	2.23	0.52
3:C:141:GLY:HA2	8:J:16:ASP:HB3	1.91	0.52
8:J:24:LEU:O	8:J:30:LEU:HB2	2.08	0.52
8:J:36:LEU:HD11	8:J:51:LEU:HD13	1.90	0.52
3:C:165:LYS:O	9:K:6:ARG:NH1	2.41	0.52
11:R:9:G:H1	12:T:19:DC:N4	2.07	0.52
1:A:260:ASP:OD1	1:A:261:ASP:N	2.40	0.52
1:A:315:LEU:HB3	1:A:316:GLN:CA	2.39	0.52
1:A:351:THR:CG2	1:A:352:VAL:H	2.20	0.52
1:A:829:VAL:C	1:A:831:THR:N	2.62	0.52
2:B:1056:SER:CB	2:B:1066:SER:O	2.57	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.91	0.52
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.25	0.52
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.52
1:A:1341:ILE:HB	4:E:182:ASP:OD2	2.09	0.52
9:K:46:ILE:O	9:K:50:LEU:N	2.42	0.52
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.93	0.52
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.92	0.52
2:B:197:PHE:CG	2:B:817:LEU:HD11	2.45	0.52
2:B:823:ALA:HA	8:J:48:ARG:NH1	2.24	0.52
1:A:453:MET:C	1:A:455:MET:N	2.63	0.52
1:A:826:ASP:N	1:A:826:ASP:OD2	2.43	0.52
2:B:1034:VAL:HG22	2:B:1059:LEU:CB	2.40	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.07	0.52
2:B:745:PRO:O	2:B:748:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HA	2:B:999:MET:CE	2.39	0.52
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.92	0.52
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.31	0.52
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.91	0.52
1:A:572:TRP:HE3	1:A:572:TRP:N	2.08	0.52
1:A:65:LEU:O	1:A:71:GLN:HA	2.09	0.52
2:B:577:ALA:HB1	2:B:589:VAL:HG12	1.92	0.52
7:I:75:CYS:SG	7:I:103:CYS:SG	3.00	0.52
1:A:802:ASN:HD21	2:B:729:ILE:H	1.56	0.51
3:C:9:LYS:O	3:C:20:PHE:HB2	2.10	0.51
6:H:84:ALA:C	6:H:86:ASP:N	2.59	0.51
1:A:827:THR:HG22	1:A:827:THR:O	2.10	0.51
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.92	0.51
2:B:557:PHE:CD2	2:B:557:PHE:C	2.84	0.51
2:B:801:LYS:HG3	2:B:802:PRO:O	2.09	0.51
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.76	0.51
2:B:110:HIS:HE1	10:L:53:HIS:CE1	2.28	0.51
10:L:60:ARG:HG3	10:L:61:THR:H	1.74	0.51
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.92	0.51
1:A:1378:GLN:HE22	1:A:1392:SER:HB2	1.75	0.51
1:A:1419:ASP:OD1	1:A:1420:ASP:N	2.44	0.51
1:A:457:ALA:O	1:A:507:VAL:HG23	2.10	0.51
1:A:343:LYS:HZ2	2:B:1197:PRO:HB3	1.76	0.51
5:F:116:ASP:OD2	5:F:117:PRO:HD2	2.11	0.51
2:B:190:TYR:HD2	8:J:63:TYR:CE2	2.29	0.51
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.76	0.51
1:A:870:GLU:HB3	4:E:204:THR:HG23	1.92	0.51
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.10	0.51
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.25	0.51
1:A:332:LYS:H	1:A:337:ARG:HB3	1.75	0.51
1:A:567:LYS:HB3	6:H:96:VAL:N	2.10	0.51
1:A:889:SER:HB2	1:A:892:ALA:CB	2.41	0.51
2:B:483:LEU:HD22	2:B:491:THR:HG23	1.93	0.51
2:B:703:ILE:HA	2:B:740:HIS:O	2.10	0.51
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.35	0.51
1:A:998:LEU:CD1	1:A:1001:ARG:HG3	2.41	0.51
2:B:185:THR:OG1	2:B:188:ASP:HB2	2.11	0.51
2:B:364:ILE:O	2:B:365:THR:HB	2.11	0.51
9:K:102:LYS:O	9:K:106:GLU:HG2	2.11	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.93	0.51
2:B:563:MET:HG3	2:B:563:MET:O	2.10	0.51
3:C:261:ALA:HA	3:C:264:GLN:HE21	1.74	0.51
6:H:36:CYS:HA	6:H:126:GLU:O	2.11	0.51
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	1.93	0.51
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.26	0.51
2:B:648:HIS:HD2	2:B:649:LYS:O	1.94	0.51
3:C:127:ARG:HG3	3:C:129:ILE:HD13	1.92	0.51
6:H:102:TYR:OH	6:H:122:LEU:HD22	2.11	0.51
1:A:329:LEU:HD13	1:A:335:ARG:HB3	1.93	0.51
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.44	0.51
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.08	0.50
1:A:423:ASP:C	1:A:424:ILE:HG12	2.31	0.50
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.11	0.50
2:B:515:HIS:CD2	2:B:516:ASN:N	2.80	0.50
3:C:75:MET:CE	3:C:239:PRO:HG3	2.41	0.50
3:C:251:LEU:O	3:C:255:VAL:HG23	2.10	0.50
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.76	0.50
9:K:63:VAL:O	9:K:63:VAL:CG2	2.59	0.50
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.24	0.50
3:C:33:LEU:HD12	3:C:37:MET:CE	2.41	0.50
12:T:23:DT:H2'	12:T:24:DC:H6	1.75	0.50
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.77	0.50
1:A:247:ARG:HG2	1:A:263:THR:OG1	2.11	0.50
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.47	0.50
1:A:563:PRO:HB2	1:A:565:ILE:O	2.11	0.50
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.41	0.50
4:E:162:ARG:HA	4:E:165:LEU:HB2	1.93	0.50
1:A:308:ILE:CG2	1:A:309:ALA:H	2.05	0.50
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.11	0.50
2:B:777:ALA:O	2:B:819:ALA:HB1	2.12	0.50
4:E:195:VAL:HG12	4:E:196:VAL:O	2.12	0.50
6:H:91:ASP:C	6:H:93:TYR:N	2.64	0.50
7:I:46:HIS:HD1	7:I:46:HIS:C	2.15	0.50
1:A:99:ILE:CD1	1:A:235:ILE:HG23	2.42	0.50
1:A:364:VAL:HG12	1:A:459:ARG:O	2.11	0.50
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.76	0.50
1:A:265:LYS:NZ	1:A:323:LYS:HG2	2.27	0.50
1:A:889:SER:HB2	1:A:892:ALA:H	1.75	0.50
2:B:981:ALA:HB3	2:B:1095:LEU:HD21	1.92	0.50
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.71	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:7:A:H61	12:T:21:DT:H3	1.60	0.50
1:A:1213:GLY:HA3	1:A:1228:TRP:CZ3	2.46	0.50
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.41	0.50
2:B:213:ILE:O	2:B:215:GLN:OE1	2.30	0.50
2:B:805:THR:CB	2:B:815:ARG:NH2	2.75	0.50
2:B:900:ALA:O	2:B:901:PRO:O	2.30	0.50
3:C:166:GLU:O	3:C:167:HIS:HB2	2.10	0.50
4:E:28:TYR:CD1	4:E:78:LEU:HD13	2.45	0.50
7:I:25:LEU:H	7:I:25:LEU:HD23	1.75	0.50
8:J:43:ARG:O	8:J:47:ARG:N	2.44	0.50
8:J:57:ILE:O	8:J:60:PHE:HB2	2.11	0.50
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.94	0.50
1:A:1351:GLU:O	1:A:1352:VAL:C	2.50	0.50
1:A:302:THR:HG21	1:A:313:GLN:OE1	2.11	0.50
2:B:1076:HIS:CD2	2:B:1076:HIS:H	2.29	0.50
2:B:224:GLN:O	2:B:238:ALA:HA	2.12	0.50
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.50
2:B:850:LEU:HD12	8:J:8:PHE:CD1	2.47	0.50
9:K:70:ARG:O	9:K:70:ARG:HG3	2.12	0.50
1:A:1258:HIS:CD2	1:A:1262:LYS:HD2	2.47	0.50
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.94	0.50
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.19	0.50
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.93	0.50
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.50
2:B:1072:MET:CE	2:B:1085:ILE:HG21	2.41	0.50
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.68	0.50
4:E:127:ILE:HD13	4:E:127:ILE:N	2.27	0.50
1:A:997:LEU:HD22	1:A:1053:PHE:CD1	2.47	0.49
1:A:456:MET:HG3	1:A:507:VAL:HG22	1.92	0.49
1:A:473:SER:O	1:A:521:MET:HB3	2.13	0.49
1:A:845:LEU:HA	1:A:848:ILE:HD13	1.93	0.49
1:A:858:ASN:ND2	1:A:858:ASN:C	2.64	0.49
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.94	0.49
2:B:698:GLU:HA	2:B:701:ILE:CD1	2.42	0.49
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.49
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.40	0.49
6:H:39:THR:OG1	6:H:124:ARG:HB3	2.12	0.49
1:A:50:ILE:HG22	1:A:52:GLY:H	1.77	0.49
1:A:909:ASP:OD2	1:A:910:PRO:HD2	2.13	0.49
2:B:487:THR:O	2:B:489:SER:N	2.45	0.49
2:B:730:ARG:HB2	2:B:730:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:821:GLN:H	2:B:851:PHE:HE2	1.60	0.49
2:B:968:VAL:HG12	2:B:969:ARG:N	2.27	0.49
1:A:330:LYS:O	1:A:334:GLY:HA3	2.12	0.49
1:A:367:PRO:HB3	1:A:466:SER:HA	1.94	0.49
1:A:727:ASP:O	1:A:731:ARG:HD3	2.13	0.49
3:C:123:ASN:ND2	3:C:125:MET:HG3	2.21	0.49
3:C:129:ILE:CG2	3:C:130:GLY:N	2.75	0.49
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.94	0.49
1:A:827:THR:HG21	11:R:11:G:N3	2.26	0.49
2:B:487:THR:HG21	2:B:819:ALA:HB2	1.93	0.49
2:B:882:THR:HG23	2:B:884:ARG:H	1.77	0.49
2:B:910:VAL:HG12	2:B:911:ILE:N	2.27	0.49
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.23	0.49
1:A:134:ARG:HD3	1:A:221:SER:O	2.13	0.49
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.94	0.49
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.94	0.49
4:E:190:LEU:HD12	4:E:214:CYS:HB2	1.95	0.49
1:A:1100:ARG:O	1:A:1101:LEU:C	2.51	0.49
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.78	0.49
1:A:1406:VAL:HA	1:A:1409:LEU:HD12	1.94	0.49
1:A:27:VAL:O	1:A:30:ILE:HG22	2.12	0.49
1:A:456:MET:CG	1:A:478:TYR:OH	2.60	0.49
2:B:708:GLU:OE2	2:B:709:ASP:HB2	2.11	0.49
2:B:862:GLN:NE2	2:B:961:LEU:HD13	2.25	0.49
6:H:145:ARG:HG3	6:H:146:ARG:HG2	1.95	0.49
7:I:7:CYS:SG	7:I:8:ARG:N	2.86	0.49
8:J:25:LEU:HD21	8:J:32:GLU:HA	1.95	0.49
1:A:760:GLN:HA	1:A:764:CYS:O	2.11	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.94	0.49
2:B:204:ILE:O	2:B:205:ILE:HD13	2.12	0.49
1:A:472:LEU:HD22	2:B:835:GLN:HB2	1.94	0.49
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.48	0.49
1:A:369:SER:O	1:A:372:LYS:HB2	2.12	0.49
2:B:1000:PRO:O	2:B:1008:PRO:HD3	2.13	0.49
2:B:797:TYR:CE1	2:B:854:LEU:CD2	2.95	0.49
6:H:60:ALA:O	6:H:61:SER:HB3	2.12	0.49
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.94	0.49
1:A:802:ASN:CG	2:B:729:ILE:H	2.16	0.49
2:B:734:HIS:O	2:B:735:ALA:CB	2.60	0.49
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.94	0.49
2:B:823:ALA:HA	8:J:48:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.48	0.49
1:A:912:LEU:HD21	1:A:1033:GLN:HG3	1.94	0.49
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.41	0.49
1:A:639:PRO:HG2	1:A:640:GLN:H	1.78	0.49
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.48	0.49
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.49
2:B:805:THR:CG2	2:B:815:ARG:HH21	2.26	0.49
2:B:816:GLU:O	8:J:56:LEU:HD21	2.11	0.49
10:L:30:ILE:HD12	10:L:57:LEU:HB2	1.95	0.49
1:A:129:LYS:O	1:A:130:ASP:HB2	2.12	0.48
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.95	0.48
1:A:538:ASP:HB2	6:H:20:TYR:HD2	1.78	0.48
2:B:34:ILE:CG1	2:B:542:MET:CE	2.90	0.48
5:F:81:THR:OG1	5:F:144:GLU:OE1	2.29	0.48
12:T:26:DA:C2	12:T:27:DT:C6	3.01	0.48
1:A:1398:MET:O	1:A:1399:ARG:C	2.52	0.48
1:A:512:VAL:HG13	1:A:512:VAL:O	2.12	0.48
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.95	0.48
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.96	0.48
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.48	0.48
6:H:62:SER:OG	6:H:63:LEU:N	2.44	0.48
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.29	0.48
12:T:20:DC:H2'	12:T:21:DT:O4'	2.13	0.48
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.13	0.48
1:A:19:PHE:O	1:A:1416:ALA:HA	2.14	0.48
2:B:986:GLN:HG3	2:B:1025:HIS:CD2	2.49	0.48
1:A:1193:LEU:N	1:A:1260:LEU:HD21	2.29	0.48
1:A:503:GLN:O	1:A:509:LEU:CD1	2.60	0.48
1:A:942:PHE:C	1:A:942:PHE:CD2	2.86	0.48
2:B:516:ASN:N	2:B:516:ASN:HD22	2.10	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.92	0.48
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.49	0.48
3:C:54:ASN:OD1	3:C:63:ILE:HD12	2.14	0.48
1:A:637:LYS:HD2	1:A:641:VAL:HG11	1.96	0.48
1:A:84:ILE:HG13	1:A:270:LEU:HD13	1.95	0.48
2:B:1074:ASN:ND2	2:B:1077:THR:H	2.11	0.48
4:E:187:TYR:CD2	4:E:187:TYR:O	2.67	0.48
4:E:180:ARG:NH2	4:E:192:ARG:HB2	2.28	0.48
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.96	0.48
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.96	0.48
2:B:826:ALA:O	2:B:1011:ILE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ASN:HB3	2:B:839:MET:HA	1.95	0.48
4:E:161:LYS:HD2	4:E:195:VAL:CG2	2.44	0.48
1:A:540:PHE:CE1	6:H:43:ASN:ND2	2.82	0.48
1:A:253:ASN:ND2	1:A:254:GLU:H	2.11	0.48
1:A:337:ARG:NH2	12:T:17:DC:OP1	2.46	0.48
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.48
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.95	0.48
1:A:793:SER:CB	1:A:794:PRO:HD2	2.43	0.48
2:B:202:TYR:N	2:B:202:TYR:CD2	2.82	0.48
2:B:458:LYS:O	2:B:462:ALA:N	2.41	0.48
3:C:75:MET:HE1	3:C:239:PRO:HG3	1.95	0.48
10:L:28:LYS:HE2	10:L:39:SER:OG	2.14	0.48
2:B:827:ILE:HA	2:B:1012:ILE:O	2.14	0.48
2:B:115:GLN:O	2:B:119:LEU:HD12	2.14	0.48
2:B:100:PRO:HD3	2:B:126:SER:HB3	1.95	0.48
3:C:251:LEU:HG	9:K:98:LEU:HD11	1.95	0.48
6:H:30:SER:HB2	6:H:36:CYS:SG	2.54	0.48
12:T:23:DT:C2	12:T:24:DC:C5	3.02	0.48
1:A:225:ASN:O	1:A:227:VAL:N	2.47	0.48
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.48	0.48
1:A:858:ASN:O	1:A:860:LEU:N	2.47	0.48
2:B:698:GLU:HA	2:B:701:ILE:HD12	1.96	0.48
2:B:879:ARG:HB2	2:B:880:THR:CB	2.44	0.48
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.46	0.48
3:C:98:VAL:CG1	3:C:99:LEU:H	2.26	0.48
3:C:69:LEU:HD23	8:J:6:ARG:HB2	1.96	0.48
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.27	0.48
1:A:106:VAL:HG11	1:A:214:ILE:HD12	1.96	0.47
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.59	0.47
2:B:236:HIS:HD2	2:B:389:ALA:HB2	1.77	0.47
2:B:551:PRO:O	2:B:554:ILE:HB	2.14	0.47
2:B:732:SER:HB3	2:B:734:HIS:HD2	1.79	0.47
7:I:10:CYS:HB2	7:I:31:THR:HG1	1.74	0.47
7:I:59:VAL:HG12	7:I:60:GLN:N	2.29	0.47
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.49	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HH11	1.78	0.47
1:A:1263:ILE:HG23	1:A:1264:GLU:N	2.28	0.47
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.75	0.47
1:A:540:PHE:CZ	6:H:121:LEU:HD21	2.48	0.47
3:C:84:ARG:HG3	3:C:85:ASP:N	2.29	0.47
1:A:786:HIS:CE1	2:B:705:MET:SD	3.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.95	0.47
3:C:14:SER:OG	3:C:17:ASN:HB2	2.14	0.47
1:A:224:PHE:HZ	1:A:234:MET:HE1	1.78	0.47
1:A:264:PHE:HE1	1:A:317:LYS:CB	2.11	0.47
1:A:363:GLN:HG3	1:A:459:ARG:NH1	2.30	0.47
1:A:575:LYS:CB	1:A:612:ILE:HD11	2.42	0.47
2:B:1027:ILE:O	2:B:1028:GLU:C	2.50	0.47
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.28	0.47
2:B:248:SER:H	2:B:418:LYS:NZ	2.03	0.47
2:B:567:GLU:N	2:B:567:GLU:CD	2.56	0.47
2:B:701:ILE:HB	2:B:739:THR:OG1	2.14	0.47
4:E:77:SER:HB3	4:E:105:PHE:HA	1.97	0.47
4:E:166:LYS:O	4:E:169:ARG:N	2.45	0.47
4:E:46:TYR:CD2	4:E:58:MET:HG3	2.49	0.47
1:A:1031:VAL:O	1:A:1031:VAL:HG22	2.14	0.47
1:A:26:GLU:O	1:A:30:ILE:HB	2.15	0.47
1:A:452:LYS:HE2	1:A:510:GLN:HE22	1.79	0.47
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.29	0.47
1:A:58:LEU:HD23	1:A:58:LEU:C	2.34	0.47
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.97	0.47
1:A:344:ARG:HB3	2:B:1118:PRO:HG2	1.97	0.47
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.15	0.47
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.98	0.47
2:B:97:VAL:HB	2:B:178:ASN:HD21	1.79	0.47
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.96	0.47
1:A:344:ARG:CZ	2:B:1129:ARG:HB2	2.44	0.47
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.97	0.47
2:B:321:GLY:C	2:B:323:VAL:H	2.18	0.47
2:B:472:ALA:O	2:B:474:SER:HB3	2.15	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.96	0.47
1:A:357:PRO:HB3	1:A:472:LEU:HD11	1.97	0.47
1:A:726:ARG:HH11	1:A:766:GLY:HA3	1.79	0.47
1:A:71:GLN:C	1:A:73:GLY:H	2.18	0.47
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.42	0.47
2:B:174:LEU:HD22	2:B:204:ILE:CD1	2.44	0.47
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.44	0.47
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.45	0.47
2:B:955:THR:HG23	10:L:54:ARG:O	2.15	0.47
1:A:1338:VAL:O	4:E:183:PRO:HB3	2.14	0.47
9:K:19:LEU:HD22	9:K:33:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:C	1:A:267:ALA:N	2.68	0.47
1:A:350:ARG:HH21	12:T:21:DT:H2''	1.79	0.47
1:A:525:GLN:O	1:A:526:ASP:C	2.52	0.47
1:A:711:ARG:NH1	7:I:91:ARG:HH12	2.13	0.47
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.30	0.47
2:B:628:THR:O	2:B:628:THR:HG23	2.14	0.47
2:B:636:PRO:CB	2:B:637:LEU:CA	2.65	0.47
2:B:975:GLN:N	2:B:978:ASP:OD2	2.40	0.47
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.97	0.47
6:H:112:ILE:N	6:H:127:GLY:O	2.31	0.47
1:A:998:LEU:HD12	1:A:1001:ARG:HG3	1.97	0.47
2:B:47:GLN:HB3	2:B:173:MET:HE2	1.97	0.47
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.97	0.47
2:B:952:VAL:CG1	2:B:953:LEU:N	2.78	0.47
3:C:189:THR:HG22	3:C:190:ASP:N	2.30	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.15	0.47
7:I:111:THR:HG22	7:I:112:SER:N	2.29	0.47
1:A:1155:ASP:OD2	1:A:1162:VAL:HG23	2.14	0.47
1:A:774:ARG:NH2	1:A:797:LYS:HD3	2.30	0.47
2:B:1110:PRO:O	2:B:1119:VAL:HG12	2.14	0.47
2:B:210:LYS:HA	2:B:481:GLN:O	2.15	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.97	0.47
6:H:109:LYS:HB2	6:H:111:LEU:N	2.29	0.47
6:H:128:ASN:O	6:H:131:ASN:ND2	2.47	0.47
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.80	0.47
1:A:457:ALA:HB3	1:A:506:ALA:CA	2.43	0.47
1:A:830:LYS:HD3	1:A:1080:THR:HA	1.97	0.47
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.47
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.80	0.47
2:B:468:GLU:HG3	2:B:469:GLN:N	2.29	0.47
2:B:658:ILE:HD12	2:B:661:LEU:HD12	1.97	0.47
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.49	0.47
3:C:93:ASP:O	3:C:127:ARG:NH2	2.47	0.47
7:I:71:SER:H	7:I:83:ASN:ND2	2.13	0.47
11:R:7:A:H2'	11:R:8:G:H5'	1.97	0.47
1:A:830:LYS:HD3	1:A:1079:MET:O	2.14	0.46
1:A:903:ASN:ND2	1:A:906:HIS:HB2	2.30	0.46
2:B:1077:THR:HG22	2:B:1079:LYS:HB2	1.97	0.46
2:B:956:THR:HG23	2:B:961:LEU:H	1.80	0.46
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.44	0.46
1:A:106:VAL:HG12	1:A:107:CYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLU:O	1:A:622:VAL:HG12	2.15	0.46
1:A:845:LEU:O	1:A:848:ILE:HD13	2.15	0.46
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.96	0.46
1:A:933:TYR:O	1:A:933:TYR:CD2	2.68	0.46
2:B:1135:ARG:NE	2:B:1139:ILE:HD11	2.30	0.46
2:B:723:VAL:O	2:B:724:ASP:C	2.54	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.50	0.46
5:F:75:PRO:O	5:F:79:ARG:HD2	2.15	0.46
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.45	0.46
11:R:9:G:H5'	11:R:10:A:OP2	2.15	0.46
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.79	0.46
1:A:582:ILE:HD12	1:A:629:LEU:HD11	1.97	0.46
1:A:630:ILE:N	1:A:630:ILE:CD1	2.71	0.46
1:A:92:HIS:O	1:A:94:GLY:N	2.49	0.46
2:B:459:TYR:HD2	2:B:459:TYR:O	1.98	0.46
3:C:148:ARG:HD2	3:C:149:LYS:H	1.81	0.46
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.62	0.46
1:A:315:LEU:HB3	1:A:317:LYS:N	2.31	0.46
1:A:49:LYS:O	1:A:50:ILE:HB	2.14	0.46
1:A:525:GLN:O	1:A:528:LEU:N	2.48	0.46
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.28	0.46
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.49	0.46
2:B:307:ASP:O	2:B:310:MET:HB3	2.15	0.46
2:B:732:SER:HB3	2:B:734:HIS:CD2	2.51	0.46
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.97	0.46
4:E:61:GLN:HE21	4:E:105:PHE:HZ	1.63	0.46
1:A:417:TYR:O	1:A:418:SER:HB3	2.15	0.46
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.30	0.46
2:B:784:ASN:OD1	2:B:788:ARG:HG3	2.15	0.46
1:A:827:THR:HG21	11:R:11:G:C1'	2.46	0.46
1:A:1019:CYS:O	1:A:1023:ARG:HG3	2.16	0.46
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.46
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
1:A:767:GLN:OE1	1:A:774:ARG:HD2	2.15	0.46
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.14	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
2:B:708:GLU:CG	2:B:709:ASP:H	2.27	0.46
7:I:10:CYS:CB	7:I:31:THR:HG1	2.29	0.46
2:B:236:HIS:NE2	2:B:389:ALA:HA	2.31	0.46
3:C:248:ILE:HG13	3:C:248:ILE:H	1.60	0.46
1:A:1427:ASN:CB	1:A:1434:ALA:HB2	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:843:GLN:HB2	2:B:993:THR:OG1	2.16	0.46
3:C:29:MET:HB3	9:K:45:LEU:HD11	1.98	0.46
1:A:339:ASN:O	1:A:343:LYS:HG2	2.16	0.46
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.81	0.46
1:A:834:THR:HG22	1:A:834:THR:O	2.15	0.46
1:A:857:ARG:HA	1:A:864:ILE:HD12	1.98	0.46
2:B:232:SER:OG	2:B:234:ILE:O	2.34	0.46
2:B:642:ASP:O	2:B:644:GLU:N	2.49	0.46
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.56	0.46
7:I:69:PRO:HG2	7:I:85:PHE:CE1	2.50	0.46
1:A:1042:PHE:O	1:A:1045:VAL:N	2.49	0.46
1:A:577:ILE:O	1:A:580:VAL:N	2.39	0.46
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.42	0.46
1:A:751:SER:CB	2:B:1015:HIS:CE1	3.00	0.46
2:B:464:GLY:HA3	2:B:478:GLY:C	2.35	0.46
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.98	0.46
2:B:600:LEU:HB3	2:B:615:MET:CE	2.46	0.46
2:B:704:ALA:HB1	2:B:710:LEU:HD13	1.74	0.46
9:K:24:ASP:OD2	9:K:74:ARG:HD2	2.15	0.46
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.98	0.45
2:B:522:VAL:HG13	2:B:537:LYS:HB2	1.97	0.45
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.52	0.45
5:F:89:GLU:O	5:F:93:ILE:HG12	2.16	0.45
7:I:63:GLY:HA3	7:I:104:LEU:CD1	2.40	0.45
1:A:830:LYS:HD3	1:A:1080:THR:OG1	2.17	0.45
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.97	0.45
1:A:472:LEU:HD22	2:B:835:GLN:CB	2.46	0.45
1:A:557:ASP:OD1	1:A:559:VAL:HG22	2.17	0.45
1:A:527:THR:HG23	1:A:653:VAL:CG2	2.46	0.45
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.97	0.45
2:B:1119:VAL:O	2:B:1126:GLY:CA	2.65	0.45
2:B:1138:MET:HB3	2:B:1147:LEU:HD12	1.98	0.45
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.99	0.45
1:A:461:LYS:O	1:A:461:LYS:HG3	2.16	0.45
2:B:287:ARG:HB3	2:B:330:ALA:HB2	1.99	0.45
2:B:545:ILE:C	2:B:634:TYR:HE2	2.20	0.45
3:C:31:ASN:O	3:C:34:ARG:N	2.49	0.45
11:R:7:A:C2'	11:R:8:G:H5'	2.46	0.45
1:A:531:ILE:O	1:A:535:THR:HB	2.16	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:HG11	1.97	0.45
2:B:345:LYS:N	2:B:347:LYS:HE3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:N	2:B:634:TYR:HE2	2.14	0.45
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.98	0.45
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.93	0.45
9:K:6:ARG:HB3	9:K:6:ARG:HH11	1.81	0.45
1:A:1434:ALA:O	1:A:1436:ILE:N	2.50	0.45
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.97	0.45
1:A:47:ARG:HH11	1:A:47:ARG:HB2	1.81	0.45
1:A:629:LEU:O	1:A:633:VAL:HG23	2.17	0.45
1:A:767:GLN:NE2	1:A:797:LYS:O	2.49	0.45
2:B:1097:HIS:HB3	2:B:1102:LYS:NZ	2.31	0.45
2:B:210:LYS:HE3	2:B:462:ALA:HA	1.97	0.45
2:B:273:LEU:HD23	2:B:274:PRO:HD2	1.98	0.45
2:B:426:LYS:HD2	2:B:430:ARG:HH22	1.82	0.45
2:B:494:HIS:HA	2:B:497:ARG:CZ	2.46	0.45
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.97	0.45
3:C:167:HIS:HD2	3:C:169:LYS:N	2.07	0.45
4:E:187:TYR:HD2	4:E:188:LEU:HG	1.80	0.45
5:F:90:ARG:HD3	5:F:155:LEU:HD11	1.97	0.45
6:H:41:ASP:O	6:H:121:LEU:HD12	2.17	0.45
1:A:1004:ASN:HD22	4:E:167:ARG:HH11	1.65	0.45
1:A:814:PHE:O	1:A:818:MET:HG3	2.16	0.45
1:A:982:THR:C	1:A:984:LYS:N	2.70	0.45
2:B:301:ILE:HG22	2:B:302:CYS:N	2.31	0.45
3:C:15:LYS:H	3:C:15:LYS:HD2	1.80	0.45
3:C:33:LEU:HD12	3:C:37:MET:HE1	1.99	0.45
3:C:43:THR:HG22	3:C:44:LEU:N	2.32	0.45
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.97	0.45
1:A:635:ARG:NH1	1:A:635:ARG:HA	2.29	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.98	0.45
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.46	0.45
1:A:660:ASN:HA	2:B:1082:MET:HB2	1.99	0.45
2:B:1162:ILE:HD11	2:B:1216:LEU:HD23	1.99	0.45
2:B:321:GLY:O	2:B:323:VAL:N	2.50	0.45
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.52	0.45
3:C:258:ILE:HD11	9:K:19:LEU:HD11	1.99	0.45
8:J:23:ASN:C	8:J:25:LEU:H	2.20	0.45
12:T:17:DC:H2'	12:T:17:DC:O2	2.16	0.45
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.17	0.45
1:A:1349:TYR:O	1:A:1350:LYS:C	2.55	0.45
1:A:760:GLN:NE2	1:A:765:VAL:O	2.49	0.45
2:B:850:LEU:O	2:B:974:PRO:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ILE:HD13	3:C:258:ILE:O	2.17	0.45
3:C:51:VAL:O	10:L:64:LEU:HD22	2.17	0.45
4:E:12:LEU:CD2	4:E:53:PRO:HB3	2.46	0.45
6:H:109:LYS:HB3	6:H:110:ASP:C	2.37	0.45
7:I:68:LEU:HA	7:I:69:PRO:HD3	1.70	0.45
8:J:7:CYS:HA	8:J:49:MET:HG2	1.98	0.45
1:A:1274:ARG:HB3	1:A:1274:ARG:NH1	2.32	0.45
2:B:1065:GLN:HG2	3:C:201:TRP:CZ3	2.52	0.45
2:B:487:THR:HG21	2:B:819:ALA:CB	2.47	0.45
3:C:196:ASP:C	3:C:198:ALA:H	2.21	0.45
3:C:29:MET:O	3:C:30:ALA:C	2.54	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.18	0.45
1:A:356:ASP:OD2	1:A:359:LEU:HG	2.16	0.45
1:A:380:VAL:HG13	1:A:385:ILE:HG23	1.99	0.45
1:A:467:THR:HG22	2:B:1099:VAL:HG11	1.99	0.45
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.17	0.45
4:E:196:VAL:HG12	4:E:197:LYS:N	2.32	0.45
4:E:79:TRP:CD1	4:E:100:ILE:HD11	2.51	0.45
8:J:36:LEU:O	8:J:41:LEU:HB2	2.16	0.45
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.99	0.45
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.44
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.99	0.44
1:A:780:VAL:O	1:A:789:LYS:HG2	2.17	0.44
1:A:494:SER:HB2	2:B:1149:GLU:OE2	2.17	0.44
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.57	0.44
2:B:1152:MET:CE	2:B:1195:HIS:HB3	2.47	0.44
2:B:186:GLU:O	2:B:187:SER:C	2.56	0.44
2:B:33:VAL:HG23	2:B:658:ILE:HD11	1.99	0.44
2:B:801:LYS:O	8:J:52:THR:HG23	2.16	0.44
3:C:29:MET:HG3	3:C:30:ALA:N	2.31	0.44
4:E:14:ARG:NH1	4:E:142:VAL:HG22	2.20	0.44
1:A:1394:THR:HG21	1:A:1398:MET:HE3	1.99	0.44
2:B:482:VAL:O	2:B:483:LEU:C	2.54	0.44
2:B:569:TYR:HE1	2:B:574:SER:HB2	1.82	0.44
2:B:597:MET:O	2:B:600:LEU:N	2.50	0.44
5:F:89:GLU:OE2	5:F:136:ARG:NE	2.50	0.44
1:A:1116:LEU:HB2	1:A:1308:THR:CG2	2.48	0.44
1:A:332:LYS:C	1:A:334:GLY:H	2.20	0.44
1:A:562:THR:HA	1:A:563:PRO:HD3	1.86	0.44
1:A:628:GLY:O	1:A:632:VAL:HG23	2.17	0.44
2:B:1177:HIS:O	2:B:1179:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HH11	2:B:169:ARG:HG2	1.73	0.44
2:B:288:ALA:HB1	2:B:331:LEU:HD13	1.98	0.44
2:B:622:LYS:HE3	7:I:57:GLY:HA2	1.99	0.44
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.16	0.44
2:B:997:GLU:HG2	3:C:39:ALA:CB	2.44	0.44
3:C:115:SER:HB3	3:C:142:VAL:HB	1.99	0.44
11:R:4:G:H2'	11:R:5:A:C8	2.53	0.44
1:A:79:GLY:O	1:A:243:PRO:HG3	2.17	0.44
1:A:27:VAL:HG12	1:A:83:HIS:HB2	1.99	0.44
2:B:1022:THR:HG23	2:B:1022:THR:O	2.18	0.44
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.99	0.44
2:B:261:ARG:HB2	2:B:264:SER:HB2	1.98	0.44
2:B:730:ARG:HB2	2:B:730:ARG:NH1	2.32	0.44
4:E:147:HIS:HD2	4:E:149:LEU:H	1.66	0.44
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.98	0.44
1:A:246:VAL:HG12	1:A:246:VAL:O	2.17	0.44
1:A:362:ASP:N	1:A:362:ASP:OD2	2.35	0.44
2:B:361:LEU:HD11	2:B:381:MET:HE3	1.99	0.44
3:C:142:VAL:H	8:J:16:ASP:CB	2.27	0.44
4:E:75:MET:CG	4:E:76:GLY:N	2.79	0.44
6:H:40:LEU:HD21	6:H:142:LEU:HD21	1.99	0.44
7:I:99:LEU:O	7:I:111:THR:HG23	2.18	0.44
7:I:75:CYS:HA	7:I:76:PRO:HD2	1.77	0.44
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.53	0.44
11:R:10:A:H5'	11:R:11:G:OP2	2.17	0.44
1:A:1100:ARG:O	1:A:1103:GLU:N	2.51	0.44
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.53	0.44
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.17	0.44
1:A:67:CYS:HB3	1:A:80:HIS:CE1	2.53	0.44
1:A:888:GLY:O	1:A:889:SER:O	2.35	0.44
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.81	0.44
2:B:654:ARG:HD3	2:B:654:ARG:HA	1.83	0.44
2:B:94:LYS:HD2	2:B:94:LYS:HA	1.84	0.44
2:B:957:ASN:H	2:B:961:LEU:HB2	1.81	0.44
2:B:976:ILE:HD12	2:B:993:THR:HG22	1.98	0.44
5:F:81:THR:HG22	5:F:136:ARG:HD3	1.99	0.44
11:R:1:A:C5	11:R:2:U:C5	3.05	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.48	0.44
2:B:482:VAL:C	2:B:483:LEU:O	2.56	0.44
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.00	0.44
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1212:VAL:HA	1:A:1273:LEU:HD21	1.98	0.44
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.17	0.44
1:A:1398:MET:O	1:A:1401:SER:N	2.45	0.44
1:A:33:ALA:O	1:A:83:HIS:CD2	2.70	0.44
2:B:1204:PHE:O	2:B:1208:MET:HB2	2.17	0.44
2:B:459:TYR:C	2:B:459:TYR:HD2	2.19	0.44
4:E:113:GLN:HA	4:E:137:GLU:CG	2.47	0.44
4:E:75:MET:HG3	4:E:76:GLY:N	2.33	0.44
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.00	0.44
10:L:46:VAL:HG22	10:L:47:ARG:N	2.25	0.44
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.82	0.44
1:A:908:LEU:HD22	1:A:1032:LEU:HD12	2.00	0.44
1:A:928:LEU:HA	1:A:931:GLU:HB3	1.99	0.44
2:B:520:GLY:O	2:B:521:LEU:HD23	2.17	0.44
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.78	0.44
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.44	0.44
7:I:14:LEU:HD22	7:I:29:CYS:HB2	1.99	0.44
1:A:1101:LEU:HG	1:A:1105:LEU:HD11	2.00	0.43
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.00	0.43
1:A:633:VAL:HG11	1:A:645:LEU:HD22	2.00	0.43
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.82	0.43
2:B:1059:LEU:HA	2:B:1062:HIS:HB2	1.99	0.43
2:B:232:SER:HA	2:B:233:PRO:HD2	1.88	0.43
2:B:473:MET:CA	2:B:474:SER:HB3	2.46	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:CB	2.35	0.43
1:A:1152:ILE:HG22	1:A:1152:ILE:O	2.18	0.43
1:A:649:ILE:O	1:A:653:VAL:HG22	2.18	0.43
1:A:900:ASP:O	1:A:907:THR:HA	2.18	0.43
7:I:78:CYS:O	7:I:79:HIS:HB2	2.19	0.43
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.38	0.43
1:A:1195:LEU:O	1:A:1237:ILE:HA	2.19	0.43
1:A:1404:GLU:HB3	1:A:1407:GLU:CG	2.49	0.43
1:A:265:LYS:O	1:A:268:ASP:N	2.51	0.43
1:A:272:ALA:HA	1:A:275:SER:HB3	2.00	0.43
1:A:741:ASN:O	1:A:744:LYS:HB2	2.18	0.43
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.22	0.43
1:A:351:THR:HG23	2:B:1103:ILE:HD13	1.99	0.43
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.17	0.43
2:B:708:GLU:C	2:B:710:LEU:N	2.71	0.43
1:A:472:LEU:HD13	2:B:835:GLN:HE22	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:205:SER:O	4:E:206:GLY:C	2.56	0.43
1:A:67:CYS:HB3	1:A:80:HIS:HE1	1.83	0.43
1:A:81:PHE:CE1	2:B:1208:MET:HG2	2.54	0.43
2:B:240:ILE:HD13	2:B:240:ILE:C	2.39	0.43
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.53	0.43
2:B:913:GLY:HA2	2:B:938:SER:CB	2.48	0.43
1:A:1006:ILE:HG12	1:A:1007:ILE:N	2.33	0.43
1:A:1209:MET:HE1	1:A:1228:TRP:HB2	2.00	0.43
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.18	0.43
1:A:1323:ASP:HA	1:A:1324:PRO:HD3	1.88	0.43
1:A:1445:ILE:HG13	1:A:1445:ILE:H	1.71	0.43
1:A:305:ASP:OD1	1:A:306:ASN:N	2.51	0.43
1:A:403:LYS:O	1:A:404:TYR:CB	2.57	0.43
1:A:660:ASN:O	2:B:1081:LEU:HD22	2.18	0.43
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.99	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.18	0.43
3:C:54:ASN:C	3:C:54:ASN:ND2	2.69	0.43
5:F:85:MET:CE	5:F:148:VAL:HG13	2.49	0.43
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.00	0.43
1:A:1341:ILE:CD1	1:A:1380:GLY:HA2	2.48	0.43
1:A:369:SER:HB3	9:K:2:ASN:ND2	2.30	0.43
1:A:456:MET:HG3	1:A:478:TYR:OH	2.18	0.43
1:A:932:GLU:O	1:A:934:LYS:N	2.51	0.43
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.89	0.43
2:B:515:HIS:H	2:B:518:HIS:CD2	2.23	0.43
3:C:262:LEU:HD21	9:K:87:LEU:HD23	2.00	0.43
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	2.00	0.43
1:A:401:GLY:H	1:A:435:HIS:HD2	1.66	0.43
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.00	0.43
2:B:57:TYR:HD1	2:B:57:TYR:N	2.15	0.43
2:B:621:GLU:HG3	2:B:623:GLU:HG3	2.00	0.43
2:B:788:ARG:CG	2:B:788:ARG:HH11	2.32	0.43
7:I:111:THR:HG22	7:I:112:SER:H	1.82	0.43
7:I:46:HIS:ND1	7:I:46:HIS:C	2.72	0.43
8:J:7:CYS:HB2	8:J:49:MET:HG2	2.01	0.43
11:R:7:A:N6	12:T:21:DT:H3	2.16	0.43
1:A:1139:GLU:OE2	1:A:1282:VAL:HG12	2.18	0.43
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	2.01	0.43
1:A:58:LEU:CD2	1:A:244:PRO:HD2	2.48	0.43
1:A:783:THR:O	2:B:516:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:PRO:CB	2:B:741:CYS:SG	3.00	0.43
6:H:137:GLN:HB2	6:H:138:GLU:H	1.69	0.43
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.49	0.43
1:A:265:LYS:HZ3	1:A:322:VAL:HG12	1.80	0.43
1:A:590:ARG:HH21	1:A:621:THR:HA	1.84	0.43
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.49	0.43
2:B:1132:GLU:HG3	2:B:1132:GLU:H	1.52	0.43
1:A:329:LEU:HD11	2:B:1203:LEU:HD12	2.01	0.43
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	2.00	0.43
2:B:199:MET:SD	2:B:200:GLY:N	2.92	0.43
2:B:240:ILE:O	2:B:240:ILE:HG23	2.18	0.43
2:B:235:SER:HA	2:B:261:ARG:HH21	1.83	0.43
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.84	0.43
3:C:204:SER:C	3:C:206:ASN:N	2.72	0.43
1:A:1209:MET:HG3	1:A:1236:LEU:HD22	2.01	0.43
1:A:313:GLN:HB3	1:A:314:ALA:H	1.58	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:511:ILE:O	1:A:519:PRO:HA	2.19	0.43
1:A:800:VAL:HG11	1:A:808:LEU:HG	2.00	0.43
2:B:1032:SER:O	2:B:1033:LYS:C	2.57	0.43
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.53	0.43
5:F:101:ILE:HD13	5:F:120:ILE:HG22	2.00	0.43
6:H:12:VAL:HG22	6:H:53:ASP:O	2.19	0.43
8:J:53:HIS:CE1	8:J:55:ASP:HA	2.54	0.43
12:T:27:DT:H2'	12:T:27:DT:O2	2.19	0.43
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.83	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.53	0.42
1:A:269:ILE:HG23	1:A:299:HIS:CB	2.49	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.03	0.42
1:A:768:GLN:CG	1:A:816:HIS:HA	2.45	0.42
1:A:899:VAL:O	1:A:899:VAL:CG1	2.67	0.42
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.44	0.42
2:B:315:LYS:N	2:B:316:PRO:CD	2.81	0.42
2:B:515:HIS:HD2	2:B:517:THR:H	1.64	0.42
3:C:178:PHE:C	3:C:178:PHE:HD2	2.23	0.42
6:H:139:ASN:O	6:H:140:ALA:CB	2.65	0.42
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.19	0.42
1:A:457:ALA:HB3	1:A:506:ALA:N	2.34	0.42
1:A:552:TRP:CD1	1:A:655:PHE:CD1	3.07	0.42
1:A:737:LEU:HB3	1:A:744:LYS:HG3	2.01	0.42
1:A:928:LEU:O	1:A:931:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:TYR:O	2:B:114:PRO:C	2.56	0.42
2:B:585:VAL:HG12	2:B:587:HIS:CD2	2.54	0.42
2:B:685:LEU:HD22	2:B:692:TYR:CE2	2.54	0.42
4:E:199:ILE:O	4:E:199:ILE:CG2	2.64	0.42
6:H:6:PHE:CG	6:H:7:ASP:N	2.86	0.42
6:H:93:TYR:CG	6:H:143:LEU:HB3	2.54	0.42
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	2.01	0.42
1:A:1436:ILE:O	1:A:1438:THR:N	2.52	0.42
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.43	0.42
1:A:840:ARG:O	1:A:841:LEU:C	2.56	0.42
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.85	0.42
1:A:907:THR:HG22	1:A:908:LEU:H	1.85	0.42
2:B:1154:ALA:O	2:B:1155:SER:CB	2.66	0.42
2:B:27:ALA:HB2	2:B:708:GLU:HG2	2.00	0.42
2:B:482:VAL:O	2:B:483:LEU:O	2.36	0.42
2:B:808:ALA:C	2:B:810:GLU:N	2.72	0.42
2:B:879:ARG:N	2:B:879:ARG:NE	2.67	0.42
4:E:83:CYS:SG	4:E:110:PHE:HE1	2.41	0.42
9:K:6:ARG:HB3	9:K:6:ARG:NH1	2.33	0.42
1:A:1203:ASN:O	1:A:1204:ASP:C	2.56	0.42
1:A:95:PHE:HB3	1:A:234:MET:HG2	2.01	0.42
1:A:388:LEU:HD13	1:A:391:LEU:HD12	2.02	0.42
1:A:451:HIS:C	1:A:453:MET:H	2.23	0.42
1:A:37:PHE:HB2	1:A:52:GLY:HA3	2.01	0.42
1:A:744:LYS:HD3	1:A:748:MET:HE3	2.01	0.42
1:A:683:ILE:HG21	1:A:801:GLU:HG2	2.01	0.42
1:A:824:LEU:O	11:R:11:G:N2	2.51	0.42
2:B:255:GLN:H	2:B:272:THR:HG22	1.84	0.42
2:B:360:PHE:O	2:B:361:LEU:C	2.57	0.42
2:B:372:SER:O	2:B:376:PHE:HD1	2.03	0.42
2:B:428:ILE:CD1	2:B:448:ILE:HD13	2.46	0.42
2:B:788:ARG:HG3	2:B:788:ARG:HH11	1.84	0.42
2:B:821:GLN:NE2	2:B:851:PHE:H	2.16	0.42
2:B:865:LYS:HB3	2:B:866:TYR:H	1.72	0.42
7:I:10:CYS:HB3	7:I:32:CYS:HB3	1.80	0.42
1:A:709:THR:CG2	7:I:94:ASP:HA	2.46	0.42
8:J:16:ASP:OD2	8:J:17:LYS:HD2	2.20	0.42
1:A:645:LEU:O	1:A:646:PHE:C	2.57	0.42
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.67	0.42
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.02	0.42
2:B:26:THR:O	2:B:29:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:523:CYS:SG	2:B:750:GLY:N	2.92	0.42
2:B:701:ILE:HG21	2:B:740:HIS:CE1	2.52	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.90	0.42
4:E:198:ILE:CD1	4:E:212:ARG:HG2	2.43	0.42
2:B:309:GLN:OE1	7:I:52:ILE:HG23	2.19	0.42
3:C:29:MET:HB3	9:K:45:LEU:CD1	2.49	0.42
1:A:402:ALA:HB1	1:A:434:ARG:HA	2.01	0.42
1:A:692:ASP:HA	1:A:695:LYS:HB2	2.01	0.42
2:B:1077:THR:HG21	2:B:1079:LYS:HB2	2.01	0.42
2:B:377:PHE:O	2:B:380:TYR:N	2.47	0.42
2:B:378:LEU:O	2:B:382:ILE:HG12	2.20	0.42
2:B:475:SER:O	2:B:476:ARG:C	2.58	0.42
3:C:99:LEU:HD13	3:C:120:ILE:HA	2.01	0.42
4:E:28:TYR:CE1	4:E:78:LEU:CD1	2.95	0.42
4:E:21:GLU:HG3	4:E:35:VAL:HG21	2.02	0.42
6:H:93:TYR:HB3	6:H:144:ILE:O	2.19	0.42
7:I:30:ARG:HE	7:I:30:ARG:HB3	1.70	0.42
10:L:61:THR:HG22	10:L:63:ARG:N	2.34	0.42
1:A:1394:THR:HG21	1:A:1398:MET:CE	2.50	0.42
2:B:638:PHE:HB2	2:B:741:CYS:O	2.19	0.42
3:C:31:ASN:O	3:C:33:LEU:N	2.52	0.42
6:H:107:VAL:HG21	6:H:126:GLU:HG3	2.02	0.42
1:A:1153:TYR:CE1	7:I:42:LEU:HD13	2.55	0.42
1:A:253:ASN:CG	1:A:254:GLU:N	2.70	0.42
1:A:613:ILE:O	6:H:117:SER:OG	2.31	0.42
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.42
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.49	0.42
2:B:612:GLU:O	2:B:632:ARG:NH2	2.52	0.42
2:B:784:ASN:HD21	2:B:788:ARG:HD3	1.85	0.42
2:B:886:LYS:HB2	2:B:890:TYR:CZ	2.54	0.42
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.54	0.42
3:C:204:SER:O	3:C:206:ASN:N	2.53	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.19	0.42
1:A:1062:GLU:OE1	1:A:1067:LEU:HD13	2.19	0.42
1:A:1209:MET:CE	1:A:1228:TRP:HB2	2.50	0.42
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.20	0.42
1:A:30:ILE:HG12	2:B:1170:THR:CG2	2.49	0.42
1:A:345:VAL:HG12	2:B:1155:SER:HB2	2.00	0.42
1:A:504:LEU:CD1	1:A:504:LEU:N	2.82	0.42
1:A:550:LEU:HD12	1:A:556:TRP:NE1	2.35	0.42
2:B:999:MET:HE3	2:B:999:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:HB3	3:C:160:LYS:HD2	2.00	0.42
6:H:82:PRO:C	6:H:84:ALA:N	2.71	0.42
9:K:74:ARG:C	9:K:75:ILE:HG13	2.38	0.42
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	2.02	0.42
1:A:549:MET:HA	1:A:552:TRP:HB2	2.02	0.42
1:A:583:PRO:O	1:A:610:GLY:CA	2.68	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.55	0.42
1:A:894:GLU:O	1:A:896:ARG:N	2.40	0.42
1:A:958:VAL:HG13	1:A:1052:GLN:HB3	2.01	0.42
2:B:1150:ARG:HA	2:B:1150:ARG:HD3	1.86	0.42
2:B:780:VAL:HA	2:B:795:ILE:HG22	2.01	0.42
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.20	0.41
1:A:15:LYS:HB3	2:B:1220:ARG:HD3	2.02	0.41
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.55	0.41
1:A:77:CYS:HA	1:A:78:PRO:HD3	1.91	0.41
1:A:884:ASP:N	1:A:884:ASP:OD2	2.51	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HE21	1.85	0.41
2:B:173:MET:O	2:B:176:SER:OG	2.29	0.41
2:B:202:TYR:CD1	2:B:209:GLU:HG2	2.55	0.41
2:B:230:ALA:C	2:B:232:SER:H	2.23	0.41
2:B:315:LYS:HG2	7:I:13:MET:HE1	2.02	0.41
2:B:473:MET:CA	2:B:474:SER:CB	2.91	0.41
1:A:1163:ILE:HG13	1:A:1163:ILE:H	1.74	0.41
1:A:1325:THR:HA	4:E:147:HIS:HA	2.01	0.41
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.33	0.41
1:A:451:HIS:O	2:B:1137:CYS:SG	2.77	0.41
1:A:652:VAL:O	1:A:655:PHE:N	2.53	0.41
2:B:1146:PHE:CD2	2:B:1146:PHE:C	2.93	0.41
2:B:190:TYR:OH	2:B:196:PRO:HG3	2.20	0.41
2:B:600:LEU:C	2:B:615:MET:HE3	2.41	0.41
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.58	0.41
2:B:805:THR:CB	2:B:815:ARG:HH21	2.32	0.41
8:J:42:LYS:HE3	8:J:43:ARG:NH2	2.35	0.41
1:A:1038:THR:O	1:A:1041:ALA:N	2.54	0.41
1:A:405:VAL:O	1:A:413:ILE:HB	2.20	0.41
1:A:56:PRO:O	1:A:57:ARG:CG	2.64	0.41
2:B:803:LEU:HD22	2:B:1035:ALA:CB	2.50	0.41
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.88	0.41
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.82	0.41
3:C:181:ASP:HA	3:C:182:PRO:HD2	1.79	0.41
3:C:232:VAL:HG21	3:C:244:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:127:ILE:H	4:E:127:ILE:HD13	1.84	0.41
5:F:85:MET:HE1	5:F:148:VAL:HG13	2.02	0.41
5:F:94:LEU:HD22	5:F:122:MET:HG2	2.01	0.41
9:K:36:GLU:HB3	9:K:37:LYS:HG2	2.00	0.41
1:A:1042:PHE:CD2	1:A:1042:PHE:C	2.94	0.41
2:B:597:MET:SD	2:B:624:LEU:HD11	2.61	0.41
3:C:105:GLY:HA3	3:C:149:LYS:O	2.19	0.41
3:C:44:LEU:HD12	3:C:160:LYS:O	2.20	0.41
6:H:26:ILE:HG23	6:H:26:ILE:O	2.21	0.41
7:I:46:HIS:O	7:I:47:GLU:HB2	2.20	0.41
9:K:50:LEU:HD23	9:K:56:VAL:HG11	2.01	0.41
2:B:463:THR:HG23	12:T:26:DA:H4'	2.02	0.41
1:A:108:MET:C	1:A:110:CYS:H	2.23	0.41
1:A:269:ILE:HG23	1:A:299:HIS:HB2	2.01	0.41
1:A:456:MET:HG2	1:A:478:TYR:OH	2.20	0.41
1:A:68:GLN:OE1	1:A:68:GLN:O	2.38	0.41
1:A:783:THR:O	1:A:784:LEU:HD23	2.21	0.41
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.83	0.41
2:B:173:MET:HB3	2:B:176:SER:HB3	2.02	0.41
2:B:44:VAL:O	2:B:47:GLN:N	2.53	0.41
2:B:739:THR:OG1	2:B:740:HIS:N	2.53	0.41
2:B:902:GLY:O	2:B:948:ILE:HG23	2.20	0.41
2:B:1060:ARG:NH1	3:C:199:LYS:O	2.47	0.41
3:C:258:ILE:HG13	9:K:35:PHE:HE2	1.84	0.41
1:A:568:PRO:HD3	6:H:94:ASP:O	2.19	0.41
1:A:401:GLY:O	1:A:402:ALA:HB2	2.20	0.41
1:A:829:VAL:O	1:A:831:THR:N	2.53	0.41
1:A:982:THR:C	1:A:984:LYS:H	2.24	0.41
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.02	0.41
2:B:973:ILE:HA	2:B:974:PRO:HD3	1.89	0.41
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.56	0.41
1:A:167:CYS:SG	1:A:167:CYS:O	2.77	0.41
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.84	0.41
1:A:858:ASN:O	1:A:861:GLY:N	2.45	0.41
1:A:892:ALA:O	1:A:896:ARG:HB2	2.21	0.41
1:A:983:ILE:O	1:A:983:ILE:CG2	2.68	0.41
2:B:1160:VAL:O	2:B:1194:ILE:HD13	2.21	0.41
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.85	0.41
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.03	0.41
2:B:637:LEU:HD22	2:B:741:CYS:O	2.20	0.41
3:C:99:LEU:HD11	3:C:120:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:95:TYR:HB3	6:H:144:ILE:HB	2.03	0.41
9:K:53:ASP:O	9:K:56:VAL:HG22	2.21	0.41
11:R:8:G:N2	12:T:21:DT:H1'	2.35	0.41
1:A:1030:ARG:C	1:A:1032:LEU:H	2.23	0.41
1:A:1316:VAL:O	1:A:1319:VAL:HB	2.20	0.41
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.89	0.41
2:B:999:MET:HG3	2:B:1008:PRO:HD2	2.02	0.41
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.85	0.41
2:B:600:LEU:HB3	2:B:615:MET:HE2	2.03	0.41
3:C:82:TYR:CE2	3:C:84:ARG:NH2	2.88	0.41
4:E:168:TYR:C	4:E:169:ARG:HG2	2.41	0.41
4:E:61:GLN:HG2	4:E:62:ALA:N	2.36	0.41
5:F:111:LEU:N	5:F:111:LEU:CD1	2.83	0.41
1:A:1062:GLU:N	5:F:88:TYR:HE1	2.19	0.41
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.41
1:A:1263:ILE:CG2	1:A:1264:GLU:N	2.83	0.41
1:A:1425:SER:O	1:A:1427:ASN:N	2.54	0.41
1:A:179:LEU:HD13	1:A:301:ALA:HB2	2.02	0.41
1:A:306:ASN:HD22	1:A:306:ASN:N	2.18	0.41
1:A:350:ARG:HB3	2:B:1128:LEU:HD11	2.03	0.41
1:A:754:SER:OG	1:A:757:ASN:ND2	2.54	0.41
1:A:814:PHE:O	1:A:817:ALA:HB3	2.20	0.41
1:A:903:ASN:O	1:A:907:THR:OG1	2.37	0.41
2:B:522:VAL:CG1	2:B:537:LYS:HB2	2.51	0.41
3:C:181:ASP:OD1	3:C:185:LYS:HG2	2.20	0.41
5:F:152:ILE:HD12	5:F:152:ILE:H	1.86	0.41
7:I:78:CYS:SG	7:I:105:SER:HB2	2.61	0.41
1:A:1154:TYR:HD2	7:I:25:LEU:HD22	1.86	0.41
7:I:14:LEU:CD2	7:I:29:CYS:HB2	2.51	0.41
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.47	0.41
1:A:350:ARG:NH2	12:T:21:DT:H2"	2.35	0.41
1:A:1152:ILE:HD13	7:I:44:TYR:HD2	1.85	0.41
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.56	0.41
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.35	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.56	0.41
3:C:90:ASP:HB3	3:C:91:HIS:H	1.78	0.41
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.03	0.41
9:K:31:VAL:O	9:K:74:ARG:HA	2.20	0.41
1:A:315:LEU:CD1	1:A:319:GLY:HA2	2.51	0.41
1:A:379:VAL:HG12	1:A:380:VAL:H	1.86	0.41
1:A:590:ARG:O	1:A:591:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:THR:C	1:A:598:LEU:N	2.74	0.41
1:A:619:LYS:O	1:A:623:GLY:HA3	2.20	0.41
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.50	0.41
2:B:1045:SER:HA	2:B:1046:PRO:HD3	1.87	0.41
2:B:301:ILE:HA	2:B:379:GLY:O	2.21	0.41
2:B:553:PRO:HA	2:B:556:THR:HG22	2.03	0.41
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.56	0.41
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.21	0.41
2:B:710:LEU:HA	2:B:710:LEU:HD23	1.77	0.41
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.54	0.41
2:B:795:ILE:HD11	2:B:854:LEU:HB2	2.03	0.41
4:E:112:TYR:CZ	4:E:116:ILE:HD11	2.55	0.41
4:E:112:TYR:O	4:E:137:GLU:HG2	2.21	0.41
7:I:55:THR:O	7:I:55:THR:HG23	2.21	0.41
7:I:68:LEU:HB3	7:I:84:VAL:HG22	2.01	0.41
1:A:9:ALA:HA	1:A:10:PRO:HD3	1.90	0.40
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.86	0.40
1:A:853:ASP:C	1:A:855:THR:H	2.24	0.40
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.22	0.40
2:B:190:TYR:HD2	8:J:63:TYR:CD2	2.38	0.40
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.40
2:B:884:ARG:O	2:B:936:ASP:HB3	2.21	0.40
4:E:89:GLY:O	4:E:91:LYS:N	2.54	0.40
5:F:81:THR:O	5:F:136:ARG:NH1	2.54	0.40
1:A:964:ILE:CD1	1:A:1037:LEU:HD21	2.47	0.40
1:A:106:VAL:HG12	1:A:107:CYS:H	1.86	0.40
1:A:1341:ILE:CD1	1:A:1379:GLY:O	2.69	0.40
1:A:399:HIS:O	1:A:435:HIS:CD2	2.74	0.40
1:A:31:SER:OG	1:A:83:HIS:CD2	2.75	0.40
2:B:57:TYR:O	2:B:60:GLN:HB3	2.21	0.40
9:K:65:HIS:C	9:K:67:PHE:N	2.75	0.40
1:A:1059:HIS:HB3	5:F:86:THR:HB	2.03	0.40
1:A:299:HIS:HA	1:A:302:THR:HB	2.03	0.40
1:A:532:ARG:O	1:A:533:LYS:C	2.59	0.40
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.86	0.40
1:A:794:PRO:HG2	1:A:795:GLU:H	1.85	0.40
2:B:803:LEU:HD22	2:B:1035:ALA:HB3	2.04	0.40
2:B:1115:THR:O	2:B:1116:ARG:C	2.59	0.40
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.52	0.40
2:B:861:ASP:OD1	2:B:862:GLN:N	2.55	0.40
3:C:234:SER:HB3	3:C:240:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:98:TYR:C	6:H:118:PHE:HD2	2.25	0.40
6:H:94:ASP:N	6:H:94:ASP:OD1	2.55	0.40
7:I:26:LEU:HD13	7:I:35:VAL:HG11	2.02	0.40
9:K:7:PHE:C	9:K:9:LEU:H	2.24	0.40
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	2.02	0.40
1:A:320:ARG:HG3	2:B:471:LYS:HG2	2.04	0.40
1:A:265:LYS:HZ2	1:A:323:LYS:HG2	1.87	0.40
1:A:353:ILE:HD13	1:A:487:MET:CE	2.52	0.40
1:A:795:GLU:H	1:A:795:GLU:HG3	1.48	0.40
2:B:979:LYS:HE3	2:B:1095:LEU:HD12	2.02	0.40
2:B:642:ASP:OD2	2:B:649:LYS:NZ	2.55	0.40
2:B:910:VAL:HG12	2:B:911:ILE:H	1.85	0.40
1:A:1350:LYS:O	1:A:1354:ASN:HB2	2.22	0.40
1:A:870:GLU:HG3	4:E:208:TYR:CG	2.57	0.40
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.69	0.40
2:B:228:LYS:NZ	2:B:234:ILE:HG13	2.36	0.40
2:B:289:LEU:HA	2:B:289:LEU:HD23	1.95	0.40
4:E:147:HIS:HB3	4:E:150:VAL:HG23	2.02	0.40
1:A:1017:LEU:HB2	4:E:205:SER:HA	2.03	0.40
5:F:82:THR:HG22	5:F:84:TYR:H	1.86	0.40
5:F:92:ARG:O	5:F:96:THR:OG1	2.25	0.40
8:J:25:LEU:HA	8:J:25:LEU:HD23	1.85	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%)	1075 (78%)	218 (16%)	90 (6%)	1	19
2	B	1088/1224 (89%)	849 (78%)	169 (16%)	70 (6%)	1	20
3	C	264/318 (83%)	211 (80%)	39 (15%)	14 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	212/215 (99%)	177 (84%)	31 (15%)	4 (2%)	8	42
5	F	82/155 (53%)	73 (89%)	6 (7%)	3 (4%)	3	29
6	H	129/146 (88%)	96 (74%)	20 (16%)	13 (10%)	0	9
7	I	117/122 (96%)	92 (79%)	18 (15%)	7 (6%)	1	20
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	20
9	K	112/120 (93%)	95 (85%)	15 (13%)	2 (2%)	8	42
10	L	44/70 (63%)	32 (73%)	9 (20%)	3 (7%)	1	18
All	All	3494/4173 (84%)	2748 (79%)	536 (15%)	210 (6%)	1	20

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	93	VAL
1	A	226	GLU
1	A	253	ASN
1	A	254	GLU
1	A	258	GLY
1	A	312	PRO
1	A	313	GLN
1	A	317	LYS
1	A	321	PRO
1	A	325	ILE
1	A	424	ILE
1	A	517	ASN
1	A	567	LYS
1	A	597	LEU
1	A	830	LYS
1	A	846	GLU
1	A	889	SER
1	A	972	HIS
1	A	998	LEU
1	A	1261	LYS
1	A	1365	TYR
1	A	1435	PRO
2	B	21	GLU
2	B	67	SER
2	B	176	SER
2	B	223	VAL
2	B	229	ALA

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Mol	Chain	Res	Type
2	B	249	ARG
2	B	466	TRP
2	B	477	ALA
2	B	479	VAL
2	B	480	SER
2	B	483	LEU
2	B	563	MET
2	B	636	PRO
2	B	643	ASP
2	B	731	VAL
2	B	735	ALA
2	B	738	PHE
2	B	809	MET
2	B	864	LYS
2	B	903	VAL
2	B	958	GLN
2	B	1066	SER
2	B	1155	SER
2	B	1176	ASN
2	B	1178	ASN
2	B	1183	LYS
4	E	90	VAL
5	F	104	ASN
6	H	32	THR
6	H	61	SER
6	H	78	SER
6	H	82	PRO
6	H	140	ALA
7	I	33	SER
7	I	54	GLU
8	J	2	ILE
8	J	6	ARG
10	L	46	VAL
1	A	46	THR
1	A	50	ILE
1	A	55	ASP
1	A	68	GLN
1	A	86	LEU
1	A	89	PRO
1	A	178	GLY
1	A	257	ARG
1	A	266	LEU

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Mol	Chain	Res	Type
1	A	315	LEU
1	A	538	ASP
1	A	543	LEU
1	A	628	GLY
1	A	774	ARG
1	A	821	ARG
1	A	859	SER
1	A	958	VAL
1	A	1221	LYS
1	A	1229	SER
1	A	1437	GLY
2	B	100	PRO
2	B	200	GLY
2	B	265	SER
2	B	365	THR
2	B	436	VAL
2	B	450	ALA
2	B	475	SER
2	B	488	TYR
2	B	709	ASP
2	B	837	ASP
2	B	901	PRO
2	B	976	ILE
2	B	1082	MET
2	B	1096	ARG
2	B	1126	GLY
2	B	1131	GLY
2	B	1156	ASP
3	C	110	THR
3	C	212	PRO
4	E	192	ARG
5	F	82	THR
6	H	108	SER
6	H	129	TYR
7	I	76	PRO
9	K	81	TYR
10	L	56	LEU
1	A	48	ALA
1	A	202	LEU
1	A	251	SER
1	A	333	GLU
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	895	LYS
2	B	45	SER
2	B	121	ASN
2	B	266	ALA
2	B	307	ASP
2	B	468	GLU
2	B	734	HIS
2	B	869	SER
3	C	167	HIS
4	E	59	SER
5	F	112	GLU
6	H	52	GLN
7	I	34	TYR
7	I	47	GLU
7	I	88	SER
8	J	29	GLU
1	A	72	GLU
1	A	308	ILE
1	A	314	ALA
1	A	418	SER
1	A	454	SER
1	A	465	TYR
1	A	1016	THR
1	A	1270	ASN
2	B	248	SER
2	B	322	PHE
2	B	454	THR
2	B	549	THR
2	B	699	GLU
2	B	724	ASP
2	B	974	PRO
2	B	1116	ARG
2	B	1153	GLU
2	B	1157	ALA
3	C	28	ALA
3	C	142	VAL
3	C	144	ILE
3	C	214	ASN
6	H	3	ASN
10	L	42	ARG
1	A	40	THR
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	130	ASP
1	A	248	PRO
1	A	324	SER
1	A	332	LYS
1	A	385	ILE
1	A	386	ASP
1	A	404	TYR
1	A	525	GLN
1	A	639	PRO
1	A	896	ARG
1	A	933	TYR
1	A	1062	GLU
1	A	1280	GLU
1	A	1384	VAL
1	A	1393	ASN
2	B	359	GLU
2	B	370	PHE
2	B	467	GLY
2	B	792	MET
2	B	1211	ASN
3	C	6	PRO
3	C	172	PRO
3	C	213	PRO
3	C	227	THR
3	C	265	MET
4	E	124	VAL
6	H	62	SER
6	H	92	ASP
6	H	135	LEU
9	K	10	PHE
1	A	149	GLU
1	A	399	HIS
1	A	492	PRO
1	A	886	ILE
1	A	1424	VAL
2	B	876	LYS
2	B	1214	PRO
3	C	253	LYS
7	I	21	GLU
1	A	168	GLY
1	A	667	GLY
1	A	986	ILE

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Mol	Chain	Res	Type
1	A	250	ILE
1	A	946	VAL
1	A	1146	VAL
2	B	611	PRO
2	B	1046	PRO
3	C	240	VAL
1	A	166	GLY
1	A	1327	ILE
6	H	85	GLY
1	A	1388	GLY
2	B	301	ILE
8	J	64	ASN
1	A	35	ILE
1	A	583	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%)	1008 (83%)	210 (17%)	2	13
2	B	960/1061 (90%)	786 (82%)	174 (18%)	1	12
3	C	234/274 (85%)	189 (81%)	45 (19%)	1	10
4	E	196/197 (100%)	169 (86%)	27 (14%)	3	22
5	F	74/137 (54%)	65 (88%)	9 (12%)	5	25
6	H	117/128 (91%)	101 (86%)	16 (14%)	3	22
7	I	113/116 (97%)	90 (80%)	23 (20%)	1	8
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	9
9	K	99/102 (97%)	86 (87%)	13 (13%)	4	23
10	L	40/57 (70%)	30 (75%)	10 (25%)	0	4
All	All	3111/3657 (85%)	2572 (83%)	539 (17%)	2	13

All (539) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	13	THR
1	A	22	PHE
1	A	28	ARG
1	A	32	VAL
1	A	40	THR
1	A	44	THR
1	A	47	ARG
1	A	49	LYS
1	A	58	LEU
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	99	ILE
1	A	102	VAL
1	A	105	CYS
1	A	108	MET
1	A	110	CYS
1	A	114	LEU
1	A	115	LEU
1	A	126	LEU
1	A	144	THR
1	A	169	ASN
1	A	179	LEU
1	A	185	TRP
1	A	222	LEU
1	A	225	ASN
1	A	230	ARG
1	A	235	ILE
1	A	250	ILE
1	A	252	PHE
1	A	263	THR
1	A	269	ILE
1	A	271	LYS
1	A	287	HIS
1	A	289	ILE
1	A	304	MET
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	325	ILE
1	A	332	LYS
1	A	337	ARG
1	A	340	LEU
1	A	350	ARG
1	A	362	ASP
1	A	368	LYS
1	A	385	ILE
1	A	388	LEU
1	A	397	ASN
1	A	403	LYS
1	A	411	ASP
1	A	412	ARG
1	A	419	LYS
1	A	424	ILE
1	A	431	LYS
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	450	LEU
1	A	452	LYS
1	A	453	MET
1	A	455	MET
1	A	456	MET
1	A	466	SER
1	A	469	ARG
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	493	GLN
1	A	494	SER
1	A	501	LEU
1	A	516	SER
1	A	518	LYS
1	A	521	MET
1	A	525	GLN
1	A	534	LEU

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Mol	Chain	Res	Type
1	A	535	THR
1	A	536	LEU
1	A	541	ILE
1	A	550	LEU
1	A	552	TRP
1	A	555	ASP
1	A	557	ASP
1	A	567	LYS
1	A	572	TRP
1	A	576	GLN
1	A	577	ILE
1	A	596	THR
1	A	597	LEU
1	A	599	SER
1	A	618	GLU
1	A	629	LEU
1	A	630	ILE
1	A	634	THR
1	A	635	ARG
1	A	658	LEU
1	A	660	ASN
1	A	662	PHE
1	A	666	ILE
1	A	675	THR
1	A	677	ARG
1	A	694	THR
1	A	695	LYS
1	A	731	ARG
1	A	740	LEU
1	A	741	ASN
1	A	747	VAL
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	783	THR
1	A	793	SER
1	A	801	GLU
1	A	805	LEU
1	A	806	ARG
1	A	808	LEU

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Mol	Chain	Res	Type
1	A	826	ASP
1	A	830	LYS
1	A	839	ARG
1	A	858	ASN
1	A	867	ILE
1	A	870	GLU
1	A	882	SER
1	A	884	ASP
1	A	885	THR
1	A	896	ARG
1	A	898	ARG
1	A	902	LEU
1	A	907	THR
1	A	911	SER
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
1	A	938	LYS
1	A	949	ASP
1	A	962	ARG
1	A	964	ILE
1	A	977	LYS
1	A	988	LEU
1	A	990	VAL
1	A	993	LEU
1	A	994	GLN
1	A	996	ASN
1	A	1004	ASN
1	A	1006	ILE
1	A	1017	LEU
1	A	1020	CYS
1	A	1022	LEU
1	A	1025	ARG
1	A	1039	LYS
1	A	1043	ASP
1	A	1058	VAL
1	A	1067	LEU
1	A	1077	THR
1	A	1092	LYS
1	A	1095	THR
1	A	1116	LEU
1	A	1118	VAL

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Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1163	ILE
1	A	1187	GLN
1	A	1193	LEU
1	A	1219	THR
1	A	1232	ASN
1	A	1237	ILE
1	A	1239	ARG
1	A	1240	CYS
1	A	1257	ASP
1	A	1263	ILE
1	A	1264	GLU
1	A	1280	GLU
1	A	1283	VAL
1	A	1284	MET
1	A	1295	THR
1	A	1299	VAL
1	A	1308	THR
1	A	1309	ASP
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1394	THR
1	A	1407	GLU
1	A	1420	ASP
1	A	1425	SER
2	B	25	ILE

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Mol	Chain	Res	Type
2	B	26	THR
2	B	28	GLU
2	B	43	LEU
2	B	45	SER
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	90	ILE
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	104	GLU
2	B	108	VAL
2	B	120	ARG
2	B	131	ASP
2	B	132	VAL
2	B	134	LYS
2	B	167	ILE
2	B	169	ARG
2	B	174	LEU
2	B	175	ARG
2	B	189	LEU
2	B	194	GLU
2	B	199	MET
2	B	202	TYR
2	B	217	ARG
2	B	222	ILE
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	239	GLU
2	B	240	ILE
2	B	244	LEU
2	B	246	LYS
2	B	249	ARG
2	B	268	THR
2	B	273	LEU
2	B	276	ILE
2	B	277	LYS

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Mol	Chain	Res	Type
2	B	294	ASP
2	B	296	GLU
2	B	298	LEU
2	B	302	CYS
2	B	305	VAL
2	B	313	MET
2	B	314	LEU
2	B	327	ARG
2	B	347	LYS
2	B	361	LEU
2	B	370	PHE
2	B	387	LEU
2	B	388	CYS
2	B	398	ARG
2	B	403	LYS
2	B	404	LYS
2	B	423	LYS
2	B	424	LEU
2	B	429	PHE
2	B	459	TYR
2	B	463	THR
2	B	466	TRP
2	B	471	LYS
2	B	474	SER
2	B	481	GLN
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	493	SER
2	B	496	ARG
2	B	513	GLN
2	B	527	THR
2	B	529	GLU
2	B	537	LYS
2	B	547	VAL
2	B	552	MET
2	B	559	SER
2	B	563	MET
2	B	570	VAL
2	B	576	ASP
2	B	608	ASP
2	B	614	SER

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Mol	Chain	Res	Type
2	B	622	LYS
2	B	637	LEU
2	B	638	PHE
2	B	642	ASP
2	B	643	ASP
2	B	649	LYS
2	B	653	VAL
2	B	655	LYS
2	B	661	LEU
2	B	664	THR
2	B	667	GLN
2	B	678	GLU
2	B	680	THR
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	730	ARG
2	B	731	VAL
2	B	737	THR
2	B	740	HIS
2	B	754	SER
2	B	755	ILE
2	B	762	ASN
2	B	771	SER
2	B	773	MET
2	B	788	ARG
2	B	791	THR
2	B	792	MET
2	B	801	LYS
2	B	822	ASN
2	B	831	SER
2	B	839	MET
2	B	844	SER
2	B	865	LYS
2	B	878	GLN
2	B	882	THR
2	B	884	ARG
2	B	886	LYS

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Mol	Chain	Res	Type
2	B	889	THR
2	B	915	THR
2	B	950	ASP
2	B	957	ASN
2	B	970	THR
2	B	971	THR
2	B	995	ARG
2	B	996	ARG
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1010	LEU
2	B	1013	ASN
2	B	1020	ARG
2	B	1029	CYS
2	B	1048	THR
2	B	1051	THR
2	B	1059	LEU
2	B	1065	GLN
2	B	1067	ARG
2	B	1084	GLN
2	B	1092	TYR
2	B	1095	LEU
2	B	1099	VAL
2	B	1113	VAL
2	B	1114	LEU
2	B	1115	THR
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1132	GLU
2	B	1138	MET
2	B	1156	ASP
2	B	1159	ARG
2	B	1166	CYS
2	B	1170	THR
2	B	1172	ILE
2	B	1177	HIS
2	B	1178	ASN
2	B	1183	LYS
2	B	1191	ILE
2	B	1194	ILE

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Mol	Chain	Res	Type
2	B	1196	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1207	LEU
2	B	1221	SER
3	C	3	GLU
3	C	4	GLU
3	C	10	ILE
3	C	15	LYS
3	C	24	ASN
3	C	26	ASP
3	C	27	LEU
3	C	33	LEU
3	C	37	MET
3	C	40	GLU
3	C	53	THR
3	C	54	ASN
3	C	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	77	ILE
3	C	81	GLU
3	C	89	GLU
3	C	90	ASP
3	C	99	LEU
3	C	111	THR
3	C	116	LYS
3	C	120	ILE
3	C	129	ILE
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	148	ARG
3	C	149	LYS
3	C	155	LEU
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	178	PHE
3	C	183	TRP
3	C	185	LYS
3	C	224	GLN

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Mol	Chain	Res	Type
3	C	226	ASP
3	C	233	GLU
3	C	240	VAL
3	C	244	VAL
3	C	258	ILE
3	C	266	ASP
3	C	267	GLN
3	C	268	ASP
4	E	2	ASP
4	E	3	GLN
4	E	24	LYS
4	E	31	THR
4	E	32	GLN
4	E	54	GLN
4	E	61	GLN
4	E	65	THR
4	E	72	PHE
4	E	83	CYS
4	E	88	VAL
4	E	94	LYS
4	E	107	THR
4	E	110	PHE
4	E	127	ILE
4	E	134	THR
4	E	146	HIS
4	E	158	SER
4	E	166	LYS
4	E	169	ARG
4	E	184	VAL
4	E	187	TYR
4	E	190	LEU
4	E	198	ILE
4	E	200	ARG
4	E	201	LYS
4	E	212	ARG
5	F	77	ASP
5	F	81	THR
5	F	90	ARG
5	F	97	ARG
5	F	104	ASN
5	F	111	LEU
5	F	120	ILE

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Mol	Chain	Res	Type
5	F	145	ASP
5	F	155	LEU
6	H	16	ASP
6	H	24	CYS
6	H	33	GLN
6	H	39	THR
6	H	46	LEU
6	H	55	LEU
6	H	77	ARG
6	H	89	LEU
6	H	94	ASP
6	H	102	TYR
6	H	110	ASP
6	H	114	VAL
6	H	121	LEU
6	H	132	LEU
6	H	135	LEU
6	H	139	ASN
7	I	7	CYS
7	I	11	ASN
7	I	12	ASN
7	I	14	LEU
7	I	19	ASP
7	I	20	LYS
7	I	22	ASN
7	I	24	ARG
7	I	26	LEU
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	52	ILE
7	I	61	ASP
7	I	64	SER
7	I	79	HIS
7	I	83	ASN
7	I	91	ARG
7	I	94	ASP
7	I	95	THR
7	I	104	LEU
7	I	106	CYS
7	I	107	SER
8	J	2	ILE

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Mol	Chain	Res	Type
8	J	3	VAL
8	J	7	CYS
8	J	10	CYS
8	J	14	VAL
8	J	24	LEU
8	J	28	ASP
8	J	29	GLU
8	J	43	ARG
8	J	47	ARG
8	J	48	ARG
8	J	59	LYS
9	K	1	MET
9	K	5	ASP
9	K	20	LYS
9	K	26	LYS
9	K	32	VAL
9	K	42	LEU
9	K	47	ARG
9	K	55	LYS
9	K	64	GLU
9	K	67	PHE
9	K	78	THR
9	K	81	TYR
9	K	113	THR
10	L	27	LEU
10	L	30	ILE
10	L	42	ARG
10	L	44	ASP
10	L	48	CYS
10	L	50	ASP
10	L	51	CYS
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 (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	54	ASN
1	A	68	GLN
1	A	80	HIS

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Mol	Chain	Res	Type
1	A	83	HIS
1	A	92	HIS
1	A	124	GLN
1	A	316	GLN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	515	GLN
1	A	545	GLN
1	A	576	GLN
1	A	660	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1173	HIS
1	A	1218	GLN
1	A	1232	ASN
1	A	1258	HIS
1	A	1364	ASN
1	A	1378	GLN
1	A	1432	GLN
2	B	46	GLN
2	B	110	HIS
2	B	121	ASN
2	B	215	GLN
2	B	300	HIS
2	B	383	ASN
2	B	395	GLN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS

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Mol	Chain	Res	Type
2	B	648	HIS
2	B	657	HIS
2	B	734	HIS
2	B	740	HIS
2	B	744	HIS
2	B	761	HIS
2	B	762	ASN
2	B	822	ASN
2	B	835	GLN
2	B	842	ASN
2	B	862	GLN
2	B	951	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1074	ASN
2	B	1084	GLN
2	B	1112	GLN
2	B	1161	HIS
2	B	1177	HIS
2	B	1178	ASN
2	B	1187	ASN
2	B	1193	GLN
2	B	1195	HIS
2	B	1211	ASN
3	C	54	ASN
3	C	73	GLN
3	C	123	ASN
3	C	140	ASN
3	C	167	HIS
3	C	264	GLN
4	E	5	ASN
4	E	8	ASN
4	E	32	GLN
4	E	54	GLN
4	E	99	HIS
4	E	104	ASN
4	E	114	ASN
4	E	147	HIS
5	F	104	ASN
6	H	52	GLN

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Mol	Chain	Res	Type
6	H	131	ASN
7	I	22	ASN
7	I	60	GLN
7	I	83	ASN
8	J	53	HIS
9	K	40	HIS
9	K	104	ASN
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/12 (83%)	6 (60%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	C
11	R	5	A
11	R	8	G
11	R	9	G
11	R	10	A
11	R	11	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1395/1733 (80%)	-0.15	27 (1%) 66 59	61, 90, 153, 177	0
2	B	1106/1224 (90%)	-0.16	18 (1%) 72 64	57, 85, 129, 160	0
3	C	266/318 (83%)	-0.36	2 (0%) 86 81	67, 83, 112, 124	0
4	E	214/215 (99%)	-0.06	6 (2%) 53 43	75, 119, 155, 165	0
5	F	84/155 (54%)	-0.32	0 100 100	72, 95, 115, 119	0
6	H	133/146 (91%)	0.01	5 (3%) 40 33	96, 109, 138, 142	0
7	I	119/122 (97%)	-0.25	1 (0%) 86 81	75, 99, 121, 136	0
8	J	65/70 (92%)	-0.42	0 100 100	66, 79, 99, 106	0
9	K	114/120 (95%)	-0.41	0 100 100	71, 87, 98, 100	0
10	L	46/70 (65%)	0.15	3 (6%) 18 14	93, 144, 156, 157	0
11	R	11/12 (91%)	-0.24	1 (9%) 9 7	65, 94, 118, 135	0
12	T	12/29 (41%)	-0.52	0 100 100	73, 91, 126, 135	0
All	All	3565/4214 (84%)	-0.18	63 (1%) 68 61	57, 90, 146, 177	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	6.0
1	A	1176	LEU	5.7
2	B	1223	ASP	5.0
4	E	118	PRO	4.9
2	B	1222	ARG	4.5
4	E	93	MET	4.4
2	B	866	TYR	4.3
4	E	119	SER	4.0
1	A	1175	SER	3.6
1	A	147	VAL	3.5
1	A	316	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	3.4
4	E	53	PRO	3.3
1	A	144	THR	3.2
1	A	69	THR	3.1
1	A	1169	ILE	3.1
1	A	318	SER	3.0
1	A	44	THR	3.0
1	A	173	THR	3.0
1	A	152	VAL	2.9
1	A	311	GLN	2.9
2	B	882	THR	2.9
1	A	426	LEU	2.9
2	B	1224	PHE	2.8
1	A	176	LYS	2.8
2	B	1173	ALA	2.8
6	H	130	ARG	2.7
1	A	146	MET	2.7
1	A	153	PRO	2.6
1	A	76	GLU	2.6
1	A	286	HIS	2.6
1	A	151	ASP	2.6
2	B	265	SER	2.6
1	A	182	VAL	2.5
10	L	44	ASP	2.5
1	A	175	ARG	2.5
1	A	313	GLN	2.5
4	E	110	PHE	2.4
1	A	150	THR	2.4
2	B	165	VAL	2.4
2	B	865	LYS	2.4
2	B	1221	SER	2.4
2	B	429	PHE	2.4
2	B	260	GLY	2.4
2	B	133	LYS	2.4
2	B	1172	ILE	2.3
7	I	39	GLY	2.3
1	A	148	CYS	2.3
2	B	92	PHE	2.2
6	H	85	GLY	2.2
3	C	210	GLU	2.2
2	B	448	ILE	2.2
1	A	168	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	212	PRO	2.1
10	L	43	THR	2.1
4	E	83	CYS	2.1
6	H	86	ASP	2.1
11	R	11	G	2.1
6	H	50	ALA	2.0
6	H	132	LEU	2.0
1	A	281	HIS	2.0
10	L	26	THR	2.0
2	B	869	SER	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	ZN	L	105	1/1	0.93	0.04	169,169,169,169	0
13	ZN	A	1735	1/1	0.94	0.05	118,118,118,118	0
13	ZN	A	1734	1/1	0.94	0.04	128,128,128,128	0
13	ZN	J	101	1/1	0.95	0.20	187,187,187,187	0
13	ZN	I	203	1/1	0.98	0.12	148,148,148,148	0
13	ZN	B	1307	1/1	0.98	0.13	141,141,141,141	0
13	ZN	C	319	1/1	0.98	0.05	83,83,83,83	0
13	ZN	I	204	1/1	0.99	0.06	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.