



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:02 PM GMT

PDB ID : 4E54  
Title : Damaged DNA induced UV-damaged DNA-binding protein (UV-DDB) dimerization and its roles in chromatinized DNA repair  
Authors : Yeh, J.I.; Du, S.  
Deposited on : 2012-03-14  
Resolution : 2.85 Å(reported)

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

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

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

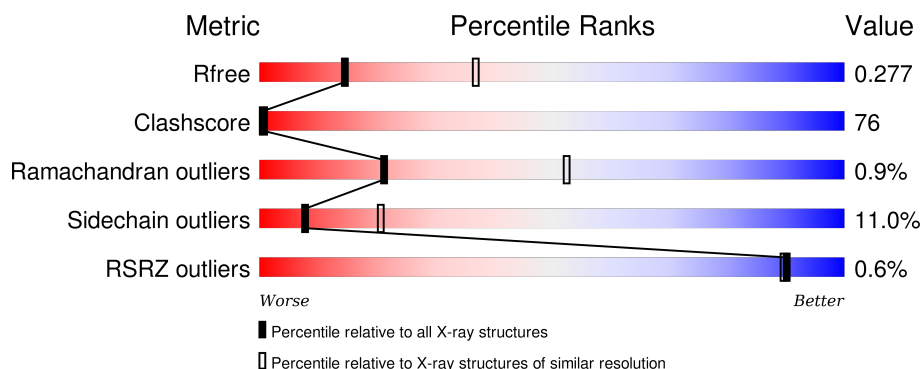
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	1150	<div> <div>40%</div> <div>53%</div> <div>6%</div> </div>
2	B	435	<div> <div>2%</div> <div>19%</div> <div>59%</div> <div>13%</div> <div>8%</div> </div>
3	F	24	<div> <div>17%</div> <div>75%</div> <div>8%</div> </div>
4	G	24	<div> <div>17%</div> <div>71%</div> <div>13%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13008 atoms, of which 33 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1140	Total	C	H	N	O	S	0	0	0
			8874	5589	33	1497	1711	44			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP Q16531
A	-8	HIS	-	EXPRESSION TAG	UNP Q16531
A	-7	HIS	-	EXPRESSION TAG	UNP Q16531
A	-6	HIS	-	EXPRESSION TAG	UNP Q16531
A	-5	HIS	-	EXPRESSION TAG	UNP Q16531
A	-4	HIS	-	EXPRESSION TAG	UNP Q16531
A	-3	HIS	-	EXPRESSION TAG	UNP Q16531
A	-2	HIS	-	EXPRESSION TAG	UNP Q16531
A	-1	HIS	-	EXPRESSION TAG	UNP Q16531
A	0	HIS	-	EXPRESSION TAG	UNP Q16531
A	1	HIS	-	EXPRESSION TAG	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3157	2001	571	565	20			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	EXPRESSION TAG	UNP Q92466
B	-6	ASP	-	EXPRESSION TAG	UNP Q92466
B	-5	TYR	-	EXPRESSION TAG	UNP Q92466
B	-4	LYS	-	EXPRESSION TAG	UNP Q92466
B	-3	ASP	-	EXPRESSION TAG	UNP Q92466

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ASP	-	EXPRESSION TAG	UNP Q92466
B	-1	ASP	-	EXPRESSION TAG	UNP Q92466
B	0	ASP	-	EXPRESSION TAG	UNP Q92466
B	1	LYS	-	EXPRESSION TAG	UNP Q92466

- Molecule 3 is a DNA chain called AP24 DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	24	Total	C	N	O	P	0	0	0
			497	236	91	146	24			

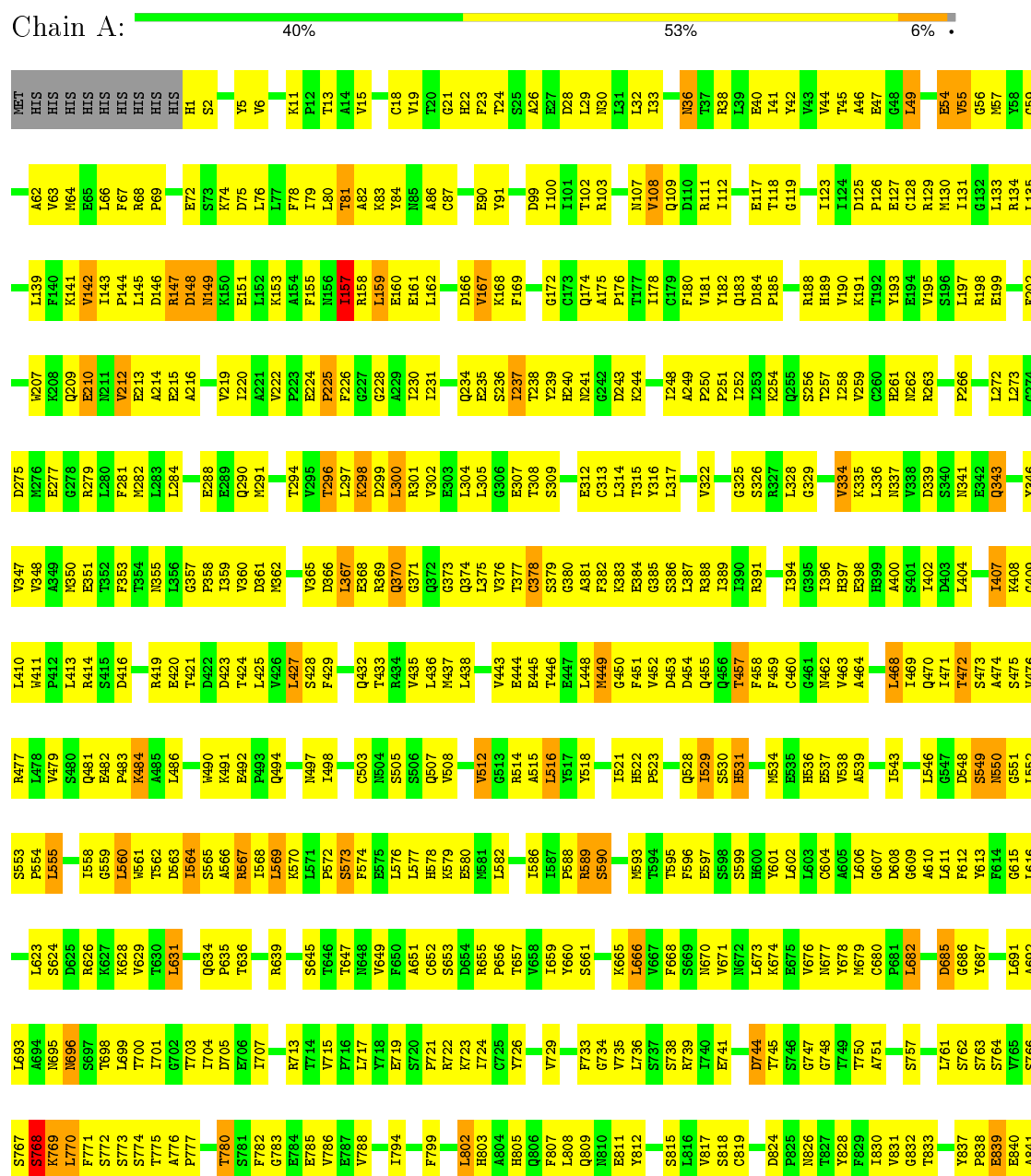
- Molecule 4 is a DNA chain called AP24 DNA complementary strand.

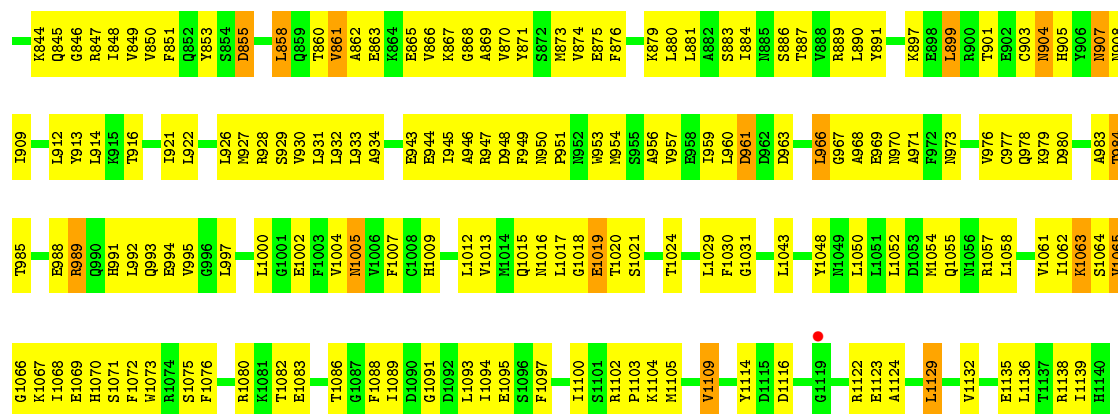
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	24	Total	C	N	O	P	0	0	0
			480	228	86	142	24			

### 3 Residue-property plots

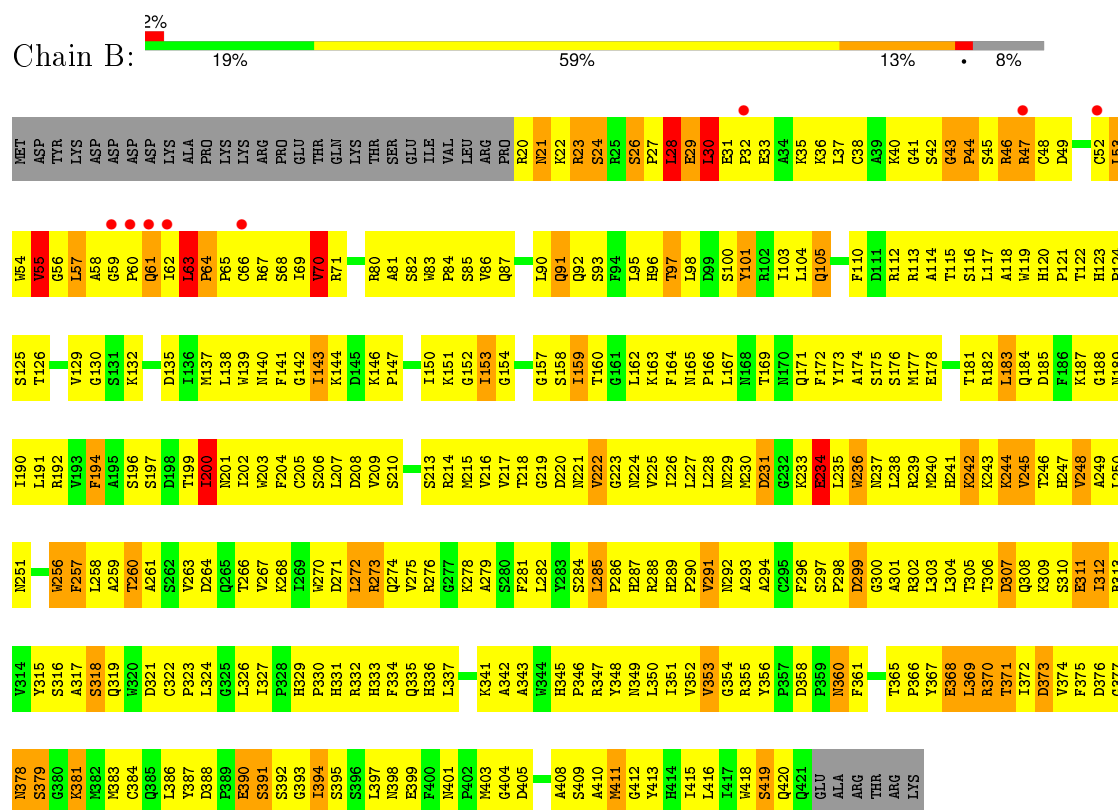
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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 damage-binding protein 1

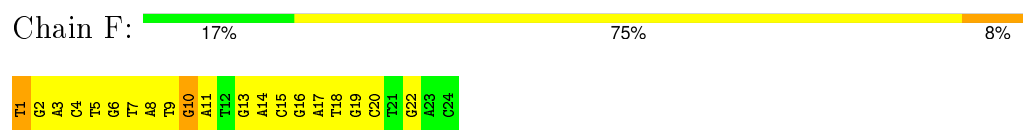




### • Molecule 2: DNA damage-binding protein 2



### • Molecule 3: AP24 DNA strand



### • Molecule 4: AP24 DNA complementary strand



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.74Å 70.88Å 191.45Å 90.00° 99.68° 90.00°	Depositor
Resolution (Å)	33.31 – 2.85 33.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.0 (33.31-2.85) 76.2 (33.31-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.233 , 0.281 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	1932 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 329.7	EDS
Estimated twinning fraction	0.190 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.14$	Xtriage
Outliers	0 of 39354 reflections	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	13008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	0.30	0/9003	0.65	6/12208 (0.0%)
2	B	0.38	3/3244 (0.1%)	0.91	12/4404 (0.3%)
3	F	0.63	1/557 (0.2%)	1.55	3/857 (0.4%)
4	G	0.97	2/524 (0.4%)	1.34	6/801 (0.7%)
All	All	0.39	6/13328 (0.0%)	0.82	27/18270 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	12	DC	O3'-P	-16.33	1.41	1.61
4	G	1	DG	OP3-P	-10.74	1.48	1.61
3	F	1	DT	OP3-P	-10.05	1.49	1.61
2	B	30	LEU	CA-C	6.24	1.69	1.52
2	B	30	LEU	N-CA	5.88	1.58	1.46
2	B	29	GLU	CA-C	-5.23	1.39	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	DT	OP1-P-OP2	-22.73	85.51	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	VAL	CA-C-N	-21.23	73.74	116.20
2	B	55	VAL	O-C-N	19.17	155.79	123.20
3	F	1	DT	O5'-P-OP2	-18.66	88.31	110.70
2	B	55	VAL	CA-C-O	-18.11	82.06	120.10
2	B	63	LEU	C-N-CD	-14.54	88.62	120.60
2	B	47	ARG	N-CA-CB	-11.71	89.52	110.60
4	G	12	DC	OP1-P-O3'	-11.06	80.86	105.20
2	B	29	GLU	N-CA-C	-10.51	82.63	111.00
4	G	12	DC	OP2-P-O3'	9.85	126.86	105.20
1	A	484	LYS	N-CA-C	9.51	136.68	111.00
4	G	1	DG	OP1-P-OP2	-8.18	107.33	119.60
4	G	7	DA	O4'-C1'-N9	7.99	113.59	108.00
1	A	747	GLY	N-CA-C	7.92	132.90	113.10
2	B	30	LEU	N-CA-C	7.28	130.66	111.00
4	G	5	DG	O4'-C1'-N9	6.88	112.82	108.00
2	B	38	CYS	N-CA-C	6.68	129.03	111.00
1	A	21	GLY	N-CA-C	-6.45	96.96	113.10
2	B	28	LEU	C-N-CA	6.08	136.91	121.70
2	B	368	GLU	N-CA-C	6.07	127.38	111.00
1	A	157	ILE	CB-CA-C	-5.95	99.69	111.60
2	B	43	GLY	C-N-CD	-5.95	107.51	120.60
1	A	769	LYS	N-CA-C	5.88	126.89	111.00
4	G	12	DC	P-O3'-C3'	-5.72	112.84	119.70
3	F	10	DG	O4'-C1'-N9	5.63	111.94	108.00
2	B	21	ASN	N-CA-C	-5.48	96.19	111.00
1	A	210	GLU	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	GLU	Peptide
1	A	148	ASP	Peptide
1	A	548	ASP	Peptide
1	A	768	SER	Peptide
2	B	200	ILE	Peptide
2	B	234	GLU	Peptide
2	B	390	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8841	33	8728	1094	2
2	B	3157	0	3128	801	2
3	F	497	0	272	41	0
4	G	480	0	267	44	0
All	All	12975	33	12395	1919	3

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 76.

All (1919) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:TRP:CD1	2:B:55:VAL:HG12	1.33	1.57
2:B:24:SER:CB	2:B:36:LYS:HE3	1.37	1.51
2:B:48:CYS:SG	2:B:52:CYS:HB3	1.48	1.49
2:B:30:LEU:CD1	2:B:31:GLU:H	1.28	1.46
2:B:52:CYS:SG	2:B:53:LEU:HD11	1.58	1.42
2:B:30:LEU:HD12	2:B:31:GLU:N	1.32	1.39
2:B:28:LEU:CD2	2:B:36:LYS:HB3	1.55	1.36
2:B:54:TRP:CD1	2:B:55:VAL:N	1.94	1.35
1:A:768:SER:HB2	1:A:769:LYS:C	1.44	1.33
2:B:308:GLN:HB3	2:B:333:HIS:CD2	1.64	1.33
2:B:52:CYS:SG	2:B:53:LEU:CD1	2.16	1.32
2:B:53:LEU:HB2	2:B:54:TRP:CA	1.59	1.31
2:B:57:LEU:O	2:B:60:PRO:HD2	1.21	1.31
1:A:602:LEU:HD13	1:A:623:LEU:CD2	1.61	1.30
2:B:60:PRO:O	2:B:64:PRO:HD2	1.28	1.30
1:A:19:VAL:HG11	1:A:64:MET:O	1.31	1.29
2:B:53:LEU:C	2:B:57:LEU:HG	1.51	1.29
2:B:24:SER:CB	2:B:36:LYS:CE	2.11	1.29
2:B:53:LEU:CB	2:B:54:TRP:HA	1.49	1.28
2:B:24:SER:OG	2:B:36:LYS:CD	1.79	1.28
1:A:427:LEU:HD21	1:A:429:PHE:CE2	1.67	1.27
2:B:60:PRO:HA	2:B:63:LEU:CD1	1.64	1.27
2:B:57:LEU:HD13	2:B:57:LEU:C	1.49	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:HIS:HB2	1:A:74:LYS:CE	1.63	1.26
2:B:28:LEU:HD21	2:B:36:LYS:CB	1.66	1.25
2:B:24:SER:OG	2:B:36:LYS:HD3	1.12	1.25
2:B:28:LEU:CD2	2:B:36:LYS:CB	2.16	1.23
2:B:54:TRP:CD1	2:B:55:VAL:CG1	2.19	1.23
2:B:28:LEU:CB	2:B:30:LEU:H	1.52	1.22
2:B:53:LEU:CA	2:B:57:LEU:HG	1.68	1.22
2:B:54:TRP:O	2:B:57:LEU:HD12	1.39	1.21
2:B:290:PRO:HB2	2:B:308:GLN:CD	1.62	1.20
1:A:824:ASP:OD2	1:A:897:LYS:NZ	1.74	1.20
2:B:23:ARG:O	2:B:27:PRO:HD2	1.40	1.20
2:B:41:GLY:O	2:B:44:PRO:HD3	1.37	1.20
2:B:53:LEU:CD2	2:B:54:TRP:HA	1.70	1.19
1:A:550:ASN:N	1:A:551:GLY:HA2	1.52	1.19
2:B:54:TRP:HD1	2:B:55:VAL:CG1	1.54	1.19
1:A:129:ARG:HD2	1:A:176:PRO:CG	1.72	1.19
1:A:980:ASP:O	1:A:989:ARG:NH2	1.73	1.19
2:B:48:CYS:SG	2:B:52:CYS:CB	2.30	1.18
1:A:512:VAL:HG12	1:A:515:ALA:HB3	1.22	1.18
2:B:46:ARG:C	2:B:48:CYS:HA	1.63	1.18
2:B:129:VAL:HG11	2:B:415:ILE:HD11	1.18	1.17
1:A:359:ILE:O	1:A:1005:ASN:OD1	1.63	1.17
1:A:375:LEU:HD11	1:A:389:ILE:CG2	1.73	1.17
2:B:46:ARG:HG3	2:B:49:ASP:CG	1.64	1.17
2:B:28:LEU:HB3	2:B:30:LEU:N	1.58	1.16
1:A:828:TYR:OH	1:A:897:LYS:NZ	1.78	1.16
1:A:416:ASP:HB3	1:A:419:ARG:NH1	1.60	1.16
2:B:46:ARG:HB2	2:B:49:ASP:H	1.09	1.15
2:B:35:LYS:O	2:B:37:LEU:HD13	1.47	1.15
1:A:248:ILE:HD12	1:A:300:LEU:HB2	1.20	1.15
2:B:53:LEU:HB2	2:B:54:TRP:C	1.68	1.14
2:B:63:LEU:HB2	2:B:64:PRO:HD2	1.14	1.14
1:A:602:LEU:HD11	1:A:616:LEU:CD1	1.77	1.14
1:A:157:ILE:HG21	1:A:202:PHE:HE2	1.11	1.14
1:A:602:LEU:HD12	1:A:616:LEU:HB2	1.21	1.13
4:G:11:3DR:C3'	4:G:12:DC:H5''	1.77	1.13
2:B:53:LEU:CD2	2:B:54:TRP:CA	2.26	1.13
1:A:144:PRO:HB3	1:A:197:LEU:HD11	1.29	1.13
2:B:63:LEU:HB2	2:B:64:PRO:CD	1.80	1.12
2:B:411:MET:HG2	2:B:412:GLY:N	1.59	1.12
1:A:394:ILE:HG23	1:A:705:ASP:OD1	1.48	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LEU:CG	2:B:54:TRP:HA	1.78	1.11
1:A:436:LEU:HD11	1:A:443:VAL:HB	1.14	1.11
2:B:53:LEU:HD13	2:B:53:LEU:N	1.66	1.11
1:A:608:ASP:OD1	1:A:610:ALA:N	1.83	1.11
2:B:46:ARG:HB2	2:B:49:ASP:N	1.66	1.11
2:B:52:CYS:C	2:B:53:LEU:HD13	1.69	1.11
1:A:536:HIS:HB2	1:A:560:LEU:HD12	1.19	1.11
1:A:67:PHE:CE1	1:A:145:LEU:HD21	1.87	1.10
1:A:248:ILE:HG22	1:A:250:PRO:HD3	1.27	1.10
4:G:11:3DR:H3'	4:G:12:DC:C5'	1.80	1.10
1:A:133:LEU:HD22	1:A:135:LEU:HD21	1.34	1.10
2:B:59:GLY:O	2:B:62:ILE:HG12	1.52	1.10
2:B:221:ASN:HA	2:B:244:LYS:HB2	1.30	1.10
2:B:60:PRO:HA	2:B:63:LEU:HD12	1.21	1.09
2:B:46:ARG:HG3	2:B:49:ASP:OD2	1.53	1.09
1:A:248:ILE:CD1	1:A:300:LEU:HB2	1.81	1.09
1:A:129:ARG:HD2	1:A:176:PRO:HG3	1.27	1.09
2:B:53:LEU:HD23	2:B:54:TRP:CG	1.88	1.09
2:B:47:ARG:N	2:B:48:CYS:HA	1.52	1.09
2:B:293:ALA:HB3	2:B:306:THR:HG22	1.30	1.08
2:B:23:ARG:HG2	2:B:24:SER:N	1.41	1.08
3:F:19:DG:H2''	3:F:20:DC:H5'	1.12	1.08
2:B:313:ARG:HD3	2:B:326:LEU:HD21	1.34	1.08
1:A:472:THR:HG23	1:A:474:ALA:H	1.15	1.08
1:A:224:GLU:HA	1:A:226:PHE:N	1.68	1.07
1:A:602:LEU:HD13	1:A:623:LEU:HD22	1.21	1.06
1:A:224:GLU:HA	1:A:226:PHE:H	0.91	1.06
1:A:22:HIS:HB2	1:A:74:LYS:HE3	1.12	1.06
2:B:332:ARG:NH2	2:B:358:ASP:HB3	1.71	1.06
1:A:1018:GLY:CA	1:A:1019:GLU:HB2	1.86	1.06
2:B:112:ARG:NH2	2:B:154:GLY:O	1.89	1.05
1:A:367:LEU:HD22	1:A:368:GLU:N	1.71	1.05
2:B:48:CYS:N	2:B:52:CYS:SG	2.30	1.05
2:B:53:LEU:HA	2:B:57:LEU:HG	1.36	1.04
1:A:602:LEU:HD11	1:A:616:LEU:HD13	1.05	1.04
1:A:427:LEU:HD21	1:A:429:PHE:CZ	1.92	1.04
1:A:299:ASP:OD1	1:A:300:LEU:N	1.90	1.04
2:B:308:GLN:CD	2:B:333:HIS:NE2	2.10	1.04
1:A:679:MET:HG2	1:A:691:LEU:HD11	1.36	1.04
2:B:62:ILE:CG1	2:B:63:LEU:HD23	1.87	1.04
2:B:24:SER:HB2	2:B:36:LYS:HE3	1.09	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LEU:HB2	2:B:54:TRP:O	1.55	1.03
1:A:436:LEU:HD11	1:A:443:VAL:CB	1.88	1.03
1:A:463:VAL:CG1	1:A:521:ILE:HD13	1.88	1.03
1:A:157:ILE:HD13	1:A:202:PHE:CZ	1.93	1.03
2:B:53:LEU:CD2	2:B:54:TRP:CB	2.37	1.03
2:B:312:ILE:CG2	2:B:327:ILE:HD12	1.89	1.02
1:A:589:ARG:HD3	1:A:589:ARG:O	1.57	1.02
2:B:62:ILE:CG1	2:B:63:LEU:CD2	2.38	1.02
2:B:312:ILE:HG21	2:B:327:ILE:HD12	1.06	1.02
2:B:57:LEU:O	2:B:60:PRO:CD	2.06	1.02
2:B:120:HIS:CE1	2:B:169:THR:HG21	1.95	1.02
1:A:536:HIS:HB2	1:A:560:LEU:CD1	1.88	1.02
2:B:62:ILE:HG12	2:B:63:LEU:CD2	1.90	1.01
2:B:332:ARG:HH22	2:B:358:ASP:HB3	1.25	1.01
1:A:507:GLN:HE22	1:A:553:SER:H	1.06	1.01
2:B:30:LEU:O	2:B:32:PRO:O	1.76	1.01
2:B:313:ARG:HD3	2:B:326:LEU:CD2	1.89	1.01
1:A:374:GLN:O	1:A:1012:LEU:HD22	1.60	1.01
1:A:129:ARG:HH11	1:A:176:PRO:HG3	1.21	1.01
2:B:172:PHE:HZ	2:B:184:GLN:HE21	1.08	1.01
2:B:31:GLU:OE2	2:B:85:SER:HB2	1.61	1.00
2:B:290:PRO:O	2:B:308:GLN:HG3	1.59	1.00
1:A:463:VAL:HG11	1:A:521:ILE:HD13	1.42	1.00
1:A:366:ASP:HA	1:A:373:GLY:CA	1.91	1.00
1:A:366:ASP:HA	1:A:373:GLY:HA3	1.02	1.00
1:A:32:LEU:HG	1:A:41:ILE:HG12	1.42	1.00
2:B:199:THR:O	2:B:200:ILE:HG13	1.60	1.00
1:A:537:GLU:O	1:A:560:LEU:HD13	1.62	0.99
1:A:1062:ILE:HG22	1:A:1063:LYS:O	1.60	0.99
2:B:40:LYS:O	2:B:44:PRO:HD2	1.62	0.99
1:A:1094:ILE:CD1	1:A:1136:LEU:HD13	1.92	0.99
2:B:28:LEU:HB3	2:B:30:LEU:HA	1.39	0.99
1:A:157:ILE:HD13	1:A:202:PHE:CE2	1.97	0.99
1:A:602:LEU:CD1	1:A:616:LEU:HD13	1.90	0.99
2:B:53:LEU:C	2:B:57:LEU:CG	2.30	0.98
2:B:32:PRO:HD2	2:B:67:ARG:NE	1.78	0.98
2:B:58:ALA:O	2:B:62:ILE:HG23	1.63	0.98
1:A:375:LEU:HD11	1:A:389:ILE:HG23	1.41	0.98
3:F:19:DG:H2''	3:F:20:DC:C5'	1.93	0.98
1:A:416:ASP:HB3	1:A:419:ARG:HH11	1.14	0.98
1:A:288:GLU:HG3	1:A:296:THR:HB	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:CB	2:B:64:PRO:HD2	1.85	0.98
1:A:427:LEU:CD2	1:A:429:PHE:CE2	2.46	0.97
2:B:41:GLY:C	2:B:44:PRO:HD3	1.83	0.97
2:B:62:ILE:HG13	2:B:63:LEU:HD23	1.45	0.97
2:B:97:THR:OG1	2:B:420:GLN:NE2	1.96	0.97
2:B:24:SER:CB	2:B:36:LYS:CD	2.41	0.97
2:B:20:ARG:O	2:B:23:ARG:HD3	1.64	0.97
2:B:47:ARG:N	2:B:48:CYS:CA	2.28	0.97
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.45	0.97
1:A:602:LEU:CD1	1:A:623:LEU:CD2	2.43	0.97
1:A:601:TYR:CZ	1:A:666:LEU:HD11	2.00	0.97
1:A:602:LEU:CD1	1:A:616:LEU:HB2	1.93	0.96
2:B:23:ARG:HG2	2:B:24:SER:H	1.03	0.96
1:A:1005:ASN:HD22	1:A:1005:ASN:H	1.13	0.96
1:A:277:GLU:OE1	1:A:279:ARG:NH1	1.98	0.96
2:B:53:LEU:HD23	2:B:54:TRP:CA	1.94	0.96
1:A:534:MET:HE1	1:A:558:ILE:CD1	1.95	0.96
1:A:151:GLU:OE1	1:A:153:LYS:NZ	1.97	0.96
2:B:24:SER:OG	2:B:36:LYS:CE	2.11	0.96
1:A:762:SER:HG	1:A:803:HIS:HD1	1.06	0.96
1:A:768:SER:HB2	1:A:769:LYS:CA	1.95	0.96
2:B:23:ARG:CG	2:B:24:SER:N	2.29	0.96
2:B:36:LYS:HG3	2:B:37:LEU:H	1.30	0.96
1:A:471:ILE:HG23	1:A:476:VAL:HG12	1.48	0.96
2:B:53:LEU:HB2	2:B:54:TRP:HA	1.20	0.95
2:B:330:PRO:O	2:B:356:TYR:N	1.98	0.95
2:B:200:ILE:HD12	2:B:201:ASN:H	1.30	0.95
1:A:147:ARG:CG	1:A:147:ARG:HH11	1.78	0.95
1:A:341:ASN:HB2	1:A:343:GLN:OE1	1.66	0.95
2:B:24:SER:HB3	2:B:36:LYS:CE	1.94	0.95
2:B:28:LEU:HB3	2:B:30:LEU:H	1.20	0.95
2:B:263:VAL:HA	2:B:290:PRO:HB3	1.47	0.95
1:A:550:ASN:H	1:A:551:GLY:HA2	1.30	0.95
2:B:270:TRP:HE3	2:B:275:VAL:HG21	1.30	0.95
2:B:114:ALA:HB1	2:B:410:ALA:HB1	1.47	0.95
3:F:7:DT:H2"	3:F:8:DA:H5"	1.48	0.95
2:B:28:LEU:CB	2:B:30:LEU:N	2.24	0.95
2:B:30:LEU:HD13	2:B:31:GLU:H	1.29	0.95
2:B:57:LEU:CD1	2:B:57:LEU:C	2.30	0.95
1:A:518:TYR:CD2	1:A:529:ILE:HG12	2.02	0.94
2:B:129:VAL:HG11	2:B:415:ILE:CD1	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:VAL:HG22	2:B:216:VAL:HG22	1.49	0.94
2:B:60:PRO:O	2:B:64:PRO:CD	2.15	0.94
2:B:53:LEU:CB	2:B:54:TRP:CA	2.26	0.94
1:A:176:PRO:HB2	1:A:195:VAL:CG1	1.97	0.94
3:F:15:DC:N4	4:G:10:DG:O6	2.00	0.94
1:A:602:LEU:HD13	1:A:623:LEU:HD21	1.45	0.94
2:B:52:CYS:SG	2:B:53:LEU:HD13	2.08	0.94
2:B:59:GLY:HA2	2:B:62:ILE:HD13	1.49	0.94
1:A:436:LEU:CD1	1:A:443:VAL:HB	1.98	0.94
2:B:28:LEU:HB3	2:B:30:LEU:CA	1.96	0.94
2:B:241:HIS:HB2	2:B:268:LYS:NZ	1.83	0.94
2:B:57:LEU:HD13	2:B:58:ALA:N	1.81	0.93
2:B:355:ARG:NH1	2:B:368:GLU:OE1	2.01	0.93
4:G:20:DA:C2'	4:G:21:DG:H5''	1.99	0.93
1:A:157:ILE:HG21	1:A:202:PHE:CE2	2.02	0.93
1:A:157:ILE:CD1	1:A:202:PHE:CE2	2.51	0.93
1:A:1016:ASN:HA	1:A:1017:LEU:CB	1.99	0.93
2:B:28:LEU:HD22	2:B:36:LYS:CB	1.98	0.93
2:B:46:ARG:HE	2:B:46:ARG:HA	1.28	0.93
1:A:580:GLU:OE2	1:A:626:ARG:NH2	2.00	0.93
2:B:53:LEU:HD22	2:B:54:TRP:CB	1.97	0.92
4:G:16:DA:H2''	4:G:17:DT:H5''	1.51	0.92
3:F:19:DG:C2'	3:F:20:DC:H5'	1.99	0.92
1:A:129:ARG:NH1	1:A:176:PRO:HG3	1.84	0.92
1:A:366:ASP:CA	1:A:373:GLY:HA3	1.96	0.92
2:B:53:LEU:HD23	2:B:54:TRP:CB	1.97	0.92
1:A:768:SER:CB	1:A:769:LYS:C	2.35	0.92
2:B:365:THR:HG23	2:B:368:GLU:OE2	1.69	0.92
1:A:432:GLN:HG3	1:A:453:ASP:O	1.67	0.92
2:B:171:GLN:HB3	2:B:183:LEU:HD11	1.51	0.92
1:A:375:LEU:HD11	1:A:389:ILE:HG22	1.51	0.92
1:A:144:PRO:CB	1:A:197:LEU:HD11	2.00	0.92
2:B:235:LEU:HD12	2:B:235:LEU:O	1.70	0.91
1:A:770:LEU:HD22	1:A:772:SER:HB2	1.51	0.91
1:A:129:ARG:HD2	1:A:176:PRO:HG2	1.51	0.91
1:A:176:PRO:HB2	1:A:195:VAL:HG13	1.52	0.91
1:A:307:GLU:OE2	1:A:383:LYS:NZ	2.02	0.91
1:A:377:THR:HA	1:A:388:ARG:O	1.69	0.90
1:A:679:MET:CG	1:A:691:LEU:HD11	1.99	0.90
2:B:43:GLY:N	2:B:44:PRO:HD2	1.86	0.90
1:A:953:TRP:CE3	2:B:83:TRP:HZ2	1.90	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:SER:HB3	2:B:36:LYS:HG2	1.53	0.90
2:B:379:SER:OG	2:B:381:LYS:HG2	1.70	0.90
2:B:46:ARG:H	2:B:48:CYS:HB2	1.36	0.90
1:A:770:LEU:HD22	1:A:772:SER:CB	2.01	0.90
2:B:308:GLN:HB3	2:B:333:HIS:NE2	1.87	0.90
1:A:370:GLN:HE22	1:A:674:LYS:CE	1.84	0.90
2:B:23:ARG:O	2:B:27:PRO:CD	2.19	0.89
2:B:57:LEU:HD22	2:B:57:LEU:O	1.73	0.89
2:B:53:LEU:HD22	2:B:54:TRP:HB2	1.50	0.89
2:B:412:GLY:O	2:B:413:TYR:HB2	1.72	0.89
1:A:281:PHE:CE1	1:A:304:LEU:HD13	2.08	0.89
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.36	0.89
2:B:52:CYS:CB	2:B:53:LEU:HD13	2.02	0.89
2:B:365:THR:O	2:B:368:GLU:HG2	1.71	0.89
1:A:5:TYR:OH	1:A:1094:ILE:HD11	1.71	0.89
1:A:1054:MET:O	1:A:1058:LEU:HD12	1.71	0.89
1:A:416:ASP:CB	1:A:419:ARG:NH1	2.35	0.89
1:A:379:SER:HB3	1:A:721:PRO:HG2	1.52	0.89
2:B:356:TYR:OH	3:F:15:DC:OP1	1.90	0.88
2:B:221:ASN:CB	2:B:244:LYS:HE2	2.02	0.88
1:A:1018:GLY:HA2	1:A:1019:GLU:HB2	1.53	0.88
3:F:17:DA:N6	4:G:8:DT:O4	2.05	0.88
2:B:28:LEU:HD22	2:B:36:LYS:HB2	1.56	0.88
2:B:36:LYS:CG	2:B:37:LEU:H	1.85	0.88
2:B:32:PRO:HD2	2:B:67:ARG:CD	2.04	0.88
1:A:472:THR:CG2	1:A:474:ALA:H	1.87	0.88
2:B:370:ARG:HD3	2:B:392:SER:O	1.75	0.87
1:A:1114:TYR:HB2	1:A:1124:ALA:HB2	1.54	0.87
1:A:68:ARG:HB2	1:A:75:ASP:OD1	1.74	0.87
1:A:951:PRO:HB3	2:B:347:ARG:CZ	2.05	0.87
2:B:308:GLN:HB3	2:B:333:HIS:HD2	1.36	0.87
2:B:256:TRP:O	2:B:272:LEU:HB3	1.75	0.87
1:A:463:VAL:HG12	1:A:464:ALA:N	1.87	0.87
1:A:570:LYS:HG2	1:A:577:LEU:HD11	1.54	0.87
1:A:536:HIS:CB	1:A:560:LEU:HD12	2.03	0.86
1:A:1020:THR:HA	1:A:1021:SER:C	1.95	0.86
1:A:160:GLU:O	1:A:162:LEU:HD12	1.75	0.86
1:A:722:ARG:NH2	1:A:812:TYR:OH	2.06	0.86
1:A:57:MET:SD	1:A:1068:ILE:HD12	2.15	0.86
1:A:370:GLN:HE22	1:A:674:LYS:HE2	1.40	0.86
1:A:22:HIS:HB2	1:A:74:LYS:HE2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PRO:C	2:B:63:LEU:HG	1.95	0.86
1:A:125:ASP:OD1	1:A:129:ARG:HG2	1.76	0.86
2:B:290:PRO:HB2	2:B:308:GLN:NE2	1.90	0.86
2:B:293:ALA:CB	2:B:306:THR:HG22	2.04	0.86
2:B:394:ILE:HD12	2:B:395:SER:H	1.39	0.86
1:A:529:ILE:HD12	1:A:530:SER:N	1.90	0.86
2:B:248:VAL:HG13	2:B:260:THR:HB	1.56	0.85
2:B:129:VAL:CG1	2:B:415:ILE:HD11	2.04	0.85
3:F:18:DT:O4	4:G:7:DA:N6	2.08	0.85
1:A:463:VAL:HG21	1:A:469:ILE:HB	1.56	0.85
1:A:370:GLN:NE2	1:A:674:LYS:CE	2.39	0.85
1:A:147:ARG:NH1	1:A:147:ARG:HB2	1.92	0.85
1:A:207:TRP:CZ2	1:A:241:ASN:HA	2.12	0.85
2:B:30:LEU:CD1	2:B:31:GLU:N	2.07	0.85
2:B:401:ASN:ND2	2:B:405:ASP:OD1	2.10	0.85
2:B:53:LEU:CD2	2:B:54:TRP:CG	2.60	0.85
1:A:1018:GLY:HA3	1:A:1019:GLU:HB2	1.58	0.85
2:B:270:TRP:CE3	2:B:275:VAL:HG21	2.12	0.85
1:A:451:PHE:HE1	1:A:479:VAL:HG21	1.40	0.85
1:A:396:ILE:CG2	1:A:673:LEU:HD11	2.06	0.85
2:B:53:LEU:CD1	2:B:53:LEU:N	2.37	0.85
1:A:419:ARG:NH2	1:A:423:ASP:CG	2.29	0.85
2:B:119:TRP:NE1	2:B:399:GLU:O	2.08	0.85
1:A:123:ILE:HD13	1:A:167:VAL:HG22	1.59	0.85
1:A:288:GLU:HG3	1:A:296:THR:CB	2.07	0.84
2:B:54:TRP:CG	2:B:55:VAL:N	2.42	0.84
4:G:11:3DR:H3'	4:G:12:DC:H5''	0.91	0.84
1:A:1071:SER:O	1:A:1072:PHE:HB3	1.76	0.84
2:B:206:SER:HB2	2:B:248:VAL:HG23	1.60	0.84
2:B:355:ARG:O	2:B:394:ILE:HD11	1.78	0.84
1:A:771:PHE:H	1:A:772:SER:HA	1.42	0.84
1:A:389:ILE:HB	1:A:713:ARG:CG	2.07	0.84
1:A:1061:VAL:HG11	1:A:1104:LYS:HD2	1.60	0.84
2:B:206:SER:HB2	2:B:248:VAL:CG2	2.08	0.84
2:B:365:THR:CG2	2:B:368:GLU:OE2	2.25	0.83
1:A:463:VAL:HG12	1:A:464:ALA:H	1.42	0.83
2:B:64:PRO:N	2:B:65:PRO:CD	2.41	0.83
1:A:67:PHE:HE1	1:A:145:LEU:HD21	1.42	0.83
4:G:20:DA:H2'	4:G:21:DG:H5''	1.58	0.83
2:B:308:GLN:CB	2:B:333:HIS:CD2	2.58	0.83
2:B:308:GLN:CG	2:B:333:HIS:NE2	2.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:THR:OG1	2:B:292:ASN:HA	1.78	0.83
1:A:550:ASN:N	1:A:551:GLY:CA	2.37	0.83
2:B:221:ASN:CA	2:B:244:LYS:HB2	2.07	0.82
2:B:114:ALA:CB	2:B:410:ALA:HB1	2.08	0.82
1:A:102:THR:HG21	1:A:1066:GLY:H	1.43	0.82
1:A:1004:VAL:HG11	1:A:1007:PHE:CE2	2.13	0.82
1:A:570:LYS:CG	1:A:577:LEU:HD11	2.08	0.82
1:A:773:SER:O	1:A:777:PRO:HA	1.78	0.82
1:A:22:HIS:CB	1:A:74:LYS:HE3	2.05	0.82
1:A:102:THR:CG2	1:A:1066:GLY:H	1.92	0.82
2:B:54:TRP:CD1	2:B:55:VAL:CB	2.62	0.82
1:A:102:THR:HG21	1:A:1066:GLY:CA	2.07	0.82
1:A:288:GLU:CG	1:A:296:THR:HB	2.08	0.82
2:B:54:TRP:NE1	2:B:55:VAL:HG12	1.95	0.82
1:A:309:SER:HA	1:A:384:GLU:OE2	1.79	0.82
1:A:443:VAL:HG23	1:A:444:GLU:H	1.45	0.82
2:B:419:SER:OG	2:B:420:GLN:N	2.05	0.82
1:A:912:LEU:HD11	1:A:926:LEU:HD13	1.61	0.82
1:A:927:MET:O	2:B:347:ARG:NH2	2.11	0.82
1:A:129:ARG:CD	1:A:176:PRO:HG3	2.09	0.81
1:A:953:TRP:CE3	2:B:83:TRP:CZ2	2.68	0.81
1:A:54:GLU:O	1:A:54:GLU:HG2	1.79	0.81
2:B:60:PRO:O	2:B:63:LEU:HB2	1.79	0.81
2:B:27:PRO:HB3	2:B:61:GLN:OE1	1.80	0.81
1:A:328:LEU:HD11	2:B:80:ARG:HD3	1.61	0.81
1:A:147:ARG:CB	1:A:147:ARG:HH11	1.93	0.81
1:A:1080:ARG:HH21	2:B:298:PRO:HB3	1.45	0.81
2:B:256:TRP:HB3	2:B:273:ARG:HD3	1.60	0.81
1:A:507:GLN:NE2	1:A:553:SER:H	1.78	0.81
1:A:102:THR:HG21	1:A:1066:GLY:N	1.96	0.81
2:B:52:CYS:CB	2:B:53:LEU:CD1	2.59	0.81
2:B:59:GLY:O	2:B:63:LEU:HD21	1.81	0.81
1:A:679:MET:HG2	1:A:691:LEU:CD1	2.11	0.81
1:A:248:ILE:HG22	1:A:250:PRO:CD	2.09	0.81
1:A:413:LEU:HD21	1:A:468:LEU:HD21	1.63	0.81
1:A:602:LEU:HD11	1:A:616:LEU:CG	2.11	0.81
2:B:184:GLN:HA	2:B:191:LEU:HD12	1.62	0.81
2:B:305:THR:HB	2:B:313:ARG:HB2	1.61	0.81
1:A:407:ILE:HD11	1:A:410:LEU:HD11	1.62	0.80
2:B:53:LEU:CA	2:B:57:LEU:CG	2.58	0.80
1:A:191:LYS:HE3	1:A:209:GLN:HE21	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:CD1	1:A:623:LEU:HD21	2.09	0.80
2:B:184:GLN:OE1	2:B:190:ILE:HG12	1.80	0.80
2:B:47:ARG:O	2:B:54:TRP:CZ3	2.34	0.80
1:A:389:ILE:HB	1:A:713:ARG:HG2	1.62	0.80
2:B:241:HIS:HB2	2:B:268:LYS:HZ1	1.46	0.80
1:A:376:VAL:HG23	1:A:1012:LEU:HD21	1.64	0.80
1:A:570:LYS:HD2	1:A:577:LEU:HD21	1.61	0.80
2:B:58:ALA:O	2:B:61:GLN:NE2	2.14	0.80
2:B:60:PRO:O	2:B:63:LEU:CB	2.30	0.80
2:B:20:ARG:O	2:B:23:ARG:CD	2.29	0.80
1:A:90:GLU:OE1	1:A:103:ARG:NE	2.15	0.80
1:A:66:LEU:HD12	1:A:66:LEU:O	1.81	0.80
2:B:59:GLY:O	2:B:63:LEU:CG	2.30	0.80
2:B:59:GLY:O	2:B:63:LEU:HG	1.82	0.79
2:B:32:PRO:O	2:B:67:ARG:NH1	2.14	0.79
1:A:343:GLN:NE2	1:A:343:GLN:H	1.79	0.79
2:B:59:GLY:O	2:B:63:LEU:CD2	2.30	0.79
2:B:64:PRO:N	2:B:65:PRO:HD3	1.96	0.79
2:B:241:HIS:CD2	2:B:268:LYS:HE2	2.16	0.79
2:B:24:SER:OG	2:B:36:LYS:HE3	1.77	0.79
2:B:46:ARG:NE	2:B:46:ARG:HA	1.97	0.79
2:B:63:LEU:N	2:B:63:LEU:HD23	1.95	0.79
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.61	0.79
1:A:909:ILE:HD13	1:A:928:ARG:HD3	1.65	0.79
1:A:112:ILE:HD12	1:A:112:ILE:O	1.81	0.79
1:A:891:TYR:CG	1:A:899:LEU:HD13	2.18	0.79
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.65	0.79
1:A:252:ILE:HD11	1:A:304:LEU:HD22	1.64	0.79
1:A:997:LEU:HD13	1:A:1083:GLU:OE2	1.83	0.79
1:A:463:VAL:CG1	1:A:464:ALA:H	1.94	0.79
1:A:534:MET:HE3	1:A:538:VAL:HG22	1.64	0.79
2:B:28:LEU:HD21	2:B:36:LYS:HB3	0.81	0.79
2:B:52:CYS:SG	2:B:53:LEU:CD2	2.71	0.79
2:B:54:TRP:N	2:B:57:LEU:HB3	1.98	0.79
2:B:115:THR:O	2:B:397:LEU:HD11	1.82	0.79
1:A:463:VAL:HG13	1:A:521:ILE:HD13	1.65	0.79
2:B:103:ILE:HD12	2:B:103:ILE:H	1.47	0.79
2:B:63:LEU:CB	2:B:64:PRO:CD	2.49	0.79
2:B:53:LEU:HD22	2:B:54:TRP:HA	1.64	0.79
2:B:117:LEU:HD12	2:B:117:LEU:O	1.83	0.79
2:B:221:ASN:HA	2:B:244:LYS:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:CG1	1:A:367:LEU:HD12	2.12	0.79
4:G:4:DA:H4'	4:G:5:DG:OP1	1.83	0.79
1:A:244:LYS:NZ	1:A:296:THR:O	2.15	0.78
1:A:49:LEU:HD21	1:A:353:PHE:HZ	1.47	0.78
2:B:29:GLU:O	2:B:29:GLU:CG	2.30	0.78
1:A:234:GLN:OE1	2:B:37:LEU:HD23	1.83	0.78
1:A:1024:THR:HG22	1:A:1043:LEU:HD23	1.65	0.78
2:B:40:LYS:O	2:B:44:PRO:CD	2.30	0.78
2:B:251:ASN:CB	2:B:257:PHE:HE2	1.96	0.78
1:A:133:LEU:HD22	1:A:135:LEU:CD2	2.11	0.78
2:B:53:LEU:CB	2:B:54:TRP:O	2.30	0.78
2:B:98:LEU:O	2:B:101:TYR:HB2	1.83	0.78
2:B:24:SER:HB3	2:B:36:LYS:CG	2.13	0.78
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.65	0.78
2:B:221:ASN:HB3	2:B:244:LYS:HE2	1.64	0.78
1:A:966:LEU:HG	1:A:1007:PHE:HE1	1.48	0.78
2:B:332:ARG:CZ	2:B:358:ASP:HB3	2.13	0.78
1:A:534:MET:CE	1:A:558:ILE:CD1	2.61	0.78
1:A:930:VAL:HG12	1:A:948:ASP:HB3	1.66	0.78
2:B:319:GLN:OE1	2:B:321:ASP:HB2	1.84	0.77
1:A:1076:PHE:HB3	1:A:1083:GLU:HG2	1.66	0.77
1:A:739:ARG:HG2	1:A:788:VAL:HG23	1.67	0.77
1:A:23:PHE:H	1:A:74:LYS:NZ	1.82	0.77
2:B:218:THR:HG22	2:B:226:ILE:HG23	1.64	0.77
2:B:394:ILE:HD12	2:B:395:SER:N	1.98	0.77
1:A:413:LEU:HD21	1:A:468:LEU:CD2	2.14	0.77
2:B:267:VAL:HG21	2:B:285:LEU:CD2	2.15	0.77
1:A:376:VAL:CG2	1:A:1012:LEU:HD21	2.15	0.77
1:A:570:LYS:NZ	1:A:577:LEU:HD11	1.98	0.77
2:B:29:GLU:O	2:B:30:LEU:HG	1.84	0.77
2:B:62:ILE:CG1	2:B:63:LEU:HD21	2.12	0.77
1:A:299:ASP:C	1:A:300:LEU:HD12	2.05	0.77
1:A:1062:ILE:CG2	1:A:1063:LYS:O	2.32	0.77
1:A:90:GLU:O	1:A:100:ILE:HD12	1.84	0.77
2:B:53:LEU:HD21	2:B:54:TRP:CE3	2.20	0.77
1:A:168:LYS:HG2	1:A:219:VAL:HG13	1.67	0.77
2:B:308:GLN:CB	2:B:333:HIS:NE2	2.47	0.76
1:A:210:GLU:CD	1:A:240:HIS:HD1	1.89	0.76
1:A:49:LEU:CD2	1:A:353:PHE:HZ	1.98	0.76
1:A:682:LEU:HD12	1:A:701:ILE:HD12	1.67	0.76
2:B:217:VAL:CG2	2:B:227:LEU:HD12	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ARG:O	2:B:276:ARG:NH2	2.18	0.76
4:G:10:DG:H2"	4:G:12:DC:OP2	1.83	0.76
1:A:977:CYS:HB3	1:A:992:LEU:HB3	1.67	0.76
2:B:47:ARG:HB3	2:B:54:TRP:HZ3	1.51	0.76
2:B:53:LEU:O	2:B:57:LEU:HG	1.86	0.76
1:A:256:SER:HB2	1:A:275:ASP:OD2	1.85	0.76
1:A:671:VAL:CG1	1:A:673:LEU:HD13	2.14	0.76
2:B:27:PRO:CB	2:B:61:GLN:OE1	2.32	0.76
2:B:33:GLU:O	2:B:35:LYS:O	2.04	0.76
2:B:57:LEU:HD13	2:B:57:LEU:O	1.85	0.76
2:B:120:HIS:NE2	2:B:169:THR:HG21	1.99	0.76
2:B:43:GLY:N	2:B:44:PRO:CD	2.49	0.76
1:A:22:HIS:O	1:A:30:ASN:HB2	1.86	0.76
2:B:240:MET:O	2:B:241:HIS:ND1	2.18	0.76
2:B:199:THR:HG23	2:B:200:ILE:N	2.01	0.76
2:B:60:PRO:O	2:B:63:LEU:HG	1.85	0.76
1:A:408:LYS:O	1:A:428:SER:HB3	1.85	0.76
2:B:29:GLU:O	2:B:29:GLU:HG2	1.84	0.76
2:B:59:GLY:O	2:B:62:ILE:CG1	2.30	0.76
1:A:770:LEU:HD13	1:A:772:SER:HB2	1.68	0.76
1:A:602:LEU:HG	1:A:616:LEU:HD22	1.67	0.76
2:B:31:GLU:CD	2:B:85:SER:HB2	2.06	0.75
2:B:218:THR:CG2	2:B:226:ILE:HG23	2.15	0.75
1:A:537:GLU:HB2	1:A:561:TRP:HB2	1.68	0.75
1:A:69:PRO:HD2	1:A:72:GLU:OE1	1.86	0.75
1:A:102:THR:CG2	1:A:1066:GLY:N	2.50	0.75
2:B:353:VAL:HG23	2:B:375:PHE:HE1	1.50	0.75
2:B:46:ARG:CG	2:B:49:ASP:CG	2.53	0.75
1:A:157:ILE:HG13	1:A:158:ARG:N	1.95	0.75
2:B:183:LEU:O	2:B:191:LEU:HD12	1.86	0.75
1:A:739:ARG:O	1:A:788:VAL:HG22	1.87	0.75
2:B:159:ILE:HD12	2:B:174:ALA:HB1	1.69	0.75
1:A:858:LEU:O	1:A:858:LEU:HD13	1.87	0.75
1:A:129:ARG:HG3	1:A:130:MET:CE	2.16	0.75
2:B:60:PRO:CA	2:B:63:LEU:CD1	2.57	0.74
2:B:308:GLN:OE1	2:B:333:HIS:NE2	2.18	0.74
1:A:1005:ASN:ND2	1:A:1031:GLY:O	2.19	0.74
1:A:951:PRO:HB3	2:B:347:ARG:NE	2.02	0.74
1:A:47:GLU:HG3	1:A:350:MET:SD	2.27	0.74
1:A:107:ASN:O	1:A:108:VAL:HG22	1.88	0.74
2:B:260:THR:HG23	2:B:268:LYS:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CE1	1:A:145:LEU:CD2	2.69	0.74
1:A:1136:LEU:O	1:A:1139:ILE:HG12	1.87	0.74
2:B:28:LEU:HD11	2:B:33:GLU:O	1.88	0.74
2:B:113:ARG:HG2	2:B:413:TYR:CE2	2.23	0.74
1:A:838:PRO:O	2:B:66:CYS:O	2.05	0.74
2:B:52:CYS:SG	2:B:53:LEU:HD21	2.28	0.74
2:B:30:LEU:O	2:B:67:ARG:NH1	2.21	0.74
2:B:329:HIS:HE1	2:B:354:GLY:O	1.71	0.74
1:A:463:VAL:CG1	1:A:464:ALA:N	2.50	0.74
2:B:53:LEU:CB	2:B:57:LEU:CD1	2.65	0.74
1:A:22:HIS:HD1	1:A:29:LEU:HA	1.52	0.74
2:B:97:THR:O	2:B:101:TYR:HD1	1.71	0.74
1:A:472:THR:HG23	1:A:474:ALA:N	1.98	0.74
2:B:162:LEU:O	2:B:163:LYS:HD3	1.88	0.74
2:B:113:ARG:HH11	2:B:113:ARG:HG3	1.52	0.74
2:B:157:GLY:HA2	2:B:178:GLU:HG3	1.69	0.74
2:B:53:LEU:HD22	2:B:54:TRP:CA	2.08	0.74
1:A:977:CYS:HA	1:A:993:GLN:O	1.87	0.74
1:A:237:ILE:N	1:A:248:ILE:O	2.19	0.73
1:A:443:VAL:HG23	1:A:444:GLU:N	2.02	0.73
2:B:215:MET:HG3	2:B:227:LEU:HD21	1.70	0.73
2:B:369:LEU:CD2	2:B:387:TYR:HE2	2.02	0.73
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.17	0.73
1:A:359:ILE:O	1:A:1005:ASN:CG	2.26	0.73
1:A:891:TYR:HB3	1:A:899:LEU:HD22	1.70	0.73
2:B:53:LEU:HB2	2:B:57:LEU:HD12	1.69	0.73
2:B:61:GLN:HG2	2:B:65:PRO:HG3	1.70	0.73
2:B:62:ILE:HD11	2:B:63:LEU:HD21	1.70	0.73
1:A:768:SER:HB2	1:A:769:LYS:O	1.88	0.73
1:A:529:ILE:HD13	1:A:572:PRO:HB2	1.70	0.73
2:B:43:GLY:O	2:B:48:CYS:HB3	1.88	0.73
2:B:47:ARG:HB3	2:B:54:TRP:CZ3	2.23	0.73
1:A:407:ILE:CD1	1:A:410:LEU:HD11	2.18	0.73
1:A:147:ARG:NH1	1:A:147:ARG:CB	2.51	0.73
2:B:260:THR:HG23	2:B:268:LYS:CG	2.18	0.73
1:A:102:THR:CG2	1:A:1066:GLY:HA2	2.19	0.73
2:B:46:ARG:CA	2:B:46:ARG:HE	2.02	0.73
1:A:127:GLU:OE1	1:A:129:ARG:NH2	2.21	0.73
1:A:107:ASN:OD1	1:A:109:GLN:HG3	1.88	0.73
2:B:290:PRO:C	2:B:308:GLN:HG3	2.08	0.73
1:A:609:GLY:O	1:A:631:LEU:HD12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:HG22	1:A:475:SER:H	1.53	0.73
2:B:160:THR:OG1	2:B:205:CYS:O	2.06	0.73
1:A:929:SER:OG	1:A:950:ASN:O	2.05	0.73
2:B:26:SER:HB3	2:B:27:PRO:HD3	1.71	0.72
2:B:220:ASP:O	2:B:245:VAL:HG23	1.89	0.72
1:A:1094:ILE:CD1	1:A:1136:LEU:CD1	2.65	0.72
2:B:313:ARG:CD	2:B:326:LEU:HD21	2.15	0.72
1:A:57:MET:HE2	1:A:1065:VAL:HG12	1.70	0.72
1:A:402:ILE:HG22	1:A:404:LEU:CD1	2.20	0.72
1:A:534:MET:HE1	1:A:558:ILE:HD11	1.70	0.72
1:A:328:LEU:HD13	1:A:382:PHE:CD2	2.24	0.72
3:F:8:DA:H2''	3:F:9:DT:O5'	1.88	0.72
1:A:568:ILE:HD11	1:A:602:LEU:HD21	1.70	0.72
1:A:951:PRO:HB3	2:B:347:ARG:NH2	2.04	0.72
1:A:414:ARG:HB2	1:A:462:ASN:OD1	1.89	0.72
1:A:568:ILE:HD11	1:A:602:LEU:CD2	2.20	0.72
1:A:1080:ARG:NH2	2:B:298:PRO:HB3	2.04	0.72
2:B:29:GLU:OE2	2:B:67:ARG:NH2	2.23	0.71
2:B:54:TRP:CD1	2:B:55:VAL:CA	2.72	0.71
1:A:111:ARG:HD3	2:B:256:TRP:CH2	2.24	0.71
2:B:218:THR:O	2:B:225:VAL:HG13	1.89	0.71
1:A:396:ILE:HG22	1:A:673:LEU:HD11	1.69	0.71
1:A:436:LEU:HD13	1:A:444:GLU:O	1.89	0.71
1:A:1013:VAL:HG21	1:A:1139:ILE:O	1.90	0.71
1:A:1070:HIS:CD2	1:A:1093:LEU:HD13	2.25	0.71
1:A:147:ARG:HB2	1:A:147:ARG:HH11	1.48	0.71
2:B:173:TYR:CZ	2:B:183:LEU:HD22	2.26	0.71
2:B:184:GLN:HB3	2:B:190:ILE:HG23	1.72	0.71
1:A:534:MET:SD	1:A:558:ILE:HD13	2.31	0.71
4:G:23:DC:H2''	4:G:24:DA:O5'	1.90	0.71
2:B:31:GLU:OE1	2:B:31:GLU:N	1.82	0.71
1:A:837:TYR:HD2	1:A:840:GLU:OE2	1.74	0.71
2:B:200:ILE:CD1	2:B:201:ASN:H	2.03	0.71
2:B:43:GLY:H	2:B:44:PRO:HD2	1.54	0.71
2:B:263:VAL:HG11	4:G:14:DT:H3'	1.72	0.71
2:B:225:VAL:HG12	2:B:226:ILE:N	2.06	0.71
1:A:570:LYS:HZ3	1:A:577:LEU:HD11	1.54	0.71
1:A:529:ILE:HD13	1:A:572:PRO:CB	2.20	0.71
1:A:300:LEU:N	1:A:300:LEU:CD1	2.54	0.71
2:B:55:VAL:HG13	2:B:56:GLY:H	1.55	0.70
2:B:32:PRO:HD2	2:B:67:ARG:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:CD1	1:A:534:MET:HE1	2.21	0.70
1:A:805:HIS:HB2	1:A:858:LEU:HD21	1.73	0.70
1:A:953:TRP:CZ3	2:B:83:TRP:HZ2	2.09	0.70
2:B:27:PRO:CG	2:B:61:GLN:OE1	2.40	0.70
1:A:248:ILE:HD12	1:A:300:LEU:CB	2.11	0.70
1:A:966:LEU:HD12	1:A:967:GLY:N	2.07	0.70
1:A:968:ALA:HB2	1:A:1007:PHE:HZ	1.55	0.70
2:B:28:LEU:HB2	2:B:30:LEU:H	1.51	0.70
2:B:60:PRO:HA	2:B:63:LEU:HD11	1.70	0.70
1:A:300:LEU:N	1:A:300:LEU:HD12	2.07	0.70
1:A:343:GLN:CD	1:A:343:GLN:H	1.94	0.70
1:A:1055:GLN:NE2	1:A:1089:ILE:HD12	2.06	0.70
1:A:989:ARG:HG2	1:A:989:ARG:HH11	1.55	0.70
2:B:227:LEU:HD22	2:B:272:LEU:CD1	2.21	0.70
1:A:595:THR:O	1:A:647:THR:HG21	1.92	0.70
2:B:53:LEU:CD2	2:B:54:TRP:CD2	2.75	0.70
3:F:3:DA:H2"	3:F:4:DC:OP1	1.90	0.70
1:A:15:VAL:HG13	1:A:33:ILE:HG23	1.74	0.70
1:A:111:ARG:HD3	2:B:256:TRP:HH2	1.56	0.70
1:A:374:GLN:HB2	1:A:1012:LEU:HA	1.74	0.70
2:B:67:ARG:O	2:B:67:ARG:HG3	1.90	0.69
1:A:770:LEU:CD2	1:A:772:SER:HB2	2.22	0.69
1:A:744:ASP:O	1:A:745:THR:OG1	2.10	0.69
2:B:297:SER:O	2:B:300:GLY:N	2.25	0.69
2:B:62:ILE:CD1	2:B:63:LEU:HD21	2.22	0.69
1:A:602:LEU:CD1	1:A:623:LEU:HD22	2.09	0.69
1:A:67:PHE:HE1	1:A:145:LEU:CD2	2.04	0.69
1:A:370:GLN:NE2	1:A:674:LYS:HE3	2.07	0.69
2:B:53:LEU:HA	2:B:57:LEU:CG	2.18	0.69
2:B:62:ILE:HG12	2:B:63:LEU:HD23	1.58	0.69
2:B:43:GLY:CA	2:B:46:ARG:O	2.40	0.69
2:B:60:PRO:O	2:B:63:LEU:CG	2.39	0.69
2:B:24:SER:HB3	2:B:36:LYS:CD	2.18	0.69
2:B:353:VAL:HG23	2:B:375:PHE:CE1	2.27	0.69
1:A:144:PRO:HB3	1:A:197:LEU:CD1	2.16	0.69
1:A:160:GLU:O	1:A:162:LEU:CD1	2.40	0.69
2:B:281:PHE:CE1	2:B:284:SER:HB2	2.27	0.69
2:B:142:GLY:C	2:B:143:ILE:HD13	2.13	0.69
1:A:23:PHE:H	1:A:74:LYS:HZ2	1.40	0.69
2:B:171:GLN:HB3	2:B:183:LEU:CD1	2.23	0.69
2:B:261:ALA:HB1	2:B:291:VAL:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:THR:CG2	2:B:200:ILE:N	2.55	0.69
1:A:370:GLN:NE2	1:A:674:LYS:HE2	2.02	0.69
1:A:1064:SER:HB3	1:A:1067:LYS:HA	1.74	0.69
2:B:256:TRP:O	2:B:272:LEU:N	2.25	0.69
1:A:673:LEU:CD2	1:A:693:LEU:HD22	2.23	0.69
1:A:290:GLN:OE1	1:A:290:GLN:N	2.24	0.69
4:G:14:DT:H2''	4:G:15:DC:O5'	1.92	0.68
1:A:374:GLN:C	1:A:1012:LEU:HD22	2.13	0.68
1:A:634:GLN:HG3	1:A:635:PRO:HD2	1.74	0.68
1:A:102:THR:CG2	1:A:1066:GLY:CA	2.70	0.68
1:A:107:ASN:O	1:A:108:VAL:CG2	2.41	0.68
2:B:54:TRP:HD1	2:B:55:VAL:N	1.55	0.68
2:B:52:CYS:CA	2:B:53:LEU:HD13	2.24	0.68
1:A:602:LEU:CG	1:A:616:LEU:HD22	2.23	0.68
1:A:679:MET:HE3	1:A:691:LEU:HD13	1.75	0.68
2:B:41:GLY:O	2:B:44:PRO:CD	2.30	0.68
1:A:326:SER:OG	1:A:329:GLY:O	2.10	0.68
1:A:926:LEU:O	1:A:953:TRP:HD1	1.76	0.68
2:B:367:TYR:O	2:B:367:TYR:CG	2.47	0.68
1:A:334:VAL:HG13	1:A:347:VAL:HG13	1.76	0.68
2:B:172:PHE:CZ	2:B:184:GLN:HG3	2.28	0.68
2:B:256:TRP:HB3	2:B:273:ARG:CD	2.22	0.68
1:A:486:LEU:C	1:A:486:LEU:HD13	2.14	0.68
1:A:389:ILE:HG12	1:A:799:PHE:CZ	2.28	0.68
1:A:1004:VAL:CG1	1:A:1007:PHE:CE2	2.77	0.68
1:A:850:VAL:HB	1:A:862:ALA:CB	2.24	0.68
1:A:402:ILE:CD1	1:A:443:VAL:HG21	2.23	0.68
1:A:24:THR:OG1	1:A:30:ASN:ND2	2.27	0.68
1:A:468:LEU:HB2	1:A:479:VAL:HG23	1.75	0.68
1:A:660:TYR:CD1	1:A:707:ILE:CG2	2.77	0.68
3:F:15:DC:N3	4:G:10:DG:N1	2.37	0.68
1:A:1055:GLN:HE21	1:A:1089:ILE:HD12	1.58	0.68
1:A:215:GLU:OE1	1:A:215:GLU:HA	1.94	0.68
2:B:60:PRO:HA	2:B:63:LEU:CG	2.23	0.68
1:A:1080:ARG:HE	2:B:298:PRO:HB3	1.59	0.68
2:B:352:VAL:HG12	2:B:374:VAL:HG22	1.76	0.68
1:A:129:ARG:HG3	1:A:130:MET:HE2	1.75	0.67
2:B:267:VAL:CG2	2:B:285:LEU:HB2	2.24	0.67
2:B:201:ASN:O	2:B:202:ILE:HG13	1.94	0.67
1:A:1094:ILE:HD11	1:A:1136:LEU:HD13	1.76	0.67
2:B:30:LEU:O	2:B:32:PRO:C	2.31	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HD12	1:A:703:THR:O	1.95	0.67
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.09	0.67
2:B:28:LEU:CD2	2:B:36:LYS:CG	2.72	0.67
1:A:472:THR:HG23	1:A:473:SER:N	2.08	0.67
2:B:267:VAL:HG21	2:B:285:LEU:HD23	1.75	0.67
1:A:308:THR:O	1:A:383:LYS:NZ	2.21	0.67
1:A:866:VAL:HG21	1:A:884:ILE:HD13	1.76	0.67
1:A:476:VAL:HG22	1:A:490:TRP:HB3	1.75	0.67
1:A:237:ILE:HG22	1:A:248:ILE:HB	1.76	0.67
2:B:372:ILE:HB	2:B:386:LEU:HB2	1.76	0.67
2:B:60:PRO:CA	2:B:63:LEU:HG	2.24	0.67
1:A:23:PHE:H	1:A:74:LYS:CE	2.06	0.67
1:A:414:ARG:NH1	1:A:420:GLU:HA	2.10	0.67
1:A:558:ILE:HG23	1:A:567:ARG:HG3	1.76	0.67
1:A:733:PHE:HB2	1:A:794:ILE:HG13	1.77	0.67
1:A:612:PHE:CZ	1:A:628:LYS:HE3	2.29	0.67
2:B:55:VAL:CG1	2:B:56:GLY:H	1.95	0.67
1:A:536:HIS:O	1:A:560:LEU:HD11	1.95	0.67
2:B:41:GLY:C	2:B:44:PRO:CD	2.60	0.67
1:A:419:ARG:O	1:A:420:GLU:HG2	1.95	0.67
2:B:368:GLU:O	2:B:369:LEU:C	2.33	0.67
1:A:1135:GLU:O	1:A:1138:ARG:HG2	1.95	0.67
1:A:597:GLU:HG3	1:A:661:SER:OG	1.95	0.67
1:A:411:TRP:CZ3	1:A:457:THR:CG2	2.78	0.67
2:B:172:PHE:CE2	2:B:184:GLN:HG3	2.30	0.67
2:B:267:VAL:O	2:B:268:LYS:HG2	1.95	0.67
2:B:53:LEU:CB	2:B:57:LEU:HD12	2.25	0.66
2:B:123:HIS:HD2	2:B:124:PRO:HD2	1.60	0.66
1:A:1004:VAL:CG1	1:A:1007:PHE:HE2	2.08	0.66
2:B:36:LYS:CG	2:B:37:LEU:N	2.55	0.66
1:A:365:VAL:HG11	1:A:367:LEU:HD12	1.76	0.66
2:B:241:HIS:HB2	2:B:268:LYS:HZ3	1.60	0.66
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.77	0.66
1:A:166:ASP:CG	1:A:219:VAL:HG12	2.16	0.66
2:B:143:ILE:HG22	2:B:144:LYS:O	1.95	0.66
2:B:238:LEU:HD12	2:B:238:LEU:O	1.95	0.66
1:A:909:ILE:CD1	1:A:928:ARG:HD3	2.24	0.66
1:A:1016:ASN:HB3	1:A:1017:LEU:C	2.15	0.66
2:B:53:LEU:C	2:B:57:LEU:CB	2.63	0.66
1:A:512:VAL:CG1	1:A:512:VAL:O	2.42	0.66
2:B:105:GLN:NE2	2:B:420:GLN:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:ILE:HG13	1:A:1095:GLU:N	2.11	0.66
1:A:771:PHE:N	1:A:772:SER:HA	2.04	0.66
1:A:419:ARG:HG3	1:A:421:THR:H	1.61	0.66
1:A:157:ILE:CD1	1:A:202:PHE:CZ	2.72	0.66
2:B:365:THR:HG23	2:B:365:THR:O	1.94	0.66
1:A:536:HIS:C	1:A:560:LEU:HD11	2.16	0.66
1:A:22:HIS:CB	1:A:74:LYS:CE	2.59	0.66
1:A:537:GLU:O	1:A:560:LEU:CD1	2.41	0.66
1:A:307:GLU:HA	1:A:307:GLU:OE1	1.96	0.66
1:A:451:PHE:CE1	1:A:479:VAL:HG21	2.28	0.66
1:A:612:PHE:CE2	1:A:628:LYS:HE3	2.31	0.66
2:B:23:ARG:CG	2:B:24:SER:H	1.95	0.66
1:A:922:LEU:HD12	1:A:931:LEU:O	1.96	0.66
1:A:182:TYR:OH	1:A:209:GLN:NE2	2.30	0.65
1:A:651:ALA:HB3	1:A:657:THR:OG1	1.96	0.65
1:A:602:LEU:CD1	1:A:616:LEU:HD22	2.26	0.65
1:A:157:ILE:HD12	1:A:202:PHE:CE2	2.31	0.65
2:B:218:THR:CG2	2:B:226:ILE:CG2	2.74	0.65
2:B:334:PHE:HE2	2:B:336:HIS:HD1	1.42	0.65
1:A:997:LEU:HD13	1:A:1083:GLU:CD	2.15	0.65
1:A:312:GLU:N	1:A:325:GLY:O	2.30	0.65
1:A:602:LEU:CD1	1:A:616:LEU:CB	2.72	0.65
1:A:679:MET:CE	1:A:691:LEU:HD13	2.27	0.65
1:A:671:VAL:HG12	1:A:673:LEU:HD13	1.77	0.65
2:B:95:LEU:HD13	2:B:383:MET:HB3	1.78	0.65
1:A:824:ASP:OD1	1:A:826:ASN:N	2.27	0.65
1:A:256:SER:OG	1:A:277:GLU:OE1	2.13	0.65
2:B:411:MET:HG2	2:B:412:GLY:CA	2.26	0.65
1:A:151:GLU:CB	1:A:153:LYS:HZ2	2.10	0.65
2:B:32:PRO:CD	2:B:67:ARG:HD2	2.27	0.65
1:A:768:SER:CB	1:A:769:LYS:O	2.44	0.65
1:A:407:ILE:HD11	1:A:410:LEU:CD1	2.25	0.65
1:A:427:LEU:HD21	1:A:429:PHE:HE2	1.52	0.65
1:A:157:ILE:CG2	1:A:202:PHE:HE2	2.01	0.65
2:B:246:THR:CB	2:B:292:ASN:HA	2.26	0.65
2:B:395:SER:OG	2:B:398:ASN:OD1	2.15	0.65
2:B:101:TYR:OH	2:B:405:ASP:O	2.12	0.65
1:A:534:MET:CE	1:A:538:VAL:HG22	2.26	0.65
2:B:63:LEU:HB2	2:B:64:PRO:HD3	1.77	0.65
2:B:315:TYR:CE1	2:B:323:PRO:HB3	2.32	0.65
2:B:53:LEU:CD2	2:B:54:TRP:CE3	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ASN:CA	2:B:244:LYS:HE2	2.27	0.65
1:A:770:LEU:HD22	1:A:772:SER:OG	1.96	0.65
1:A:475:SER:HB2	1:A:490:TRP:O	1.97	0.65
1:A:67:PHE:HB2	1:A:128:CYS:SG	2.37	0.65
1:A:224:GLU:HB3	1:A:225:PRO:HA	1.79	0.65
2:B:97:THR:HG1	2:B:420:GLN:HE22	1.45	0.65
2:B:82:SER:HB2	2:B:84:PRO:HD2	1.79	0.65
3:F:11:DA:H5'	3:F:11:DA:C8	2.32	0.65
2:B:54:TRP:O	2:B:57:LEU:CD1	2.31	0.64
2:B:249:ALA:O	2:B:258:LEU:HD12	1.97	0.64
1:A:858:LEU:H	1:A:858:LEU:HD12	1.62	0.64
2:B:20:ARG:O	2:B:23:ARG:N	2.30	0.64
2:B:116:SER:O	2:B:129:VAL:HG23	1.97	0.64
2:B:227:LEU:HD22	2:B:272:LEU:HD13	1.78	0.64
2:B:31:GLU:OE1	2:B:31:GLU:H	1.10	0.64
1:A:968:ALA:HB2	1:A:1007:PHE:CZ	2.32	0.64
1:A:840:GLU:HG3	1:A:840:GLU:O	1.96	0.64
1:A:438:LEU:HD23	1:A:443:VAL:HG12	1.79	0.64
2:B:304:LEU:HA	2:B:313:ARG:O	1.97	0.64
1:A:803:HIS:NE2	1:A:858:LEU:HD11	2.12	0.64
2:B:210:SER:HB3	2:B:213:SER:OG	1.98	0.64
1:A:427:LEU:CD2	1:A:429:PHE:HE2	2.07	0.64
3:F:7:DT:C2'	3:F:8:DA:H5''	2.27	0.64
2:B:302:ARG:HD3	2:B:316:SER:HA	1.80	0.64
2:B:372:ILE:HD12	2:B:372:ILE:N	2.13	0.64
1:A:733:PHE:CD2	1:A:794:ILE:HD11	2.32	0.64
2:B:24:SER:HB3	2:B:36:LYS:HE3	1.54	0.64
1:A:946:ALA:HB2	1:A:989:ARG:O	1.98	0.64
1:A:871:TYR:HE1	2:B:70:VAL:HG23	1.63	0.64
2:B:32:PRO:HD2	2:B:67:ARG:CZ	2.28	0.64
1:A:989:ARG:HG2	1:A:989:ARG:NH1	2.12	0.64
2:B:181:THR:HG23	2:B:204:PHE:CD2	2.33	0.64
2:B:287:HIS:HD2	2:B:291:VAL:HG11	1.63	0.64
4:G:4:DA:H2''	4:G:5:DG:H8	1.63	0.64
1:A:102:THR:HG21	1:A:1066:GLY:HA2	1.80	0.64
1:A:36:ASN:ND2	1:A:1002:GLU:OE2	2.31	0.64
1:A:775:THR:HG23	1:A:775:THR:O	1.97	0.64
2:B:287:HIS:CD2	2:B:291:VAL:HG11	2.32	0.64
1:A:953:TRP:HB2	1:A:970:ASN:HD22	1.63	0.64
1:A:118:THR:O	1:A:118:THR:HG22	1.98	0.64
2:B:28:LEU:CB	2:B:30:LEU:HA	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:GLY:O	2:B:48:CYS:CB	2.44	0.63
1:A:733:PHE:HB2	1:A:794:ILE:CG1	2.28	0.63
2:B:62:ILE:HG12	2:B:63:LEU:HD21	1.73	0.63
1:A:419:ARG:HH21	1:A:423:ASP:H	1.46	0.63
2:B:358:ASP:OD1	2:B:361:PHE:HB2	1.98	0.63
1:A:601:TYR:CE1	1:A:666:LEU:HD21	2.32	0.63
1:A:468:LEU:O	1:A:479:VAL:HG22	1.99	0.63
1:A:536:HIS:C	1:A:560:LEU:CD1	2.66	0.63
1:A:1000:LEU:HD22	1:A:1002:GLU:HB2	1.81	0.63
1:A:907:ASN:HD21	1:A:944:GLU:CD	2.02	0.63
1:A:281:PHE:CE1	1:A:304:LEU:CD1	2.81	0.63
2:B:35:LYS:O	2:B:37:LEU:CD1	2.37	0.63
2:B:55:VAL:HG22	2:B:56:GLY:N	2.12	0.63
2:B:53:LEU:HB3	2:B:57:LEU:CD1	2.27	0.63
1:A:539:ALA:N	1:A:559:GLY:O	2.20	0.63
2:B:20:ARG:C	2:B:23:ARG:HD3	2.18	0.63
1:A:512:VAL:HG13	1:A:512:VAL:O	1.98	0.63
1:A:416:ASP:CB	1:A:419:ARG:HH12	2.10	0.63
2:B:247:HIS:HD2	2:B:294:ALA:H	1.46	0.63
2:B:53:LEU:HB3	2:B:57:LEU:HD11	1.80	0.63
1:A:23:PHE:N	1:A:74:LYS:HE3	2.14	0.63
1:A:5:TYR:OH	1:A:1094:ILE:CD1	2.46	0.63
1:A:774:SER:O	1:A:775:THR:HG22	1.99	0.63
2:B:36:LYS:HD2	2:B:37:LEU:N	2.14	0.63
1:A:616:LEU:HD13	1:A:623:LEU:HD21	1.81	0.63
1:A:416:ASP:H	1:A:419:ARG:HH12	1.45	0.63
1:A:207:TRP:CE2	1:A:241:ASN:HA	2.34	0.63
1:A:1069:GLU:O	1:A:1071:SER:O	2.17	0.63
1:A:802:LEU:HD22	1:A:853:TYR:OH	1.99	0.63
2:B:28:LEU:CA	2:B:30:LEU:H	2.10	0.62
2:B:53:LEU:HD23	2:B:54:TRP:CD2	2.30	0.62
2:B:62:ILE:HG13	2:B:63:LEU:CD2	2.18	0.62
2:B:221:ASN:HB3	2:B:244:LYS:CE	2.29	0.62
1:A:358:PRO:O	1:A:379:SER:O	2.17	0.62
2:B:116:SER:OG	2:B:159:ILE:O	2.15	0.62
2:B:343:ALA:HB1	2:B:399:GLU:OE2	1.99	0.62
2:B:44:PRO:N	2:B:45:SER:HA	2.14	0.62
1:A:23:PHE:H	1:A:74:LYS:HE3	1.63	0.62
2:B:184:GLN:HA	2:B:191:LEU:CD1	2.30	0.62
2:B:117:LEU:HD12	2:B:117:LEU:C	2.19	0.62
1:A:534:MET:CE	1:A:558:ILE:HD11	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.81	0.62
2:B:369:LEU:HD23	2:B:387:TYR:HE2	1.64	0.62
1:A:450:GLY:O	1:A:477:ARG:HD3	2.00	0.62
1:A:518:TYR:CD2	1:A:529:ILE:CG1	2.81	0.62
2:B:82:SER:CB	2:B:84:PRO:HD2	2.29	0.62
1:A:207:TRP:CH2	1:A:240:HIS:O	2.53	0.62
1:A:212:VAL:HG22	1:A:213:GLU:H	1.64	0.62
1:A:251:PRO:HA	1:A:254:LYS:CD	2.29	0.62
2:B:137:MET:CE	2:B:415:ILE:HD12	2.30	0.62
1:A:370:GLN:HE22	1:A:674:LYS:HE3	1.59	0.62
1:A:139:LEU:HG	2:B:318:SER:HB3	1.80	0.62
1:A:234:GLN:OE1	2:B:37:LEU:CD2	2.48	0.62
2:B:53:LEU:C	2:B:57:LEU:HB3	2.21	0.62
2:B:225:VAL:CG1	2:B:226:ILE:N	2.62	0.62
2:B:312:ILE:HG21	2:B:327:ILE:CD1	2.02	0.61
2:B:221:ASN:HA	2:B:244:LYS:HE2	1.80	0.61
1:A:507:GLN:HE22	1:A:553:SER:N	1.89	0.61
1:A:11:LYS:HD3	1:A:38:ARG:HD2	1.81	0.61
2:B:55:VAL:HG13	2:B:56:GLY:N	2.14	0.61
2:B:307:ASP:OD1	2:B:311:GLU:N	2.33	0.61
2:B:355:ARG:O	2:B:394:ILE:CD1	2.48	0.61
2:B:202:ILE:HG12	2:B:221:ASN:OD1	2.00	0.61
1:A:81:THR:HG22	1:A:83:LYS:H	1.65	0.61
1:A:398:GLU:OE1	1:A:700:THR:HG21	2.00	0.61
1:A:334:VAL:CG1	1:A:347:VAL:HG13	2.29	0.61
4:G:4:DA:C2'	4:G:5:DG:H8	2.12	0.61
1:A:570:LYS:HG2	1:A:577:LEU:CD1	2.30	0.61
1:A:252:ILE:CD1	1:A:304:LEU:HD22	2.30	0.61
1:A:980:ASP:OD2	1:A:988:GLU:HB3	2.00	0.61
1:A:359:ILE:HG23	1:A:378:CYS:HB3	1.81	0.61
2:B:334:PHE:CD1	3:F:14:DA:H4'	2.35	0.61
2:B:55:VAL:O	2:B:58:ALA:HB2	2.00	0.61
1:A:407:ILE:HD12	1:A:427:LEU:HD12	1.81	0.61
1:A:744:ASP:OD1	1:A:748:GLY:O	2.19	0.61
2:B:32:PRO:CD	2:B:67:ARG:CD	2.76	0.61
2:B:260:THR:CG2	2:B:268:LYS:HG3	2.30	0.61
1:A:631:LEU:HD13	1:A:636:THR:OG1	1.99	0.61
2:B:203:TRP:CZ3	2:B:221:ASN:ND2	2.68	0.61
1:A:176:PRO:O	1:A:195:VAL:HG12	2.01	0.61
1:A:49:LEU:HD21	1:A:353:PHE:CZ	2.33	0.61
1:A:220:ILE:HG12	1:A:261:HIS:ND1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LEU:C	2:B:30:LEU:HD12	2.18	0.60
2:B:53:LEU:O	2:B:57:LEU:CG	2.48	0.60
1:A:237:ILE:HG23	1:A:237:ILE:O	2.01	0.60
1:A:1019:GLU:OE1	1:A:1138:ARG:NH2	2.34	0.60
1:A:149:ASN:O	1:A:149:ASN:ND2	2.34	0.60
2:B:57:LEU:C	2:B:60:PRO:HD2	2.16	0.60
2:B:165:ASN:ND2	2:B:183:LEU:HD21	2.16	0.60
1:A:145:LEU:O	1:A:146:ASP:C	2.40	0.60
1:A:601:TYR:CD1	1:A:666:LEU:HD21	2.35	0.60
1:A:117:GLU:HG3	2:B:84:PRO:HB3	1.83	0.60
1:A:815:SER:OG	1:A:832:GLY:HA3	2.01	0.60
1:A:695:ASN:OD1	1:A:698:THR:HG22	2.00	0.60
2:B:46:ARG:CA	2:B:48:CYS:HA	2.31	0.60
1:A:81:THR:CG2	1:A:83:LYS:H	2.12	0.60
1:A:768:SER:HB2	1:A:770:LEU:N	2.14	0.60
1:A:889:ARG:NH1	1:A:904:ASN:OD1	2.35	0.60
2:B:138:LEU:O	2:B:147:PRO:HB3	2.02	0.60
1:A:387:LEU:HB2	1:A:715:VAL:HG23	1.83	0.60
1:A:419:ARG:HH21	1:A:423:ASP:N	1.99	0.60
2:B:261:ALA:HB1	2:B:291:VAL:CG2	2.30	0.60
1:A:80:LEU:CD2	1:A:133:LEU:HD21	2.32	0.60
1:A:905:HIS:NE2	1:A:907:ASN:ND2	2.49	0.60
1:A:649:VAL:HB	1:A:659:ILE:HB	1.83	0.60
2:B:53:LEU:HD23	2:B:54:TRP:C	2.21	0.60
1:A:961:ASP:OD1	1:A:961:ASP:N	2.33	0.60
2:B:182:ARG:HH21	2:B:184:GLN:NE2	2.00	0.60
1:A:930:VAL:CG1	1:A:948:ASP:HB3	2.32	0.60
1:A:367:LEU:HD11	1:A:375:LEU:HD22	1.84	0.60
1:A:67:PHE:CZ	1:A:145:LEU:HD21	2.35	0.60
2:B:173:TYR:OH	2:B:230:MET:SD	2.57	0.60
1:A:570:LYS:CD	1:A:577:LEU:HD11	2.32	0.60
1:A:580:GLU:OE2	1:A:626:ARG:CZ	2.50	0.60
1:A:1080:ARG:NE	2:B:298:PRO:HB3	2.16	0.60
1:A:284:LEU:HD22	1:A:301:ARG:HH21	1.66	0.60
2:B:24:SER:CB	2:B:36:LYS:HG2	2.29	0.60
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.67	0.60
1:A:166:ASP:OD2	1:A:219:VAL:HG12	2.02	0.60
1:A:129:ARG:HG3	1:A:130:MET:HE3	1.83	0.59
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.83	0.59
1:A:162:LEU:CD2	2:B:324:LEU:HD11	2.32	0.59
3:F:9:DT:H2'	3:F:10:DG:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:HIS:CD2	2:B:121:PRO:HD2	2.37	0.59
1:A:216:ALA:HB1	1:A:231:ILE:CG2	2.31	0.59
1:A:396:ILE:CD1	1:A:703:THR:O	2.49	0.59
1:A:410:LEU:O	1:A:639:ARG:NH2	2.35	0.59
2:B:159:ILE:CD1	2:B:174:ALA:HB1	2.32	0.59
2:B:251:ASN:HB2	2:B:257:PHE:HE2	1.65	0.59
2:B:267:VAL:HG22	2:B:285:LEU:H	1.67	0.59
2:B:332:ARG:NH1	2:B:358:ASP:HB3	2.17	0.59
2:B:386:LEU:HB3	2:B:418:TRP:CH2	2.38	0.59
1:A:1135:GLU:HA	1:A:1138:ARG:CZ	2.33	0.59
2:B:52:CYS:O	2:B:53:LEU:HD22	2.02	0.59
1:A:343:GLN:N	1:A:343:GLN:NE2	2.50	0.59
1:A:518:TYR:HD2	1:A:529:ILE:CD1	2.15	0.59
1:A:1071:SER:O	1:A:1072:PHE:CB	2.50	0.59
2:B:35:LYS:NZ	2:B:65:PRO:HA	2.16	0.59
2:B:123:HIS:ND1	2:B:126:THR:OG1	2.36	0.59
2:B:113:ARG:NE	2:B:336:HIS:O	2.35	0.59
2:B:199:THR:O	2:B:200:ILE:CG1	2.46	0.59
1:A:1094:ILE:HD12	1:A:1136:LEU:CD1	2.32	0.59
2:B:399:GLU:OE2	2:B:399:GLU:HA	2.02	0.59
1:A:290:GLN:HG2	1:A:291:MET:N	2.17	0.59
1:A:402:ILE:HD13	1:A:443:VAL:HG21	1.83	0.59
1:A:476:VAL:CG2	1:A:490:TRP:HB3	2.31	0.59
2:B:370:ARG:O	2:B:370:ARG:HG2	2.02	0.59
1:A:516:LEU:CD1	1:A:534:MET:CE	2.80	0.59
2:B:159:ILE:HA	2:B:175:SER:O	2.03	0.59
1:A:158:ARG:HD3	2:B:319:GLN:HB2	1.85	0.59
2:B:202:ILE:HA	2:B:221:ASN:HD21	1.68	0.59
1:A:928:ARG:HD2	2:B:405:ASP:OD2	2.02	0.59
1:A:1094:ILE:HD13	1:A:1136:LEU:HD13	1.81	0.59
2:B:173:TYR:CE1	2:B:183:LEU:HD22	2.38	0.59
1:A:80:LEU:HD13	1:A:86:ALA:HB2	1.85	0.59
1:A:463:VAL:CG1	1:A:521:ILE:HG21	2.33	0.59
1:A:63:VAL:O	1:A:79:ILE:HA	2.03	0.59
1:A:837:TYR:CD2	1:A:840:GLU:OE2	2.56	0.59
1:A:444:GLU:HG2	1:A:445:GLU:H	1.67	0.58
2:B:267:VAL:HG22	2:B:285:LEU:HB2	1.84	0.58
1:A:463:VAL:HG11	1:A:521:ILE:HG21	1.83	0.58
1:A:927:MET:SD	2:B:348:TYR:OH	2.60	0.58
1:A:926:LEU:HD21	2:B:90:LEU:CD2	2.33	0.58
1:A:1080:ARG:HH21	2:B:298:PRO:CB	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:LEU:O	1:A:1132:VAL:CG1	2.51	0.58
2:B:311:GLU:O	2:B:312:ILE:HD12	2.03	0.58
1:A:360:VAL:HA	1:A:1005:ASN:OD1	2.03	0.58
1:A:367:LEU:HD22	1:A:368:GLU:H	1.65	0.58
2:B:158:SER:O	2:B:177:MET:N	2.36	0.58
1:A:57:MET:HE3	1:A:79:ILE:CD1	2.32	0.58
1:A:682:LEU:CD1	1:A:701:ILE:HD12	2.33	0.58
2:B:28:LEU:HD21	2:B:36:LYS:CG	2.34	0.58
2:B:369:LEU:HD22	2:B:387:TYR:HE2	1.68	0.58
2:B:103:ILE:HD12	2:B:103:ILE:N	2.18	0.58
1:A:484:LYS:O	1:A:484:LYS:HG3	2.02	0.58
1:A:19:VAL:HG22	1:A:64:MET:CE	2.33	0.58
1:A:360:VAL:CA	1:A:1005:ASN:OD1	2.52	0.58
2:B:267:VAL:HG21	2:B:285:LEU:HD22	1.85	0.58
1:A:237:ILE:CG2	1:A:248:ILE:HB	2.34	0.58
1:A:570:LYS:HZ3	1:A:577:LEU:CD1	2.16	0.58
1:A:432:GLN:HG2	1:A:433:THR:N	2.18	0.58
1:A:679:MET:CG	1:A:691:LEU:CD1	2.78	0.58
1:A:989:ARG:O	1:A:989:ARG:HD3	2.03	0.58
1:A:49:LEU:CD2	1:A:353:PHE:CZ	2.85	0.58
1:A:660:TYR:CD1	1:A:707:ILE:HG21	2.39	0.58
1:A:414:ARG:O	1:A:481:GLN:NE2	2.36	0.58
2:B:183:LEU:C	2:B:191:LEU:HD12	2.23	0.58
1:A:1052:LEU:HD13	1:A:1089:ILE:HD11	1.85	0.58
1:A:890:LEU:HB3	1:A:903:CYS:HB3	1.84	0.58
1:A:185:PRO:HA	2:B:21:ASN:HB3	1.85	0.58
2:B:28:LEU:C	2:B:30:LEU:N	2.54	0.58
2:B:52:CYS:SG	2:B:53:LEU:CG	2.92	0.58
2:B:227:LEU:HB2	2:B:236:TRP:CD1	2.39	0.58
2:B:251:ASN:HB2	2:B:257:PHE:CE2	2.39	0.58
2:B:29:GLU:O	2:B:29:GLU:CD	2.42	0.58
2:B:369:LEU:HD12	2:B:369:LEU:H	1.68	0.58
2:B:401:ASN:O	2:B:404:GLY:N	2.36	0.58
1:A:151:GLU:HB3	1:A:153:LYS:HZ2	1.67	0.58
1:A:100:ILE:HG23	1:A:100:ILE:O	2.03	0.58
1:A:183:GLN:HB2	1:A:188:ARG:HG2	1.86	0.58
1:A:367:LEU:CD2	1:A:368:GLU:N	2.59	0.57
1:A:375:LEU:CD1	1:A:389:ILE:HG23	2.25	0.57
1:A:157:ILE:HD12	1:A:202:PHE:CD2	2.38	0.57
1:A:328:LEU:HD13	1:A:382:PHE:CE2	2.39	0.57
2:B:54:TRP:NE1	2:B:55:VAL:CG1	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:C	1:A:1005:ASN:OD1	2.41	0.57
1:A:673:LEU:HD21	1:A:693:LEU:HD22	1.84	0.57
2:B:33:GLU:O	2:B:35:LYS:N	2.37	0.57
1:A:24:THR:HG23	1:A:91:TYR:CE2	2.38	0.57
1:A:736:LEU:HD21	1:A:831:VAL:HG23	1.86	0.57
2:B:132:LYS:HZ3	2:B:158:SER:HB2	1.68	0.57
1:A:288:GLU:HB3	1:A:298:LYS:HG2	1.86	0.57
1:A:1064:SER:OG	1:A:1068:ILE:N	2.38	0.57
1:A:660:TYR:CE1	1:A:707:ILE:CG2	2.87	0.57
2:B:227:LEU:CD2	2:B:272:LEU:HD13	2.35	0.57
2:B:114:ALA:HB1	2:B:410:ALA:CB	2.30	0.57
2:B:332:ARG:NH2	2:B:358:ASP:CB	2.58	0.57
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.87	0.57
1:A:536:HIS:CB	1:A:560:LEU:CD1	2.75	0.57
2:B:119:TRP:CZ2	2:B:408:ALA:CB	2.88	0.57
2:B:182:ARG:HE	2:B:184:GLN:CD	2.08	0.57
1:A:891:TYR:CD1	1:A:899:LEU:HD13	2.39	0.57
1:A:682:LEU:HD12	1:A:701:ILE:CD1	2.33	0.57
2:B:215:MET:CG	2:B:227:LEU:HD21	2.34	0.57
1:A:849:VAL:CG1	1:A:860:THR:HG23	2.35	0.57
2:B:53:LEU:CB	2:B:54:TRP:C	2.59	0.57
2:B:159:ILE:HG13	2:B:175:SER:O	2.05	0.57
2:B:251:ASN:CB	2:B:257:PHE:CE2	2.85	0.57
2:B:20:ARG:C	2:B:22:LYS:N	2.53	0.56
2:B:28:LEU:HD13	2:B:35:LYS:HB2	1.87	0.56
2:B:45:SER:O	2:B:46:ARG:NE	2.38	0.56
1:A:549:SER:C	1:A:551:GLY:HA2	2.21	0.56
2:B:32:PRO:CG	2:B:67:ARG:HD2	2.34	0.56
2:B:43:GLY:O	2:B:46:ARG:N	2.39	0.56
2:B:55:VAL:CG2	2:B:56:GLY:N	2.59	0.56
1:A:402:ILE:HG22	1:A:404:LEU:HD12	1.87	0.56
1:A:473:SER:O	1:A:497:ASN:HA	2.06	0.56
1:A:157:ILE:HG13	1:A:158:ARG:C	2.26	0.56
2:B:261:ALA:HB1	2:B:291:VAL:O	2.05	0.56
1:A:947:ARG:HD3	1:A:949:PHE:HE1	1.70	0.56
2:B:377:GLY:C	2:B:379:SER:H	2.07	0.56
1:A:726:TYR:HB2	1:A:733:PHE:CE1	2.40	0.56
1:A:411:TRP:CH2	1:A:457:THR:CG2	2.88	0.56
2:B:274:GLN:O	2:B:274:GLN:HG2	2.05	0.56
1:A:490:TRP:NE1	1:A:528:GLN:OE1	2.37	0.56
1:A:389:ILE:HD13	1:A:713:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:PHE:CD2	1:A:991:HIS:CE1	2.94	0.56
1:A:162:LEU:CD2	2:B:324:LEU:CD1	2.84	0.56
2:B:24:SER:CB	2:B:36:LYS:CG	2.79	0.56
1:A:770:LEU:CD1	1:A:772:SER:HB2	2.34	0.56
2:B:200:ILE:HD12	2:B:201:ASN:N	2.10	0.56
1:A:629:VAL:HG11	1:A:668:PHE:CE1	2.41	0.56
2:B:153:ILE:O	2:B:153:ILE:HD12	2.04	0.56
1:A:881:LEU:HD21	1:A:921:ILE:HG21	1.87	0.56
1:A:516:LEU:HD12	1:A:534:MET:HE1	1.87	0.56
1:A:398:GLU:OE2	1:A:400:ALA:O	2.23	0.56
4:G:16:DA:H2''	4:G:17:DT:C5'	2.33	0.56
2:B:116:SER:HB2	2:B:130:GLY:HA3	1.88	0.56
2:B:388:ASP:O	2:B:391:SER:O	2.24	0.56
1:A:536:HIS:CG	1:A:562:THR:HB	2.41	0.56
1:A:966:LEU:HD12	1:A:967:GLY:H	1.69	0.56
1:A:396:ILE:HG21	1:A:673:LEU:HD11	1.87	0.56
1:A:416:ASP:N	1:A:419:ARG:HH12	2.03	0.56
4:G:4:DA:C2'	4:G:5:DG:C8	2.89	0.56
1:A:516:LEU:HD12	1:A:534:MET:CE	2.35	0.56
1:A:739:ARG:HG2	1:A:788:VAL:CG2	2.36	0.56
2:B:91:GLN:O	2:B:95:LEU:HG	2.06	0.56
4:G:15:DC:H2''	4:G:16:DA:H5'	1.88	0.56
1:A:538:VAL:HG22	1:A:558:ILE:HD11	1.88	0.56
1:A:1102:ARG:HG2	1:A:1102:ARG:HH11	1.70	0.56
1:A:907:ASN:OD1	1:A:907:ASN:O	2.22	0.56
1:A:1129:LEU:O	1:A:1132:VAL:HG13	2.06	0.56
1:A:761:LEU:C	1:A:761:LEU:HD23	2.25	0.56
1:A:44:VAL:HG23	1:A:44:VAL:O	2.05	0.56
1:A:335:LYS:HB3	1:A:348:VAL:CG2	2.36	0.56
2:B:37:LEU:HD12	2:B:37:LEU:N	2.21	0.55
1:A:33:ILE:HD12	1:A:42:TYR:HE2	1.71	0.55
2:B:248:VAL:HG12	2:B:258:LEU:HD11	1.88	0.55
2:B:246:THR:HG1	2:B:292:ASN:HA	1.70	0.55
1:A:733:PHE:HD2	1:A:794:ILE:HD11	1.70	0.55
2:B:299:ASP:HB3	2:B:301:ALA:H	1.71	0.55
2:B:60:PRO:CA	2:B:63:LEU:CG	2.84	0.55
1:A:443:VAL:CG2	1:A:444:GLU:H	2.16	0.55
2:B:257:PHE:HB2	2:B:270:TRP:O	2.06	0.55
2:B:214:ARG:HG2	2:B:230:MET:CE	2.37	0.55
2:B:32:PRO:CG	2:B:67:ARG:CD	2.85	0.55
1:A:768:SER:OG	1:A:769:LYS:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:LEU:HD11	1:A:616:LEU:CD2	2.34	0.55
2:B:97:THR:O	2:B:101:TYR:CD1	2.58	0.55
1:A:762:SER:OG	1:A:803:HIS:ND1	2.20	0.55
1:A:79:ILE:CG1	1:A:87:CYS:SG	2.94	0.55
1:A:212:VAL:HG22	1:A:213:GLU:N	2.21	0.55
1:A:335:LYS:HB3	1:A:348:VAL:HG23	1.87	0.55
2:B:32:PRO:HG2	2:B:67:ARG:HD3	1.89	0.55
1:A:767:SER:O	1:A:768:SER:OG	2.21	0.55
1:A:602:LEU:HD11	1:A:616:LEU:HD22	1.88	0.55
2:B:225:VAL:HG23	2:B:240:MET:HG3	1.88	0.55
4:G:10:DG:C2'	4:G:12:DC:OP2	2.55	0.55
1:A:22:HIS:HB3	1:A:28:ASP:O	2.06	0.55
1:A:463:VAL:CG2	1:A:469:ILE:HB	2.31	0.55
1:A:601:TYR:CZ	1:A:666:LEU:CD1	2.82	0.55
1:A:328:LEU:HD13	1:A:382:PHE:HD2	1.70	0.55
2:B:47:ARG:C	2:B:54:TRP:CZ3	2.80	0.55
1:A:680:CYS:SG	1:A:692:ALA:HB3	2.47	0.55
2:B:306:THR:HG21	2:B:341:LYS:HA	1.87	0.55
3:F:5:DT:C2	3:F:6:DG:C8	2.95	0.55
2:B:23:ARG:O	2:B:27:PRO:CG	2.55	0.55
1:A:389:ILE:HB	1:A:713:ARG:HG3	1.87	0.55
1:A:934:ALA:HB3	1:A:945:ILE:HD11	1.88	0.55
1:A:780:THR:HB	1:A:782:PHE:H	1.72	0.55
2:B:43:GLY:HA2	2:B:46:ARG:O	2.06	0.55
1:A:22:HIS:O	1:A:30:ASN:CB	2.53	0.55
1:A:715:VAL:HG11	1:A:799:PHE:HB3	1.89	0.55
2:B:335:GLN:OE1	3:F:13:DG:N2	2.40	0.55
2:B:169:THR:O	2:B:169:THR:HG22	2.05	0.55
1:A:803:HIS:NE2	1:A:858:LEU:CD1	2.70	0.55
2:B:119:TRP:CZ2	2:B:408:ALA:HB2	2.42	0.55
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.88	0.55
1:A:534:MET:CE	1:A:558:ILE:HD13	2.37	0.55
3:F:1:DT:H5'	3:F:1:DT:O2	2.07	0.55
1:A:290:GLN:HG2	1:A:291:MET:H	1.72	0.55
1:A:411:TRP:CZ3	1:A:457:THR:HG22	2.42	0.55
1:A:881:LEU:HD13	1:A:890:LEU:HD13	1.89	0.55
2:B:20:ARG:O	2:B:23:ARG:CG	2.55	0.54
2:B:303:LEU:HB3	2:B:315:TYR:HB2	1.89	0.54
4:G:21:DG:H8	4:G:21:DG:H5''	1.72	0.54
3:F:1:DT:H2'	3:F:1:DT:O2	2.05	0.54
1:A:881:LEU:HD21	1:A:921:ILE:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:ARG:NH1	1:A:1109:VAL:O	2.40	0.54
2:B:37:LEU:CD1	2:B:37:LEU:N	2.71	0.54
2:B:206:SER:HB2	2:B:248:VAL:HG22	1.85	0.54
2:B:365:THR:HG22	2:B:368:GLU:OE2	2.07	0.54
1:A:611:LEU:HD22	1:A:631:LEU:HD21	1.88	0.54
1:A:631:LEU:CD1	1:A:636:THR:OG1	2.55	0.54
1:A:238:THR:HG23	1:A:240:HIS:CD2	2.41	0.54
3:F:1:DT:H2"	3:F:2:DG:C8	2.42	0.54
1:A:44:VAL:HG11	1:A:317:LEU:HD13	1.89	0.54
1:A:361:ASP:CB	1:A:723:LYS:HA	2.37	0.54
2:B:52:CYS:HB2	2:B:53:LEU:CD1	2.36	0.54
3:F:22:DG:N2	4:G:4:DA:C2	2.75	0.54
1:A:558:ILE:HG22	1:A:567:ARG:O	2.08	0.54
1:A:858:LEU:CD1	1:A:858:LEU:O	2.55	0.54
1:A:357:GLY:HA2	1:A:358:PRO:C	2.26	0.54
1:A:380:GLY:C	1:A:385:GLY:HA2	2.28	0.54
2:B:92:GLN:O	2:B:92:GLN:HG3	2.07	0.54
2:B:290:PRO:HB2	2:B:308:GLN:CG	2.38	0.54
1:A:436:LEU:HD11	1:A:443:VAL:C	2.28	0.54
2:B:313:ARG:HH11	2:B:326:LEU:HD21	1.72	0.54
1:A:1013:VAL:HG21	1:A:1139:ILE:C	2.27	0.54
1:A:419:ARG:NH2	1:A:423:ASP:OD1	2.40	0.54
2:B:223:GLY:HA3	2:B:241:HIS:O	2.08	0.54
4:G:20:DA:H2'	4:G:21:DG:C8	2.43	0.54
2:B:379:SER:HG	2:B:381:LYS:HG2	1.71	0.54
1:A:57:MET:SD	1:A:1068:ILE:CD1	2.93	0.54
1:A:739:ARG:CG	1:A:788:VAL:CG2	2.85	0.54
1:A:850:VAL:HB	1:A:862:ALA:HB3	1.90	0.54
2:B:334:PHE:HB3	2:B:337:LEU:CB	2.38	0.54
4:G:20:DA:H2"	4:G:21:DG:OP1	2.08	0.54
1:A:512:VAL:CG1	1:A:515:ALA:HB3	2.15	0.54
2:B:104:LEU:HD11	2:B:416:LEU:HD23	1.90	0.54
2:B:267:VAL:CG1	2:B:287:HIS:NE2	2.71	0.54
2:B:117:LEU:HD23	2:B:397:LEU:HB3	1.89	0.54
1:A:589:ARG:CD	1:A:589:ARG:O	2.45	0.54
2:B:59:GLY:O	2:B:62:ILE:CD1	2.55	0.54
2:B:376:ASP:OD2	2:B:377:GLY:O	2.26	0.54
2:B:377:GLY:O	2:B:378:ASN:HB3	2.07	0.54
2:B:62:ILE:HG12	2:B:63:LEU:N	2.23	0.54
2:B:207:LEU:HD12	2:B:208:ASP:H	1.72	0.54
2:B:312:ILE:O	2:B:312:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HD12	1:A:141:LYS:HD2	1.89	0.54
1:A:147:ARG:NH1	1:A:147:ARG:CG	2.50	0.53
1:A:367:LEU:HD22	1:A:368:GLU:CA	2.38	0.53
3:F:4:DC:H2"	3:F:5:DT:O5'	2.08	0.53
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.43	0.53
2:B:185:ASP:OD2	2:B:187:LYS:HB2	2.08	0.53
2:B:36:LYS:CD	2:B:37:LEU:N	2.71	0.53
1:A:368:GLU:CD	1:A:391:ARG:HE	2.11	0.53
2:B:229:ASN:O	2:B:231:ASP:N	2.41	0.53
2:B:332:ARG:HG3	2:B:332:ARG:HH21	1.73	0.53
1:A:612:PHE:CZ	1:A:628:LYS:CE	2.91	0.53
2:B:164:PHE:O	2:B:166:PRO:HD3	2.08	0.53
2:B:57:LEU:C	2:B:60:PRO:CD	2.76	0.53
2:B:369:LEU:CD2	2:B:387:TYR:CE2	2.88	0.53
1:A:811:GLU:CD	1:A:847:ARG:HH21	2.10	0.53
1:A:828:TYR:CZ	1:A:897:LYS:NZ	2.73	0.53
1:A:1005:ASN:N	1:A:1005:ASN:HD22	1.89	0.53
2:B:209:VAL:CG2	2:B:216:VAL:HG22	2.32	0.53
2:B:241:HIS:CB	2:B:268:LYS:NZ	2.66	0.53
2:B:397:LEU:O	2:B:398:ASN:ND2	2.41	0.53
1:A:666:LEU:N	1:A:666:LEU:CD1	2.71	0.53
1:A:475:SER:HB3	1:A:491:LYS:HG2	1.90	0.53
1:A:416:ASP:CB	1:A:419:ARG:HH11	2.03	0.53
2:B:227:LEU:H	2:B:236:TRP:CB	2.22	0.53
2:B:240:MET:SD	2:B:270:TRP:CE2	3.01	0.53
1:A:83:LYS:NZ	1:A:1072:PHE:O	2.38	0.53
1:A:554:PRO:HD2	1:A:555:LEU:HD22	1.91	0.53
1:A:198:ARG:O	1:A:199:GLU:HB2	2.08	0.53
1:A:913:TYR:HB3	1:A:957:VAL:HG22	1.91	0.53
2:B:241:HIS:CD2	2:B:268:LYS:CE	2.89	0.53
1:A:369:ARG:O	1:A:370:GLN:OE1	2.27	0.53
1:A:833:THR:O	1:A:870:VAL:HG23	2.07	0.53
1:A:1:HIS:HD2	1:A:995:VAL:HG11	1.74	0.53
1:A:444:GLU:CG	1:A:445:GLU:H	2.20	0.53
2:B:329:HIS:CE1	2:B:355:ARG:HA	2.43	0.53
2:B:330:PRO:HG2	2:B:355:ARG:NH1	2.24	0.53
2:B:143:ILE:O	2:B:144:LYS:HB2	2.08	0.53
1:A:907:ASN:ND2	1:A:944:GLU:OE1	2.42	0.53
2:B:52:CYS:C	2:B:53:LEU:CD1	2.60	0.53
2:B:47:ARG:O	2:B:54:TRP:CE3	2.60	0.53
2:B:369:LEU:HB3	2:B:387:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:GLY:HA2	2:B:178:GLU:CG	2.39	0.53
2:B:125:SER:O	2:B:140:ASN:HA	2.08	0.53
1:A:147:ARG:HG2	1:A:147:ARG:NH1	2.13	0.53
1:A:23:PHE:HD1	1:A:75:ASP:O	1.92	0.53
1:A:387:LEU:HB2	1:A:715:VAL:CG2	2.38	0.53
2:B:291:VAL:O	2:B:291:VAL:CG2	2.56	0.53
1:A:374:GLN:CB	1:A:1012:LEU:HA	2.39	0.53
1:A:1082:THR:HG22	1:A:1083:GLU:N	2.24	0.53
2:B:217:VAL:HG23	2:B:227:LEU:HD12	1.91	0.53
3:F:18:DT:H2"	3:F:19:DG:OP2	2.09	0.53
1:A:112:ILE:CD1	2:B:317:ALA:HB1	2.39	0.53
1:A:736:LEU:HD21	1:A:831:VAL:CG2	2.39	0.53
2:B:264:ASP:OD2	2:B:266:THR:OG1	2.13	0.53
1:A:608:ASP:OD1	1:A:609:GLY:N	2.41	0.52
1:A:79:ILE:HG13	1:A:87:CYS:SG	2.49	0.52
1:A:191:LYS:HD3	1:A:193:TYR:CZ	2.44	0.52
1:A:850:VAL:HB	1:A:862:ALA:HB2	1.90	0.52
1:A:1105:MET:O	1:A:1109:VAL:HG23	2.09	0.52
2:B:23:ARG:O	2:B:27:PRO:HG2	2.10	0.52
1:A:22:HIS:ND1	1:A:29:LEU:HA	2.23	0.52
1:A:197:LEU:O	1:A:197:LEU:HD23	2.09	0.52
1:A:949:PHE:CD2	1:A:991:HIS:ND1	2.77	0.52
1:A:381:ALA:N	1:A:385:GLY:HA2	2.24	0.52
1:A:102:THR:HG22	1:A:1066:GLY:HA2	1.91	0.52
1:A:954:MET:CE	1:A:957:VAL:HG12	2.39	0.52
2:B:122:THR:OG1	2:B:123:HIS:N	2.43	0.52
1:A:570:LYS:O	1:A:574:PHE:N	2.40	0.52
1:A:408:LYS:NZ	1:A:678:TYR:OH	2.39	0.52
2:B:57:LEU:CD2	2:B:57:LEU:O	2.53	0.52
1:A:80:LEU:HD22	1:A:133:LEU:HD21	1.92	0.52
2:B:202:ILE:CG2	2:B:203:TRP:N	2.72	0.52
1:A:569:LEU:CD1	1:A:569:LEU:N	2.72	0.52
1:A:1080:ARG:CZ	2:B:298:PRO:HB3	2.38	0.52
1:A:398:GLU:CD	1:A:700:THR:HG23	2.30	0.52
2:B:54:TRP:C	2:B:57:LEU:HD12	2.22	0.52
2:B:293:ALA:HB3	2:B:306:THR:CG2	2.22	0.52
2:B:83:TRP:N	2:B:84:PRO:CD	2.72	0.52
1:A:162:LEU:HD22	2:B:324:LEU:HD11	1.91	0.52
1:A:1052:LEU:CD1	1:A:1089:ILE:HD11	2.40	0.52
1:A:555:LEU:N	1:A:555:LEU:HD22	2.24	0.52
1:A:828:TYR:OH	1:A:897:LYS:CE	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:SER:N	1:A:550:ASN:HA	2.24	0.52
1:A:157:ILE:O	1:A:157:ILE:HG12	2.10	0.52
2:B:162:LEU:HD12	2:B:173:TYR:O	2.10	0.52
2:B:217:VAL:HB	2:B:227:LEU:CD1	2.39	0.52
1:A:413:LEU:HB3	1:A:424:THR:HB	1.91	0.52
1:A:22:HIS:ND1	1:A:28:ASP:O	2.42	0.52
1:A:365:VAL:HG12	1:A:367:LEU:H	1.74	0.52
2:B:246:THR:N	2:B:261:ALA:O	2.43	0.52
1:A:536:HIS:ND1	1:A:562:THR:HB	2.25	0.52
1:A:926:LEU:HD21	2:B:90:LEU:HD22	1.91	0.52
1:A:960:LEU:C	1:A:961:ASP:OD1	2.48	0.52
1:A:873:MET:HA	1:A:881:LEU:O	2.10	0.52
2:B:53:LEU:O	2:B:57:LEU:CB	2.58	0.52
1:A:22:HIS:CB	1:A:74:LYS:HE2	2.34	0.52
1:A:1018:GLY:CA	1:A:1019:GLU:CB	2.66	0.52
4:G:19:DC:H1'	4:G:20:DA:C8	2.45	0.52
1:A:484:LYS:O	1:A:484:LYS:CG	2.57	0.52
1:A:458:PHE:HE2	1:A:498:ILE:O	1.93	0.52
1:A:518:TYR:O	1:A:529:ILE:HG13	2.09	0.52
1:A:766:SER:HB3	1:A:808:LEU:CD2	2.40	0.52
2:B:387:TYR:CD1	2:B:388:ASP:N	2.78	0.52
1:A:117:GLU:N	1:A:117:GLU:OE2	2.42	0.52
1:A:922:LEU:HD11	1:A:930:VAL:CG2	2.39	0.52
2:B:260:THR:OG1	2:B:261:ALA:N	2.43	0.51
4:G:21:DG:H8	4:G:21:DG:C5'	2.23	0.51
2:B:184:GLN:HB3	2:B:190:ILE:HA	1.91	0.51
2:B:225:VAL:O	2:B:237:ASN:HA	2.10	0.51
1:A:251:PRO:HA	1:A:254:LYS:HD3	1.91	0.51
1:A:883:SER:OG	1:A:914:LEU:HD11	2.10	0.51
1:A:22:HIS:CE1	1:A:29:LEU:HG	2.44	0.51
1:A:477:ARG:HG2	1:A:477:ARG:NH1	2.24	0.51
1:A:328:LEU:HA	1:A:358:PRO:HD3	1.91	0.51
1:A:337:ASN:O	1:A:346:TYR:HD1	1.94	0.51
1:A:411:TRP:HB2	1:A:460:CYS:SG	2.51	0.51
1:A:1116:ASP:OD2	1:A:1122:ARG:NH1	2.26	0.51
1:A:876:PHE:O	1:A:879:LYS:HB2	2.10	0.51
1:A:244:LYS:CE	1:A:296:THR:O	2.58	0.51
1:A:601:TYR:OH	1:A:666:LEU:HD11	2.11	0.51
1:A:685:ASP:N	1:A:685:ASP:OD1	2.44	0.51
2:B:334:PHE:HB3	2:B:337:LEU:HB3	1.92	0.51
1:A:144:PRO:CG	1:A:197:LEU:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:LYS:NZ	2:B:158:SER:HB2	2.25	0.51
2:B:126:THR:HA	2:B:139:TRP:O	2.11	0.51
1:A:262:ASN:CG	1:A:315:THR:HA	2.31	0.51
2:B:369:LEU:HD23	2:B:387:TYR:CE2	2.45	0.51
1:A:463:VAL:HG21	1:A:469:ILE:CB	2.36	0.51
2:B:83:TRP:CE2	2:B:87:GLN:HB2	2.45	0.51
1:A:26:ALA:HA	1:A:74:LYS:HD3	1.92	0.51
2:B:245:VAL:HA	2:B:261:ALA:O	2.11	0.51
2:B:240:MET:SD	2:B:270:TRP:NE1	2.83	0.51
2:B:247:HIS:CD2	2:B:294:ALA:H	2.28	0.51
2:B:393:GLY:HA3	2:B:411:MET:CE	2.40	0.51
1:A:970:ASN:OD1	1:A:971:ALA:N	2.44	0.51
1:A:739:ARG:CG	1:A:788:VAL:HG23	2.39	0.51
1:A:84:TYR:O	1:A:107:ASN:O	2.28	0.51
2:B:162:LEU:HD11	2:B:172:PHE:HB2	1.91	0.51
2:B:184:GLN:CA	2:B:191:LEU:HD12	2.36	0.51
1:A:671:VAL:HG12	1:A:673:LEU:CD1	2.41	0.51
1:A:44:VAL:CG1	1:A:317:LEU:HD13	2.41	0.51
1:A:176:PRO:HB2	1:A:195:VAL:HG12	1.88	0.51
3:F:13:DG:N7	3:F:14:DA:C6	2.79	0.51
1:A:1135:GLU:O	1:A:1138:ARG:CG	2.58	0.51
1:A:81:THR:HG22	1:A:83:LYS:N	2.26	0.51
1:A:943:GLU:O	1:A:945:ILE:HD12	2.11	0.51
1:A:248:ILE:HD11	1:A:300:LEU:HB2	1.87	0.50
1:A:516:LEU:HD22	1:A:574:PHE:CE1	2.46	0.50
1:A:238:THR:HG21	1:A:240:HIS:NE2	2.26	0.50
2:B:241:HIS:HD2	2:B:268:LYS:HE2	1.70	0.50
1:A:686:GLY:C	1:A:687:TYR:CD1	2.84	0.50
1:A:398:GLU:OE2	1:A:700:THR:HG23	2.12	0.50
1:A:837:TYR:HB2	1:A:840:GLU:HG2	1.92	0.50
2:B:69:ILE:O	2:B:70:VAL:HB	2.11	0.50
2:B:40:LYS:O	2:B:40:LYS:HG3	2.12	0.50
2:B:59:GLY:CA	2:B:62:ILE:HD13	2.32	0.50
1:A:1048:TYR:CE2	1:A:1052:LEU:HD22	2.46	0.50
1:A:866:VAL:HG11	1:A:884:ILE:HD13	1.94	0.50
1:A:602:LEU:CD1	1:A:616:LEU:CG	2.84	0.50
3:F:3:DA:H3'	3:F:4:DC:C6	2.47	0.50
2:B:58:ALA:O	2:B:62:ILE:CG2	2.47	0.50
1:A:402:ILE:HD11	1:A:443:VAL:HG21	1.93	0.50
1:A:774:SER:O	1:A:775:THR:CG2	2.59	0.50
1:A:212:VAL:O	1:A:213:GLU:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:PHE:HA	2:B:219:GLY:O	2.12	0.50
1:A:589:ARG:HD3	1:A:589:ARG:C	2.28	0.50
1:A:518:TYR:CD2	1:A:529:ILE:CD1	2.95	0.50
1:A:738:SER:HA	1:A:788:VAL:O	2.12	0.50
1:A:129:ARG:NH1	1:A:176:PRO:CG	2.69	0.50
1:A:472:THR:CG2	1:A:474:ALA:N	2.67	0.50
1:A:374:GLN:HB2	1:A:1012:LEU:CA	2.41	0.50
2:B:86:VAL:O	2:B:90:LEU:HG	2.11	0.50
1:A:13:THR:OG1	1:A:355:ASN:OD1	2.19	0.50
1:A:609:GLY:O	1:A:631:LEU:CD1	2.57	0.50
1:A:726:TYR:HB2	1:A:733:PHE:HE1	1.77	0.50
2:B:208:ASP:OD1	2:B:209:VAL:N	2.44	0.50
2:B:310:SER:O	2:B:311:GLU:HB2	2.11	0.50
1:A:1054:MET:C	1:A:1058:LEU:HD12	2.32	0.50
1:A:1080:ARG:HE	2:B:298:PRO:CB	2.25	0.50
2:B:367:TYR:O	2:B:367:TYR:CD2	2.65	0.50
2:B:42:SER:O	2:B:45:SER:O	2.30	0.49
2:B:158:SER:HB3	2:B:177:MET:HB2	1.94	0.49
1:A:32:LEU:CD1	1:A:41:ILE:HG23	2.42	0.49
2:B:21:ASN:OD1	2:B:22:LYS:N	2.45	0.49
1:A:19:VAL:HG22	1:A:64:MET:HE3	1.93	0.49
1:A:436:LEU:HD11	1:A:443:VAL:CA	2.42	0.49
1:A:365:VAL:HG12	1:A:367:LEU:HD12	1.91	0.49
2:B:218:THR:HG23	2:B:226:ILE:CG2	2.41	0.49
1:A:396:ILE:HG22	1:A:673:LEU:CD1	2.39	0.49
1:A:693:LEU:C	1:A:693:LEU:HD12	2.32	0.49
1:A:282:MET:HB2	1:A:305:LEU:HD21	1.94	0.49
1:A:315:THR:O	1:A:315:THR:HG23	2.12	0.49
1:A:6:VAL:O	1:A:1091:GLY:N	2.41	0.49
2:B:104:LEU:HD21	2:B:416:LEU:HG	1.94	0.49
2:B:331:HIS:HA	2:B:356:TYR:HB3	1.94	0.49
1:A:930:VAL:CG1	1:A:948:ASP:CB	2.90	0.49
1:A:449:MET:HB3	1:A:484:LYS:O	2.13	0.49
1:A:1005:ASN:H	1:A:1005:ASN:ND2	1.94	0.49
2:B:251:ASN:HB3	2:B:257:PHE:HE2	1.74	0.49
2:B:327:ILE:HG21	2:B:375:PHE:CD2	2.46	0.49
1:A:1094:ILE:HD12	1:A:1136:LEU:HD12	1.93	0.49
1:A:956:ALA:HB3	1:A:1007:PHE:CE2	2.47	0.49
2:B:43:GLY:O	2:B:46:ARG:O	2.30	0.49
2:B:62:ILE:CG1	2:B:63:LEU:N	2.75	0.49
1:A:402:ILE:HG22	1:A:404:LEU:HD11	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:O	1:A:721:PRO:HD2	2.11	0.49
1:A:281:PHE:CD1	1:A:304:LEU:HD13	2.45	0.49
1:A:468:LEU:HB2	1:A:479:VAL:CG2	2.41	0.49
1:A:336:LEU:HA	1:A:346:TYR:O	2.13	0.49
1:A:419:ARG:O	1:A:420:GLU:CG	2.60	0.49
2:B:241:HIS:CB	2:B:268:LYS:HZ1	2.22	0.49
2:B:135:ASP:OD1	2:B:152:GLY:N	2.38	0.49
1:A:980:ASP:O	1:A:989:ARG:CZ	2.54	0.49
2:B:98:LEU:HD12	2:B:101:TYR:CD1	2.48	0.49
1:A:119:GLY:O	1:A:134:ARG:NH2	2.36	0.49
2:B:64:PRO:N	2:B:65:PRO:HD2	2.28	0.49
2:B:372:ILE:HD12	2:B:372:ILE:H	1.76	0.49
1:A:239:TYR:CZ	1:A:297:LEU:HD22	2.47	0.49
1:A:616:LEU:HD13	1:A:623:LEU:CD2	2.43	0.49
2:B:226:ILE:HD11	2:B:234:GLU:OE1	2.12	0.49
2:B:270:TRP:HH2	2:B:279:ALA:HA	1.78	0.49
2:B:54:TRP:NE1	2:B:55:VAL:CB	2.76	0.49
3:F:13:DG:H2''	3:F:14:DA:H5'	1.95	0.49
1:A:135:LEU:CD1	1:A:141:LYS:HD2	2.43	0.49
1:A:1007:PHE:CD2	1:A:1007:PHE:N	2.81	0.49
1:A:839:GLU:HA	2:B:63:LEU:O	2.13	0.48
2:B:54:TRP:NE1	2:B:55:VAL:HB	2.28	0.48
2:B:214:ARG:HA	2:B:230:MET:HE2	1.95	0.48
2:B:227:LEU:N	2:B:236:TRP:CD1	2.81	0.48
1:A:947:ARG:CG	1:A:949:PHE:CE1	2.96	0.48
1:A:722:ARG:NH2	1:A:812:TYR:CZ	2.80	0.48
1:A:880:LEU:HD23	1:A:899:LEU:HD11	1.95	0.48
1:A:251:PRO:HA	1:A:254:LYS:HD2	1.95	0.48
1:A:783:GLY:O	1:A:785:GLU:N	2.46	0.48
1:A:129:ARG:CG	1:A:130:MET:HE3	2.44	0.48
2:B:221:ASN:OD1	2:B:222:VAL:N	2.46	0.48
2:B:401:ASN:OD1	2:B:404:GLY:N	2.45	0.48
1:A:288:GLU:CD	1:A:296:THR:HG21	2.33	0.48
1:A:377:THR:CA	1:A:388:ARG:O	2.51	0.48
1:A:861:VAL:HG22	1:A:862:ALA:N	2.26	0.48
2:B:352:VAL:HA	2:B:373:ASP:O	2.13	0.48
1:A:976:VAL:O	1:A:994:GLU:HA	2.13	0.48
2:B:334:PHE:HD1	3:F:14:DA:H4'	1.78	0.48
1:A:1076:PHE:HB3	1:A:1083:GLU:CG	2.39	0.48
1:A:398:GLU:OE1	1:A:700:THR:CG2	2.61	0.48
1:A:741:GLU:HB3	1:A:750:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:ILE:HD13	2:B:188:GLY:HA3	1.95	0.48
1:A:32:LEU:HD12	1:A:41:ILE:HG23	1.95	0.48
1:A:244:LYS:HB3	1:A:244:LYS:HE3	1.52	0.48
1:A:190:VAL:HG21	1:A:231:ILE:HD11	1.95	0.48
4:G:24:DA:N3	4:G:24:DA:H2'	2.28	0.48
2:B:44:PRO:N	2:B:45:SER:CA	2.76	0.48
2:B:308:GLN:OE1	2:B:333:HIS:CD2	2.66	0.48
1:A:22:HIS:HA	1:A:30:ASN:H	1.78	0.48
3:F:15:DC:H2''	3:F:16:DG:C8	2.49	0.48
4:G:11:3DR:H3'	4:G:12:DC:C4'	2.43	0.48
1:A:151:GLU:HB2	1:A:153:LYS:HZ2	1.78	0.48
1:A:348:VAL:HG23	1:A:348:VAL:O	2.12	0.48
1:A:131:ILE:HB	1:A:143:ILE:HB	1.94	0.48
2:B:214:ARG:HG2	2:B:230:MET:HE2	1.94	0.48
3:F:19:DG:OP2	3:F:19:DG:H8	1.95	0.48
2:B:98:LEU:HA	2:B:101:TYR:CD1	2.49	0.48
1:A:963:ASP:O	1:A:978:GLN:HA	2.13	0.48
1:A:74:LYS:NZ	1:A:75:ASP:H	2.11	0.48
2:B:118:ALA:HB2	2:B:162:LEU:HG	1.96	0.48
2:B:329:HIS:CE1	2:B:353:VAL:HB	2.49	0.48
2:B:370:ARG:NH1	3:F:16:DG:OP2	2.46	0.48
1:A:151:GLU:HB2	1:A:153:LYS:NZ	2.28	0.48
1:A:930:VAL:HG12	1:A:948:ASP:CB	2.42	0.48
1:A:290:GLN:CG	1:A:291:MET:H	2.27	0.48
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.48	0.48
1:A:379:SER:HA	1:A:386:SER:O	2.14	0.48
1:A:123:ILE:HD13	1:A:167:VAL:CG2	2.38	0.48
1:A:615:GLY:N	1:A:624:SER:O	2.43	0.48
1:A:699:LEU:HD23	1:A:699:LEU:C	2.34	0.48
1:A:645:SER:O	1:A:645:SER:OG	2.30	0.48
2:B:32:PRO:HG2	2:B:67:ARG:CD	2.43	0.48
1:A:404:LEU:O	1:A:407:ILE:HG22	2.14	0.48
1:A:436:LEU:CD1	1:A:443:VAL:C	2.82	0.48
2:B:137:MET:HE1	2:B:415:ILE:HD12	1.96	0.48
2:B:218:THR:HG23	2:B:226:ILE:HG22	1.96	0.48
1:A:1070:HIS:HD2	1:A:1093:LEU:HD13	1.75	0.48
2:B:62:ILE:O	2:B:65:PRO:HD2	2.14	0.47
1:A:928:ARG:HG2	1:A:947:ARG:HH21	1.79	0.47
1:A:907:ASN:ND2	1:A:944:GLU:CD	2.67	0.47
1:A:679:MET:HG3	1:A:691:LEU:HD11	1.90	0.47
1:A:470:GLN:OE1	1:A:477:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HG21	1:A:1031:GLY:HA3	1.95	0.47
2:B:336:HIS:CD2	4:G:10:DG:C4	3.02	0.47
4:G:4:DA:C4'	4:G:5:DG:OP1	2.57	0.47
1:A:1013:VAL:CG2	1:A:1139:ILE:O	2.60	0.47
1:A:558:ILE:CG2	1:A:567:ARG:HG3	2.43	0.47
1:A:1007:PHE:N	1:A:1007:PHE:HD2	2.12	0.47
2:B:119:TRP:HZ2	2:B:408:ALA:N	2.11	0.47
1:A:183:GLN:CB	1:A:188:ARG:HG2	2.44	0.47
1:A:411:TRP:CH2	1:A:457:THR:HG22	2.49	0.47
1:A:559:GLY:HA2	1:A:565:SER:O	2.14	0.47
2:B:20:ARG:O	2:B:21:ASN:C	2.53	0.47
2:B:40:LYS:O	2:B:44:PRO:CG	2.62	0.47
1:A:768:SER:CB	1:A:769:LYS:CA	2.80	0.47
2:B:370:ARG:CD	2:B:392:SER:O	2.53	0.47
1:A:558:ILE:O	1:A:566:ALA:HA	2.14	0.47
2:B:332:ARG:NH1	2:B:356:TYR:CE2	2.83	0.47
2:B:369:LEU:O	2:B:371:THR:HG22	2.14	0.47
1:A:558:ILE:HG21	1:A:569:LEU:HD11	1.95	0.47
1:A:518:TYR:CG	1:A:529:ILE:HG12	2.48	0.47
1:A:432:GLN:HG2	1:A:433:THR:H	1.78	0.47
1:A:261:HIS:HA	1:A:272:LEU:O	2.15	0.47
1:A:954:MET:HE1	1:A:957:VAL:HG12	1.95	0.47
2:B:46:ARG:CB	2:B:49:ASP:H	2.01	0.47
1:A:22:HIS:O	1:A:23:PHE:HB3	2.14	0.47
2:B:250:LEU:HD23	2:B:258:LEU:HD13	1.96	0.47
2:B:394:ILE:O	2:B:411:MET:HG3	2.14	0.47
1:A:398:GLU:CD	1:A:700:THR:CG2	2.83	0.47
1:A:945:ILE:N	1:A:945:ILE:HD12	2.29	0.47
2:B:36:LYS:C	2:B:36:LYS:HD2	2.34	0.47
2:B:35:LYS:CD	2:B:65:PRO:HA	2.43	0.47
1:A:33:ILE:HD12	1:A:42:TYR:CE2	2.49	0.47
2:B:215:MET:CE	2:B:272:LEU:HD21	2.45	0.47
1:A:172:GLY:HA2	1:A:224:GLU:OE1	2.15	0.47
1:A:151:GLU:CB	1:A:153:LYS:NZ	2.77	0.47
1:A:107:ASN:C	1:A:108:VAL:HG22	2.35	0.47
1:A:452:VAL:CG1	1:A:454:ASP:H	2.28	0.47
1:A:55:VAL:HG23	1:A:56:GLY:N	2.30	0.47
2:B:290:PRO:HB2	2:B:308:GLN:OE1	2.10	0.47
1:A:715:VAL:HG11	1:A:799:PHE:CB	2.45	0.47
1:A:368:GLU:OE2	1:A:391:ARG:NE	2.48	0.47
1:A:237:ILE:CG2	1:A:237:ILE:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:ARG:O	2:B:413:TYR:CD1	2.68	0.47
1:A:634:GLN:HG3	1:A:635:PRO:CD	2.44	0.47
1:A:601:TYR:CE1	1:A:666:LEU:CD2	2.97	0.47
1:A:569:LEU:HD12	1:A:569:LEU:N	2.29	0.47
1:A:383:LYS:HE3	1:A:384:GLU:OE2	2.13	0.47
1:A:848:ILE:HG12	1:A:873:MET:SD	2.55	0.47
1:A:1050:LEU:HD13	1:A:1050:LEU:O	2.14	0.47
2:B:242:LYS:HE3	2:B:242:LYS:HB3	1.60	0.47
1:A:74:LYS:HZ3	1:A:75:ASP:H	1.63	0.47
2:B:260:THR:O	2:B:267:VAL:O	2.32	0.47
1:A:764:SER:O	1:A:805:HIS:HD2	1.98	0.47
1:A:112:ILE:HD13	2:B:317:ALA:HB1	1.96	0.47
1:A:139:LEU:HG	2:B:318:SER:CB	2.44	0.47
1:A:696:ASN:N	1:A:696:ASN:OD1	2.41	0.47
2:B:289:HIS:HB3	2:B:290:PRO:CD	2.45	0.47
4:G:20:DA:H2"	4:G:21:DG:H5"	1.91	0.47
2:B:206:SER:HB3	2:B:247:HIS:CA	2.44	0.47
1:A:244:LYS:HE2	1:A:296:THR:O	2.15	0.47
1:A:601:TYR:OH	1:A:666:LEU:CD1	2.62	0.47
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.80	0.47
1:A:846:GLY:HA3	1:A:868:GLY:O	2.16	0.47
2:B:43:GLY:C	2:B:46:ARG:N	2.68	0.46
3:F:10:DG:OP2	3:F:10:DG:H2'	2.15	0.46
1:A:679:MET:CE	1:A:691:LEU:CD1	2.93	0.46
2:B:313:ARG:NH1	2:B:326:LEU:HD11	2.30	0.46
1:A:558:ILE:CG2	1:A:569:LEU:HD11	2.45	0.46
1:A:971:ALA:HB3	1:A:973:ASN:ND2	2.29	0.46
1:A:281:PHE:HE1	1:A:304:LEU:HD13	1.71	0.46
1:A:335:LYS:HB2	1:A:335:LYS:HZ3	1.80	0.46
1:A:652:CYS:SG	1:A:676:VAL:HG12	2.55	0.46
1:A:126:PRO:HD3	1:A:169:PHE:HB3	1.95	0.46
1:A:586:ILE:HD12	1:A:608:ASP:HB3	1.97	0.46
1:A:570:LYS:CG	1:A:577:LEU:CD1	2.86	0.46
1:A:362:MET:HB2	1:A:377:THR:O	2.15	0.46
1:A:290:GLN:CG	1:A:291:MET:N	2.79	0.46
1:A:775:THR:O	1:A:776:ALA:HB3	2.15	0.46
2:B:304:LEU:HD22	2:B:351:ILE:HG12	1.96	0.46
1:A:81:THR:HG23	1:A:82:ALA:N	2.30	0.46
1:A:448:LEU:HG	1:A:484:LYS:NZ	2.30	0.46
1:A:1097:PHE:O	1:A:1100:ILE:HG22	2.16	0.46
1:A:855:ASP:N	1:A:855:ASP:OD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:HD11	1:A:604:CYS:SG	2.55	0.46
2:B:173:TYR:CD2	2:B:209:VAL:HG21	2.50	0.46
2:B:257:PHE:CD2	2:B:257:PHE:C	2.87	0.46
1:A:529:ILE:CD1	1:A:530:SER:N	2.72	0.46
1:A:739:ARG:HG3	1:A:788:VAL:CG2	2.45	0.46
1:A:290:GLN:OE1	1:A:294:THR:CB	2.63	0.46
1:A:802:LEU:HD13	1:A:853:TYR:OH	2.15	0.46
1:A:849:VAL:HG13	1:A:860:THR:HG23	1.97	0.46
1:A:845:GLN:HE21	1:A:865:GLU:CD	2.17	0.46
2:B:68:SER:O	2:B:71:ARG:HB2	2.15	0.46
2:B:57:LEU:C	2:B:59:GLY:N	2.66	0.46
1:A:365:VAL:HG12	1:A:367:LEU:CD1	2.46	0.46
2:B:261:ALA:CB	2:B:291:VAL:HG23	2.45	0.46
1:A:947:ARG:NH1	1:A:949:PHE:HD1	2.14	0.46
1:A:1065:VAL:HG12	1:A:1065:VAL:O	2.16	0.46
1:A:182:TYR:CE2	1:A:189:HIS:HB2	2.51	0.46
2:B:60:PRO:CA	2:B:63:LEU:HD12	2.15	0.46
4:G:19:DC:C4'	4:G:20:DA:OP1	2.64	0.46
1:A:432:GLN:CG	1:A:433:THR:N	2.79	0.46
1:A:190:VAL:CG1	1:A:210:GLU:HG3	2.45	0.46
1:A:871:TYR:CE1	2:B:70:VAL:HG23	2.49	0.46
1:A:546:LEU:HD11	1:A:593:MET:HB3	1.98	0.46
1:A:472:THR:CG2	1:A:473:SER:N	2.79	0.46
2:B:401:ASN:OD1	2:B:405:ASP:N	2.48	0.46
1:A:926:LEU:HD21	2:B:90:LEU:HD21	1.98	0.46
1:A:55:VAL:HG23	1:A:56:GLY:O	2.15	0.46
2:B:192:ARG:HB3	2:B:192:ARG:CZ	2.45	0.46
1:A:407:ILE:HD11	1:A:410:LEU:HD21	1.97	0.46
1:A:953:TRP:CH2	2:B:347:ARG:HG3	2.50	0.46
1:A:408:LYS:CE	1:A:678:TYR:OH	2.63	0.46
1:A:486:LEU:C	1:A:486:LEU:CD1	2.82	0.46
2:B:227:LEU:H	2:B:236:TRP:HB3	1.79	0.46
2:B:369:LEU:HD22	2:B:387:TYR:CE2	2.50	0.46
1:A:534:MET:CE	1:A:538:VAL:CG2	2.93	0.46
2:B:30:LEU:C	2:B:67:ARG:HH22	2.19	0.46
1:A:409:GLY:C	1:A:410:LEU:HD22	2.36	0.46
1:A:473:SER:O	1:A:498:ILE:N	2.47	0.46
1:A:596:PHE:CZ	1:A:649:VAL:HG23	2.51	0.46
2:B:163:LYS:HD3	2:B:163:LYS:HA	1.61	0.45
2:B:368:GLU:O	2:B:369:LEU:O	2.32	0.45
2:B:419:SER:HG	2:B:420:GLN:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:CG2	1:A:1012:LEU:HD11	2.46	0.45
2:B:119:TRP:HZ2	2:B:408:ALA:H	1.63	0.45
1:A:1129:LEU:O	1:A:1132:VAL:HG12	2.17	0.45
1:A:22:HIS:CD2	1:A:74:LYS:HE2	2.51	0.45
2:B:207:LEU:HD12	2:B:208:ASP:N	2.31	0.45
2:B:236:TRP:O	2:B:237:ASN:CB	2.64	0.45
1:A:567:ARG:NH2	1:A:579:LYS:HD2	2.31	0.45
1:A:57:MET:SD	1:A:1065:VAL:O	2.74	0.45
1:A:408:LYS:HA	1:A:678:TYR:CE2	2.51	0.45
1:A:444:GLU:CG	1:A:445:GLU:N	2.78	0.45
1:A:66:LEU:HB2	1:A:76:LEU:O	2.16	0.45
1:A:49:LEU:HD11	1:A:351:GLU:OE1	2.17	0.45
1:A:687:TYR:N	1:A:687:TYR:CD1	2.85	0.45
2:B:36:LYS:O	2:B:37:LEU:HB2	2.17	0.45
2:B:256:TRP:O	2:B:272:LEU:CB	2.58	0.45
1:A:13:THR:HB	1:A:355:ASN:HA	1.99	0.45
1:A:983:ALA:C	1:A:984:THR:OG1	2.55	0.45
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.98	0.45
2:B:236:TRP:HA	2:B:236:TRP:CE3	2.51	0.45
1:A:394:ILE:HG21	1:A:704:ILE:HD11	1.98	0.45
1:A:1018:GLY:HA3	1:A:1019:GLU:CB	2.35	0.45
1:A:516:LEU:O	1:A:531:HIS:ND1	2.44	0.45
1:A:518:TYR:HB3	1:A:529:ILE:HD11	1.99	0.45
1:A:1020:THR:HA	1:A:1021:SER:O	2.16	0.45
1:A:81:THR:CG2	1:A:82:ALA:N	2.79	0.45
1:A:411:TRP:CE2	1:A:459:PHE:HA	2.51	0.45
1:A:448:LEU:CD1	1:A:484:LYS:HE2	2.47	0.45
1:A:913:TYR:HB3	1:A:957:VAL:CG2	2.46	0.45
1:A:841:ALA:HA	2:B:68:SER:HB2	1.98	0.45
2:B:26:SER:HB3	2:B:27:PRO:CD	2.44	0.45
1:A:57:MET:HE3	1:A:79:ILE:HD12	1.99	0.45
3:F:1:DT:H72	4:G:23:DC:N4	2.32	0.45
1:A:907:ASN:O	1:A:907:ASN:CG	2.55	0.45
1:A:588:PRO:HA	1:A:606:LEU:HA	1.98	0.45
2:B:35:LYS:HD3	2:B:65:PRO:HA	1.99	0.45
1:A:147:ARG:NE	1:A:147:ARG:HA	2.31	0.45
1:A:68:ARG:NH2	1:A:72:GLU:O	2.50	0.45
1:A:824:ASP:OD1	1:A:826:ASN:HB2	2.16	0.45
1:A:947:ARG:NH1	2:B:124:PRO:HG2	2.31	0.45
2:B:383:MET:O	2:B:384:CYS:HB2	2.16	0.45
1:A:845:GLN:NE2	1:A:865:GLU:OE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PRO:C	2:B:63:LEU:CG	2.77	0.45
1:A:404:LEU:HD23	1:A:429:PHE:HZ	1.82	0.45
1:A:368:GLU:CD	1:A:391:ARG:NE	2.70	0.45
1:A:188:ARG:HD2	1:A:214:ALA:O	2.16	0.45
2:B:272:LEU:HD12	2:B:272:LEU:O	2.17	0.45
2:B:332:ARG:HH22	2:B:358:ASP:CB	2.13	0.45
2:B:132:LYS:O	2:B:158:SER:HA	2.17	0.45
1:A:374:GLN:C	1:A:1012:LEU:CD2	2.85	0.45
1:A:362:MET:HE1	1:A:1030:PHE:HA	1.99	0.45
2:B:83:TRP:N	2:B:84:PRO:HD2	2.31	0.45
1:A:402:ILE:CG2	1:A:404:LEU:HD11	2.46	0.45
1:A:127:GLU:CD	1:A:129:ARG:HH21	2.21	0.45
2:B:207:LEU:HD12	2:B:217:VAL:O	2.17	0.45
2:B:342:ALA:HB2	2:B:353:VAL:HG13	1.99	0.45
2:B:202:ILE:C	2:B:203:TRP:HE3	2.20	0.45
2:B:96:HIS:O	2:B:97:THR:HB	2.17	0.45
1:A:432:GLN:CG	1:A:433:THR:H	2.30	0.45
1:A:674:LYS:HD3	1:A:674:LYS:HA	1.57	0.45
1:A:396:ILE:HG13	1:A:397:HIS:N	2.32	0.45
2:B:217:VAL:HB	2:B:227:LEU:HD12	1.99	0.44
1:A:379:SER:HB3	1:A:721:PRO:CG	2.35	0.44
1:A:238:THR:CG2	1:A:240:HIS:CD2	3.00	0.44
2:B:345:HIS:ND1	2:B:346:PRO:HD2	2.32	0.44
1:A:72:GLU:OE2	1:A:147:ARG:NH2	2.49	0.44
1:A:129:ARG:CD	1:A:176:PRO:CG	2.67	0.44
2:B:310:SER:O	2:B:311:GLU:CB	2.65	0.44
2:B:203:TRP:N	2:B:203:TRP:CE3	2.86	0.44
1:A:57:MET:CE	1:A:79:ILE:HD11	2.47	0.44
1:A:45:THR:OG1	1:A:46:ALA:N	2.48	0.44
1:A:665:LYS:HE2	1:A:665:LYS:HB3	1.78	0.44
1:A:367:LEU:CD2	1:A:368:GLU:HG3	2.46	0.44
1:A:966:LEU:HG	1:A:1007:PHE:CE1	2.38	0.44
1:A:912:LEU:CD1	1:A:926:LEU:HD13	2.41	0.44
1:A:503:CYS:SG	1:A:508:VAL:HG22	2.57	0.44
1:A:959:ILE:O	1:A:1009:HIS:CE1	2.70	0.44
1:A:770:LEU:HD12	1:A:770:LEU:C	2.37	0.44
2:B:129:VAL:CG1	2:B:415:ILE:CD1	2.79	0.44
2:B:332:ARG:HG3	2:B:332:ARG:NH2	2.32	0.44
1:A:57:MET:CE	1:A:1065:VAL:O	2.65	0.44
2:B:334:PHE:HD2	2:B:337:LEU:H	1.65	0.44
1:A:947:ARG:HH12	2:B:403:MET:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLU:HA	1:A:863:GLU:OE1	2.18	0.44
2:B:63:LEU:N	2:B:63:LEU:CD2	2.57	0.44
3:F:19:DG:C2'	3:F:20:DC:C5'	2.77	0.44
1:A:408:LYS:HE3	1:A:678:TYR:OH	2.18	0.44
3:F:4:DC:C2'	3:F:5:DT:O5'	2.65	0.44
1:A:744:ASP:N	1:A:744:ASP:OD1	2.39	0.44
1:A:314:LEU:HD22	1:A:322:VAL:HG11	2.00	0.44
1:A:771:PHE:CB	1:A:772:SER:HA	2.48	0.44
1:A:367:LEU:CD2	1:A:368:GLU:CG	2.95	0.44
4:G:20:DA:H2'	4:G:21:DG:H8	1.81	0.44
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.52	0.44
1:A:503:CYS:CA	1:A:543:ILE:HD11	2.45	0.44
1:A:729:VAL:CG1	1:A:729:VAL:O	2.66	0.44
1:A:367:LEU:HD13	1:A:367:LEU:H	1.83	0.44
2:B:285:LEU:HD11	2:B:321:ASP:HA	1.99	0.44
2:B:117:LEU:HB3	2:B:397:LEU:HD13	1.99	0.44
1:A:608:ASP:OD2	1:A:610:ALA:CB	2.66	0.44
1:A:819:CYS:HB2	1:A:875:GLU:HG3	2.00	0.44
2:B:46:ARG:CA	2:B:46:ARG:NE	2.68	0.44
2:B:184:GLN:CB	2:B:190:ILE:HA	2.48	0.44
4:G:11:3DR:H3'	4:G:12:DC:O4'	2.18	0.44
2:B:177:MET:HG3	2:B:203:TRP:CD1	2.52	0.44
1:A:803:HIS:CD2	1:A:858:LEU:HG	2.53	0.44
1:A:700:THR:CG2	1:A:701:ILE:N	2.80	0.44
1:A:188:ARG:NH1	1:A:215:GLU:OE1	2.51	0.44
2:B:189:ASN:OD1	2:B:189:ASN:N	2.50	0.44
2:B:41:GLY:O	2:B:42:SER:OG	2.30	0.43
1:A:476:VAL:HG23	1:A:476:VAL:O	2.18	0.43
1:A:367:LEU:HD11	1:A:375:LEU:CD2	2.47	0.43
1:A:288:GLU:CG	1:A:298:LYS:HG2	2.48	0.43
2:B:239:ARG:HE	2:B:239:ARG:HB2	1.56	0.43
1:A:142:VAL:HG21	1:A:155:PHE:CE1	2.53	0.43
2:B:302:ARG:HA	2:B:315:TYR:O	2.18	0.43
3:F:18:DT:C2	3:F:19:DG:C8	3.06	0.43
4:G:19:DC:H1'	4:G:20:DA:N7	2.33	0.43
1:A:969:GLU:HG2	1:A:970:ASN:N	2.33	0.43
2:B:83:TRP:CZ3	2:B:86:VAL:HB	2.53	0.43
2:B:142:GLY:O	2:B:143:ILE:HD13	2.17	0.43
1:A:74:LYS:HG3	1:A:75:ASP:N	2.33	0.43
1:A:376:VAL:HG23	1:A:1012:LEU:CD2	2.43	0.43
1:A:1000:LEU:HD23	1:A:1000:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:CYS:SG	2:B:322:CYS:O	2.75	0.43
2:B:334:PHE:HB3	2:B:337:LEU:HB2	2.00	0.43
1:A:563:ASP:O	1:A:564:ILE:C	2.57	0.43
1:A:687:TYR:CD2	1:A:701:ILE:CG2	3.01	0.43
2:B:194:PHE:N	2:B:194:PHE:CD2	2.86	0.43
1:A:436:LEU:CG	1:A:443:VAL:HB	2.47	0.43
1:A:419:ARG:HH22	1:A:423:ASP:CG	2.17	0.43
3:F:22:DG:N2	4:G:4:DA:N1	2.65	0.43
1:A:373:GLY:O	1:A:374:GLN:CD	2.56	0.43
1:A:382:PHE:C	1:A:384:GLU:N	2.72	0.43
2:B:185:ASP:O	2:B:188:GLY:N	2.38	0.43
2:B:31:GLU:OE2	2:B:85:SER:CB	2.50	0.43
2:B:54:TRP:HD1	2:B:55:VAL:H	0.81	0.43
2:B:285:LEU:HG	2:B:315:TYR:CE1	2.54	0.43
1:A:239:TYR:CE2	1:A:297:LEU:HD22	2.54	0.43
1:A:673:LEU:HD21	1:A:693:LEU:CD2	2.48	0.43
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.43	0.43
2:B:141:PHE:O	2:B:143:ILE:HG12	2.19	0.43
1:A:652:CYS:HB3	1:A:676:VAL:O	2.18	0.43
1:A:367:LEU:HD22	1:A:367:LEU:C	2.36	0.43
2:B:113:ARG:CG	2:B:113:ARG:NH1	2.80	0.43
2:B:199:THR:HG23	2:B:200:ILE:O	2.19	0.43
1:A:534:MET:HE3	1:A:538:VAL:CG2	2.40	0.43
1:A:162:LEU:N	1:A:162:LEU:HD12	2.34	0.43
1:A:207:TRP:CZ2	1:A:228:GLY:HA2	2.53	0.43
1:A:629:VAL:HG21	1:A:668:PHE:CE2	2.54	0.43
1:A:886:SER:HB2	1:A:908:ASN:O	2.19	0.43
1:A:62:ALA:HB3	1:A:80:LEU:O	2.18	0.43
1:A:78:PHE:HE1	1:A:86:ALA:HB1	1.84	0.43
2:B:293:ALA:CB	2:B:306:THR:CG2	2.86	0.43
1:A:653:SER:O	1:A:656:PRO:HD3	2.19	0.43
1:A:305:LEU:HD13	1:A:336:LEU:HD13	2.00	0.43
1:A:841:ALA:O	2:B:68:SER:OG	2.18	0.43
1:A:809:GLN:O	1:A:809:GLN:HG3	2.18	0.43
1:A:602:LEU:O	1:A:613:TYR:HA	2.19	0.43
2:B:238:LEU:HD22	2:B:276:ARG:O	2.18	0.43
2:B:354:GLY:HA3	2:B:395:SER:O	2.19	0.43
1:A:238:THR:HG23	1:A:240:HIS:HD2	1.80	0.43
1:A:891:TYR:CD2	1:A:899:LEU:HD13	2.53	0.43
1:A:44:VAL:CG2	1:A:44:VAL:O	2.67	0.43
1:A:954:MET:CE	1:A:957:VAL:CG1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:CD1	1:A:604:CYS:SG	3.07	0.43
2:B:33:GLU:HB3	2:B:37:LEU:HD11	2.01	0.43
2:B:44:PRO:O	2:B:48:CYS:SG	2.77	0.43
2:B:62:ILE:HG12	2:B:63:LEU:H	1.83	0.43
2:B:288:ARG:C	2:B:289:HIS:CD2	2.92	0.43
1:A:178:ILE:HD11	1:A:202:PHE:HE1	1.84	0.43
1:A:281:PHE:CD1	1:A:304:LEU:CD1	3.01	0.43
1:A:305:LEU:HD13	1:A:336:LEU:CD1	2.48	0.43
1:A:263:ARG:HH11	1:A:266:PRO:HA	1.83	0.43
1:A:184:ASP:CB	1:A:185:PRO:CD	2.89	0.42
2:B:54:TRP:HE1	2:B:55:VAL:HB	1.83	0.42
2:B:190:ILE:H	2:B:190:ILE:HG13	1.62	0.42
2:B:358:ASP:OD2	2:B:360:ASN:ND2	2.52	0.42
1:A:564:ILE:HG22	1:A:564:ILE:O	2.19	0.42
1:A:464:ALA:HB2	1:A:505:SER:O	2.19	0.42
1:A:90:GLU:O	1:A:100:ILE:CD1	2.62	0.42
1:A:807:PHE:HB3	1:A:811:GLU:OE1	2.18	0.42
1:A:129:ARG:HH11	1:A:176:PRO:CG	2.11	0.42
1:A:176:PRO:CB	1:A:195:VAL:CG1	2.84	0.42
1:A:472:THR:O	1:A:498:ILE:HD12	2.20	0.42
1:A:1005:ASN:HD21	1:A:1031:GLY:C	2.22	0.42
2:B:96:HIS:O	2:B:97:THR:CB	2.66	0.42
1:A:1072:PHE:O	1:A:1075:SER:HB2	2.19	0.42
3:F:2:DG:H2'	3:F:3:DA:O4'	2.19	0.42
1:A:282:MET:HB2	1:A:305:LEU:HD11	2.01	0.42
2:B:218:THR:HG22	2:B:226:ILE:O	2.18	0.42
2:B:267:VAL:CG2	2:B:285:LEU:HD22	2.48	0.42
1:A:307:GLU:CD	1:A:383:LYS:NZ	2.71	0.42
1:A:984:THR:HB	1:A:985:THR:H	1.54	0.42
1:A:435:VAL:HB	1:A:446:THR:O	2.19	0.42
2:B:217:VAL:HG21	2:B:227:LEU:HD12	1.98	0.42
2:B:267:VAL:HG12	2:B:287:HIS:NE2	2.34	0.42
1:A:608:ASP:OD1	1:A:610:ALA:CB	2.67	0.42
1:A:537:GLU:HB2	1:A:561:TRP:CB	2.45	0.42
2:B:202:ILE:HG23	2:B:221:ASN:OD1	2.20	0.42
2:B:205:CYS:HB2	2:B:244:LYS:NZ	2.34	0.42
1:A:305:LEU:O	1:A:346:TYR:N	2.44	0.42
2:B:68:SER:O	2:B:71:ARG:CB	2.67	0.42
1:A:30:ASN:OD1	1:A:42:TYR:O	2.38	0.42
2:B:225:VAL:HG12	2:B:236:TRP:HD1	1.85	0.42
4:G:7:DA:H2''	4:G:8:DT:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HD13	1:A:534:MET:CE	2.49	0.42
1:A:1004:VAL:HG13	1:A:1030:PHE:HB2	2.00	0.42
1:A:1102:ARG:HB3	1:A:1103:PRO:CD	2.49	0.42
2:B:146:LYS:HA	2:B:147:PRO:HD3	1.71	0.42
1:A:811:GLU:OE2	1:A:847:ARG:NE	2.48	0.42
1:A:954:MET:HE1	1:A:957:VAL:CG1	2.50	0.42
1:A:897:LYS:HD2	1:A:897:LYS:HA	1.78	0.42
1:A:534:MET:HE1	1:A:558:ILE:HD12	1.90	0.42
4:G:19:DC:H4'	4:G:20:DA:OP1	2.17	0.42
1:A:468:LEU:CB	1:A:479:VAL:CG2	2.96	0.42
2:B:352:VAL:CG1	2:B:374:VAL:HG22	2.48	0.42
2:B:35:LYS:HD3	2:B:65:PRO:CA	2.50	0.42
1:A:470:GLN:O	1:A:477:ARG:HG2	2.20	0.42
2:B:224:ASN:HA	2:B:240:MET:H	1.83	0.42
2:B:251:ASN:HB3	2:B:257:PHE:CE2	2.53	0.42
2:B:306:THR:HG23	2:B:306:THR:O	2.20	0.42
1:A:1075:SER:HB3	1:A:1083:GLU:O	2.20	0.42
2:B:28:LEU:CA	2:B:30:LEU:N	2.78	0.42
2:B:47:ARG:HB2	2:B:48:CYS:C	2.40	0.42
2:B:57:LEU:CD1	2:B:58:ALA:N	2.65	0.42
2:B:32:PRO:CD	2:B:67:ARG:CZ	2.97	0.42
1:A:129:ARG:CG	1:A:130:MET:CE	2.95	0.42
1:A:375:LEU:HD21	1:A:389:ILE:HG23	2.02	0.42
1:A:157:ILE:HG13	1:A:158:ARG:CA	2.50	0.42
1:A:590:SER:OG	1:A:636:THR:O	2.31	0.42
1:A:666:LEU:N	1:A:666:LEU:HD12	2.34	0.42
1:A:596:PHE:HZ	1:A:649:VAL:CG2	2.33	0.42
2:B:345:HIS:ND1	2:B:346:PRO:CD	2.83	0.42
1:A:492:GLU:CD	1:A:494:GLN:H	2.22	0.42
1:A:74:LYS:HA	1:A:74:LYS:HD2	1.83	0.42
2:B:278:LYS:O	2:B:279:ALA:HB3	2.20	0.42
2:B:199:THR:CG2	2:B:200:ILE:H	2.32	0.42
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.81	0.42
2:B:40:LYS:HD2	2:B:40:LYS:HA	1.81	0.42
2:B:415:ILE:C	2:B:416:LEU:HD12	2.39	0.42
1:A:1000:LEU:HD22	1:A:1002:GLU:CB	2.49	0.42
1:A:815:SER:O	1:A:831:VAL:HA	2.20	0.42
1:A:983:ALA:O	1:A:984:THR:OG1	2.37	0.42
2:B:196:SER:OG	2:B:197:SER:N	2.53	0.42
1:A:22:HIS:HE1	1:A:29:LEU:HG	1.84	0.41
1:A:824:ASP:OD2	1:A:828:TYR:OH	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:SER:OG	2:B:219:GLY:HA3	2.20	0.41
2:B:330:PRO:HD3	2:B:361:PHE:CZ	2.55	0.41
2:B:244:LYS:HE2	2:B:244:LYS:HB2	1.59	0.41
1:A:190:VAL:HG13	1:A:190:VAL:O	2.19	0.41
1:A:181:VAL:HA	1:A:189:HIS:O	2.20	0.41
1:A:166:ASP:O	1:A:180:PHE:HA	2.19	0.41
2:B:290:PRO:CB	2:B:308:GLN:NE2	2.74	0.41
1:A:639:ARG:HG2	1:A:679:MET:SD	2.60	0.41
1:A:410:LEU:HB3	1:A:680:CYS:SG	2.60	0.41
1:A:455:GLN:HB2	1:A:472:THR:OG1	2.19	0.41
1:A:1005:ASN:ND2	1:A:1031:GLY:C	2.72	0.41
2:B:183:LEU:HG	2:B:191:LEU:HD13	2.02	0.41
1:A:805:HIS:ND1	1:A:851:PHE:CE2	2.88	0.41
1:A:57:MET:CE	1:A:1065:VAL:HG12	2.43	0.41
3:F:4:DC:H2"	3:F:5:DT:OP1	2.20	0.41
1:A:1100:ILE:CG2	1:A:1105:MET:HG3	2.50	0.41
1:A:497:ASN:O	1:A:512:VAL:HG23	2.20	0.41
2:B:217:VAL:CB	2:B:227:LEU:HD12	2.49	0.41
2:B:371:THR:OG1	2:B:372:ILE:N	2.52	0.41
1:A:366:ASP:CG	1:A:373:GLY:H	2.24	0.41
1:A:369:ARG:O	1:A:371:GLY:N	2.51	0.41
1:A:336:LEU:CD2	1:A:347:VAL:HG22	2.50	0.41
1:A:830:ILE:HG12	1:A:850:VAL:HG22	2.01	0.41
1:A:1116:ASP:HB3	1:A:1122:ARG:HH22	1.86	0.41
1:A:655:ARG:NH1	1:A:1015:GLN:O	2.40	0.41
2:B:54:TRP:HD1	2:B:55:VAL:HG12	0.86	0.41
1:A:111:ARG:HD3	2:B:256:TRP:CZ2	2.55	0.41
2:B:171:GLN:CB	2:B:183:LEU:HD11	2.35	0.41
2:B:309:LYS:O	2:B:331:HIS:O	2.39	0.41
2:B:334:PHE:HE2	2:B:336:HIS:ND1	2.14	0.41
2:B:365:THR:CG2	2:B:365:THR:O	2.65	0.41
1:A:382:PHE:C	1:A:384:GLU:H	2.23	0.41
1:A:2:SER:HB3	1:A:995:VAL:HG21	2.01	0.41
2:B:349:ASN:O	2:B:350:LEU:HG	2.21	0.41
3:F:8:DA:H61	4:G:17:DT:H3	1.69	0.41
1:A:425:LEU:HB2	1:A:438:LEU:HD11	2.01	0.41
1:A:22:HIS:CG	1:A:74:LYS:HE2	2.56	0.41
2:B:165:ASN:HD22	2:B:183:LEU:HD21	1.82	0.41
1:A:947:ARG:NH1	1:A:949:PHE:CD1	2.88	0.41
1:A:805:HIS:CE1	1:A:851:PHE:CE2	3.09	0.41
1:A:529:ILE:HD12	1:A:530:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HG12	1:A:454:ASP:H	1.84	0.41
1:A:677:ASN:HD22	1:A:696:ASN:N	2.19	0.41
1:A:19:VAL:CG2	1:A:64:MET:HE3	2.50	0.41
2:B:358:ASP:OD1	2:B:361:PHE:N	2.53	0.41
2:B:393:GLY:HA3	2:B:411:MET:HE3	2.01	0.41
1:A:463:VAL:CG2	1:A:469:ILE:CG2	2.99	0.41
1:A:329:GLY:HA3	1:A:384:GLU:HB3	2.02	0.41
1:A:46:ALA:O	1:A:47:GLU:C	2.59	0.41
2:B:366:PRO:HA	2:B:367:TYR:HA	1.70	0.41
1:A:867:LYS:HG3	1:A:867:LYS:O	2.21	0.41
1:A:932:LEU:HD21	1:A:979:LYS:HD3	2.02	0.41
2:B:53:LEU:CD2	2:B:54:TRP:HB2	2.19	0.41
2:B:31:GLU:HG2	2:B:81:ALA:HB1	2.02	0.41
2:B:229:ASN:O	2:B:230:MET:C	2.59	0.41
2:B:285:LEU:HA	2:B:286:PRO:HD2	1.95	0.41
1:A:560:LEU:O	1:A:564:ILE:HA	2.21	0.41
1:A:222:VAL:HG22	1:A:230:ILE:HD12	2.03	0.41
1:A:522:HIS:HB3	1:A:523:PRO:HD2	2.02	0.41
1:A:74:LYS:HZ2	1:A:75:ASP:HB2	1.85	0.41
2:B:332:ARG:HH12	2:B:358:ASP:HB3	1.83	0.41
1:A:660:TYR:CE1	1:A:707:ILE:HG22	2.55	0.41
2:B:29:GLU:O	2:B:30:LEU:CG	2.64	0.41
2:B:27:PRO:HG3	2:B:61:GLN:OE1	2.19	0.41
2:B:315:TYR:CD1	2:B:323:PRO:HB3	2.55	0.41
2:B:221:ASN:HA	2:B:244:LYS:CA	2.51	0.41
2:B:203:TRP:HZ2	4:G:13:DA:OP2	2.04	0.41
1:A:464:ALA:N	1:A:505:SER:O	2.54	0.41
1:A:567:ARG:HA	1:A:578:HIS:O	2.21	0.41
1:A:573:SER:O	1:A:574:PHE:HB2	2.20	0.41
1:A:1016:ASN:CB	1:A:1017:LEU:C	2.86	0.41
1:A:385:GLY:HA3	1:A:719:GLU:O	2.21	0.41
1:A:207:TRP:HZ2	1:A:241:ASN:OD1	2.03	0.41
1:A:479:VAL:O	1:A:479:VAL:HG23	2.21	0.41
2:B:239:ARG:NH1	3:F:6:DG:OP2	2.31	0.41
2:B:69:ILE:O	2:B:70:VAL:CB	2.69	0.41
1:A:236:SER:HA	1:A:249:ALA:HA	2.02	0.41
1:A:1097:PHE:CZ	1:A:1105:MET:HG2	2.56	0.41
1:A:361:ASP:OD2	1:A:724:ILE:N	2.39	0.41
1:A:932:LEU:HD21	1:A:979:LYS:CD	2.51	0.41
2:B:259:ALA:HB3	2:B:296:PHE:CE1	2.56	0.41
1:A:18:CYS:HB2	1:A:313:CYS:HB2	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:CD1	1:A:770:LEU:C	2.89	0.41
1:A:437:MET:O	1:A:443:VAL:HA	2.21	0.41
4:G:6:DC:N4	4:G:7:DA:N6	2.68	0.41
1:A:589:ARG:CD	1:A:589:ARG:C	2.89	0.41
1:A:296:THR:O	1:A:297:LEU:CB	2.68	0.41
2:B:83:TRP:CE3	2:B:86:VAL:HB	2.55	0.41
1:A:929:SER:HB3	1:A:930:VAL:H	1.60	0.41
2:B:143:ILE:HG22	2:B:144:LYS:C	2.42	0.41
1:A:869:ALA:O	1:A:884:ILE:HA	2.20	0.41
1:A:1050:LEU:HD13	1:A:1050:LEU:C	2.40	0.41
1:A:174:GLN:HG3	1:A:175:ALA:N	2.36	0.41
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.56	0.40
1:A:472:THR:HB	1:A:477:ARG:HH12	1.85	0.40
1:A:608:ASP:OD2	1:A:610:ALA:HB3	2.21	0.40
2:B:123:HIS:HA	2:B:124:PRO:HD3	1.65	0.40
1:A:529:ILE:HD12	1:A:530:SER:CA	2.50	0.40
1:A:249:ALA:O	1:A:254:LYS:NZ	2.53	0.40
2:B:290:PRO:O	2:B:308:GLN:CG	2.49	0.40
3:F:13:DG:H2''	3:F:14:DA:O4'	2.21	0.40
1:A:32:LEU:HA	1:A:40:GLU:O	2.21	0.40
1:A:1024:THR:HG22	1:A:1043:LEU:CD2	2.45	0.40
1:A:1089:ILE:HA	1:A:1089:ILE:HD13	1.81	0.40
1:A:874:VAL:HG13	1:A:881:LEU:HB3	2.03	0.40
1:A:817:VAL:HG12	1:A:818:SER:N	2.36	0.40
2:B:167:LEU:CD1	2:B:167:LEU:N	2.84	0.40
1:A:159:LEU:HD22	1:A:161:GLU:O	2.21	0.40
1:A:715:VAL:HG23	1:A:715:VAL:O	2.22	0.40
2:B:240:MET:CE	2:B:270:TRP:CZ2	3.04	0.40
2:B:245:VAL:HG12	2:B:260:THR:OG1	2.22	0.40
2:B:307:ASP:OD1	2:B:311:GLU:HB2	2.20	0.40
2:B:356:TYR:HD1	2:B:394:ILE:HG12	1.85	0.40
1:A:463:VAL:HG13	1:A:505:SER:O	2.21	0.40
1:A:298:LYS:HD3	1:A:298:LYS:HA	1.80	0.40
1:A:305:LEU:O	1:A:346:TYR:HB2	2.22	0.40
1:A:262:ASN:HB2	1:A:314:LEU:O	2.22	0.40
1:A:6:VAL:CG2	1:A:1088:PHE:HD1	2.35	0.40
1:A:438:LEU:CD2	1:A:443:VAL:HG12	2.48	0.40
2:B:225:VAL:HG12	2:B:236:TRP:CD1	2.56	0.40
2:B:332:ARG:NH1	2:B:358:ASP:CB	2.84	0.40
2:B:120:HIS:HD2	2:B:122:THR:H	1.70	0.40
1:A:529:ILE:HD13	1:A:572:PRO:HB3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:MET:HE2	1:A:957:VAL:HG12	2.03	0.40
1:A:258:ILE:HD13	1:A:273:LEU:HD13	2.03	0.40
2:B:289:HIS:HB3	2:B:290:PRO:HD2	2.02	0.40
1:A:378:CYS:O	1:A:387:LEU:HA	2.22	0.40
4:G:9:DC:H2"	4:G:10:DG:H5"	2.04	0.40
1:A:343:GLN:N	1:A:343:GLN:CD	2.68	0.40
1:A:687:TYR:CD2	1:A:701:ILE:HG22	2.57	0.40
1:A:861:VAL:CG2	1:A:862:ALA:N	2.85	0.40
1:A:724:ILE:HA	1:A:734:GLY:O	2.21	0.40
1:A:316:TYR:HD1	1:A:322:VAL:HG22	1.86	0.40

All (3) 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)
2:B:42:SER:OG	2:B:187:LYS:O[1_565]	1.68	0.52
1:A:514:ARG:NH2	1:A:855:ASP:O[2_646]	1.98	0.22
1:A:243:ASP:OD2	2:B:233:LYS:NZ[1_565]	1.98	0.22

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1138/1150 (99%)	1055 (93%)	74 (6%)	9 (1%)	24	56
2	B	400/435 (92%)	335 (84%)	60 (15%)	5 (1%)	15	42
All	All	1538/1585 (97%)	1390 (90%)	134 (9%)	14 (1%)	21	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	44	PRO

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Mol	Chain	Res	Type
2	B	70	VAL
2	B	200	ILE
2	B	64	PRO
1	A	298	LYS
1	A	1109	VAL
2	B	369	LEU
1	A	36	ASN
1	A	370	GLN
1	A	564	ILE
1	A	529	ILE
1	A	1065	VAL
1	A	108	VAL
1	A	225	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	976/1009 (97%)	895 (92%)	81 (8%)	14	36
2	B	347/379 (92%)	283 (82%)	64 (18%)	2	5
All	All	1323/1388 (95%)	1178 (89%)	145 (11%)	8	21

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	54	GLU
1	A	55	VAL
1	A	81	THR
1	A	99	ASP
1	A	142	VAL
1	A	147	ARG
1	A	148	ASP
1	A	149	ASN
1	A	157	ILE

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	167	VAL
1	A	212	VAL
1	A	235	GLU
1	A	237	ILE
1	A	257	THR
1	A	259	VAL
1	A	296	THR
1	A	300	LEU
1	A	302	VAL
1	A	334	VAL
1	A	339	ASP
1	A	343	GLN
1	A	367	LEU
1	A	378	CYS
1	A	407	ILE
1	A	427	LEU
1	A	449	MET
1	A	457	THR
1	A	468	LEU
1	A	472	THR
1	A	512	VAL
1	A	516	LEU
1	A	531	HIS
1	A	549	SER
1	A	550	ASN
1	A	552	LEU
1	A	555	LEU
1	A	560	LEU
1	A	567	ARG
1	A	569	LEU
1	A	573	SER
1	A	576	LEU
1	A	589	ARG
1	A	590	SER
1	A	599	SER
1	A	631	LEU
1	A	666	LEU
1	A	670	ASN
1	A	682	LEU
1	A	685	ASP
1	A	696	ASN

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Mol	Chain	Res	Type
1	A	744	ASP
1	A	757	SER
1	A	763	SER
1	A	768	SER
1	A	770	LEU
1	A	780	THR
1	A	786	VAL
1	A	802	LEU
1	A	839	GLU
1	A	844	LYS
1	A	855	ASP
1	A	858	LEU
1	A	861	VAL
1	A	887	THR
1	A	899	LEU
1	A	901	THR
1	A	904	ASN
1	A	907	ASN
1	A	916	THR
1	A	961	ASP
1	A	966	LEU
1	A	984	THR
1	A	989	ARG
1	A	1005	ASN
1	A	1029	LEU
1	A	1063	LYS
1	A	1086	THR
1	A	1123	GLU
1	A	1129	LEU
2	B	23	ARG
2	B	24	SER
2	B	26	SER
2	B	28	LEU
2	B	30	LEU
2	B	46	ARG
2	B	53	LEU
2	B	55	VAL
2	B	57	LEU
2	B	61	GLN
2	B	63	LEU
2	B	70	VAL
2	B	91	GLN

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Mol	Chain	Res	Type
2	B	93	SER
2	B	97	THR
2	B	100	SER
2	B	101	TYR
2	B	105	GLN
2	B	110	PHE
2	B	143	ILE
2	B	151	LYS
2	B	153	ILE
2	B	159	ILE
2	B	176	SER
2	B	183	LEU
2	B	194	PHE
2	B	222	VAL
2	B	228	LEU
2	B	231	ASP
2	B	234	GLU
2	B	236	TRP
2	B	242	LYS
2	B	243	LYS
2	B	244	LYS
2	B	245	VAL
2	B	248	VAL
2	B	256	TRP
2	B	257	PHE
2	B	260	THR
2	B	271	ASP
2	B	272	LEU
2	B	273	ARG
2	B	282	LEU
2	B	285	LEU
2	B	291	VAL
2	B	299	ASP
2	B	307	ASP
2	B	311	GLU
2	B	312	ILE
2	B	318	SER
2	B	353	VAL
2	B	360	ASN
2	B	370	ARG
2	B	371	THR
2	B	373	ASP

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Mol	Chain	Res	Type
2	B	378	ASN
2	B	379	SER
2	B	381	LYS
2	B	390	GLU
2	B	391	SER
2	B	394	ILE
2	B	409	SER
2	B	411	MET
2	B	419	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	30	ASN
1	A	203	ASN
1	A	209	GLN
1	A	507	GLN
1	A	522	HIS
1	A	677	ASN
1	A	727	GLN
1	A	790	ASN
1	A	805	HIS
1	A	810	ASN
1	A	907	ASN
1	A	908	ASN
1	A	999	HIS
1	A	1015	GLN
2	B	120	HIS
2	B	247	HIS
2	B	289	HIS
2	B	349	ASN
2	B	360	ASN
2	B	398	ASN
2	B	420	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	3DR	G	11	4	7,11,12	3.33	2 (28%)	8,14,17	1.05	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3DR	G	11	4	-	0/3/15/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	11	3DR	C2'-C3'	-7.70	1.39	1.52
4	G	11	3DR	O4'-C4'	-3.28	1.38	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	11	3DR	O5'-C5'-C4'	2.23	117.30	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	11	3DR	5	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1140/1150 (99%)	-0.89	1 (0%) 95 95	2, 36, 59, 90	0
2	B	402/435 (92%)	-0.71	8 (1%) 68 64	6, 37, 66, 115	0
3	F	24/24 (100%)	-0.92	0 100 100	34, 47, 56, 58	0
4	G	23/24 (95%)	-0.96	0 100 100	26, 45, 53, 56	0
All	All	1589/1633 (97%)	-0.85	9 (0%) 90 89	2, 36, 61, 115	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	32	PRO	3.6
2	B	52	CYS	3.2
2	B	62	ILE	3.2
2	B	66	CYS	2.9
2	B	47	ARG	2.9
2	B	61	GLN	2.7
1	A	1119	GLY	2.5
2	B	60	PRO	2.4
2	B	59	GLY	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	3DR	G	11	11/12	0.91	0.17	-	31,33,39,40	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.