



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:44 am BST

PDB ID : 3GTG  
Title : Backtracked RNA polymerase II complex with 12mer RNA  
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.  
Deposited on : 2009-03-27  
Resolution : 3.78 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

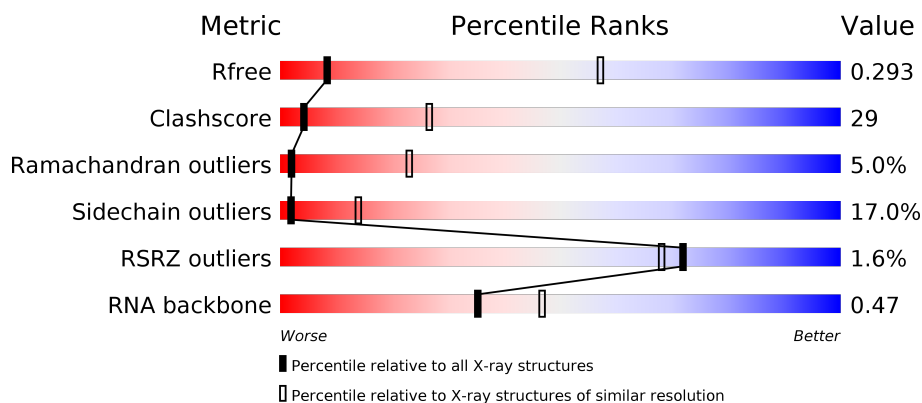
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.78 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.






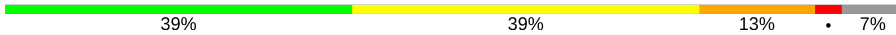





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1038 (3.96-3.60)
Clashscore	141614	1100 (3.96-3.60)
Ramachandran outliers	138981	1062 (3.96-3.60)
Sidechain outliers	138945	1058 (3.96-3.60)
RSRZ outliers	127900	1009 (3.98-3.58)
RNA backbone	3102	1035 (4.52-3.00)

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	 2% 38% 35% 9% 17%
2	B	1224	 2% 41% 42% 10% 6%
3	C	318	 % 36% 37% 11% 15%
4	E	215	 63% 32% 5%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	12	
12	T	29	
13	N	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	A	1734	-	-	X	-
14	ZN	B	1307	-	-	X	-
14	ZN	J	101	-	-	X	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 30067 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	1442	Total	C	N	O	S	0	0	0
			11332	7133	1982	2156	61			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1153	Total	C	N	O	S	0	0	0
			9167	5794	1604	1713	56			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2135	1344	355	423	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	215	Total	C	N	O	S	0	0	0
			1757	1114	310	322	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	85	Total	C	N	O	S	0	0	0
			684	437	116	128	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	136	Total	C	N	O	S	0	0	0
			1087	684	183	215	5			

- 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\*G)-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		

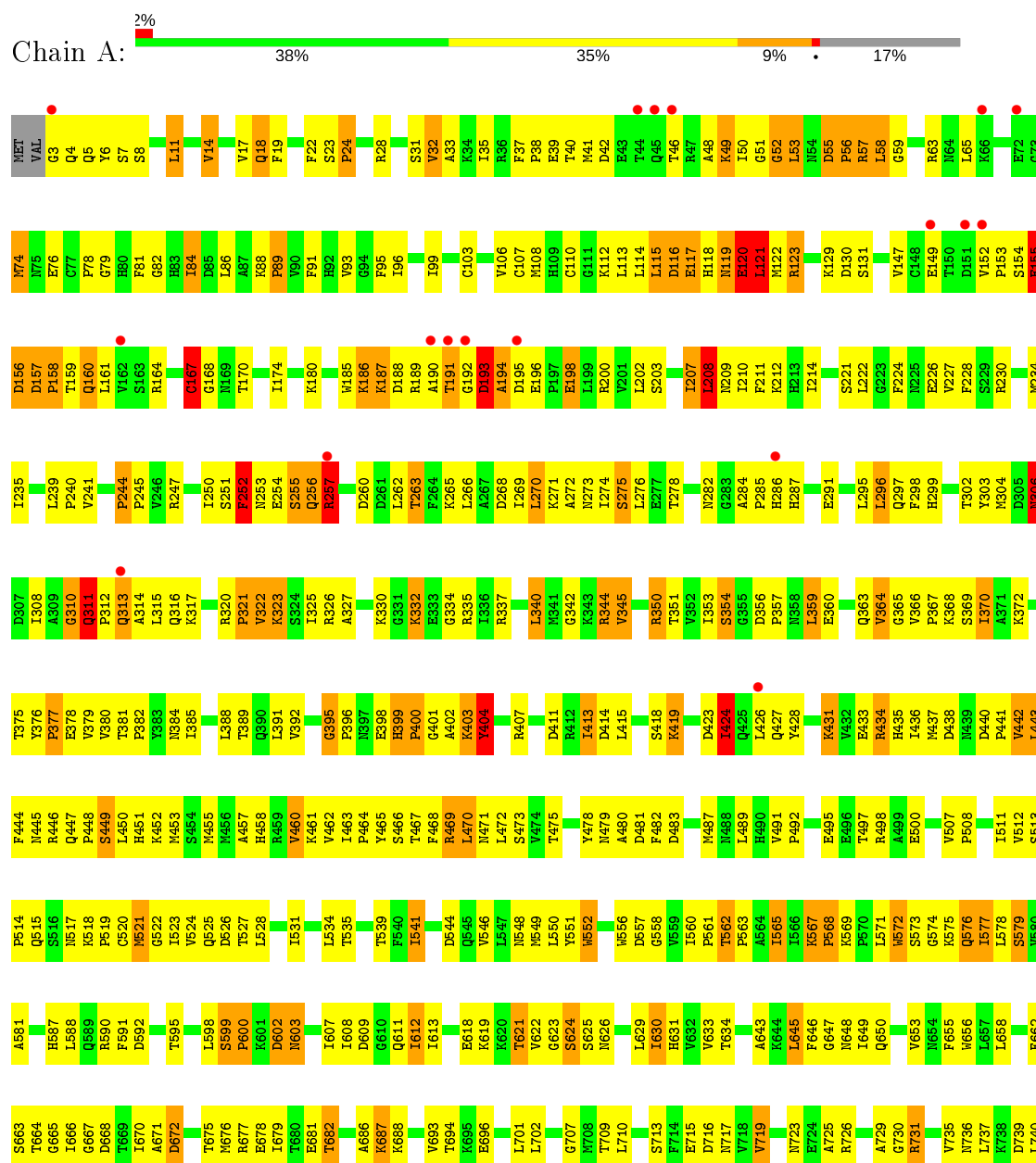
- Molecule 16 is water.

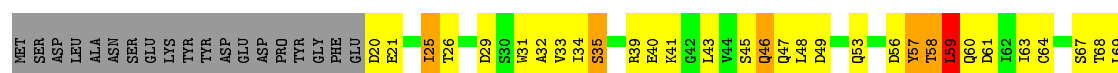
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	1	Total	O	0	0
			1	1		

### 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



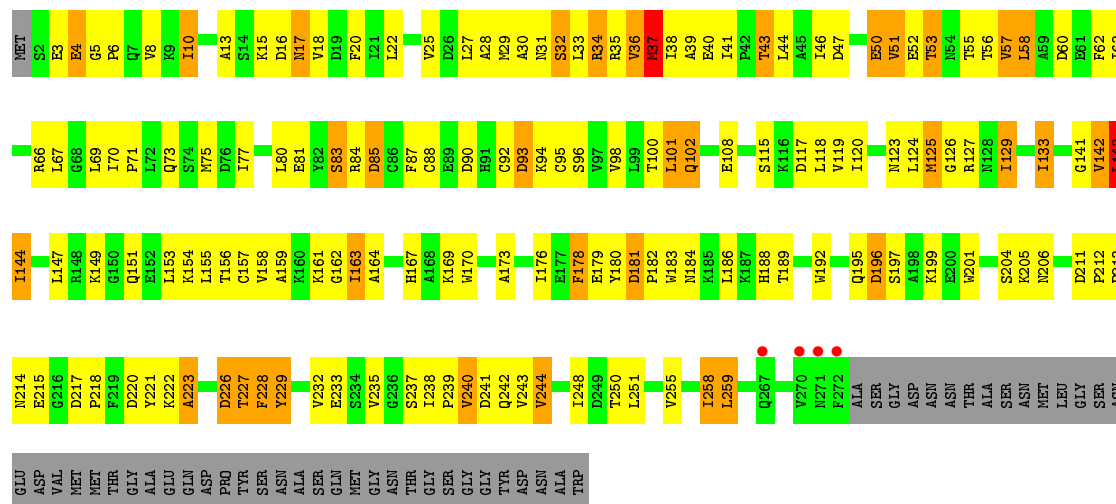




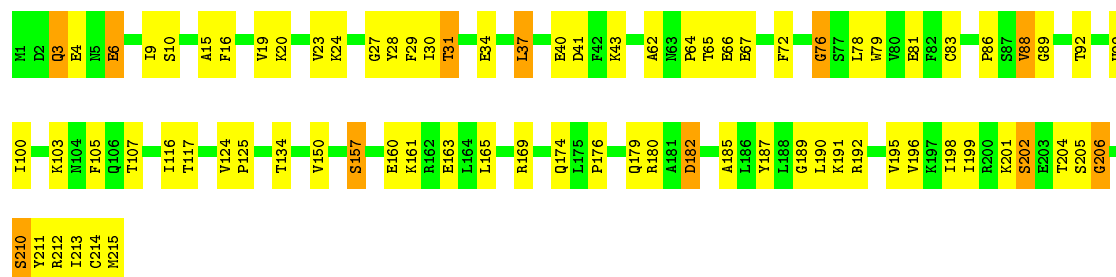




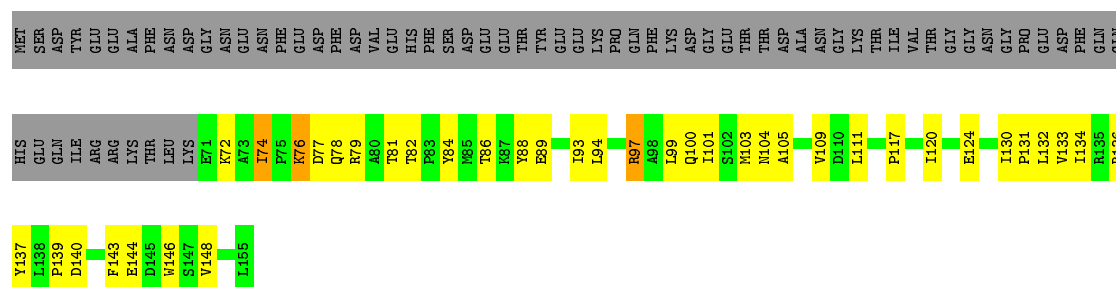
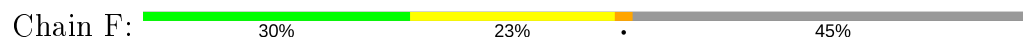
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



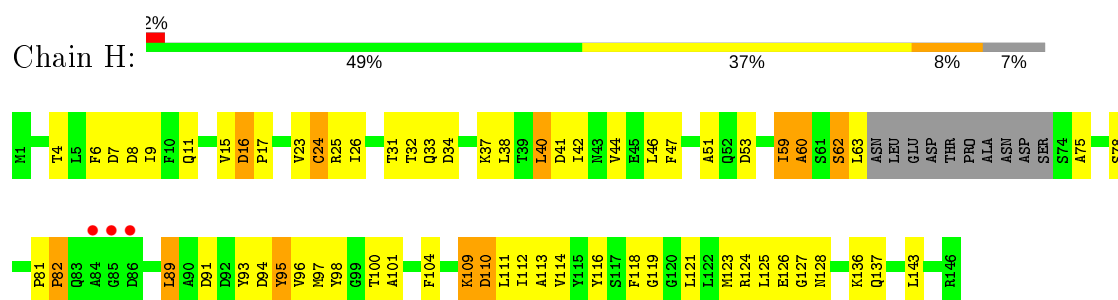
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



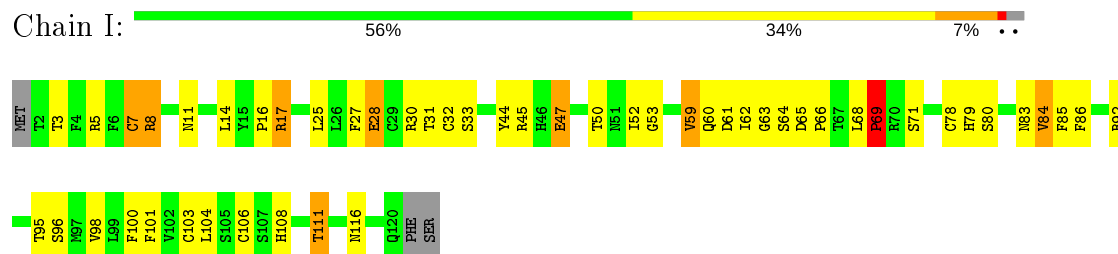
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



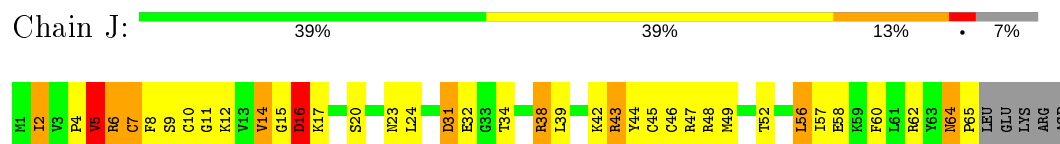
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



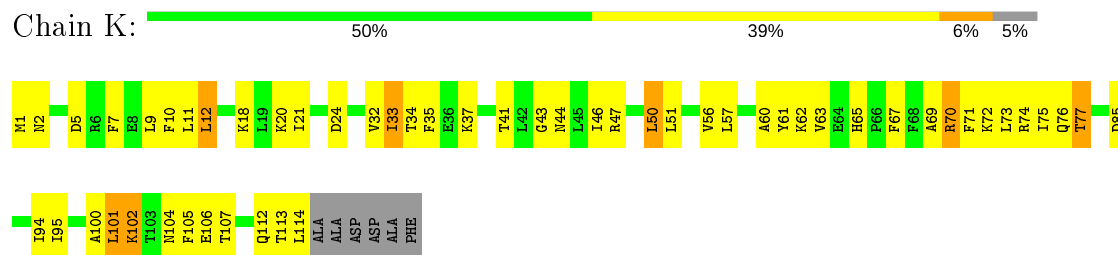
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



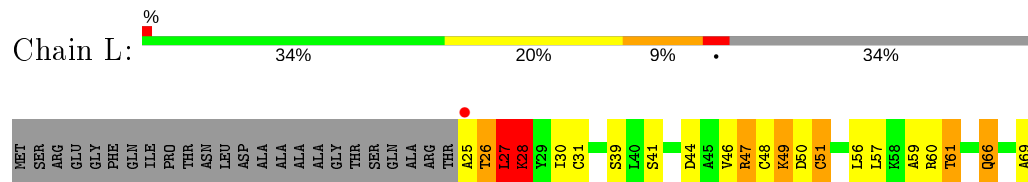
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



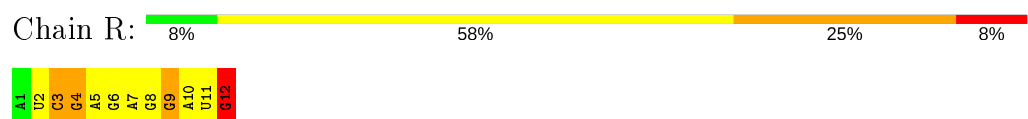
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



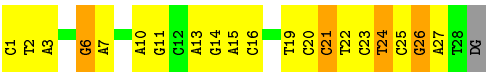
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



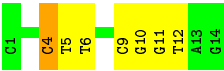
- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*G)-3')



● 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, $\alpha$ , $\beta$ , $\gamma$	170.96 Å   223.00 Å   195.41 Å 90.00°   102.28°   90.00°	Depositor
Resolution (Å)	50.00 – 3.78 42.41 – 3.79	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-3.78) 95.5 (42.41-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.76 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.253   ,   0.300 0.254   ,   0.293	Depositor DCC
$R_{free}$ test set	3441 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 78.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	30067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.53	0/11536	0.76	14/15605 (0.1%)
2	B	0.60	0/9347	0.79	15/12609 (0.1%)
3	C	0.63	0/2174	0.76	1/2946 (0.0%)
4	E	0.47	0/1793	0.64	1/2413 (0.0%)
5	F	0.47	0/696	0.74	1/940 (0.1%)
6	H	0.47	0/1105	0.79	2/1495 (0.1%)
7	I	0.53	0/989	0.72	0/1331
8	J	0.67	0/541	0.91	2/727 (0.3%)
9	K	0.65	0/937	0.71	1/1265 (0.1%)
10	L	0.58	0/365	0.90	2/485 (0.4%)
11	R	0.95	0/292	1.67	5/455 (1.1%)
12	T	0.96	1/634 (0.2%)	1.67	13/975 (1.3%)
13	N	0.91	0/317	1.53	4/488 (0.8%)
All	All	0.58	1/30726 (0.0%)	0.82	61/41734 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	23	DC	C1'-N1	5.72	1.56	1.49

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	59	ILE	CB-CA-C	-9.58	92.45	111.60
12	T	24	DT	O4'-C1'-N1	9.42	114.59	108.00
1	A	885	THR	N-CA-CB	-9.25	92.73	110.30
2	B	974	PRO	N-CA-C	-9.20	88.18	112.10
12	T	25	DC	O4'-C1'-N1	9.20	114.44	108.00
1	A	885	THR	N-CA-C	7.87	132.25	111.00
6	H	60	ALA	N-CA-C	-7.58	90.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	24	DT	N3-C4-O4	7.11	124.16	119.90
12	T	23	DC	O4'-C1'-N1	6.88	112.82	108.00
1	A	208	LEU	CA-CB-CG	6.80	130.95	115.30
1	A	1176	LEU	N-CA-C	6.70	129.10	111.00
2	B	74	LEU	CA-CB-CG	6.65	130.59	115.30
1	A	121	LEU	CA-CB-CG	6.62	130.52	115.30
10	L	28	LYS	N-CA-CB	-6.59	98.73	110.60
2	B	981	ALA	N-CA-C	6.53	128.62	111.00
10	L	27	LEU	CB-CA-C	-6.38	98.09	110.20
12	T	6	DG	P-O3'-C3'	6.33	127.30	119.70
2	B	975	GLN	N-CA-C	-6.16	94.38	111.00
11	R	3	C	O4'-C1'-N1	6.16	113.12	108.20
13	N	9	DC	O4'-C1'-N1	6.12	112.28	108.00
1	A	306	ASN	N-CA-C	6.07	127.40	111.00
3	C	37	MET	CB-CA-C	-6.05	98.30	110.40
12	T	24	DT	C5-C4-O4	-6.01	120.69	124.90
2	B	763	GLN	CB-CA-C	5.96	122.31	110.40
11	R	9	G	O4'-C1'-N9	-5.92	103.47	108.20
2	B	416	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	624	SER	N-CA-C	-5.90	95.08	111.00
12	T	20	DC	O4'-C4'-C3'	-5.83	102.17	104.50
2	B	976	ILE	N-CA-C	5.82	126.71	111.00
12	T	1	DC	P-O3'-C3'	5.77	126.62	119.70
8	J	31	ASP	CB-CA-C	5.71	121.83	110.40
13	N	6	DT	O4'-C1'-N1	5.71	112.00	108.00
1	A	884	ASP	CB-CA-C	5.70	121.80	110.40
11	R	12	G	C4-C5-N7	-5.68	108.53	110.80
11	R	12	G	N9-C4-C5	5.66	107.66	105.40
1	A	257	ARG	CB-CA-C	-5.65	99.10	110.40
12	T	21	DC	C4'-C3'-C2'	-5.61	98.05	103.10
2	B	1026	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	167	CYS	N-CA-C	-5.55	96.01	111.00
12	T	22	DT	O4'-C4'-C3'	-5.55	102.28	104.50
1	A	168	GLY	N-CA-C	5.53	126.93	113.10
2	B	1017	ILE	N-CA-CB	5.50	123.45	110.80
1	A	317	LYS	CB-CA-C	5.48	121.36	110.40
2	B	782	LEU	CA-CB-CG	5.42	127.77	115.30
5	F	76	LYS	N-CA-CB	5.34	120.22	110.60
2	B	1211	ASN	N-CA-C	5.34	125.41	111.00
9	K	9	LEU	CB-CA-C	5.28	120.22	110.20
2	B	981	ALA	CB-CA-C	-5.27	102.20	110.10
2	B	230	ALA	N-CA-C	5.26	125.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	37	LEU	CA-CB-CG	5.22	127.30	115.30
2	B	229	ALA	CB-CA-C	-5.21	102.28	110.10
11	R	9	G	C5'-C4'-O4'	5.18	115.32	109.10
8	J	5	VAL	CB-CA-C	-5.18	101.55	111.40
13	N	10	DG	P-O3'-C3'	5.18	125.92	119.70
12	T	10	DA	O4'-C1'-N9	5.16	111.61	108.00
1	A	1015	VAL	CB-CA-C	-5.12	101.66	111.40
13	N	4	DC	O4'-C1'-N1	5.12	111.58	108.00
12	T	1	DC	O4'-C1'-N1	5.07	111.55	108.00
1	A	805	LEU	CA-CB-CG	5.06	126.94	115.30
12	T	26	DG	O4'-C1'-N9	5.05	111.53	108.00
2	B	763	GLN	N-CA-C	-5.03	97.41	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	11332	0	11392	764	1
2	B	9167	0	9178	660	0
3	C	2135	0	2090	155	1
4	E	1757	0	1781	55	0
5	F	684	0	703	27	0
6	H	1087	0	1062	46	0
7	I	971	0	929	30	0
8	J	532	0	545	55	0
9	K	919	0	929	57	0
10	L	363	0	387	24	0
11	R	260	0	132	22	0
12	T	566	0	316	15	0
13	N	284	0	161	3	0
14	A	2	0	0	3	0
14	B	1	0	0	2	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	1	0	0	2	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	R	1	0	0	0	0
All	All	30067	0	29605	1752	1

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 29.

All (1752) 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	1.52	1.43
2:B:439:ALA:CB	2:B:440:HIS:HA	1.41	1.42
1:A:399:HIS:CD2	1:A:400:PRO:HD3	1.62	1.34
1:A:1081:LEU:CD2	1:A:1082:ASN:H	1.47	1.27
2:B:439:ALA:HB3	2:B:440:HIS:CA	1.66	1.24
2:B:636:PRO:CB	2:B:637:LEU:HA	1.66	1.23
1:A:1081:LEU:HD22	1:A:1082:ASN:N	1.53	1.23
1:A:115:LEU:HD12	1:A:122:MET:CE	1.73	1.18
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.22	1.14
1:A:49:LYS:HB3	1:A:55:ASP:OD2	1.46	1.14
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.49	1.13
10:L:48:CYS:HB3	10:L:51:CYS:SG	1.88	1.13
2:B:863:GLU:HA	2:B:864:LYS:HB2	1.25	1.13
1:A:399:HIS:CG	1:A:400:PRO:CD	2.33	1.12
1:A:399:HIS:CB	1:A:400:PRO:HD3	1.79	1.11
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.11
2:B:955:THR:HG22	2:B:956:THR:H	0.95	1.10
2:B:636:PRO:CB	2:B:637:LEU:CA	2.30	1.09
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.25	1.09
1:A:399:HIS:CB	1:A:400:PRO:CD	2.30	1.09
1:A:1081:LEU:HD22	1:A:1082:ASN:H	0.95	1.08
1:A:666:ILE:HD11	2:B:1026:LEU:HB3	1.13	1.08
2:B:77:HIS:CA	2:B:78:THR:HB	1.84	1.08
2:B:77:HIS:HA	2:B:78:THR:HB	1.17	1.08
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.34	1.08
1:A:399:HIS:HB3	1:A:400:PRO:CD	1.84	1.07
1:A:630:ILE:HD12	1:A:630:ILE:H	1.13	1.07
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.35	1.07
2:B:878:GLN:HG2	2:B:879:ARG:H	1.17	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HA	1:A:120:GLU:OE2	1.54	1.06
1:A:50:ILE:HG12	1:A:51:GLY:H	1.16	1.06
1:A:49:LYS:HB2	1:A:50:ILE:C	1.75	1.05
2:B:636:PRO:HB2	2:B:637:LEU:CB	1.86	1.05
1:A:272:ALA:C	1:A:296:LEU:HD11	1.77	1.04
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.39	1.04
1:A:252:PHE:HD1	1:A:256:GLN:HG2	1.19	1.03
3:C:3:GLU:HG3	3:C:4:GLU:H	1.20	1.03
2:B:979:LYS:HD3	2:B:1097:HIS:HD2	1.19	1.03
1:A:115:LEU:CD1	1:A:122:MET:HB2	1.88	1.02
2:B:769:TYR:OH	11:R:12:G:H2'	1.59	1.02
1:A:256:GLN:O	1:A:256:GLN:HG3	1.59	1.02
1:A:1081:LEU:HD13	1:A:1082:ASN:N	1.73	1.02
1:A:310:GLY:N	1:A:311:GLN:HB3	1.75	1.01
1:A:40:THR:H	1:A:41:MET:HB2	1.22	1.01
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.42	1.01
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.90	1.01
1:A:115:LEU:HD12	1:A:122:MET:HE2	1.40	0.99
1:A:254:GLU:HG2	2:B:918:ILE:HD12	1.42	0.99
1:A:666:ILE:HD11	2:B:1026:LEU:CB	1.94	0.98
1:A:107:CYS:HG	14:A:1734:ZN:ZN	0.66	0.98
3:C:3:GLU:HB3	9:K:104:ASN:HD21	1.27	0.97
2:B:906:SER:HA	2:B:946:ASN:CB	1.94	0.97
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.44	0.97
1:A:666:ILE:CD1	2:B:1026:LEU:HB3	1.94	0.97
12:T:15:DA:H2''	12:T:16:DC:H5''	1.46	0.97
10:L:25:ALA:O	10:L:27:LEU:HG	1.64	0.97
2:B:863:GLU:HA	2:B:864:LYS:CB	1.93	0.96
2:B:973:ILE:CG2	2:B:974:PRO:HD2	1.95	0.96
2:B:955:THR:CG2	2:B:956:THR:H	1.78	0.96
1:A:320:ARG:HB3	1:A:321:PRO:HD2	1.48	0.96
2:B:955:THR:HG22	2:B:956:THR:N	1.79	0.96
1:A:1084:PHE:H	1:A:1084:PHE:HD1	0.96	0.95
2:B:60:GLN:O	2:B:63:ILE:HG22	1.67	0.95
2:B:979:LYS:HD3	2:B:1097:HIS:CD2	2.02	0.95
2:B:638:PHE:CD1	2:B:743:ILE:HD13	2.00	0.95
1:A:187:LYS:O	1:A:189:ARG:HG3	1.66	0.94
2:B:994:TYR:HB2	2:B:999:MET:CE	1.98	0.94
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.30	0.94
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.29	0.94
10:L:26:THR:C	10:L:27:LEU:HG	1.84	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:4:G:H2'	11:R:5:A:H8	1.33	0.93
1:A:155:GLU:OE2	1:A:155:GLU:HA	1.67	0.93
2:B:863:GLU:CA	2:B:864:LYS:HB2	1.98	0.93
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.50	0.93
1:A:901:LEU:H	1:A:926:GLN:HE21	1.15	0.93
1:A:1062:GLU:HG2	5:F:88:TYR:OH	1.67	0.92
1:A:916:GLY:O	1:A:919:ILE:HB	1.69	0.92
1:A:310:GLY:CA	1:A:311:GLN:HB3	2.00	0.92
1:A:767:GLN:HG3	1:A:799:PHE:HB2	1.52	0.92
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.52	0.92
1:A:399:HIS:CD2	1:A:400:PRO:CD	2.49	0.91
2:B:78:THR:O	2:B:78:THR:HG23	1.68	0.91
1:A:1192:LEU:HG	1:A:1193:LEU:H	1.36	0.91
1:A:49:LYS:HB2	1:A:50:ILE:CA	2.01	0.91
1:A:252:PHE:HD1	1:A:256:GLN:CG	1.84	0.90
1:A:1084:PHE:N	1:A:1084:PHE:HD1	1.69	0.90
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.07	0.90
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.54	0.90
1:A:1386:ARG:HA	1:A:1390:ASN:HD21	1.35	0.90
2:B:784:ASN:ND2	2:B:788:ARG:HD2	1.87	0.90
2:B:906:SER:HA	2:B:946:ASN:HB3	1.54	0.89
1:A:1081:LEU:CG	1:A:1082:ASN:H	1.86	0.89
1:A:253:ASN:HA	1:A:255:SER:H	1.36	0.89
1:A:55:ASP:H	1:A:56:PRO:HD2	1.38	0.89
1:A:356:ASP:HB3	1:A:359:LEU:HD12	1.55	0.88
1:A:120:GLU:O	1:A:122:MET:N	2.05	0.88
1:A:1084:PHE:CD1	1:A:1084:PHE:N	2.38	0.88
1:A:272:ALA:CB	1:A:296:LEU:CD1	2.51	0.88
2:B:549:THR:HG22	2:B:550:ASP:H	1.38	0.88
8:J:46:CYS:HG	14:J:101:ZN:ZN	0.61	0.87
2:B:439:ALA:CB	2:B:440:HIS:CA	2.30	0.87
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.55	0.87
1:A:834:THR:HG21	1:A:1077:THR:HA	1.53	0.87
1:A:1386:ARG:HH22	12:T:15:DA:H8	1.21	0.87
1:A:160:GLN:NE2	1:A:160:GLN:H	1.73	0.86
1:A:252:PHE:CD1	1:A:256:GLN:HG2	2.09	0.86
1:A:470:LEU:HD21	1:A:487:MET:CE	2.05	0.86
1:A:115:LEU:CD1	1:A:122:MET:CB	2.53	0.86
2:B:638:PHE:CE1	2:B:743:ILE:HD13	2.10	0.86
2:B:879:ARG:CZ	2:B:879:ARG:HA	2.05	0.86
1:A:1431:GLY:HA3	2:B:1152:MET:HE1	1.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.56	0.86
2:B:878:GLN:CG	2:B:879:ARG:H	1.88	0.86
9:K:43:GLY:HA2	9:K:71:PHE:CE1	2.10	0.86
1:A:399:HIS:HB3	1:A:400:PRO:HD2	1.58	0.86
1:A:1085:HIS:HD2	1:A:1086:PHE:N	1.73	0.86
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.40	0.86
2:B:715:ALA:H	2:B:716:ASN:HA	1.40	0.85
1:A:1081:LEU:CD1	1:A:1082:ASN:N	2.39	0.85
2:B:956:THR:HA	2:B:961:LEU:O	1.77	0.85
2:B:1185:CYS:HG	14:B:1307:ZN:ZN	0.56	0.84
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.58	0.84
1:A:272:ALA:O	1:A:296:LEU:HD21	1.77	0.84
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.57	0.84
1:A:118:HIS:HB2	1:A:123:ARG:HG2	1.60	0.84
1:A:1386:ARG:NH2	12:T:15:DA:H8	1.75	0.84
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.84
1:A:272:ALA:HB1	1:A:296:LEU:HD13	1.57	0.83
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.08	0.83
1:A:1081:LEU:CD2	1:A:1082:ASN:N	2.26	0.83
1:A:1084:PHE:CE2	1:A:1086:PHE:O	2.31	0.83
1:A:272:ALA:HB1	1:A:296:LEU:CD1	2.07	0.83
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.92	0.83
2:B:76:GLN:O	2:B:77:HIS:HB2	1.78	0.83
1:A:192:GLY:O	1:A:193:ASP:HB3	1.74	0.83
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.60	0.83
1:A:286:HIS:HB3	1:A:287:HIS:HB2	1.61	0.83
2:B:878:GLN:HG2	2:B:879:ARG:N	1.90	0.83
2:B:906:SER:HA	2:B:946:ASN:HB2	1.60	0.83
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.59	0.83
2:B:85:SER:HA	2:B:86:ARG:HB3	1.58	0.83
2:B:71:LEU:HG	2:B:72:GLU:N	1.92	0.83
1:A:668:ASP:HB3	1:A:743:VAL:CG2	2.08	0.82
9:K:43:GLY:CA	9:K:71:PHE:CE1	2.62	0.82
1:A:1085:HIS:CD2	1:A:1086:PHE:N	2.47	0.82
1:A:253:ASN:HB3	1:A:254:GLU:HA	1.61	0.82
1:A:419:LYS:NZ	1:A:419:LYS:HB3	1.95	0.82
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.62	0.82
1:A:160:GLN:NE2	1:A:160:GLN:HA	1.94	0.82
2:B:604:ARG:HD3	2:B:691:GLU:OE2	1.79	0.82
2:B:78:THR:H	2:B:79:THR:HB	1.44	0.82
1:A:272:ALA:O	1:A:296:LEU:HD11	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:46:VAL:HG12	10:L:47:ARG:H	1.43	0.82
8:J:9:SER:OG	8:J:45:CYS:HB2	1.79	0.81
1:A:160:GLN:NE2	1:A:160:GLN:CA	2.43	0.81
1:A:310:GLY:H	1:A:311:GLN:HB3	1.43	0.81
1:A:115:LEU:CD1	1:A:122:MET:CG	2.59	0.81
1:A:276:LEU:HD13	1:A:296:LEU:CD2	2.11	0.81
2:B:77:HIS:HA	2:B:78:THR:CB	1.97	0.81
1:A:115:LEU:HD12	1:A:122:MET:CG	2.11	0.81
2:B:973:ILE:HG22	2:B:974:PRO:CD	2.10	0.81
1:A:320:ARG:HB3	1:A:321:PRO:CD	2.10	0.81
4:E:15:ALA:O	4:E:19:VAL:HG23	1.81	0.81
1:A:1189:SER:HB3	1:A:1241:ARG:HB3	1.63	0.80
8:J:32:GLU:CD	8:J:32:GLU:H	1.85	0.80
1:A:351:THR:HG22	1:A:468:PHE:CD1	2.17	0.80
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.64	0.80
2:B:849:GLY:HA2	2:B:852:ARG:HG3	1.64	0.80
1:A:254:GLU:CG	2:B:918:ILE:HD12	2.10	0.79
1:A:445:ASN:HB3	1:A:455:MET:HG2	1.64	0.79
1:A:821:ARG:O	1:A:825:ILE:HG12	1.82	0.79
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.64	0.79
1:A:50:ILE:HG12	1:A:51:GLY:N	1.94	0.79
1:A:345:VAL:HG12	2:B:1154:ALA:O	1.82	0.79
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.46	0.79
2:B:526:GLU:OE2	2:B:752:ALA:HB3	1.82	0.79
2:B:803:LEU:N	2:B:822:ASN:HD21	1.81	0.79
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.43	0.79
1:A:160:GLN:NE2	1:A:160:GLN:N	2.31	0.79
1:A:208:LEU:HB2	1:A:235:ILE:HD11	1.65	0.78
1:A:49:LYS:CB	1:A:55:ASP:OD2	2.30	0.78
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.64	0.78
2:B:445:LYS:HA	2:B:447:ALA:H	1.47	0.78
1:A:58:LEU:HD11	1:A:244:PRO:HD2	1.66	0.78
2:B:1174:LYS:HB2	2:B:1179:GLN:O	1.84	0.78
2:B:581:PHE:HA	2:B:585:VAL:O	1.84	0.77
2:B:603:LEU:HB3	2:B:609:ILE:HG12	1.65	0.77
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.33	0.77
2:B:994:TYR:HB2	2:B:999:MET:HE1	1.67	0.77
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.04	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.32	0.77
8:J:20:SER:O	8:J:24:LEU:HG	1.84	0.77
1:A:107:CYS:SG	14:A:1734:ZN:ZN	1.74	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.49	0.77
1:A:192:GLY:O	1:A:193:ASP:CB	2.33	0.77
1:A:630:ILE:H	1:A:630:ILE:CD1	1.89	0.77
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.85	0.77
1:A:573:SER:O	1:A:576:GLN:HB2	1.83	0.77
2:B:516:ASN:H	2:B:516:ASN:HD22	1.31	0.77
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.64	0.76
1:A:157:ASP:OD1	1:A:158:PRO:HD3	1.85	0.76
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.85	0.76
2:B:486:TYR:OH	2:B:1096:ARG:HG2	1.86	0.76
9:K:70:ARG:O	9:K:70:ARG:HG3	1.85	0.76
3:C:3:GLU:HG3	3:C:4:GLU:N	1.98	0.76
2:B:78:THR:H	2:B:79:THR:CB	1.99	0.76
10:L:25:ALA:O	10:L:27:LEU:CG	2.33	0.76
1:A:115:LEU:CD1	1:A:122:MET:HG2	2.15	0.76
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.66	0.75
1:A:203:SER:O	1:A:207:ILE:HD11	1.87	0.75
7:I:7:CYS:SG	7:I:8:ARG:O	2.44	0.75
1:A:115:LEU:HD13	1:A:122:MET:CB	2.15	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.22	0.75
5:F:74:ILE:HD13	5:F:74:ILE:H	1.51	0.75
1:A:821:ARG:HH12	2:B:514:LEU:HD13	1.50	0.75
10:L:48:CYS:CB	10:L:51:CYS:SG	2.64	0.75
3:C:101:LEU:HD13	3:C:117:ASP:O	1.87	0.75
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.21	0.75
6:H:109:LYS:HB3	6:H:111:LEU:H	1.52	0.75
1:A:917:SER:O	1:A:918:GLU:HG3	1.86	0.74
2:B:744:HIS:HD2	2:B:746:SER:OG	1.70	0.74
1:A:185:TRP:HB2	1:A:198:GLU:HG3	1.68	0.74
2:B:655:LYS:O	2:B:658:ILE:HG22	1.86	0.74
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.70	0.74
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.76	0.74
3:C:124:LEU:O	3:C:126:GLY:N	2.20	0.74
11:R:11:U:C5	11:R:12:G:C5	2.75	0.74
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.53	0.74
2:B:941:LEU:HD13	2:B:942:ARG:H	1.53	0.73
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.69	0.73
3:C:31:ASN:O	3:C:35:ARG:HG3	1.87	0.73
2:B:78:THR:N	2:B:79:THR:HB	2.03	0.73
3:C:124:LEU:C	3:C:126:GLY:H	1.90	0.73
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:LEU:HD23	2:B:484:ASN:H	1.53	0.73
2:B:762:ASN:OD1	2:B:984:HIS:HD2	1.72	0.73
1:A:91:PHE:H	1:A:297:GLN:HE22	1.34	0.73
2:B:591:ARG:O	2:B:592:ASN:HB3	1.87	0.73
1:A:767:GLN:HG3	1:A:799:PHE:CB	2.19	0.73
1:A:50:ILE:CG1	1:A:51:GLY:H	1.99	0.73
1:A:272:ALA:CB	1:A:296:LEU:HD11	2.19	0.72
1:A:55:ASP:H	1:A:56:PRO:CD	2.02	0.72
1:A:534:LEU:O	1:A:574:GLY:HA3	1.89	0.72
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.02	0.72
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.02	0.72
1:A:1431:GLY:HA3	2:B:1152:MET:CE	2.20	0.72
1:A:1081:LEU:CD1	1:A:1082:ASN:H	1.99	0.72
10:L:25:ALA:O	10:L:27:LEU:CD2	2.38	0.72
10:L:26:THR:O	10:L:27:LEU:HG	1.90	0.72
2:B:745:PRO:O	2:B:748:ILE:HG12	1.90	0.72
1:A:519:PRO:O	1:A:624:SER:HB2	1.90	0.72
1:A:1085:HIS:CD2	1:A:1086:PHE:HB2	2.25	0.72
1:A:49:LYS:H	1:A:50:ILE:HA	1.55	0.72
1:A:630:ILE:HD12	1:A:630:ILE:N	1.98	0.72
1:A:24:PRO:O	1:A:28:ARG:HB2	1.89	0.71
1:A:49:LYS:HB2	1:A:50:ILE:O	1.90	0.71
2:B:1115:THR:HB	2:B:1117:GLN:H	1.55	0.71
2:B:85:SER:CA	2:B:86:ARG:HB3	2.20	0.71
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.72	0.71
2:B:32:ALA:HB3	2:B:658:ILE:HD11	1.72	0.71
2:B:843:GLN:HG2	2:B:993:THR:HB	1.71	0.71
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.71	0.71
8:J:56:LEU:O	8:J:60:PHE:HD2	1.72	0.71
2:B:493:SER:HA	2:B:751:VAL:HG11	1.73	0.71
2:B:78:THR:HA	2:B:79:THR:O	1.90	0.71
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.73	0.71
6:H:109:LYS:HA	6:H:110:ASP:CB	2.19	0.71
1:A:115:LEU:HD13	1:A:122:MET:HG2	1.71	0.71
3:C:62:PHE:O	3:C:66:ARG:HG3	1.90	0.71
2:B:115:GLN:OE1	2:B:115:GLN:HA	1.90	0.71
2:B:77:HIS:CB	2:B:78:THR:HB	2.21	0.71
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.20	0.71
8:J:5:VAL:HA	8:J:15:GLY:H	1.55	0.71
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.26	0.70
1:A:793:SER:CB	1:A:794:PRO:HD2	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:17:LYS:HB3	8:J:39:LEU:HD23	1.73	0.70
1:A:1383:SER:O	1:A:1388:GLY:HA3	1.91	0.70
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.21	0.70
2:B:530:GLY:HA3	11:R:12:G:H22	1.55	0.70
2:B:176:SER:O	2:B:182:SER:HB3	1.91	0.70
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.73	0.70
1:A:565:ILE:HG13	6:H:97:MET:HG2	1.74	0.70
2:B:439:ALA:HB3	2:B:440:HIS:HA	0.71	0.70
2:B:796:LEU:O	2:B:799:PRO:HD3	1.91	0.70
2:B:498:THR:HG22	2:B:499:ASN:N	2.06	0.70
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.13	0.70
1:A:115:LEU:HD12	1:A:122:MET:HB2	1.70	0.70
1:A:1390:ASN:C	1:A:1392:SER:H	1.95	0.70
1:A:58:LEU:C	1:A:58:LEU:HD22	2.11	0.70
8:J:6:ARG:HG2	8:J:11:GLY:O	1.91	0.70
10:L:26:THR:O	10:L:27:LEU:CG	2.40	0.70
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.06	0.69
1:A:40:THR:N	1:A:41:MET:HB2	2.01	0.69
1:A:679:ILE:O	1:A:682:THR:HG22	1.92	0.69
6:H:109:LYS:CB	6:H:111:LEU:H	2.05	0.69
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.31	0.69
1:A:195:ASP:CG	1:A:196:GLU:H	1.95	0.69
9:K:43:GLY:HA2	9:K:71:PHE:HE1	1.58	0.69
2:B:644:GLU:HG3	2:B:654:ARG:HH22	1.56	0.69
1:A:39:GLU:O	1:A:53:LEU:HD13	1.91	0.69
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.58	0.69
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.10	0.69
2:B:973:ILE:CG2	2:B:974:PRO:CD	2.68	0.69
8:J:7:CYS:SG	8:J:10:CYS:HB2	2.33	0.69
12:T:2:DT:H2"	12:T:3:DA:C8	2.27	0.69
1:A:115:LEU:HD12	1:A:122:MET:HE3	1.74	0.69
2:B:905:VAL:N	2:B:947:GLY:O	2.25	0.69
1:A:253:ASN:HA	1:A:255:SER:N	2.06	0.69
2:B:1185:CYS:SG	14:B:1307:ZN:ZN	1.75	0.69
2:B:78:THR:CG2	2:B:78:THR:O	2.41	0.69
1:A:457:ALA:O	1:A:507:VAL:HG23	1.92	0.69
1:A:1081:LEU:HD13	1:A:1082:ASN:CA	2.22	0.68
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.21	0.68
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.73	0.68
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.59	0.68
1:A:167:CYS:SG	14:A:1734:ZN:ZN	1.82	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:O	1:A:468:PHE:HA	1.92	0.68
2:B:1084:GLN:CD	2:B:1084:GLN:H	1.97	0.68
3:C:93:ASP:O	3:C:127:ARG:NH2	2.27	0.68
2:B:596:LEU:O	2:B:600:LEU:HD23	1.94	0.68
1:A:354:SER:O	1:A:469:ARG:HA	1.94	0.68
1:A:847:ASP:HB3	1:A:1424:VAL:HG23	1.76	0.68
2:B:864:LYS:HA	2:B:864:LYS:HE2	1.75	0.68
5:F:82:THR:HG22	5:F:84:TYR:H	1.59	0.68
7:I:71:SER:HB3	7:I:85:PHE:HE2	1.58	0.68
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.74	0.68
1:A:392:VAL:HG11	1:A:424:ILE:HG21	1.76	0.67
1:A:455:MET:HE1	2:B:1134:GLU:HB3	1.75	0.67
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.76	0.67
3:C:167:HIS:CD2	3:C:169:LYS:H	2.12	0.67
1:A:41:MET:HG3	1:A:42:ASP:H	1.58	0.67
1:A:251:SER:O	1:A:252:PHE:HB3	1.93	0.67
1:A:765:VAL:CG2	1:A:800:VAL:HB	2.24	0.67
3:C:142:VAL:O	3:C:143:LEU:HB2	1.95	0.67
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.59	0.67
1:A:185:TRP:HB2	1:A:198:GLU:CG	2.23	0.67
1:A:886:ILE:HD11	1:A:943:LEU:CB	2.21	0.67
10:L:26:THR:O	10:L:27:LEU:HD12	1.95	0.67
2:B:1152:MET:O	2:B:1157:ALA:HB2	1.95	0.67
2:B:516:ASN:ND2	2:B:516:ASN:H	1.91	0.67
3:C:51:VAL:HG13	3:C:155:LEU:HD21	1.75	0.67
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.30	0.67
2:B:706:GLN:O	2:B:710:LEU:HB2	1.95	0.67
3:C:73:GLN:HE21	3:C:75:MET:H	1.43	0.67
2:B:911:ILE:O	2:B:912:ILE:HG13	1.94	0.67
3:C:124:LEU:C	3:C:126:GLY:N	2.48	0.67
4:E:89:GLY:HA2	4:E:117:THR:OG1	1.95	0.67
1:A:1013:ASP:HA	1:A:1016:THR:OG1	1.95	0.66
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.77	0.66
1:A:120:GLU:CA	1:A:120:GLU:OE2	2.36	0.66
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.95	0.66
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.16	0.66
2:B:827:ILE:CD1	2:B:1086:PHE:CD2	2.78	0.66
3:C:51:VAL:HG13	3:C:155:LEU:CD2	2.25	0.66
3:C:10:ILE:HB	9:K:112:GLN:HE21	1.60	0.66
11:R:8:G:H2'	11:R:9:G:H8	1.60	0.66
1:A:356:ASP:CB	1:A:359:LEU:HD12	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLY:O	1:A:668:ASP:HB2	1.94	0.66
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.60	0.66
2:B:1033:LYS:HA	2:B:1089:PRO:HG2	1.76	0.66
2:B:759:PRO:HB3	2:B:767:ASN:OD1	1.95	0.66
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.77	0.66
1:A:1169:ILE:H	1:A:1170:ILE:HG22	1.60	0.66
3:C:13:ALA:HA	3:C:17:ASN:O	1.95	0.66
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.30	0.66
1:A:115:LEU:CD1	1:A:122:MET:HE2	2.21	0.66
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.76	0.66
1:A:306:ASN:H	1:A:306:ASN:HD22	1.44	0.66
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.31	0.66
2:B:762:ASN:HB2	2:B:767:ASN:ND2	2.11	0.66
3:C:108:GLU:OE1	3:C:149:LYS:HE2	1.96	0.66
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.77	0.66
8:J:38:ARG:HH11	8:J:38:ARG:HB2	1.61	0.66
1:A:445:ASN:HD21	1:A:447:GLN:NE2	1.94	0.65
3:C:220:ASP:OD2	3:C:223:ALA:HB2	1.97	0.65
1:A:115:LEU:HD12	1:A:122:MET:CB	2.26	0.65
1:A:1072:ILE:HD11	1:A:1368:MET:HG2	1.77	0.65
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.78	0.65
2:B:728:ARG:HH21	2:B:1048:THR:H	1.44	0.65
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.27	0.65
3:C:8:VAL:CG2	9:K:101:LEU:HD21	2.25	0.65
2:B:716:ASN:O	2:B:717:GLU:HB2	1.96	0.65
5:F:74:ILE:N	5:F:74:ILE:CD1	2.59	0.65
1:A:1119:TYR:CD1	1:A:1326:ARG:HB3	2.31	0.65
1:A:155:GLU:CA	1:A:155:GLU:OE2	2.43	0.65
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.77	0.65
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.78	0.65
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.58	0.65
3:C:178:PHE:HD2	3:C:179:GLU:N	1.93	0.65
1:A:115:LEU:O	1:A:116:ASP:CG	2.36	0.65
1:A:272:ALA:O	1:A:296:LEU:CD2	2.43	0.65
3:C:66:ARG:HH12	8:J:4:PRO:HA	1.61	0.65
10:L:26:THR:OG1	10:L:27:LEU:N	2.30	0.65
1:A:157:ASP:N	1:A:158:PRO:HD2	2.12	0.65
1:A:719:VAL:O	1:A:723:ASN:ND2	2.29	0.65
1:A:110:CYS:HG	1:A:167:CYS:HG	1.39	0.65
3:C:58:LEU:CD2	8:J:57:ILE:HD13	2.27	0.65
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.64
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.80	0.64
4:E:213:ILE:HG12	4:E:214:CYS:H	1.63	0.64
8:J:7:CYS:SG	8:J:10:CYS:N	2.62	0.64
1:A:284:ALA:N	1:A:285:PRO:HD3	2.11	0.64
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.79	0.64
3:C:8:VAL:HG21	9:K:101:LEU:CD2	2.28	0.64
1:A:255:SER:HB2	1:A:257:ARG:HA	1.80	0.64
1:A:1081:LEU:CG	1:A:1082:ASN:N	2.48	0.64
1:A:419:LYS:HZ3	1:A:419:LYS:HB3	1.59	0.64
1:A:445:ASN:HB3	1:A:455:MET:CG	2.27	0.64
1:A:272:ALA:O	1:A:296:LEU:CD1	2.45	0.64
1:A:834:THR:CG2	1:A:1077:THR:HA	2.27	0.64
1:A:115:LEU:HD12	1:A:122:MET:SD	2.37	0.64
1:A:156:ASP:OD2	1:A:160:GLN:HG2	1.97	0.64
1:A:1434:ALA:O	1:A:1436:ILE:N	2.31	0.64
1:A:398:GLU:O	1:A:399:HIS:C	2.35	0.64
2:B:58:THR:O	2:B:61:ASP:N	2.30	0.64
2:B:77:HIS:CA	2:B:78:THR:CB	2.66	0.64
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.80	0.64
1:A:115:LEU:HD13	1:A:122:MET:CG	2.26	0.64
1:A:1390:ASN:O	1:A:1392:SER:N	2.30	0.64
1:A:118:HIS:O	1:A:120:GLU:N	2.30	0.64
1:A:306:ASN:HD22	1:A:306:ASN:N	1.96	0.64
1:A:364:VAL:HG13	1:A:366:VAL:HG23	1.78	0.64
1:A:497:THR:HG23	2:B:1146:PHE:CD1	2.33	0.64
2:B:168:GLY:H	2:B:450:ALA:HB1	1.63	0.64
3:C:43:THR:HG23	3:C:44:LEU:H	1.63	0.64
11:R:4:G:H2'	11:R:5:A:C8	2.24	0.64
1:A:40:THR:H	1:A:41:MET:CB	2.05	0.63
1:A:58:LEU:HD22	1:A:59:GLY:N	2.13	0.63
1:A:252:PHE:CD1	1:A:256:GLN:CG	2.76	0.63
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.80	0.63
8:J:10:CYS:HG	8:J:46:CYS:HG	1.47	0.63
1:A:157:ASP:N	1:A:158:PRO:CD	2.58	0.63
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.11	0.63
2:B:417:PHE:HE1	2:B:453:ILE:HG21	1.63	0.63
3:C:226:ASP:O	3:C:227:THR:CB	2.47	0.63
8:J:6:ARG:HA	8:J:12:LYS:O	1.98	0.63
1:A:889:SER:C	1:A:891:ALA:H	2.02	0.63
2:B:1097:HIS:NE2	11:R:9:G:H4'	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ALA:HB3	1:A:296:LEU:CD1	2.27	0.63
1:A:440:ASP:H	1:A:460:VAL:HG23	1.63	0.63
2:B:122:LEU:HD22	2:B:958:GLN:HE21	1.63	0.63
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.98	0.63
1:A:147:VAL:HG12	1:A:170:THR:HG22	1.81	0.63
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.33	0.63
1:A:1089:VAL:HG13	1:A:1090:ALA:N	2.15	0.62
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.34	0.62
3:C:178:PHE:C	3:C:178:PHE:HD2	2.02	0.62
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.64	0.62
1:A:188:ASP:O	1:A:189:ARG:HG2	2.00	0.62
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.14	0.62
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.62
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.29	0.62
2:B:762:ASN:HB2	2:B:767:ASN:HD21	1.65	0.62
2:B:769:TYR:OH	11:R:12:G:C2'	2.43	0.62
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.14	0.62
3:C:226:ASP:O	3:C:227:THR:HB	2.00	0.62
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.80	0.62
2:B:979:LYS:CD	2:B:1097:HIS:HD2	2.04	0.62
4:E:88:VAL:HG23	4:E:116:ILE:HA	1.82	0.62
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.34	0.62
1:A:399:HIS:CG	1:A:400:PRO:N	2.67	0.62
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.62
1:A:1189:SER:CB	1:A:1241:ARG:HB3	2.29	0.62
1:A:310:GLY:HA2	1:A:311:GLN:HB3	1.81	0.62
1:A:807:GLY:HA3	2:B:728:ARG:HH11	1.65	0.61
2:B:57:TYR:O	2:B:58:THR:C	2.38	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD12	1.82	0.61
1:A:55:ASP:N	1:A:56:PRO:CD	2.62	0.61
1:A:575:LYS:NZ	1:A:602:ASP:OD2	2.31	0.61
2:B:637:LEU:CD1	2:B:740:HIS:HB3	2.29	0.61
3:C:3:GLU:CG	3:C:4:GLU:H	2.04	0.61
3:C:8:VAL:HG21	9:K:101:LEU:HD21	1.83	0.61
10:L:26:THR:O	10:L:27:LEU:CD1	2.48	0.61
1:A:360:GLU:HB2	1:A:363:GLN:CD	2.21	0.61
2:B:492:LEU:HB3	2:B:751:VAL:HG21	1.82	0.61
2:B:861:ASP:OD2	2:B:914:LYS:HE2	1.99	0.61
3:C:228:PHE:N	3:C:228:PHE:CD1	2.66	0.61
11:R:11:U:H5	11:R:12:G:C4	2.18	0.61
1:A:1377:THR:HB	4:E:176:PRO:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HB2	1:A:50:ILE:HA	1.81	0.61
2:B:1115:THR:O	2:B:1198:TYR:HD2	1.81	0.61
2:B:872:GLU:CD	2:B:916:THR:HB	2.21	0.61
3:C:142:VAL:HG23	8:J:15:GLY:HA3	1.82	0.61
1:A:254:GLU:HG2	2:B:918:ILE:CD1	2.24	0.61
1:A:313:GLN:HB2	1:A:314:ALA:CA	2.29	0.61
1:A:356:ASP:OD2	9:K:65:HIS:CE1	2.53	0.61
1:A:399:HIS:O	1:A:401:GLY:N	2.33	0.61
2:B:471:LYS:HB2	2:B:472:ALA:HA	1.81	0.61
2:B:619:ILE:HG21	7:I:62:ILE:HA	1.81	0.61
2:B:77:HIS:ND1	2:B:78:THR:HB	2.15	0.61
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.29	0.61
8:J:6:ARG:H	8:J:14:VAL:H	1.48	0.61
3:C:73:GLN:HE21	3:C:75:MET:N	1.97	0.61
6:H:110:ASP:HB3	6:H:111:LEU:HD12	1.82	0.61
1:A:48:ALA:C	1:A:49:LYS:HD2	2.21	0.61
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.34	0.61
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.16	0.61
1:A:115:LEU:CD1	1:A:122:MET:CE	2.65	0.61
1:A:313:GLN:HB2	1:A:314:ALA:HA	1.82	0.61
2:B:1051:THR:O	2:B:1055:ILE:HG12	2.00	0.61
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.82	0.61
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.82	0.61
2:B:1156:ASP:CB	2:B:1198:TYR:H	2.13	0.61
3:C:178:PHE:C	3:C:178:PHE:CD2	2.73	0.61
2:B:530:GLY:HA3	11:R:12:G:N2	2.16	0.61
1:A:55:ASP:O	1:A:57:ARG:N	2.34	0.61
4:E:19:VAL:O	4:E:23:VAL:HG23	2.00	0.61
6:H:104:PHE:HE1	6:H:136:LYS:HG2	1.66	0.61
10:L:60:ARG:HG3	10:L:61:THR:H	1.66	0.60
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.60
2:B:439:ALA:HB1	2:B:440:HIS:HA	1.70	0.60
3:C:55:THR:OG1	3:C:151:GLN:HA	2.00	0.60
8:J:7:CYS:HG	8:J:10:CYS:H	1.46	0.60
6:H:104:PHE:CE1	6:H:136:LYS:HG2	2.35	0.60
3:C:3:GLU:CB	9:K:104:ASN:HD21	2.08	0.60
1:A:946:VAL:HG22	4:E:201:LYS:HB3	1.82	0.60
2:B:58:THR:O	2:B:59:LEU:C	2.40	0.60
1:A:120:GLU:C	1:A:122:MET:H	2.03	0.60
1:A:1431:GLY:O	2:B:1152:MET:HE2	2.01	0.60
1:A:91:PHE:H	1:A:297:GLN:NE2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.30	0.60
2:B:33:VAL:HG11	2:B:638:PHE:CZ	2.37	0.60
1:A:1177:LEU:H	1:A:1178:ASP:HB3	1.66	0.60
1:A:185:TRP:O	1:A:186:LYS:HG2	2.01	0.60
1:A:265:LYS:HA	1:A:268:ASP:HB2	1.84	0.60
2:B:861:ASP:OD1	2:B:862:GLN:N	2.35	0.60
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.67	0.60
3:C:32:SER:O	3:C:36:VAL:HG12	2.01	0.60
9:K:43:GLY:HA3	9:K:71:PHE:CE1	2.37	0.60
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.82	0.60
3:C:235:VAL:HG11	8:J:6:ARG:HH21	1.67	0.60
9:K:46:ILE:O	9:K:50:LEU:HB2	2.02	0.60
10:L:41:SER:O	10:L:44:ASP:HB2	2.01	0.60
2:B:1115:THR:O	2:B:1198:TYR:CD2	2.55	0.60
1:A:316:GLN:HG2	1:A:322:VAL:HG13	1.83	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.83	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.59
1:A:185:TRP:HH2	1:A:200:ARG:HH11	1.48	0.59
1:A:623:GLY:O	1:A:625:SER:N	2.36	0.59
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.17	0.59
1:A:1386:ARG:NH2	12:T:15:DA:C8	2.64	0.59
1:A:252:PHE:O	1:A:256:GLN:HG2	2.02	0.59
2:B:441:ASP:O	2:B:443:ASN:N	2.34	0.59
2:B:994:TYR:HB2	2:B:999:MET:HE3	1.81	0.59
1:A:262:LEU:O	1:A:266:LEU:HD23	2.03	0.59
1:A:451:HIS:HB3	1:A:453:MET:H	1.68	0.59
1:A:455:MET:CE	2:B:1130:PHE:HE1	2.16	0.59
1:A:767:GLN:CG	1:A:799:PHE:HB2	2.29	0.59
2:B:20:ASP:O	2:B:21:GLU:HG2	2.02	0.59
2:B:301:ILE:HG22	2:B:302:CYS:N	2.18	0.59
1:A:1021:LEU:CD1	1:A:1025:ARG:HE	2.16	0.59
1:A:160:GLN:N	1:A:160:GLN:CD	2.55	0.59
1:A:424:ILE:O	1:A:424:ILE:HG23	2.03	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.35	0.59
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.83	0.59
2:B:977:GLY:O	2:B:1099:VAL:HG13	2.02	0.59
2:B:978:ASP:O	2:B:980:PHE:HD1	1.85	0.59
2:B:762:ASN:OD1	2:B:984:HIS:CD2	2.53	0.59
4:E:198:ILE:HD11	4:E:212:ARG:HD2	1.82	0.59
2:B:769:TYR:HE1	11:R:12:G:HO2'	1.51	0.59
1:A:599:SER:HB2	1:A:603:ASN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:O	2:B:275:TYR:HB2	2.03	0.59
2:B:474:SER:O	2:B:475:SER:O	2.21	0.59
5:F:74:ILE:H	5:F:74:ILE:CD1	2.14	0.59
1:A:377:PRO:HB3	1:A:431:LYS:HD3	1.84	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.85	0.59
3:C:43:THR:CG2	3:C:44:LEU:N	2.65	0.59
3:C:8:VAL:CG2	9:K:101:LEU:CD2	2.80	0.59
1:A:364:VAL:O	1:A:364:VAL:HG13	2.01	0.58
2:B:211:VAL:CG2	2:B:483:LEU:HG	2.33	0.58
2:B:715:ALA:N	2:B:716:ASN:HA	2.10	0.58
2:B:77:HIS:ND1	2:B:78:THR:HG21	2.18	0.58
1:A:1151:GLU:HG3	1:A:1194:ARG:HB3	1.85	0.58
1:A:1168:GLU:HG2	1:A:1171:GLN:HB3	1.85	0.58
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.84	0.58
2:B:792:MET:O	2:B:793:ALA:HB2	2.03	0.58
2:B:878:GLN:O	2:B:879:ARG:NH2	2.36	0.58
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.33	0.58
2:B:978:ASP:OD1	2:B:1099:VAL:HG22	2.03	0.58
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.18	0.58
1:A:483:ASP:HB3	2:B:837:ASP:HB3	1.85	0.58
6:H:38:LEU:HD12	6:H:124:ARG:O	2.04	0.58
1:A:915:SER:O	1:A:917:SER:O	2.21	0.58
4:E:31:THR:HG23	4:E:34:GLU:HB2	1.86	0.58
2:B:863:GLU:CA	2:B:864:LYS:CB	2.71	0.58
4:E:23:VAL:HB	4:E:30:ILE:HD11	1.86	0.58
6:H:114:VAL:HG22	6:H:125:LEU:HB3	1.86	0.58
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.69	0.58
2:B:202:TYR:CD1	2:B:209:GLU:HB3	2.39	0.58
2:B:555:ILE:HA	2:B:558:LEU:HD12	1.86	0.58
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.04	0.58
4:E:16:PHE:CE2	4:E:20:LYS:HE2	2.39	0.58
7:I:17:ARG:NH1	7:I:28:GLU:HG2	2.18	0.58
2:B:354:ASP:HA	2:B:357:GLN:HB2	1.86	0.57
2:B:487:THR:HG22	2:B:488:TYR:N	2.19	0.57
1:A:670:ILE:HG22	1:A:671:ALA:H	1.69	0.57
4:E:78:LEU:HD12	4:E:107:THR:HB	1.85	0.57
3:C:58:LEU:HD23	8:J:57:ILE:HD13	1.86	0.57
1:A:1029:ARG:O	1:A:1033:GLN:HB2	2.04	0.57
1:A:402:ALA:O	1:A:415:LEU:HD12	2.04	0.57
6:H:109:LYS:HG2	6:H:111:LEU:HB2	1.85	0.57
2:B:638:PHE:CE1	2:B:743:ILE:CD1	2.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:GLN:NE2	2:B:976:ILE:HG22	2.20	0.57
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.68	0.57
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.86	0.57
2:B:77:HIS:ND1	2:B:78:THR:CB	2.67	0.57
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.39	0.57
1:A:567:LYS:NZ	6:H:46:LEU:HB2	2.20	0.57
2:B:436:VAL:HA	2:B:437:GLU:C	2.25	0.57
2:B:79:THR:HG22	2:B:80:GLU:H	1.69	0.57
1:A:726:ARG:O	1:A:730:GLY:N	2.36	0.57
2:B:487:THR:HG22	2:B:488:TYR:H	1.69	0.57
3:C:142:VAL:HG13	3:C:143:LEU:H	1.69	0.57
1:A:186:LYS:NZ	1:A:194:ALA:HB1	2.20	0.57
2:B:860:MET:SD	2:B:861:ASP:N	2.78	0.57
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.44	0.57
10:L:28:LYS:HG3	10:L:39:SER:OG	2.04	0.57
1:A:1085:HIS:HD2	1:A:1086:PHE:H	1.52	0.57
8:J:48:ARG:O	8:J:52:THR:OG1	2.23	0.57
1:A:676:MET:HA	1:A:679:ILE:HD12	1.86	0.57
2:B:526:GLU:C	2:B:527:THR:HG22	2.26	0.57
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.05	0.57
2:B:636:PRO:CB	2:B:637:LEU:HB3	2.23	0.56
1:A:577:ILE:HG13	1:A:578:LEU:N	2.18	0.56
1:A:915:SER:HB3	1:A:919:ILE:HG13	1.86	0.56
2:B:766:ARG:HE	2:B:1020:ARG:HB2	1.70	0.56
1:A:658:LEU:HD13	2:B:831:SER:N	2.20	0.56
13:N:4:DC:H2"	13:N:5:DT:OP2	2.05	0.56
2:B:417:PHE:CE1	2:B:453:ILE:HG21	2.40	0.56
2:B:216:GLU:N	2:B:499:ASN:O	2.36	0.56
2:B:765:PRO:O	2:B:769:TYR:HB2	2.05	0.56
1:A:1089:VAL:HG13	1:A:1090:ALA:H	1.69	0.56
1:A:419:LYS:HZ2	1:A:419:LYS:HB3	1.70	0.56
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.36	0.56
9:K:102:LYS:O	9:K:106:GLU:HG2	2.06	0.56
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.35	0.56
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.87	0.56
2:B:591:ARG:O	2:B:592:ASN:CB	2.52	0.56
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.40	0.56
1:A:579:SER:HB3	1:A:611:GLN:HA	1.87	0.56
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.87	0.56
2:B:827:ILE:HD11	2:B:1086:PHE:CD2	2.40	0.56
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.86	0.56
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.34	0.56
1:A:901:LEU:N	1:A:926:GLN:HE21	1.94	0.56
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.38	0.56
1:A:1085:HIS:CD2	1:A:1085:HIS:C	2.78	0.56
1:A:330:LYS:O	1:A:334:GLY:HA3	2.06	0.56
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.88	0.56
3:C:248:ILE:CD1	9:K:101:LEU:HD13	2.36	0.56
2:B:964:VAL:HG12	2:B:965:LYS:N	2.21	0.56
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.72	0.55
1:A:803:SER:OG	1:A:806:ARG:HG3	2.06	0.55
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.87	0.55
2:B:635:ARG:O	2:B:636:PRO:C	2.44	0.55
2:B:839:MET:HG2	2:B:989:THR:O	2.07	0.55
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.87	0.55
1:A:1243:VAL:HG13	1:A:1244:ARG:HB2	1.87	0.55
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.87	0.55
1:A:455:MET:HE2	2:B:1130:PHE:HE1	1.70	0.55
2:B:498:THR:CG2	2:B:499:ASN:N	2.69	0.55
2:B:856:PHE:HB3	2:B:967:ARG:HD2	1.88	0.55
8:J:45:CYS:O	8:J:48:ARG:HG3	2.06	0.55
1:A:513:SER:C	1:A:515:GLN:H	2.07	0.55
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.87	0.55
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.89	0.55
1:A:1449:SER:HA	1:A:1450:LEU:C	2.27	0.55
1:A:157:ASP:CB	1:A:158:PRO:HD3	2.36	0.55
1:A:715:GLU:O	1:A:719:VAL:HG23	2.06	0.55
2:B:1033:LYS:CA	2:B:1089:PRO:HG2	2.36	0.55
4:E:157:SER:OG	4:E:160:GLU:HB2	2.06	0.55
1:A:1407:GLU:HA	1:A:1410:PHE:HB2	1.87	0.55
2:B:825:VAL:O	2:B:1087:PHE:HA	2.06	0.55
2:B:648:HIS:CD2	2:B:649:LYS:H	2.24	0.55
2:B:795:ILE:HG22	2:B:796:LEU:H	1.71	0.55
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.21	0.55
2:B:525:ALA:O	2:B:527:THR:HG22	2.06	0.55
9:K:69:ALA:O	9:K:70:ARG:HB3	2.06	0.55
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.26	0.55
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.20	0.55
1:A:1390:ASN:C	1:A:1392:SER:N	2.59	0.55
1:A:203:SER:O	1:A:207:ILE:CD1	2.54	0.55
2:B:383:ASN:O	2:B:387:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HA	6:H:110:ASP:HB3	1.88	0.55
1:A:1119:TYR:HD1	1:A:1326:ARG:HB3	1.70	0.55
1:A:672:ASP:H	1:A:736:ASN:HD21	1.55	0.55
2:B:826:ALA:O	2:B:1011:ILE:HA	2.07	0.55
2:B:710:LEU:HD13	2:B:733:HIS:HB3	1.89	0.55
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.07	0.55
7:I:59:VAL:HB	7:I:61:ASP:H	1.72	0.55
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.72	0.55
1:A:18:GLN:NE2	1:A:228:PHE:CD1	2.75	0.55
1:A:663:SER:O	1:A:742:ASN:CG	2.46	0.55
2:B:73:GLN:HG3	2:B:86:ARG:HG3	1.89	0.55
1:A:195:ASP:O	1:A:196:GLU:C	2.46	0.54
2:B:1150:ARG:O	2:B:1151:LEU:HD12	2.07	0.54
2:B:983:ARG:HG3	2:B:1093:GLN:OE1	2.06	0.54
2:B:57:TYR:O	2:B:59:LEU:N	2.40	0.54
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.88	0.54
5:F:81:THR:HG23	5:F:144:GLU:OE1	2.07	0.54
1:A:187:LYS:O	1:A:189:ARG:CG	2.50	0.54
1:A:527:THR:HG21	1:A:650:GLN:HG2	1.89	0.54
1:A:889:SER:C	1:A:891:ALA:N	2.59	0.54
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.42	0.54
2:B:77:HIS:CG	2:B:78:THR:HB	2.42	0.54
2:B:849:GLY:CA	2:B:852:ARG:HG3	2.36	0.54
2:B:998:ASP:OD2	3:C:35:ARG:NH2	2.39	0.54
1:A:901:LEU:HD12	1:A:926:GLN:HG2	1.88	0.54
2:B:728:ARG:NH2	2:B:1048:THR:H	2.05	0.54
1:A:203:SER:O	1:A:207:ILE:CG1	2.55	0.54
2:B:118:ARG:HA	2:B:207:GLY:HA2	1.89	0.54
2:B:745:PRO:C	2:B:747:MET:H	2.11	0.54
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.89	0.54
3:C:142:VAL:HG22	3:C:143:LEU:N	2.21	0.54
3:C:33:LEU:O	3:C:37:MET:HE3	2.08	0.54
2:B:469:GLN:O	2:B:470:LYS:HB2	2.07	0.54
2:B:879:ARG:HA	2:B:879:ARG:NE	2.21	0.54
8:J:16:ASP:OD1	8:J:16:ASP:N	2.41	0.54
1:A:350:ARG:O	1:A:351:THR:HB	2.07	0.54
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.43	0.54
1:A:1431:GLY:CA	2:B:1152:MET:HE1	2.33	0.54
2:B:976:ILE:O	2:B:990:ILE:O	2.24	0.54
1:A:49:LYS:HD2	1:A:49:LYS:N	2.22	0.54
1:A:696:GLU:HG2	1:A:701:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.42	0.54
2:B:878:GLN:CG	2:B:879:ARG:N	2.59	0.54
1:A:1086:PHE:HE1	1:A:1092:LYS:HG2	1.73	0.54
1:A:1429:ILE:O	1:A:1429:ILE:HG22	2.06	0.54
1:A:901:LEU:H	1:A:926:GLN:NE2	1.95	0.54
2:B:1153:GLU:N	2:B:1153:GLU:OE2	2.41	0.54
2:B:363:HIS:O	2:B:364:ILE:HB	2.08	0.54
3:C:36:VAL:HA	3:C:40:GLU:HB2	1.90	0.54
3:C:63:ILE:O	3:C:66:ARG:N	2.40	0.54
1:A:567:LYS:O	1:A:569:LYS:N	2.41	0.54
1:A:253:ASN:CB	1:A:254:GLU:HA	2.32	0.53
1:A:819:GLY:O	1:A:820:GLY:C	2.47	0.53
2:B:1175:LEU:HD23	2:B:1176:ASN:H	1.73	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.90	0.53
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.90	0.53
2:B:863:GLU:HA	2:B:864:LYS:CG	2.37	0.53
1:A:302:THR:HG21	1:A:314:ALA:HB3	1.89	0.53
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.07	0.53
3:C:178:PHE:CD2	3:C:179:GLU:N	2.76	0.53
8:J:7:CYS:SG	8:J:7:CYS:O	2.54	0.53
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.43	0.53
1:A:353:ILE:HD13	1:A:487:MET:CE	2.26	0.53
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.44	0.53
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.43	0.53
2:B:706:GLN:HB2	2:B:710:LEU:HD23	1.91	0.53
8:J:10:CYS:HB2	8:J:46:CYS:SG	2.49	0.53
11:R:6:G:H2'	11:R:7:A:H8	1.73	0.53
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.43	0.53
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.74	0.53
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.53
1:A:1146:VAL:O	1:A:1197:LEU:HD22	2.08	0.53
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.90	0.53
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.90	0.53
2:B:978:ASP:HB2	2:B:980:PHE:CE1	2.43	0.53
1:A:956:LEU:HD23	1:A:957:PRO:CD	2.39	0.53
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.44	0.53
1:A:1086:PHE:HE1	1:A:1092:LYS:CG	2.21	0.53
1:A:364:VAL:CG1	1:A:364:VAL:O	2.57	0.53
1:A:468:PHE:CE2	1:A:489:LEU:HD13	2.44	0.53
2:B:486:TYR:CZ	2:B:1096:ARG:HG2	2.43	0.53
1:A:49:LYS:N	1:A:50:ILE:HA	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:TYR:N	3:C:229:TYR:CD1	2.76	0.53
9:K:65:HIS:O	9:K:67:PHE:N	2.42	0.53
1:A:1080:THR:CG2	1:A:1098:VAL:HG23	2.38	0.53
1:A:819:GLY:O	1:A:822:GLU:N	2.40	0.53
1:A:419:LYS:NZ	1:A:419:LYS:CB	2.70	0.53
1:A:447:GLN:HG3	1:A:449:SER:OG	2.09	0.53
1:A:458:HIS:NE2	1:A:507:VAL:HG21	2.24	0.53
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.39	0.53
6:H:95:TYR:HD2	6:H:96:VAL:N	2.07	0.53
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.91	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.91	0.52
2:B:459:TYR:C	2:B:459:TYR:CD2	2.82	0.52
2:B:85:SER:CA	2:B:86:ARG:CB	2.84	0.52
3:C:228:PHE:HD1	3:C:228:PHE:N	2.08	0.52
5:F:74:ILE:HD13	5:F:74:ILE:N	2.19	0.52
6:H:37:LYS:H	6:H:126:GLU:HB3	1.74	0.52
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.50	0.52
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.91	0.52
1:A:1128:GLN:HB3	1:A:1304:TRP:CE2	2.45	0.52
1:A:1389:PHE:O	1:A:1390:ASN:OD1	2.27	0.52
1:A:208:LEU:CB	1:A:235:ILE:HD11	2.37	0.52
1:A:534:LEU:HA	1:A:539:THR:HG21	1.90	0.52
1:A:815:PHE:O	1:A:818:MET:HB2	2.09	0.52
4:E:79:TRP:NE1	4:E:81:GLU:HG3	2.25	0.52
5:F:132:LEU:O	5:F:148:VAL:HG23	2.09	0.52
7:I:17:ARG:HH12	7:I:28:GLU:HG2	1.75	0.52
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.09	0.52
1:A:1349:TYR:O	1:A:1350:LYS:C	2.46	0.52
1:A:962:ARG:O	1:A:966:ASN:HB2	2.09	0.52
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.52
3:C:80:LEU:HD21	3:C:95:CYS:O	2.09	0.52
1:A:11:LEU:HA	2:B:1193:GLN:O	2.08	0.52
1:A:55:ASP:HA	1:A:58:LEU:O	2.10	0.52
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.92	0.52
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.49	0.52
1:A:74:MET:HG3	1:A:74:MET:O	2.10	0.52
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.71	0.52
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.91	0.52
1:A:512:VAL:HA	1:A:519:PRO:HA	1.90	0.52
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.40	0.52
2:B:1112:GLN:HG2	2:B:1119:VAL:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:MET:SD	2:B:1210:MET:HG3	2.50	0.52
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.92	0.52
2:B:915:THR:HB	2:B:934:LYS:HB3	1.91	0.52
2:B:95:ILE:O	2:B:95:ILE:HG23	2.10	0.52
3:C:220:ASP:OD2	3:C:223:ALA:CB	2.57	0.52
1:A:663:SER:O	1:A:742:ASN:OD1	2.27	0.52
2:B:1008:PRO:HG3	2:B:1087:PHE:CE1	2.45	0.52
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.91	0.52
2:B:488:TYR:C	2:B:490:SER:H	2.13	0.52
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.91	0.52
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.92	0.52
2:B:1074:ASN:HB3	2:B:1077:THR:HG22	1.92	0.52
2:B:498:THR:HG22	2:B:499:ASN:H	1.74	0.52
2:B:58:THR:O	2:B:60:GLN:N	2.43	0.52
2:B:764:SER:HB2	2:B:765:PRO:HD3	1.92	0.52
2:B:911:ILE:CG2	2:B:912:ILE:HG13	2.40	0.52
1:A:469:ARG:NH2	2:B:991:GLY:O	2.43	0.52
1:A:664:THR:OG1	2:B:1014:PRO:HB2	2.10	0.52
2:B:386:LEU:C	2:B:388:CYS:H	2.12	0.52
2:B:784:ASN:OD1	2:B:784:ASN:N	2.42	0.52
8:J:46:CYS:SG	14:J:101:ZN:ZN	1.79	0.52
11:R:5:A:H2'	11:R:6:G:C8	2.45	0.52
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.24	0.51
1:A:272:ALA:CA	1:A:296:LEU:HD11	2.40	0.51
2:B:827:ILE:HD11	2:B:1086:PHE:HD2	1.73	0.51
1:A:455:MET:CE	2:B:1130:PHE:CE1	2.93	0.51
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.45	0.51
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.44	0.51
1:A:446:ARG:NH1	1:A:478:TYR:O	2.42	0.51
1:A:686:ALA:HB1	1:A:725:ALA:HB2	1.92	0.51
2:B:1060:ARG:HD2	2:B:1064:TYR:O	2.10	0.51
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.11	0.51
1:A:464:PRO:C	1:A:465:TYR:HD1	2.13	0.51
2:B:497:ARG:HE	2:B:538:ASN:HD21	1.57	0.51
2:B:402:GLY:HA3	2:B:695:ALA:HB3	1.90	0.51
5:F:81:THR:CG2	5:F:144:GLU:OE1	2.58	0.51
6:H:95:TYR:HD2	6:H:95:TYR:C	2.12	0.51
7:I:100:PHE:CE2	7:I:111:THR:HG23	2.45	0.51
1:A:886:ILE:O	1:A:944:ARG:NH2	2.39	0.51
3:C:144:ILE:N	3:C:144:ILE:HD13	2.25	0.51
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLU:HG2	5:F:88:TYR:CZ	2.44	0.51
1:A:1086:PHE:O	1:A:1087:ALA:HB3	2.11	0.51
1:A:915:SER:HB3	1:A:919:ILE:CG1	2.41	0.51
2:B:1032:SER:O	2:B:1033:LYS:C	2.49	0.51
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.93	0.51
2:B:874:PHE:CZ	2:B:964:VAL:HG23	2.44	0.51
3:C:71:PRO:HB2	3:C:133:ILE:HD12	1.90	0.51
4:E:191:LYS:HG2	4:E:192:ARG:H	1.75	0.51
4:E:64:PRO:HG3	4:E:76:GLY:HA2	1.91	0.51
12:T:26:DG:N2	12:T:27:DA:H1'	2.25	0.51
1:A:354:SER:OG	1:A:467:THR:HG21	2.11	0.51
3:C:35:ARG:HH11	3:C:35:ARG:HB3	1.75	0.51
1:A:942:PHE:C	1:A:942:PHE:CD2	2.84	0.51
2:B:994:TYR:CB	2:B:999:MET:CE	2.81	0.51
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.25	0.51
11:R:11:U:H5	11:R:12:G:C5	2.23	0.51
1:A:775:ILE:HB	1:A:797:LYS:C	2.31	0.51
2:B:1002:THR:HG21	2:B:1006:ILE:HG13	1.92	0.51
2:B:349:ILE:O	2:B:353:LYS:N	2.39	0.51
1:A:821:ARG:NH1	2:B:514:LEU:HD13	2.22	0.51
3:C:173:ALA:O	3:C:233:GLU:O	2.28	0.51
4:E:88:VAL:HG21	4:E:116:ILE:HD13	1.91	0.51
1:A:556:TRP:O	1:A:558:GLY:N	2.43	0.51
1:A:572:TRP:HE3	1:A:572:TRP:N	2.08	0.51
1:A:578:LEU:O	1:A:581:ALA:HB3	2.11	0.51
3:C:88:CYS:SG	3:C:88:CYS:O	2.69	0.51
5:F:82:THR:O	5:F:136:ARG:NH1	2.44	0.51
1:A:403:LYS:HG3	1:A:404:TYR:CE1	2.46	0.51
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.45	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.93	0.51
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.75	0.51
12:T:11:DG:H1	13:N:4:DC:H42	1.59	0.51
2:B:731:VAL:O	2:B:732:SER:CB	2.59	0.50
1:A:1081:LEU:HD13	1:A:1082:ASN:CB	2.41	0.50
1:A:326:ARG:HE	1:A:1406:VAL:HG21	1.75	0.50
1:A:444:PHE:CZ	1:A:470:LEU:HD23	2.46	0.50
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.93	0.50
2:B:1204:PHE:O	2:B:1208:MET:HG3	2.11	0.50
2:B:531:GLN:HG2	2:B:531:GLN:O	2.11	0.50
2:B:731:VAL:O	2:B:732:SER:HB3	2.11	0.50
2:B:780:VAL:HG12	2:B:817:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:994:TYR:CB	2:B:999:MET:HE3	2.41	0.50
6:H:41:ASP:CB	6:H:121:LEU:HB3	2.41	0.50
6:H:95:TYR:CD2	6:H:95:TYR:C	2.84	0.50
1:A:278:THR:HG23	1:A:282:ASN:HD22	1.76	0.50
1:A:320:ARG:CB	1:A:321:PRO:CD	2.81	0.50
1:A:39:GLU:HB3	1:A:41:MET:CB	2.35	0.50
1:A:572:TRP:N	1:A:572:TRP:CE3	2.79	0.50
2:B:114:PRO:HG2	2:B:181:LEU:HD21	1.94	0.50
2:B:345:LYS:HG2	2:B:348:ARG:NH2	2.26	0.50
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.75	0.50
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.12	0.50
2:B:25:ILE:HG22	2:B:26:THR:N	2.26	0.50
2:B:529:GLU:HA	2:B:533:CYS:HB2	1.92	0.50
2:B:603:LEU:HB3	2:B:609:ILE:CG1	2.38	0.50
4:E:205:SER:O	4:E:206:GLY:C	2.49	0.50
6:H:109:LYS:CA	6:H:111:LEU:H	2.24	0.50
1:A:193:ASP:O	1:A:194:ALA:O	2.30	0.50
2:B:472:ALA:HB1	2:B:476:ARG:H	1.77	0.50
2:B:840:ILE:HD12	2:B:1011:ILE:HD12	1.93	0.50
4:E:179:GLN:O	4:E:182:ASP:HB2	2.11	0.50
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.12	0.50
1:A:1177:LEU:HB3	1:A:1178:ASP:HB2	1.94	0.50
1:A:1391:ARG:O	1:A:1391:ARG:HG3	2.12	0.50
1:A:158:PRO:HA	1:A:159:THR:OG1	2.12	0.50
1:A:376:TYR:CZ	1:A:498:ARG:HD2	2.46	0.50
1:A:470:LEU:CD2	1:A:487:MET:HE1	2.41	0.50
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.12	0.50
1:A:6:TYR:O	2:B:1175:LEU:HD21	2.11	0.50
1:A:403:LYS:HG3	1:A:404:TYR:HE1	1.77	0.50
2:B:126:SER:HB2	2:B:172:ILE:HD11	1.92	0.50
2:B:174:LEU:HD11	2:B:204:ILE:HD13	1.93	0.50
2:B:785:TYR:C	2:B:785:TYR:CD1	2.84	0.50
3:C:100:THR:HG22	3:C:119:VAL:HG12	1.94	0.50
3:C:96:SER:HB2	3:C:158:VAL:HG12	1.93	0.50
3:C:35:ARG:HB3	3:C:35:ARG:NH1	2.27	0.50
1:A:870:GLU:OE1	4:E:202:SER:HB2	2.12	0.50
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.94	0.50
1:A:306:ASN:HB2	1:A:313:GLN:OE1	2.10	0.50
1:A:398:GLU:O	1:A:399:HIS:O	2.30	0.50
2:B:1025:HIS:HD1	2:B:1025:HIS:C	2.14	0.50
2:B:680:THR:O	2:B:683:SER:OG	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:ASP:O	2:B:980:PHE:CD1	2.63	0.50
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.94	0.50
1:A:103:CYS:HB3	1:A:174:ILE:HD13	1.94	0.50
1:A:1088:GLY:O	1:A:1089:VAL:HG12	2.12	0.50
1:A:185:TRP:CH2	1:A:200:ARG:HD2	2.47	0.50
1:A:195:ASP:CG	1:A:196:GLU:N	2.64	0.50
1:A:195:ASP:OD1	1:A:196:GLU:N	2.45	0.50
1:A:313:GLN:HB2	1:A:314:ALA:HB2	1.94	0.50
1:A:451:HIS:HB3	1:A:453:MET:N	2.27	0.50
1:A:453:MET:HG2	1:A:520:CYS:SG	2.52	0.50
1:A:524:VAL:HG12	1:A:525:GLN:HG3	1.94	0.50
1:A:814:PHE:O	1:A:817:ALA:HB3	2.11	0.50
1:A:114:LEU:O	1:A:115:LEU:O	2.30	0.49
1:A:185:TRP:O	1:A:186:LYS:CG	2.60	0.49
1:A:224:PHE:HZ	1:A:234:MET:CE	2.25	0.49
1:A:256:GLN:O	1:A:256:GLN:CG	2.43	0.49
2:B:1108:ARG:HG2	2:B:1109:GLY:H	1.76	0.49
3:C:63:ILE:O	3:C:66:ARG:HB2	2.12	0.49
1:A:1436:ILE:O	1:A:1438:THR:N	2.44	0.49
1:A:573:SER:H	1:A:576:GLN:HG3	1.76	0.49
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.92	0.49
2:B:1132:GLU:O	2:B:1134:GLU:N	2.45	0.49
2:B:127:GLY:HA2	2:B:169:ARG:HG2	1.93	0.49
2:B:640:VAL:HG13	2:B:650:GLU:O	2.12	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
2:B:911:ILE:O	2:B:911:ILE:HG23	2.11	0.49
3:C:53:THR:O	3:C:153:LEU:HA	2.12	0.49
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.95	0.49
1:A:367:PRO:HA	1:A:463:ILE:O	2.12	0.49
2:B:386:LEU:O	2:B:388:CYS:N	2.46	0.49
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.93	0.49
2:B:628:THR:O	2:B:628:THR:HG22	2.12	0.49
2:B:635:ARG:O	2:B:636:PRO:O	2.30	0.49
3:C:127:ARG:HG3	3:C:129:ILE:HG21	1.94	0.49
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.10	0.49
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.47	0.49
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.48	0.49
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.28	0.49
1:A:441:PRO:HD3	1:A:498:ARG:NH2	2.27	0.49
1:A:956:LEU:CD2	1:A:957:PRO:HD2	2.42	0.49
2:B:1065:GLN:HA	2:B:1065:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.13	0.49
2:B:581:PHE:N	2:B:581:PHE:CD1	2.80	0.49
2:B:77:HIS:ND1	2:B:78:THR:CG2	2.75	0.49
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.78	0.49
1:A:1187:GLN:HB3	1:A:1188:GLN:HA	1.94	0.49
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.13	0.49
1:A:413:ILE:CD1	1:A:413:ILE:N	2.76	0.49
1:A:468:PHE:HE2	1:A:489:LEU:HD13	1.76	0.49
1:A:1431:GLY:O	2:B:1152:MET:CE	2.60	0.49
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.28	0.49
2:B:976:ILE:HG23	2:B:977:GLY:H	1.76	0.49
4:E:199:ILE:O	4:E:199:ILE:HG22	2.12	0.49
9:K:35:PHE:CD1	9:K:35:PHE:N	2.81	0.49
1:A:369:SER:HB2	9:K:2:ASN:OD1	2.13	0.49
1:A:399:HIS:O	1:A:400:PRO:C	2.51	0.49
1:A:78:PRO:O	2:B:1201:LYS:HE2	2.12	0.49
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.47	0.49
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.76	0.49
1:A:265:LYS:HZ3	1:A:265:LYS:HB2	1.78	0.49
1:A:567:LYS:CB	1:A:568:PRO:CD	2.80	0.49
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.27	0.49
1:A:118:HIS:O	1:A:122:MET:HB3	2.13	0.49
1:A:272:ALA:O	1:A:275:SER:HB3	2.13	0.49
1:A:464:PRO:O	1:A:465:TYR:HB2	2.13	0.49
1:A:807:GLY:HA3	2:B:728:ARG:NH1	2.28	0.49
2:B:364:ILE:O	2:B:365:THR:HB	2.12	0.49
2:B:530:GLY:CA	11:R:12:G:H22	2.23	0.49
2:B:807:ARG:O	2:B:810:GLU:HB3	2.13	0.49
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.94	0.49
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.13	0.49
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.95	0.49
1:A:443:LEU:O	1:A:489:LEU:HA	2.12	0.49
1:A:626:ASN:O	1:A:631:HIS:ND1	2.45	0.49
2:B:363:HIS:C	2:B:365:THR:H	2.16	0.49
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.45	0.49
10:L:60:ARG:HG3	10:L:61:THR:N	2.27	0.49
1:A:649:ILE:O	1:A:653:VAL:HG23	2.13	0.49
2:B:515:HIS:H	2:B:518:HIS:CD2	2.30	0.49
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.47	0.49
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.77	0.48
2:B:1132:GLU:O	2:B:1133:MET:C	2.50	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:H	2:B:899:ILE:HD12	1.77	0.48
1:A:513:SER:O	1:A:515:GLN:N	2.46	0.48
1:A:666:ILE:N	1:A:666:ILE:HD12	2.27	0.48
1:A:909:ASP:HB3	1:A:912:LEU:HG	1.95	0.48
2:B:874:PHE:CE1	2:B:964:VAL:HG23	2.47	0.48
3:C:222:LYS:O	3:C:223:ALA:HB2	2.12	0.48
4:E:191:LYS:O	4:E:214:CYS:HB3	2.14	0.48
6:H:42:ILE:HG23	6:H:95:TYR:HE1	1.78	0.48
1:A:49:LYS:CB	1:A:50:ILE:HA	2.35	0.48
1:A:33:ALA:HB3	1:A:82:GLY:HA3	1.95	0.48
2:B:792:MET:O	2:B:793:ALA:CB	2.61	0.48
2:B:857:ARG:NH2	2:B:942:ARG:NH2	2.62	0.48
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.94	0.48
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.95	0.48
1:A:1169:ILE:HB	1:A:1170:ILE:HB	1.94	0.48
1:A:360:GLU:HB2	1:A:363:GLN:OE1	2.13	0.48
1:A:56:PRO:O	1:A:57:ARG:HB2	2.11	0.48
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.48
2:B:256:VAL:HG11	2:B:382:ILE:CD1	2.44	0.48
2:B:636:PRO:O	2:B:692:TYR:HA	2.13	0.48
2:B:773:MET:C	2:B:775:LYS:N	2.66	0.48
2:B:979:LYS:HB2	2:B:1097:HIS:HB2	1.95	0.48
2:B:977:GLY:HA2	2:B:990:ILE:O	2.13	0.48
4:E:62:ALA:N	4:E:78:LEU:O	2.44	0.48
1:A:255:SER:HA	1:A:256:GLN:C	2.34	0.48
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.94	0.48
2:B:525:ALA:O	2:B:768:THR:HG23	2.14	0.48
3:C:238:ILE:HG22	3:C:239:PRO:O	2.13	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
3:C:58:LEU:HB3	3:C:62:PHE:HD2	1.78	0.48
1:A:118:HIS:O	1:A:119:ASN:C	2.52	0.48
1:A:351:THR:HG22	1:A:468:PHE:HD1	1.70	0.48
1:A:571:LEU:C	1:A:572:TRP:CE3	2.87	0.48
2:B:1051:THR:HB	2:B:1054:GLY:H	1.77	0.48
2:B:498:THR:CG2	2:B:499:ASN:H	2.26	0.48
2:B:604:ARG:CD	2:B:691:GLU:OE2	2.58	0.48
3:C:58:LEU:HD21	8:J:57:ILE:HD13	1.96	0.48
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.49	0.48
1:A:492:PRO:HA	2:B:1149:GLU:OE1	2.14	0.48
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.48
2:B:449:ASN:C	2:B:451:LYS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:GLN:H	2:B:710:LEU:HG	1.79	0.48
2:B:893:LEU:HD11	2:B:910:VAL:HG12	1.95	0.48
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.96	0.48
10:L:30:ILE:O	10:L:56:LEU:HD23	2.14	0.48
1:A:152:VAL:CG2	1:A:153:PRO:HD2	2.43	0.48
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.29	0.48
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.78	0.48
6:H:6:PHE:CG	6:H:7:ASP:N	2.82	0.48
1:A:568:PRO:HD3	6:H:94:ASP:O	2.14	0.48
6:H:8:ASP:CG	6:H:9:ILE:H	2.17	0.48
3:C:163:ILE:HD13	9:K:10:PHE:CE1	2.49	0.48
1:A:360:GLU:HA	1:A:360:GLU:OE2	2.14	0.48
1:A:471:ASN:HD22	1:A:473:SER:H	1.62	0.48
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.96	0.48
1:A:549:MET:O	1:A:552:TRP:HB2	2.14	0.48
2:B:215:GLN:HE22	2:B:499:ASN:HB3	1.78	0.48
6:H:6:PHE:HD2	6:H:59:ILE:HG12	1.79	0.48
2:B:769:TYR:HH	11:R:12:G:H2'	1.74	0.48
1:A:38:PRO:HG3	1:A:274:ILE:CD1	2.43	0.47
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.13	0.47
2:B:1142:GLY:HA3	5:F:88:TYR:HE2	1.78	0.47
2:B:1166:CYS:SG	2:B:1167:GLY:N	2.87	0.47
2:B:1196:ILE:HG13	2:B:1200:ALA:HB3	1.96	0.47
2:B:232:SER:C	2:B:261:ARG:HH21	2.18	0.47
3:C:34:ARG:O	3:C:38:ILE:HG12	2.14	0.47
6:H:41:ASP:HB3	6:H:121:LEU:HB3	1.96	0.47
1:A:535:THR:O	1:A:575:LYS:HE2	2.14	0.47
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.96	0.47
2:B:1024:ALA:O	2:B:1027:ILE:N	2.47	0.47
2:B:211:VAL:HG21	2:B:483:LEU:HG	1.96	0.47
2:B:636:PRO:CB	2:B:637:LEU:CB	2.71	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.67	0.47
2:B:779:GLY:O	2:B:795:ILE:HG23	2.15	0.47
2:B:795:ILE:HD12	2:B:795:ILE:H	1.80	0.47
2:B:810:GLU:HG3	2:B:811:TYR:CD2	2.50	0.47
3:C:102:GLN:HB3	3:C:154:LYS:HE2	1.96	0.47
3:C:127:ARG:HG3	3:C:129:ILE:CG2	2.44	0.47
1:A:156:ASP:N	1:A:156:ASP:OD1	2.32	0.47
2:B:1016:ALA:O	2:B:1017:ILE:HD13	2.14	0.47
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.13	0.47
2:B:48:LEU:O	2:B:49:ASP:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:SER:N	2:B:86:ARG:HB3	2.30	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.13	0.47
1:A:1081:LEU:CD1	1:A:1082:ASN:ND2	2.78	0.47
1:A:1168:GLU:HA	1:A:1171:GLN:HB2	1.94	0.47
1:A:546:VAL:O	1:A:550:LEU:HD22	2.13	0.47
1:A:861:GLY:HA3	4:E:174:GLN:HE21	1.79	0.47
1:A:663:SER:HA	2:B:1014:PRO:HG3	1.97	0.47
2:B:979:LYS:CD	2:B:1097:HIS:CD2	2.87	0.47
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.11	0.47
3:C:84:ARG:HD2	9:K:11:LEU:HD21	1.97	0.47
1:A:1287:TYR:CD2	1:A:1305:VAL:HG21	2.50	0.47
1:A:40:THR:HB	1:A:41:MET:HA	1.96	0.47
2:B:549:THR:HG22	2:B:550:ASP:N	2.20	0.47
2:B:90:ILE:CG2	2:B:91:SER:N	2.77	0.47
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.47	0.47
1:A:1434:ALA:HA	1:A:1435:PRO:HD2	1.70	0.47
1:A:154:SER:O	1:A:156:ASP:N	2.48	0.47
1:A:107:CYS:SG	1:A:167:CYS:SG	3.11	0.47
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.96	0.47
2:B:1155:SER:HB3	2:B:1156:ASP:H	1.55	0.47
3:C:37:MET:HG2	3:C:176:ILE:HD11	1.96	0.47
1:A:666:ILE:HG22	1:A:670:ILE:HD11	1.97	0.47
2:B:1210:MET:O	2:B:1210:MET:HG2	2.15	0.47
2:B:773:MET:C	2:B:775:LYS:H	2.17	0.47
4:E:198:ILE:N	4:E:210:SER:O	2.44	0.47
7:I:84:VAL:CG2	7:I:85:PHE:N	2.78	0.47
2:B:1149:GLU:C	2:B:1151:LEU:H	2.18	0.47
2:B:190:TYR:CE1	8:J:62:ARG:HD3	2.50	0.47
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.15	0.47
10:L:46:VAL:HG12	10:L:47:ARG:N	2.21	0.47
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.80	0.47
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.15	0.47
1:A:276:LEU:HD13	1:A:296:LEU:HD23	1.95	0.47
1:A:424:ILE:O	1:A:424:ILE:CG2	2.62	0.47
2:B:334:ILE:O	2:B:334:ILE:HG22	2.14	0.47
2:B:583:ASN:HD21	2:B:628:THR:HB	1.79	0.47
2:B:637:LEU:O	2:B:690:VAL:HA	2.13	0.47
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.97	0.47
9:K:65:HIS:HD2	9:K:67:PHE:HB2	1.72	0.47
9:K:32:VAL:HA	9:K:73:LEU:O	2.15	0.47
1:A:313:GLN:HB2	1:A:314:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:C	1:A:58:LEU:CD2	2.83	0.47
1:A:804:TYR:OH	2:B:763:GLN:HB2	2.15	0.47
2:B:121:ASN:HD22	2:B:121:ASN:N	2.13	0.47
2:B:476:ARG:C	2:B:478:GLY:H	2.18	0.47
1:A:265:LYS:NZ	1:A:265:LYS:HB2	2.30	0.47
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.79	0.47
2:B:809:MET:HA	2:B:812:LEU:HD12	1.97	0.47
3:C:142:VAL:HG23	8:J:5:VAL:HG13	1.96	0.47
1:A:413:ILE:HD12	1:A:413:ILE:N	2.29	0.46
1:A:492:PRO:HB3	1:A:497:THR:CG2	2.45	0.46
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.14	0.46
2:B:1030:LEU:O	2:B:1031:LEU:C	2.53	0.46
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.96	0.46
2:B:820:GLY:O	2:B:821:GLN:HG3	2.15	0.46
3:C:248:ILE:HD13	9:K:101:LEU:HD13	1.96	0.46
12:T:26:DG:C2	12:T:27:DA:H1'	2.50	0.46
1:A:1021:LEU:HD11	1:A:1025:ARG:HE	1.80	0.46
1:A:1111:MET:HE2	1:A:1114:PRO:HA	1.98	0.46
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.96	0.46
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.29	0.46
1:A:760:GLN:HE21	1:A:765:VAL:HA	1.80	0.46
4:E:185:ALA:HB1	4:E:190:LEU:HD23	1.96	0.46
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.46	0.46
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.80	0.46
1:A:946:VAL:HG12	1:A:947:PHE:N	2.29	0.46
1:A:956:LEU:HD23	1:A:957:PRO:HD2	1.96	0.46
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.15	0.46
3:C:37:MET:HB3	3:C:38:ILE:H	1.61	0.46
1:A:95:PHE:HB3	1:A:234:MET:SD	2.56	0.46
2:B:173:MET:HB2	2:B:203:PHE:CZ	2.50	0.46
1:A:1444:MET:HB2	5:F:133:VAL:CG1	2.45	0.46
1:A:310:GLY:CA	1:A:311:GLN:CB	2.80	0.46
1:A:465:TYR:CD1	1:A:465:TYR:N	2.84	0.46
2:B:1074:ASN:HB3	2:B:1077:THR:CG2	2.45	0.46
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.49	0.46
2:B:386:LEU:C	2:B:388:CYS:N	2.69	0.46
2:B:515:HIS:HD2	2:B:517:THR:H	1.63	0.46
2:B:549:THR:CG2	2:B:550:ASP:H	2.18	0.46
2:B:488:TYR:HE2	2:B:812:LEU:O	1.97	0.46
3:C:204:SER:O	3:C:206:ASN:N	2.48	0.46
3:C:69:LEU:HD12	8:J:6:ARG:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:O	1:A:1105:LEU:HD12	2.16	0.46
1:A:118:HIS:CB	1:A:123:ARG:HB3	2.45	0.46
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.98	0.46
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.46
1:A:370:ILE:CG2	2:B:1105:ALA:HB2	2.42	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.46	0.46
6:H:93:TYR:CD1	6:H:143:LEU:HD23	2.50	0.46
7:I:52:ILE:HG13	7:I:53:GLY:H	1.81	0.46
1:A:1086:PHE:CE1	1:A:1092:LYS:HG2	2.51	0.46
1:A:112:LYS:HG2	1:A:113:LEU:N	2.30	0.46
1:A:190:ALA:O	1:A:191:THR:OG1	2.30	0.46
1:A:368:LYS:O	1:A:372:LYS:N	2.49	0.46
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.97	0.46
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.51	0.46
2:B:1093:GLN:H	2:B:1093:GLN:HG2	1.52	0.46
2:B:636:PRO:O	2:B:691:GLU:O	2.33	0.46
2:B:754:SER:O	2:B:806:THR:OG1	2.27	0.46
4:E:27:GLY:O	4:E:65:THR:HG22	2.14	0.46
8:J:57:ILE:O	8:J:60:PHE:HB2	2.15	0.46
1:A:563:PRO:HB3	1:A:572:TRP:CD2	2.51	0.46
1:A:4:GLN:O	1:A:5:GLN:HG3	2.15	0.46
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.45	0.46
2:B:289:LEU:O	2:B:327:ARG:NH2	2.47	0.46
8:J:10:CYS:CB	8:J:46:CYS:SG	3.03	0.46
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.98	0.46
1:A:118:HIS:C	1:A:120:GLU:N	2.70	0.46
1:A:1344:GLY:O	1:A:1347:ALA:N	2.46	0.46
1:A:466:SER:HB3	2:B:1103:ILE:CD1	2.46	0.46
1:A:841:LEU:HD21	1:A:1105:LEU:HD22	1.97	0.46
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.46	0.46
6:H:16:ASP:HA	6:H:17:PRO:HD3	1.83	0.46
8:J:43:ARG:HB2	8:J:45:CYS:SG	2.56	0.46
3:C:15:LYS:HE3	9:K:114:LEU:HD22	1.98	0.46
9:K:21:ILE:HD12	9:K:33:ILE:HG12	1.98	0.46
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.79	0.46
1:A:323:LYS:HD3	1:A:323:LYS:HA	1.70	0.46
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.46
1:A:890:ASP:OD2	1:A:1296:GLY:HA2	2.16	0.46
2:B:459:TYR:C	2:B:459:TYR:HD2	2.19	0.46
2:B:642:ASP:C	2:B:644:GLU:H	2.20	0.46
2:B:748:ILE:HG12	2:B:748:ILE:H	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:860:MET:O	2:B:861:ASP:HB2	2.15	0.46
3:C:176:ILE:O	3:C:176:ILE:HG22	2.14	0.46
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.51	0.46
8:J:5:VAL:HA	8:J:15:GLY:N	2.28	0.46
9:K:100:ALA:O	9:K:101:LEU:C	2.54	0.46
1:A:1008:GLN:HA	1:A:1011:GLN:HB3	1.98	0.45
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.16	0.45
1:A:1075:PRO:O	1:A:1076:ALA:C	2.54	0.45
1:A:495:GLU:O	1:A:498:ARG:HB2	2.16	0.45
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.97	0.45
2:B:879:ARG:O	2:B:880:THR:OG1	2.27	0.45
2:B:911:ILE:C	2:B:912:ILE:HG13	2.35	0.45
3:C:241:ASP:O	3:C:244:VAL:HG13	2.17	0.45
1:A:208:LEU:HD13	1:A:209:ASN:N	2.32	0.45
1:A:265:LYS:HE2	1:A:303:TYR:HA	1.98	0.45
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.81	0.45
1:A:779:PHE:CZ	2:B:517:THR:HA	2.51	0.45
2:B:1188:LYS:HB2	2:B:1189:ILE:HD12	1.98	0.45
3:C:235:VAL:HG11	8:J:6:ARG:NH2	2.29	0.45
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.50	0.45
9:K:57:LEU:HD12	9:K:76:GLN:HG2	1.98	0.45
12:T:6:DG:H2'	12:T:7:DA:C8	2.51	0.45
1:A:157:ASP:CG	1:A:158:PRO:HD3	2.36	0.45
1:A:491:VAL:HA	1:A:492:PRO:HD2	1.61	0.45
2:B:41:LYS:HB3	2:B:45:SER:HB3	1.97	0.45
2:B:78:THR:HA	2:B:79:THR:C	2.36	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.81	0.45
2:B:879:ARG:HA	2:B:879:ARG:NH1	2.30	0.45
2:B:874:PHE:CE1	2:B:964:VAL:CG2	3.00	0.45
9:K:11:LEU:C	9:K:12:LEU:HG	2.35	0.45
1:A:567:LYS:C	1:A:569:LYS:H	2.20	0.45
1:A:55:ASP:CA	1:A:58:LEU:O	2.65	0.45
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.31	0.45
2:B:795:ILE:HD12	2:B:795:ILE:N	2.31	0.45
7:I:68:LEU:HA	7:I:69:PRO:HD2	1.56	0.45
7:I:96:SER:HB2	7:I:98:VAL:HG23	1.97	0.45
2:B:1202:LEU:O	2:B:1205:GLN:HB2	2.16	0.45
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.47	0.45
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.49	0.45
2:B:78:THR:N	2:B:79:THR:CB	2.72	0.45
3:C:142:VAL:HG13	3:C:144:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:28:TYR:HA	4:E:64:PRO:HA	1.98	0.45
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.52	0.45
6:H:109:LYS:HB3	6:H:111:LEU:N	2.27	0.45
6:H:98:TYR:C	6:H:118:PHE:HD2	2.20	0.45
1:A:399:HIS:CD2	1:A:400:PRO:CG	2.99	0.45
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.54	0.45
1:A:912:LEU:HD22	1:A:1036:ARG:NH2	2.32	0.45
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.81	0.45
1:A:500:GLU:OE1	2:B:1145:SER:N	2.49	0.45
2:B:440:HIS:C	2:B:442:PHE:N	2.70	0.45
2:B:721:LEU:HA	2:B:722:ASP:HA	1.77	0.45
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.98	0.45
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.31	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.99	0.45
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.47	0.45
2:B:554:ILE:O	2:B:557:PHE:HB3	2.17	0.45
3:C:242:GLN:OE1	3:C:242:GLN:HA	2.16	0.45
3:C:41:ILE:HD11	3:C:243:VAL:HG13	1.97	0.45
3:C:44:LEU:HD22	3:C:129:ILE:HG13	1.99	0.45
1:A:129:LYS:O	1:A:130:ASP:HB2	2.16	0.45
1:A:590:ARG:NH2	1:A:621:THR:HA	2.32	0.45
2:B:778:MET:HE2	2:B:1094:ARG:HD3	1.97	0.45
2:B:344:LYS:HG2	2:B:347:LYS:HD2	1.98	0.45
2:B:422:LYS:O	2:B:425:THR:HG22	2.17	0.45
3:C:176:ILE:HG12	3:C:232:VAL:HG13	1.98	0.45
3:C:5:GLY:HA3	3:C:6:PRO:HD2	1.77	0.45
5:F:77:ASP:OD1	5:F:78:GLN:HG3	2.17	0.45
7:I:7:CYS:O	7:I:11:ASN:HA	2.17	0.45
1:A:315:LEU:H	1:A:315:LEU:HD22	1.81	0.45
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	2.47	0.45
1:A:41:MET:HG3	1:A:42:ASP:N	2.29	0.45
1:A:511:ILE:HG12	1:A:521:MET:HG3	1.97	0.45
1:A:541:ILE:HG21	1:A:549:MET:CE	2.47	0.45
2:B:192:LEU:O	2:B:193:LYS:HB2	2.16	0.45
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.34	0.45
2:B:439:ALA:HB3	2:B:440:HIS:CG	2.52	0.45
7:I:32:CYS:SG	7:I:33:SER:N	2.87	0.45
1:A:278:THR:O	1:A:282:ASN:HB2	2.17	0.45
1:A:401:GLY:C	1:A:435:HIS:CD2	2.90	0.45
1:A:403:LYS:C	1:A:404:TYR:CD1	2.91	0.45
2:B:345:LYS:HE2	2:B:348:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.99	0.45
6:H:110:ASP:O	6:H:128:ASN:ND2	2.50	0.45
6:H:23:VAL:CG1	6:H:24:CYS:N	2.80	0.45
2:B:953:LEU:HA	10:L:56:LEU:O	2.17	0.45
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.17	0.44
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.57	0.44
2:B:471:LYS:CB	2:B:472:ALA:HA	2.47	0.44
2:B:831:SER:OG	2:B:832:GLY:N	2.50	0.44
2:B:964:VAL:HG12	2:B:965:LYS:H	1.81	0.44
3:C:258:ILE:O	3:C:259:LEU:C	2.55	0.44
1:A:1085:HIS:O	1:A:1086:PHE:CG	2.71	0.44
1:A:1383:SER:OG	1:A:1388:GLY:N	2.51	0.44
1:A:389:THR:HA	1:A:426:LEU:HD12	2.00	0.44
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.32	0.44
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	2.00	0.44
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.32	0.44
2:B:121:ASN:HD21	2:B:965:LYS:HE3	1.83	0.44
2:B:221:ASN:OD1	2:B:242:SER:HA	2.17	0.44
2:B:634:TYR:HA	2:B:693:ILE:O	2.16	0.44
2:B:905:VAL:HG12	2:B:906:SER:N	2.32	0.44
2:B:975:GLN:HE21	2:B:975:GLN:HB3	1.52	0.44
4:E:213:ILE:HG12	4:E:214:CYS:N	2.30	0.44
5:F:101:ILE:HB	5:F:117:PRO:HB3	1.99	0.44
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	2.00	0.44
2:B:440:HIS:O	2:B:442:PHE:N	2.50	0.44
2:B:530:GLY:HA2	2:B:533:CYS:HB2	2.00	0.44
2:B:698:GLU:O	2:B:701:ILE:HD13	2.16	0.44
2:B:765:PRO:O	2:B:769:TYR:N	2.49	0.44
2:B:76:GLN:O	2:B:77:HIS:CB	2.55	0.44
2:B:857:ARG:NH2	12:T:24:DT:OP1	2.51	0.44
3:C:43:THR:CG2	3:C:44:LEU:H	2.26	0.44
10:L:26:THR:O	10:L:27:LEU:O	2.34	0.44
1:A:118:HIS:HB2	1:A:123:ARG:CG	2.40	0.44
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.17	0.44
1:A:380:VAL:HG11	1:A:427:GLN:O	2.18	0.44
2:B:1033:LYS:N	2:B:1089:PRO:HG2	2.33	0.44
2:B:215:GLN:NE2	2:B:499:ASN:HB3	2.32	0.44
2:B:365:THR:HG21	2:B:370:PHE:CG	2.53	0.44
2:B:589:VAL:HG12	2:B:590:HIS:N	2.32	0.44
2:B:640:VAL:HG12	2:B:641:GLU:N	2.32	0.44
2:B:40:GLU:HG3	2:B:681:TRP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:MET:HA	2:B:776:GLN:NE2	2.33	0.44
4:E:160:GLU:O	4:E:163:GLU:HB3	2.18	0.44
4:E:213:ILE:CG1	4:E:214:CYS:H	2.28	0.44
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.98	0.44
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.81	0.44
10:L:41:SER:O	10:L:44:ASP:CB	2.66	0.44
1:A:1021:LEU:HD12	1:A:1025:ARG:HE	1.80	0.44
1:A:442:VAL:O	1:A:457:ALA:HA	2.17	0.44
1:A:531:ILE:O	1:A:531:ILE:HG12	2.17	0.44
1:A:599:SER:HA	1:A:600:PRO:HD2	1.71	0.44
1:A:645:LEU:O	1:A:649:ILE:HG13	2.17	0.44
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.52	0.44
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.53	0.44
2:B:739:THR:HB	2:B:740:HIS:ND1	2.31	0.44
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.53	0.44
9:K:113:THR:O	9:K:114:LEU:HB2	2.18	0.44
12:T:14:DG:H2'	12:T:15:DA:C4	2.52	0.44
1:A:185:TRP:HB2	1:A:198:GLU:HG2	1.99	0.44
1:A:323:LYS:HG3	1:A:327:ALA:CB	2.47	0.44
1:A:367:PRO:HB3	1:A:465:TYR:O	2.18	0.44
1:A:716:ASP:O	1:A:717:ASN:C	2.56	0.44
1:A:824:LEU:HD22	2:B:529:GLU:OE1	2.18	0.44
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.66	0.44
2:B:973:ILE:O	2:B:974:PRO:C	2.56	0.44
3:C:51:VAL:HG13	3:C:155:LEU:HD23	1.98	0.44
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.98	0.44
7:I:85:PHE:O	7:I:86:PHE:HB3	2.17	0.44
1:A:1189:SER:HB2	1:A:1242:VAL:O	2.17	0.44
1:A:800:VAL:HG13	1:A:812:GLU:CD	2.38	0.44
2:B:1110:PRO:HB2	2:B:1119:VAL:HG22	1.99	0.44
2:B:781:PHE:HE2	2:B:785:TYR:HB2	1.82	0.44
7:I:78:CYS:O	7:I:79:HIS:HB2	2.18	0.44
8:J:57:ILE:O	8:J:58:GLU:C	2.56	0.44
11:R:5:A:H2'	11:R:6:G:H8	1.82	0.44
1:A:662:PHE:HD2	2:B:829:CYS:SG	2.40	0.44
1:A:709:THR:HG22	1:A:710:LEU:N	2.33	0.44
2:B:1156:ASP:OD2	2:B:1156:ASP:N	2.49	0.44
2:B:473:MET:HA	2:B:474:SER:HA	1.84	0.44
2:B:64:CYS:HA	2:B:67:SER:HB3	1.99	0.44
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.18	0.44
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:CB	1:A:448:PRO:HA	2.47	0.44
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.52	0.44
2:B:293:PRO:O	2:B:297:ILE:HG12	2.17	0.44
2:B:522:VAL:HG12	2:B:523:CYS:N	2.32	0.44
2:B:986:GLN:HG3	2:B:1025:HIS:CD2	2.52	0.44
3:C:115:SER:OG	3:C:141:GLY:HA3	2.18	0.44
1:A:1173:HIS:CG	1:A:1173:HIS:O	2.70	0.43
1:A:116:ASP:O	1:A:117:GLU:O	2.36	0.43
1:A:1331:SER:OG	1:A:1333:ILE:HG23	2.18	0.43
1:A:23:SER:HA	1:A:24:PRO:HD2	1.67	0.43
1:A:340:LEU:HD22	1:A:1429:ILE:HG23	2.00	0.43
1:A:49:LYS:CB	1:A:50:ILE:O	2.64	0.43
1:A:548:ASN:HA	9:K:60:ALA:HB1	1.99	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HG12	1.99	0.43
2:B:260:GLY:O	2:B:267:ARG:HD3	2.18	0.43
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.18	0.43
8:J:9:SER:HB3	8:J:48:ARG:HH21	1.84	0.43
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.53	0.43
1:A:440:ASP:HB2	1:A:460:VAL:HG21	1.99	0.43
1:A:473:SER:OG	1:A:522:GLY:O	2.28	0.43
2:B:401:PHE:O	2:B:404:LYS:HG3	2.18	0.43
2:B:764:SER:CB	2:B:765:PRO:HD3	2.47	0.43
9:K:10:PHE:CD2	9:K:10:PHE:N	2.86	0.43
13:N:11:DG:H2"	13:N:12:DT:H5"	2.00	0.43
1:A:1084:PHE:CD2	1:A:1086:PHE:O	2.69	0.43
1:A:1344:GLY:O	1:A:1345:ARG:C	2.56	0.43
1:A:188:ASP:C	1:A:189:ARG:HG2	2.39	0.43
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.18	0.43
1:A:86:LEU:HD23	1:A:273:ASN:ND2	2.34	0.43
1:A:11:LEU:HD13	2:B:1195:HIS:HD2	1.82	0.43
2:B:430:ARG:HA	2:B:433:GLN:HE21	1.83	0.43
2:B:822:ASN:HD22	8:J:52:THR:CG2	2.29	0.43
4:E:9:ILE:HG23	4:E:10:SER:H	1.82	0.43
6:H:26:ILE:HG22	6:H:40:LEU:O	2.18	0.43
11:R:7:A:C2	11:R:8:G:C4	3.06	0.43
12:T:13:DA:H2"	12:T:14:DG:C8	2.53	0.43
1:A:1353:TYR:C	1:A:1355:VAL:H	2.21	0.43
1:A:365:GLY:N	1:A:469:ARG:O	2.43	0.43
1:A:810:PRO:HA	2:B:1047:PHE:CE2	2.53	0.43
4:E:24:LYS:HB3	4:E:30:ILE:HD12	2.00	0.43
9:K:35:PHE:H	9:K:35:PHE:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:O	1:A:186:LYS:CB	2.67	0.43
1:A:676:MET:O	1:A:677:ARG:C	2.56	0.43
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.54	0.43
2:B:955:THR:CG2	2:B:956:THR:N	2.52	0.43
1:A:1383:SER:C	1:A:1388:GLY:HA3	2.38	0.43
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.00	0.43
2:B:414:ALA:C	2:B:416:LEU:H	2.22	0.43
2:B:46:GLN:OE1	2:B:47:GLN:N	2.52	0.43
2:B:597:MET:O	2:B:600:LEU:HB2	2.19	0.43
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.83	0.43
3:C:258:ILE:HG22	3:C:259:LEU:N	2.33	0.43
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.18	0.43
1:A:1280:GLU:O	1:A:1281:ARG:C	2.57	0.43
1:A:1377:THR:HB	4:E:176:PRO:CA	2.48	0.43
1:A:1402:PHE:CZ	1:A:1403:GLU:OE2	2.72	0.43
1:A:678:GLU:CA	1:A:681:GLU:HG2	2.34	0.43
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.97	0.43
1:A:31:SER:HB2	1:A:81:PHE:O	2.18	0.43
2:B:211:VAL:HG12	2:B:212:LEU:N	2.34	0.43
2:B:729:ILE:O	2:B:729:ILE:HG22	2.19	0.43
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.83	0.43
3:C:143:LEU:HG	8:J:2:ILE:HD11	2.01	0.43
12:T:6:DG:H4'	12:T:7:DA:OP1	2.19	0.43
1:A:1319:VAL:HB	1:A:1322:ILE:HD12	2.01	0.43
1:A:295:LEU:O	1:A:298:PHE:HB3	2.18	0.43
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.00	0.43
1:A:775:ILE:HB	1:A:797:LYS:O	2.19	0.43
1:A:820:GLY:O	1:A:823:GLY:N	2.51	0.43
1:A:855:THR:HG22	1:A:866:PHE:O	2.19	0.43
2:B:1002:THR:CG2	2:B:1006:ILE:CG1	2.96	0.43
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.84	0.43
6:H:114:VAL:CG2	6:H:125:LEU:HB3	2.49	0.43
1:A:622:VAL:O	1:A:630:ILE:HD11	2.19	0.43
1:A:675:THR:HG22	1:A:679:ILE:HD11	2.01	0.43
2:B:1154:ALA:O	2:B:1155:SER:CB	2.66	0.43
2:B:237:VAL:HG13	2:B:256:VAL:O	2.18	0.43
9:K:44:ASN:HB2	9:K:61:TYR:OH	2.18	0.43
1:A:379:VAL:HG12	1:A:380:VAL:H	1.84	0.43
1:A:513:SER:C	1:A:515:GLN:N	2.72	0.43
1:A:769:SER:O	1:A:770:VAL:HB	2.18	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:764:SER:O	2:B:767:ASN:N	2.51	0.43
2:B:798:TYR:N	2:B:799:PRO:HD3	2.34	0.43
2:B:879:ARG:HH12	2:B:883:LEU:HB2	1.84	0.43
2:B:938:SER:O	2:B:940:PRO:HD3	2.19	0.43
2:B:99:LYS:O	2:B:101:MET:HG3	2.18	0.43
3:C:238:ILE:CG2	3:C:242:GLN:CB	2.93	0.43
3:C:27:LEU:C	3:C:29:MET:H	2.22	0.43
3:C:27:LEU:HD12	3:C:228:PHE:CE2	2.43	0.43
8:J:45:CYS:SG	8:J:46:CYS:N	2.92	0.43
9:K:56:VAL:HG13	9:K:77:THR:HG23	2.01	0.43
10:L:48:CYS:SG	10:L:49:LYS:N	2.92	0.43
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.33	0.42
1:A:846:GLU:HG2	1:A:1424:VAL:HG21	2.01	0.42
1:A:575:LYS:O	1:A:579:SER:OG	2.36	0.42
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.49	0.42
2:B:248:SER:HA	2:B:418:LYS:HD3	2.01	0.42
2:B:461:LEU:HD12	2:B:480:SER:HB2	2.01	0.42
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.83	0.42
3:C:52:GLU:OE2	3:C:154:LYS:HG2	2.19	0.42
3:C:227:THR:C	3:C:228:PHE:CD1	2.92	0.42
4:E:99:HIS:CD2	4:E:103:LYS:HD2	2.53	0.42
1:A:1243:VAL:HG13	1:A:1244:ARG:CB	2.48	0.42
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.83	0.42
1:A:253:ASN:CA	1:A:255:SER:H	2.19	0.42
1:A:447:GLN:HA	1:A:448:PRO:C	2.40	0.42
1:A:619:LYS:O	1:A:623:GLY:N	2.52	0.42
1:A:853:ASP:O	1:A:854:ASN:HB2	2.19	0.42
2:B:115:GLN:O	2:B:119:LEU:HG	2.18	0.42
2:B:203:PHE:C	2:B:204:ILE:HD12	2.39	0.42
2:B:25:ILE:HG23	2:B:29:ASP:HB2	2.01	0.42
2:B:603:LEU:HD12	2:B:609:ILE:HD11	2.01	0.42
2:B:906:SER:O	2:B:907:GLY:C	2.57	0.42
2:B:973:ILE:HG22	2:B:974:PRO:N	2.34	0.42
2:B:979:LYS:O	2:B:980:PHE:CD1	2.71	0.42
3:C:29:MET:O	3:C:30:ALA:C	2.57	0.42
4:E:29:PHE:C	4:E:30:ILE:HG13	2.40	0.42
5:F:97:ARG:HD3	5:F:100:GLN:OE1	2.18	0.42
8:J:64:ASN:HB3	8:J:65:PRO:HD3	2.01	0.42
8:J:7:CYS:HB2	8:J:49:MET:HE3	2.01	0.42
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.52	0.42
1:A:311:GLN:H	1:A:313:GLN:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:HA	1:A:38:PRO:HD3	1.84	0.42
1:A:775:ILE:HA	1:A:775:ILE:HD13	1.88	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.19	0.42
2:B:1070:GLU:O	2:B:1071:VAL:C	2.57	0.42
3:C:3:GLU:HB3	9:K:104:ASN:ND2	2.11	0.42
7:I:100:PHE:CD2	7:I:111:THR:HG23	2.55	0.42
7:I:62:ILE:C	7:I:64:SER:H	2.22	0.42
11:R:11:U:H3'	11:R:12:G:H5'	2.01	0.42
11:R:9:G:C2	12:T:21:DC:N3	2.88	0.42
1:A:19:PHE:O	1:A:1416:ALA:HA	2.18	0.42
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.20	0.42
1:A:202:LEU:HB3	1:A:207:ILE:HD11	2.00	0.42
1:A:33:ALA:HB3	1:A:82:GLY:CA	2.50	0.42
1:A:996:ASN:OD1	1:A:996:ASN:N	2.52	0.42
2:B:1182:CYS:HB3	2:B:1185:CYS:HB2	2.01	0.42
2:B:476:ARG:HD3	2:B:476:ARG:H	1.84	0.42
2:B:755:ILE:HA	2:B:755:ILE:HD13	1.76	0.42
2:B:879:ARG:HH12	2:B:883:LEU:CB	2.32	0.42
2:B:872:GLU:O	2:B:914:LYS:HB2	2.17	0.42
3:C:35:ARG:HB2	9:K:41:THR:HG23	2.02	0.42
6:H:4:THR:HA	6:H:60:ALA:CB	2.48	0.42
1:A:1394:THR:HB	1:A:1395:GLY:H	1.70	0.42
1:A:507:VAL:CG1	1:A:521:MET:HE3	2.49	0.42
1:A:979:SER:OG	1:A:981:LEU:HD12	2.17	0.42
2:B:1020:ARG:HG2	2:B:1020:ARG:H	1.59	0.42
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.19	0.42
2:B:223:VAL:HG21	2:B:384:ARG:HG3	1.99	0.42
2:B:440:HIS:C	2:B:442:PHE:H	2.23	0.42
3:C:108:GLU:OE1	3:C:108:GLU:HA	2.20	0.42
3:C:98:VAL:HG22	3:C:158:VAL:HG13	2.01	0.42
9:K:7:PHE:CD1	9:K:7:PHE:C	2.93	0.42
2:B:1133:MET:HG3	12:T:19:DT:H4'	2.02	0.42
1:A:497:THR:CG2	2:B:1146:PHE:CD1	2.90	0.42
2:B:174:LEU:CD1	2:B:204:ILE:CD1	2.98	0.42
2:B:304:ASP:C	2:B:306:ASN:H	2.22	0.42
2:B:436:VAL:O	2:B:436:VAL:HG13	2.18	0.42
6:H:62:SER:O	6:H:63:LEU:C	2.58	0.42
1:A:239:LEU:HD13	1:A:240:PRO:O	2.19	0.42
1:A:649:ILE:HG13	1:A:649:ILE:H	1.73	0.42
1:A:956:LEU:HD23	1:A:957:PRO:HD3	2.01	0.42
2:B:102:VAL:HG12	2:B:112:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.67	0.42
2:B:1132:GLU:C	2:B:1134:GLU:N	2.72	0.42
2:B:202:TYR:C	2:B:203:PHE:CD1	2.93	0.42
2:B:225:VAL:H	2:B:396:ASP:HB2	1.84	0.42
2:B:416:LEU:HD21	2:B:460:ALA:CB	2.50	0.42
2:B:941:LEU:HD13	2:B:942:ARG:N	2.27	0.42
3:C:56:THR:HG22	3:C:147:LEU:HD21	2.02	0.42
4:E:64:PRO:HD3	4:E:76:GLY:O	2.20	0.42
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.74	0.42
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	2.01	0.42
1:A:446:ARG:NH1	1:A:479:ASN:HB3	2.35	0.42
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.35	0.42
2:B:1168:LEU:HD22	2:B:1214:PRO:HD2	2.01	0.42
2:B:436:VAL:HA	2:B:438:GLU:O	2.20	0.42
2:B:520:GLY:C	2:B:521:LEU:HG	2.39	0.42
2:B:90:ILE:HG22	2:B:91:SER:H	1.84	0.42
3:C:184:ASN:HD21	3:C:189:THR:H	1.68	0.42
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.88	0.42
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.90	0.42
1:A:1072:ILE:HD11	1:A:1368:MET:CG	2.49	0.42
1:A:17:VAL:HB	1:A:1419:ASP:HB3	2.01	0.42
1:A:310:GLY:HA2	1:A:311:GLN:CB	2.46	0.42
2:B:622:LYS:HE2	7:I:59:VAL:HG13	2.02	0.42
2:B:521:LEU:HD22	2:B:633:VAL:HB	2.00	0.42
2:B:901:PRO:HB3	2:B:950:ASP:O	2.19	0.42
2:B:842:ASN:HA	2:B:994:TYR:O	2.20	0.42
3:C:180:TYR:O	3:C:181:ASP:O	2.37	0.42
1:A:1027:ALA:O	1:A:1030:ARG:HB2	2.20	0.42
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.41	0.42
1:A:1148:ILE:HA	1:A:1148:ILE:HD13	1.98	0.42
1:A:1394:THR:HG22	1:A:1398:MET:HE1	2.02	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.57	0.42
1:A:284:ALA:N	1:A:285:PRO:CD	2.82	0.42
1:A:655:PHE:O	1:A:656:TRP:C	2.57	0.42
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.85	0.42
1:A:917:SER:C	1:A:919:ILE:H	2.24	0.42
2:B:1025:HIS:ND1	2:B:1025:HIS:C	2.72	0.42
2:B:778:MET:O	2:B:819:ALA:HA	2.20	0.42
3:C:15:LYS:H	3:C:15:LYS:HD2	1.85	0.42
8:J:44:TYR:HA	8:J:47:ARG:HD2	2.01	0.42
9:K:32:VAL:O	9:K:32:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:TRP:O	1:A:1045:VAL:C	2.59	0.41
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.19	0.41
1:A:1377:THR:HB	4:E:176:PRO:HB3	2.01	0.41
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.75	0.41
1:A:451:HIS:HB3	1:A:453:MET:HB2	2.02	0.41
1:A:527:THR:O	1:A:531:ILE:HG22	2.20	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.20	0.41
1:A:91:PHE:HB3	1:A:96:ILE:HD11	2.02	0.41
2:B:1006:ILE:H	2:B:1006:ILE:HG12	1.60	0.41
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.35	0.41
2:B:273:LEU:HA	2:B:274:PRO:HD3	1.80	0.41
2:B:293:PRO:HB2	7:I:11:ASN:O	2.20	0.41
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.85	0.41
6:H:100:THR:HG22	6:H:101:ALA:O	2.20	0.41
7:I:16:PRO:HB3	7:I:25:LEU:HD11	2.02	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.35	0.41
1:A:320:ARG:O	1:A:321:PRO:C	2.59	0.41
1:A:353:ILE:HD12	1:A:482:PHE:CE2	2.55	0.41
1:A:915:SER:CB	1:A:919:ILE:HG13	2.48	0.41
2:B:1096:ARG:O	2:B:1097:HIS:C	2.57	0.41
2:B:1162:ILE:O	2:B:1191:ILE:HG23	2.20	0.41
2:B:45:SER:OG	2:B:46:GLN:N	2.53	0.41
2:B:515:HIS:CD2	2:B:516:ASN:N	2.88	0.41
2:B:522:VAL:HG11	2:B:537:LYS:HD2	2.03	0.41
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.36	0.41
2:B:798:TYR:CE2	8:J:4:PRO:HB3	2.55	0.41
2:B:844:SER:HB2	2:B:996:ARG:H	1.85	0.41
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.83	0.41
3:C:83:SER:OG	3:C:95:CYS:SG	2.77	0.41
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	2.20	0.41
1:A:511:ILE:O	1:A:519:PRO:HA	2.20	0.41
1:A:815:PHE:O	1:A:818:MET:N	2.53	0.41
2:B:620:ARG:HD2	7:I:68:LEU:HD11	2.02	0.41
9:K:21:ILE:CD1	9:K:33:ILE:HG12	2.50	0.41
1:A:287:HIS:ND1	1:A:291:GLU:OE2	2.54	0.41
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.86	0.41
1:A:3:GLY:C	1:A:4:GLN:HG3	2.41	0.41
1:A:414:ASP:O	1:A:418:SER:HB2	2.21	0.41
1:A:560:ILE:HA	1:A:561:PRO:HD3	1.92	0.41
1:A:57:ARG:HA	1:A:57:ARG:HD3	1.59	0.41
2:B:1207:LEU:HA	2:B:1210:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.88	0.41
2:B:486:TYR:CE2	2:B:777:ALA:O	2.74	0.41
2:B:796:LEU:O	2:B:797:TYR:C	2.59	0.41
2:B:959:ASP:OD1	2:B:959:ASP:N	2.54	0.41
4:E:198:ILE:HD11	4:E:212:ARG:CD	2.50	0.41
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.03	0.41
1:A:55:ASP:O	1:A:56:PRO:C	2.58	0.41
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.21	0.41
1:A:992:ASP:O	1:A:995:GLU:HB2	2.21	0.41
1:A:99:ILE:O	1:A:103:CYS:SG	2.76	0.41
2:B:254:LEU:HD21	2:B:381:MET:SD	2.60	0.41
2:B:35:SER:HB3	2:B:811:TYR:CE2	2.55	0.41
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.36	0.41
3:C:133:ILE:HD11	3:C:237:SER:HA	2.02	0.41
1:A:35:ILE:HG13	1:A:241:VAL:HG21	2.03	0.41
1:A:658:LEU:HD13	2:B:831:SER:H	1.82	0.41
2:B:1172:ILE:HG22	2:B:1174:LYS:HG3	2.01	0.41
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.50	0.41
2:B:816:GLU:O	8:J:56:LEU:HD21	2.19	0.41
2:B:85:SER:H	2:B:86:ARG:HB3	1.85	0.41
2:B:910:VAL:CG1	2:B:911:ILE:N	2.83	0.41
4:E:40:GLU:O	4:E:41:ASP:HB2	2.21	0.41
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.35	0.41
6:H:81:PRO:HA	6:H:82:PRO:HD3	1.99	0.41
7:I:103:CYS:SG	7:I:106:CYS:N	2.93	0.41
1:A:120:GLU:O	1:A:121:LEU:C	2.59	0.41
3:C:10:ILE:HG23	3:C:20:PHE:HB3	2.01	0.41
3:C:255:VAL:O	3:C:258:ILE:HB	2.20	0.41
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.84	0.41
1:A:687:LYS:HG2	1:A:794:PRO:HG3	2.02	0.41
2:B:1024:ALA:O	2:B:1028:GLU:N	2.45	0.41
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.50	0.41
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.02	0.41
2:B:301:ILE:HG12	2:B:382:ILE:HB	2.02	0.41
2:B:476:ARG:HG2	2:B:477:ALA:N	2.35	0.41
2:B:214:ALA:O	2:B:499:ASN:N	2.53	0.41
2:B:905:VAL:HG12	2:B:906:SER:H	1.85	0.41
6:H:112:ILE:HG22	6:H:127:GLY:O	2.20	0.41
8:J:44:TYR:CD1	8:J:44:TYR:C	2.94	0.41
9:K:43:GLY:HA3	9:K:71:PHE:CD1	2.56	0.41
1:A:1006:ILE:H	1:A:1006:ILE:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:GLU:HA	1:A:1302:PRO:HD3	1.95	0.41
1:A:335:ARG:HE	2:B:1202:LEU:HD11	1.85	0.41
1:A:48:ALA:O	1:A:49:LYS:HD2	2.21	0.41
1:A:977:LYS:HA	1:A:978:PRO:HD3	1.77	0.41
2:B:1080:LYS:HB2	3:C:180:TYR:OH	2.21	0.41
3:C:50:GLU:HG2	10:L:66:GLN:HG3	2.03	0.41
6:H:31:THR:C	6:H:33:GLN:H	2.24	0.41
2:B:850:LEU:HD12	8:J:8:PHE:CD1	2.56	0.41
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.36	0.41
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.60	0.41
1:A:211:PHE:HA	1:A:214:ILE:HG12	2.02	0.41
1:A:463:ILE:HA	1:A:464:PRO:HD3	1.81	0.41
1:A:495:GLU:OE1	1:A:498:ARG:HD3	2.21	0.41
1:A:779:PHE:O	1:A:782:ARG:O	2.39	0.41
1:A:871:ASP:OD1	1:A:873:MET:HB2	2.21	0.41
2:B:1017:ILE:HD13	2:B:1017:ILE:HA	1.76	0.41
2:B:204:ILE:N	2:B:204:ILE:HD12	2.35	0.41
2:B:218:SER:HA	2:B:404:LYS:HB3	2.03	0.41
2:B:412:LEU:HB3	2:B:466:TRP:HE1	1.85	0.41
2:B:852:ARG:HD3	2:B:973:ILE:HG23	2.03	0.41
2:B:90:ILE:CG2	2:B:91:SER:H	2.33	0.41
3:C:46:ILE:HG22	3:C:47:ASP:N	2.36	0.41
11:R:11:U:O4	11:R:12:G:C6	2.74	0.41
1:A:323:LYS:HG3	1:A:327:ALA:HB1	2.03	0.41
1:A:395:GLY:HA2	1:A:396:PRO:HD3	1.86	0.41
1:A:766:GLY:HA2	1:A:799:PHE:HE1	1.86	0.41
1:A:939:ASP:O	1:A:940:ARG:C	2.58	0.41
2:B:1092:TYR:C	2:B:1093:GLN:O	2.57	0.41
2:B:1132:GLU:HA	2:B:1135:ARG:HB3	2.03	0.41
3:C:43:THR:HG23	3:C:44:LEU:N	2.28	0.41
1:A:1198:ASP:OD1	1:A:1198:ASP:N	2.54	0.40
1:A:270:LEU:O	1:A:274:ILE:HG13	2.21	0.40
1:A:779:PHE:HD1	1:A:783:THR:O	2.05	0.40
1:A:939:ASP:O	1:A:942:PHE:N	2.54	0.40
2:B:1022:THR:OG1	2:B:1025:HIS:HB3	2.21	0.40
2:B:1158:PHE:HB2	2:B:1198:TYR:HB2	2.03	0.40
2:B:494:HIS:HA	2:B:497:ARG:NH1	2.36	0.40
3:C:27:LEU:O	3:C:29:MET:N	2.54	0.40
5:F:103:MET:O	5:F:105:ALA:N	2.54	0.40
1:A:1169:ILE:N	1:A:1170:ILE:HG22	2.32	0.40
1:A:444:PHE:CE2	1:A:470:LEU:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:THR:HA	1:A:563:PRO:HD3	1.91	0.40
1:A:707:GLY:HA2	1:A:1281:ARG:HB2	2.03	0.40
1:A:866:PHE:CZ	4:E:211:TYR:HB2	2.57	0.40
2:B:855:PHE:CE2	2:B:857:ARG:HG3	2.56	0.40
5:F:137:TYR:CD2	5:F:143:PHE:HB3	2.56	0.40
5:F:93:ILE:O	5:F:94:LEU:C	2.58	0.40
11:R:2:U:H2'	11:R:3:C:C6	2.56	0.40
1:A:84:ILE:HG22	1:A:239:LEU:HB3	2.02	0.40
1:A:517:ASN:O	1:A:517:ASN:OD1	2.39	0.40
1:A:912:LEU:HD22	1:A:1036:ARG:HH21	1.84	0.40
2:B:1008:PRO:HG3	2:B:1087:PHE:CD1	2.56	0.40
2:B:1082:MET:HA	3:C:189:THR:HA	2.04	0.40
2:B:573:GLN:O	2:B:575:PRO:HD3	2.22	0.40
2:B:798:TYR:OH	3:C:66:ARG:NH1	2.48	0.40
2:B:843:GLN:HA	2:B:843:GLN:OE1	2.21	0.40
2:B:95:ILE:CG2	2:B:95:ILE:O	2.69	0.40
3:C:15:LYS:C	3:C:16:ASP:OD2	2.60	0.40
1:A:32:VAL:HB	1:A:57:ARG:CB	2.52	0.40
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.56	0.40
1:A:986:ILE:O	1:A:990:VAL:HG23	2.20	0.40
2:B:1206:GLU:O	2:B:1207:LEU:C	2.59	0.40
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.56	0.40
2:B:333:PHE:C	2:B:335:GLY:H	2.25	0.40
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.22	0.40
5:F:109:VAL:HG23	5:F:124:GLU:HG2	2.02	0.40
6:H:15:VAL:HG12	6:H:51:ALA:HB2	2.03	0.40
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.34	0.40
1:A:1248:LEU:H	1:A:1248:LEU:HD23	1.86	0.40
1:A:1389:PHE:O	1:A:1390:ASN:CG	2.60	0.40
1:A:160:GLN:CD	1:A:160:GLN:H	2.17	0.40
1:A:320:ARG:CB	1:A:321:PRO:HD2	2.32	0.40
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.57	0.40
1:A:811:GLN:O	1:A:812:GLU:C	2.60	0.40
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.79	0.40
2:B:361:LEU:O	2:B:363:HIS:O	2.39	0.40
2:B:445:LYS:CA	2:B:447:ALA:H	2.27	0.40
2:B:488:TYR:C	2:B:490:SER:N	2.75	0.40
2:B:898:LEU:CD1	2:B:952:VAL:HG11	2.46	0.40
3:C:80:LEU:O	3:C:161:LYS:HD2	2.21	0.40
4:E:9:ILE:HG23	4:E:10:SER:N	2.36	0.40
4:E:3:GLN:HA	4:E:6:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:84:VAL:HG22	7:I:85:PHE:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:SER:OG	3:C:87:PHE:O[2_555]	2.17	0.03

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1438/1733 (83%)	1054 (73%)	303 (21%)	81 (6%)	2	21
2	B	1145/1224 (94%)	855 (75%)	231 (20%)	59 (5%)	2	22
3	C	269/318 (85%)	207 (77%)	48 (18%)	14 (5%)	2	22
4	E	213/215 (99%)	175 (82%)	33 (16%)	5 (2%)	6	38
5	F	83/155 (54%)	66 (80%)	14 (17%)	3 (4%)	3	30
6	H	132/146 (90%)	104 (79%)	22 (17%)	6 (4%)	2	24
7	I	117/122 (96%)	84 (72%)	29 (25%)	4 (3%)	3	31
8	J	63/70 (90%)	48 (76%)	12 (19%)	3 (5%)	2	23
9	K	112/120 (93%)	86 (77%)	24 (21%)	2 (2%)	8	42
10	L	44/70 (63%)	31 (70%)	9 (20%)	4 (9%)	1	11
All	All	3616/4173 (87%)	2710 (75%)	725 (20%)	181 (5%)	2	23

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	116	ASP
1	A	117	GLU
1	A	119	ASN
1	A	121	LEU
1	A	155	GLU
1	A	158	PRO
1	A	193	ASP
1	A	194	ALA
1	A	399	HIS
1	A	400	PRO
1	A	568	PRO
1	A	770	VAL
1	A	1089	VAL
1	A	1170	ILE
1	A	1394	THR
1	A	1435	PRO
2	B	58	THR
2	B	74	LEU
2	B	78	THR
2	B	439	ALA
2	B	475	SER
2	B	483	LEU
2	B	636	PRO
2	B	712	PRO
2	B	732	SER
2	B	793	ALA
2	B	830	TYR
2	B	864	LYS
2	B	1046	PRO
2	B	1155	SER
3	C	125	MET
3	C	143	LEU
3	C	182	PRO
3	C	223	ALA
5	F	72	LYS
5	F	104	ASN
9	K	70	ARG
1	A	55	ASP
1	A	186	LYS
1	A	191	THR
1	A	255	SER

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Mol	Chain	Res	Type
1	A	395	GLY
1	A	404	TYR
1	A	423	ASP
1	A	557	ASP
1	A	592	ASP
1	A	846	GLU
1	A	884	ASP
1	A	922	ASP
1	A	958	VAL
1	A	1085	HIS
1	A	1221	LYS
1	A	1391	ARG
1	A	1437	GLY
2	B	59	LEU
2	B	76	GLN
2	B	79	THR
2	B	365	THR
2	B	468	GLU
2	B	746	SER
2	B	782	LEU
2	B	1108	ARG
2	B	1133	MET
3	C	60	ASP
3	C	196	ASP
3	C	227	THR
4	E	206	GLY
6	H	75	ALA
6	H	82	PRO
7	I	47	GLU
10	L	47	ARG
1	A	89	PRO
1	A	332	LYS
1	A	1172	LEU
1	A	1247	SER
1	A	1379	GLY
2	B	260	GLY
2	B	334	ILE
2	B	442	PHE
2	B	450	ALA
2	B	470	LYS
2	B	575	PRO
2	B	643	ASP

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Mol	Chain	Res	Type
2	B	981	ALA
2	B	1017	ILE
3	C	142	VAL
3	C	205	LYS
4	E	76	GLY
4	E	187	TYR
6	H	34	ASP
7	I	3	THR
7	I	116	ASN
8	J	6	ARG
10	L	27	LEU
10	L	51	CYS
1	A	311	GLN
1	A	321	PRO
1	A	424	ILE
1	A	567	LYS
1	A	591	PHE
1	A	972	HIS
1	A	1091	SER
1	A	1156	PRO
1	A	1252	THR
2	B	77	HIS
2	B	441	ASP
2	B	489	SER
2	B	958	GLN
6	H	109	LYS
7	I	69	PRO
8	J	16	ASP
10	L	59	ALA
1	A	120	GLU
1	A	149	GLU
1	A	252	PHE
1	A	364	VAL
1	A	377	PRO
1	A	599	SER
1	A	600	PRO
1	A	609	ASP
1	A	731	ARG
1	A	742	ASN
1	A	890	ASP
1	A	955	PRO
1	A	1087	ALA

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Mol	Chain	Res	Type
1	A	1354	ASN
2	B	387	LEU
2	B	518	HIS
2	B	527	THR
2	B	592	ASN
2	B	676	VAL
2	B	717	GLU
2	B	784	ASN
2	B	907	GLY
2	B	1150	ARG
2	B	1214	PRO
3	C	28	ALA
3	C	90	ASP
3	C	181	ASP
3	C	214	ASN
6	H	32	THR
1	A	52	GLY
1	A	1255	GLU
1	A	1388	GLY
1	A	1390	ASN
1	A	1429	ILE
2	B	305	VAL
2	B	467	GLY
2	B	875	GLU
6	H	119	GLY
8	J	64	ASN
9	K	37	LYS
1	A	79	GLY
1	A	250	ILE
1	A	385	ILE
1	A	719	VAL
1	A	1107	VAL
1	A	1190	PRO
1	A	1327	ILE
2	B	290	GLY
2	B	436	VAL
2	B	671	GLY
2	B	912	ILE
3	C	240	VAL
4	E	189	GLY
5	F	139	PRO
1	A	310	GLY

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Mol	Chain	Res	Type
1	A	325	ILE
2	B	70	ILE
1	A	24	PRO
1	A	312	PRO
2	B	479	VAL
2	B	1103	ILE
1	A	514	PRO
2	B	25	ILE
2	B	976	ILE
4	E	86	PRO
1	A	244	PRO
2	B	251	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1258/1520 (83%)	1041 (83%)	217 (17%)	2	13
2	B	1000/1061 (94%)	822 (82%)	178 (18%)	2	12
3	C	238/274 (87%)	188 (79%)	50 (21%)	1	7
4	E	196/197 (100%)	174 (89%)	22 (11%)	6	29
5	F	74/137 (54%)	66 (89%)	8 (11%)	6	30
6	H	119/128 (93%)	107 (90%)	12 (10%)	7	32
7	I	113/116 (97%)	96 (85%)	17 (15%)	3	18
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	3197/3657 (87%)	2654 (83%)	543 (17%)	2	14

All (543) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER

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Mol	Chain	Res	Type
1	A	8	SER
1	A	11	LEU
1	A	14	VAL
1	A	18	GLN
1	A	32	VAL
1	A	46	THR
1	A	49	LYS
1	A	53	LEU
1	A	57	ARG
1	A	58	LEU
1	A	63	ARG
1	A	65	LEU
1	A	74	MET
1	A	76	GLU
1	A	84	ILE
1	A	93	VAL
1	A	108	MET
1	A	120	GLU
1	A	121	LEU
1	A	123	ARG
1	A	131	SER
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP
1	A	160	GLN
1	A	161	LEU
1	A	164	ARG
1	A	167	CYS
1	A	180	LYS
1	A	187	LYS
1	A	193	ASP
1	A	198	GLU
1	A	207	ILE
1	A	208	LEU
1	A	210	ILE
1	A	212	LYS
1	A	221	SER
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	230	ARG
1	A	252	PHE

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	257	ARG
1	A	260	ASP
1	A	263	THR
1	A	270	LEU
1	A	271	LYS
1	A	275	SER
1	A	296	LEU
1	A	306	ASN
1	A	308	ILE
1	A	311	GLN
1	A	313	GLN
1	A	322	VAL
1	A	323	LYS
1	A	332	LYS
1	A	337	ARG
1	A	340	LEU
1	A	344	ARG
1	A	345	VAL
1	A	350	ARG
1	A	354	SER
1	A	359	LEU
1	A	370	ILE
1	A	403	LYS
1	A	404	TYR
1	A	411	ASP
1	A	413	ILE
1	A	419	LYS
1	A	424	ILE
1	A	431	LYS
1	A	434	ARG
1	A	437	MET
1	A	442	VAL
1	A	443	LEU
1	A	449	SER
1	A	450	LEU
1	A	452	LYS
1	A	460	VAL
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP

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Mol	Chain	Res	Type
1	A	518	LYS
1	A	521	MET
1	A	541	ILE
1	A	552	TRP
1	A	562	THR
1	A	565	ILE
1	A	572	TRP
1	A	576	GLN
1	A	577	ILE
1	A	579	SER
1	A	595	THR
1	A	602	ASP
1	A	603	ASN
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	630	ILE
1	A	634	THR
1	A	645	LEU
1	A	646	PHE
1	A	672	ASP
1	A	682	THR
1	A	687	LYS
1	A	688	LYS
1	A	693	VAL
1	A	694	THR
1	A	702	LEU
1	A	713	SER
1	A	735	VAL
1	A	739	ASP
1	A	740	LEU
1	A	760	GLN
1	A	767	GLN
1	A	768	GLN
1	A	771	GLU
1	A	774	ARG
1	A	775	ILE
1	A	783	THR
1	A	793	SER
1	A	795	GLU
1	A	805	LEU
1	A	808	LEU

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Mol	Chain	Res	Type
1	A	809	THR
1	A	827	THR
1	A	858	ASN
1	A	859	SER
1	A	867	ILE
1	A	883	LEU
1	A	884	ASP
1	A	885	THR
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	908	LEU
1	A	918	GLU
1	A	919	ILE
1	A	920	LEU
1	A	929	LEU
1	A	961	ARG
1	A	963	ILE
1	A	982	THR
1	A	988	LEU
1	A	1000	LEU
1	A	1001	ARG
1	A	1006	ILE
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1031	VAL
1	A	1033	GLN
1	A	1035	TYR
1	A	1037	LEU
1	A	1039	LYS
1	A	1047	SER
1	A	1048	ASN
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1080	THR
1	A	1081	LEU
1	A	1083	THR
1	A	1084	PHE
1	A	1085	HIS

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Mol	Chain	Res	Type
1	A	1089	VAL
1	A	1116	LEU
1	A	1118	VAL
1	A	1128	GLN
1	A	1141	THR
1	A	1142	THR
1	A	1146	VAL
1	A	1163	ILE
1	A	1170	ILE
1	A	1178	ASP
1	A	1222	ASN
1	A	1223	ASP
1	A	1227	ILE
1	A	1229	SER
1	A	1235	LYS
1	A	1237	ILE
1	A	1243	VAL
1	A	1248	LEU
1	A	1251	GLU
1	A	1257	ASP
1	A	1259	MET
1	A	1264	GLU
1	A	1267	MET
1	A	1280	GLU
1	A	1281	ARG
1	A	1291	VAL
1	A	1314	SER
1	A	1322	ILE
1	A	1327	ILE
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1355	VAL
1	A	1366	ARG
1	A	1382	THR
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1401	SER
1	A	1403	GLU

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Mol	Chain	Res	Type
1	A	1406	VAL
1	A	1420	ASP
1	A	1426	GLU
1	A	1448	GLU
1	A	1450	LEU
1	A	1451	VAL
2	B	35	SER
2	B	39	ARG
2	B	43	LEU
2	B	46	GLN
2	B	57	TYR
2	B	59	LEU
2	B	68	THR
2	B	69	LEU
2	B	71	LEU
2	B	74	LEU
2	B	79	THR
2	B	80	GLU
2	B	87	LYS
2	B	88	TYR
2	B	89	GLU
2	B	90	ILE
2	B	96	TYR
2	B	108	VAL
2	B	112	LEU
2	B	120	ARG
2	B	121	ASN
2	B	164	LYS
2	B	176	SER
2	B	199	MET
2	B	206	ASN
2	B	222	ILE
2	B	244	LEU
2	B	246	LYS
2	B	253	THR
2	B	254	LEU
2	B	264	SER
2	B	268	THR
2	B	279	ASP
2	B	283	VAL
2	B	302	CYS
2	B	305	VAL

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Mol	Chain	Res	Type
2	B	310	MET
2	B	313	MET
2	B	315	LYS
2	B	317	CYS
2	B	323	VAL
2	B	327	ARG
2	B	333	PHE
2	B	337	ARG
2	B	353	LYS
2	B	354	ASP
2	B	355	ILE
2	B	364	ILE
2	B	391	ASP
2	B	394	ASP
2	B	396	ASP
2	B	397	ASP
2	B	398	ARG
2	B	404	LYS
2	B	408	LEU
2	B	416	LEU
2	B	419	THR
2	B	420	LEU
2	B	425	THR
2	B	427	ASP
2	B	440	HIS
2	B	445	LYS
2	B	459	TYR
2	B	463	THR
2	B	466	TRP
2	B	469	GLN
2	B	470	LYS
2	B	476	ARG
2	B	479	VAL
2	B	483	LEU
2	B	489	SER
2	B	490	SER
2	B	502	ILE
2	B	516	ASN
2	B	526	GLU
2	B	527	THR
2	B	531	GLN
2	B	533	CYS

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Mol	Chain	Res	Type
2	B	539	LEU
2	B	542	MET
2	B	544	CYS
2	B	556	THR
2	B	570	VAL
2	B	581	PHE
2	B	603	LEU
2	B	624	LEU
2	B	625	LYS
2	B	626	ILE
2	B	635	ARG
2	B	637	LEU
2	B	643	ASP
2	B	644	GLU
2	B	678	GLU
2	B	679	TYR
2	B	684	LEU
2	B	701	ILE
2	B	709	ASP
2	B	710	LEU
2	B	730	ARG
2	B	736	THR
2	B	739	THR
2	B	748	ILE
2	B	763	GLN
2	B	764	SER
2	B	769	TYR
2	B	771	SER
2	B	776	GLN
2	B	782	LEU
2	B	790	ASP
2	B	794	ASN
2	B	795	ILE
2	B	801	LYS
2	B	806	THR
2	B	822	ASN
2	B	824	ILE
2	B	840	ILE
2	B	843	GLN
2	B	844	SER
2	B	845	SER
2	B	856	PHE

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Mol	Chain	Res	Type
2	B	857	ARG
2	B	864	LYS
2	B	865	LYS
2	B	871	THR
2	B	873	THR
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU
2	B	886	LYS
2	B	899	ILE
2	B	911	ILE
2	B	941	LEU
2	B	942	ARG
2	B	943	SER
2	B	953	LEU
2	B	959	ASP
2	B	963	PHE
2	B	970	THR
2	B	975	GLN
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1010	LEU
2	B	1011	ILE
2	B	1012	ILE
2	B	1019	SER
2	B	1022	THR
2	B	1028	GLU
2	B	1037	LEU
2	B	1051	THR
2	B	1060	ARG
2	B	1065	GLN
2	B	1071	VAL
2	B	1082	MET
2	B	1087	PHE
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1103	ILE

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Mol	Chain	Res	Type
2	B	1113	VAL
2	B	1115	THR
2	B	1116	ARG
2	B	1122	ARG
2	B	1124	ARG
2	B	1133	MET
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1155	SER
2	B	1159	ARG
2	B	1194	ILE
2	B	1196	ILE
2	B	1203	LEU
3	C	4	GLU
3	C	10	ILE
3	C	17	ASN
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	32	SER
3	C	34	ARG
3	C	36	VAL
3	C	37	MET
3	C	43	THR
3	C	50	GLU
3	C	51	VAL
3	C	53	THR
3	C	57	VAL
3	C	58	LEU
3	C	77	ILE
3	C	81	GLU
3	C	83	SER
3	C	85	ASP
3	C	92	CYS
3	C	93	ASP
3	C	94	LYS
3	C	101	LEU
3	C	102	GLN
3	C	118	LEU

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Mol	Chain	Res	Type
3	C	120	ILE
3	C	129	ILE
3	C	133	ILE
3	C	143	LEU
3	C	144	ILE
3	C	156	THR
3	C	163	ILE
3	C	178	PHE
3	C	183	TRP
3	C	195	GLN
3	C	196	ASP
3	C	197	SER
3	C	199	LYS
3	C	211	ASP
3	C	215	GLU
3	C	221	TYR
3	C	226	ASP
3	C	228	PHE
3	C	229	TYR
3	C	240	VAL
3	C	244	VAL
3	C	250	THR
3	C	258	ILE
3	C	259	LEU
4	E	3	GLN
4	E	4	GLU
4	E	6	GLU
4	E	31	THR
4	E	37	LEU
4	E	43	LYS
4	E	66	GLU
4	E	67	GLU
4	E	72	PHE
4	E	83	CYS
4	E	88	VAL
4	E	92	THR
4	E	134	THR
4	E	150	VAL
4	E	157	SER
4	E	165	LEU
4	E	169	ARG
4	E	182	ASP

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Mol	Chain	Res	Type
4	E	196	VAL
4	E	202	SER
4	E	204	THR
4	E	210	SER
5	F	74	ILE
5	F	76	LYS
5	F	79	ARG
5	F	97	ARG
5	F	99	LEU
5	F	111	LEU
5	F	120	ILE
5	F	140	ASP
6	H	11	GLN
6	H	16	ASP
6	H	24	CYS
6	H	40	LEU
6	H	44	VAL
6	H	53	ASP
6	H	62	SER
6	H	78	SER
6	H	89	LEU
6	H	95	TYR
6	H	110	ASP
6	H	137	GLN
7	I	5	ARG
7	I	7	CYS
7	I	8	ARG
7	I	17	ARG
7	I	28	GLU
7	I	30	ARG
7	I	31	THR
7	I	50	THR
7	I	59	VAL
7	I	60	GLN
7	I	69	PRO
7	I	80	SER
7	I	83	ASN
7	I	84	VAL
7	I	92	ARG
7	I	95	THR
7	I	111	THR
8	J	2	ILE

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Mol	Chain	Res	Type
8	J	5	VAL
8	J	7	CYS
8	J	14	VAL
8	J	16	ASP
8	J	23	ASN
8	J	31	ASP
8	J	34	THR
8	J	38	ARG
8	J	42	LYS
8	J	43	ARG
8	J	56	LEU
9	K	1	MET
9	K	5	ASP
9	K	12	LEU
9	K	18	LYS
9	K	20	LYS
9	K	33	ILE
9	K	34	THR
9	K	50	LEU
9	K	51	LEU
9	K	63	VAL
9	K	75	ILE
9	K	77	THR
9	K	85	ASP
9	K	94	ILE
9	K	95	ILE
9	K	101	LEU
9	K	102	LYS
9	K	107	THR
10	L	26	THR
10	L	27	LEU
10	L	28	LYS
10	L	31	CYS
10	L	49	LYS
10	L	50	ASP
10	L	57	LEU
10	L	61	THR
10	L	66	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	160	GLN
1	A	273	ASN
1	A	281	HIS
1	A	297	GLN
1	A	306	ASN
1	A	339	ASN
1	A	399	HIS
1	A	435	HIS
1	A	447	GLN
1	A	471	ASN
1	A	490	HIS
1	A	503	GLN
1	A	517	ASN
1	A	659	HIS
1	A	723	ASN
1	A	741	ASN
1	A	742	ASN
1	A	760	GLN
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1082	ASN
1	A	1085	HIS
1	A	1222	ASN
1	A	1278	ASN
1	A	1354	ASN
1	A	1387	HIS
1	A	1427	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	215	GLN
2	B	236	HIS
2	B	278	GLN
2	B	395	GLN
2	B	433	GLN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	648	HIS

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Mol	Chain	Res	Type
2	B	744	HIS
2	B	762	ASN
2	B	770	GLN
2	B	794	ASN
2	B	822	ASN
2	B	862	GLN
2	B	958	GLN
2	B	975	GLN
2	B	984	HIS
2	B	1025	HIS
2	B	1084	GLN
2	B	1141	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1195	HIS
3	C	31	ASN
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	184	ASN
3	C	188	HIS
3	C	195	GLN
3	C	203	GLN
4	E	8	ASN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
6	H	11	GLN
6	H	137	GLN
7	I	60	GLN
9	K	65	HIS
9	K	104	ASN
9	K	112	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/12 (91%)	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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	1442/1733 (83%)	-0.28	30 (2%) 63 59	72, 131, 247, 370	0
2	B	1153/1224 (94%)	-0.23	21 (1%) 68 65	71, 114, 240, 374	0
3	C	271/318 (85%)	-0.42	4 (1%) 73 70	80, 106, 165, 306	0
4	E	215/215 (100%)	-0.33	0 100 100	106, 165, 276, 316	0
5	F	85/155 (54%)	-0.33	0 100 100	107, 137, 170, 200	0
6	H	136/146 (93%)	-0.14	3 (2%) 62 57	126, 169, 276, 299	0
7	I	119/122 (97%)	-0.34	0 100 100	109, 150, 180, 237	0
8	J	65/70 (92%)	-0.51	0 100 100	80, 94, 135, 153	0
9	K	114/120 (95%)	-0.46	0 100 100	83, 112, 136, 139	0
10	L	46/70 (65%)	-0.18	1 (2%) 62 57	99, 175, 228, 246	0
11	R	12/12 (100%)	-0.54	0 100 100	104, 119, 182, 208	0
12	T	28/29 (96%)	-0.10	0 100 100	102, 222, 413, 422	0
13	N	14/14 (100%)	-0.13	0 100 100	270, 329, 352, 379	0
All	All	3700/4228 (87%)	-0.28	59 (1%) 72 68	71, 128, 251, 422	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1250	ALA	6.4
2	B	882	THR	6.0
1	A	1249	ASP	5.4
1	A	44	THR	5.3
2	B	441	ASP	4.8
1	A	1248	LEU	4.6
1	A	1247	SER	4.3
1	A	191	THR	4.2
2	B	443	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	83	ASN	4.1
6	H	84	ALA	3.6
1	A	1086	PHE	3.6
1	A	257	ARG	3.6
1	A	45	GLN	3.6
2	B	869	SER	3.5
2	B	717	GLU	3.3
2	B	75	ALA	3.3
6	H	86	ASP	3.1
1	A	1251	GLU	3.0
2	B	720	ASP	3.0
2	B	341	LEU	3.0
1	A	66	LYS	3.0
1	A	3	GLY	3.0
1	A	46	THR	2.9
1	A	72	GLU	2.9
2	B	85	SER	2.9
1	A	1252	THR	2.7
2	B	719	ASN	2.7
2	B	106	ASP	2.7
2	B	343	ILE	2.7
1	A	1087	ALA	2.7
1	A	1245	PRO	2.6
1	A	1091	SER	2.6
6	H	85	GLY	2.6
1	A	190	ALA	2.5
2	B	342	GLY	2.5
1	A	1126	ALA	2.5
10	L	25	ALA	2.5
1	A	149	GLU	2.5
2	B	79	THR	2.5
1	A	152	VAL	2.4
3	C	272	PHE	2.4
2	B	1161	HIS	2.3
1	A	1246	LYS	2.3
2	B	440	HIS	2.3
2	B	84	ILE	2.3
1	A	192	GLY	2.3
1	A	426	LEU	2.3
3	C	271	ASN	2.2
3	C	267	GLN	2.2
2	B	714	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	195	ASP	2.2
1	A	162	VAL	2.2
1	A	151	ASP	2.2
2	B	339	THR	2.2
3	C	270	VAL	2.1
1	A	313	GLN	2.1
1	A	286	HIS	2.1
2	B	709	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
14	ZN	J	101	1/1	0.75	0.16	218,218,218,218	0
14	ZN	B	1307	1/1	0.90	0.03	163,163,163,163	0
14	ZN	A	1734	1/1	0.92	0.04	232,232,232,232	0
14	ZN	L	105	1/1	0.94	0.10	155,155,155,155	0
14	ZN	A	1735	1/1	0.97	0.08	136,136,136,136	0
14	ZN	I	204	1/1	0.98	0.06	125,125,125,125	0
14	ZN	I	203	1/1	0.99	0.09	103,103,103,103	0
14	ZN	C	319	1/1	0.99	0.11	118,118,118,118	0
15	MG	A	1736	1/1	0.99	0.14	113,113,113,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.