



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:45 am BST

PDB ID : 3GTO  
Title : Backtracked RNA polymerase II complex with 15mer RNA  
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.  
Deposited on : 2009-03-27  
Resolution : 4.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

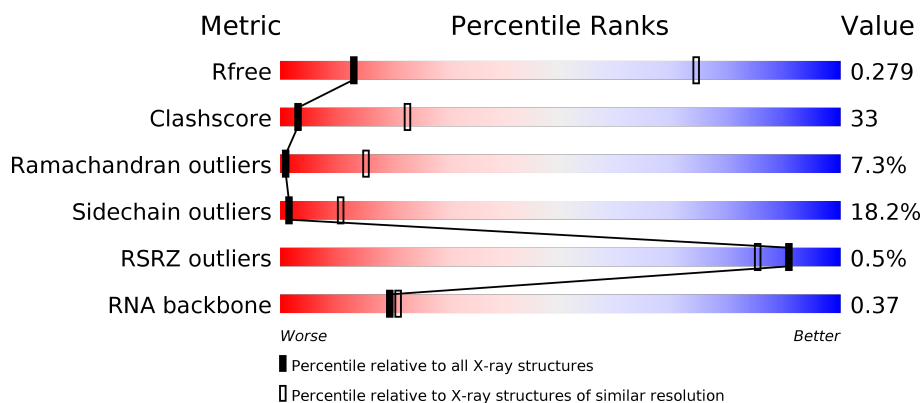
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.






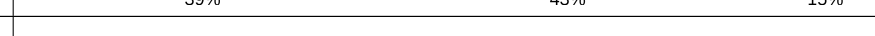
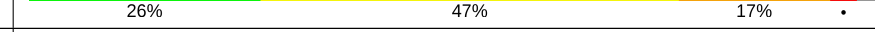
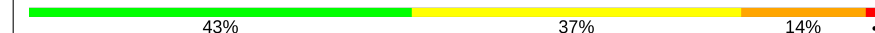


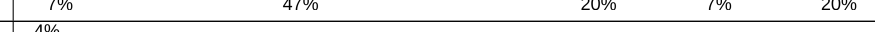
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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  $\geq 3$ , 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>32%</div> <div>35%</div> <div>12%</div> <div>20%</div> </div>
2	B	1224	<div> <div>36%</div> <div>42%</div> <div>11%</div> <div>10%</div> </div>
3	C	318	<div> <div>34%</div> <div>39%</div> <div>9%</div> <div>16%</div> </div>
4	E	215	<div> <div>47%</div> <div>40%</div> <div>10%</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	15	
12	T	28	
13	N	14	

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 29259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			260	117	52	80	11			

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

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

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

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

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

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

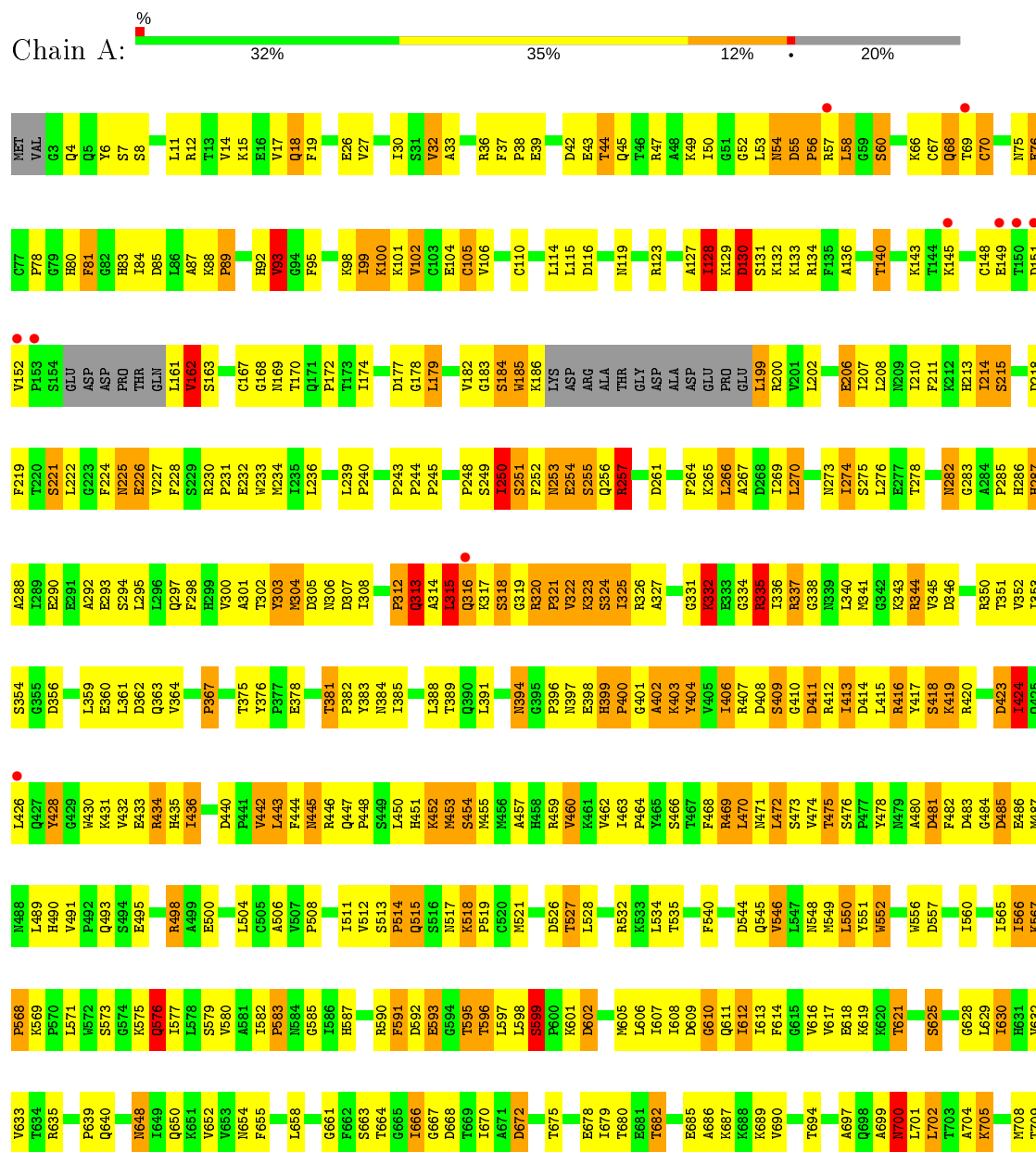
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

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

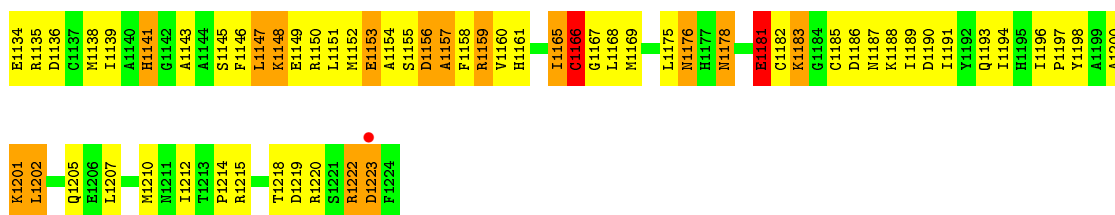
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





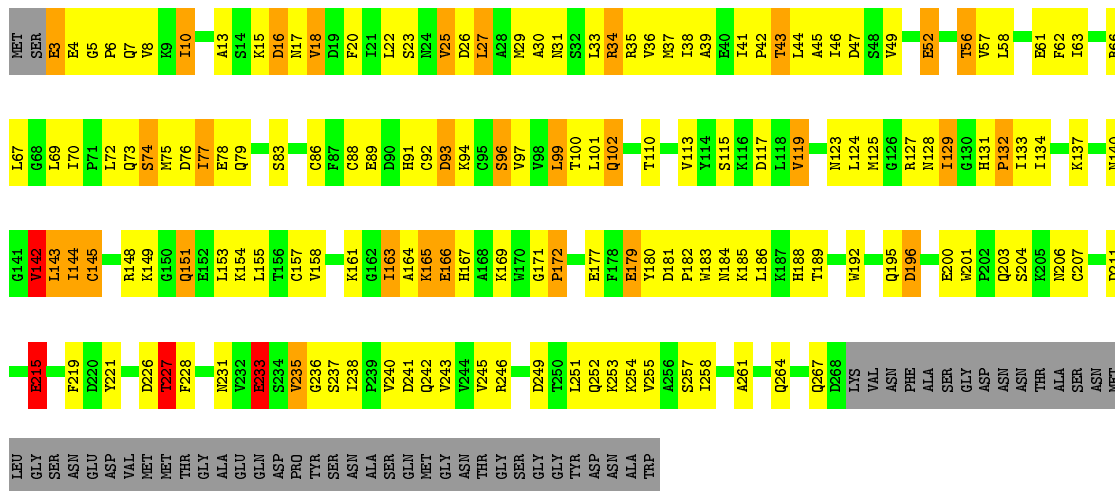






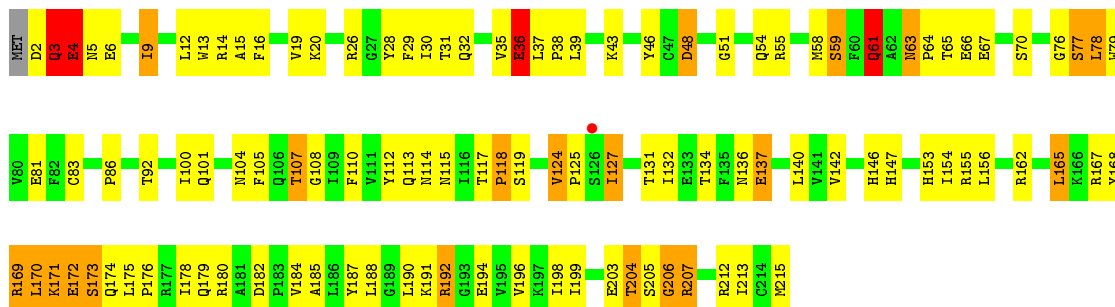
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 34% 39% 9% 16%



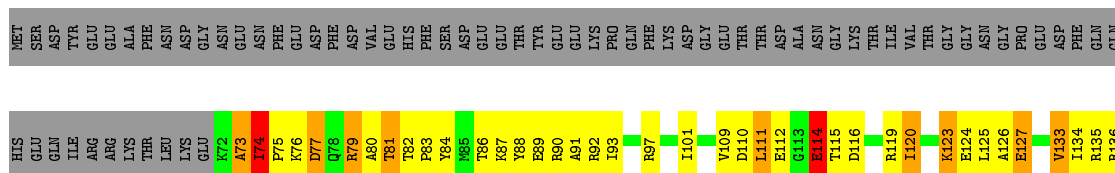
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 47% 40% 10% 3%



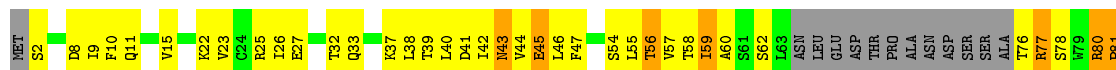
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 26% 21% 6% 46%

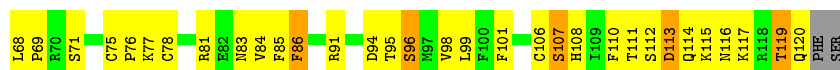




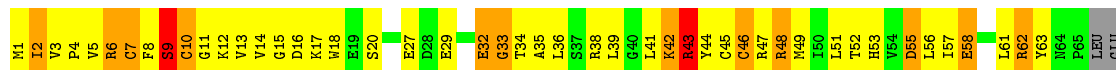
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



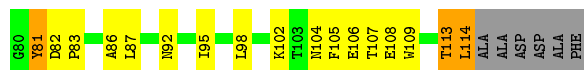
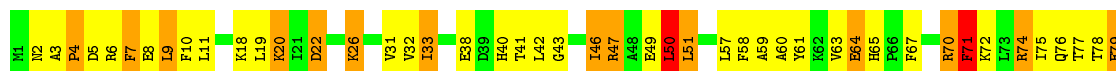
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



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



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

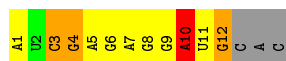
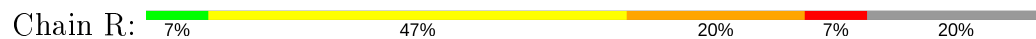


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

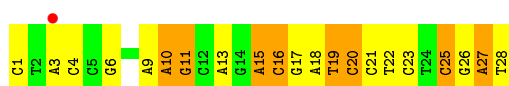




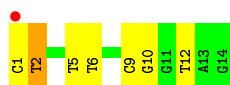
- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*GP\*CP\*AP\*C)-3')



- Molecule 12: DNA (28-MER)



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.85Å 222.80Å 194.98Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 49.45 – 4.00	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-4.00) 93.6 (49.45-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.269 , 0.290 0.264 , 0.279	Depositor DCC
$R_{free}$ test set	2847 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	29259	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	43/11163 (0.4%)	0.81	10/15091 (0.1%)
2	B	1.13	48/8963 (0.5%)	0.88	19/12086 (0.2%)
3	C	1.16	11/2133 (0.5%)	0.84	0/2891
4	E	1.12	9/1788 (0.5%)	0.80	3/2406 (0.1%)
5	F	1.14	3/691 (0.4%)	0.87	0/933
6	H	1.01	3/1086 (0.3%)	0.84	0/1470
7	I	1.26	9/989 (0.9%)	0.95	5/1331 (0.4%)
8	J	1.28	9/541 (1.7%)	0.97	3/727 (0.4%)
9	K	1.08	3/937 (0.3%)	0.80	1/1265 (0.1%)
10	L	1.09	0/365	0.93	0/485
11	R	1.25	1/292 (0.3%)	1.79	5/455 (1.1%)
12	T	1.39	1/634 (0.2%)	1.90	22/975 (2.3%)
13	N	1.83	8/317 (2.5%)	1.67	6/488 (1.2%)
All	All	1.11	148/29899 (0.5%)	0.91	74/40603 (0.2%)

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
3	C	0	1
6	H	0	1
7	I	0	1
All	All	0	3

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	574	SER	CB-OG	12.89	1.59	1.42
4	E	137	GLU	CD-OE1	11.71	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	54	GLU	CD-OE1	11.17	1.38	1.25
1	A	1426	GLU	CD-OE1	10.61	1.37	1.25
2	B	598	GLU	CD-OE2	10.45	1.37	1.25
1	A	1426	GLU	CD-OE2	10.34	1.37	1.25
13	N	2	DT	P-O5'	9.68	1.69	1.59
2	B	742	GLU	CD-OE1	9.61	1.36	1.25
13	N	1	DC	N1-C6	9.32	1.42	1.37
4	E	4	GLU	CD-OE1	9.29	1.35	1.25
3	C	74	SER	CB-OG	9.28	1.54	1.42
9	K	38	GLU	CD-OE1	9.15	1.35	1.25
8	J	29	GLU	CD-OE2	9.08	1.35	1.25
2	B	1070	GLU	CB-CG	8.96	1.69	1.52
1	A	1165	GLU	CD-OE1	8.68	1.35	1.25
4	E	155	ARG	CZ-NH1	8.58	1.44	1.33
4	E	137	GLU	CD-OE2	8.55	1.35	1.25
1	A	1194	ARG	CZ-NH1	8.40	1.44	1.33
8	J	29	GLU	CD-OE1	8.40	1.34	1.25
2	B	116	GLU	CD-OE1	8.33	1.34	1.25
8	J	9	SER	CB-OG	8.29	1.53	1.42
11	R	10	A	P-O5'	8.03	1.67	1.59
13	N	1	DC	N3-C4	7.91	1.39	1.33
8	J	58	GLU	CD-OE1	7.78	1.34	1.25
1	A	1293	SER	CB-OG	7.58	1.52	1.42
8	J	20	SER	CB-OG	7.55	1.52	1.42
5	F	114	GLU	CD-OE1	7.47	1.33	1.25
8	J	33	GLY	C-O	7.43	1.35	1.23
5	F	127	GLU	CD-OE1	7.43	1.33	1.25
1	A	1277	GLU	CD-OE1	7.38	1.33	1.25
3	C	52	GLU	CD-OE1	7.33	1.33	1.25
1	A	593	GLU	CD-OE1	7.32	1.33	1.25
2	B	844	SER	CB-OG	7.25	1.51	1.42
8	J	58	GLU	CD-OE2	7.15	1.33	1.25
1	A	43	GLU	CD-OE2	7.07	1.33	1.25
12	T	3	DA	O5'-C5'	6.95	1.59	1.42
3	C	233	GLU	CD-OE2	6.87	1.33	1.25
1	A	846	GLU	CD-OE2	6.85	1.33	1.25
1	A	678	GLU	CD-OE1	6.83	1.33	1.25
2	B	935	ARG	CZ-NH1	6.77	1.41	1.33
2	B	1061	GLU	CD-OE1	6.71	1.33	1.25
9	K	64	GLU	CD-OE1	6.70	1.33	1.25
2	B	368	GLU	CD-OE2	6.70	1.33	1.25
5	F	127	GLU	CD-OE2	6.59	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	327	ARG	CZ-NH2	6.56	1.41	1.33
1	A	678	GLU	CD-OE2	6.55	1.32	1.25
2	B	986	GLN	CG-CD	6.53	1.66	1.51
4	E	207	ARG	CZ-NH1	6.49	1.41	1.33
2	B	39	ARG	CZ-NH1	6.46	1.41	1.33
13	N	6	DT	C5-C7	6.42	1.53	1.50
4	E	36	GLU	CD-OE2	6.40	1.32	1.25
2	B	543	SER	CB-OG	6.40	1.50	1.42
3	C	86	CYS	CB-SG	6.39	1.93	1.82
1	A	625	SER	CB-OG	6.38	1.50	1.42
1	A	1196	GLU	CD-OE1	6.34	1.32	1.25
3	C	204	SER	CB-OG	6.34	1.50	1.42
1	A	1165	GLU	CG-CD	6.33	1.61	1.51
2	B	635	ARG	CZ-NH1	6.31	1.41	1.33
2	B	731	VAL	C-O	6.31	1.35	1.23
3	C	257	SER	CB-OG	6.30	1.50	1.42
3	C	179	GLU	CB-CG	6.30	1.64	1.52
4	E	81	GLU	CD-OE1	6.29	1.32	1.25
3	C	52	GLU	CD-OE2	6.24	1.32	1.25
2	B	182	SER	CB-OG	6.20	1.50	1.42
2	B	384	ARG	CZ-NH1	6.18	1.41	1.33
1	A	1117	THR	CB-OG1	6.15	1.55	1.43
2	B	967	ARG	CZ-NH1	6.09	1.41	1.33
7	I	96	SER	CB-OG	6.08	1.50	1.42
2	B	480	SER	CB-OG	6.06	1.50	1.42
1	A	771	GLU	CD-OE1	6.05	1.32	1.25
1	A	66	LYS	CE-NZ	6.04	1.64	1.49
13	N	12	DT	O5'-C5'	6.00	1.57	1.42
1	A	43	GLU	CD-OE1	5.98	1.32	1.25
2	B	245	GLU	CG-CD	5.97	1.60	1.51
13	N	6	DT	N1-C6	5.96	1.42	1.38
2	B	823	ALA	C-O	5.93	1.34	1.23
2	B	696	GLU	CD-OE1	5.92	1.32	1.25
2	B	742	GLU	CD-OE2	5.88	1.32	1.25
2	B	1183	LYS	CD-CE	5.87	1.66	1.51
1	A	36	ARG	CZ-NH1	5.83	1.40	1.33
1	A	1415	SER	CB-OG	5.83	1.49	1.42
1	A	350	ARG	CZ-NH1	5.82	1.40	1.33
4	E	81	GLU	CD-OE2	5.80	1.32	1.25
2	B	372	SER	CB-OG	5.75	1.49	1.42
1	A	682	THR	C-O	5.75	1.34	1.23
13	N	1	DC	C4-C5	5.72	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	43	ARG	CZ-NH1	5.72	1.40	1.33
2	B	1117	GLN	CD-NE2	5.70	1.47	1.32
1	A	332	LYS	CE-NZ	5.70	1.63	1.49
2	B	696	GLU	CD-OE2	5.70	1.31	1.25
1	A	1151	GLU	CD-OE1	5.69	1.31	1.25
1	A	870	GLU	C-O	5.68	1.34	1.23
1	A	934	LYS	CE-NZ	5.67	1.63	1.49
6	H	136	LYS	CE-NZ	-5.67	1.34	1.49
1	A	1074	GLU	CD-OE1	5.65	1.31	1.25
13	N	1	DC	N1-C2	5.65	1.45	1.40
2	B	797	TYR	CE1-CZ	5.63	1.45	1.38
2	B	486	TYR	CE1-CZ	5.63	1.45	1.38
6	H	45	GLU	CD-OE1	5.63	1.31	1.25
2	B	430	ARG	CZ-NH1	5.60	1.40	1.33
3	C	215	GLU	CD-OE2	5.58	1.31	1.25
2	B	700	SER	CB-OG	5.55	1.49	1.42
3	C	96	SER	CA-CB	5.55	1.61	1.52
7	I	61	ASP	CG-OD1	5.52	1.38	1.25
1	A	1301	GLU	CD-OE1	5.51	1.31	1.25
1	A	1297	GLU	CD-OE1	5.50	1.31	1.25
1	A	1423	GLY	C-O	5.49	1.32	1.23
7	I	24	ARG	CZ-NH1	5.47	1.40	1.33
2	B	368	GLU	CD-OE1	5.45	1.31	1.25
1	A	354	SER	CB-OG	5.43	1.49	1.42
1	A	1301	GLU	CD-OE2	5.43	1.31	1.25
2	B	1061	GLU	CD-OE2	5.40	1.31	1.25
7	I	45	ARG	CZ-NH1	5.36	1.40	1.33
2	B	1009	ASP	CB-CG	5.33	1.62	1.51
1	A	226	GLU	CD-OE2	5.31	1.31	1.25
1	A	85	ASP	CG-OD1	5.29	1.37	1.25
7	I	81	ARG	CZ-NH1	5.29	1.40	1.33
2	B	797	TYR	CG-CD2	5.28	1.46	1.39
1	A	599	SER	CB-OG	5.27	1.49	1.42
2	B	187	SER	CB-OG	5.26	1.49	1.42
7	I	47	GLU	CG-CD	5.21	1.59	1.51
2	B	906	SER	CB-OG	5.19	1.49	1.42
1	A	1404	GLU	CD-OE1	5.19	1.31	1.25
1	A	149	GLU	CD-OE2	5.17	1.31	1.25
1	A	179	LEU	C-O	5.17	1.33	1.23
2	B	641	GLU	CD-OE2	5.17	1.31	1.25
2	B	468	GLU	CG-CD	5.14	1.59	1.51
2	B	598	GLU	CD-OE1	5.13	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1148	LYS	CD-CE	5.10	1.64	1.51
7	I	115	LYS	CD-CE	5.10	1.64	1.51
2	B	1028	GLU	CG-CD	5.09	1.59	1.51
1	A	900	ASP	C-O	5.07	1.32	1.23
1	A	593	GLU	CD-OE2	5.07	1.31	1.25
9	K	26	LYS	CE-NZ	5.07	1.61	1.49
2	B	1181	GLU	CD-OE2	5.07	1.31	1.25
2	B	678	GLU	CD-OE2	5.05	1.31	1.25
2	B	531	GLN	CD-NE2	5.05	1.45	1.32
2	B	666	TYR	CE1-CZ	5.04	1.45	1.38
3	C	166	GLU	CD-OE1	5.04	1.31	1.25
6	H	127	GLY	C-O	5.04	1.31	1.23
2	B	957	ASN	CG-OD1	5.03	1.35	1.24
4	E	61	GLN	CD-NE2	5.03	1.45	1.32
7	I	12	ASN	CG-ND2	5.02	1.45	1.32
1	A	177	ASP	CG-OD1	5.02	1.36	1.25
1	A	700	ASN	CG-OD1	5.02	1.34	1.24
8	J	46	CYS	C-O	5.01	1.32	1.23
1	A	1025	ARG	NE-CZ	5.01	1.39	1.33
2	B	486	TYR	CG-CD2	5.00	1.45	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	16	DC	O4'-C4'-C3'	-10.87	99.48	106.00
1	A	1173	HIS	N-CA-C	9.95	137.86	111.00
1	A	1172	LEU	N-CA-C	9.54	136.75	111.00
12	T	16	DC	O4'-C1'-N1	8.87	114.21	108.00
12	T	27	DA	O4'-C4'-C3'	-8.83	100.70	106.00
4	E	155	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	B	327	ARG	NE-CZ-NH2	-7.92	116.34	120.30
4	E	207	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	B	1222	ARG	NE-CZ-NH2	7.53	124.06	120.30
12	T	21	DC	C4'-C3'-C2'	-7.51	96.34	103.10
2	B	39	ARG	NE-CZ-NH2	-7.50	116.55	120.30
12	T	11	DG	O4'-C1'-N9	7.46	113.22	108.00
2	B	635	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	36	ARG	NE-CZ-NH1	7.39	124.00	120.30
11	R	10	A	O4'-C1'-N9	-7.37	102.30	108.20
13	N	10	DG	P-O3'-C3'	7.36	128.53	119.70
1	A	731	ARG	NE-CZ-NH1	7.31	123.96	120.30
2	B	852	ARG	NE-CZ-NH2	-7.15	116.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	LEU	CB-CA-C	-7.14	96.63	110.20
11	R	3	C	O4'-C1'-N1	6.97	113.78	108.20
8	J	43	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	1173	HIS	N-CA-CB	-6.90	98.17	110.60
13	N	6	DT	O4'-C1'-N1	6.90	112.83	108.00
2	B	935	ARG	NE-CZ-NH2	-6.88	116.86	120.30
12	T	25	DC	O4'-C1'-N1	6.88	112.81	108.00
12	T	19	DT	N3-C2-O2	-6.84	118.20	122.30
13	N	9	DC	O4'-C1'-N1	6.83	112.78	108.00
8	J	10	CYS	CA-CB-SG	6.78	126.20	114.00
11	R	12	G	C3'-C2'-C1'	6.50	106.70	101.50
12	T	6	DG	P-O3'-C3'	6.47	127.46	119.70
12	T	19	DT	C4-C5-C7	6.28	122.77	119.00
12	T	15	DA	P-O3'-C3'	6.21	127.16	119.70
12	T	3	DA	C5'-C4'-C3'	6.19	125.25	114.10
12	T	4	DC	O4'-C1'-N1	6.19	112.33	108.00
12	T	23	DC	O4'-C4'-C3'	-6.15	102.04	104.50
4	E	155	ARG	NE-CZ-NH1	6.12	123.36	120.30
2	B	967	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	731	ARG	NE-CZ-NH2	-6.07	117.26	120.30
2	B	39	ARG	NE-CZ-NH1	5.95	123.28	120.30
13	N	2	DT	P-O3'-C3'	5.88	126.75	119.70
7	I	10	CYS	CA-CB-SG	5.83	124.49	114.00
12	T	22	DT	C4'-C3'-C2'	-5.82	97.86	103.10
2	B	1096	ARG	NE-CZ-NH1	5.82	123.21	120.30
12	T	20	DC	N1-C2-O2	5.75	122.35	118.90
7	I	81	ARG	NE-CZ-NH2	-5.71	117.45	120.30
12	T	27	DA	C4'-C3'-C2'	-5.71	97.96	103.10
2	B	1010	LEU	CB-CG-CD1	-5.69	101.32	111.00
2	B	384	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	637	LEU	CA-CB-CG	5.56	128.09	115.30
11	R	12	G	C8-N9-C4	-5.50	104.20	106.40
12	T	1	DC	N3-C4-N4	-5.50	114.15	118.00
2	B	967	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	36	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	1098	MET	CG-SD-CE	5.40	108.84	100.20
1	A	1194	ARG	NE-CZ-NH2	-5.40	117.60	120.30
8	J	43	ARG	NE-CZ-NH1	5.37	122.98	120.30
12	T	27	DA	O4'-C1'-N9	5.36	111.75	108.00
12	T	16	DC	C4'-C3'-C2'	-5.34	98.30	103.10
7	I	113	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	1116	LEU	CA-CB-CG	5.31	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	539	LEU	CA-CB-CG	5.29	127.47	115.30
2	B	430	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	B	1011	ILE	CB-CA-C	-5.26	101.08	111.60
7	I	24	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	782	LEU	CA-CB-CG	5.24	127.35	115.30
9	K	74	ARG	NE-CZ-NH2	-5.22	117.69	120.30
12	T	3	DA	O4'-C4'-C3'	-5.21	102.42	104.50
11	R	8	G	C5'-C4'-O4'	5.21	115.35	109.10
7	I	81	ARG	NE-CZ-NH1	5.17	122.89	120.30
13	N	6	DT	C4-C5-C7	5.11	122.07	119.00
12	T	10	DA	O4'-C1'-N9	5.02	111.52	108.00
12	T	1	DC	C5-C4-N4	5.02	123.71	120.20
2	B	1098	MET	CB-CG-SD	-5.01	97.36	112.40
13	N	1	DC	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	172	PRO	Peptide
6	H	136	LYS	Peptide
7	I	77	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11071	924	0
2	B	8792	0	8824	632	0
3	C	2095	0	2052	131	0
4	E	1752	0	1776	91	0
5	F	679	0	701	45	0
6	H	1068	0	1040	64	0
7	I	971	0	928	46	0
8	J	532	0	544	65	0
9	K	919	0	929	64	0
10	L	363	0	387	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	260	0	132	15	0
12	T	566	0	316	21	0
13	N	284	0	161	5	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	1	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	1	0
15	A	1	0	0	0	0
All	All	29259	0	28861	1940	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 33.

All (1940) 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)
1:A:399:HIS:CG	1:A:400:PRO:HD3	1.44	1.48
1:A:315:LEU:HB2	1:A:316:GLN:C	1.39	1.43
1:A:315:LEU:HB2	1:A:316:GLN:CA	1.51	1.38
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.59	1.30
1:A:1111:MET:CG	1:A:1114:PRO:HG3	1.64	1.27
2:B:865:LYS:HG2	2:B:866:TYR:N	1.44	1.24
1:A:1116:LEU:HD23	1:A:1329:THR:CG2	1.68	1.22
1:A:256:GLN:HA	1:A:257:ARG:CB	1.60	1.21
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.76	1.21
1:A:320:ARG:N	1:A:320:ARG:HD2	1.45	1.19
2:B:864:LYS:HG3	2:B:865:LYS:N	1.59	1.18
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.81	1.16
1:A:399:HIS:CG	1:A:400:PRO:CD	2.29	1.16
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.26	1.15
1:A:399:HIS:CB	1:A:400:PRO:HD3	1.75	1.15
1:A:315:LEU:CD2	1:A:316:GLN:HA	1.77	1.14
1:A:323:LYS:HD3	1:A:323:LYS:N	1.50	1.14
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.29	1.14
2:B:865:LYS:CG	2:B:866:TYR:H	1.61	1.14
1:A:1116:LEU:HD23	1:A:1329:THR:HG22	1.30	1.12
1:A:129:LYS:O	1:A:130:ASP:HB2	1.45	1.12
1:A:253:ASN:HA	1:A:256:GLN:O	1.48	1.11
1:A:590:ARG:HH11	1:A:590:ARG:HG3	0.99	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.29	1.11
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.12	1.11
1:A:399:HIS:CB	1:A:400:PRO:CD	2.29	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.12	1.10
1:A:399:HIS:HB3	1:A:400:PRO:CD	1.83	1.08
2:B:882:THR:HG21	2:B:935:ARG:HA	1.30	1.08
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.27	1.08
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.31	1.07
1:A:315:LEU:H	1:A:315:LEU:HD13	1.20	1.07
1:A:573:SER:O	1:A:576:GLN:HB2	1.52	1.07
1:A:315:LEU:HB2	1:A:317:LYS:N	1.68	1.07
11:R:4:G:H2'	11:R:5:A:H8	1.07	1.07
2:B:976:ILE:O	2:B:990:ILE:HB	1.56	1.06
1:A:315:LEU:CB	1:A:316:GLN:CA	2.30	1.06
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.84	1.06
11:R:4:G:H2'	11:R:5:A:C8	1.89	1.06
1:A:213:HIS:O	1:A:214:ILE:O	1.72	1.06
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.32	1.06
1:A:49:LYS:HD3	1:A:55:ASP:OD1	1.54	1.05
1:A:315:LEU:CB	1:A:316:GLN:HA	1.84	1.05
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.87	1.05
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.71	1.04
1:A:315:LEU:HB3	1:A:318:SER:N	1.71	1.04
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.04
1:A:805:LEU:HD13	1:A:805:LEU:C	1.78	1.03
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.75	1.03
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.36	1.03
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.39	1.03
1:A:630:ILE:HD12	1:A:630:ILE:H	1.19	1.03
1:A:67:CYS:HB3	1:A:70:CYS:SG	1.97	1.02
1:A:805:LEU:O	1:A:805:LEU:HD13	1.60	1.02
1:A:320:ARG:CD	1:A:320:ARG:H	1.62	1.02
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.88	1.02
1:A:315:LEU:HB3	1:A:318:SER:H	0.85	1.01
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	0.85	1.01
1:A:351:THR:CG2	2:B:1103:ILE:HD12	1.89	1.00
1:A:344:ARG:HH11	1:A:344:ARG:HG3	1.25	1.00
1:A:319:GLY:CA	1:A:320:ARG:HH11	1.75	1.00
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.40	1.00
1:A:446:ARG:NE	1:A:480:ALA:HB2	1.77	0.99
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:HB3	1:A:257:ARG:N	1.77	0.99
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.78	0.99
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.93	0.98
1:A:1111:MET:SD	1:A:1114:PRO:HG3	2.02	0.98
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.41	0.98
1:A:320:ARG:H	1:A:320:ARG:HD2	0.84	0.98
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.05	0.98
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.28	0.98
1:A:315:LEU:CB	1:A:316:GLN:C	2.33	0.97
1:A:573:SER:H	1:A:576:GLN:HG3	1.23	0.97
2:B:1149:GLU:HG3	2:B:1153:GLU:HG2	1.47	0.96
1:A:322:VAL:C	1:A:323:LYS:HD3	1.85	0.96
4:E:86:PRO:CB	4:E:114:ASN:HD22	1.77	0.96
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.26	0.96
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.79	0.96
2:B:864:LYS:HG3	2:B:865:LYS:H	1.27	0.95
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.48	0.95
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.46	0.95
2:B:363:HIS:O	2:B:364:ILE:HB	1.67	0.94
1:A:567:LYS:HB3	6:H:96:VAL:H	1.32	0.94
1:A:253:ASN:CB	1:A:257:ARG:N	2.30	0.94
1:A:401:GLY:N	1:A:435:HIS:HD2	1.65	0.93
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.35	0.93
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.49	0.93
2:B:864:LYS:HZ3	2:B:867:GLY:N	1.67	0.93
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.51	0.93
2:B:955:THR:HG22	2:B:956:THR:H	1.34	0.92
1:A:315:LEU:CB	1:A:318:SER:H	1.81	0.92
1:A:315:LEU:HD23	1:A:316:GLN:HA	1.49	0.92
2:B:98:THR:O	2:B:126:SER:HB3	1.70	0.92
3:C:56:THR:HG21	3:C:145:CYS:SG	2.10	0.91
1:A:256:GLN:CB	1:A:257:ARG:HB3	2.00	0.91
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.68	0.91
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.00	0.91
1:A:741:ASN:HD22	1:A:744:LYS:H	1.13	0.91
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.69	0.91
1:A:630:ILE:HD12	1:A:630:ILE:N	1.85	0.91
2:B:864:LYS:CG	2:B:865:LYS:H	1.83	0.91
1:A:1111:MET:HG2	1:A:1114:PRO:HG3	1.53	0.90
1:A:315:LEU:CB	1:A:317:LYS:N	2.33	0.90
1:A:319:GLY:CA	1:A:320:ARG:NH1	2.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:H	1:A:435:HIS:HD2	1.19	0.90
1:A:855:THR:CG2	1:A:857:ARG:HE	1.85	0.90
2:B:913:GLY:HA2	2:B:938:SER:CB	2.01	0.90
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.01	0.90
1:A:805:LEU:C	1:A:805:LEU:CD1	2.39	0.90
1:A:315:LEU:CD1	1:A:319:GLY:HA2	2.02	0.90
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.35	0.90
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.50	0.89
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.38	0.89
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.13	0.89
5:F:109:VAL:HG12	5:F:110:ASP:H	1.37	0.88
1:A:351:THR:HG22	1:A:352:VAL:N	1.88	0.88
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.09	0.88
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.56	0.87
3:C:142:VAL:HG13	3:C:143:LEU:N	1.89	0.87
8:J:7:CYS:SG	8:J:10:CYS:N	2.46	0.87
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.61	0.87
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.75	0.87
2:B:955:THR:HG22	2:B:956:THR:N	1.88	0.86
7:I:111:THR:HG22	7:I:113:ASP:H	1.37	0.86
1:A:406:ILE:N	1:A:406:ILE:HD12	1.91	0.86
1:A:751:SER:HB2	2:B:1015:HIS:HE1	1.39	0.86
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.74	0.85
1:A:315:LEU:HD12	1:A:319:GLY:CA	2.05	0.85
2:B:635:ARG:O	2:B:636:PRO:O	1.93	0.85
2:B:864:LYS:HE2	2:B:870:ILE:O	1.76	0.85
1:A:630:ILE:H	1:A:630:ILE:CD1	1.89	0.85
2:B:293:PRO:O	2:B:297:ILE:HG12	1.75	0.85
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.59	0.84
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.40	0.84
1:A:253:ASN:CB	1:A:256:GLN:C	2.46	0.84
8:J:42:LYS:O	8:J:47:ARG:HD2	1.78	0.84
1:A:320:ARG:CD	1:A:320:ARG:N	2.30	0.84
1:A:323:LYS:O	1:A:324:SER:HB3	1.76	0.84
2:B:899:ILE:HD11	2:B:911:ILE:HG12	1.58	0.84
7:I:17:ARG:HG2	7:I:18:GLU:H	1.43	0.84
1:A:399:HIS:HB3	1:A:400:PRO:HD2	1.57	0.84
1:A:830:LYS:HD3	1:A:1079:MET:O	1.78	0.84
1:A:315:LEU:HD13	1:A:315:LEU:N	1.91	0.83
2:B:975:GLN:HG2	2:B:976:ILE:H	1.43	0.83
1:A:590:ARG:HH11	1:A:590:ARG:CG	1.85	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.60	0.83
2:B:880:THR:O	2:B:881:ASN:HB2	1.75	0.83
2:B:37:PHE:O	2:B:38:PHE:HB2	1.75	0.83
1:A:319:GLY:HA3	1:A:320:ARG:NH1	1.93	0.83
1:A:257:ARG:HG2	1:A:257:ARG:O	1.78	0.83
9:K:113:THR:O	9:K:114:LEU:HB2	1.78	0.83
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.13	0.83
7:I:7:CYS:SG	7:I:8:ARG:O	2.36	0.83
1:A:590:ARG:O	1:A:591:PHE:CD1	2.31	0.82
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.08	0.82
9:K:65:HIS:HD2	9:K:67:PHE:H	1.23	0.82
1:A:518:LYS:HG3	1:A:519:PRO:HD2	1.61	0.82
1:A:265:LYS:C	1:A:267:ALA:H	1.83	0.82
1:A:1111:MET:SD	1:A:1114:PRO:CG	2.68	0.82
1:A:889:SER:HB2	1:A:892:ALA:H	1.42	0.82
1:A:777:PHE:CE2	1:A:781:ASP:O	2.33	0.82
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.45	0.81
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.60	0.81
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.09	0.81
1:A:1215:ARG:HH12	1:A:1272:THR:HG22	1.45	0.81
1:A:55:ASP:H	1:A:56:PRO:HD2	1.44	0.81
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.63	0.81
11:R:3:C:H42	12:T:26:DG:H1	1.29	0.81
1:A:239:LEU:HD12	1:A:240:PRO:CD	2.08	0.81
2:B:803:LEU:N	2:B:822:ASN:HD21	1.78	0.81
1:A:253:ASN:HB2	1:A:256:GLN:C	2.01	0.81
1:A:276:LEU:HD11	1:A:292:ALA:HB3	1.61	0.81
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.44	0.81
1:A:344:ARG:NH1	1:A:344:ARG:HG3	1.93	0.80
2:B:875:GLU:O	2:B:877:PRO:HD3	1.81	0.80
9:K:70:ARG:O	9:K:71:PHE:HB3	1.81	0.80
2:B:351:TYR:O	2:B:355:ILE:HG13	1.82	0.80
1:A:67:CYS:CB	1:A:70:CYS:SG	2.70	0.80
1:A:765:VAL:HG21	1:A:800:VAL:HB	1.63	0.80
2:B:636:PRO:HB3	2:B:743:ILE:CG1	2.10	0.80
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	1.80	0.80
1:A:351:THR:HG22	1:A:352:VAL:H	1.47	0.80
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.63	0.80
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.12	0.80
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.80
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.63	0.79
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.17	0.79
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.48	0.79
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.46	0.79
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.17	0.79
1:A:249:SER:O	1:A:250:ILE:CG1	2.30	0.79
1:A:346:ASP:H	2:B:1154:ALA:HB1	1.47	0.79
2:B:706:GLN:O	2:B:710:LEU:HB2	1.82	0.79
1:A:316:GLN:O	1:A:316:GLN:CG	2.31	0.78
1:A:319:GLY:HA2	1:A:320:ARG:NH1	1.97	0.78
2:B:708:GLU:HG3	2:B:709:ASP:H	1.48	0.78
2:B:864:LYS:HE3	2:B:871:THR:HG23	1.66	0.78
1:A:283:GLY:O	1:A:285:PRO:HD3	1.84	0.78
1:A:913:LEU:HD11	1:A:981:LEU:O	1.84	0.78
1:A:261:ASP:HB3	1:A:323:LYS:HE3	1.64	0.78
2:B:64:CYS:HA	2:B:67:SER:HB2	1.65	0.78
1:A:401:GLY:H	1:A:435:HIS:CD2	2.01	0.78
2:B:552:MET:HG3	2:B:553:PRO:HD3	1.65	0.78
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.66	0.77
1:A:315:LEU:HD23	1:A:316:GLN:CA	2.14	0.77
2:B:567:GLU:CD	2:B:567:GLU:H	1.86	0.77
1:A:319:GLY:HA3	1:A:320:ARG:HH11	1.49	0.77
1:A:182:VAL:HG12	1:A:183:GLY:H	1.48	0.77
1:A:323:LYS:O	1:A:324:SER:CB	2.32	0.77
12:T:15:DA:H2''	12:T:16:DC:O5'	1.85	0.77
1:A:344:ARG:HH11	1:A:344:ARG:CG	1.95	0.77
3:C:91:HIS:HB2	3:C:96:SER:OG	1.84	0.77
1:A:323:LYS:N	1:A:323:LYS:CD	2.34	0.76
2:B:980:PHE:O	2:B:981:ALA:HB2	1.85	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.68	0.76
4:E:86:PRO:HB3	4:E:114:ASN:ND2	2.00	0.76
1:A:1111:MET:CG	1:A:1114:PRO:CG	2.57	0.76
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.41	0.76
1:A:182:VAL:HG12	1:A:183:GLY:N	1.99	0.76
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.67	0.76
1:A:590:ARG:O	1:A:591:PHE:HB2	1.84	0.76
3:C:101:LEU:HD12	3:C:117:ASP:O	1.84	0.76
1:A:590:ARG:O	1:A:591:PHE:CB	2.32	0.76
3:C:133:ILE:HD13	3:C:236:GLY:O	1.86	0.76
1:A:315:LEU:CG	1:A:316:GLN:HA	2.16	0.76
2:B:471:LYS:HG3	2:B:472:ALA:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.66	0.75
6:H:145:ARG:O	6:H:146:ARG:OXT	2.04	0.75
1:A:255:SER:O	1:A:256:GLN:HG3	1.87	0.75
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.02	0.75
2:B:1096:ARG:HG3	2:B:1097:HIS:CD2	2.20	0.75
2:B:1148:LYS:O	2:B:1152:MET:HB2	1.87	0.75
5:F:82:THR:HG22	5:F:84:TYR:HB2	1.67	0.75
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.68	0.75
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.68	0.74
1:A:315:LEU:HD12	1:A:318:SER:C	2.08	0.74
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.45	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.71	0.74
8:J:7:CYS:HG	8:J:10:CYS:H	1.35	0.74
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.70	0.74
4:E:86:PRO:CB	4:E:114:ASN:ND2	2.50	0.74
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.68	0.74
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.74
1:A:151:ASP:CG	1:A:163:SER:HA	2.08	0.74
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.68	0.74
2:B:64:CYS:HA	2:B:67:SER:CB	2.18	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.69	0.74
1:A:1111:MET:SD	1:A:1114:PRO:CB	2.75	0.74
1:A:532:ARG:HH22	1:A:745:GLN:HE21	1.36	0.74
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.13	0.74
8:J:35:ALA:O	8:J:39:LEU:HD12	1.88	0.74
4:E:86:PRO:HB3	4:E:114:ASN:HD22	1.52	0.73
1:A:255:SER:C	1:A:256:GLN:HG3	2.08	0.73
2:B:956:THR:HA	2:B:961:LEU:O	1.87	0.73
1:A:249:SER:O	1:A:250:ILE:HG12	1.87	0.73
4:E:15:ALA:HA	4:E:140:LEU:O	1.88	0.73
1:A:446:ARG:HE	1:A:480:ALA:HB2	1.51	0.73
2:B:494:HIS:HD2	2:B:497:ARG:NH1	1.86	0.73
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.70	0.73
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.24	0.73
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.70	0.73
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.71	0.72
1:A:253:ASN:CA	1:A:256:GLN:O	2.32	0.72
1:A:446:ARG:HD2	1:A:480:ALA:CB	2.19	0.72
2:B:1004:GLU:O	3:C:177:GLU:HG2	1.88	0.72
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.71	0.72
11:R:4:G:C2'	11:R:5:A:H8	1.95	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:SER:O	3:C:77:ILE:HB	1.88	0.72
4:E:77:SER:HB2	4:E:105:PHE:HA	1.70	0.72
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.71	0.72
8:J:45:CYS:SG	8:J:46:CYS:N	2.62	0.72
1:A:802:ASN:HD21	2:B:729:ILE:H	1.35	0.72
2:B:955:THR:CG2	2:B:956:THR:H	2.02	0.72
12:T:26:DG:N3	12:T:27:DA:H1'	2.04	0.72
1:A:1407:GLU:H	1:A:1407:GLU:CD	1.93	0.72
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.53	0.72
2:B:649:LYS:O	2:B:650:GLU:HB2	1.90	0.72
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.70	0.72
2:B:31:TRP:CZ2	2:B:744:HIS:CD2	2.78	0.72
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.71	0.72
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.24	0.72
1:A:151:ASP:OD1	1:A:163:SER:HB2	1.90	0.72
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.30	0.72
1:A:249:SER:C	1:A:250:ILE:HG23	2.09	0.71
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.89	0.71
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.72	0.71
10:L:51:CYS:HG	14:L:105:ZN:ZN	1.04	0.71
2:B:591:ARG:O	2:B:592:ASN:HB3	1.89	0.71
1:A:485:ASP:N	1:A:485:ASP:OD1	2.21	0.71
2:B:980:PHE:O	2:B:981:ALA:CB	2.37	0.71
1:A:364:VAL:HG12	1:A:459:ARG:O	1.89	0.71
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.72	0.71
6:H:44:VAL:O	6:H:44:VAL:HG12	1.91	0.71
1:A:1342:GLU:HG2	4:E:212:ARG:HH12	1.54	0.71
1:A:413:ILE:CD1	1:A:413:ILE:N	2.54	0.71
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.25	0.71
2:B:636:PRO:CB	2:B:637:LEU:HA	2.21	0.71
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.72	0.71
1:A:1111:MET:SD	1:A:1114:PRO:CA	2.79	0.71
9:K:18:LYS:O	9:K:19:LEU:HD23	1.90	0.71
1:A:1116:LEU:H	1:A:1308:THR:HB	1.55	0.71
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.73	0.71
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.54	0.71
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.73	0.71
1:A:315:LEU:HD12	1:A:319:GLY:N	2.04	0.70
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.23	0.70
1:A:276:LEU:CD1	1:A:292:ALA:HB3	2.20	0.70
1:A:315:LEU:H	1:A:315:LEU:CD1	1.93	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.27	0.70
2:B:744:HIS:CD2	2:B:746:SER:OG	2.44	0.70
2:B:1094:ARG:HH22	2:B:1098:MET:HG2	1.53	0.70
12:T:13:DA:H61	13:N:2:DT:C7	2.04	0.70
2:B:485:ARG:HH11	2:B:485:ARG:HG2	1.56	0.70
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.08	0.70
2:B:881:ASN:HB2	2:B:933:SER:N	2.06	0.70
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.74	0.70
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.26	0.70
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.74	0.70
2:B:610:ASN:OD1	2:B:612:GLU:HB2	1.92	0.70
3:C:142:VAL:HG13	3:C:143:LEU:H	1.57	0.70
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.74	0.70
1:A:316:GLN:O	1:A:316:GLN:HG3	1.91	0.70
1:A:855:THR:HG21	1:A:857:ARG:NE	2.02	0.70
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.73	0.69
2:B:302:CYS:SG	2:B:310:MET:HG2	2.32	0.69
8:J:48:ARG:HH21	8:J:49:MET:CE	2.04	0.69
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.32	0.69
1:A:250:ILE:O	1:A:251:SER:HB3	1.93	0.69
3:C:219:PHE:CD2	6:H:45:GLU:HG2	2.27	0.69
10:L:40:LEU:HD22	10:L:44:ASP:OD2	1.93	0.69
1:A:401:GLY:O	1:A:402:ALA:HB2	1.91	0.69
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.75	0.69
1:A:925:LEU:O	1:A:929:LEU:HB2	1.93	0.69
2:B:1099:VAL:HG12	2:B:1103:ILE:CD1	2.16	0.69
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.08	0.69
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.74	0.69
8:J:6:ARG:HB3	8:J:11:GLY:O	1.92	0.69
1:A:413:ILE:HD13	1:A:413:ILE:N	2.06	0.69
4:E:77:SER:CB	4:E:105:PHE:HA	2.23	0.69
1:A:304:MET:HG3	2:B:1210:MET:HG3	1.74	0.69
4:E:173:SER:O	4:E:174:GLN:HG2	1.92	0.69
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.08	0.69
1:A:445:ASN:HB2	1:A:454:SER:O	1.92	0.69
3:C:124:LEU:O	3:C:127:ARG:HG2	1.93	0.69
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.09	0.68
1:A:1132:LYS:O	1:A:1135:ARG:HB3	1.91	0.68
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.74	0.68
7:I:68:LEU:HB3	7:I:84:VAL:HG22	1.74	0.68
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:H	1:A:926:GLN:NE2	1.91	0.68
2:B:859:TYR:OH	2:B:941:LEU:HD22	1.92	0.68
2:B:955:THR:HG23	10:L:54:ARG:O	1.93	0.68
2:B:1027:ILE:O	2:B:1029:CYS:N	2.26	0.68
1:A:256:GLN:HB3	1:A:257:ARG:HB3	1.75	0.68
1:A:128:ILE:HG22	1:A:134:ARG:HG3	1.75	0.68
1:A:152:VAL:O	1:A:162:VAL:HG23	1.94	0.68
3:C:142:VAL:CG1	3:C:143:LEU:N	2.57	0.68
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.23	0.68
1:A:27:VAL:O	1:A:30:ILE:HG22	1.94	0.68
3:C:167:HIS:HD2	3:C:169:LYS:H	1.39	0.68
3:C:3:GLU:HA	9:K:104:ASN:HD21	1.58	0.68
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.59	0.68
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.94	0.68
1:A:249:SER:O	1:A:250:ILE:HG23	1.94	0.68
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.08	0.67
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.76	0.67
4:E:199:ILE:O	4:E:199:ILE:HG22	1.94	0.67
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.28	0.67
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.59	0.67
1:A:413:ILE:HD13	1:A:413:ILE:H	1.59	0.67
2:B:628:THR:O	2:B:628:THR:HG22	1.95	0.67
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.42	0.67
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.77	0.67
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.59	0.67
2:B:975:GLN:HG2	2:B:976:ILE:N	2.10	0.67
5:F:109:VAL:HG12	5:F:110:ASP:N	2.09	0.67
1:A:1116:LEU:CD2	1:A:1329:THR:HG22	2.18	0.67
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.24	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.08	0.67
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.82	0.67
1:A:590:ARG:O	1:A:591:PHE:CG	2.47	0.67
2:B:494:HIS:CD2	2:B:497:ARG:NH1	2.63	0.67
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.60	0.67
4:E:46:TYR:CE2	4:E:58:MET:HA	2.30	0.67
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.25	0.67
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.10	0.67
1:A:629:LEU:HD23	1:A:633:VAL:HG23	1.77	0.67
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.74	0.67
2:B:549:THR:HG22	2:B:550:ASP:H	1.59	0.67
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:32:GLU:CD	8:J:32:GLU:H	1.96	0.67
1:A:315:LEU:HD22	1:A:316:GLN:HA	1.76	0.66
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.26	0.66
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.75	0.66
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.76	0.66
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.77	0.66
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.76	0.66
2:B:560:GLU:O	2:B:561:TRP:CD1	2.48	0.66
2:B:865:LYS:CG	2:B:866:TYR:N	2.31	0.66
4:E:29:PHE:O	4:E:30:ILE:HG13	1.95	0.66
1:A:1398:MET:O	1:A:1400:CYS:N	2.29	0.66
2:B:101:MET:HE3	2:B:169:ARG:HH12	1.58	0.66
2:B:108:VAL:HG12	2:B:109:THR:H	1.60	0.66
3:C:172:PRO:O	3:C:235:VAL:HG23	1.96	0.66
6:H:22:LYS:O	6:H:23:VAL:HG23	1.95	0.66
1:A:115:LEU:HD11	1:A:145:LYS:HE3	1.77	0.66
2:B:884:ARG:O	2:B:936:ASP:HB3	1.96	0.66
1:A:565:ILE:HD13	6:H:46:LEU:CD1	2.26	0.66
2:B:980:PHE:O	2:B:1095:LEU:HD12	1.93	0.66
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.30	0.66
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.34	0.66
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.29	0.66
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.78	0.66
6:H:26:ILE:HG22	6:H:40:LEU:O	1.96	0.66
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.78	0.66
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.64	0.66
3:C:88:CYS:SG	14:C:319:ZN:ZN	1.84	0.66
1:A:401:GLY:N	1:A:435:HIS:CD2	2.57	0.66
1:A:590:ARG:NH1	1:A:590:ARG:CG	2.52	0.66
1:A:629:LEU:HD23	1:A:633:VAL:CG2	2.26	0.66
2:B:591:ARG:O	2:B:592:ASN:CB	2.42	0.66
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.04	0.66
1:A:1400:CYS:O	1:A:1405:THR:HG23	1.96	0.66
1:A:628:GLY:O	1:A:632:VAL:HG23	1.95	0.66
2:B:474:SER:C	2:B:476:ARG:H	1.98	0.66
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.43	0.66
1:A:53:LEU:O	1:A:56:PRO:CD	2.44	0.66
1:A:1215:ARG:NH1	1:A:1272:THR:HG22	2.10	0.65
1:A:472:LEU:HD21	2:B:835:GLN:HB3	1.78	0.65
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.60	0.65
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:LEU:O	6:H:91:ASP:N	2.27	0.65
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.60	0.65
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.12	0.65
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.32	0.65
2:B:899:ILE:CD1	2:B:911:ILE:HG12	2.25	0.65
1:A:408:ASP:O	1:A:410:GLY:N	2.30	0.65
1:A:901:LEU:HA	1:A:907:THR:HG23	1.79	0.65
2:B:649:LYS:O	2:B:650:GLU:CB	2.45	0.65
1:A:1386:ARG:HD3	1:A:1403:GLU:HG2	1.79	0.65
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.27	0.65
2:B:816:GLU:OE1	2:B:816:GLU:N	2.30	0.65
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.79	0.65
4:E:172:GLU:O	4:E:174:GLN:N	2.30	0.65
6:H:43:ASN:CG	6:H:46:LEU:HD12	2.17	0.65
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.97	0.65
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.11	0.65
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.77	0.64
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.79	0.64
1:A:751:SER:CB	2:B:1015:HIS:HE1	2.08	0.64
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.96	0.64
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.64
2:B:711:GLU:H	2:B:712:PRO:HD3	1.62	0.64
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.78	0.64
2:B:378:LEU:O	2:B:382:ILE:HG12	1.97	0.64
4:E:171:LYS:O	4:E:173:SER:N	2.30	0.64
6:H:58:THR:HG22	6:H:59:ILE:N	2.11	0.64
8:J:58:GLU:HA	8:J:61:LEU:HD12	1.80	0.64
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.26	0.64
1:A:675:THR:HG22	1:A:679:ILE:HD11	1.78	0.64
2:B:522:VAL:HG13	2:B:538:ASN:O	1.97	0.64
1:A:404:TYR:HA	1:A:413:ILE:O	1.98	0.64
1:A:672:ASP:CB	1:A:736:ASN:HD21	2.09	0.64
1:A:896:ARG:HD2	1:A:897:TYR:HE1	1.62	0.64
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.27	0.64
1:A:388:LEU:HD22	1:A:432:VAL:HG11	1.79	0.64
1:A:406:ILE:HD12	1:A:406:ILE:H	1.62	0.64
2:B:108:VAL:HG12	2:B:109:THR:N	2.12	0.64
2:B:550:ASP:OD2	2:B:552:MET:CG	2.46	0.64
2:B:635:ARG:O	2:B:636:PRO:C	2.36	0.64
2:B:830:TYR:O	2:B:832:GLY:N	2.30	0.64
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.78	0.64
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.97	0.64
1:A:464:PRO:HG2	9:K:67:PHE:CD1	2.33	0.64
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	2.13	0.64
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.79	0.64
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.79	0.64
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.80	0.64
2:B:1103:ILE:N	2:B:1103:ILE:HD13	2.11	0.64
4:E:3:GLN:HG3	4:E:4:GLU:N	2.12	0.64
1:A:105:CYS:O	1:A:114:LEU:HG	1.98	0.64
2:B:451:LYS:HA	2:B:454:THR:HB	1.79	0.64
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.28	0.64
6:H:84:ALA:O	6:H:86:ASP:N	2.30	0.64
1:A:55:ASP:O	1:A:57:ARG:N	2.31	0.64
8:J:1:MET:N	8:J:56:LEU:H	1.96	0.64
1:A:777:PHE:CD2	1:A:781:ASP:O	2.52	0.63
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.80	0.63
7:I:35:VAL:HG12	7:I:36:GLU:N	2.13	0.63
2:B:276:ILE:HG22	2:B:278:GLN:H	1.63	0.63
2:B:168:GLY:H	2:B:450:ALA:HB1	1.63	0.63
1:A:1067:LEU:HD12	1:A:1067:LEU:O	1.99	0.63
1:A:324:SER:O	1:A:326:ARG:N	2.32	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
1:A:475:THR:HG22	1:A:476:SER:N	2.13	0.63
1:A:802:ASN:ND2	2:B:729:ILE:H	1.95	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.79	0.63
1:A:265:LYS:O	1:A:267:ALA:N	2.31	0.63
1:A:440:ASP:H	1:A:460:VAL:HG23	1.63	0.63
3:C:184:ASN:HD21	3:C:189:THR:H	1.46	0.63
1:A:351:THR:CG2	1:A:352:VAL:N	2.60	0.63
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.11	0.63
1:A:955:PRO:O	1:A:956:LEU:HG	1.99	0.63
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.34	0.63
2:B:864:LYS:NZ	2:B:867:GLY:N	2.45	0.63
2:B:1148:LYS:O	2:B:1152:MET:N	2.31	0.63
2:B:879:ARG:CZ	2:B:879:ARG:H	2.11	0.63
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.80	0.63
1:A:1154:TYR:CE2	1:A:1156:PRO:HG3	2.34	0.63
1:A:264:PHE:CE1	1:A:317:LYS:HB3	2.34	0.63
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.14	0.63
1:A:1116:LEU:HD23	1:A:1329:THR:HG21	1.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.81	0.62
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.80	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.99	0.62
2:B:1084:GLN:HE21	3:C:192:TRP:HB2	1.64	0.62
2:B:420:LEU:O	2:B:423:LYS:HB3	1.99	0.62
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.63	0.62
6:H:113:ALA:HA	6:H:125:LEU:O	1.99	0.62
1:A:302:THR:HG21	1:A:313:GLN:HE22	1.63	0.62
1:A:577:ILE:O	1:A:580:VAL:HG23	2.00	0.62
1:A:821:ARG:O	1:A:825:ILE:HG12	2.00	0.62
3:C:100:THR:HB	3:C:119:VAL:HG12	1.81	0.62
3:C:73:GLN:HE21	3:C:75:MET:H	1.47	0.62
2:B:552:MET:HG3	2:B:553:PRO:CD	2.29	0.62
2:B:803:LEU:H	2:B:822:ASN:HD21	1.47	0.62
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	2.14	0.62
1:A:324:SER:O	1:A:325:ILE:C	2.38	0.62
2:B:865:LYS:HG2	2:B:866:TYR:H	0.66	0.62
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.00	0.62
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.81	0.62
1:A:55:ASP:N	1:A:56:PRO:CD	2.62	0.62
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	1.82	0.62
1:A:518:LYS:CG	1:A:519:PRO:HD2	2.30	0.62
1:A:253:ASN:HA	1:A:256:GLN:C	2.19	0.62
1:A:53:LEU:O	1:A:56:PRO:HD3	2.00	0.62
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.15	0.62
1:A:320:ARG:CB	1:A:321:PRO:HA	2.30	0.62
1:A:787:PHE:CZ	1:A:796:SER:HB2	2.35	0.62
1:A:845:LEU:O	1:A:848:ILE:HG12	1.99	0.62
2:B:1082:MET:HA	3:C:189:THR:HA	1.81	0.62
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.82	0.61
1:A:253:ASN:HB3	1:A:257:ARG:H	1.61	0.61
1:A:253:ASN:HB2	1:A:257:ARG:N	2.10	0.61
1:A:261:ASP:HB3	1:A:323:LYS:CE	2.30	0.61
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.83	0.61
1:A:754:SER:H	1:A:757:ASN:HD22	1.46	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.82	0.61
2:B:211:VAL:O	2:B:480:SER:HA	2.00	0.61
1:A:332:LYS:C	1:A:334:GLY:H	2.04	0.61
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.64	0.61
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.67	0.61
2:B:784:ASN:ND2	2:B:788:ARG:HD2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.82	0.61
5:F:82:THR:CG2	5:F:84:TYR:HB2	2.30	0.61
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.40	0.61
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.83	0.61
5:F:111:LEU:H	5:F:111:LEU:HD13	1.65	0.61
2:B:1096:ARG:HG2	2:B:1096:ARG:NH1	2.04	0.61
1:A:1025:ARG:CG	1:A:1025:ARG:HH11	2.14	0.61
1:A:568:PRO:HB3	3:C:221:TYR:CZ	2.36	0.61
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.83	0.61
8:J:44:TYR:CA	8:J:47:ARG:HB2	2.18	0.61
1:A:1111:MET:SD	1:A:1114:PRO:HA	2.41	0.61
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.52	0.61
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.83	0.61
1:A:833:GLU:HG2	1:A:1102:LYS:HE3	1.83	0.61
1:A:765:VAL:HG21	1:A:800:VAL:CB	2.30	0.61
1:A:98:LYS:O	1:A:101:LYS:N	2.33	0.61
2:B:589:VAL:CG1	2:B:590:HIS:N	2.64	0.60
3:C:172:PRO:C	3:C:235:VAL:HG23	2.21	0.60
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.01	0.60
2:B:322:PHE:CD1	2:B:322:PHE:O	2.55	0.60
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.65	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.40	0.60
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.66	0.60
2:B:622:LYS:HE2	7:I:59:VAL:HG22	1.82	0.60
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.01	0.60
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.00	0.60
1:A:648:ASN:O	1:A:652:VAL:HG23	2.02	0.60
2:B:475:SER:C	2:B:477:ALA:N	2.53	0.60
2:B:640:VAL:O	2:B:640:VAL:HG12	2.00	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
3:C:185:LYS:HE3	3:C:211:ASP:O	2.01	0.60
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.02	0.60
1:A:672:ASP:H	1:A:736:ASN:ND2	1.99	0.60
2:B:1096:ARG:HG3	2:B:1097:HIS:CG	2.37	0.60
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.16	0.60
1:A:129:LYS:O	1:A:130:ASP:CB	2.32	0.60
1:A:442:VAL:HG11	1:A:489:LEU:HD21	1.83	0.60
2:B:273:LEU:HD11	2:B:285:ILE:CD1	2.31	0.60
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.36	0.60
6:H:44:VAL:O	6:H:44:VAL:CG1	2.49	0.60
1:A:55:ASP:H	1:A:56:PRO:CD	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1012:ILE:HD13	2:B:1092:TYR:OH	2.02	0.60
2:B:801:LYS:O	8:J:52:THR:CG2	2.50	0.60
1:A:883:LEU:HD11	1:A:1017:LEU:HD21	1.84	0.60
1:A:567:LYS:O	1:A:569:LYS:N	2.34	0.60
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.60	0.60
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.36	0.60
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.32	0.60
10:L:41:SER:O	10:L:44:ASP:HB2	2.02	0.60
1:A:1437:GLY:HA3	5:F:88:TYR:CD2	2.36	0.60
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.67	0.60
9:K:20:LYS:HD3	9:K:22:ASP:OD2	2.02	0.60
2:B:322:PHE:HZ	7:I:30:ARG:HH11	1.48	0.59
4:E:171:LYS:O	4:E:172:GLU:C	2.40	0.59
1:A:754:SER:N	1:A:757:ASN:HD22	1.99	0.59
1:A:949:ASP:N	1:A:949:ASP:OD1	2.26	0.59
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.35	0.59
2:B:957:ASN:HD22	2:B:959:ASP:H	1.49	0.59
1:A:182:VAL:CG1	1:A:183:GLY:H	2.14	0.59
1:A:685:GLU:O	1:A:689:LYS:HB2	2.02	0.59
3:C:73:GLN:NE2	3:C:237:SER:O	2.35	0.59
4:E:2:ASP:O	4:E:3:GLN:HB3	2.02	0.59
1:A:675:THR:HG22	1:A:679:ILE:CD1	2.33	0.59
3:C:41:ILE:HG13	3:C:172:PRO:HG3	1.84	0.59
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.02	0.59
1:A:303:TYR:CG	1:A:303:TYR:O	2.56	0.59
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.84	0.59
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.84	0.59
2:B:315:LYS:N	2:B:316:PRO:HD2	2.18	0.59
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.85	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.03	0.59
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.68	0.59
2:B:1027:ILE:O	2:B:1030:LEU:N	2.36	0.59
2:B:501:PRO:O	2:B:502:ILE:HB	2.03	0.59
2:B:779:GLY:O	2:B:795:ILE:HG23	2.02	0.59
1:A:315:LEU:CD1	1:A:319:GLY:CA	2.72	0.59
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.68	0.59
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.83	0.59
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.85	0.59
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.83	0.59
4:E:86:PRO:CA	4:E:114:ASN:HD22	2.14	0.59
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CD2	1:A:400:PRO:CD	2.71	0.59
2:B:1131:GLY:O	2:B:1134:GLU:N	2.34	0.59
3:C:13:ALA:HA	3:C:17:ASN:O	2.02	0.59
1:A:265:LYS:HD2	1:A:303:TYR:HB2	1.85	0.59
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.84	0.59
2:B:789:MET:CE	2:B:965:LYS:HB3	2.32	0.59
2:B:830:TYR:O	2:B:831:SER:C	2.40	0.59
4:E:77:SER:HB2	4:E:105:PHE:CA	2.33	0.59
6:H:139:ASN:O	6:H:140:ALA:CB	2.51	0.59
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.85	0.58
1:A:1398:MET:C	1:A:1400:CYS:H	2.05	0.58
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.85	0.58
1:A:470:LEU:HD21	1:A:487:MET:CE	2.32	0.58
1:A:567:LYS:CB	6:H:95:TYR:HA	2.33	0.58
1:A:787:PHE:CE1	1:A:796:SER:HB2	2.38	0.58
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.85	0.58
2:B:400:HIS:CE1	2:B:517:THR:HG21	2.38	0.58
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.84	0.58
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.85	0.58
2:B:1103:ILE:HD13	2:B:1103:ILE:H	1.68	0.58
2:B:550:ASP:OD2	2:B:552:MET:HG3	2.03	0.58
8:J:9:SER:OG	8:J:48:ARG:NH2	2.36	0.58
1:A:253:ASN:CA	1:A:256:GLN:C	2.70	0.58
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.85	0.58
3:C:93:ASP:O	3:C:127:ARG:NH2	2.36	0.58
2:B:986:GLN:OE1	2:B:986:GLN:CA	2.49	0.58
2:B:179:CYS:SG	2:B:180:TYR:N	2.76	0.58
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.85	0.58
8:J:7:CYS:HB3	8:J:46:CYS:SG	2.43	0.58
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.86	0.58
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.50	0.58
2:B:383:ASN:O	2:B:387:LEU:HB2	2.03	0.58
2:B:515:HIS:H	2:B:518:HIS:CD2	2.22	0.58
2:B:975:GLN:CG	2:B:976:ILE:H	2.16	0.58
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.69	0.58
6:H:127:GLY:HA3	6:H:130:ARG:NH2	2.19	0.58
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.03	0.58
1:A:399:HIS:CG	1:A:400:PRO:N	2.72	0.58
1:A:869:GLY:O	4:E:204:THR:HG21	2.03	0.58
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.58
2:B:98:THR:O	2:B:126:SER:CB	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.03	0.58
1:A:151:ASP:OD2	1:A:163:SER:HA	2.04	0.58
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.85	0.58
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.16	0.58
2:B:128:LEU:HB2	2:B:167:ILE:O	2.04	0.58
2:B:864:LYS:HZ3	2:B:867:GLY:CA	2.15	0.58
2:B:864:LYS:CE	2:B:870:ILE:O	2.51	0.58
2:B:703:ILE:HA	2:B:740:HIS:O	2.04	0.58
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.69	0.58
1:A:352:VAL:CG2	2:B:1099:VAL:HG13	2.32	0.58
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.85	0.57
2:B:474:SER:C	2:B:476:ARG:N	2.57	0.57
2:B:783:THR:HG22	8:J:63:TYR:CE1	2.34	0.57
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.85	0.57
2:B:733:HIS:O	2:B:735:ALA:N	2.35	0.57
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.68	0.57
4:E:153:HIS:O	4:E:154:ILE:HD13	2.04	0.57
1:A:99:ILE:HA	1:A:102:VAL:HG23	1.87	0.57
1:A:182:VAL:CG1	1:A:183:GLY:N	2.67	0.57
1:A:256:GLN:HB3	1:A:257:ARG:CD	2.33	0.57
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.33	0.57
3:C:43:THR:HG23	3:C:44:LEU:N	2.19	0.57
8:J:7:CYS:SG	8:J:9:SER:N	2.77	0.57
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.57
1:A:807:GLY:O	2:B:728:ARG:HD3	2.04	0.57
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.34	0.57
2:B:596:LEU:O	2:B:600:LEU:HD23	2.05	0.57
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.68	0.57
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.87	0.57
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.86	0.57
1:A:777:PHE:CD2	1:A:781:ASP:C	2.78	0.57
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.69	0.57
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.68	0.57
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.85	0.57
1:A:256:GLN:HA	1:A:257:ARG:HB2	1.74	0.57
1:A:323:LYS:HD3	1:A:323:LYS:H	1.60	0.57
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.86	0.57
2:B:384:ARG:HH22	2:B:621:GLU:HG3	1.69	0.57
1:A:1342:GLU:CG	4:E:212:ARG:NH1	2.62	0.57
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.40	0.57
2:B:638:PHE:O	2:B:740:HIS:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:C	9:K:9:LEU:H	2.08	0.57
1:A:11:LEU:HA	2:B:1193:GLN:O	2.04	0.57
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.58	0.57
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.86	0.57
11:R:9:G:O2'	11:R:10:A:H5'	2.04	0.57
1:A:119:ASN:O	1:A:123:ARG:HG3	2.04	0.57
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.20	0.57
1:A:635:ARG:HE	1:A:877:HIS:HA	1.70	0.57
2:B:636:PRO:CB	2:B:637:LEU:CA	2.83	0.57
2:B:736:THR:O	2:B:736:THR:HG22	2.05	0.57
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.87	0.57
2:B:1096:ARG:CG	2:B:1096:ARG:HH11	2.09	0.56
2:B:34:ILE:HD13	2:B:542:MET:HE1	1.87	0.56
2:B:519:TRP:O	2:B:519:TRP:CD1	2.58	0.56
11:R:9:G:C2'	11:R:10:A:H5'	2.33	0.56
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.19	0.56
1:A:249:SER:O	1:A:250:ILE:HD13	2.04	0.56
1:A:814:PHE:O	1:A:817:ALA:HB3	2.06	0.56
3:C:79:GLN:HE21	3:C:127:ARG:HB3	1.68	0.56
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.66	0.56
1:A:32:VAL:HB	1:A:57:ARG:CB	2.34	0.56
2:B:65:GLU:OE1	2:B:65:GLU:N	2.38	0.56
2:B:778:MET:CE	2:B:853:SER:HB3	2.34	0.56
12:T:27:DA:N3	12:T:27:DA:H2'	2.19	0.56
1:A:172:PRO:HB2	1:A:174:ILE:HG12	1.87	0.56
1:A:408:ASP:O	1:A:409:SER:C	2.44	0.56
1:A:567:LYS:HB3	6:H:96:VAL:N	2.12	0.56
2:B:650:GLU:HG3	2:B:651:LEU:N	2.20	0.56
3:C:39:ALA:O	3:C:164:ALA:HB3	2.05	0.56
3:C:69:LEU:O	8:J:6:ARG:NH1	2.32	0.56
1:A:185:TRP:O	1:A:186:LYS:HB2	2.05	0.56
2:B:541:LEU:HB2	2:B:747:MET:CE	2.35	0.56
1:A:361:LEU:HD21	1:A:521:MET:HE1	1.88	0.56
1:A:55:ASP:N	1:A:56:PRO:HD2	2.15	0.56
2:B:1060:ARG:C	2:B:1062:HIS:H	2.07	0.56
1:A:402:ALA:O	1:A:415:LEU:CD1	2.53	0.56
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.87	0.56
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.05	0.56
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.24	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.38	0.56
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.69	0.56
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.36	0.56
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.35	0.56
6:H:42:ILE:HG23	6:H:95:TYR:CE1	2.40	0.56
1:A:320:ARG:CB	1:A:321:PRO:CA	2.84	0.56
1:A:962:ARG:O	1:A:964:ILE:N	2.39	0.56
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.36	0.56
1:A:596:THR:C	1:A:598:LEU:H	2.08	0.56
1:A:809:THR:HB	1:A:810:PRO:HD2	1.87	0.56
2:B:863:GLU:O	2:B:864:LYS:C	2.43	0.56
12:T:26:DG:C2	12:T:27:DA:H1'	2.39	0.56
1:A:179:LEU:HD11	1:A:298:PHE:HD1	1.70	0.55
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.55
1:A:705:LYS:HE3	1:A:713:SER:HB2	1.87	0.55
2:B:976:ILE:HG23	2:B:977:GLY:N	2.21	0.55
1:A:791:ASP:OD1	1:A:791:ASP:C	2.44	0.55
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.87	0.55
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.72	0.55
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.40	0.55
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.18	0.55
3:C:167:HIS:CD2	3:C:169:LYS:H	2.22	0.55
4:E:171:LYS:H	4:E:174:GLN:HG3	1.70	0.55
4:E:3:GLN:CG	4:E:5:ASN:H	2.18	0.55
1:A:213:HIS:O	1:A:214:ILE:C	2.40	0.55
2:B:175:ARG:CG	2:B:175:ARG:HH11	2.20	0.55
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.88	0.55
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.87	0.55
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.89	0.55
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.36	0.55
1:A:929:LEU:HD21	1:A:983:ILE:CG2	2.36	0.55
2:B:1017:ILE:H	2:B:1018:PRO:HD3	1.71	0.55
2:B:983:ARG:C	2:B:984:HIS:CG	2.80	0.55
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.20	0.55
1:A:130:ASP:C	1:A:132:LYS:H	2.09	0.55
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.60	0.55
1:A:249:SER:O	1:A:250:ILE:CD1	2.54	0.55
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.22	0.55
1:A:661:GLY:N	2:B:1081:LEU:HD22	2.21	0.55
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.36	0.55
3:C:99:LEU:HD23	3:C:99:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HB2	1:A:321:PRO:CA	2.36	0.55
1:A:352:VAL:HG12	1:A:353:ILE:N	2.22	0.55
1:A:376:TYR:CD2	1:A:376:TYR:C	2.80	0.55
1:A:406:ILE:N	1:A:406:ILE:CD1	2.62	0.55
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.73	0.55
2:B:1027:ILE:O	2:B:1028:GLU:C	2.45	0.55
1:A:446:ARG:HG3	1:A:487:MET:HG2	1.89	0.55
2:B:169:ARG:O	2:B:171:PRO:HD3	2.07	0.55
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.88	0.55
7:I:85:PHE:O	7:I:86:PHE:HB3	2.07	0.55
1:A:315:LEU:HD12	1:A:318:SER:O	2.06	0.55
1:A:694:THR:HA	1:A:714:PHE:HE1	1.70	0.55
1:A:33:ALA:HB3	1:A:83:HIS:H	1.72	0.55
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.72	0.55
2:B:95:ILE:CD1	2:B:130:VAL:HG22	2.36	0.55
11:R:5:A:C2	11:R:6:G:C5	2.95	0.55
1:A:472:LEU:HD21	2:B:835:GLN:CB	2.37	0.55
2:B:203:PHE:C	2:B:204:ILE:HD12	2.27	0.55
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.87	0.55
1:A:1111:MET:HG3	1:A:1114:PRO:CG	2.30	0.54
1:A:344:ARG:O	2:B:1155:SER:HB2	2.06	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.54
2:B:426:LYS:HD2	2:B:430:ARG:HH22	1.71	0.54
2:B:780:VAL:O	2:B:817:LEU:HD23	2.07	0.54
3:C:251:LEU:O	3:C:255:VAL:HG23	2.06	0.54
7:I:71:SER:HB3	7:I:85:PHE:CE2	2.43	0.54
1:A:903:ASN:O	1:A:907:THR:OG1	2.26	0.54
2:B:364:ILE:O	2:B:365:THR:HB	2.07	0.54
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.89	0.54
8:J:7:CYS:HA	8:J:49:MET:HG2	1.89	0.54
1:A:320:ARG:HB2	1:A:321:PRO:HB3	1.89	0.54
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.96	0.54
3:C:66:ARG:NH2	8:J:3:VAL:O	2.40	0.54
2:B:101:MET:CE	2:B:169:ARG:HH12	2.19	0.54
2:B:604:ARG:HA	2:B:609:ILE:O	2.07	0.54
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.07	0.54
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.12	0.54
1:A:352:VAL:HG21	2:B:1099:VAL:HG13	1.89	0.54
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.07	0.54
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.21	0.54
4:E:168:TYR:O	4:E:170:LEU:HG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:76:LYS:O	5:F:79:ARG:HD2	2.07	0.54
1:A:568:PRO:HD3	6:H:94:ASP:O	2.06	0.54
7:I:27:PHE:O	7:I:35:VAL:HG13	2.08	0.54
2:B:792:MET:HE1	2:B:857:ARG:NH2	2.22	0.54
4:E:168:TYR:HB3	4:E:170:LEU:HD11	1.90	0.54
4:E:36:GLU:O	4:E:38:PRO:HD3	2.07	0.54
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.88	0.54
9:K:65:HIS:HD2	9:K:67:PHE:N	2.01	0.54
3:C:165:LYS:O	9:K:6:ARG:NH1	2.40	0.54
5:F:109:VAL:HG11	5:F:123:LYS:HG2	1.90	0.54
9:K:49:GLU:C	9:K:51:LEU:H	2.09	0.54
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.90	0.54
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.89	0.54
1:A:383:TYR:HB3	5:F:115:THR:HB	1.89	0.54
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.88	0.54
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.43	0.54
1:A:805:LEU:CD2	2:B:1052:VAL:HG21	2.38	0.54
4:E:127:ILE:HG12	4:E:127:ILE:O	2.08	0.54
4:E:191:LYS:H	4:E:194:GLU:HB2	1.72	0.54
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.89	0.54
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.90	0.54
3:C:143:LEU:C	3:C:143:LEU:HD12	2.28	0.54
1:A:332:LYS:H	1:A:337:ARG:HB3	1.71	0.53
1:A:402:ALA:O	1:A:415:LEU:HD12	2.08	0.53
1:A:893:PHE:C	1:A:893:PHE:CD2	2.81	0.53
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.89	0.53
1:A:709:THR:HG23	7:I:94:ASP:HA	1.90	0.53
1:A:257:ARG:CG	1:A:257:ARG:O	2.51	0.53
1:A:471:ASN:O	1:A:472:LEU:C	2.47	0.53
2:B:329:THR:HA	2:B:332:ASP:CB	2.38	0.53
3:C:242:GLN:O	3:C:246:ARG:HG3	2.08	0.53
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.90	0.53
1:A:1398:MET:C	1:A:1400:CYS:N	2.61	0.53
1:A:351:THR:HG21	1:A:466:SER:O	2.08	0.53
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.08	0.53
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.24	0.53
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.44	0.53
9:K:40:HIS:HE1	9:K:63:VAL:CG2	2.21	0.53
1:A:482:PHE:HD1	2:B:835:GLN:O	1.91	0.53
1:A:504:LEU:HD11	5:F:91:ALA:HB2	1.91	0.53
1:A:526:ASP:OD2	2:B:829:CYS:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:CB	2:B:649:LYS:HG3	2.23	0.53
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.90	0.53
9:K:65:HIS:CD2	9:K:67:PHE:H	2.14	0.53
1:A:599:SER:C	1:A:601:LYS:H	2.12	0.53
1:A:822:GLU:O	1:A:826:ASP:OD2	2.27	0.53
2:B:361:LEU:O	2:B:363:HIS:O	2.26	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HB	1.89	0.53
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.29	0.53
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.72	0.53
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.48	0.53
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.42	0.53
1:A:401:GLY:O	1:A:402:ALA:CB	2.56	0.53
4:E:15:ALA:O	4:E:19:VAL:HG23	2.08	0.53
9:K:46:ILE:O	9:K:50:LEU:HB2	2.08	0.53
1:A:1410:PHE:O	1:A:1413:GLY:N	2.41	0.53
1:A:590:ARG:HH21	1:A:621:THR:HA	1.74	0.53
1:A:528:LEU:HD23	1:A:751:SER:HA	1.91	0.53
2:B:913:GLY:HA2	2:B:938:SER:HB2	1.87	0.53
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.49	0.53
2:B:778:MET:O	2:B:819:ALA:HB1	2.08	0.53
3:C:43:THR:CG2	3:C:44:LEU:N	2.72	0.53
3:C:5:GLY:O	3:C:7:GLN:HG2	2.09	0.53
8:J:7:CYS:CB	8:J:46:CYS:SG	2.97	0.53
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.17	0.53
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.91	0.53
8:J:2:ILE:O	8:J:2:ILE:HG23	2.09	0.53
8:J:7:CYS:CA	8:J:49:MET:HE3	2.38	0.53
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.09	0.52
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.74	0.52
2:B:592:ASN:N	2:B:593:PRO:CD	2.71	0.52
4:E:153:HIS:CD2	4:E:198:ILE:HG12	2.43	0.52
1:A:765:VAL:HG23	1:A:766:GLY:H	1.74	0.52
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.91	0.52
2:B:954:VAL:O	10:L:55:ILE:O	2.27	0.52
1:A:252:PHE:O	1:A:252:PHE:HD1	1.91	0.52
1:A:49:LYS:HD3	1:A:55:ASP:CG	2.28	0.52
1:A:361:LEU:HD21	1:A:521:MET:CE	2.39	0.52
1:A:880:LYS:CG	1:A:880:LYS:O	2.57	0.52
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.74	0.52
2:B:983:ARG:O	2:B:984:HIS:CG	2.62	0.52
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:PRO:O	1:A:313:GLN:HB2	2.10	0.52
1:A:535:THR:HG22	1:A:616:VAL:HA	1.91	0.52
1:A:858:ASN:HD22	1:A:858:ASN:C	2.12	0.52
1:A:894:GLU:C	1:A:896:ARG:H	2.13	0.52
4:E:6:GLU:O	4:E:9:ILE:HG22	2.09	0.52
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.39	0.52
1:A:403:LYS:HA	1:A:415:LEU:HB2	1.91	0.52
1:A:639:PRO:HG2	1:A:640:GLN:HG2	1.92	0.52
1:A:885:THR:O	1:A:940:ARG:HG3	2.09	0.52
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.92	0.52
2:B:737:THR:HG21	7:I:66:PRO:HA	1.91	0.52
3:C:58:LEU:HD21	8:J:57:ILE:CD1	2.40	0.52
5:F:111:LEU:H	5:F:111:LEU:CD1	2.22	0.52
6:H:58:THR:HG22	6:H:59:ILE:H	1.74	0.52
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.91	0.52
2:B:864:LYS:HD3	2:B:870:ILE:O	2.10	0.52
1:A:127:ALA:O	1:A:128:ILE:C	2.48	0.52
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.25	0.52
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.52
4:E:30:ILE:HG22	4:E:31:THR:O	2.09	0.52
4:E:2:ASP:O	4:E:3:GLN:CB	2.57	0.52
7:I:99:LEU:O	7:I:111:THR:HG23	2.09	0.52
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.90	0.52
1:A:161:LEU:O	1:A:162:VAL:O	2.27	0.52
1:A:265:LYS:NZ	1:A:323:LYS:HE2	2.25	0.52
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.92	0.52
1:A:648:ASN:OD1	1:A:648:ASN:N	2.43	0.52
2:B:176:SER:O	2:B:182:SER:HB2	2.10	0.52
3:C:16:ASP:O	3:C:233:GLU:HA	2.10	0.52
1:A:1021:LEU:O	1:A:1024:SER:N	2.43	0.52
1:A:417:TYR:O	1:A:418:SER:HB3	2.10	0.52
2:B:363:HIS:O	2:B:364:ILE:CB	2.47	0.52
2:B:516:ASN:H	2:B:516:ASN:HD22	1.56	0.52
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.10	0.52
1:A:1341:ILE:HB	4:E:182:ASP:OD2	2.09	0.52
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.74	0.51
2:B:912:ILE:O	2:B:938:SER:HB2	2.10	0.51
1:A:134:ARG:HD2	1:A:221:SER:O	2.11	0.51
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.92	0.51
2:B:204:ILE:N	2:B:204:ILE:HD12	2.25	0.51
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:CG2	2:B:935:ARG:HA	2.22	0.51
8:J:1:MET:N	8:J:56:LEU:N	2.58	0.51
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.91	0.51
1:A:863:VAL:O	1:A:864:ILE:HD13	2.10	0.51
6:H:84:ALA:C	6:H:86:ASP:N	2.64	0.51
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.91	0.51
1:A:251:SER:OG	1:A:252:PHE:N	2.42	0.51
1:A:265:LYS:HZ1	1:A:323:LYS:HE2	1.75	0.51
1:A:471:ASN:O	1:A:473:SER:N	2.44	0.51
1:A:39:GLU:O	1:A:53:LEU:HB2	2.09	0.51
1:A:803:SER:OG	1:A:806:ARG:HD2	2.10	0.51
2:B:323:VAL:O	2:B:324:ILE:HG13	2.10	0.51
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.91	0.51
2:B:475:SER:C	2:B:477:ALA:H	2.14	0.51
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.75	0.51
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.25	0.51
1:A:1437:GLY:CA	5:F:88:TYR:CD2	2.93	0.51
1:A:256:GLN:HB3	1:A:257:ARG:HD3	1.90	0.51
1:A:514:PRO:O	1:A:515:GLN:C	2.49	0.51
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.93	0.51
1:A:705:LYS:HG3	1:A:713:SER:HB3	1.92	0.51
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.76	0.51
2:B:64:CYS:HA	2:B:67:SER:HB3	1.92	0.51
3:C:226:ASP:O	3:C:227:THR:O	2.29	0.51
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.92	0.51
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.10	0.51
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.08	0.51
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.92	0.51
1:A:401:GLY:CA	1:A:435:HIS:CD2	2.94	0.51
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.40	0.51
1:A:802:ASN:HD21	2:B:729:ILE:N	2.05	0.51
2:B:978:ASP:OD1	2:B:1099:VAL:HG23	2.11	0.51
7:I:106:CYS:O	7:I:107:SER:C	2.49	0.51
1:A:321:PRO:O	1:A:322:VAL:HG22	2.10	0.51
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.51
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.26	0.51
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.46	0.51
6:H:115:TYR:CE2	6:H:124:ARG:HG3	2.45	0.51
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.93	0.51
1:A:92:HIS:ND1	1:A:236:LEU:HD21	2.25	0.51
1:A:319:GLY:HA2	1:A:320:ARG:HH11	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.31	0.51
2:B:778:MET:CE	2:B:1094:ARG:HH11	2.24	0.51
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.44	0.51
1:A:526:ASP:OD2	2:B:829:CYS:HB2	2.10	0.51
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.17	0.51
1:A:475:THR:CG2	1:A:476:SER:N	2.74	0.51
2:B:696:GLU:O	2:B:699:GLU:HB2	2.11	0.51
3:C:3:GLU:HA	9:K:104:ASN:ND2	2.25	0.51
3:C:42:PRO:HA	3:C:163:ILE:HG23	1.92	0.51
1:A:1021:LEU:O	1:A:1022:LEU:C	2.48	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.75	0.51
1:A:1434:ALA:O	1:A:1436:ILE:N	2.44	0.51
1:A:249:SER:O	1:A:250:ILE:CB	2.59	0.51
1:A:794:PRO:O	1:A:797:LYS:N	2.41	0.51
1:A:857:ARG:HB3	1:A:862:ASN:O	2.11	0.51
2:B:814:PHE:C	2:B:816:GLU:H	2.14	0.51
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.93	0.50
2:B:1065:GLN:HE21	2:B:1069:PHE:H	1.59	0.50
1:A:705:LYS:HE3	1:A:713:SER:CB	2.41	0.50
6:H:41:ASP:HB3	6:H:121:LEU:HD22	1.93	0.50
3:C:66:ARG:NH2	8:J:4:PRO:HA	2.26	0.50
9:K:51:LEU:CD1	9:K:59:ALA:HB3	2.41	0.50
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.44	0.50
1:A:49:LYS:NZ	1:A:60:SER:HA	2.26	0.50
1:A:965:GLN:HA	1:A:968:GLN:HG2	1.93	0.50
2:B:902:GLY:O	10:L:65:VAL:HG11	2.11	0.50
1:A:794:PRO:HA	1:A:797:LYS:HB2	1.93	0.50
2:B:313:MET:HG3	2:B:390:LEU:HD21	1.94	0.50
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.41	0.50
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.44	0.50
10:L:34:CYS:O	10:L:35:SER:HB2	2.10	0.50
1:A:351:THR:CG2	1:A:352:VAL:H	2.18	0.50
1:A:76:GLU:CD	2:B:1159:ARG:HH12	2.15	0.50
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.50
1:A:658:LEU:HD22	2:B:831:SER:HA	1.92	0.50
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.92	0.50
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.41	0.50
4:E:113:GLN:HB3	4:E:137:GLU:OE1	2.11	0.50
9:K:32:VAL:HB	9:K:74:ARG:HG3	1.93	0.50
1:A:1061:GLY:O	1:A:1062:GLU:C	2.50	0.50
1:A:1116:LEU:CD2	1:A:1329:THR:CG2	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PRO:O	1:A:286:HIS:HB2	2.10	0.50
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.47	0.50
1:A:99:ILE:HG12	1:A:234:MET:SD	2.51	0.50
2:B:62:ILE:HD12	2:B:418:LYS:HE2	1.94	0.50
1:A:1166:ASP:CG	1:A:1194:ARG:HH21	2.15	0.50
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.11	0.50
2:B:176:SER:O	2:B:182:SER:CB	2.60	0.50
2:B:647:GLY:O	2:B:648:HIS:O	2.30	0.50
4:E:3:GLN:HG2	4:E:5:ASN:H	1.76	0.50
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.12	0.50
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.12	0.50
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.94	0.50
1:A:880:LYS:O	1:A:880:LYS:HG2	2.12	0.50
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.93	0.50
4:E:165:LEU:HD13	4:E:170:LEU:O	2.11	0.50
9:K:6:ARG:O	9:K:8:GLU:N	2.45	0.50
1:A:100:LYS:O	1:A:104:GLU:HG3	2.12	0.50
1:A:184:SER:HA	1:A:199:LEU:HD13	1.93	0.50
1:A:590:ARG:HG2	1:A:591:PHE:H	1.77	0.50
1:A:765:VAL:HG21	1:A:800:VAL:CG1	2.41	0.50
2:B:648:HIS:O	2:B:649:LYS:O	2.30	0.50
2:B:864:LYS:CG	2:B:865:LYS:N	2.36	0.50
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.50
11:R:3:C:H2'	11:R:4:G:C8	2.46	0.50
1:A:909:ASP:OD1	1:A:911:SER:HB3	2.11	0.49
2:B:840:ILE:HB	2:B:1011:ILE:HD12	1.93	0.49
2:B:1168:LEU:HD21	2:B:1214:PRO:HD2	1.93	0.49
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.12	0.49
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.42	0.49
2:B:863:GLU:O	2:B:864:LYS:O	2.30	0.49
6:H:109:LYS:HB3	6:H:110:ASP:C	2.31	0.49
1:A:273:ASN:C	1:A:275:SER:H	2.15	0.49
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.43	0.49
1:A:672:ASP:N	1:A:736:ASN:HD21	2.11	0.49
1:A:666:ILE:HG23	2:B:1026:LEU:HD12	1.94	0.49
2:B:982:SER:O	2:B:1093:GLN:HG3	2.12	0.49
6:H:59:ILE:O	6:H:60:ALA:HB3	2.12	0.49
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.92	0.49
1:A:902:LEU:CG	1:A:926:GLN:HG3	2.42	0.49
2:B:1060:ARG:C	2:B:1062:HIS:N	2.65	0.49
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.94	0.49
5:F:83:PRO:HG2	5:F:84:TYR:HD1	1.77	0.49
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.93	0.49
1:A:100:LYS:HD3	1:A:104:GLU:OE1	2.12	0.49
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.61	0.49
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.13	0.49
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.13	0.49
1:A:290:GLU:HA	1:A:293:GLU:HG3	1.93	0.49
1:A:314:ALA:HA	1:A:320:ARG:HA	1.95	0.49
1:A:500:GLU:HG2	2:B:1143:ALA:HB1	1.94	0.49
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.27	0.49
1:A:605:MET:HE3	1:A:606:LEU:H	1.77	0.49
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.25	0.49
2:B:515:HIS:H	2:B:518:HIS:HD2	1.58	0.49
2:B:807:ARG:CG	2:B:807:ARG:HH11	2.17	0.49
5:F:114:GLU:OE2	5:F:119:ARG:HG2	2.12	0.49
1:A:711:ARG:HH12	7:I:95:THR:HB	1.77	0.49
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.95	0.49
1:A:962:ARG:O	1:A:963:ILE:C	2.51	0.49
2:B:745:PRO:O	2:B:747:MET:N	2.46	0.49
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.48	0.49
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.77	0.49
5:F:116:ASP:HB3	5:F:119:ARG:HB2	1.93	0.49
7:I:35:VAL:CG1	7:I:36:GLU:N	2.76	0.49
1:A:1111:MET:SD	1:A:1114:PRO:HB3	2.50	0.49
1:A:406:ILE:HD13	1:A:431:LYS:CB	2.42	0.49
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.95	0.49
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.94	0.49
1:A:991:LYS:O	1:A:994:GLN:HB3	2.11	0.49
2:B:211:VAL:HG12	2:B:212:LEU:N	2.27	0.49
2:B:581:PHE:HB2	2:B:625:LYS:HG2	1.95	0.49
6:H:80:ARG:O	6:H:81:PRO:O	2.30	0.49
12:T:16:DC:C6	12:T:17:DG:C8	3.01	0.49
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.95	0.49
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.15	0.49
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.78	0.49
1:A:316:GLN:O	1:A:316:GLN:HG2	2.11	0.49
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.95	0.49
1:A:579:SER:HB3	1:A:611:GLN:HA	1.94	0.49
1:A:672:ASP:N	1:A:736:ASN:ND2	2.60	0.49
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1149:GLU:HG3	2:B:1153:GLU:CG	2.30	0.49
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.48	0.49
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.49
2:B:566:LEU:HD22	2:B:586:TRP:O	2.13	0.49
8:J:7:CYS:CB	8:J:49:MET:HE3	2.43	0.49
1:A:252:PHE:CD1	1:A:252:PHE:C	2.85	0.49
1:A:544:ASP:N	1:A:544:ASP:OD1	2.46	0.49
2:B:592:ASN:H	2:B:593:PRO:HD3	1.78	0.49
8:J:45:CYS:O	8:J:48:ARG:HG3	2.13	0.49
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.12	0.49
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.13	0.49
1:A:451:HIS:HB3	1:A:453:MET:N	2.28	0.49
1:A:483:ASP:OD1	11:R:11:U:P	2.71	0.49
1:A:822:GLU:O	1:A:826:ASP:CG	2.51	0.49
2:B:174:LEU:O	2:B:175:ARG:CB	2.60	0.49
1:A:472:LEU:CD2	2:B:835:GLN:HB3	2.41	0.49
4:E:78:LEU:HD12	4:E:107:THR:HB	1.95	0.49
1:A:249:SER:O	1:A:250:ILE:CG2	2.60	0.48
1:A:791:ASP:OD1	1:A:793:SER:OG	2.30	0.48
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.35	0.48
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.95	0.48
7:I:19:ASP:HB3	7:I:24:ARG:H	1.78	0.48
8:J:15:GLY:C	8:J:17:LYS:H	2.16	0.48
1:A:206:GLU:O	1:A:210:ILE:HG12	2.13	0.48
1:A:32:VAL:HB	1:A:57:ARG:HB3	1.95	0.48
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.32	0.48
1:A:755:PHE:O	1:A:758:ILE:N	2.46	0.48
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.48	0.48
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.43	0.48
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.95	0.48
5:F:80:ALA:O	5:F:81:THR:C	2.51	0.48
1:A:367:PRO:HG3	1:A:466:SER:C	2.34	0.48
2:B:483:LEU:O	2:B:484:ASN:HB2	2.13	0.48
2:B:864:LYS:NZ	2:B:867:GLY:CA	2.75	0.48
1:A:396:PRO:O	1:A:397:ASN:C	2.52	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.48	0.48
1:A:410:GLY:O	1:A:411:ASP:O	2.30	0.48
2:B:124:TYR:HH	2:B:179:CYS:HG	1.60	0.48
2:B:209:GLU:OE2	2:B:485:ARG:HD2	2.14	0.48
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.13	0.48
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HD23	1:A:316:GLN:CB	2.43	0.48
2:B:639:ILE:HG22	2:B:640:VAL:N	2.27	0.48
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.96	0.48
10:L:48:CYS:SG	10:L:49:LYS:N	2.85	0.48
1:A:18:GLN:HE21	1:A:1418:LEU:HD13	1.78	0.48
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.12	0.48
1:A:446:ARG:HE	1:A:480:ALA:CB	2.24	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.96	0.48
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.96	0.48
4:E:205:SER:O	4:E:207:ARG:N	2.47	0.48
4:E:35:VAL:C	4:E:37:LEU:H	2.17	0.48
1:A:464:PRO:HG2	9:K:67:PHE:CE1	2.49	0.48
1:A:815:PHE:O	1:A:818:MET:N	2.46	0.48
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.48	0.48
3:C:31:ASN:O	3:C:33:LEU:N	2.47	0.48
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.48
1:A:53:LEU:O	1:A:56:PRO:HD2	2.13	0.48
1:A:787:PHE:CE2	1:A:796:SER:HB2	2.48	0.48
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.96	0.48
2:B:235:SER:OG	2:B:236:HIS:CD2	2.66	0.48
2:B:329:THR:HA	2:B:332:ASP:HB2	1.96	0.48
2:B:476:ARG:O	2:B:478:GLY:N	2.47	0.48
3:C:249:ASP:O	3:C:253:LYS:HG3	2.12	0.48
4:E:108:GLY:HA3	4:E:132:ILE:HG12	1.96	0.48
4:E:12:LEU:HG	4:E:12:LEU:O	2.13	0.48
6:H:38:LEU:HD12	6:H:124:ARG:O	2.14	0.48
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.78	0.48
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.48	0.48
1:A:545:GLN:O	1:A:546:VAL:C	2.52	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.96	0.48
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.95	0.48
1:A:1215:ARG:O	1:A:1218:GLN:HB2	2.14	0.48
1:A:254:GLU:HA	1:A:255:SER:HA	1.64	0.48
1:A:320:ARG:HB2	1:A:321:PRO:CB	2.43	0.48
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.96	0.48
1:A:596:THR:C	1:A:598:LEU:N	2.67	0.48
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.29	0.48
1:A:928:LEU:HA	1:A:931:GLU:HB3	1.96	0.48
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.78	0.48
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.48	0.48
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.78	0.47
1:A:608:ILE:CG1	1:A:613:ILE:HG13	2.44	0.47
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.49	0.47
2:B:485:ARG:NH1	2:B:485:ARG:HG2	2.27	0.47
2:B:745:PRO:C	2:B:747:MET:H	2.16	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.64	0.47
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.29	0.47
3:C:148:ARG:O	3:C:151:GLN:HG3	2.14	0.47
3:C:167:HIS:HD2	3:C:169:LYS:N	2.09	0.47
4:E:112:TYR:O	4:E:137:GLU:HG3	2.14	0.47
6:H:80:ARG:HB3	6:H:81:PRO:HD2	1.95	0.47
7:I:106:CYS:O	7:I:108:HIS:N	2.47	0.47
8:J:3:VAL:CG2	8:J:18:TRP:CG	2.97	0.47
11:R:3:C:H2'	11:R:4:G:H8	1.78	0.47
1:A:445:ASN:HD21	1:A:447:GLN:HE21	1.62	0.47
1:A:518:LYS:CB	1:A:519:PRO:HD2	2.44	0.47
1:A:755:PHE:O	1:A:757:ASN:N	2.48	0.47
1:A:76:GLU:OE2	2:B:1159:ARG:NH1	2.44	0.47
2:B:361:LEU:CD2	2:B:377:PHE:HD2	2.27	0.47
2:B:416:LEU:CD2	2:B:457:LEU:HD23	2.43	0.47
2:B:633:VAL:O	2:B:694:ASP:HB2	2.14	0.47
2:B:773:MET:C	2:B:775:LYS:N	2.66	0.47
3:C:18:VAL:O	3:C:231:ASN:HA	2.15	0.47
3:C:196:ASP:O	3:C:200:GLU:HB2	2.14	0.47
6:H:104:PHE:N	6:H:104:PHE:CD1	2.82	0.47
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.96	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.45	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
2:B:424:LEU:O	2:B:428:ILE:HG12	2.13	0.47
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.78	0.47
2:B:563:MET:HG3	2:B:563:MET:O	2.13	0.47
5:F:125:LEU:C	5:F:127:GLU:H	2.16	0.47
6:H:43:ASN:ND2	6:H:46:LEU:HD12	2.30	0.47
1:A:294:SER:O	1:A:298:PHE:HB2	2.15	0.47
1:A:385:ILE:HD11	1:A:428:TYR:CZ	2.49	0.47
1:A:367:PRO:HB3	1:A:466:SER:HA	1.96	0.47
1:A:556:TRP:CZ2	1:A:560:ILE:HD13	2.49	0.47
2:B:777:ALA:HA	2:B:1095:LEU:HD23	1.97	0.47
2:B:779:GLY:O	2:B:795:ILE:HA	2.15	0.47
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.29	0.47
9:K:49:GLU:C	9:K:51:LEU:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:O	1:A:132:LYS:N	2.48	0.47
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.49	0.47
2:B:365:THR:OG1	2:B:367:LEU:HG	2.14	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.14	0.47
5:F:109:VAL:CG1	5:F:110:ASP:H	2.17	0.47
1:A:1059:HIS:CE1	5:F:87:LYS:H	2.32	0.47
8:J:53:HIS:HE1	8:J:55:ASP:OD1	1.96	0.47
1:A:1111:MET:HG3	1:A:1114:PRO:CD	2.44	0.47
1:A:1104:ILE:HD13	1:A:1332:PHE:CE2	2.50	0.47
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.15	0.47
1:A:535:THR:CG2	1:A:616:VAL:HA	2.44	0.47
2:B:260:GLY:O	2:B:267:ARG:HD3	2.14	0.47
2:B:577:ALA:HB1	2:B:589:VAL:HG13	1.96	0.47
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.28	0.47
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.50	0.47
2:B:805:THR:HG21	2:B:815:ARG:HD3	1.96	0.47
2:B:957:ASN:ND2	2:B:958:GLN:N	2.63	0.47
1:A:276:LEU:CD1	1:A:292:ALA:CB	2.91	0.47
6:H:84:ALA:C	6:H:86:ASP:H	2.18	0.47
1:A:700:ASN:ND2	7:I:116:ASN:HD21	2.13	0.47
7:I:32:CYS:SG	7:I:34:TYR:CB	3.03	0.47
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.30	0.47
1:A:1072:ILE:HG22	1:A:1072:ILE:O	2.14	0.47
1:A:947:PHE:CD2	1:A:954:TRP:NE1	2.82	0.47
1:A:951:GLU:OE2	1:A:951:GLU:HA	2.14	0.47
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.95	0.47
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.12	0.47
9:K:92:ASN:O	9:K:95:ILE:N	2.47	0.47
1:A:133:LYS:HA	1:A:136:ALA:HB3	1.97	0.47
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.96	0.47
1:A:848:ILE:O	1:A:1065:GLY:N	2.37	0.47
2:B:45:SER:OG	2:B:46:GLN:N	2.48	0.47
2:B:552:MET:O	2:B:555:ILE:HB	2.15	0.47
2:B:708:GLU:HG3	2:B:709:ASP:N	2.24	0.47
3:C:185:LYS:CE	3:C:211:ASP:O	2.63	0.47
4:E:168:TYR:CB	4:E:170:LEU:HD11	2.45	0.47
1:A:446:ARG:HH12	1:A:448:PRO:HD2	1.79	0.47
1:A:590:ARG:O	1:A:591:PHE:HD1	1.95	0.47
2:B:1013:ASN:C	2:B:1015:HIS:H	2.19	0.47
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.29	0.47
6:H:76:THR:O	6:H:77:ARG:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1039:GLY:HA2	8:J:51:LEU:HD22	1.96	0.47
9:K:57:LEU:HB2	9:K:76:GLN:HG2	1.97	0.47
1:A:583:PRO:O	1:A:610:GLY:HA2	2.15	0.46
1:A:700:ASN:HD22	7:I:116:ASN:HD21	1.64	0.46
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.51	0.46
1:A:805:LEU:HD21	2:B:1052:VAL:HG21	1.96	0.46
1:A:809:THR:H	1:A:812:GLU:HB2	1.81	0.46
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.04	0.46
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.45	0.46
9:K:102:LYS:O	9:K:106:GLU:HG2	2.15	0.46
1:A:286:HIS:O	1:A:288:ALA:N	2.42	0.46
1:A:320:ARG:N	1:A:320:ARG:HH11	2.13	0.46
1:A:407:ARG:HA	1:A:430:TRP:CD1	2.50	0.46
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.61	0.46
2:B:490:SER:OG	2:B:491:THR:N	2.48	0.46
2:B:519:TRP:C	2:B:519:TRP:CD1	2.88	0.46
2:B:592:ASN:H	2:B:593:PRO:CD	2.27	0.46
2:B:769:TYR:O	2:B:772:ALA:N	2.49	0.46
2:B:814:PHE:C	2:B:816:GLU:N	2.67	0.46
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.81	0.46
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.28	0.46
1:A:55:ASP:O	1:A:56:PRO:C	2.52	0.46
1:A:741:ASN:ND2	1:A:744:LYS:H	1.95	0.46
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.96	0.46
2:B:541:LEU:HB2	2:B:747:MET:HE1	1.97	0.46
2:B:573:GLN:O	2:B:575:PRO:HD3	2.16	0.46
2:B:586:TRP:NE1	2:B:588:GLY:O	2.48	0.46
9:K:40:HIS:HE1	9:K:63:VAL:HG22	1.78	0.46
12:T:27:DA:N3	12:T:28:DT:H5'	2.31	0.46
1:A:1325:THR:HA	4:E:147:HIS:HA	1.97	0.46
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.97	0.46
1:A:549:MET:O	1:A:552:TRP:HB2	2.16	0.46
1:A:591:PHE:HD2	1:A:595:THR:HB	1.80	0.46
1:A:609:ASP:C	1:A:611:GLN:H	2.19	0.46
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.98	0.46
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.53	0.46
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.64	0.46
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.46
2:B:451:LYS:O	2:B:452:THR:C	2.53	0.46
3:C:102:GLN:HA	3:C:153:LEU:O	2.16	0.46
4:E:175:LEU:HB2	4:E:213:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:22:LYS:HD3	6:H:45:GLU:OE1	2.16	0.46
7:I:40:SER:HB2	7:I:41:PRO:CD	2.45	0.46
1:A:252:PHE:CD1	1:A:252:PHE:O	2.69	0.46
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.97	0.46
1:A:360:GLU:O	1:A:363:GLN:HB2	2.16	0.46
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.44	0.46
1:A:68:GLN:C	1:A:70:CYS:H	2.18	0.46
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.81	0.46
1:A:793:SER:O	1:A:794:PRO:C	2.54	0.46
2:B:199:MET:N	2:B:199:MET:SD	2.82	0.46
1:A:997:LEU:O	1:A:1053:PHE:CE2	2.68	0.46
1:A:403:LYS:HB2	1:A:404:TYR:CD1	2.50	0.46
1:A:755:PHE:O	1:A:756:ILE:C	2.54	0.46
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.13	0.46
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.80	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.46
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.98	0.46
12:T:13:DA:H61	13:N:2:DT:H71	1.79	0.46
1:A:239:LEU:CD1	1:A:240:PRO:HD2	2.35	0.46
1:A:573:SER:N	1:A:576:GLN:HG3	2.07	0.46
1:A:857:ARG:HA	1:A:864:ILE:HG12	1.97	0.46
2:B:1023:VAL:O	2:B:1024:ALA:C	2.54	0.46
2:B:555:ILE:CD1	2:B:587:HIS:CE1	2.99	0.46
2:B:600:LEU:HD12	2:B:615:MET:SD	2.56	0.46
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.81	0.46
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.51	0.46
5:F:83:PRO:O	5:F:151:LEU:HD23	2.16	0.46
8:J:32:GLU:CD	8:J:32:GLU:N	2.68	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.79	0.46
1:A:322:VAL:CA	1:A:323:LYS:HD3	2.46	0.46
1:A:442:VAL:CG1	1:A:491:VAL:HG22	2.45	0.46
1:A:67:CYS:O	1:A:70:CYS:SG	2.74	0.46
1:A:839:ARG:O	1:A:843:LYS:HB2	2.16	0.46
2:B:34:ILE:HD13	2:B:542:MET:CE	2.45	0.46
2:B:603:LEU:O	2:B:608:ASP:N	2.48	0.46
2:B:681:TRP:O	2:B:684:LEU:HB2	2.16	0.46
3:C:33:LEU:HG	3:C:37:MET:CE	2.46	0.46
1:A:303:TYR:O	1:A:303:TYR:CD1	2.68	0.46
1:A:596:THR:O	1:A:598:LEU:N	2.48	0.46
1:A:774:ARG:NH2	1:A:794:PRO:HA	2.31	0.46
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.36	0.46
1:A:251:SER:HB2	11:R:1:A:N3	2.31	0.46
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.87	0.46
1:A:332:LYS:O	1:A:334:GLY:N	2.48	0.46
1:A:629:LEU:CD2	1:A:633:VAL:HG21	2.46	0.46
1:A:968:GLN:O	1:A:968:GLN:HG3	2.16	0.46
2:B:370:PHE:CD2	2:B:373:ARG:HG3	2.51	0.46
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.98	0.46
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.98	0.46
3:C:43:THR:HG23	3:C:44:LEU:H	1.80	0.46
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.80	0.46
10:L:26:THR:O	10:L:26:THR:HG22	2.16	0.46
10:L:60:ARG:HG3	10:L:61:THR:N	2.31	0.46
1:A:140:THR:HA	1:A:143:LYS:HE3	1.98	0.45
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.16	0.45
1:A:396:PRO:O	1:A:398:GLU:O	2.34	0.45
1:A:585:GLY:N	1:A:609:ASP:OD1	2.40	0.45
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.98	0.45
1:A:694:THR:HA	1:A:714:PHE:CE1	2.50	0.45
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.31	0.45
1:A:412:ARG:HH22	2:B:1108:ARG:NH2	2.13	0.45
2:B:175:ARG:CG	2:B:175:ARG:NH1	2.77	0.45
2:B:288:ALA:O	2:B:331:LEU:HD11	2.16	0.45
8:J:6:ARG:HA	8:J:12:LYS:O	2.15	0.45
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.81	0.45
1:A:315:LEU:CB	1:A:317:LYS:H	2.26	0.45
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.16	0.45
1:A:590:ARG:HG2	1:A:591:PHE:N	2.31	0.45
1:A:922:ASP:OD1	1:A:923:LEU:N	2.46	0.45
2:B:208:SER:OG	2:B:210:LYS:HE2	2.16	0.45
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.45
2:B:955:THR:CG2	2:B:956:THR:N	2.58	0.45
7:I:40:SER:HB2	7:I:41:PRO:HD3	1.97	0.45
8:J:8:PHE:H	8:J:49:MET:HE3	1.80	0.45
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.98	0.45
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.76	0.45
1:A:482:PHE:HB2	2:B:836:GLU:O	2.17	0.45
1:A:838:GLN:O	1:A:839:ARG:C	2.55	0.45
2:B:95:ILE:HG13	2:B:129:PHE:O	2.16	0.45
2:B:190:TYR:CD2	8:J:62:ARG:HB3	2.52	0.45
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.17	0.45
2:B:763:GLN:O	2:B:766:ARG:HB2	2.16	0.45
4:E:67:GLU:O	4:E:70:SER:HB3	2.17	0.45
4:E:169:ARG:HG3	5:F:140:ASP:HB3	1.97	0.45
6:H:26:ILE:N	6:H:40:LEU:O	2.50	0.45
10:L:38:LEU:HD21	10:L:49:LYS:HG2	1.98	0.45
1:A:1392:SER:O	1:A:1394:THR:N	2.48	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.45
2:B:430:ARG:CD	2:B:434:ARG:HH22	2.29	0.45
2:B:515:HIS:CD2	2:B:517:THR:H	2.34	0.45
2:B:589:VAL:CG1	2:B:590:HIS:H	2.30	0.45
2:B:800:GLN:HG2	8:J:52:THR:HG22	1.98	0.45
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.98	0.45
7:I:111:THR:HG22	7:I:112:SER:N	2.32	0.45
7:I:32:CYS:SG	7:I:34:TYR:HB2	2.57	0.45
1:A:320:ARG:H	1:A:320:ARG:HH11	1.64	0.45
1:A:575:LYS:CG	1:A:612:ILE:HD11	2.47	0.45
1:A:661:GLY:CA	2:B:1081:LEU:HD22	2.46	0.45
1:A:699:ALA:O	1:A:701:LEU:N	2.49	0.45
1:A:99:ILE:HG13	1:A:99:ILE:H	1.49	0.45
2:B:48:LEU:O	2:B:49:ASP:C	2.55	0.45
2:B:796:LEU:HB3	2:B:799:PRO:CD	2.22	0.45
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.97	0.45
10:L:61:THR:HG21	10:L:63:ARG:HG3	1.98	0.45
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.45
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.98	0.45
1:A:391:LEU:O	1:A:394:ASN:N	2.49	0.45
1:A:550:LEU:HD13	1:A:550:LEU:HA	1.79	0.45
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.98	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
2:B:1148:LYS:O	2:B:1152:MET:CB	2.62	0.45
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.43	0.45
2:B:575:PRO:C	2:B:577:ALA:H	2.19	0.45
2:B:779:GLY:C	2:B:795:ILE:HG23	2.37	0.45
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.98	0.45
7:I:62:ILE:C	7:I:64:SER:H	2.19	0.45
1:A:545:GLN:HB3	1:A:549:MET:HE3	1.98	0.45
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.28	0.45
1:A:412:ARG:NH2	2:B:1108:ARG:NH2	2.65	0.45
2:B:1149:GLU:CG	2:B:1153:GLU:HG2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:GLU:C	2:B:321:GLY:H	2.19	0.45
2:B:361:LEU:N	2:B:362:PRO:HD3	2.32	0.45
2:B:737:THR:O	2:B:738:PHE:C	2.56	0.45
2:B:983:ARG:O	2:B:984:HIS:CD2	2.70	0.45
1:A:1117:THR:N	1:A:1328:TYR:O	2.50	0.45
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.99	0.45
3:C:99:LEU:CD2	3:C:99:LEU:N	2.79	0.45
12:T:13:DA:H61	13:N:2:DT:H73	1.77	0.45
12:T:9:DA:C5	12:T:10:DA:C6	3.05	0.45
12:T:26:DG:C2	12:T:27:DA:C8	3.05	0.45
1:A:219:PHE:CE1	1:A:230:ARG:HG2	2.52	0.45
1:A:239:LEU:HD12	1:A:240:PRO:N	2.31	0.45
1:A:324:SER:O	1:A:327:ALA:N	2.49	0.45
1:A:557:ASP:HA	9:K:26:LYS:CE	2.45	0.45
1:A:68:GLN:O	1:A:70:CYS:N	2.50	0.45
1:A:746:MET:HG2	1:A:751:SER:OG	2.17	0.45
2:B:321:GLY:C	2:B:323:VAL:H	2.21	0.45
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.34	0.45
2:B:647:GLY:O	2:B:648:HIS:C	2.55	0.45
1:A:1342:GLU:CG	4:E:212:ARG:HH11	2.25	0.45
10:L:25:ALA:N	10:L:27:LEU:HD22	2.32	0.45
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.17	0.45
1:A:587:HIS:HA	1:A:607:ILE:O	2.17	0.45
1:A:768:GLN:CG	1:A:816:HIS:HA	2.47	0.45
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.82	0.45
2:B:1027:ILE:C	2:B:1029:CYS:N	2.69	0.45
2:B:202:TYR:H	2:B:202:TYR:HD2	1.63	0.45
2:B:773:MET:C	2:B:775:LYS:H	2.20	0.45
3:C:56:THR:CG2	3:C:145:CYS:SG	2.95	0.45
5:F:111:LEU:N	5:F:111:LEU:CD1	2.79	0.45
2:B:845:SER:HB2	8:J:8:PHE:HB3	1.99	0.45
1:A:382:PRO:N	1:A:428:TYR:HE2	2.14	0.44
1:A:629:LEU:HD23	1:A:633:VAL:HG21	1.99	0.44
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.34	0.44
2:B:870:ILE:O	2:B:870:ILE:HG22	2.16	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.44
4:E:108:GLY:O	4:E:132:ILE:HG23	2.17	0.44
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.98	0.44
12:T:18:DA:H2'	12:T:19:DT:C6	2.52	0.44
12:T:9:DA:C6	12:T:10:DA:N1	2.85	0.44
1:A:81:PHE:HE2	1:A:240:PRO:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:HD12	1:A:556:TRP:CD1	2.52	0.44
1:A:881:GLN:CD	1:A:959:ASN:HA	2.37	0.44
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.32	0.44
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.33	0.44
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.52	0.44
11:R:3:C:N4	12:T:26:DG:H1	2.08	0.44
1:A:1067:LEU:HD12	1:A:1071:SER:OG	2.18	0.44
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.15	0.44
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.99	0.44
1:A:445:ASN:CB	1:A:455:MET:HG2	2.46	0.44
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.83	0.44
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.99	0.44
2:B:329:THR:HA	2:B:332:ASP:HB3	1.98	0.44
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.44
2:B:859:TYR:CD1	2:B:859:TYR:N	2.86	0.44
3:C:251:LEU:HG	9:K:98:LEU:HD11	1.99	0.44
5:F:81:THR:O	5:F:82:THR:C	2.55	0.44
6:H:57:VAL:HG22	6:H:144:ILE:HG12	1.99	0.44
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.52	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.98	0.44
1:A:423:ASP:C	1:A:424:ILE:HG13	2.37	0.44
1:A:599:SER:OG	1:A:614:PHE:CD1	2.66	0.44
1:A:774:ARG:NH1	1:A:797:LYS:HD2	2.32	0.44
1:A:1030:ARG:O	1:A:1031:VAL:C	2.55	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.98	0.44
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.62	0.44
1:A:947:PHE:HD2	1:A:954:TRP:CE2	2.36	0.44
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.99	0.44
2:B:552:MET:N	2:B:553:PRO:HD2	2.33	0.44
3:C:29:MET:O	3:C:30:ALA:C	2.55	0.44
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.47	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.00	0.44
1:A:343:LYS:NZ	2:B:1156:ASP:OD2	2.50	0.44
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.45	0.44
2:B:44:VAL:O	2:B:45:SER:C	2.55	0.44
4:E:184:VAL:O	4:E:187:TYR:N	2.50	0.44
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.53	0.44
8:J:36:LEU:HD11	8:J:51:LEU:HB2	2.00	0.44
8:J:36:LEU:HD23	8:J:36:LEU:HA	1.85	0.44
11:R:6:G:H2'	11:R:7:A:H8	1.83	0.44
1:A:1340:GLY:O	1:A:1342:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HD11	2:B:285:ILE:HD12	2.00	0.44
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.98	0.44
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.99	0.44
5:F:116:ASP:HB3	5:F:119:ARG:CB	2.47	0.44
9:K:83:PRO:O	9:K:86:ALA:HB3	2.18	0.44
1:A:315:LEU:N	1:A:315:LEU:HD22	2.33	0.44
1:A:32:VAL:HB	1:A:57:ARG:HB2	2.00	0.44
1:A:336:ILE:HA	1:A:340:LEU:HD12	2.00	0.44
1:A:341:MET:HE1	1:A:843:LYS:HZ1	1.82	0.44
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.92	0.44
4:E:176:PRO:O	4:E:212:ARG:HA	2.18	0.44
1:A:466:SER:HB3	9:K:2:ASN:ND2	2.33	0.44
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.33	0.44
1:A:219:PHE:CZ	1:A:230:ARG:HG2	2.53	0.44
1:A:353:ILE:HD11	1:A:481:ASP:O	2.18	0.44
1:A:474:VAL:HG22	1:A:478:TYR:CE1	2.53	0.44
1:A:53:LEU:HB3	1:A:54:ASN:H	1.52	0.44
1:A:809:THR:O	1:A:812:GLU:HB2	2.18	0.44
2:B:791:THR:O	2:B:792:MET:CB	2.66	0.44
2:B:881:ASN:CB	2:B:933:SER:N	2.80	0.44
2:B:843:GLN:N	2:B:994:TYR:O	2.43	0.44
2:B:999:MET:HG2	2:B:1008:PRO:HD2	2.00	0.44
1:A:265:LYS:HD2	1:A:303:TYR:CB	2.48	0.43
1:A:352:VAL:CG1	1:A:353:ILE:N	2.81	0.43
1:A:463:ILE:HB	1:A:464:PRO:CD	2.47	0.43
2:B:1051:THR:HB	2:B:1054:GLY:H	1.82	0.43
2:B:806:THR:H	2:B:809:MET:HG3	1.83	0.43
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.18	0.43
2:B:956:THR:CA	2:B:961:LEU:O	2.63	0.43
4:E:199:ILE:O	4:E:199:ILE:CG2	2.65	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.17	0.43
1:A:962:ARG:C	1:A:964:ILE:N	2.69	0.43
2:B:1103:ILE:H	2:B:1103:ILE:CD1	2.29	0.43
2:B:542:MET:SD	2:B:636:PRO:HG3	2.58	0.43
2:B:766:ARG:HA	2:B:769:TYR:CD1	2.52	0.43
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.53	0.43
8:J:56:LEU:O	8:J:57:ILE:C	2.54	0.43
12:T:25:DC:H2'	12:T:26:DG:H8	1.83	0.43
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.83	0.43
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.18	0.43
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:CA	1:A:257:ARG:CB	2.38	0.43
1:A:315:LEU:N	1:A:315:LEU:CD1	2.63	0.43
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.01	0.43
1:A:815:PHE:O	1:A:816:HIS:C	2.56	0.43
2:B:1033:LYS:O	2:B:1036:ALA:HB3	2.18	0.43
2:B:1118:PRO:HD3	2:B:1155:SER:HA	2.00	0.43
7:I:96:SER:HB2	7:I:98:VAL:HG23	2.00	0.43
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.84	0.43
1:A:1261:LYS:C	1:A:1263:ILE:N	2.72	0.43
1:A:1379:GLY:O	4:E:179:GLN:HG2	2.18	0.43
1:A:250:ILE:O	1:A:251:SER:CB	2.64	0.43
1:A:402:ALA:O	1:A:415:LEU:HD13	2.19	0.43
1:A:389:THR:OG1	1:A:426:LEU:HD12	2.19	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HG12	2.00	0.43
1:A:709:THR:HB	1:A:712:GLU:HG3	2.00	0.43
1:A:809:THR:CB	1:A:810:PRO:HD2	2.47	0.43
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.43
2:B:333:PHE:O	2:B:333:PHE:CG	2.72	0.43
5:F:125:LEU:O	5:F:127:GLU:N	2.51	0.43
5:F:76:LYS:O	5:F:79:ARG:CD	2.67	0.43
7:I:75:CYS:HB3	7:I:110:PHE:HE2	1.82	0.43
8:J:7:CYS:HA	8:J:49:MET:HE3	2.00	0.43
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.31	0.43
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.82	0.43
1:A:152:VAL:O	1:A:162:VAL:CG2	2.65	0.43
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.33	0.43
1:A:729:ALA:HA	1:A:732:LEU:HB2	2.01	0.43
2:B:701:ILE:HG12	2:B:702:LEU:N	2.34	0.43
6:H:58:THR:CG2	6:H:59:ILE:N	2.79	0.43
8:J:15:GLY:O	8:J:17:LYS:N	2.50	0.43
1:A:315:LEU:HB3	1:A:317:LYS:N	2.22	0.43
1:A:598:LEU:O	1:A:599:SER:C	2.57	0.43
1:A:924:LYS:HB2	1:A:924:LYS:NZ	2.33	0.43
2:B:1056:SER:CB	2:B:1066:SER:O	2.67	0.43
2:B:637:LEU:HD22	2:B:741:CYS:O	2.17	0.43
2:B:697:GLU:O	2:B:698:GLU:C	2.56	0.43
2:B:755:ILE:HA	2:B:755:ILE:HD13	1.86	0.43
2:B:763:GLN:HG2	2:B:764:SER:N	2.33	0.43
3:C:41:ILE:HD11	3:C:243:VAL:HG13	2.01	0.43
4:E:136:ASN:OD1	4:E:137:GLU:N	2.50	0.43
4:E:3:GLN:HG3	4:E:5:ASN:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:32:CYS:SG	7:I:33:SER:N	2.91	0.43
12:T:26:DG:N2	12:T:27:DA:H1'	2.34	0.43
1:A:130:ASP:C	1:A:132:LYS:N	2.71	0.43
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.84	0.43
1:A:508:PRO:O	1:A:511:ILE:HG13	2.18	0.43
1:A:686:ALA:O	1:A:690:VAL:HG23	2.18	0.43
1:A:796:SER:O	1:A:796:SER:OG	2.31	0.43
1:A:943:LEU:C	1:A:945:GLU:N	2.72	0.43
2:B:1056:SER:HB3	2:B:1066:SER:O	2.18	0.43
2:B:108:VAL:CG1	2:B:109:THR:N	2.81	0.43
2:B:981:ALA:CB	2:B:1095:LEU:HD11	2.49	0.43
4:E:26:ARG:HD3	4:E:188:LEU:HA	2.01	0.43
6:H:102:TYR:HE2	6:H:116:TYR:C	2.22	0.43
7:I:99:LEU:HB2	7:I:101:PHE:CE1	2.53	0.43
7:I:50:THR:HG22	7:I:52:ILE:HG22	2.00	0.43
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.55	0.43
1:A:172:PRO:HB3	1:A:183:GLY:HA3	2.01	0.43
1:A:590:ARG:HB3	1:A:605:MET:N	2.34	0.43
1:A:787:PHE:CD1	1:A:796:SER:HB2	2.53	0.43
2:B:126:SER:O	2:B:169:ARG:HA	2.19	0.43
2:B:394:ASP:OD2	7:I:91:ARG:HB3	2.18	0.43
2:B:481:GLN:HB2	2:B:494:HIS:HE1	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.33	0.43
6:H:9:ILE:HG12	6:H:56:THR:HG23	2.01	0.43
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.54	0.43
10:L:68:GLU:HG3	10:L:68:GLU:H	1.57	0.43
11:R:5:A:N3	11:R:6:G:C8	2.87	0.43
1:A:1072:ILE:HD11	1:A:1368:MET:CA	2.47	0.43
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.34	0.43
2:B:104:GLU:HG2	2:B:104:GLU:H	1.66	0.43
2:B:1084:GLN:N	2:B:1084:GLN:CD	2.72	0.43
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.19	0.43
2:B:40:GLU:OE2	2:B:681:TRP:HB3	2.19	0.43
2:B:95:ILE:HA	2:B:129:PHE:O	2.19	0.43
1:A:700:ASN:HD22	7:I:116:ASN:ND2	2.16	0.43
7:I:17:ARG:HG2	7:I:18:GLU:N	2.21	0.43
10:L:46:VAL:HG12	10:L:47:ARG:H	1.83	0.43
1:A:1398:MET:O	1:A:1401:SER:N	2.44	0.43
1:A:922:ASP:O	1:A:923:LEU:HG	2.19	0.43
1:A:982:THR:C	1:A:984:LYS:N	2.71	0.43
2:B:1168:LEU:HB3	2:B:1169:MET:H	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:ARG:HD3	2:B:566:LEU:HD23	2.01	0.43
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.43
3:C:182:PRO:HG3	3:C:206:ASN:O	2.18	0.43
3:C:30:ALA:O	3:C:33:LEU:HB3	2.19	0.43
1:A:1059:HIS:CE1	5:F:86:THR:HA	2.53	0.43
7:I:69:PRO:HG2	7:I:85:PHE:CE1	2.53	0.43
12:T:19:DT:H2'	12:T:20:DC:O4'	2.19	0.43
1:A:106:VAL:HG11	1:A:214:ILE:HD11	2.00	0.42
1:A:902:LEU:H	1:A:902:LEU:HG	1.69	0.42
2:B:1149:GLU:HG2	2:B:1153:GLU:HB2	2.01	0.42
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.53	0.42
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.19	0.42
7:I:21:GLU:H	7:I:21:GLU:HG3	1.62	0.42
9:K:78:THR:HG22	9:K:79:GLU:N	2.34	0.42
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.51	0.42
1:A:1146:VAL:O	1:A:1197:LEU:HD23	2.19	0.42
1:A:282:ASN:HB3	1:A:283:GLY:H	1.60	0.42
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.84	0.42
2:B:92:PHE:HB3	2:B:130:VAL:HG11	2.01	0.42
2:B:195:CYS:CB	2:B:782:LEU:HD22	2.49	0.42
2:B:458:LYS:O	2:B:462:ALA:HB2	2.18	0.42
2:B:637:LEU:HD23	2:B:742:GLU:OE2	2.18	0.42
3:C:115:SER:HB3	3:C:142:VAL:HG12	2.01	0.42
3:C:180:TYR:O	3:C:181:ASP:HB3	2.19	0.42
4:E:16:PHE:O	4:E:19:VAL:N	2.51	0.42
4:E:12:LEU:HD22	4:E:55:ARG:NH2	2.34	0.42
8:J:1:MET:O	8:J:2:ILE:O	2.37	0.42
9:K:102:LYS:O	9:K:106:GLU:CG	2.67	0.42
1:A:1025:ARG:CG	1:A:1025:ARG:NH1	2.77	0.42
1:A:416:ARG:HG2	1:A:416:ARG:H	1.52	0.42
1:A:805:LEU:HD12	1:A:806:ARG:N	2.35	0.42
1:A:913:LEU:HG	1:A:915:SER:H	1.84	0.42
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.35	0.42
2:B:976:ILE:HD11	2:B:992:ILE:HA	2.02	0.42
4:E:13:TRP:CE3	4:E:39:LEU:HD13	2.54	0.42
8:J:7:CYS:HB2	8:J:49:MET:HE3	2.01	0.42
1:A:1336:MET:CE	1:A:1380:GLY:HA2	2.49	0.42
1:A:332:LYS:H	1:A:337:ARG:CB	2.33	0.42
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.42
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.42
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.84	0.42
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.02	0.42
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.42
2:B:551:PRO:O	2:B:554:ILE:HB	2.20	0.42
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.73	0.42
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.54	0.42
9:K:61:TYR:HA	9:K:72:LYS:O	2.19	0.42
1:A:1390:ASN:ND2	1:A:1402:PHE:HB3	2.35	0.42
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.02	0.42
1:A:219:PHE:HB3	1:A:224:PHE:HB2	2.00	0.42
1:A:332:LYS:C	1:A:334:GLY:N	2.71	0.42
1:A:535:THR:HG21	1:A:617:VAL:H	1.84	0.42
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.51	0.42
4:E:114:ASN:O	4:E:115:ASN:HB3	2.19	0.42
6:H:26:ILE:CG2	6:H:40:LEU:HB3	2.49	0.42
9:K:57:LEU:HD12	9:K:76:GLN:HG2	2.01	0.42
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.19	0.42
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	2.01	0.42
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	2.01	0.42
1:A:75:ASN:HA	2:B:1116:ARG:HH12	1.84	0.42
1:A:756:ILE:O	1:A:760:GLN:HG3	2.19	0.42
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.20	0.42
1:A:954:TRP:HE3	1:A:955:PRO:HD2	1.84	0.42
2:B:1020:ARG:HG2	2:B:1020:ARG:H	1.64	0.42
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.34	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.78	0.42
2:B:840:ILE:HG23	2:B:992:ILE:HG22	2.02	0.42
1:A:1067:LEU:HD12	1:A:1067:LEU:C	2.40	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.54	0.42
1:A:442:VAL:HG12	1:A:491:VAL:HG22	2.01	0.42
2:B:276:ILE:CG2	2:B:277:LYS:N	2.83	0.42
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.97	0.42
9:K:63:VAL:HG23	9:K:63:VAL:O	2.19	0.42
1:A:1313:LEU:O	1:A:1315:GLU:N	2.53	0.42
1:A:253:ASN:HB2	1:A:256:GLN:CA	2.48	0.42
1:A:848:ILE:HD13	1:A:858:ASN:HB3	2.01	0.42
1:A:346:ASP:N	2:B:1154:ALA:HB1	2.24	0.42
2:B:43:LEU:HD11	2:B:811:TYR:O	2.20	0.42
2:B:534:GLY:O	2:B:537:LYS:HD3	2.20	0.42
2:B:58:THR:O	2:B:62:ILE:HG12	2.20	0.42
2:B:594:ALA:HB2	7:I:61:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:PHE:CD2	2:B:914:LYS:HB3	2.55	0.42
1:A:1271:ILE:HG22	1:A:1273:LEU:HD12	2.01	0.42
1:A:408:ASP:C	1:A:410:GLY:N	2.73	0.42
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.01	0.42
1:A:833:GLU:O	1:A:834:THR:C	2.58	0.42
1:A:884:ASP:OD2	1:A:884:ASP:N	2.50	0.42
1:A:996:ASN:C	1:A:998:LEU:N	2.73	0.42
2:B:801:LYS:O	8:J:52:THR:HG23	2.20	0.42
3:C:131:HIS:O	3:C:132:PRO:C	2.57	0.42
4:E:100:ILE:HG12	4:E:105:PHE:HD1	1.83	0.42
6:H:77:ARG:O	6:H:78:SER:C	2.57	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.93	0.42
9:K:4:PRO:HG2	9:K:4:PRO:O	2.20	0.42
9:K:7:PHE:C	9:K:9:LEU:N	2.74	0.42
10:L:34:CYS:O	10:L:35:SER:CB	2.68	0.42
12:T:11:DG:N2	13:N:5:DT:O2	2.53	0.42
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	2.01	0.42
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.75	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
2:B:762:ASN:HD21	2:B:1022:THR:HA	1.85	0.42
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.85	0.42
2:B:708:GLU:O	2:B:710:LEU:N	2.53	0.42
3:C:10:ILE:HG21	3:C:13:ALA:HB2	2.01	0.42
10:L:32:ALA:HB3	10:L:55:ILE:HD12	2.02	0.42
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.60	0.41
1:A:512:VAL:HG13	1:A:512:VAL:O	2.20	0.41
1:A:566:ILE:O	1:A:567:LYS:O	2.37	0.41
1:A:675:THR:C	1:A:679:ILE:HD12	2.40	0.41
2:B:1096:ARG:HG3	2:B:1097:HIS:N	2.35	0.41
2:B:1099:VAL:H	2:B:1099:VAL:HG23	1.55	0.41
2:B:1138:MET:HG3	2:B:1146:PHE:CE2	2.55	0.41
2:B:1147:LEU:O	2:B:1151:LEU:HB2	2.20	0.41
2:B:430:ARG:HD3	2:B:434:ARG:NH2	2.34	0.41
2:B:899:ILE:HD11	2:B:911:ILE:CG1	2.40	0.41
3:C:78:GLU:OE1	3:C:246:ARG:HD3	2.19	0.41
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.48	0.41
6:H:23:VAL:HG21	6:H:121:LEU:HD21	2.01	0.41
6:H:39:THR:O	6:H:123:MET:HA	2.20	0.41
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.55	0.41
1:A:215:SER:HB3	1:A:218:ASP:OD2	2.20	0.41
1:A:225:ASN:O	1:A:227:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ASN:HA	9:K:60:ALA:HB1	2.02	0.41
1:A:826:ASP:N	1:A:826:ASP:OD2	2.45	0.41
2:B:37:PHE:HD1	2:B:681:TRP:CE2	2.38	0.41
2:B:65:GLU:CD	2:B:66:ASP:H	2.24	0.41
5:F:74:ILE:HA	5:F:74:ILE:HD13	1.90	0.41
6:H:123:MET:HE1	6:H:142:LEU:HD13	2.02	0.41
1:A:1059:HIS:ND1	5:F:87:LYS:HG2	2.35	0.41
1:A:1166:ASP:OD1	1:A:1194:ARG:NH2	2.44	0.41
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.20	0.41
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.41
1:A:518:LYS:CB	1:A:519:PRO:CD	2.99	0.41
2:B:99:LYS:HA	2:B:100:PRO:HD2	1.76	0.41
2:B:377:PHE:O	2:B:380:TYR:N	2.51	0.41
2:B:412:LEU:O	2:B:413:LEU:C	2.57	0.41
2:B:778:MET:HE1	2:B:853:SER:HB3	2.01	0.41
2:B:956:THR:HB	10:L:46:VAL:HG21	2.03	0.41
3:C:41:ILE:HG13	3:C:172:PRO:CG	2.48	0.41
4:E:191:LYS:HE3	4:E:191:LYS:HB2	1.84	0.41
1:A:567:LYS:HB3	6:H:95:TYR:HA	2.01	0.41
1:A:551:TYR:OH	9:K:32:VAL:HG21	2.21	0.41
12:T:9:DA:C6	12:T:10:DA:C6	3.08	0.41
1:A:1021:LEU:O	1:A:1023:ARG:N	2.54	0.41
1:A:423:ASP:HB3	1:A:424:ILE:H	1.26	0.41
1:A:794:PRO:O	1:A:796:SER:N	2.54	0.41
2:B:1033:LYS:N	2:B:1089:PRO:HG2	2.35	0.41
2:B:1200:ALA:O	2:B:1201:LYS:C	2.57	0.41
2:B:386:LEU:C	2:B:388:CYS:N	2.74	0.41
2:B:516:ASN:ND2	2:B:516:ASN:H	2.17	0.41
2:B:554:ILE:O	2:B:555:ILE:C	2.59	0.41
2:B:639:ILE:CG2	2:B:640:VAL:N	2.83	0.41
2:B:658:ILE:O	2:B:661:LEU:HB2	2.20	0.41
2:B:710:LEU:O	2:B:711:GLU:HB3	2.21	0.41
2:B:911:ILE:O	2:B:912:ILE:HG13	2.20	0.41
4:E:124:VAL:H	4:E:125:PRO:CD	2.34	0.41
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.21	0.41
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.56	0.41
1:A:278:THR:HG22	1:A:278:THR:O	2.19	0.41
1:A:609:ASP:O	1:A:611:GLN:N	2.53	0.41
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.68	0.41
2:B:384:ARG:HH22	2:B:621:GLU:CG	2.32	0.41
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:93:TYR:CD2	6:H:145:ARG:HD3	2.56	0.41
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.84	0.41
1:A:1414:ALA:C	1:A:1416:ALA:H	2.24	0.41
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.91	0.41
1:A:353:ILE:HG13	1:A:485:ASP:O	2.20	0.41
1:A:809:THR:HB	1:A:810:PRO:CD	2.51	0.41
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.79	0.41
2:B:309:GLN:OE1	7:I:52:ILE:HG23	2.21	0.41
3:C:31:ASN:C	3:C:33:LEU:N	2.73	0.41
4:E:59:SER:O	4:E:79:TRP:CH2	2.73	0.41
4:E:63:ASN:HB3	4:E:64:PRO:HD3	1.99	0.41
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.03	0.41
8:J:36:LEU:O	8:J:41:LEU:HB2	2.21	0.41
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.02	0.41
1:A:274:ILE:HG22	1:A:274:ILE:O	2.21	0.41
1:A:345:VAL:HA	2:B:1118:PRO:HG2	2.02	0.41
1:A:406:ILE:HG22	1:A:407:ARG:N	2.36	0.41
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.79	0.41
1:A:446:ARG:HD3	1:A:478:TYR:O	2.20	0.41
1:A:911:SER:O	1:A:978:PRO:HB3	2.21	0.41
2:B:276:ILE:HG22	2:B:277:LYS:N	2.36	0.41
2:B:60:GLN:O	2:B:63:ILE:HG22	2.20	0.41
2:B:879:ARG:HB2	2:B:880:THR:H	1.33	0.41
5:F:125:LEU:C	5:F:127:GLU:N	2.74	0.41
7:I:33:SER:O	7:I:34:TYR:C	2.59	0.41
8:J:2:ILE:O	8:J:2:ILE:CG2	2.69	0.41
1:A:1261:LYS:C	1:A:1263:ILE:H	2.24	0.41
1:A:1349:TYR:O	1:A:1350:LYS:C	2.59	0.41
1:A:844:ALA:HB2	1:A:1389:PHE:CZ	2.56	0.41
1:A:68:GLN:O	1:A:68:GLN:CD	2.59	0.41
1:A:805:LEU:CD1	1:A:806:ARG:N	2.82	0.41
2:B:248:SER:HB3	2:B:249:ARG:H	1.65	0.41
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.56	0.41
4:E:179:GLN:O	4:E:182:ASP:HB2	2.21	0.41
1:A:1121:GLU:HG3	1:A:1122:PRO:HD2	2.02	0.41
1:A:1408:ILE:O	1:A:1412:ALA:HB2	2.20	0.41
1:A:214:ILE:HA	1:A:214:ILE:HD13	1.84	0.41
1:A:335:ARG:HE	1:A:335:ARG:HA	1.86	0.41
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.56	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG22	2.02	0.41
2:B:1053:GLU:HB3	2:B:1057:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1055:ILE:HD13	2:B:1055:ILE:HA	1.94	0.41
2:B:1131:GLY:O	2:B:1132:GLU:C	2.58	0.41
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.56	0.41
2:B:520:GLY:HA3	2:B:635:ARG:CD	2.51	0.41
3:C:33:LEU:HG	3:C:37:MET:HE3	2.03	0.41
1:A:955:PRO:C	1:A:956:LEU:HG	2.41	0.41
2:B:1158:PHE:CD2	2:B:1198:TYR:HD1	2.38	0.41
2:B:519:TRP:O	2:B:519:TRP:HD1	2.02	0.41
1:A:384:ASN:O	1:A:385:ILE:C	2.59	0.41
1:A:965:GLN:HG3	1:A:965:GLN:H	1.65	0.41
2:B:1155:SER:OG	2:B:1156:ASP:N	2.53	0.41
2:B:62:ILE:HG23	2:B:418:LYS:HG2	2.03	0.41
2:B:655:LYS:O	2:B:658:ILE:HG22	2.21	0.41
2:B:762:ASN:HD22	2:B:763:GLN:H	1.69	0.41
2:B:975:GLN:CG	2:B:976:ILE:N	2.78	0.41
5:F:73:ALA:O	5:F:74:ILE:HG12	2.21	0.41
5:F:75:PRO:O	5:F:77:ASP:O	2.39	0.41
6:H:91:ASP:O	6:H:91:ASP:CG	2.59	0.41
7:I:111:THR:CG2	7:I:112:SER:N	2.84	0.41
9:K:40:HIS:CE1	9:K:63:VAL:CG2	3.03	0.41
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.20	0.40
1:A:381:THR:HG22	1:A:384:ASN:CG	2.41	0.40
1:A:491:VAL:O	1:A:493:GLN:NE2	2.54	0.40
1:A:532:ARG:O	1:A:535:THR:N	2.50	0.40
1:A:590:ARG:CG	1:A:591:PHE:H	2.33	0.40
1:A:929:LEU:CD2	1:A:983:ILE:CG2	2.99	0.40
1:A:4:GLN:HE22	2:B:1159:ARG:H	1.67	0.40
2:B:405:ARG:HB3	2:B:631:GLY:HA3	2.03	0.40
1:A:598:LEU:HD13	6:H:25:ARG:HH12	1.86	0.40
6:H:82:PRO:C	6:H:84:ALA:H	2.25	0.40
7:I:119:THR:O	7:I:120:GLN:HG2	2.21	0.40
9:K:108:GLU:O	9:K:109:TRP:C	2.59	0.40
10:L:53:HIS:O	10:L:55:ILE:N	2.50	0.40
11:R:6:G:N3	11:R:7:A:C8	2.90	0.40
1:A:1053:PHE:O	1:A:1055:ARG:N	2.53	0.40
1:A:214:ILE:HG22	1:A:215:SER:O	2.22	0.40
1:A:32:VAL:HB	1:A:57:ARG:HD2	2.02	0.40
1:A:664:THR:OG1	2:B:1014:PRO:HB2	2.21	0.40
1:A:794:PRO:O	1:A:795:GLU:C	2.59	0.40
2:B:205:ILE:O	2:B:208:SER:N	2.48	0.40
2:B:235:SER:OG	2:B:236:HIS:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:O	2:B:488:TYR:C	2.59	0.40
2:B:859:TYR:CZ	2:B:941:LEU:HD22	2.55	0.40
3:C:31:ASN:O	3:C:34:ARG:N	2.54	0.40
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.51	0.40
12:T:17:DG:N3	12:T:17:DG:H2'	2.36	0.40
1:A:444:PHE:O	1:A:478:TYR:CE2	2.75	0.40
1:A:666:ILE:HG23	2:B:1026:LEU:CD1	2.52	0.40
2:B:174:LEU:HA	2:B:174:LEU:HD12	1.90	0.40
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.56	0.40
2:B:99:LYS:HB3	2:B:180:TYR:CE2	2.56	0.40
3:C:76:ASP:O	3:C:79:GLN:HG2	2.22	0.40
7:I:15:TYR:N	7:I:15:TYR:CD1	2.89	0.40
13:N:2:DT:O2	13:N:2:DT:H2'	2.22	0.40
1:A:1048:ASN:O	1:A:1049:ILE:C	2.60	0.40
1:A:265:LYS:C	1:A:267:ALA:N	2.53	0.40
1:A:442:VAL:O	1:A:457:ALA:HA	2.21	0.40
2:B:115:GLN:O	2:B:119:LEU:HD12	2.21	0.40
2:B:291:ILE:CG2	2:B:297:ILE:HD13	2.50	0.40
2:B:839:MET:O	2:B:990:ILE:HA	2.21	0.40
2:B:992:ILE:HG21	2:B:994:TYR:CE2	2.56	0.40
1:A:1049:ILE:O	1:A:1050:GLU:C	2.60	0.40
1:A:1404:GLU:HB3	1:A:1407:GLU:HG2	2.02	0.40
2:B:1156:ASP:HB3	2:B:1157:ALA:H	1.55	0.40
2:B:287:ARG:HA	2:B:291:ILE:O	2.20	0.40
2:B:426:LYS:HG3	2:B:430:ARG:HH12	1.87	0.40
2:B:745:PRO:O	2:B:748:ILE:HG12	2.22	0.40
2:B:821:GLN:HE22	2:B:851:PHE:H	1.69	0.40
3:C:46:ILE:H	3:C:46:ILE:HG12	1.58	0.40
3:C:46:ILE:HD12	3:C:157:CYS:HB3	2.02	0.40
4:E:117:THR:HA	4:E:118:PRO:HD2	1.88	0.40
8:J:35:ALA:O	8:J:39:LEU:CD1	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1038 (75%)	233 (17%)	112 (8%)	1	13
2	B	1088/1224 (89%)	822 (76%)	188 (17%)	78 (7%)	1	16
3	C	264/318 (83%)	209 (79%)	48 (18%)	7 (3%)	5	34
4	E	212/215 (99%)	162 (76%)	39 (18%)	11 (5%)	2	21
5	F	82/155 (53%)	65 (79%)	13 (16%)	4 (5%)	2	22
6	H	129/146 (88%)	97 (75%)	21 (16%)	11 (8%)	1	12
7	I	117/122 (96%)	83 (71%)	25 (21%)	9 (8%)	1	14
8	J	63/70 (90%)	45 (71%)	14 (22%)	4 (6%)	1	18
9	K	112/120 (93%)	89 (80%)	16 (14%)	7 (6%)	1	18
10	L	44/70 (63%)	24 (54%)	9 (20%)	11 (25%)	0	1
All	All	3494/4173 (84%)	2634 (75%)	606 (17%)	254 (7%)	1	15

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	55	ASP
1	A	56	PRO
1	A	93	VAL
1	A	130	ASP
1	A	162	VAL
1	A	214	ILE
1	A	248	PRO
1	A	250	ILE
1	A	251	SER
1	A	253	ASN
1	A	257	ARG
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	325	ILE
1	A	331	GLY
1	A	399	HIS
1	A	402	ALA
1	A	411	ASP
1	A	428	TYR

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Mol	Chain	Res	Type
1	A	567	LYS
1	A	568	PRO
1	A	591	PHE
1	A	700	ASN
1	A	846	GLU
1	A	998	LEU
1	A	1036	ARG
1	A	1255	GLU
1	A	1393	ASN
2	B	100	PRO
2	B	176	SER
2	B	229	ALA
2	B	249	ARG
2	B	436	VAL
2	B	466	TRP
2	B	477	ALA
2	B	484	ASN
2	B	531	GLN
2	B	592	ASN
2	B	636	PRO
2	B	648	HIS
2	B	649	LYS
2	B	650	GLU
2	B	711	GLU
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	831	SER
2	B	864	LYS
2	B	865	LYS
2	B	981	ALA
2	B	1046	PRO
2	B	1157	ALA
2	B	1181	GLU
3	C	142	VAL
3	C	149	LYS
3	C	227	THR
4	E	3	GLN
4	E	59	SER
4	E	172	GLU
4	E	173	SER
5	F	74	ILE

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Mol	Chain	Res	Type
6	H	77	ARG
6	H	81	PRO
6	H	140	ALA
7	I	20	LYS
7	I	47	GLU
7	I	107	SER
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
10	L	26	THR
10	L	35	SER
1	A	50	ILE
1	A	68	GLN
1	A	226	GLU
1	A	266	LEU
1	A	312	PRO
1	A	313	GLN
1	A	409	SER
1	A	472	LEU
1	A	515	GLN
1	A	517	ASN
1	A	592	ASP
1	A	597	LEU
1	A	610	GLY
1	A	756	ILE
1	A	972	HIS
1	A	986	ILE
1	A	1048	ASN
1	A	1054	LEU
1	A	1341	ILE
1	A	1388	GLY
1	A	1399	ARG
2	B	53	GLN
2	B	58	THR
2	B	475	SER
2	B	516	ASN
2	B	540	SER
2	B	708	GLU
2	B	709	ASP
2	B	1028	GLU
2	B	1166	CYS
2	B	1176	ASN

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Mol	Chain	Res	Type
3	C	110	THR
4	E	192	ARG
4	E	206	GLY
5	F	81	THR
6	H	32	THR
6	H	82	PRO
6	H	85	GLY
6	H	134	ASN
7	I	21	GLU
7	I	34	TYR
7	I	86	PHE
8	J	16	ASP
9	K	81	TYR
10	L	54	ARG
10	L	55	ILE
10	L	64	LEU
1	A	69	THR
1	A	76	GLU
1	A	89	PRO
1	A	128	ILE
1	A	131	SER
1	A	167	CYS
1	A	178	GLY
1	A	282	ASN
1	A	424	ILE
1	A	593	GLU
1	A	708	MET
1	A	755	PHE
1	A	810	PRO
1	A	895	LYS
1	A	903	ASN
1	A	922	ASP
1	A	957	PRO
1	A	963	ILE
1	A	1022	LEU
1	A	1062	GLU
1	A	1188	GLN
1	A	1223	ASP
1	A	1261	LYS
1	A	1270	ASN
1	A	1274	ARG
1	A	1314	SER

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Mol	Chain	Res	Type
1	A	1327	ILE
1	A	1398	MET
1	A	1435	PRO
2	B	21	GLU
2	B	67	SER
2	B	248	SER
2	B	333	PHE
2	B	555	ILE
2	B	563	MET
2	B	738	PHE
2	B	879	ARG
2	B	881	ASN
2	B	958	GLN
2	B	1047	PHE
2	B	1156	ASP
2	B	1167	GLY
2	B	1201	LYS
3	C	215	GLU
4	E	36	GLU
5	F	73	ALA
5	F	126	ALA
6	H	62	SER
7	I	54	GLU
9	K	5	ASP
9	K	46	ILE
10	L	45	ALA
1	A	287	HIS
1	A	318	SER
1	A	404	TYR
1	A	484	GLY
1	A	923	LEU
1	A	994	GLN
1	A	1021	LEU
1	A	1221	LYS
1	A	1438	THR
2	B	45	SER
2	B	266	ALA
2	B	367	LEU
2	B	418	LYS
2	B	712	PRO
2	B	746	SER
2	B	876	LYS

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Mol	Chain	Res	Type
2	B	878	GLN
2	B	891	ASP
2	B	997	GLU
2	B	1186	ASP
2	B	1222	ARG
2	B	1223	ASP
4	E	124	VAL
6	H	43	ASN
6	H	90	ALA
9	K	7	PHE
10	L	37	LYS
10	L	59	ALA
1	A	87	ALA
1	A	274	ILE
1	A	332	LYS
1	A	335	ARG
1	A	418	SER
1	A	514	PRO
1	A	576	GLN
1	A	958	VAL
2	B	365	THR
2	B	483	LEU
2	B	488	TYR
2	B	791	THR
2	B	792	MET
2	B	799	PRO
2	B	1021	MET
2	B	1061	GLU
3	C	6	PRO
3	C	144	ILE
10	L	39	SER
10	L	56	LEU
1	A	367	PRO
1	A	546	VAL
1	A	583	PRO
1	A	795	GLU
1	A	1122	PRO
1	A	1424	VAL
2	B	575	PRO
2	B	613	VAL
2	B	647	GLY
2	B	1027	ILE

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Mol	Chain	Res	Type
2	B	1178	ASN
4	E	76	GLY
7	I	63	GLY
9	K	4	PRO
9	K	50	LEU
10	L	53	HIS
1	A	400	PRO
2	B	1017	ILE
4	E	51	GLY
8	J	33	GLY
1	A	829	VAL
1	A	1437	GLY
4	E	118	PRO
6	H	59	ILE
1	A	916	GLY
2	B	1103	ILE
2	B	1165	ILE
7	I	76	PRO
1	A	599	SER
1	A	1049	ILE
1	A	1107	VAL
1	A	321	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%)	987 (81%)	231 (19%)	1	9
2	B	960/1061 (90%)	790 (82%)	170 (18%)	2	12
3	C	234/274 (85%)	188 (80%)	46 (20%)	1	8
4	E	196/197 (100%)	164 (84%)	32 (16%)	2	15
5	F	74/137 (54%)	63 (85%)	11 (15%)	3	17
6	H	117/128 (91%)	97 (83%)	20 (17%)	2	13
7	I	113/116 (97%)	95 (84%)	18 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	J	60/65 (92%)	48 (80%)	12 (20%)	1	8
9	K	99/102 (97%)	81 (82%)	18 (18%)	1	11
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	6
All	All	3111/3657 (85%)	2544 (82%)	567 (18%)	1	11

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

Mol	Chain	Res	Type
1	A	6	TYR
1	A	8	SER
1	A	12	ARG
1	A	18	GLN
1	A	26	GLU
1	A	32	VAL
1	A	44	THR
1	A	47	ARG
1	A	58	LEU
1	A	60	SER
1	A	70	CYS
1	A	80	HIS
1	A	81	PHE
1	A	84	ILE
1	A	93	VAL
1	A	99	ILE
1	A	100	LYS
1	A	102	VAL
1	A	105	CYS
1	A	110	CYS
1	A	116	ASP
1	A	128	ILE
1	A	130	ASP
1	A	140	THR
1	A	162	VAL
1	A	169	ASN
1	A	170	THR
1	A	184	SER
1	A	185	TRP
1	A	199	LEU
1	A	206	GLU
1	A	208	LEU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	250	ILE
1	A	254	GLU
1	A	255	SER
1	A	257	ARG
1	A	266	LEU
1	A	270	LEU
1	A	287	HIS
1	A	295	LEU
1	A	297	GLN
1	A	303	TYR
1	A	304	MET
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	323	LYS
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	381	THR
1	A	394	ASN
1	A	403	LYS
1	A	406	ILE
1	A	413	ILE
1	A	416	ARG
1	A	419	LYS
1	A	423	ASP
1	A	424	ILE
1	A	434	ARG
1	A	436	ILE
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	453	MET

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Mol	Chain	Res	Type
1	A	454	SER
1	A	460	VAL
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	485	ASP
1	A	486	GLU
1	A	498	ARG
1	A	513	SER
1	A	518	LYS
1	A	527	THR
1	A	534	LEU
1	A	550	LEU
1	A	552	TRP
1	A	566	ILE
1	A	576	GLN
1	A	595	THR
1	A	596	THR
1	A	599	SER
1	A	602	ASP
1	A	612	ILE
1	A	618	GLU
1	A	619	LYS
1	A	621	THR
1	A	625	SER
1	A	630	ILE
1	A	648	ASN
1	A	663	SER
1	A	666	ILE
1	A	672	ASP
1	A	680	THR
1	A	682	THR
1	A	687	LYS
1	A	702	LEU
1	A	705	LYS
1	A	720	ARG
1	A	728	LYS
1	A	732	LEU
1	A	740	LEU
1	A	752	LYS
1	A	764	CYS

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Mol	Chain	Res	Type
1	A	768	GLN
1	A	771	GLU
1	A	774	ARG
1	A	781	ASP
1	A	782	ARG
1	A	783	THR
1	A	788	SER
1	A	796	SER
1	A	797	LYS
1	A	801	GLU
1	A	803	SER
1	A	805	LEU
1	A	821	ARG
1	A	826	ASP
1	A	829	VAL
1	A	830	LYS
1	A	831	THR
1	A	838	GLN
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	879	GLU
1	A	880	LYS
1	A	885	THR
1	A	886	ILE
1	A	895	LYS
1	A	896	ARG
1	A	897	TYR
1	A	902	LEU
1	A	905	ASP
1	A	907	THR
1	A	911	SER
1	A	918	GLU
1	A	924	LYS
1	A	929	LEU
1	A	949	ASP
1	A	969	GLN
1	A	982	THR
1	A	988	LEU
1	A	990	VAL
1	A	996	ASN
1	A	998	LEU

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Mol	Chain	Res	Type
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1037	LEU
1	A	1048	ASN
1	A	1058	VAL
1	A	1067	LEU
1	A	1074	GLU
1	A	1081	LEU
1	A	1094	VAL
1	A	1095	THR
1	A	1110	ASN
1	A	1111	MET
1	A	1118	VAL
1	A	1120	LEU
1	A	1127	ASP
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG
1	A	1146	VAL
1	A	1160	SER
1	A	1161	THR
1	A	1165	GLU
1	A	1172	LEU
1	A	1173	HIS
1	A	1187	GLN
1	A	1193	LEU
1	A	1199	ARG
1	A	1217	LYS
1	A	1219	THR
1	A	1222	ASN
1	A	1231	ASP
1	A	1232	ASN
1	A	1235	LYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1273	LEU
1	A	1274	ARG
1	A	1276	VAL
1	A	1280	GLU

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Mol	Chain	Res	Type
1	A	1281	ARG
1	A	1285	MET
1	A	1291	VAL
1	A	1299	VAL
1	A	1300	LYS
1	A	1301	GLU
1	A	1312	ASN
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1336	MET
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1355	VAL
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1405	THR
1	A	1407	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1428	VAL
2	B	28	GLU
2	B	40	GLU
2	B	66	ASP
2	B	67	SER
2	B	95	ILE
2	B	98	THR
2	B	104	GLU
2	B	106	ASP
2	B	109	THR
2	B	119	LEU
2	B	120	ARG
2	B	126	SER

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Mol	Chain	Res	Type
2	B	175	ARG
2	B	177	LYS
2	B	187	SER
2	B	188	ASP
2	B	199	MET
2	B	202	TYR
2	B	222	ILE
2	B	225	VAL
2	B	244	LEU
2	B	246	LYS
2	B	248	SER
2	B	249	ARG
2	B	261	ARG
2	B	264	SER
2	B	268	THR
2	B	283	VAL
2	B	313	MET
2	B	319	GLU
2	B	327	ARG
2	B	347	LYS
2	B	348	ARG
2	B	354	ASP
2	B	387	LEU
2	B	391	ASP
2	B	393	LYS
2	B	398	ARG
2	B	404	LYS
2	B	408	LEU
2	B	416	LEU
2	B	424	LEU
2	B	425	THR
2	B	426	LYS
2	B	427	ASP
2	B	429	PHE
2	B	432	MET
2	B	437	GLU
2	B	459	TYR
2	B	461	LEU
2	B	463	THR
2	B	468	GLU
2	B	473	MET
2	B	479	VAL

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Mol	Chain	Res	Type
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	489	SER
2	B	490	SER
2	B	513	GLN
2	B	527	THR
2	B	537	LYS
2	B	542	MET
2	B	549	THR
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	582	VAL
2	B	591	ARG
2	B	595	ARG
2	B	600	LEU
2	B	614	SER
2	B	633	VAL
2	B	637	LEU
2	B	641	GLU
2	B	644	GLU
2	B	651	LEU
2	B	668	ASP
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	728	ARG
2	B	737	THR
2	B	740	HIS
2	B	742	GLU
2	B	751	VAL
2	B	762	ASN
2	B	764	SER
2	B	790	ASP
2	B	791	THR
2	B	794	ASN
2	B	800	GLN
2	B	807	ARG
2	B	812	LEU
2	B	822	ASN

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Mol	Chain	Res	Type
2	B	825	VAL
2	B	829	CYS
2	B	830	TYR
2	B	847	ASP
2	B	861	ASP
2	B	864	LYS
2	B	865	LYS
2	B	866	TYR
2	B	868	MET
2	B	869	SER
2	B	872	GLU
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	892	LYS
2	B	895	ASP
2	B	899	ILE
2	B	905	VAL
2	B	906	SER
2	B	911	ILE
2	B	944	THR
2	B	951	GLN
2	B	953	LEU
2	B	957	ASN
2	B	959	ASP
2	B	971	THR
2	B	973	ILE
2	B	976	ILE
2	B	983	ARG
2	B	986	GLN
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1050	ILE
2	B	1051	THR
2	B	1062	HIS
2	B	1077	THR
2	B	1082	MET
2	B	1090	THR
2	B	1093	GLN
2	B	1096	ARG
2	B	1098	MET
2	B	1099	VAL
2	B	1103	ILE
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1132	GLU
2	B	1141	HIS
2	B	1145	SER
2	B	1147	LEU
2	B	1153	GLU
2	B	1159	ARG
2	B	1165	ILE
2	B	1166	CYS
2	B	1178	ASN
2	B	1183	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1218	THR
2	B	1219	ASP
2	B	1223	ASP
3	C	3	GLU
3	C	4	GLU
3	C	10	ILE
3	C	15	LYS
3	C	16	ASP
3	C	18	VAL
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG

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Mol	Chain	Res	Type
3	C	36	VAL
3	C	38	ILE
3	C	43	THR
3	C	49	VAL
3	C	56	THR
3	C	62	PHE
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	93	ASP
3	C	99	LEU
3	C	102	GLN
3	C	119	VAL
3	C	129	ILE
3	C	132	PRO
3	C	134	ILE
3	C	137	LYS
3	C	140	ASN
3	C	142	VAL
3	C	143	LEU
3	C	145	CYS
3	C	151	GLN
3	C	163	ILE
3	C	165	LYS
3	C	166	GLU
3	C	183	TRP
3	C	195	GLN
3	C	196	ASP
3	C	203	GLN
3	C	215	GLU
3	C	227	THR
3	C	233	GLU
3	C	235	VAL
3	C	240	VAL
3	C	254	LYS
3	C	267	GLN
4	E	3	GLN
4	E	4	GLU
4	E	9	ILE
4	E	32	GLN
4	E	43	LYS
4	E	48	ASP

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Mol	Chain	Res	Type
4	E	61	GLN
4	E	63	ASN
4	E	65	THR
4	E	66	GLU
4	E	77	SER
4	E	78	LEU
4	E	83	CYS
4	E	92	THR
4	E	101	GLN
4	E	104	ASN
4	E	107	THR
4	E	110	PHE
4	E	119	SER
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	146	HIS
4	E	156	LEU
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	170	LEU
4	E	171	LYS
4	E	192	ARG
4	E	196	VAL
4	E	204	THR
5	F	74	ILE
5	F	77	ASP
5	F	79	ARG
5	F	90	ARG
5	F	97	ARG
5	F	111	LEU
5	F	112	GLU
5	F	114	GLU
5	F	120	ILE
5	F	123	LYS
5	F	133	VAL
6	H	2	SER
6	H	11	GLN
6	H	27	GLU
6	H	33	GLN
6	H	37	LYS

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Mol	Chain	Res	Type
6	H	54	SER
6	H	55	LEU
6	H	56	THR
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	89	LEU
6	H	95	TYR
6	H	102	TYR
6	H	104	PHE
6	H	110	ASP
6	H	121	LEU
6	H	132	LEU
6	H	136	LYS
6	H	139	ASN
7	I	3	THR
7	I	5	ARG
7	I	8	ARG
7	I	10	CYS
7	I	11	ASN
7	I	12	ASN
7	I	13	MET
7	I	28	GLU
7	I	30	ARG
7	I	37	GLU
7	I	50	THR
7	I	52	ILE
7	I	62	ILE
7	I	78	CYS
7	I	83	ASN
7	I	114	GLN
7	I	117	LYS
7	I	119	THR
8	J	7	CYS
8	J	9	SER
8	J	14	VAL
8	J	27	GLU
8	J	32	GLU
8	J	34	THR
8	J	38	ARG
8	J	42	LYS
8	J	43	ARG

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Mol	Chain	Res	Type
8	J	48	ARG
8	J	55	ASP
8	J	62	ARG
9	K	9	LEU
9	K	20	LYS
9	K	22	ASP
9	K	31	VAL
9	K	33	ILE
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	64	GLU
9	K	70	ARG
9	K	71	PHE
9	K	75	ILE
9	K	77	THR
9	K	79	GLU
9	K	81	TYR
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	46	VAL
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	65	VAL
10	L	66	GLN
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	ASN
1	A	80	HIS
1	A	169	ASN
1	A	171	GLN
1	A	282	ASN
1	A	313	GLN
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	517	ASN
1	A	654	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	858	ASN
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	968	GLN
1	A	1033	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1278	ASN
1	A	1312	ASN
1	A	1330	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	236	HIS
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	762	ASN
2	B	794	ASN
2	B	822	ASN
2	B	834	ASN
2	B	862	GLN

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Mol	Chain	Res	Type
2	B	957	ASN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1179	GLN
2	B	1193	GLN
2	B	1211	ASN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	188	HIS
3	C	203	GLN
4	E	32	GLN
4	E	61	GLN
4	E	63	ASN
4	E	114	ASN
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	134	ASN
6	H	137	GLN
7	I	11	ASN
7	I	60	GLN
7	I	83	ASN
7	I	116	ASN
8	J	53	HIS
9	K	40	HIS
9	K	65	HIS
9	K	92	ASN
10	L	53	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/15 (73%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	12	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1395/1733 (80%)	-0.37	11 (0%) 86 79	76, 116, 186, 214	0
2	B	1106/1224 (90%)	-0.40	2 (0%) 95 93	72, 109, 156, 180	0
3	C	266/318 (83%)	-0.53	0 100 100	83, 106, 145, 154	0
4	E	214/215 (99%)	-0.44	1 (0%) 91 85	104, 151, 192, 196	0
5	F	84/155 (54%)	-0.50	0 100 100	99, 123, 142, 147	0
6	H	133/146 (91%)	-0.25	1 (0%) 86 79	123, 143, 165, 167	0
7	I	119/122 (97%)	-0.47	0 100 100	113, 132, 150, 160	0
8	J	65/70 (92%)	-0.64	0 100 100	77, 94, 126, 131	0
9	K	114/120 (95%)	-0.49	0 100 100	87, 108, 124, 131	0
10	L	46/70 (65%)	-0.26	0 100 100	100, 161, 179, 181	0
11	R	12/15 (80%)	0.10	0 100 100	100, 128, 185, 192	0
12	T	28/28 (100%)	-0.15	1 (3%) 42 34	102, 210, 322, 325	0
13	N	14/14 (100%)	0.23	1 (7%) 16 13	287, 311, 317, 318	0
All	All	3596/4230 (85%)	-0.40	17 (0%) 91 85	72, 116, 181, 325	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	5.0
1	A	1176	LEU	4.3
1	A	150	THR	3.7
1	A	153	PRO	3.0
1	A	316	GLN	2.9
12	T	3	DA	2.8
1	A	152	VAL	2.7
1	A	151	ASP	2.6
13	N	1	DC	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	2.4
1	A	57	ARG	2.4
1	A	145	LYS	2.4
4	E	126	SER	2.3
6	H	86	ASP	2.3
2	B	250	PHE	2.3
2	B	1223	ASP	2.3
1	A	426	LEU	2.2

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	A	1736	1/1	0.80	0.15	92,92,92,92	0
14	ZN	A	1734	1/1	0.90	0.05	212,212,212,212	0
14	ZN	A	1735	1/1	0.97	0.07	155,155,155,155	0
14	ZN	L	105	1/1	0.98	0.05	169,169,169,169	0
14	ZN	I	203	1/1	0.99	0.05	123,123,123,123	0
14	ZN	B	1307	1/1	0.99	0.07	158,158,158,158	0
14	ZN	I	204	1/1	0.99	0.05	131,131,131,131	0
14	ZN	J	101	1/1	0.99	0.12	93,93,93,93	0
14	ZN	C	319	1/1	1.00	0.05	97,97,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.