



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:33 PM GMT

PDB ID : 1G4A  
Title : CRYSTAL STRUCTURES OF THE HSLVU PEPTIDASE-ATPASE COMPLEX REVEAL AN ATP-DEPENDENT PROTEOLYSIS MECHANISM  
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Deposited on : 2000-10-26  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

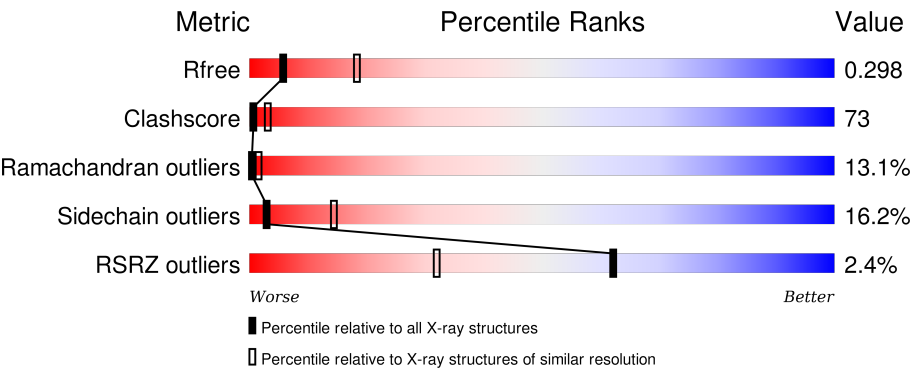
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	E	443	<div><div></div><div><div>21%</div><div>44%</div><div>14%</div><div>•</div><div>20%</div></div></div>
1	F	443	<div><div>2%</div><div><div>20%</div><div>48%</div><div>11%</div><div>•</div><div>20%</div></div></div>
2	A	175	<div><div>5%</div><div><div>19%</div><div>54%</div><div>25%</div><div>••</div></div></div>
2	B	175	<div><div></div><div><div>11%</div><div>58%</div><div>27%</div><div>••</div></div></div>
2	C	175	<div><div>3%</div><div><div>18%</div><div>58%</div><div>21%</div><div>••</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	175	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>18%</div><div>62%</div><div>17%</div><div>..</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

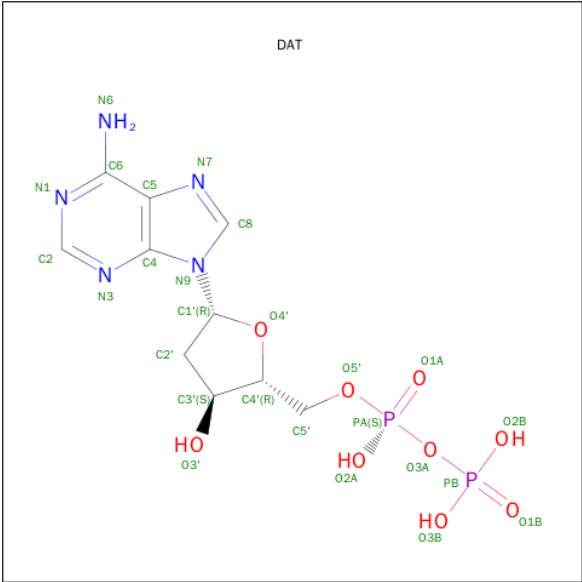
- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	356	Total	C	N	O	S	0	0	0
			2796	1747	492	546	11			
1	F	356	Total	C	N	O	S	0	0	0
			2796	1747	492	546	11			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	A	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	D	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	C	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			

- Molecule 3 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (three-letter code: DAT) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>9</sub>P<sub>2</sub>).

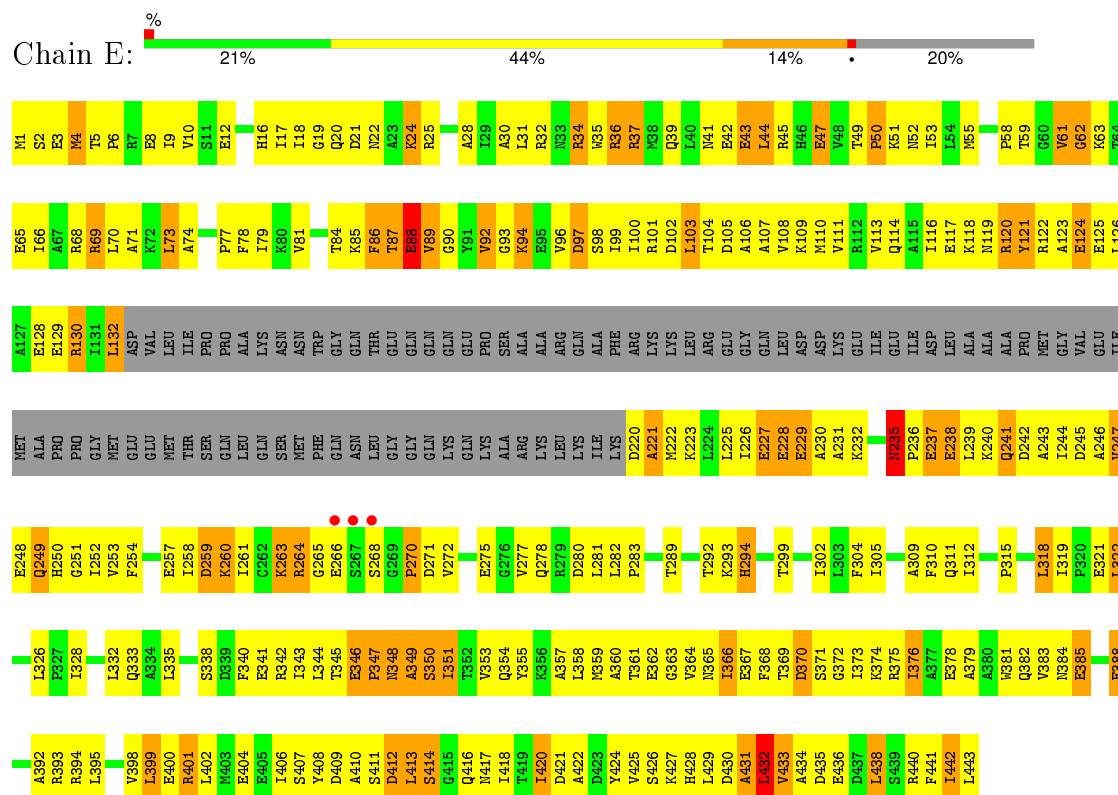


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
3	F	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

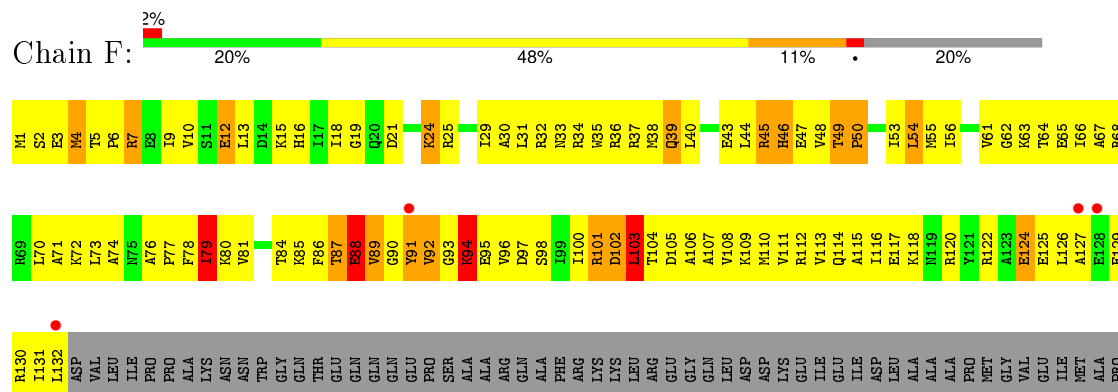
### 3 Residue-property plots

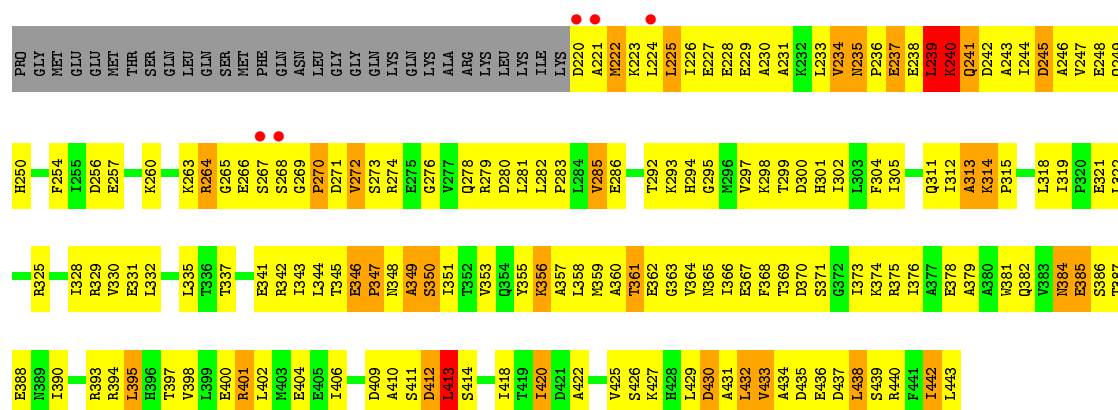
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

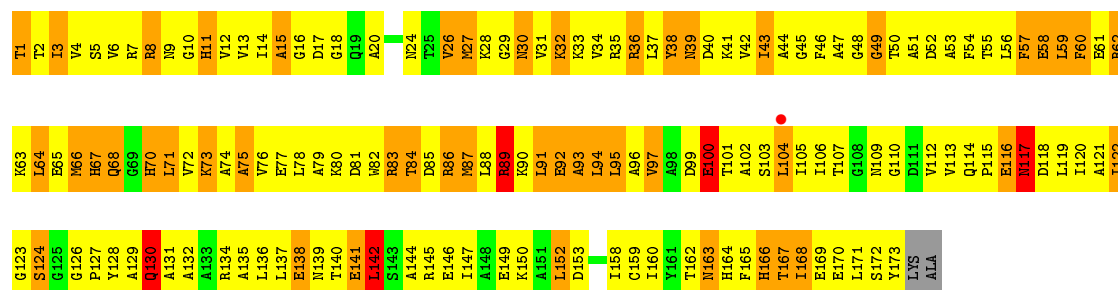
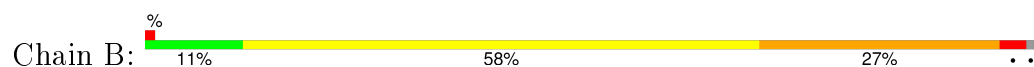


#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

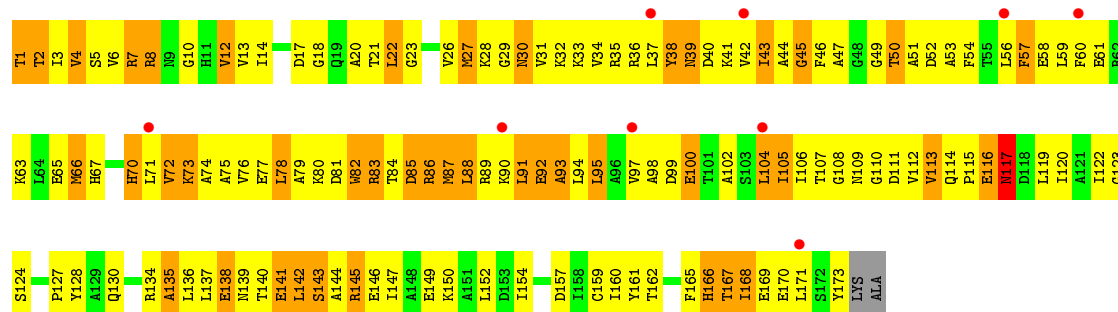
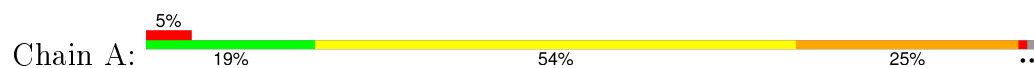




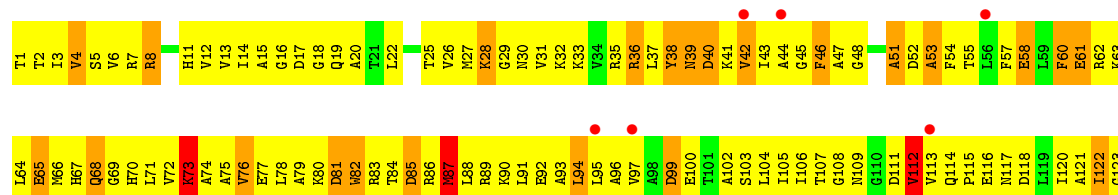
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

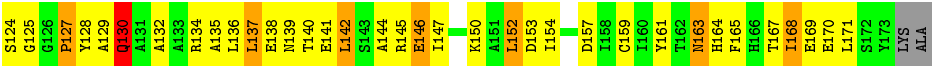
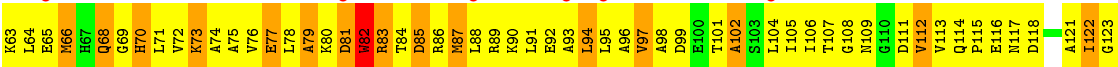
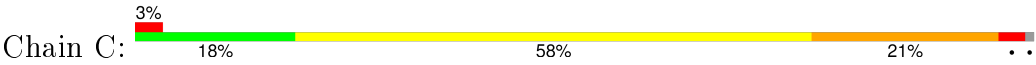


• Molecule 2: ATP-DEPENDENT PROTEASE HSLV





● Molecule 2: ATP-DEPENDENT PROTEASE HSLV





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.00Å 170.00Å 161.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	85.00 – 3.00 85.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	85.7 (85.00-3.00) 85.7 (85.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.257 , 0.294 0.263 , 0.298	Depositor DCC
$R_{free}$ test set	4647 reflections (11.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 14.9	EDS
Estimated twinning fraction	0.426 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 46550 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	10920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.30% 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: DAT

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	E	0.47	0/2829	0.76	0/3816
1	F	0.47	0/2829	0.75	0/3816
2	A	0.43	0/1336	0.76	0/1806
2	B	0.45	0/1336	0.77	1/1806 (0.1%)
2	C	0.44	0/1336	0.78	1/1806 (0.1%)
2	D	0.43	0/1336	0.74	0/1806
All	All	0.46	0/11002	0.76	2/14856 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	22	LEU	CA-CB-CG	6.38	129.96	115.30
2	B	117	ASN	N-CA-C	-5.55	96.01	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2796	0	2848	348	0
1	F	2796	0	2848	387	0
2	A	1319	0	1335	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1319	0	1335	270	0
2	C	1319	0	1335	216	0
2	D	1319	0	1335	231	0
3	E	26	0	12	3	0
3	F	26	0	12	1	0
All	All	10920	0	11060	1594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 73.

All (1594) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:THR:HG22	1:F:388:GLU:H	1.12	1.12
1:E:130:ARG:HH11	1:E:130:ARG:HB2	1.09	1.11
2:C:41:LYS:NZ	2:C:41:LYS:H	1.49	1.09
2:B:115:PRO:HD2	2:B:120:ILE:HD11	1.31	1.07
2:C:82:TRP:HE1	2:C:108:GLY:HA2	1.20	1.07
2:B:44:ALA:HB2	2:B:97:VAL:HA	1.32	1.06
2:D:8:ARG:HB3	2:D:144:ALA:HB2	1.37	1.05
1:E:104:THR:HA	1:E:247:VAL:HG21	1.33	1.04
2:C:81:ASP:HB3	2:C:87:MET:SD	1.98	1.04
2:A:91:LEU:H	2:A:91:LEU:HD22	1.21	1.04
1:E:103:LEU:HG	1:E:247:VAL:HG13	1.40	1.03
2:C:63:LYS:HD2	2:C:78:LEU:HG	1.42	1.01
1:E:128:GLU:HG2	1:E:132:LEU:HD11	1.39	0.99
1:F:374:LYS:HE2	1:F:378:GLU:OE2	1.60	0.99
2:D:63:LYS:HG3	2:D:78:LEU:HG	1.44	0.99
1:E:223:LYS:HD2	1:E:226:ILE:HG13	1.45	0.97
1:E:383:VAL:HB	1:E:394:ARG:HD3	1.47	0.97
2:B:96:ALA:O	2:B:97:VAL:HG23	1.64	0.96
2:D:70:HIS:HB3	2:D:73:LYS:HD2	1.45	0.96
2:A:115:PRO:HD2	2:A:120:ILE:HD11	1.46	0.96
2:A:36:ARG:HA	2:A:44:ALA:H	1.30	0.96
2:D:28:LYS:HD2	2:D:31:VAL:HG22	1.46	0.95
2:C:41:LYS:N	2:C:41:LYS:HZ3	1.63	0.95
1:F:351:ILE:H	1:F:351:ILE:HD12	1.30	0.95
2:B:140:THR:HB	2:B:142:LEU:HD11	1.47	0.95
2:C:71:LEU:HB2	2:C:99:ASP:OD1	1.66	0.95
2:A:116:GLU:O	2:A:117:ASN:HB2	1.65	0.95
2:B:163:ASN:ND2	2:B:165:PHE:H	1.66	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HZ3	2:B:32:LYS:HB2	1.30	0.93
1:F:115:ALA:HA	1:F:118:LYS:HB2	1.51	0.92
1:F:79:ILE:HG21	1:F:103:LEU:HB2	1.51	0.92
2:D:47:ALA:HB3	2:D:94:LEU:HD13	1.51	0.92
1:E:130:ARG:HB2	1:E:130:ARG:NH1	1.84	0.92
1:E:432:LEU:HD11	1:E:442:ILE:HD11	1.51	0.92
2:C:44:ALA:HB2	2:C:97:VAL:HG13	1.49	0.91
2:B:7:ARG:HH12	2:B:102:ALA:N	1.69	0.91
2:A:22:LEU:HD23	2:A:23:GLY:H	1.35	0.90
2:D:32:LYS:HD2	2:D:167:THR:HG21	1.54	0.89
1:F:375:ARG:HG2	1:F:375:ARG:HH11	1.35	0.88
1:F:438:LEU:HD22	1:F:442:ILE:HD12	1.54	0.88
2:B:28:LYS:HG2	2:B:30:ASN:H	1.38	0.88
2:A:2:THR:OG1	2:A:162:THR:HG21	1.73	0.88
2:C:86:ARG:HA	2:C:89:ARG:HD2	1.55	0.88
2:C:36:ARG:HG2	2:C:38:TYR:H	1.38	0.88
2:B:13:VAL:HB	2:B:170:GLU:HG3	1.53	0.87
2:D:37:LEU:HD22	2:D:61:GLU:HB2	1.54	0.87
2:B:75:ALA:HB1	2:B:112:VAL:HG21	1.58	0.86
1:F:240:LYS:HG3	1:F:241:GLN:H	1.38	0.85
2:B:2:THR:OG1	2:B:162:THR:HG21	1.75	0.85
2:A:75:ALA:HB1	2:A:112:VAL:HG21	1.56	0.85
1:F:387:THR:HG22	1:F:388:GLU:N	1.90	0.85
1:E:249:GLN:HG2	1:E:250:HIS:N	1.92	0.85
1:F:220:ASP:N	1:F:224:LEU:H	1.74	0.84
1:E:220:ASP:OD1	1:E:222:MET:HG3	1.77	0.84
1:F:382:GLN:HG2	1:F:433:VAL:CG2	2.08	0.83
1:F:34:ARG:HG3	1:F:35:TRP:H	1.43	0.83
2:A:79:ALA:HB2	2:A:112:VAL:HG23	1.60	0.83
2:C:122:ILE:H	2:C:122:ILE:HD13	1.42	0.83
2:D:83:ARG:HD2	2:D:89:ARG:HD2	1.61	0.83
2:C:83:ARG:HA	2:C:83:ARG:HH11	1.43	0.83
2:D:60:PHE:HA	2:D:78:LEU:HD11	1.61	0.82
2:C:63:LYS:HA	2:C:66:MET:SD	2.19	0.82
2:B:116:GLU:O	2:B:117:ASN:HB2	1.76	0.82
2:D:73:LYS:HE2	2:D:73:LYS:H	1.44	0.82
1:F:102:ASP:C	1:F:104:THR:H	1.79	0.82
2:D:103:SER:HB3	2:D:120:ILE:HD11	1.61	0.82
2:D:106:ILE:HG22	2:D:108:GLY:H	1.45	0.82
1:F:55:MET:HE1	1:F:66:ILE:HD12	1.62	0.82
2:C:163:ASN:C	2:C:163:ASN:HD22	1.82	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:H	2:A:111:ASP:HB3	1.42	0.81
2:C:5:SER:HB2	2:C:14:ILE:HG12	1.60	0.81
2:C:82:TRP:HE1	2:C:108:GLY:CA	1.93	0.81
2:B:32:LYS:HB2	2:B:32:LYS:NZ	1.94	0.81
1:F:21:ASP:O	1:F:25:ARG:HG3	1.80	0.81
2:B:89:ARG:HB3	2:B:89:ARG:HH11	1.45	0.81
2:A:149:GLU:OE2	2:A:168:ILE:HD13	1.81	0.81
2:D:83:ARG:HA	2:D:89:ARG:HD2	1.63	0.81
2:C:70:HIS:CG	2:C:73:LYS:HB2	2.16	0.81
1:E:20:GLN:HE22	1:E:333:GLN:H	1.25	0.81
1:E:69:ARG:HH11	1:E:69:ARG:HG3	1.46	0.80
1:E:106:ALA:O	1:E:110:MET:HB2	1.80	0.80
1:F:413:LEU:HD13	1:F:418:ILE:HD11	1.62	0.80
2:B:13:VAL:HG21	2:B:168:ILE:HG22	1.63	0.80
1:F:31:LEU:HD22	1:F:70:LEU:HD11	1.62	0.80
2:C:39:ASN:N	2:C:39:ASN:HD22	1.80	0.80
2:C:74:ALA:O	2:C:78:LEU:HB2	1.82	0.80
1:F:103:LEU:HD13	1:F:103:LEU:O	1.81	0.80
2:B:60:PHE:CZ	2:B:64:LEU:HA	2.17	0.80
1:F:34:ARG:HG3	1:F:35:TRP:N	1.97	0.80
2:D:71:LEU:HD12	2:D:99:ASP:HB2	1.63	0.79
1:F:34:ARG:NH1	1:F:250:HIS:HB3	1.95	0.79
2:B:89:ARG:HB3	2:B:89:ARG:NH1	1.97	0.79
2:D:37:LEU:O	2:D:39:ASN:N	2.14	0.79
2:A:145:ARG:O	2:A:149:GLU:HG3	1.82	0.79
2:B:159:CYS:SG	2:B:162:THR:HG23	2.22	0.79
1:F:45:ARG:HE	1:F:46:HIS:HD2	1.31	0.79
2:D:37:LEU:HD21	2:D:57:PHE:O	1.83	0.78
1:F:3:GLU:O	1:F:4:MET:HG2	1.83	0.78
1:E:96:VAL:HG21	1:E:280:ASP:O	1.83	0.78
1:F:382:GLN:HG2	1:F:433:VAL:HG23	1.65	0.78
2:A:43:ILE:HG13	2:A:171:LEU:HB2	1.65	0.78
2:A:82:TRP:HZ3	2:A:89:ARG:HA	1.48	0.78
2:A:34:VAL:HA	2:A:45:GLY:HA2	1.64	0.78
2:D:152:LEU:HD13	2:D:166:HIS:HD2	1.49	0.78
2:B:4:VAL:HG22	2:B:121:ALA:HB1	1.65	0.78
1:F:220:ASP:N	1:F:223:LYS:HB3	1.99	0.78
1:F:358:LEU:O	1:F:361:THR:HG22	1.83	0.77
2:A:91:LEU:H	2:A:91:LEU:CD2	1.96	0.77
1:F:32:ARG:HG3	1:F:36:ARG:HD3	1.65	0.77
1:F:34:ARG:HH22	1:F:74:ALA:HB1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:VAL:HG23	2:D:15:ALA:HB3	1.65	0.77
1:E:235:ASN:H	1:E:236:PRO:HD3	1.47	0.77
2:B:90:LYS:HB3	2:A:83:ARG:HH21	1.49	0.77
2:C:36:ARG:HG2	2:C:37:LEU:H	1.50	0.77
2:B:88:LEU:H	2:B:88:LEU:HD23	1.49	0.77
2:D:88:LEU:HD22	2:C:84:THR:HB	1.65	0.77
1:E:20:GLN:HA	1:E:20:GLN:HE21	1.49	0.77
1:F:45:ARG:HH11	1:F:45:ARG:HG3	1.49	0.77
2:A:136:LEU:HD13	2:D:135:ALA:HB1	1.66	0.77
2:C:90:LYS:O	2:C:91:LEU:HD13	1.83	0.77
2:A:91:LEU:HD22	2:A:91:LEU:N	1.98	0.76
1:F:34:ARG:NH2	1:F:74:ALA:HB1	2.00	0.76
2:D:44:ALA:HB2	2:D:97:VAL:HG12	1.66	0.76
1:E:258:ILE:O	1:E:261:ILE:HB	1.84	0.76
1:F:9:ILE:HD13	1:F:31:LEU:HD23	1.67	0.76
1:F:55:MET:CE	1:F:63:LYS:HA	2.15	0.76
2:A:75:ALA:HB1	2:A:112:VAL:CG2	2.16	0.76
2:D:13:VAL:HG21	2:D:145:ARG:HA	1.68	0.76
1:E:362:GLU:OE1	1:F:36:ARG:HD2	1.84	0.76
2:C:71:LEU:O	2:C:74:ALA:HB3	1.86	0.76
1:F:108:VAL:HA	1:F:111:VAL:HG23	1.68	0.76
2:C:53:ALA:O	2:C:55:THR:N	2.19	0.75
2:A:38:TYR:C	2:A:40:ASP:H	1.88	0.75
2:C:41:LYS:N	2:C:41:LYS:NZ	2.29	0.75
1:F:351:ILE:N	1:F:351:ILE:HD12	2.02	0.75
2:B:163:ASN:C	2:B:163:ASN:HD22	1.90	0.75
2:C:17:ASP:O	2:C:33:LYS:HG3	1.87	0.75
2:A:28:LYS:HG2	2:A:29:GLY:N	2.01	0.75
1:E:77:PRO:HB3	1:E:107:ALA:HB2	1.69	0.75
1:E:442:ILE:HA	1:F:329:ARG:HG3	1.68	0.75
1:F:96:VAL:HG21	1:F:280:ASP:O	1.87	0.74
2:C:39:ASN:H	2:C:39:ASN:HD22	1.33	0.74
2:A:105:ILE:HG23	2:A:113:VAL:HG13	1.69	0.74
2:B:90:LYS:HE3	2:A:83:ARG:HH21	1.49	0.74
1:F:222:MET:HA	1:F:226:ILE:HG23	1.69	0.74
1:E:263:LYS:C	1:E:263:LYS:HD3	2.07	0.74
2:D:86:ARG:HA	2:D:86:ARG:HE	1.52	0.74
2:A:58:GLU:O	2:A:61:GLU:HB3	1.87	0.74
2:D:14:ILE:HD12	2:D:43:ILE:HG22	1.69	0.74
1:F:235:ASN:O	1:F:239:LEU:HG	1.87	0.74
1:F:387:THR:HG23	1:F:440:ARG:CZ	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:SER:HA	2:D:13:VAL:O	1.87	0.74
2:A:20:ALA:HB2	2:A:31:VAL:HG21	1.68	0.74
1:E:1:MET:C	1:E:3:GLU:H	1.91	0.74
2:B:76:VAL:O	2:B:80:LYS:HG2	1.88	0.74
1:E:21:ASP:O	1:E:25:ARG:HG3	1.88	0.74
2:B:80:LYS:C	2:B:82:TRP:H	1.90	0.74
2:C:134:ARG:O	2:C:138:GLU:HG2	1.87	0.74
1:E:109:LYS:HD3	1:E:109:LYS:O	1.88	0.73
1:F:19:GLY:O	1:F:24:LYS:NZ	2.22	0.73
1:F:240:LYS:CG	1:F:241:GLN:H	2.00	0.73
2:A:12:VAL:HG13	2:A:171:LEU:HB3	1.70	0.73
2:D:7:ARG:HG3	2:D:12:VAL:HG22	1.70	0.73
2:C:57:PHE:O	2:C:60:PHE:HB2	1.89	0.73
2:B:70:HIS:O	2:B:74:ALA:HB3	1.89	0.73
1:E:9:ILE:HD13	1:E:31:LEU:HD23	1.70	0.73
2:C:1:THR:HA	2:C:17:ASP:OD1	1.89	0.72
1:E:123:ALA:HB1	1:E:229:GLU:HG3	1.71	0.72
2:A:1:THR:HB	2:A:162:THR:HG22	1.70	0.72
2:B:7:ARG:HG3	2:B:12:VAL:HG22	1.71	0.72
2:A:100:GLU:H	2:A:100:GLU:CD	1.92	0.72
1:F:21:ASP:OD1	1:F:25:ARG:HD2	1.89	0.72
2:B:64:LEU:H	2:B:64:LEU:HD12	1.52	0.72
2:A:82:TRP:CE2	2:A:108:GLY:HA3	2.25	0.72
2:C:21:THR:HG21	2:C:161:TYR:HD2	1.54	0.72
2:D:63:LYS:HA	2:D:66:MET:SD	2.29	0.72
1:F:413:LEU:HD23	1:F:413:LEU:H	1.53	0.72
2:C:63:LYS:CD	2:C:78:LEU:HG	2.19	0.72
2:D:136:LEU:C	2:D:138:GLU:H	1.93	0.72
1:E:235:ASN:H	1:E:236:PRO:CD	2.03	0.71
2:C:86:ARG:O	2:C:87:MET:HG2	1.90	0.71
2:B:34:VAL:HA	2:B:45:GLY:HA2	1.71	0.71
1:F:53:ILE:N	1:F:53:ILE:HD12	2.05	0.71
2:C:123:GLY:C	2:C:125:GLY:H	1.94	0.71
2:D:52:ASP:O	2:D:54:PHE:N	2.23	0.71
1:F:5:THR:HG22	1:F:32:ARG:NH2	2.05	0.71
2:A:18:GLY:O	2:A:31:VAL:HG23	1.90	0.71
1:E:61:VAL:HG23	1:E:62:GLY:H	1.53	0.71
2:A:28:LYS:HD3	2:A:30:ASN:OD1	1.91	0.71
1:E:244:ILE:HD12	1:E:248:GLU:OE2	1.91	0.71
2:C:42:VAL:HA	2:C:98:ALA:O	1.90	0.71
2:B:13:VAL:HG11	2:B:145:ARG:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:28:LYS:HG2	2:A:29:GLY:H	1.56	0.71
1:E:372:GLY:O	1:E:376:ILE:HG12	1.89	0.71
2:B:158:ILE:HD11	2:C:127:PRO:HB3	1.73	0.71
2:C:41:LYS:H	2:C:41:LYS:HZ3	0.77	0.71
1:F:61:VAL:HG12	1:F:335:LEU:HD13	1.73	0.71
1:E:102:ASP:C	1:E:104:THR:H	1.95	0.70
1:E:432:LEU:HB3	1:E:443:LEU:HD11	1.72	0.70
2:B:90:LYS:HE3	2:A:83:ARG:NH2	2.04	0.70
1:E:104:THR:O	1:E:108:VAL:HG23	1.90	0.70
2:B:140:THR:CB	2:B:142:LEU:HD11	2.22	0.70
2:B:1:THR:HB	2:B:33:LYS:HE3	1.72	0.70
1:E:260:LYS:HA	1:E:260:LYS:HE2	1.74	0.70
1:E:375:ARG:HA	1:E:378:GLU:OE1	1.91	0.70
2:C:35:ARG:NH1	2:C:37:LEU:HA	2.07	0.70
2:B:88:LEU:HG	2:B:89:ARG:HG2	1.73	0.70
2:D:28:LYS:CD	2:D:31:VAL:HG22	2.19	0.70
2:B:36:ARG:NH1	2:B:40:ASP:OD2	2.25	0.70
2:A:38:TYR:HB3	2:A:42:VAL:HG21	1.73	0.70
2:A:119:LEU:C	2:A:120:ILE:HD12	2.12	0.70
2:A:80:LYS:C	2:A:82:TRP:H	1.95	0.70
2:B:13:VAL:CG2	2:B:168:ILE:HG22	2.22	0.70
2:B:160:ILE:HD11	2:D:19:GLN:NE2	2.07	0.70
1:E:412:ASP:O	1:E:414:SER:N	2.24	0.70
2:D:8:ARG:HB3	2:D:144:ALA:CB	2.19	0.69
1:F:45:ARG:HE	1:F:46:HIS:CD2	2.10	0.69
2:C:62:ARG:O	2:C:65:GLU:HB2	1.92	0.69
2:C:15:ALA:HA	2:C:168:ILE:HG23	1.74	0.69
1:E:315:PRO:HA	1:E:318:LEU:HD12	1.75	0.69
1:E:401:ARG:O	1:E:401:ARG:HD3	1.92	0.69
2:A:67:HIS:HB3	2:A:70:HIS:HB2	1.75	0.69
2:C:77:GLU:H	2:C:77:GLU:CD	1.96	0.69
1:E:335:LEU:HD12	1:E:392:ALA:HB2	1.73	0.69
2:B:88:LEU:HD12	2:B:89:ARG:HE	1.58	0.69
1:F:89:VAL:HG21	1:F:274:ARG:NH2	2.07	0.69
1:F:412:ASP:O	1:F:414:SER:N	2.24	0.69
2:D:15:ALA:HB1	2:D:152:LEU:HD12	1.73	0.69
1:F:21:ASP:HA	1:F:24:LYS:HG3	1.73	0.69
1:F:34:ARG:HD3	1:F:250:HIS:CD2	2.27	0.69
1:F:6:PRO:O	1:F:10:VAL:HG23	1.93	0.69
1:E:239:LEU:O	1:E:240:LYS:HD3	1.92	0.69
1:E:259:ASP:C	1:E:261:ILE:H	1.97	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:HD13	1:E:442:ILE:H	1.57	0.68
1:E:441:PHE:HD1	1:F:56:ILE:HD13	1.57	0.68
1:F:266:GLU:HG3	1:F:267:SER:H	1.56	0.68
1:E:302:ILE:HB	1:E:304:PHE:CE1	2.28	0.68
1:E:277:VAL:O	1:E:281:LEU:HG	1.93	0.68
2:C:39:ASN:ND2	2:C:40:ASP:H	1.90	0.68
1:E:84:THR:O	1:E:87:THR:HG22	1.94	0.68
1:F:68:ARG:HG3	1:F:78:PHE:CE2	2.29	0.68
2:B:84:THR:O	2:B:84:THR:HG22	1.92	0.68
2:C:13:VAL:HG11	2:C:145:ARG:HA	1.75	0.68
2:C:36:ARG:HD2	2:C:38:TYR:CG	2.28	0.68
2:B:13:VAL:HB	2:B:170:GLU:CG	2.22	0.68
1:E:20:GLN:O	1:E:24:LYS:HG2	1.94	0.68
1:E:402:LEU:HD11	1:E:425:VAL:HA	1.76	0.68
1:F:103:LEU:HD13	1:F:247:VAL:HG22	1.76	0.68
2:D:84:THR:HG22	2:D:85:ASP:H	1.57	0.68
2:B:38:TYR:C	2:B:40:ASP:H	1.97	0.68
2:B:58:GLU:O	2:B:60:PHE:N	2.27	0.68
1:E:79:ILE:HG21	1:E:103:LEU:HB2	1.74	0.68
2:B:73:LYS:HA	2:B:77:GLU:CD	2.14	0.68
1:F:108:VAL:HG22	1:F:243:ALA:HB1	1.76	0.67
1:E:69:ARG:HH11	1:E:69:ARG:CG	2.05	0.67
2:D:7:ARG:NH1	2:D:12:VAL:HG21	2.08	0.67
2:C:6:VAL:O	2:C:144:ALA:HB1	1.94	0.67
2:A:38:TYR:C	2:A:40:ASP:N	2.46	0.67
2:D:58:GLU:O	2:D:61:GLU:HB3	1.92	0.67
2:B:150:LYS:HD3	2:C:139:ASN:HD21	1.59	0.67
2:C:87:MET:CG	2:C:88:LEU:H	2.07	0.67
1:E:18:ILE:HD13	1:E:342:ARG:HB2	1.77	0.67
2:B:137:LEU:HD13	2:B:147:ILE:HG13	1.76	0.67
2:D:88:LEU:HD23	2:D:91:LEU:HD21	1.74	0.67
2:A:61:GLU:O	2:A:65:GLU:HG3	1.94	0.67
1:E:438:LEU:HD22	1:E:442:ILE:HD12	1.76	0.67
1:F:264:ARG:HD2	1:F:312:ILE:CG1	2.25	0.67
1:F:390:ILE:HD11	1:F:394:ARG:HA	1.75	0.67
2:A:75:ALA:O	2:A:79:ALA:N	2.21	0.67
2:B:50:THR:N	2:A:111:ASP:HB3	2.10	0.67
1:E:278:GLN:HE22	1:E:318:LEU:CA	2.08	0.67
2:B:8:ARG:HG3	2:B:9:ASN:N	2.10	0.66
1:F:375:ARG:HG2	1:F:375:ARG:NH1	2.09	0.66
2:D:44:ALA:HB2	2:D:97:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:HG13	1:E:245:ASP:N	2.10	0.66
2:B:94:LEU:H	2:B:94:LEU:HD12	1.60	0.66
2:C:37:LEU:HD13	2:C:61:GLU:HG2	1.76	0.66
2:B:15:ALA:HB2	2:B:168:ILE:HG23	1.76	0.66
1:F:319:ILE:HG13	1:F:319:ILE:O	1.95	0.66
2:B:51:ALA:C	2:B:54:PHE:H	1.98	0.66
2:D:14:ILE:O	2:D:168:ILE:HG13	1.95	0.66
1:F:7:ARG:HH11	1:F:7:ARG:HG2	1.61	0.66
1:E:438:LEU:HD13	1:E:442:ILE:HD11	1.78	0.66
2:C:93:ALA:C	2:C:94:LEU:HD23	2.16	0.66
1:E:108:VAL:O	1:E:111:VAL:HG22	1.96	0.66
2:D:121:ALA:CB	2:D:130:GLN:HB2	2.26	0.66
2:D:85:ASP:O	2:D:86:ARG:HB2	1.95	0.66
2:C:122:ILE:N	2:C:122:ILE:HD13	2.10	0.65
1:F:68:ARG:HG3	1:F:78:PHE:HE2	1.62	0.65
2:C:86:ARG:H	2:C:87:MET:HE3	1.61	0.65
2:D:72:VAL:C	2:D:74:ALA:H	2.00	0.65
2:C:163:ASN:C	2:C:163:ASN:ND2	2.50	0.65
2:C:106:ILE:C	2:C:108:GLY:H	1.99	0.65
1:F:34:ARG:HH11	1:F:250:HIS:HB3	1.60	0.65
1:F:94:LYS:HE2	1:F:94:LYS:HA	1.79	0.65
2:A:88:LEU:HD22	2:A:91:LEU:HB2	1.77	0.65
2:A:42:VAL:HG12	2:A:42:VAL:O	1.97	0.65
2:D:99:ASP:CG	2:D:100:GLU:H	1.99	0.65
1:E:6:PRO:O	1:E:10:VAL:HG23	1.95	0.65
1:F:267:SER:HA	2:D:87:MET:HG3	1.79	0.65
2:C:70:HIS:CE1	2:C:72:VAL:HB	2.30	0.65
1:E:122:ARG:O	1:E:125:GLU:HG2	1.97	0.65
2:B:32:LYS:NZ	2:B:32:LYS:CB	2.59	0.65
2:C:2:THR:HG21	2:C:129:ALA:HB2	1.78	0.65
1:E:432:LEU:CD1	1:E:442:ILE:HD11	2.25	0.64
2:C:37:LEU:HB3	2:C:61:GLU:HG2	1.79	0.64
2:B:70:HIS:O	2:B:74:ALA:O	2.14	0.64
1:E:350:SER:O	1:E:354:GLN:HG3	1.97	0.64
1:E:246:ALA:C	1:E:248:GLU:H	2.00	0.64
2:C:132:ALA:HB1	2:C:154:ILE:HD12	1.78	0.64
2:B:60:PHE:CE2	2:B:64:LEU:HA	2.32	0.64
2:D:38:TYR:O	2:D:40:ASP:N	2.30	0.64
1:E:123:ALA:HA	1:E:126:LEU:HD12	1.80	0.64
2:D:85:ASP:HB3	2:D:87:MET:SD	2.38	0.64
2:C:106:ILE:O	2:C:108:GLY:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:THR:HA	2:D:17:ASP:OD1	1.98	0.64
2:C:140:THR:HG21	2:C:142:LEU:HD12	1.80	0.64
2:A:95:LEU:H	2:A:95:LEU:HD23	1.61	0.64
2:C:37:LEU:O	2:C:39:ASN:N	2.31	0.64
2:B:4:VAL:HG22	2:B:121:ALA:CB	2.27	0.64
1:E:278:GLN:NE2	1:E:319:ILE:H	1.95	0.64
1:F:384:ASN:ND2	1:F:390:ILE:H	1.95	0.64
2:B:5:SER:HB2	2:B:14:ILE:HA	1.79	0.64
1:F:240:LYS:HG3	1:F:241:GLN:N	2.12	0.64
2:D:15:ALA:HB2	2:D:168:ILE:HD12	1.79	0.64
1:F:278:GLN:NE2	1:F:319:ILE:H	1.95	0.64
2:A:142:LEU:O	2:A:143:SER:HB3	1.98	0.64
2:B:37:LEU:HG	2:B:61:GLU:OE1	1.98	0.64
2:B:90:LYS:HB3	2:A:83:ARG:NH2	2.12	0.64
2:C:81:ASP:HA	2:C:85:ASP:CG	2.18	0.64
2:B:86:ARG:HB2	2:B:86:ARG:HH11	1.61	0.64
2:C:5:SER:HA	2:C:13:VAL:O	1.98	0.64
1:E:20:GLN:HA	1:E:20:GLN:NE2	2.12	0.64
1:E:61:VAL:O	3:E:905:DAT:N7	2.31	0.64
2:B:119:LEU:C	2:B:120:ILE:HD12	2.18	0.63
2:A:38:TYR:HB3	2:A:42:VAL:CG2	2.28	0.63
2:B:8:ARG:HB3	2:B:144:ALA:HB2	1.80	0.63
1:F:387:THR:CG2	1:F:388:GLU:H	1.96	0.63
2:D:143:SER:HB3	2:D:146:GLU:HG2	1.80	0.63
2:A:3:ILE:CG1	2:A:47:ALA:HB2	2.29	0.63
2:A:138:GLU:C	2:A:139:ASN:HD22	2.02	0.63
1:F:240:LYS:O	1:F:241:GLN:C	2.35	0.63
1:E:241:GLN:O	1:E:245:ASP:OD1	2.17	0.63
2:A:135:ALA:O	2:D:136:LEU:HD21	1.98	0.63
1:F:409:ASP:O	1:F:411:SER:N	2.32	0.63
1:F:124:GLU:C	1:F:126:LEU:H	2.02	0.63
2:D:82:TRP:CD2	2:D:108:GLY:O	2.51	0.63
1:E:17:ILE:HB	1:E:24:LYS:HE3	1.81	0.63
2:A:28:LYS:HD3	2:A:30:ASN:CG	2.19	0.63
2:B:44:ALA:CB	2:B:97:VAL:HA	2.20	0.63
1:E:108:VAL:C	1:E:110:MET:N	2.52	0.63
2:A:71:LEU:HD11	2:A:97:VAL:HG23	1.80	0.63
2:D:44:ALA:HA	2:D:96:ALA:O	1.98	0.63
1:F:351:ILE:CD1	1:F:351:ILE:H	2.09	0.63
2:D:105:ILE:HB	2:D:113:VAL:HG22	1.81	0.63
2:A:28:LYS:HG2	2:A:30:ASN:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LYS:C	2:B:82:TRP:N	2.51	0.63
2:C:82:TRP:NE1	2:C:108:GLY:HA2	2.03	0.62
1:E:432:LEU:HB3	1:E:443:LEU:CD1	2.29	0.62
2:D:105:ILE:O	2:D:112:VAL:HA	1.99	0.62
2:C:15:ALA:HB1	2:C:152:LEU:HD12	1.81	0.62
2:C:44:ALA:HB2	2:C:97:VAL:CG1	2.27	0.62
2:D:136:LEU:O	2:D:138:GLU:N	2.32	0.62
2:B:6:VAL:O	2:B:144:ALA:HB1	1.99	0.62
2:A:80:LYS:C	2:A:82:TRP:N	2.53	0.62
2:A:71:LEU:HG	2:A:104:LEU:HD21	1.81	0.62
2:A:1:THR:N	2:A:33:LYS:HE2	2.14	0.62
2:B:74:ALA:O	2:B:75:ALA:HB2	1.99	0.62
1:E:259:ASP:O	1:E:261:ILE:N	2.33	0.62
2:D:85:ASP:O	2:D:87:MET:HE1	2.00	0.62
2:B:78:LEU:HD23	2:B:106:ILE:HD13	1.80	0.62
1:F:228:GLU:O	1:F:231:ALA:HB3	1.99	0.62
1:E:43:GLU:HG3	1:E:44:LEU:N	2.14	0.62
2:A:74:ALA:O	2:A:78:LEU:HB2	2.00	0.62
2:B:149:GLU:CD	2:B:168:ILE:HD13	2.19	0.62
1:F:376:ILE:O	1:F:379:ALA:HB3	1.99	0.62
1:F:97:ASP:OD2	1:F:98:SER:N	2.32	0.62
2:C:54:PHE:O	2:C:57:PHE:HB3	2.00	0.62
2:B:38:TYR:O	2:B:40:ASP:N	2.32	0.62
2:D:6:VAL:O	2:D:144:ALA:HB1	1.98	0.62
2:D:102:ALA:HB1	2:D:114:GLN:OE1	2.00	0.62
2:C:105:ILE:HG22	2:C:106:ILE:N	2.15	0.62
2:D:63:LYS:O	2:D:66:MET:HG2	2.00	0.62
1:F:312:ILE:O	1:F:313:ALA:HB2	2.00	0.62
2:A:22:LEU:CD2	2:A:23:GLY:H	2.09	0.62
1:E:96:VAL:HG11	1:E:280:ASP:HB3	1.82	0.62
1:F:88:GLU:C	1:F:90:GLY:H	2.02	0.62
2:C:39:ASN:N	2:C:39:ASN:ND2	2.48	0.62
2:D:54:PHE:O	2:D:57:PHE:HB3	1.99	0.62
2:B:95:LEU:HD23	2:B:95:LEU:H	1.64	0.62
2:C:70:HIS:ND1	2:C:72:VAL:HB	2.15	0.61
2:A:35:ARG:H	2:A:45:GLY:HA2	1.64	0.61
2:D:64:LEU:O	2:D:68:GLN:N	2.33	0.61
2:B:141:GLU:O	2:B:142:LEU:O	2.18	0.61
1:F:102:ASP:C	1:F:104:THR:N	2.51	0.61
2:B:7:ARG:HG3	2:B:12:VAL:CG2	2.29	0.61
2:D:32:LYS:HD2	2:D:167:THR:CG2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLN:HG3	1:E:312:ILE:H	1.65	0.61
2:D:74:ALA:HB1	2:D:78:LEU:HD12	1.81	0.61
2:B:72:VAL:C	2:B:74:ALA:H	2.03	0.61
2:D:82:TRP:NE1	2:D:109:ASN:HA	2.14	0.61
2:D:100:GLU:HB2	2:D:173:TYR:HD1	1.65	0.61
2:C:136:LEU:C	2:C:138:GLU:H	2.03	0.61
2:B:39:ASN:HA	2:B:62:ARG:NH2	2.14	0.61
2:B:114:GLN:HG2	2:B:116:GLU:OE1	2.00	0.61
2:B:3:ILE:O	2:B:121:ALA:HA	2.01	0.61
1:F:34:ARG:HH11	1:F:250:HIS:CB	2.13	0.61
1:F:89:VAL:HG21	1:F:274:ARG:CZ	2.30	0.61
1:E:55:MET:HE2	1:E:332:LEU:HD21	1.82	0.61
2:A:140:THR:HG22	2:A:141:GLU:N	2.16	0.61
2:B:39:ASN:H	2:B:62:ARG:NH2	1.98	0.61
2:C:45:GLY:O	2:C:95:LEU:HD12	2.00	0.61
2:B:60:PHE:CE1	2:B:64:LEU:HG	2.34	0.61
1:F:390:ILE:HD11	1:F:394:ARG:CA	2.31	0.61
2:C:63:LYS:C	2:C:65:GLU:H	2.02	0.61
1:E:242:ASP:HA	1:E:245:ASP:OD1	2.01	0.61
2:A:36:ARG:NE	2:A:40:ASP:OD2	2.32	0.61
2:B:86:ARG:HE	2:A:84:THR:HG21	1.65	0.61
1:E:229:GLU:HB2	1:E:232:LYS:HZ3	1.65	0.61
1:F:130:ARG:O	1:F:131:ILE:HD13	2.01	0.61
2:A:71:LEU:O	2:A:74:ALA:HB3	2.01	0.61
2:B:17:ASP:HA	2:B:165:PHE:O	2.00	0.61
1:F:438:LEU:HD22	1:F:442:ILE:CD1	2.30	0.61
2:D:71:LEU:CD1	2:D:99:ASP:HB2	2.30	0.60
2:D:86:ARG:HA	2:D:86:ARG:NE	2.15	0.60
1:E:349:ALA:O	1:E:350:SER:O	2.19	0.60
2:C:82:TRP:NE1	2:C:108:GLY:C	2.54	0.60
1:E:108:VAL:C	1:E:110:MET:H	2.02	0.60
1:E:88:GLU:OE2	1:E:92:VAL:N	2.27	0.60
2:B:65:GLU:HB2	2:B:66:MET:SD	2.41	0.60
2:D:35:ARG:HB3	2:D:57:PHE:HE1	1.65	0.60
1:E:432:LEU:HD11	1:E:442:ILE:CD1	2.28	0.60
1:F:235:ASN:H	1:F:236:PRO:HD3	1.65	0.60
1:E:245:ASP:HA	1:E:248:GLU:HB3	1.83	0.60
1:E:278:GLN:HE22	1:E:318:LEU:HA	1.66	0.60
2:D:35:ARG:HB3	2:D:57:PHE:CE1	2.37	0.60
1:F:122:ARG:HH21	1:F:125:GLU:HG3	1.66	0.60
2:A:3:ILE:HD12	2:A:34:VAL:HG12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:GLY:O	1:E:24:LYS:NZ	2.34	0.60
1:F:271:ASP:O	1:F:274:ARG:HG2	2.02	0.60
2:D:46:PHE:HE1	2:D:48:GLY:O	1.84	0.60
2:C:37:LEU:HB3	2:C:61:GLU:CG	2.31	0.60
1:E:299:THR:HA	1:E:302:ILE:HG12	1.84	0.60
2:A:75:ALA:CB	2:A:112:VAL:HG21	2.28	0.60
1:E:49:THR:O	1:E:50:PRO:O	2.20	0.60
1:F:432:LEU:HD11	1:F:442:ILE:HD11	1.84	0.60
2:A:140:THR:HB	2:A:142:LEU:CD1	2.32	0.60
2:C:75:ALA:O	2:C:79:ALA:HB3	2.02	0.60
1:F:39:GLN:CD	1:F:39:GLN:C	2.61	0.60
2:A:84:THR:C	2:A:86:ARG:H	2.05	0.60
1:F:73:LEU:HD23	1:F:73:LEU:C	2.22	0.60
2:D:52:ASP:OD2	2:D:53:ALA:N	2.35	0.59
2:D:52:ASP:O	2:D:55:THR:N	2.33	0.59
1:F:226:ILE:HG13	1:F:227:GLU:N	2.17	0.59
2:D:82:TRP:CD1	2:D:83:ARG:N	2.70	0.59
2:B:115:PRO:O	2:B:116:GLU:C	2.40	0.59
1:E:125:GLU:O	1:E:129:GLU:HG2	2.01	0.59
1:E:229:GLU:HB2	1:E:232:LYS:NZ	2.17	0.59
2:D:82:TRP:HD1	2:D:83:ARG:N	2.01	0.59
2:B:42:VAL:O	2:B:43:ILE:HG23	2.02	0.59
2:D:71:LEU:O	2:D:74:ALA:HB3	2.02	0.59
2:D:60:PHE:O	2:D:62:ARG:N	2.34	0.59
2:C:5:SER:CB	2:C:14:ILE:HG12	2.29	0.59
2:D:84:THR:O	2:D:85:ASP:HB2	2.02	0.59
2:B:160:ILE:HD12	2:D:160:ILE:O	2.03	0.59
1:E:103:LEU:HG	1:E:247:VAL:CG1	2.23	0.59
1:E:226:ILE:O	1:E:229:GLU:HB3	2.02	0.59
1:F:432:LEU:HG	1:F:443:LEU:HD22	1.84	0.59
1:F:55:MET:HE1	1:F:63:LYS:HA	1.82	0.59
2:C:136:LEU:O	2:C:138:GLU:N	2.36	0.59
2:C:60:PHE:O	2:C:64:LEU:HD13	2.01	0.59
2:A:38:TYR:O	2:A:40:ASP:N	2.35	0.59
1:E:249:GLN:NE2	1:E:250:HIS:ND1	2.51	0.59
2:D:88:LEU:HD22	2:C:84:THR:CB	2.31	0.59
1:F:374:LYS:O	1:F:378:GLU:HG3	2.03	0.59
1:F:375:ARG:HD3	1:F:426:SER:OG	2.03	0.59
2:D:70:HIS:HB3	2:D:73:LYS:CD	2.28	0.59
1:E:61:VAL:HG23	1:E:62:GLY:N	2.16	0.59
2:C:37:LEU:HD22	2:C:61:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:HE3	2:A:113:VAL:HG23	1.84	0.59
2:A:35:ARG:O	2:A:44:ALA:O	2.20	0.59
2:B:51:ALA:HA	2:B:54:PHE:CB	2.33	0.59
2:A:14:ILE:N	2:A:14:ILE:HD12	2.17	0.59
1:E:96:VAL:HG23	1:E:97:ASP:N	2.18	0.59
2:A:142:LEU:O	2:A:143:SER:CB	2.51	0.59
1:F:5:THR:OG1	1:F:7:ARG:HG3	2.02	0.59
2:B:18:GLY:O	2:B:31:VAL:HG23	2.02	0.59
2:C:105:ILE:C	2:C:106:ILE:HD12	2.22	0.58
1:F:67:ALA:HA	1:F:70:LEU:HB3	1.85	0.58
2:D:82:TRP:CD1	2:D:109:ASN:HA	2.38	0.58
1:E:254:PHE:HA	1:E:305:ILE:O	2.03	0.58
2:C:71:LEU:HG	2:C:99:ASP:HB2	1.85	0.58
1:E:237:GLU:O	1:E:240:LYS:HB2	2.02	0.58
1:F:366:ILE:HD13	1:F:418:ILE:HB	1.85	0.58
2:A:7:ARG:O	2:A:144:ALA:HB2	2.03	0.58
1:F:112:ARG:O	1:F:116:ILE:HG23	2.03	0.58
2:A:63:LYS:HE3	2:A:77:GLU:HB3	1.86	0.58
2:B:28:LYS:HG2	2:B:29:GLY:N	2.17	0.58
2:C:27:MET:O	2:C:29:GLY:N	2.37	0.58
1:E:5:THR:HG22	1:E:32:ARG:NH2	2.18	0.58
2:B:52:ASP:HB2	2:A:110:GLY:HA3	1.85	0.58
1:F:282:LEU:HD21	1:F:321:GLU:HB2	1.85	0.58
1:E:110:MET:HA	1:E:113:VAL:HG12	1.83	0.58
1:F:102:ASP:O	1:F:104:THR:N	2.36	0.58
1:E:90:GLY:O	1:F:91:TYR:HA	2.03	0.58
2:B:35:ARG:N	2:B:44:ALA:O	2.31	0.58
2:A:32:LYS:HG2	2:A:167:THR:HG21	1.86	0.58
1:F:375:ARG:HA	1:F:378:GLU:OE1	2.04	0.58
2:C:13:VAL:HG23	2:C:169:GLU:O	2.04	0.58
1:E:73:LEU:C	1:E:73:LEU:HD12	2.24	0.58
2:C:82:TRP:NE1	2:C:108:GLY:CA	2.64	0.58
2:B:51:ALA:HA	2:B:54:PHE:HB3	1.84	0.58
1:F:103:LEU:O	1:F:247:VAL:HG22	2.03	0.58
2:C:13:VAL:HG22	2:C:14:ILE:N	2.19	0.58
2:A:8:ARG:NH1	2:A:141:GLU:O	2.36	0.58
2:A:78:LEU:O	2:A:82:TRP:HB2	2.04	0.58
2:D:62:ARG:HA	2:D:65:GLU:OE2	2.04	0.58
2:B:34:VAL:HG22	2:B:45:GLY:HA3	1.85	0.58
1:F:240:LYS:O	1:F:243:ALA:N	2.36	0.58
2:B:72:VAL:O	2:B:74:ALA:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:THR:HG22	2:D:85:ASP:N	2.19	0.58
1:F:278:GLN:HE22	1:F:318:LEU:CA	2.17	0.58
1:F:122:ARG:NH2	1:F:125:GLU:HG3	2.19	0.58
2:D:2:THR:HG21	2:D:129:ALA:HB2	1.86	0.58
2:C:36:ARG:HG2	2:C:37:LEU:N	2.19	0.57
1:E:229:GLU:CD	1:E:229:GLU:C	2.63	0.57
1:F:344:LEU:O	1:F:350:SER:OG	2.22	0.57
1:F:264:ARG:HD2	1:F:312:ILE:HG12	1.86	0.57
1:F:381:TRP:CH2	1:F:385:GLU:HG3	2.39	0.57
1:F:108:VAL:C	1:F:110:MET:N	2.58	0.57
2:B:7:ARG:NH1	2:B:102:ALA:N	2.48	0.57
1:E:355:TYR:OH	1:E:400:GLU:HB2	2.04	0.57
2:C:23:GLY:C	2:C:24:ASN:HD22	2.06	0.57
2:C:39:ASN:HB3	2:C:61:GLU:OE1	2.04	0.57
1:F:341:GLU:OE1	1:F:374:LYS:HG3	2.03	0.57
2:D:37:LEU:HD11	2:D:60:PHE:CB	2.34	0.57
2:B:75:ALA:HB1	2:B:112:VAL:CG2	2.33	0.57
1:F:226:ILE:HG13	1:F:227:GLU:H	1.69	0.57
2:D:80:LYS:O	2:D:82:TRP:N	2.37	0.57
2:C:52:ASP:OD2	2:C:91:LEU:HD12	2.03	0.57
2:C:127:PRO:O	2:C:130:GLN:HB3	2.04	0.57
2:A:82:TRP:O	2:A:84:THR:N	2.37	0.57
1:F:236:PRO:O	1:F:238:GLU:N	2.36	0.57
1:F:9:ILE:CD1	1:F:31:LEU:HD23	2.33	0.57
2:A:71:LEU:HD22	2:A:99:ASP:OD2	2.04	0.57
2:B:51:ALA:CA	2:B:54:PHE:HB3	2.34	0.57
1:E:275:GLU:O	1:E:278:GLN:HB2	2.05	0.57
2:A:140:THR:HG22	2:A:141:GLU:H	1.70	0.57
2:B:20:ALA:HB2	2:B:31:VAL:HG21	1.85	0.57
2:C:101:THR:O	2:C:102:ALA:HB2	2.05	0.57
2:D:37:LEU:CD2	2:D:61:GLU:HB2	2.29	0.57
1:F:115:ALA:HA	1:F:118:LYS:CB	2.28	0.57
1:E:376:ILE:O	1:E:379:ALA:HB3	2.05	0.57
2:A:160:ILE:HG13	2:A:161:TYR:CD2	2.40	0.57
1:E:223:LYS:NZ	1:E:226:ILE:HG21	2.20	0.57
2:B:149:GLU:OE2	2:B:168:ILE:HD13	2.05	0.57
1:F:227:GLU:HA	1:F:230:ALA:HB3	1.86	0.57
1:F:90:GLY:O	1:F:91:TYR:CG	2.57	0.57
2:B:82:TRP:O	2:B:83:ARG:HG2	2.03	0.57
2:B:150:LYS:HD3	2:C:139:ASN:ND2	2.19	0.57
2:C:35:ARG:HD2	2:C:57:PHE:HZ	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:ILE:HG13	2:A:47:ALA:HB2	1.87	0.57
2:A:44:ALA:HB1	2:A:57:PHE:CZ	2.40	0.57
2:B:32:LYS:HG3	2:B:167:THR:HG21	1.87	0.57
1:F:240:LYS:HA	1:F:294:HIS:CD2	2.38	0.57
1:F:278:GLN:HE22	1:F:319:ILE:H	1.50	0.57
2:A:6:VAL:HG11	2:A:147:ILE:HB	1.87	0.57
2:B:38:TYR:C	2:B:40:ASP:N	2.58	0.56
2:D:28:LYS:O	2:D:31:VAL:HG23	2.05	0.56
1:F:33:ASN:HA	1:F:36:ARG:HB2	1.87	0.56
1:F:387:THR:HG23	1:F:440:ARG:NH1	2.19	0.56
2:A:79:ALA:HB2	2:A:112:VAL:CG2	2.31	0.56
1:F:45:ARG:HH11	1:F:45:ARG:CG	2.19	0.56
2:D:37:LEU:C	2:D:39:ASN:H	2.08	0.56
1:F:106:ALA:O	1:F:110:MET:HB2	2.05	0.56
1:F:244:ILE:O	1:F:247:VAL:N	2.38	0.56
1:E:3:GLU:O	1:E:4:MET:HB2	2.05	0.56
1:E:265:GLY:HA2	1:E:312:ILE:HG22	1.88	0.56
1:E:335:LEU:CD1	1:E:392:ALA:HB2	2.35	0.56
2:A:140:THR:HB	2:A:142:LEU:HD12	1.86	0.56
1:F:268:SER:C	1:F:270:PRO:HD3	2.25	0.56
1:E:102:ASP:C	1:E:104:THR:N	2.58	0.56
2:B:54:PHE:HE2	2:A:80:LYS:NZ	2.04	0.56
1:F:425:VAL:O	1:F:429:LEU:HB2	2.06	0.56
2:D:93:ALA:C	2:D:94:LEU:HD12	2.26	0.56
2:D:94:LEU:HD12	2:D:94:LEU:N	2.20	0.56
2:B:11:HIS:N	2:B:11:HIS:ND1	2.54	0.56
2:B:163:ASN:HD22	2:B:165:PHE:H	1.53	0.56
1:E:1:MET:O	1:E:3:GLU:N	2.38	0.56
1:F:104:THR:O	1:F:108:VAL:HG23	2.06	0.56
1:F:442:ILE:HD13	1:F:442:ILE:H	1.70	0.56
2:C:4:VAL:O	2:C:14:ILE:HA	2.06	0.56
2:C:43:ILE:HD13	2:C:169:GLU:O	2.04	0.56
2:B:85:ASP:O	2:B:87:MET:HG2	2.06	0.56
2:A:115:PRO:O	2:A:116:GLU:C	2.44	0.56
2:B:54:PHE:CE2	2:A:80:LYS:NZ	2.74	0.56
2:D:66:MET:C	2:D:68:GLN:H	2.08	0.56
2:B:4:VAL:HG13	2:B:121:ALA:HB2	1.87	0.56
1:E:442:ILE:HA	1:F:329:ARG:CG	2.35	0.56
1:F:413:LEU:HD23	1:F:413:LEU:N	2.18	0.56
1:E:88:GLU:C	1:E:90:GLY:H	2.08	0.56
2:C:150:LYS:O	2:C:154:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:GLY:O	2:D:95:LEU:HD13	2.05	0.56
2:C:72:VAL:C	2:C:74:ALA:H	2.08	0.56
1:E:102:ASP:O	1:E:104:THR:N	2.38	0.56
1:F:103:LEU:HD11	1:F:247:VAL:HG13	1.88	0.56
1:F:240:LYS:CG	1:F:241:GLN:N	2.68	0.56
1:F:100:ILE:HG12	1:F:299:THR:CG2	2.36	0.56
2:C:44:ALA:HA	2:C:96:ALA:O	2.06	0.56
2:B:41:LYS:HB2	2:B:41:LYS:NZ	2.21	0.56
2:C:70:HIS:CD2	2:C:73:LYS:HB2	2.39	0.56
2:C:86:ARG:HG3	2:C:87:MET:HE2	1.87	0.56
2:B:88:LEU:O	2:B:91:LEU:N	2.29	0.56
1:F:382:GLN:CG	1:F:433:VAL:HG23	2.35	0.56
2:B:7:ARG:HA	2:B:12:VAL:HG22	1.87	0.56
1:E:338:SER:O	1:E:342:ARG:HG3	2.06	0.56
1:E:264:ARG:HA	1:E:264:ARG:NE	2.20	0.56
2:B:60:PHE:O	2:B:61:GLU:OE2	2.23	0.55
1:F:243:ALA:O	1:F:246:ALA:HB3	2.06	0.55
2:C:142:LEU:HD22	2:C:146:GLU:HG2	1.87	0.55
1:E:100:ILE:C	1:E:102:ASP:H	2.09	0.55
1:E:121:TYR:HD1	1:E:122:ARG:H	1.55	0.55
1:F:268:SER:O	1:F:270:PRO:HD3	2.05	0.55
1:F:375:ARG:CG	1:F:375:ARG:HH11	2.13	0.55
1:F:312:ILE:HB	2:D:62:ARG:HD2	1.87	0.55
1:F:312:ILE:O	1:F:312:ILE:HG23	2.06	0.55
2:D:106:ILE:C	2:D:108:GLY:H	2.08	0.55
1:E:35:TRP:O	1:E:39:GLN:HG3	2.06	0.55
2:C:18:GLY:HA3	2:C:165:PHE:HD2	1.71	0.55
2:B:52:ASP:N	2:A:110:GLY:O	2.39	0.55
2:B:52:ASP:OD2	2:B:91:LEU:HD22	2.06	0.55
1:F:312:ILE:HG12	1:F:312:ILE:O	2.06	0.55
1:E:235:ASN:N	1:E:236:PRO:CD	2.69	0.55
2:A:135:ALA:HB2	2:D:154:ILE:HD12	1.86	0.55
1:E:42:GLU:O	1:E:45:ARG:HB3	2.06	0.55
1:F:402:LEU:HD13	1:F:429:LEU:HD13	1.89	0.55
2:C:47:ALA:HB3	2:C:94:LEU:HG	1.89	0.55
1:E:282:LEU:HD21	1:E:321:GLU:HB2	1.89	0.55
1:F:117:GLU:HA	1:F:120:ARG:HB2	1.89	0.55
2:C:63:LYS:HD2	2:C:78:LEU:CG	2.28	0.55
2:B:64:LEU:N	2:B:64:LEU:HD12	2.20	0.55
1:F:104:THR:O	1:F:108:VAL:N	2.40	0.55
2:C:82:TRP:O	2:C:82:TRP:CE3	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:76:VAL:O	2:A:80:LYS:HG2	2.06	0.55
2:B:49:GLY:HA3	2:B:52:ASP:HB2	1.89	0.55
1:F:237:GLU:O	1:F:240:LYS:HG2	2.06	0.55
1:F:90:GLY:O	1:F:91:TYR:CB	2.54	0.55
1:F:436:GLU:O	1:F:440:ARG:HG3	2.07	0.55
2:C:111:ASP:O	2:C:112:VAL:HG13	2.07	0.55
2:C:86:ARG:CA	2:C:89:ARG:HD2	2.33	0.55
2:B:70:HIS:N	2:B:70:HIS:CD2	2.75	0.55
1:E:25:ARG:O	1:E:28:ALA:HB3	2.06	0.55
1:E:282:LEU:HD21	1:E:321:GLU:CB	2.37	0.55
2:A:67:HIS:CE1	2:A:73:LYS:HE2	2.42	0.55
2:A:6:VAL:HG21	2:A:137:LEU:HD21	1.87	0.55
2:D:52:ASP:O	2:D:53:ALA:C	2.45	0.55
2:B:80:LYS:O	2:B:82:TRP:N	2.39	0.55
2:B:95:LEU:H	2:B:95:LEU:CD2	2.19	0.55
2:A:63:LYS:HD2	2:A:77:GLU:OE1	2.07	0.55
1:F:126:LEU:HA	1:F:129:GLU:HB2	1.89	0.55
1:E:258:ILE:O	1:E:259:ASP:O	2.24	0.55
1:E:278:GLN:HE22	1:E:319:ILE:H	1.54	0.55
2:C:123:GLY:C	2:C:125:GLY:N	2.57	0.55
1:F:278:GLN:HE22	1:F:319:ILE:N	2.05	0.55
1:F:436:GLU:O	1:F:439:SER:HB3	2.07	0.54
2:B:28:LYS:HG2	2:B:30:ASN:N	2.17	0.54
1:F:100:ILE:HG12	1:F:299:THR:HG22	1.89	0.54
2:A:1:THR:O	2:A:2:THR:OG1	2.20	0.54
1:E:65:GLU:HG2	3:E:905:DAT:H2'2	1.89	0.54
2:D:13:VAL:HG12	2:D:170:GLU:HB3	1.88	0.54
2:D:4:VAL:O	2:D:14:ILE:HA	2.06	0.54
1:F:264:ARG:HD2	1:F:312:ILE:HG13	1.88	0.54
1:F:87:THR:HG23	1:F:89:VAL:HG23	1.89	0.54
1:E:104:THR:HA	1:E:247:VAL:CG2	2.24	0.54
1:E:342:ARG:HB3	1:E:346:GLU:HG3	1.90	0.54
1:E:340:PHE:HB3	1:E:395:LEU:HD21	1.87	0.54
2:C:105:ILE:HG22	2:C:106:ILE:H	1.73	0.54
2:D:73:LYS:HE2	2:D:73:LYS:N	2.19	0.54
2:B:51:ALA:N	2:A:110:GLY:O	2.33	0.54
1:E:240:LYS:HA	1:E:294:HIS:NE2	2.22	0.54
1:F:130:ARG:NH2	1:F:225:LEU:HD11	2.23	0.54
2:D:83:ARG:NH1	2:D:89:ARG:NE	2.55	0.54
1:E:97:ASP:OD2	1:E:97:ASP:C	2.45	0.54
1:E:34:ARG:HA	1:E:34:ARG:NE	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ALA:N	2:C:111:ASP:OD1	2.40	0.54
2:B:42:VAL:HG12	2:B:43:ILE:N	2.23	0.54
1:E:69:ARG:NH1	1:E:69:ARG:CG	2.65	0.54
1:E:278:GLN:CD	1:E:319:ILE:HG23	2.28	0.54
1:F:43:GLU:HG3	1:F:44:LEU:N	2.22	0.54
2:C:80:LYS:HG2	2:C:85:ASP:OD2	2.07	0.54
1:F:87:THR:O	1:F:88:GLU:C	2.46	0.54
1:F:266:GLU:HG3	1:F:267:SER:N	2.23	0.54
2:C:66:MET:O	2:C:68:GLN:HG2	2.08	0.54
2:A:81:ASP:O	2:A:85:ASP:HB2	2.08	0.54
2:A:85:ASP:O	2:A:86:ARG:HB3	2.08	0.54
1:F:328:ILE:O	1:F:329:ARG:HD3	2.07	0.54
1:F:5:THR:HB	1:F:6:PRO:HD2	1.90	0.54
1:F:7:ARG:NH1	1:F:7:ARG:HG2	2.21	0.54
2:B:158:ILE:HG13	2:D:25:THR:HB	1.90	0.54
2:A:59:LEU:HD22	2:A:87:MET:SD	2.47	0.54
2:B:86:ARG:NH1	2:B:86:ARG:HB2	2.22	0.53
2:D:17:ASP:O	2:D:33:LYS:HD2	2.09	0.53
2:D:105:ILE:HD11	2:D:120:ILE:HG23	1.90	0.53
1:E:93:GLY:O	1:E:94:LYS:HB2	2.07	0.53
1:F:245:ASP:O	1:F:249:GLN:HB2	2.08	0.53
2:C:82:TRP:CZ3	2:C:89:ARG:HA	2.44	0.53
2:A:13:VAL:HG21	2:A:168:ILE:HG22	1.89	0.53
2:C:24:ASN:N	2:C:24:ASN:HD22	2.05	0.53
1:E:408:TYR:CE2	1:F:25:ARG:NH2	2.74	0.53
2:B:7:ARG:NH2	2:B:99:ASP:O	2.41	0.53
1:E:238:GLU:O	1:E:242:ASP:HB3	2.07	0.53
2:A:136:LEU:CD1	2:D:135:ALA:HB1	2.36	0.53
1:E:319:ILE:HG12	1:E:322:LEU:HD22	1.90	0.53
1:E:346:GLU:HB2	1:E:347:PRO:CD	2.37	0.53
2:A:34:VAL:CA	2:A:45:GLY:HA2	2.34	0.53
1:F:108:VAL:C	1:F:110:MET:H	2.10	0.53
1:F:62:GLY:O	1:F:63:LYS:C	2.44	0.53
2:B:55:THR:OG1	2:A:80:LYS:HB2	2.09	0.53
1:F:34:ARG:CG	1:F:35:TRP:H	2.20	0.53
2:D:3:ILE:HB	2:D:122:ILE:HG13	1.90	0.53
2:C:87:MET:HG3	2:C:88:LEU:H	1.73	0.53
2:A:79:ALA:CB	2:A:112:VAL:HG23	2.35	0.53
2:D:38:TYR:O	2:D:38:TYR:CD2	2.62	0.53
2:B:68:GLN:HB3	2:B:70:HIS:NE2	2.24	0.53
1:E:1:MET:C	1:E:3:GLU:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLN:HG3	1:E:312:ILE:HG12	1.91	0.53
2:B:152:LEU:HD13	2:B:166:HIS:CE1	2.44	0.53
1:E:421:ASP:N	1:E:421:ASP:OD2	2.41	0.53
2:C:55:THR:OG1	2:C:88:LEU:HD12	2.09	0.53
1:E:107:ALA:HB3	1:E:247:VAL:HG22	1.90	0.53
2:B:12:VAL:O	2:B:171:LEU:N	2.42	0.53
1:F:223:LYS:HG2	1:F:224:LEU:HD23	1.90	0.53
1:F:49:THR:O	1:F:50:PRO:O	2.27	0.53
2:B:52:ASP:OD1	2:A:83:ARG:NH1	2.42	0.53
2:D:37:LEU:HD11	2:D:60:PHE:HB2	1.91	0.53
2:B:67:HIS:O	2:B:68:GLN:O	2.28	0.53
1:E:21:ASP:OD1	1:E:25:ARG:HD2	2.09	0.53
1:F:394:ARG:O	1:F:398:VAL:HG12	2.10	0.53
1:E:400:GLU:O	1:E:404:GLU:HG2	2.09	0.53
2:C:82:TRP:HZ3	2:C:89:ARG:HA	1.75	0.52
2:D:63:LYS:CG	2:D:78:LEU:HG	2.30	0.52
1:F:401:ARG:NH2	1:F:442:ILE:HG13	2.23	0.52
2:A:1:THR:H3	2:A:33:LYS:HE2	1.73	0.52
2:C:141:GLU:O	2:C:142:LEU:HB2	2.08	0.52
2:D:171:LEU:N	2:D:171:LEU:HD23	2.24	0.52
1:F:382:GLN:HG2	1:F:433:VAL:HG21	1.88	0.52
1:E:229:GLU:HA	1:E:232:LYS:NZ	2.24	0.52
2:A:150:LYS:O	2:A:154:ILE:HD13	2.09	0.52
2:B:115:PRO:HD2	2:B:120:ILE:CD1	2.22	0.52
2:D:16:GLY:CA	2:D:152:LEU:HD11	2.39	0.52
1:F:30:ALA:CB	1:F:53:ILE:HD11	2.40	0.52
2:A:33:LYS:O	2:A:46:PHE:O	2.27	0.52
1:F:221:ALA:O	1:F:222:MET:HB2	2.08	0.52
1:F:226:ILE:O	1:F:230:ALA:N	2.42	0.52
2:A:17:ASP:HA	2:A:165:PHE:O	2.09	0.52
1:F:229:GLU:C	1:F:231:ALA:H	2.13	0.52
1:F:122:ARG:NH2	1:F:125:GLU:CD	2.63	0.52
1:F:281:LEU:O	1:F:282:LEU:C	2.48	0.52
2:C:32:LYS:HG3	2:C:167:THR:HG21	1.91	0.52
1:E:102:ASP:O	1:E:105:ASP:N	2.42	0.52
1:E:227:GLU:C	1:E:229:GLU:H	2.12	0.52
1:F:244:ILE:C	1:F:246:ALA:H	2.13	0.52
1:E:240:LYS:HD2	1:E:294:HIS:CE1	2.44	0.52
2:C:94:LEU:HD23	2:C:94:LEU:N	2.25	0.52
2:D:106:ILE:HD12	2:D:106:ILE:N	2.25	0.52
1:F:88:GLU:OE2	1:F:92:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:VAL:HG12	2:B:80:LYS:HE2	1.91	0.52
2:B:57:PHE:O	2:B:61:GLU:CG	2.57	0.52
1:E:108:VAL:O	1:E:110:MET:N	2.42	0.52
2:B:27:MET:CG	2:B:28:LYS:H	2.22	0.52
1:E:128:GLU:HG3	1:E:132:LEU:HD21	1.91	0.52
1:E:229:GLU:OE2	1:E:230:ALA:N	2.43	0.52
1:F:103:LEU:CD1	1:F:247:VAL:HG13	2.39	0.52
2:C:136:LEU:O	2:C:140:THR:HG22	2.10	0.52
1:E:311:GLN:HG3	1:E:312:ILE:N	2.24	0.52
1:F:355:TYR:OH	1:F:400:GLU:HB2	2.09	0.52
2:B:86:ARG:HE	2:A:84:THR:CG2	2.21	0.52
2:B:49:GLY:HA3	2:B:52:ASP:CB	2.40	0.52
2:B:15:ALA:HA	2:B:167:THR:O	2.09	0.52
1:F:86:PHE:CE2	1:F:96:VAL:HA	2.45	0.52
2:D:81:ASP:O	2:D:87:MET:HB2	2.10	0.52
2:C:146:GLU:OE1	2:C:150:LYS:HE2	2.09	0.52
1:E:366:ILE:HD11	1:E:406:ILE:HD13	1.90	0.52
1:E:130:ARG:NH1	1:E:130:ARG:CB	2.68	0.52
2:D:43:ILE:O	2:D:97:VAL:HA	2.10	0.52
1:F:438:LEU:O	1:F:442:ILE:HD13	2.10	0.52
2:D:105:ILE:HB	2:D:113:VAL:CG2	2.39	0.52
2:B:127:PRO:HB2	2:C:128:TYR:HE1	1.75	0.52
1:F:332:LEU:N	1:F:332:LEU:HD12	2.23	0.52
2:A:152:LEU:HD23	2:A:166:HIS:CD2	2.45	0.52
2:A:51:ALA:O	2:A:54:PHE:HB3	2.10	0.52
2:B:51:ALA:O	2:B:55:THR:N	2.40	0.52
2:D:70:HIS:CB	2:D:73:LYS:HD2	2.31	0.52
1:F:263:LYS:HE2	1:F:269:GLY:CA	2.39	0.52
2:B:3:ILE:HD11	2:B:33:LYS:HB3	1.91	0.52
1:F:273:SER:OG	1:F:274:ARG:HD3	2.08	0.52
1:F:97:ASP:C	1:F:97:ASP:OD2	2.47	0.52
1:E:413:LEU:CD1	1:E:418:ILE:HD11	2.40	0.52
2:C:106:ILE:HG22	2:C:108:GLY:H	1.75	0.52
2:B:39:ASN:HA	2:B:62:ARG:HH22	1.73	0.52
2:B:136:LEU:HD21	2:C:135:ALA:O	2.10	0.52
1:F:360:ALA:O	1:F:363:GLY:N	2.43	0.52
2:B:36:ARG:HG2	2:B:43:ILE:HG22	1.91	0.52
1:E:360:ALA:O	1:E:363:GLY:N	2.43	0.52
1:F:55:MET:HE2	1:F:63:LYS:HA	1.91	0.52
1:E:315:PRO:HA	1:E:318:LEU:CD1	2.40	0.52
1:E:375:ARG:HE	1:E:422:ALA:HB1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:ASN:OD1	2:C:30:ASN:O	2.28	0.52
2:A:1:THR:O	2:A:162:THR:HG21	2.10	0.51
1:E:52:ASN:HB2	1:E:326:LEU:HD23	1.92	0.51
2:A:1:THR:O	2:A:162:THR:CG2	2.59	0.51
1:E:238:GLU:C	1:E:240:LYS:H	2.13	0.51
2:D:80:LYS:C	2:D:82:TRP:H	2.13	0.51
2:B:82:TRP:HZ3	2:B:106:ILE:HG22	1.73	0.51
2:C:136:LEU:C	2:C:138:GLU:N	2.63	0.51
1:F:56:ILE:CD1	1:F:315:PRO:HG2	2.41	0.51
2:A:140:THR:CG2	2:A:142:LEU:HG	2.40	0.51
1:E:50:PRO:O	1:E:51:LYS:HD3	2.10	0.51
1:E:103:LEU:HD22	1:E:253:VAL:CG2	2.41	0.51
2:D:36:ARG:O	2:D:36:ARG:HG2	2.06	0.51
1:F:237:GLU:C	1:F:239:LEU:HD12	2.29	0.51
2:D:82:TRP:CD1	2:D:82:TRP:C	2.84	0.51
2:B:95:LEU:HD23	2:B:95:LEU:N	2.25	0.51
1:E:426:SER:HB3	1:E:430:ASP:OD1	2.11	0.51
1:F:94:LYS:HA	1:F:94:LYS:CE	2.41	0.51
1:F:357:ALA:O	1:F:360:ALA:HB3	2.11	0.51
2:A:34:VAL:HA	2:A:45:GLY:CA	2.38	0.51
2:C:87:MET:CG	2:C:88:LEU:N	2.73	0.51
1:E:107:ALA:HB3	1:E:247:VAL:CG2	2.40	0.51
1:E:97:ASP:OD2	1:E:98:SER:N	2.44	0.51
1:E:259:ASP:C	1:E:261:ILE:N	2.64	0.51
1:E:226:ILE:O	1:E:229:GLU:OE2	2.28	0.51
1:F:102:ASP:O	1:F:105:ASP:N	2.44	0.51
2:B:160:ILE:CG2	2:D:160:ILE:HD12	2.41	0.51
1:E:263:LYS:HG2	1:E:271:ASP:O	2.10	0.51
1:F:292:THR:OG1	1:F:293:LYS:N	2.43	0.51
2:D:27:MET:O	2:D:29:GLY:N	2.44	0.51
1:E:381:TRP:CH2	1:E:385:GLU:HG3	2.46	0.51
1:E:103:LEU:HD22	1:E:253:VAL:HG22	1.93	0.51
2:A:38:TYR:CE1	2:A:65:GLU:HA	2.46	0.51
2:B:24:ASN:ND2	2:D:161:TYR:HE1	2.09	0.51
2:A:127:PRO:HB2	2:D:128:TYR:HE1	1.76	0.51
2:B:129:ALA:O	2:B:131:ALA:N	2.44	0.51
2:A:37:LEU:O	2:A:42:VAL:HB	2.11	0.51
1:E:383:VAL:CB	1:E:394:ARG:HD3	2.32	0.51
1:F:68:ARG:HA	1:F:78:PHE:CE2	2.46	0.51
2:B:10:GLY:O	2:B:173:TYR:CD1	2.65	0.51
2:B:104:LEU:N	2:B:104:LEU:HD23	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:67:HIS:CB	2:A:70:HIS:HB2	2.40	0.50
2:B:57:PHE:O	2:B:61:GLU:OE2	2.29	0.50
1:E:68:ARG:HG3	1:E:78:PHE:CE2	2.46	0.50
2:D:30:ASN:O	2:D:30:ASN:OD1	2.29	0.50
2:B:60:PHE:CZ	2:B:64:LEU:HG	2.46	0.50
2:B:27:MET:HG3	2:B:28:LYS:H	1.76	0.50
1:E:417:ASN:OD1	1:E:417:ASN:O	2.29	0.50
2:B:42:VAL:HG12	2:B:43:ILE:H	1.76	0.50
2:A:38:TYR:CZ	2:A:65:GLU:HA	2.45	0.50
1:F:31:LEU:O	1:F:34:ARG:HG2	2.11	0.50
2:B:7:ARG:NE	2:B:12:VAL:HG21	2.27	0.50
2:D:103:SER:HB3	2:D:120:ILE:CD1	2.39	0.50
2:D:106:ILE:HG22	2:D:108:GLY:N	2.21	0.50
2:C:13:VAL:HG22	2:C:168:ILE:HG22	1.93	0.50
2:B:103:SER:HB2	2:B:118:ASP:HB3	1.93	0.50
2:B:96:ALA:O	2:B:97:VAL:CG2	2.49	0.50
2:D:36:ARG:O	2:D:38:TYR:N	2.44	0.50
1:F:311:GLN:HG3	1:F:312:ILE:H	1.77	0.50
1:F:21:ASP:HA	1:F:24:LYS:CG	2.41	0.50
2:C:127:PRO:O	2:C:128:TYR:C	2.49	0.50
2:D:1:THR:HA	2:D:17:ASP:CG	2.32	0.50
2:B:1:THR:HG21	2:B:47:ALA:HA	1.93	0.50
1:E:438:LEU:O	1:E:442:ILE:HD13	2.12	0.50
1:F:53:ILE:HG13	1:F:328:ILE:HB	1.93	0.50
1:F:131:ILE:HG13	1:F:221:ALA:HA	1.93	0.50
2:C:83:ARG:HH11	2:C:83:ARG:CA	2.19	0.50
2:B:57:PHE:O	2:B:58:GLU:C	2.50	0.50
2:A:119:LEU:O	2:A:120:ILE:HD12	2.11	0.50
2:B:88:LEU:O	2:B:89:ARG:C	2.49	0.50
1:F:35:TRP:N	1:F:38:MET:HE1	2.26	0.50
1:E:62:GLY:O	1:E:66:ILE:HG13	2.11	0.50
2:C:41:LYS:N	2:C:41:LYS:HD2	2.26	0.50
1:E:357:ALA:O	1:E:360:ALA:HB3	2.12	0.50
1:F:244:ILE:HG12	1:F:297:VAL:HG22	1.94	0.50
1:F:299:THR:HA	1:F:302:ILE:HG13	1.94	0.50
1:E:344:LEU:O	1:E:350:SER:OG	2.30	0.50
1:E:351:ILE:N	1:E:351:ILE:HD13	2.27	0.50
1:E:368:PHE:N	1:E:368:PHE:CD1	2.80	0.50
1:E:252:ILE:N	1:E:252:ILE:HD12	2.27	0.50
1:F:369:THR:HG22	1:F:370:ASP:N	2.25	0.50
2:A:42:VAL:O	2:A:43:ILE:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:312:ILE:HG13	2:D:62:ARG:HD3	1.94	0.49
1:F:263:LYS:HD3	1:F:264:ARG:N	2.26	0.49
1:E:55:MET:CE	1:E:63:LYS:HA	2.41	0.49
1:E:61:VAL:HG22	1:E:63:LYS:HZ2	1.77	0.49
2:C:70:HIS:ND1	2:C:73:LYS:HB2	2.26	0.49
1:E:223:LYS:HG3	1:E:223:LYS:O	2.11	0.49
1:F:105:ASP:O	1:F:109:LYS:N	2.43	0.49
1:E:346:GLU:O	1:E:347:PRO:C	2.50	0.49
2:B:107:THR:HG22	2:B:109:ASN:H	1.76	0.49
2:C:111:ASP:OD2	2:C:112:VAL:N	2.44	0.49
2:A:54:PHE:C	2:A:56:LEU:H	2.14	0.49
1:F:312:ILE:O	1:F:313:ALA:CB	2.60	0.49
1:E:429:LEU:O	1:E:433:VAL:HG22	2.12	0.49
2:A:26:VAL:O	2:A:27:MET:O	2.30	0.49
1:E:30:ALA:CB	1:E:53:ILE:HD11	2.42	0.49
2:C:106:ILE:C	2:C:108:GLY:N	2.65	0.49
2:A:97:VAL:O	2:A:98:ALA:HB2	2.13	0.49
1:F:10:VAL:HG13	1:F:24:LYS:HB2	1.93	0.49
1:F:220:ASP:N	1:F:224:LEU:N	2.53	0.49
1:E:278:GLN:HE22	1:E:319:ILE:N	2.10	0.49
2:A:28:LYS:HG2	2:A:30:ASN:ND2	2.27	0.49
2:A:135:ALA:HB2	2:D:154:ILE:CD1	2.43	0.49
2:B:160:ILE:HD11	2:D:19:GLN:HE22	1.74	0.49
1:E:441:PHE:CD1	1:F:56:ILE:HD13	2.43	0.49
1:F:285:VAL:HG13	1:F:285:VAL:O	2.11	0.49
2:A:112:VAL:C	2:A:113:VAL:HG12	2.32	0.49
2:A:112:VAL:HG12	2:A:113:VAL:N	2.27	0.49
2:D:74:ALA:O	2:D:78:LEU:N	2.45	0.49
1:E:223:LYS:O	1:E:223:LYS:CG	2.60	0.49
1:E:438:LEU:HD22	1:E:442:ILE:CD1	2.43	0.49
1:E:240:LYS:O	1:E:243:ALA:HB3	2.11	0.49
2:C:36:ARG:NH1	2:C:38:TYR:CZ	2.81	0.49
2:B:123:GLY:O	2:B:124:SER:C	2.49	0.49
1:F:108:VAL:HA	1:F:111:VAL:CG2	2.42	0.49
2:C:39:ASN:ND2	2:C:40:ASP:N	2.60	0.49
2:A:71:LEU:HD23	2:A:102:ALA:HB3	1.95	0.49
1:F:240:LYS:NZ	1:F:294:HIS:O	2.46	0.49
2:B:160:ILE:CD1	2:D:19:GLN:HE22	2.26	0.49
1:E:368:PHE:CD2	1:E:420:ILE:HD13	2.48	0.49
2:C:37:LEU:HD22	2:C:61:GLU:CG	2.42	0.49
1:F:429:LEU:O	1:F:433:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:PRO:HB2	1:F:103:LEU:HD21	1.95	0.49
1:F:302:ILE:HB	1:F:304:PHE:CE1	2.48	0.49
1:F:223:LYS:HB2	1:F:223:LYS:NZ	2.27	0.49
1:E:43:GLU:HG3	1:E:44:LEU:HG	1.94	0.49
1:F:360:ALA:O	1:F:362:GLU:N	2.46	0.49
1:E:47:GLU:HA	1:E:47:GLU:OE1	2.13	0.49
1:E:268:SER:C	1:E:270:PRO:HD3	2.33	0.49
2:C:41:LYS:O	2:C:42:VAL:HB	2.13	0.49
2:D:72:VAL:O	2:D:74:ALA:N	2.45	0.49
2:B:1:THR:OG1	2:B:2:THR:N	2.46	0.49
1:E:359:MET:SD	1:F:36:ARG:NH2	2.86	0.49
2:B:99:ASP:O	2:B:101:THR:N	2.46	0.49
1:F:432:LEU:C	1:F:434:ALA:H	2.16	0.49
1:F:89:VAL:HG12	1:F:89:VAL:O	2.13	0.49
1:F:384:ASN:HD21	1:F:390:ILE:HG12	1.77	0.49
1:E:43:GLU:O	1:E:45:ARG:N	2.46	0.49
2:D:13:VAL:HB	2:D:168:ILE:HD11	1.95	0.49
1:E:10:VAL:HG13	1:E:24:LYS:HB2	1.94	0.49
2:C:105:ILE:O	2:C:112:VAL:HA	2.13	0.48
2:A:49:GLY:O	2:A:50:THR:C	2.52	0.48
1:F:221:ALA:O	1:F:222:MET:CB	2.61	0.48
2:A:20:ALA:HB2	2:A:31:VAL:CG2	2.42	0.48
2:A:107:THR:C	2:A:109:ASN:H	2.16	0.48
1:E:345:THR:HG23	1:E:373:ILE:CD1	2.42	0.48
1:E:79:ILE:CG2	1:E:103:LEU:HB2	2.42	0.48
2:D:72:VAL:C	2:D:74:ALA:N	2.66	0.48
2:D:104:LEU:C	2:D:105:ILE:HG13	2.32	0.48
1:E:96:VAL:CG2	1:E:97:ASP:N	2.75	0.48
2:A:67:HIS:O	2:A:70:HIS:HD2	1.96	0.48
1:F:18:ILE:HD11	1:F:347:PRO:HD3	1.95	0.48
1:F:387:THR:CG2	1:F:388:GLU:N	2.63	0.48
2:B:37:LEU:HB3	2:B:61:GLU:HB3	1.95	0.48
1:F:62:GLY:O	1:F:66:ILE:HG13	2.14	0.48
1:E:84:THR:HA	1:E:261:ILE:HD11	1.95	0.48
1:E:4:MET:HG2	1:E:8:GLU:CB	2.42	0.48
2:D:136:LEU:C	2:D:138:GLU:N	2.60	0.48
1:E:369:THR:O	1:E:372:GLY:N	2.46	0.48
1:F:384:ASN:HD21	1:F:390:ILE:H	1.59	0.48
2:C:41:LYS:N	2:C:41:LYS:CD	2.76	0.48
1:F:127:ALA:CB	1:F:226:ILE:HG22	2.44	0.48
1:F:364:VAL:HG22	1:F:413:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLU:OE1	1:F:93:GLY:N	2.46	0.48
1:F:96:VAL:HG23	1:F:97:ASP:N	2.27	0.48
2:C:18:GLY:HA2	2:C:31:VAL:O	2.14	0.48
1:E:34:ARG:NH1	1:E:37:ARG:HE	2.12	0.48
1:F:427:LYS:HG2	1:F:427:LYS:O	2.13	0.48
2:C:38:TYR:O	2:C:39:ASN:C	2.51	0.48
2:C:66:MET:C	2:C:68:GLN:H	2.16	0.48
2:D:60:PHE:C	2:D:64:LEU:HD23	2.33	0.48
1:E:341:GLU:OE1	1:E:374:LYS:HE2	2.13	0.48
2:A:138:GLU:C	2:A:139:ASN:ND2	2.65	0.48
2:B:62:ARG:HE	2:B:62:ARG:HA	1.77	0.48
1:E:117:GLU:O	1:E:119:ASN:N	2.46	0.48
2:A:123:GLY:O	2:A:124:SER:C	2.51	0.48
2:A:43:ILE:HG12	2:A:171:LEU:HD22	1.95	0.48
2:A:4:VAL:HG13	2:A:4:VAL:O	2.13	0.48
1:E:258:ILE:C	1:E:259:ASP:O	2.51	0.48
2:A:67:HIS:ND1	2:A:73:LYS:HE2	2.29	0.48
1:F:315:PRO:O	1:F:318:LEU:HD12	2.13	0.48
1:E:117:GLU:HA	1:E:120:ARG:HB2	1.96	0.48
2:C:48:GLY:O	2:C:49:GLY:C	2.51	0.48
2:C:58:GLU:OE1	2:C:62:ARG:NH2	2.47	0.48
2:B:53:ALA:O	2:B:57:PHE:HB2	2.14	0.48
1:E:77:PRO:CB	1:E:107:ALA:HB2	2.39	0.48
2:A:3:ILE:HD12	2:A:34:VAL:CG1	2.44	0.48
1:E:394:ARG:O	1:E:398:VAL:HG23	2.14	0.48
1:E:432:LEU:O	1:E:434:ALA:N	2.46	0.48
2:C:94:LEU:HD12	2:C:122:ILE:HB	1.96	0.48
1:F:406:ILE:CD1	1:F:418:ILE:HG21	2.43	0.48
1:F:272:VAL:O	1:F:273:SER:C	2.52	0.48
2:D:85:ASP:O	2:D:86:ARG:CB	2.62	0.48
2:A:6:VAL:CG2	2:A:137:LEU:HD21	2.44	0.48
1:F:49:THR:HG21	1:F:325:ARG:HH12	1.77	0.48
1:F:435:ASP:O	1:F:437:ASP:N	2.39	0.48
2:B:44:ALA:HB2	2:B:97:VAL:CA	2.23	0.48
2:A:38:TYR:HB2	2:A:61:GLU:OE2	2.14	0.48
2:D:58:GLU:HA	2:D:61:GLU:HB3	1.96	0.48
2:D:76:VAL:O	2:D:80:LYS:HB2	2.14	0.48
2:C:59:LEU:CD2	2:C:78:LEU:HD22	2.44	0.48
2:B:163:ASN:C	2:B:163:ASN:ND2	2.63	0.48
2:D:37:LEU:HD22	2:D:61:GLU:CB	2.36	0.48
2:B:123:GLY:O	2:B:126:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:ILE:HG23	1:F:328:ILE:HG22	1.95	0.48
1:F:278:GLN:HE22	1:F:318:LEU:HA	1.78	0.48
2:B:36:ARG:HH11	2:B:36:ARG:HB3	1.78	0.48
2:A:56:LEU:HD11	2:A:88:LEU:CD1	2.44	0.48
2:D:16:GLY:C	2:D:152:LEU:HD11	2.34	0.48
1:E:384:ASN:OD1	1:E:394:ARG:HD2	2.14	0.48
2:B:140:THR:CG2	2:B:142:LEU:HD11	2.43	0.48
2:B:1:THR:HB	2:B:33:LYS:CE	2.43	0.48
1:E:401:ARG:NH2	1:E:442:ILE:HB	2.29	0.48
1:F:19:GLY:O	1:F:24:LYS:CE	2.62	0.48
2:B:79:ALA:O	2:B:110:GLY:HA2	2.14	0.48
2:A:30:ASN:HA	2:A:165:PHE:CE2	2.49	0.48
2:A:28:LYS:CG	2:A:30:ASN:ND2	2.77	0.48
2:D:51:ALA:HB1	2:C:109:ASN:O	2.14	0.47
2:B:119:LEU:HD23	2:B:130:GLN:OE1	2.14	0.47
2:B:57:PHE:O	2:B:61:GLU:CD	2.53	0.47
1:F:103:LEU:O	1:F:247:VAL:CG2	2.61	0.47
1:E:319:ILE:O	1:E:319:ILE:HG13	2.14	0.47
1:F:71:ALA:O	1:F:72:LYS:C	2.53	0.47
2:D:41:LYS:HD2	2:D:171:LEU:CD1	2.44	0.47
2:A:104:LEU:HA	2:A:113:VAL:O	2.13	0.47
2:A:112:VAL:CG1	2:A:113:VAL:N	2.77	0.47
2:A:53:ALA:O	2:A:57:PHE:HB2	2.14	0.47
1:E:123:ALA:HB1	1:E:229:GLU:CG	2.42	0.47
1:F:77:PRO:HB2	1:F:103:LEU:CD2	2.44	0.47
2:A:149:GLU:CD	2:A:168:ILE:HD13	2.33	0.47
2:D:30:ASN:HA	2:D:165:PHE:CD2	2.49	0.47
2:D:115:PRO:HB2	2:D:118:ASP:CA	2.44	0.47
1:E:105:ASP:HA	1:E:108:VAL:HB	1.96	0.47
2:A:81:ASP:HA	2:A:85:ASP:OD2	2.13	0.47
2:D:15:ALA:CB	2:D:152:LEU:HD12	2.43	0.47
2:D:37:LEU:HD11	2:D:60:PHE:HB3	1.97	0.47
2:D:60:PHE:CE2	2:D:97:VAL:HG21	2.50	0.47
1:F:113:VAL:O	1:F:113:VAL:HG12	2.13	0.47
2:A:1:THR:HB	2:A:162:THR:CG2	2.42	0.47
1:E:245:ASP:O	1:E:249:GLN:HB3	2.15	0.47
2:D:82:TRP:CD1	2:D:89:ARG:HG3	2.49	0.47
1:E:17:ILE:HB	1:E:24:LYS:CE	2.44	0.47
1:E:16:HIS:CG	1:E:69:ARG:HD2	2.49	0.47
2:B:61:GLU:O	2:B:64:LEU:HD13	2.14	0.47
2:A:116:GLU:O	2:A:117:ASN:CB	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:72:VAL:O	2:A:75:ALA:N	2.28	0.47
2:B:88:LEU:HD12	2:B:89:ARG:NE	2.26	0.47
2:D:62:ARG:O	2:D:65:GLU:OE2	2.33	0.47
2:D:1:THR:O	2:D:123:GLY:HA3	2.14	0.47
1:F:109:LYS:O	1:F:113:VAL:HG23	2.14	0.47
1:F:5:THR:HB	1:F:6:PRO:CD	2.45	0.47
2:B:74:ALA:O	2:B:75:ALA:CB	2.63	0.47
1:F:90:GLY:O	1:F:91:TYR:HB2	2.14	0.47
2:C:60:PHE:O	2:C:62:ARG:N	2.48	0.47
1:F:124:GLU:C	1:F:126:LEU:N	2.67	0.47
1:F:96:VAL:CG2	1:F:97:ASP:N	2.78	0.47
1:E:43:GLU:C	1:E:45:ARG:H	2.16	0.47
1:F:44:LEU:HA	1:F:47:GLU:HB2	1.96	0.47
2:C:58:GLU:O	2:C:62:ARG:HG2	2.14	0.47
2:D:99:ASP:CG	2:D:100:GLU:N	2.67	0.47
1:E:227:GLU:C	1:E:229:GLU:N	2.68	0.47
1:F:108:VAL:CA	1:F:111:VAL:HG23	2.41	0.47
2:A:13:VAL:C	2:A:14:ILE:HD12	2.34	0.47
1:F:274:ARG:C	1:F:276:GLY:H	2.18	0.47
2:C:141:GLU:O	2:C:147:ILE:HD11	2.14	0.47
1:E:393:ARG:HG3	3:E:905:DAT:H5'1	1.96	0.47
2:A:154:ILE:O	2:A:157:ASP:HB2	2.14	0.47
2:A:82:TRP:CZ3	2:A:89:ARG:HA	2.39	0.47
2:A:7:ARG:NH2	2:A:102:ALA:O	2.47	0.47
2:D:71:LEU:O	2:D:74:ALA:CB	2.63	0.47
2:D:124:SER:C	2:D:126:GLY:H	2.18	0.47
1:F:235:ASN:N	1:F:236:PRO:HD3	2.30	0.47
1:E:239:LEU:O	1:E:240:LYS:CD	2.62	0.47
1:E:96:VAL:O	1:E:98:SER:N	2.48	0.47
1:E:257:GLU:O	1:E:259:ASP:O	2.33	0.47
1:F:360:ALA:C	1:F:362:GLU:H	2.17	0.47
1:E:427:LYS:HG2	1:E:427:LYS:O	2.14	0.47
2:B:86:ARG:HD3	2:A:84:THR:O	2.15	0.47
2:C:7:ARG:NH1	2:C:118:ASP:OD1	2.47	0.47
1:F:343:ILE:O	1:F:351:ILE:CD1	2.63	0.47
1:F:244:ILE:CG2	1:F:248:GLU:HG3	2.44	0.47
2:D:94:LEU:HD22	2:D:122:ILE:HG21	1.96	0.47
2:B:7:ARG:HH12	2:B:102:ALA:H	1.58	0.47
1:F:274:ARG:C	1:F:276:GLY:N	2.68	0.47
1:E:335:LEU:HD13	1:E:343:ILE:CD1	2.45	0.47
2:A:139:ASN:N	2:A:139:ASN:ND2	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ASP:OD2	2:B:166:HIS:CE1	2.68	0.47
1:F:353:VAL:HA	1:F:356:LYS:HD3	1.97	0.47
2:B:117:ASN:HD22	2:B:117:ASN:HA	1.51	0.47
1:F:227:GLU:O	1:F:230:ALA:HB3	2.14	0.47
1:E:263:LYS:O	1:E:263:LYS:HD3	2.13	0.47
2:D:19:GLN:HG3	2:D:26:VAL:HG21	1.96	0.47
2:B:94:LEU:N	2:B:94:LEU:HD12	2.28	0.47
1:F:376:ILE:O	1:F:379:ALA:N	2.48	0.47
2:C:35:ARG:HD2	2:C:36:ARG:O	2.15	0.47
2:C:63:LYS:C	2:C:65:GLU:N	2.68	0.47
1:E:442:ILE:HA	1:F:329:ARG:CB	2.44	0.47
1:F:126:LEU:HA	1:F:129:GLU:CB	2.45	0.47
1:F:85:LYS:HE2	1:F:86:PHE:CE1	2.50	0.47
1:E:260:LYS:CA	1:E:260:LYS:HE2	2.43	0.47
2:C:55:THR:O	2:C:57:PHE:N	2.48	0.46
2:D:37:LEU:HD13	2:D:61:GLU:N	2.31	0.46
1:F:9:ILE:O	1:F:13:LEU:HG	2.14	0.46
2:C:44:ALA:HB2	2:C:97:VAL:HA	1.97	0.46
1:E:220:ASP:O	1:E:221:ALA:HB2	2.16	0.46
1:F:45:ARG:HG2	1:F:45:ARG:O	2.15	0.46
1:F:88:GLU:C	1:F:90:GLY:N	2.69	0.46
1:E:4:MET:HG2	1:E:8:GLU:HB3	1.96	0.46
2:D:30:ASN:O	2:D:165:PHE:CE2	2.69	0.46
2:C:35:ARG:HH11	2:C:37:LEU:HA	1.77	0.46
2:B:57:PHE:HA	2:B:57:PHE:HD2	1.67	0.46
2:A:39:ASN:C	2:A:41:LYS:H	2.18	0.46
2:B:140:THR:HB	2:B:142:LEU:CD1	2.33	0.46
2:C:88:LEU:HD23	2:C:88:LEU:HA	1.85	0.46
2:D:37:LEU:HB3	2:D:39:ASN:ND2	2.30	0.46
1:F:100:ILE:C	1:F:102:ASP:H	2.19	0.46
2:C:44:ALA:CB	2:C:97:VAL:HA	2.45	0.46
2:D:82:TRP:NE1	2:D:89:ARG:HG2	2.31	0.46
1:F:45:ARG:NH1	1:F:45:ARG:CG	2.77	0.46
1:F:267:SER:HA	2:D:87:MET:CE	2.45	0.46
1:E:332:LEU:N	1:E:332:LEU:HD12	2.30	0.46
1:F:318:LEU:O	1:F:319:ILE:C	2.54	0.46
1:E:402:LEU:HD12	1:E:429:LEU:HG	1.97	0.46
2:B:73:LYS:HA	2:B:77:GLU:OE2	2.16	0.46
2:C:36:ARG:O	2:C:37:LEU:HG	2.14	0.46
2:B:44:ALA:HB1	2:B:96:ALA:O	2.16	0.46
1:E:110:MET:O	1:E:113:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:HD3	2:B:30:ASN:C	2.36	0.46
2:D:83:ARG:HD2	2:D:83:ARG:HA	1.78	0.46
1:E:335:LEU:HD13	1:E:343:ILE:HD11	1.97	0.46
1:F:278:GLN:HE21	1:F:322:LEU:HD12	1.80	0.46
1:E:355:TYR:CE1	1:E:399:LEU:HD13	2.50	0.46
1:E:309:ALA:O	1:E:310:PHE:HB2	2.15	0.46
1:F:345:THR:CG2	1:F:373:ILE:HD12	2.45	0.46
1:F:257:GLU:HG2	1:F:260:LYS:HB2	1.97	0.46
2:C:40:ASP:O	2:C:41:LYS:O	2.32	0.46
2:C:69:GLY:O	2:C:71:LEU:N	2.48	0.46
2:B:122:ILE:H	2:B:122:ILE:HD13	1.80	0.46
2:D:106:ILE:C	2:D:108:GLY:N	2.69	0.46
1:F:122:ARG:O	1:F:125:GLU:HG2	2.16	0.46
2:D:152:LEU:HD13	2:D:166:HIS:CD2	2.39	0.46
2:D:37:LEU:C	2:D:39:ASN:N	2.68	0.46
1:F:406:ILE:HD12	1:F:418:ILE:HG21	1.96	0.46
1:F:349:ALA:O	1:F:350:SER:O	2.34	0.46
1:E:348:ASN:C	1:E:348:ASN:ND2	2.69	0.46
1:E:77:PRO:HB2	1:E:103:LEU:HD11	1.97	0.46
2:A:34:VAL:HG22	2:A:167:THR:HB	1.97	0.46
2:B:51:ALA:O	2:B:54:PHE:HB3	2.15	0.46
2:D:89:ARG:C	2:D:90:LYS:HG3	2.36	0.46
1:F:84:THR:O	1:F:87:THR:HG22	2.16	0.46
1:E:364:VAL:CG2	1:E:413:LEU:HB2	2.45	0.46
1:E:409:ASP:O	1:E:411:SER:N	2.49	0.46
1:E:43:GLU:HA	1:E:43:GLU:OE2	2.15	0.46
2:D:46:PHE:C	2:D:46:PHE:CD1	2.88	0.46
2:A:82:TRP:CG	2:A:108:GLY:HA2	2.51	0.46
2:A:60:PHE:CE2	2:A:97:VAL:HG21	2.51	0.46
2:D:31:VAL:O	2:D:33:LYS:N	2.49	0.46
2:B:13:VAL:HA	2:B:169:GLU:O	2.16	0.46
2:D:106:ILE:HG13	2:D:111:ASP:O	2.16	0.46
1:E:63:LYS:HG2	1:E:332:LEU:HD22	1.98	0.46
2:D:51:ALA:HB2	2:C:111:ASP:HB2	1.98	0.46
2:D:62:ARG:HG3	2:D:63:LYS:N	2.30	0.46
2:D:64:LEU:N	2:D:64:LEU:HD22	2.31	0.46
1:F:432:LEU:C	1:F:434:ALA:N	2.68	0.46
2:C:15:ALA:CA	2:C:168:ILE:HG23	2.42	0.46
1:F:85:LYS:C	1:F:87:THR:H	2.19	0.46
1:E:369:THR:O	1:E:370:ASP:C	2.52	0.46
2:C:2:THR:CG2	2:C:129:ALA:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:ALA:HB3	2:D:27:MET:HG3	1.98	0.46
2:C:66:MET:C	2:C:68:GLN:N	2.69	0.46
2:B:101:THR:O	2:B:101:THR:CG2	2.63	0.46
2:D:83:ARG:NH1	2:D:89:ARG:HE	2.14	0.46
2:C:163:ASN:ND2	2:C:164:HIS:N	2.64	0.46
1:E:87:THR:O	1:E:88:GLU:C	2.53	0.46
1:E:422:ALA:C	1:E:424:TYR:H	2.19	0.46
1:F:409:ASP:O	1:F:412:ASP:N	2.41	0.46
1:F:54:LEU:HD11	1:F:315:PRO:HB3	1.98	0.46
2:D:130:GLN:HA	2:D:133:ALA:HB3	1.98	0.46
1:F:360:ALA:C	1:F:362:GLU:N	2.69	0.46
2:B:173:TYR:HD1	2:B:173:TYR:O	1.98	0.46
1:E:365:ASN:O	1:E:417:ASN:HA	2.16	0.46
1:F:388:GLU:OE1	1:F:440:ARG:NH2	2.49	0.45
2:C:37:LEU:C	2:C:39:ASN:H	2.20	0.45
2:C:41:LYS:O	2:C:42:VAL:CB	2.63	0.45
1:F:70:LEU:O	1:F:70:LEU:HG	2.16	0.45
2:C:44:ALA:CB	2:C:97:VAL:HG13	2.33	0.45
1:E:261:ILE:O	1:E:261:ILE:HG22	2.15	0.45
1:E:374:LYS:O	1:E:378:GLU:HG3	2.16	0.45
2:A:56:LEU:HD11	2:A:88:LEU:HD12	1.97	0.45
2:B:55:THR:OG1	2:A:80:LYS:CB	2.64	0.45
2:D:37:LEU:CD1	2:D:60:PHE:HB3	2.45	0.45
1:E:24:LYS:O	1:E:28:ALA:HB2	2.16	0.45
1:F:1:MET:HG2	1:F:3:GLU:HG3	1.98	0.45
1:E:257:GLU:CD	1:F:279:ARG:HH21	2.20	0.45
2:B:135:ALA:O	2:B:139:ASN:ND2	2.43	0.45
2:B:128:TYR:HD2	2:B:158:ILE:HG23	1.80	0.45
2:A:66:MET:SD	2:A:67:HIS:N	2.90	0.45
2:A:8:ARG:NH2	2:A:137:LEU:O	2.50	0.45
1:F:282:LEU:O	1:F:283:PRO:C	2.55	0.45
2:B:58:GLU:O	2:B:61:GLU:HG2	2.17	0.45
1:F:429:LEU:O	1:F:430:ASP:C	2.52	0.45
1:E:442:ILE:CB	1:F:329:ARG:HB2	2.46	0.45
1:F:122:ARG:CZ	1:F:125:GLU:CD	2.85	0.45
1:E:103:LEU:HG	1:E:103:LEU:O	2.15	0.45
2:B:122:ILE:CD1	2:B:122:ILE:H	2.29	0.45
1:F:103:LEU:HD13	1:F:247:VAL:CG2	2.46	0.45
2:B:171:LEU:HD12	2:B:172:SER:H	1.81	0.45
2:A:145:ARG:NH1	2:A:170:GLU:OE1	2.49	0.45
1:F:65:GLU:HA	1:F:65:GLU:OE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ARG:NH2	1:F:314:LYS:HE2	2.32	0.45
2:C:47:ALA:HB3	2:C:94:LEU:CD1	2.46	0.45
1:F:64:THR:HG21	1:F:80:LYS:NZ	2.31	0.45
1:F:298:LYS:HE2	1:F:300:ASP:OD1	2.17	0.45
1:F:12:GLU:HA	1:F:15:LYS:HD3	1.98	0.45
2:C:36:ARG:CG	2:C:37:LEU:H	2.15	0.45
2:C:86:ARG:HH11	2:C:86:ARG:HG3	1.82	0.45
2:A:100:GLU:N	2:A:100:GLU:CD	2.64	0.45
2:C:24:ASN:ND2	2:C:24:ASN:N	2.65	0.45
1:E:108:VAL:HA	1:E:111:VAL:HG22	1.98	0.45
2:D:94:LEU:CD2	2:D:122:ILE:HG21	2.47	0.45
1:E:413:LEU:HD23	1:E:413:LEU:H	1.82	0.45
2:B:5:SER:CB	2:B:14:ILE:HA	2.45	0.45
2:C:104:LEU:N	2:C:104:LEU:HD12	2.32	0.45
2:C:80:LYS:O	2:C:82:TRP:N	2.50	0.45
1:E:107:ALA:CB	1:E:247:VAL:HG22	2.47	0.45
2:A:35:ARG:N	2:A:45:GLY:HA2	2.30	0.45
2:B:54:PHE:C	2:B:56:LEU:H	2.20	0.45
2:B:91:LEU:O	2:B:92:GLU:O	2.35	0.45
1:F:426:SER:HB3	1:F:430:ASP:OD1	2.16	0.45
2:D:62:ARG:HG3	2:D:63:LYS:H	1.82	0.45
2:C:16:GLY:C	2:C:152:LEU:HD11	2.38	0.45
1:E:360:ALA:O	1:E:362:GLU:N	2.49	0.45
1:F:244:ILE:C	1:F:246:ALA:N	2.71	0.45
1:F:242:ASP:O	1:F:246:ALA:N	2.49	0.45
1:F:88:GLU:O	1:F:90:GLY:N	2.50	0.45
1:E:402:LEU:HD13	1:E:429:LEU:HD11	1.98	0.45
1:F:55:MET:CE	1:F:66:ILE:HD12	2.42	0.45
2:A:5:SER:HA	2:A:13:VAL:O	2.17	0.45
1:E:5:THR:HB	1:E:6:PRO:HD2	1.98	0.45
1:E:41:ASN:C	1:E:43:GLU:N	2.70	0.45
1:E:43:GLU:CA	1:E:43:GLU:OE2	2.65	0.45
2:B:104:LEU:HA	2:B:113:VAL:O	2.17	0.45
1:F:101:ARG:C	1:F:102:ASP:OD1	2.55	0.44
2:C:121:ALA:CB	2:C:130:GLN:HE21	2.30	0.44
1:E:413:LEU:N	1:E:413:LEU:HD23	2.33	0.44
1:E:413:LEU:O	1:E:416:GLN:HB3	2.17	0.44
2:C:46:PHE:HE1	2:C:48:GLY:O	2.00	0.44
1:E:244:ILE:C	1:E:246:ALA:N	2.69	0.44
1:E:81:VAL:HG21	1:E:99:ILE:HG12	2.00	0.44
2:C:63:LYS:CG	2:C:78:LEU:HG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:VAL:HA	2:B:170:GLU:HA	1.99	0.44
1:F:244:ILE:O	1:F:246:ALA:N	2.51	0.44
2:B:7:ARG:CG	2:B:12:VAL:HG22	2.46	0.44
1:E:20:GLN:NE2	1:E:333:GLN:H	2.05	0.44
1:E:96:VAL:CG1	1:E:280:ASP:HB3	2.47	0.44
1:F:122:ARG:NH2	1:F:125:GLU:CG	2.80	0.44
2:D:45:GLY:O	2:D:95:LEU:HA	2.17	0.44
2:A:84:THR:O	2:A:84:THR:HG22	2.17	0.44
2:B:163:ASN:HD21	2:B:165:PHE:HB3	1.83	0.44
2:D:35:ARG:HG3	2:D:36:ARG:N	2.33	0.44
2:C:115:PRO:O	2:C:117:ASN:N	2.51	0.44
2:A:13:VAL:HG23	2:A:169:GLU:O	2.17	0.44
1:F:366:ILE:HG22	1:F:367:GLU:N	2.32	0.44
1:E:258:ILE:CG2	1:E:259:ASP:N	2.80	0.44
2:B:82:TRP:C	2:B:83:ARG:HG2	2.38	0.44
2:B:39:ASN:N	2:B:62:ARG:NH2	2.64	0.44
2:D:143:SER:OG	2:D:144:ALA:N	2.50	0.44
2:D:8:ARG:CB	2:D:144:ALA:HB2	2.27	0.44
1:E:258:ILE:HG12	1:E:318:LEU:HD21	2.00	0.44
1:E:92:VAL:HG13	1:F:92:VAL:O	2.18	0.44
2:A:89:ARG:H	2:A:91:LEU:CD2	2.31	0.44
2:B:88:LEU:H	2:B:88:LEU:CD2	2.26	0.44
1:F:29:ILE:O	1:F:30:ALA:C	2.56	0.44
1:F:34:ARG:HG3	1:F:38:MET:HE1	2.00	0.44
2:B:150:LYS:CD	2:C:139:ASN:HD21	2.26	0.44
2:A:160:ILE:HG13	2:A:161:TYR:CE2	2.52	0.44
1:E:81:VAL:CG1	1:E:86:PHE:HE2	2.31	0.44
2:A:71:LEU:CD2	2:A:102:ALA:HB3	2.48	0.44
2:A:104:LEU:H	2:A:104:LEU:HD12	1.83	0.44
1:F:233:LEU:O	1:F:234:VAL:C	2.56	0.44
2:A:2:THR:HA	2:A:122:ILE:O	2.17	0.44
1:E:239:LEU:HD23	1:E:239:LEU:O	2.17	0.44
1:E:87:THR:HA	1:E:277:VAL:HG21	2.00	0.44
1:E:374:LYS:HB2	1:E:374:LYS:HE3	1.77	0.44
1:E:375:ARG:HG3	1:E:422:ALA:HB1	1.99	0.44
2:B:9:ASN:HD22	2:B:9:ASN:HA	1.67	0.44
1:E:53:ILE:HG13	1:E:328:ILE:HB	2.00	0.44
1:F:65:GLU:HG2	3:F:906:DAT:H2'2	1.98	0.44
1:E:100:ILE:HG13	1:E:299:THR:CG2	2.48	0.44
1:E:128:GLU:CG	1:E:132:LEU:HD21	2.47	0.44
2:D:145:ARG:HH11	2:D:145:ARG:HG2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:LYS:HE3	2:B:167:THR:CG2	2.48	0.44
1:E:244:ILE:O	1:E:248:GLU:N	2.51	0.44
1:E:88:GLU:O	1:E:90:GLY:N	2.51	0.44
1:E:342:ARG:C	1:E:344:LEU:N	2.72	0.44
1:F:282:LEU:HB2	1:F:283:PRO:HD3	1.98	0.44
2:A:85:ASP:O	2:A:86:ARG:CB	2.66	0.44
2:C:145:ARG:NE	2:C:170:GLU:OE1	2.51	0.44
1:E:85:LYS:HG3	1:F:280:ASP:OD1	2.18	0.44
2:A:30:ASN:ND2	2:A:30:ASN:N	2.65	0.44
2:A:139:ASN:HD22	2:A:139:ASN:N	2.16	0.44
2:D:127:PRO:O	2:D:128:TYR:C	2.56	0.44
1:E:100:ILE:O	1:E:104:THR:HG23	2.18	0.43
2:A:144:ALA:C	2:A:146:GLU:H	2.21	0.43
2:A:72:VAL:O	2:A:74:ALA:N	2.51	0.43
1:F:220:ASP:C	1:F:222:MET:H	2.21	0.43
2:C:141:GLU:O	2:C:142:LEU:O	2.36	0.43
1:E:265:GLY:HA2	1:E:312:ILE:CG2	2.47	0.43
2:B:26:VAL:O	2:B:26:VAL:HG22	2.18	0.43
2:C:38:TYR:C	2:C:40:ASP:N	2.60	0.43
2:B:79:ALA:HB2	2:B:112:VAL:HG23	2.00	0.43
2:B:39:ASN:CA	2:B:62:ARG:NH2	2.79	0.43
2:C:86:ARG:H	2:C:87:MET:CE	2.30	0.43
2:D:72:VAL:HB	2:D:73:LYS:NZ	2.33	0.43
2:C:117:ASN:O	2:C:118:ASP:HB2	2.18	0.43
1:F:431:ALA:O	1:F:432:LEU:HB2	2.18	0.43
2:C:47:ALA:HB3	2:C:94:LEU:CG	2.48	0.43
2:B:50:THR:HB	2:A:111:ASP:CB	2.48	0.43
1:E:85:LYS:C	1:E:87:THR:H	2.21	0.43
1:F:267:SER:CA	2:D:87:MET:HG3	2.48	0.43
1:E:409:ASP:O	1:E:412:ASP:N	2.44	0.43
1:F:56:ILE:HD11	1:F:315:PRO:HG2	1.99	0.43
1:E:225:LEU:HA	1:E:228:GLU:HB3	2.01	0.43
1:E:104:THR:HG22	1:E:247:VAL:HG11	2.01	0.43
1:F:312:ILE:HB	2:D:62:ARG:CD	2.49	0.43
1:E:122:ARG:O	1:E:126:LEU:HG	2.19	0.43
1:E:223:LYS:CD	1:E:226:ILE:HG13	2.32	0.43
1:E:432:LEU:CB	1:E:443:LEU:HD11	2.43	0.43
2:A:59:LEU:CD2	2:A:87:MET:SD	3.07	0.43
1:F:49:THR:HG21	1:F:325:ARG:NH1	2.33	0.43
2:B:134:ARG:HH11	2:B:134:ARG:HG2	1.83	0.43
1:F:292:THR:HG22	1:F:295:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4:VAL:HA	2:A:120:ILE:O	2.18	0.43
2:A:81:ASP:HA	2:A:85:ASP:CG	2.37	0.43
2:B:27:MET:HE3	2:A:105:ILE:HD13	2.00	0.43
1:E:227:GLU:O	1:E:230:ALA:N	2.39	0.43
1:F:21:ASP:HA	1:F:24:LYS:HE2	1.99	0.43
1:F:432:LEU:CD1	1:F:442:ILE:HD11	2.49	0.43
1:E:281:LEU:O	1:E:282:LEU:C	2.55	0.43
1:E:358:LEU:HD11	1:F:48:VAL:HG11	2.01	0.43
2:C:51:ALA:O	2:C:53:ALA:N	2.43	0.43
2:B:30:ASN:HA	2:B:165:PHE:CD2	2.54	0.43
1:F:382:GLN:HE21	1:F:386:SER:HB3	1.84	0.43
2:D:16:GLY:N	2:D:152:LEU:HD11	2.34	0.43
1:E:431:ALA:O	1:E:434:ALA:HB3	2.17	0.43
1:E:408:TYR:HE2	1:F:25:ARG:HH21	1.61	0.43
2:D:89:ARG:O	2:D:91:LEU:HD13	2.18	0.43
1:E:278:GLN:OE1	1:E:319:ILE:HG23	2.19	0.43
1:E:413:LEU:O	1:E:414:SER:C	2.57	0.43
2:B:144:ALA:C	2:B:146:GLU:N	2.71	0.43
2:D:117:ASN:O	2:D:118:ASP:HB2	2.18	0.43
2:C:7:ARG:NH1	2:C:118:ASP:HB3	2.33	0.43
2:B:1:THR:O	2:B:2:THR:OG1	2.35	0.43
1:F:74:ALA:C	1:F:76:ALA:H	2.22	0.43
2:D:106:ILE:O	2:D:108:GLY:N	2.51	0.43
2:C:21:THR:HG21	2:C:161:TYR:CD2	2.44	0.43
1:F:346:GLU:O	1:F:347:PRO:C	2.56	0.43
2:B:44:ALA:HB1	2:B:96:ALA:C	2.39	0.43
1:E:231:ALA:O	1:E:232:LYS:C	2.56	0.43
1:E:241:GLN:HG3	1:E:242:ASP:N	2.34	0.43
1:F:223:LYS:HG2	1:F:224:LEU:CD2	2.48	0.43
2:B:150:LYS:CE	2:C:139:ASN:HD21	2.31	0.43
1:F:397:THR:OG1	1:F:398:VAL:N	2.51	0.43
1:F:47:GLU:OE2	1:F:47:GLU:HA	2.19	0.43
2:A:150:LYS:HE3	2:D:139:ASN:HD21	1.84	0.43
1:E:420:ILE:HG12	1:E:420:ILE:O	2.18	0.43
2:A:10:GLY:O	2:A:173:TYR:CE1	2.72	0.43
1:F:436:GLU:HA	1:F:439:SER:CB	2.49	0.43
2:B:160:ILE:HG22	2:D:160:ILE:HD12	2.00	0.43
2:A:63:LYS:HG2	2:A:74:ALA:HA	2.01	0.42
2:A:72:VAL:C	2:A:74:ALA:N	2.73	0.42
2:B:49:GLY:C	2:B:51:ALA:N	2.71	0.42
2:D:1:THR:O	2:D:124:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:ARG:CZ	1:F:35:TRP:CZ3	3.01	0.42
1:F:35:TRP:CZ3	1:F:36:ARG:HG3	2.54	0.42
1:E:249:GLN:CG	1:E:250:HIS:N	2.69	0.42
2:C:90:LYS:HB3	2:C:90:LYS:NZ	2.34	0.42
1:E:58:PRO:HG2	1:E:61:VAL:CG1	2.49	0.42
2:B:134:ARG:O	2:B:138:GLU:HB2	2.18	0.42
2:A:52:ASP:OD2	2:A:88:LEU:HD21	2.19	0.42
2:D:60:PHE:O	2:D:61:GLU:C	2.58	0.42
2:D:37:LEU:CD1	2:D:61:GLU:H	2.32	0.42
1:E:88:GLU:C	1:E:90:GLY:N	2.72	0.42
2:B:158:ILE:O	2:D:25:THR:HA	2.18	0.42
1:F:369:THR:CG2	1:F:370:ASP:N	2.82	0.42
1:F:353:VAL:HG12	1:F:353:VAL:O	2.19	0.42
1:E:436:GLU:O	1:E:440:ARG:HG3	2.19	0.42
2:B:38:TYR:CE1	2:B:64:LEU:HB2	2.55	0.42
2:A:54:PHE:HA	2:A:57:PHE:HB2	2.01	0.42
2:B:15:ALA:HB2	2:B:168:ILE:CG2	2.48	0.42
2:B:33:LYS:O	2:B:45:GLY:CA	2.67	0.42
1:F:235:ASN:N	1:F:236:PRO:CD	2.82	0.42
1:F:237:GLU:O	1:F:239:LEU:HD12	2.19	0.42
1:F:240:LYS:O	1:F:242:ASP:N	2.52	0.42
1:F:30:ALA:HB2	1:F:53:ILE:HD11	2.02	0.42
1:E:315:PRO:O	1:E:318:LEU:HD12	2.20	0.42
2:C:42:VAL:HG11	2:C:64:LEU:CD2	2.49	0.42
2:C:85:ASP:HB2	2:C:87:MET:HE3	2.02	0.42
2:D:60:PHE:O	2:D:64:LEU:HD23	2.19	0.42
1:E:432:LEU:O	1:E:435:ASP:N	2.51	0.42
1:E:366:ILE:HD12	1:E:418:ILE:HB	2.01	0.42
1:F:39:GLN:C	1:F:39:GLN:OE1	2.58	0.42
1:F:39:GLN:O	1:F:39:GLN:CD	2.58	0.42
1:F:368:PHE:CD2	1:F:420:ILE:HD13	2.54	0.42
2:A:37:LEU:O	2:A:38:TYR:O	2.37	0.42
2:B:48:GLY:O	2:B:49:GLY:C	2.58	0.42
2:D:145:ARG:NH1	2:D:145:ARG:HG2	2.34	0.42
2:D:52:ASP:C	2:D:54:PHE:N	2.71	0.42
2:D:75:ALA:O	2:D:79:ALA:HB3	2.19	0.42
1:F:233:LEU:O	1:F:235:ASN:ND2	2.52	0.42
2:C:121:ALA:HB3	2:C:130:GLN:NE2	2.35	0.42
1:F:39:GLN:O	1:F:40:LEU:HG	2.19	0.42
2:B:41:LYS:HG2	2:B:100:GLU:HG3	2.01	0.42
2:B:90:LYS:CE	2:A:83:ARG:NH2	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:MET:HE1	2:A:105:ILE:HD11	2.01	0.42
2:D:5:SER:HB2	2:D:14:ILE:HG12	2.01	0.42
1:F:21:ASP:CA	1:F:24:LYS:HG3	2.47	0.42
1:E:61:VAL:CG2	1:E:63:LYS:HZ2	2.32	0.42
2:B:94:LEU:H	2:B:94:LEU:CD1	2.31	0.42
2:B:16:GLY:C	2:B:152:LEU:HD11	2.39	0.42
2:D:41:LYS:O	2:D:42:VAL:CB	2.68	0.42
2:B:57:PHE:O	2:B:61:GLU:HG2	2.20	0.42
1:E:302:ILE:HB	1:E:304:PHE:CZ	2.55	0.42
2:A:113:VAL:O	2:A:115:PRO:HD3	2.20	0.42
1:E:407:SER:OG	1:F:36:ARG:NH2	2.53	0.42
1:F:34:ARG:NH1	1:F:250:HIS:CB	2.70	0.42
1:F:34:ARG:O	1:F:38:MET:SD	2.78	0.42
1:E:238:GLU:C	1:E:240:LYS:N	2.73	0.42
1:E:244:ILE:C	1:E:246:ALA:H	2.23	0.42
2:D:111:ASP:C	2:D:112:VAL:HG12	2.39	0.42
1:E:260:LYS:NZ	1:E:312:ILE:HG13	2.34	0.42
1:F:16:HIS:O	1:F:347:PRO:HB3	2.19	0.42
1:F:346:GLU:HB2	1:F:347:PRO:CD	2.49	0.42
2:A:106:ILE:N	2:A:106:ILE:HD12	2.34	0.42
2:B:37:LEU:O	2:B:40:ASP:N	2.50	0.42
2:A:114:GLN:NE2	2:A:116:GLU:OE2	2.49	0.42
2:A:40:ASP:O	2:A:43:ILE:HD13	2.20	0.42
2:D:37:LEU:CD1	2:D:61:GLU:N	2.83	0.42
1:F:100:ILE:O	1:F:102:ASP:N	2.46	0.42
1:F:101:ARG:O	1:F:102:ASP:OD1	2.37	0.42
1:E:31:LEU:HD22	1:E:70:LEU:HD11	2.02	0.42
1:E:364:VAL:HG21	1:E:413:LEU:HB2	2.02	0.42
1:E:41:ASN:HB2	1:E:43:GLU:HB3	2.01	0.42
1:F:369:THR:HG22	1:F:371:SER:H	1.85	0.42
1:F:81:VAL:O	1:F:256:ASP:N	2.52	0.42
2:C:109:ASN:C	2:C:111:ASP:N	2.70	0.42
2:B:37:LEU:O	2:B:40:ASP:HA	2.19	0.42
2:A:40:ASP:OD2	2:A:40:ASP:O	2.36	0.42
2:A:63:LYS:CE	2:A:77:GLU:HB3	2.49	0.42
1:E:36:ARG:O	1:E:39:GLN:HG3	2.20	0.42
2:A:136:LEU:HD11	2:D:135:ALA:O	2.19	0.42
2:B:135:ALA:HB2	2:C:132:ALA:HB1	2.02	0.42
2:B:173:TYR:CD1	2:B:173:TYR:O	2.73	0.42
1:F:402:LEU:HD13	1:F:429:LEU:CD1	2.49	0.42
2:D:66:MET:CG	2:D:67:HIS:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ILE:HB	1:F:329:ARG:HB2	2.00	0.42
2:A:159:CYS:HB3	2:A:162:THR:HG1	1.85	0.42
1:E:351:ILE:O	1:E:354:GLN:HB2	2.20	0.42
1:E:43:GLU:C	1:E:45:ARG:N	2.73	0.42
1:F:344:LEU:HD21	1:F:395:LEU:HG	2.02	0.42
2:D:143:SER:HB3	2:D:146:GLU:CG	2.48	0.41
2:A:41:LYS:C	2:A:43:ILE:H	2.23	0.41
1:E:227:GLU:O	1:E:229:GLU:N	2.52	0.41
2:A:1:THR:H1	2:A:33:LYS:HE2	1.85	0.41
1:E:70:LEU:O	1:E:73:LEU:HG	2.20	0.41
2:A:92:GLU:O	2:A:93:ALA:HB2	2.20	0.41
2:D:44:ALA:HA	2:D:97:VAL:HA	2.02	0.41
1:F:34:ARG:HD3	1:F:250:HIS:CG	2.55	0.41
2:A:13:VAL:HG11	2:A:145:ARG:HA	2.02	0.41
2:A:134:ARG:O	2:A:136:LEU:N	2.53	0.41
1:F:37:ARG:C	1:F:39:GLN:N	2.73	0.41
2:B:92:GLU:O	2:B:93:ALA:HB2	2.20	0.41
1:F:244:ILE:HG22	1:F:248:GLU:HG3	2.02	0.41
2:D:82:TRP:CE2	2:D:108:GLY:O	2.73	0.41
2:C:19:GLN:HB2	2:C:163:ASN:CG	2.41	0.41
2:C:46:PHE:C	2:C:46:PHE:CD1	2.93	0.41
2:A:10:GLY:O	2:A:173:TYR:CD1	2.73	0.41
2:B:140:THR:HG22	2:B:142:LEU:HG	2.01	0.41
1:F:71:ALA:HB1	1:F:78:PHE:HB2	2.01	0.41
1:E:71:ALA:O	1:E:74:ALA:N	2.52	0.41
2:B:59:LEU:O	2:B:60:PHE:CB	2.68	0.41
1:E:77:PRO:HB2	1:E:103:LEU:CD1	2.50	0.41
2:B:163:ASN:HD22	2:B:164:HIS:N	2.16	0.41
2:B:28:LYS:HD3	2:B:30:ASN:OD1	2.19	0.41
2:D:64:LEU:N	2:D:64:LEU:CD2	2.84	0.41
2:D:1:THR:N	2:D:161:TYR:O	2.48	0.41
2:D:28:LYS:HB2	2:C:113:VAL:HG13	2.01	0.41
1:F:77:PRO:HB3	1:F:107:ALA:HB2	2.02	0.41
1:F:131:ILE:O	1:F:132:LEU:HB3	2.20	0.41
1:E:282:LEU:HD21	1:E:321:GLU:HB3	2.02	0.41
2:C:123:GLY:O	2:C:125:GLY:N	2.53	0.41
1:E:43:GLU:CG	1:E:44:LEU:N	2.73	0.41
1:F:353:VAL:O	1:F:353:VAL:CG1	2.67	0.41
2:C:86:ARG:C	2:C:87:MET:HG2	2.40	0.41
1:F:385:GLU:OE2	2:D:70:HIS:CE1	2.74	0.41
2:B:3:ILE:HG12	2:B:46:PHE:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:GLN:HA	2:C:29:GLY:HA2	2.03	0.41
2:A:14:ILE:N	2:A:14:ILE:CD1	2.83	0.41
1:E:282:LEU:O	1:E:283:PRO:C	2.59	0.41
1:F:37:ARG:O	1:F:39:GLN:N	2.54	0.41
1:E:292:THR:OG1	1:E:293:LYS:N	2.53	0.41
2:C:105:ILE:CG2	2:C:106:ILE:N	2.83	0.41
2:C:70:HIS:CE1	2:C:73:LYS:HB2	2.55	0.41
2:C:85:ASP:OD1	2:C:85:ASP:N	2.53	0.41
2:B:34:VAL:HG12	2:B:169:GLU:HG3	2.02	0.41
2:B:72:VAL:C	2:B:74:ALA:N	2.71	0.41
1:F:365:ASN:ND2	1:F:367:GLU:OE2	2.49	0.41
1:E:96:VAL:C	1:E:98:SER:N	2.74	0.41
1:F:278:GLN:OE1	1:F:319:ILE:HG23	2.20	0.41
2:B:129:ALA:O	2:B:132:ALA:N	2.54	0.41
1:E:388:GLU:CD	1:E:440:ARG:NH2	2.74	0.41
2:C:124:SER:O	2:C:159:CYS:SG	2.67	0.41
1:E:428:HIS:O	1:E:429:LEU:HD23	2.20	0.41
1:F:254:PHE:HA	1:F:305:ILE:O	2.20	0.41
2:C:88:LEU:C	2:C:89:ARG:HG3	2.41	0.41
2:B:44:ALA:HB3	2:B:57:PHE:CZ	2.55	0.41
2:B:90:LYS:O	2:A:83:ARG:NH2	2.50	0.41
2:B:3:ILE:HB	2:B:122:ILE:CD1	2.50	0.41
1:F:108:VAL:O	1:F:111:VAL:N	2.53	0.41
1:E:250:HIS:O	1:E:250:HIS:CG	2.74	0.41
1:F:227:GLU:O	1:F:230:ALA:N	2.53	0.41
2:D:105:ILE:CD1	2:D:120:ILE:HG23	2.50	0.41
1:E:92:VAL:HG12	1:E:93:GLY:N	2.34	0.41
1:E:258:ILE:HG23	1:E:259:ASP:N	2.36	0.41
2:C:138:GLU:O	2:C:139:ASN:OD1	2.39	0.41
2:B:158:ILE:CG1	2:D:25:THR:HB	2.51	0.41
1:F:342:ARG:HD2	1:F:346:GLU:CD	2.41	0.41
2:B:100:GLU:HG3	2:B:100:GLU:H	1.61	0.41
1:F:371:SER:HB3	1:F:422:ALA:HB2	2.03	0.41
2:B:119:LEU:O	2:B:120:ILE:HD12	2.21	0.41
1:F:220:ASP:HB2	1:F:223:LYS:HB3	2.03	0.41
2:C:13:VAL:CG2	2:C:14:ILE:N	2.84	0.41
1:E:271:ASP:HB3	1:E:272:VAL:H	1.41	0.41
1:E:350:SER:HB3	1:E:353:VAL:CG2	2.51	0.41
1:F:286:GLU:HG3	1:F:325:ARG:NH2	2.36	0.41
2:D:171:LEU:HG	2:D:172:SER:N	2.36	0.41
1:E:77:PRO:HD2	1:E:251:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ILE:CD1	2:B:3:ILE:N	2.83	0.40
1:F:124:GLU:HA	1:F:127:ALA:HB3	2.03	0.40
1:F:45:ARG:HG3	1:F:45:ARG:NH1	2.24	0.40
2:B:66:MET:HB2	2:B:73:LYS:HZ3	1.86	0.40
1:F:384:ASN:HD22	1:F:384:ASN:HA	1.66	0.40
1:F:390:ILE:HD12	1:F:393:ARG:HB3	2.03	0.40
1:E:43:GLU:HG3	1:E:44:LEU:H	1.84	0.40
2:B:136:LEU:C	2:B:138:GLU:N	2.72	0.40
2:D:158:ILE:O	2:D:158:ILE:HG12	2.20	0.40
2:C:78:LEU:O	2:C:80:LYS:N	2.55	0.40
2:B:59:LEU:O	2:B:60:PHE:HB3	2.20	0.40
2:A:116:GLU:OE2	2:A:116:GLU:HA	2.20	0.40
2:A:3:ILE:HG12	2:A:47:ALA:HB2	2.03	0.40
2:D:55:THR:C	2:D:57:PHE:H	2.24	0.40
2:D:37:LEU:HD11	2:D:61:GLU:H	1.86	0.40
2:D:75:ALA:HA	2:D:79:ALA:H	1.86	0.40
2:B:160:ILE:HD13	2:B:160:ILE:HA	1.96	0.40
1:E:114:GLN:HG2	1:E:114:GLN:O	2.21	0.40
1:E:103:LEU:CG	1:E:103:LEU:O	2.69	0.40
1:E:247:VAL:HG12	1:E:247:VAL:O	2.21	0.40
2:A:49:GLY:O	2:A:52:ASP:N	2.55	0.40
1:E:124:GLU:C	1:E:126:LEU:H	2.24	0.40
1:F:25:ARG:O	1:F:29:ILE:HG13	2.22	0.40
1:E:32:ARG:HG3	1:E:36:ARG:HE	1.86	0.40
1:E:55:MET:HE1	1:E:66:ILE:HD12	2.03	0.40
2:D:18:GLY:O	2:D:29:GLY:C	2.59	0.40
2:A:128:TYR:CE1	2:D:128:TYR:CE1	3.09	0.40
2:D:70:HIS:HB3	2:D:73:LYS:HB2	2.03	0.40
2:D:71:LEU:HD23	2:D:71:LEU:C	2.41	0.40
2:C:113:VAL:O	2:C:115:PRO:HD3	2.21	0.40
2:B:140:THR:HG22	2:B:141:GLU:N	2.36	0.40
1:F:32:ARG:HG3	1:F:36:ARG:CD	2.43	0.40
1:F:76:ALA:HB1	1:F:77:PRO:CD	2.50	0.40
2:C:43:ILE:HD13	2:C:169:GLU:C	2.41	0.40
1:F:292:THR:CG2	1:F:295:GLY:O	2.69	0.40
2:D:153:ASP:OD1	2:D:164:HIS:HD2	2.05	0.40
2:A:94:LEU:HD22	2:A:94:LEU:N	2.36	0.40
2:C:37:LEU:HD22	2:C:61:GLU:CB	2.49	0.40
2:D:78:LEU:HB3	2:D:79:ALA:H	1.70	0.40
1:E:229:GLU:HA	1:E:232:LYS:HZ3	1.85	0.40
2:B:2:THR:HG23	2:B:126:GLY:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:HB	2:A:111:ASP:HA	2.04	0.40
1:F:88:GLU:CD	1:F:92:VAL:H	2.25	0.40
2:B:78:LEU:O	2:B:82:TRP:HB3	2.22	0.40
1:F:56:ILE:O	1:F:331:GLU:HA	2.21	0.40
2:B:144:ALA:C	2:B:146:GLU:H	2.23	0.40
2:A:140:THR:HG22	2:A:142:LEU:HG	2.03	0.40
1:F:347:PRO:O	1:F:350:SER:N	2.54	0.40
1:E:116:ILE:O	1:E:120:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	352/443 (80%)	248 (70%)	61 (17%)	43 (12%)	0	2
1	F	352/443 (80%)	245 (70%)	69 (20%)	38 (11%)	0	2
2	A	171/175 (98%)	101 (59%)	46 (27%)	24 (14%)	0	1
2	B	171/175 (98%)	94 (55%)	48 (28%)	29 (17%)	0	1
2	C	171/175 (98%)	103 (60%)	42 (25%)	26 (15%)	0	1
2	D	171/175 (98%)	108 (63%)	41 (24%)	22 (13%)	0	1
All	All	1388/1586 (88%)	899 (65%)	307 (22%)	182 (13%)	0	1

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	50	PRO
1	E	94	LYS
1	E	221	ALA
1	E	259	ASP

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Mol	Chain	Res	Type
1	E	350	SER
1	E	410	ALA
1	E	413	LEU
1	F	2	SER
1	F	50	PRO
1	F	91	TYR
1	F	222	MET
1	F	234	VAL
1	F	237	GLU
1	F	239	LEU
1	F	240	LYS
1	F	313	ALA
1	F	348	ASN
1	F	349	ALA
1	F	350	SER
1	F	410	ALA
1	F	412	ASP
1	F	413	LEU
1	F	432	LEU
2	B	15	ALA
2	B	38	TYR
2	B	39	ASN
2	B	59	LEU
2	B	64	LEU
2	B	68	GLN
2	B	75	ALA
2	B	92	GLU
2	B	100	GLU
2	B	142	LEU
2	A	27	MET
2	A	38	TYR
2	A	43	ILE
2	A	83	ARG
2	A	90	LYS
2	A	93	ALA
2	A	143	SER
2	D	28	LYS
2	D	38	TYR
2	D	42	VAL
2	D	51	ALA
2	D	53	ALA
2	D	61	GLU

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Mol	Chain	Res	Type
2	D	81	ASP
2	D	112	VAL
2	C	28	LYS
2	C	38	TYR
2	C	41	LYS
2	C	42	VAL
2	C	61	GLU
2	C	68	GLN
2	C	82	TRP
2	C	107	THR
1	E	36	ARG
1	E	43	GLU
1	E	44	LEU
1	E	88	GLU
1	E	89	VAL
1	E	103	LEU
1	E	118	LYS
1	E	120	ARG
1	E	247	VAL
1	E	349	ALA
1	E	412	ASP
1	E	414	SER
1	E	432	LEU
1	E	433	VAL
1	F	4	MET
1	F	88	GLU
1	F	89	VAL
1	F	103	LEU
1	F	225	LEU
1	F	241	GLN
1	F	270	PRO
1	F	272	VAL
2	B	49	GLY
2	B	71	LEU
2	B	89	ARG
2	B	93	ALA
2	B	94	LEU
2	B	97	VAL
2	B	117	ASN
2	B	130	GLN
2	A	2	THR
2	A	7	ARG

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Mol	Chain	Res	Type
2	A	8	ARG
2	A	70	HIS
2	A	72	VAL
2	A	117	ASN
2	D	39	ASN
2	D	68	GLN
2	D	73	LYS
2	D	137	LEU
2	D	171	LEU
2	C	27	MET
2	C	37	LEU
2	C	40	ASP
2	C	57	PHE
2	C	70	HIS
2	C	76	VAL
2	C	81	ASP
2	C	116	GLU
2	C	130	GLN
2	C	137	LEU
1	E	61	VAL
1	E	97	ASP
1	E	101	ARG
1	E	237	GLU
1	E	270	PRO
1	E	346	GLU
1	E	361	THR
1	E	431	ALA
1	F	94	LYS
1	F	101	ARG
1	F	245	ASP
1	F	361	THR
2	B	27	MET
2	B	60	PHE
2	B	73	LYS
2	B	81	ASP
2	B	84	THR
2	B	116	GLU
2	B	141	GLU
2	A	39	ASN
2	A	50	THR
2	A	135	ALA
2	A	142	LEU

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Mol	Chain	Res	Type
2	D	40	ASP
2	D	99	ASP
2	C	54	PHE
2	C	79	ALA
2	C	92	GLU
2	C	142	LEU
1	E	2	SER
1	E	4	MET
1	E	62	GLY
1	E	86	PHE
1	E	228	GLU
1	E	235	ASN
1	E	260	LYS
1	E	264	ARG
1	E	266	GLU
1	F	347	PRO
2	B	63	LYS
2	B	66	MET
2	A	86	ARG
2	A	88	LEU
2	A	145	ARG
2	D	60	PHE
2	D	85	ASP
2	D	107	THR
2	D	116	GLU
2	C	52	ASP
2	C	146	GLU
1	E	37	ARG
1	E	249	GLN
1	E	347	PRO
1	F	265	GLY
1	F	285	VAL
1	F	356	LYS
2	B	124	SER
2	A	130	GLN
2	D	87	MET
2	C	102	ALA
2	C	127	PRO
1	F	95	GLU
1	F	430	ASP
2	B	70	HIS
2	A	73	LYS

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Mol	Chain	Res	Type
2	A	4	VAL
1	F	79	ILE
1	F	235	ASN
1	F	346	GLU
2	D	76	VAL
1	E	376	ILE
1	F	92	VAL
2	A	45	GLY
2	D	69	GLY
1	E	92	VAL

### 5.3.2 Protein sidechains [i](#)

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	E	305/377 (81%)	265 (87%)	40 (13%)	5	22
1	F	305/377 (81%)	271 (89%)	34 (11%)	8	29
2	A	135/136 (99%)	110 (82%)	25 (18%)	2	10
2	B	135/136 (99%)	102 (76%)	33 (24%)	1	4
2	C	135/136 (99%)	103 (76%)	32 (24%)	1	4
2	D	135/136 (99%)	113 (84%)	22 (16%)	3	14
All	All	1150/1298 (89%)	964 (84%)	186 (16%)	3	14

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	GLU
1	E	22	ASN
1	E	24	LYS
1	E	34	ARG
1	E	47	GLU
1	E	59	THR
1	E	69	ARG
1	E	73	LEU

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Mol	Chain	Res	Type
1	E	87	THR
1	E	88	GLU
1	E	89	VAL
1	E	121	TYR
1	E	124	GLU
1	E	130	ARG
1	E	132	LEU
1	E	227	GLU
1	E	229	GLU
1	E	235	ASN
1	E	238	GLU
1	E	241	GLN
1	E	263	LYS
1	E	289	THR
1	E	294	HIS
1	E	318	LEU
1	E	322	LEU
1	E	348	ASN
1	E	351	ILE
1	E	366	ILE
1	E	367	GLU
1	E	370	ASP
1	E	371	SER
1	E	382	GLN
1	E	385	GLU
1	E	388	GLU
1	E	399	LEU
1	E	401	ARG
1	E	420	ILE
1	E	432	LEU
1	E	438	LEU
1	E	442	ILE
1	F	7	ARG
1	F	12	GLU
1	F	24	LYS
1	F	39	GLN
1	F	45	ARG
1	F	46	HIS
1	F	49	THR
1	F	54	LEU
1	F	79	ILE
1	F	87	THR

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Mol	Chain	Res	Type
1	F	88	GLU
1	F	94	LYS
1	F	102	ASP
1	F	103	LEU
1	F	114	GLN
1	F	124	GLU
1	F	239	LEU
1	F	240	LYS
1	F	264	ARG
1	F	301	HIS
1	F	314	LYS
1	F	330	VAL
1	F	337	THR
1	F	359	MET
1	F	384	ASN
1	F	385	GLU
1	F	395	LEU
1	F	401	ARG
1	F	404	GLU
1	F	413	LEU
1	F	420	ILE
1	F	433	VAL
1	F	438	LEU
1	F	442	ILE
2	B	1	THR
2	B	3	ILE
2	B	8	ARG
2	B	11	HIS
2	B	26	VAL
2	B	30	ASN
2	B	32	LYS
2	B	36	ARG
2	B	43	ILE
2	B	57	PHE
2	B	58	GLU
2	B	62	ARG
2	B	67	HIS
2	B	71	LEU
2	B	83	ARG
2	B	86	ARG
2	B	87	MET
2	B	89	ARG

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Mol	Chain	Res	Type
2	B	91	LEU
2	B	95	LEU
2	B	100	GLU
2	B	104	LEU
2	B	105	ILE
2	B	117	ASN
2	B	122	ILE
2	B	130	GLN
2	B	138	GLU
2	B	142	LEU
2	B	152	LEU
2	B	163	ASN
2	B	166	HIS
2	B	167	THR
2	B	168	ILE
2	A	1	THR
2	A	12	VAL
2	A	21	THR
2	A	22	LEU
2	A	30	ASN
2	A	57	PHE
2	A	66	MET
2	A	78	LEU
2	A	82	TRP
2	A	85	ASP
2	A	87	MET
2	A	91	LEU
2	A	92	GLU
2	A	95	LEU
2	A	100	GLU
2	A	104	LEU
2	A	105	ILE
2	A	113	VAL
2	A	116	GLU
2	A	117	ASN
2	A	138	GLU
2	A	141	GLU
2	A	166	HIS
2	A	167	THR
2	A	168	ILE
2	D	4	VAL
2	D	8	ARG

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Mol	Chain	Res	Type
2	D	11	HIS
2	D	22	LEU
2	D	36	ARG
2	D	46	PHE
2	D	58	GLU
2	D	65	GLU
2	D	73	LYS
2	D	77	GLU
2	D	82	TRP
2	D	87	MET
2	D	92	GLU
2	D	94	LEU
2	D	112	VAL
2	D	122	ILE
2	D	152	LEU
2	D	153	ASP
2	D	157	ASP
2	D	167	THR
2	D	170	GLU
2	D	173	TYR
2	C	4	VAL
2	C	8	ARG
2	C	11	HIS
2	C	32	LYS
2	C	35	ARG
2	C	38	TYR
2	C	39	ASN
2	C	41	LYS
2	C	46	PHE
2	C	59	LEU
2	C	60	PHE
2	C	61	GLU
2	C	66	MET
2	C	73	LYS
2	C	77	GLU
2	C	82	TRP
2	C	83	ARG
2	C	85	ASP
2	C	87	MET
2	C	94	LEU
2	C	97	VAL
2	C	112	VAL

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Mol	Chain	Res	Type
2	C	114	GLN
2	C	122	ILE
2	C	130	GLN
2	C	137	LEU
2	C	152	LEU
2	C	153	ASP
2	C	157	ASP
2	C	163	ASN
2	C	168	ILE
2	C	171	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	GLN
1	E	22	ASN
1	E	241	GLN
1	E	249	GLN
1	E	278	GLN
1	E	323	GLN
1	E	333	GLN
1	E	348	ASN
1	E	354	GLN
1	E	417	ASN
1	F	33	ASN
1	F	41	ASN
1	F	46	HIS
1	F	235	ASN
1	F	278	GLN
1	F	311	GLN
1	F	333	GLN
1	F	382	GLN
1	F	384	ASN
1	F	416	GLN
1	F	417	ASN
2	B	9	ASN
2	B	24	ASN
2	B	163	ASN
2	A	30	ASN
2	A	39	ASN
2	A	70	HIS
2	A	117	ASN

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Mol	Chain	Res	Type
2	D	11	HIS
2	D	39	ASN
2	D	109	ASN
2	D	164	HIS
2	D	166	HIS
2	C	24	ASN
2	C	39	ASN
2	C	109	ASN
2	C	130	GLN
2	C	139	ASN
2	C	163	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	$\# Z  > 2$
3	DAT	E	905	-	22,28,28	1.02	2 (9%)	28,43,43	0.98	2 (7%)
3	DAT	F	906	-	22,28,28	0.89	0	28,43,43	1.01	2 (7%)

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
3	DAT	E	905	-	-	0/12/28/28	0/3/3/3
3	DAT	F	906	-	-	0/12/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	905	DAT	C2-N3	2.12	1.36	1.32
3	E	905	DAT	C2-N1	2.41	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	906	DAT	C2'-C3'-C4'	2.02	106.96	102.77
3	E	905	DAT	C2'-C3'-C4'	2.21	107.36	102.77
3	F	906	DAT	O2B-PB-O1B	2.52	118.68	110.58
3	E	905	DAT	O2B-PB-O1B	2.64	119.08	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	905	DAT	3	0
3	F	906	DAT	1	0

## 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	E	356/443 (80%)	-0.08	3 (0%) 87 67	17, 42, 78, 90	0
1	F	356/443 (80%)	0.03	9 (2%) 61 30	23, 43, 75, 84	0
2	A	173/175 (98%)	0.31	9 (5%) 31 12	25, 56, 77, 86	0
2	B	173/175 (98%)	0.09	1 (0%) 90 73	28, 54, 80, 90	0
2	C	173/175 (98%)	0.23	6 (3%) 48 21	26, 61, 82, 95	0
2	D	173/175 (98%)	0.15	6 (3%) 48 21	21, 62, 84, 100	0
All	All	1404/1586 (88%)	0.08	34 (2%) 62 32	17, 48, 79, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	267	SER	5.4
1	F	220	ASP	4.6
2	A	42	VAL	4.6
2	D	95	LEU	4.3
2	D	42	VAL	4.2
1	F	221	ALA	4.0
1	E	268	SER	3.8
1	F	268	SER	3.8
2	A	37	LEU	3.6
2	A	97	VAL	3.5
1	E	267	SER	3.4
1	F	128	GLU	3.2
1	E	266	GLU	3.0
2	C	88	LEU	3.0
2	D	56	LEU	2.9
2	A	56	LEU	2.9
1	F	91	TYR	2.8
2	B	104	LEU	2.8
2	C	104	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	97	VAL	2.7
2	C	95	LEU	2.7
2	D	44	ALA	2.6
2	A	104	LEU	2.5
1	F	224	LEU	2.5
2	C	93	ALA	2.4
2	C	81	ASP	2.3
2	A	60	PHE	2.3
2	A	71	LEU	2.2
2	D	113	VAL	2.2
2	C	65	GLU	2.2
2	A	171	LEU	2.2
1	F	127	ALA	2.1
1	F	132	LEU	2.1
2	A	90	LYS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	DAT	E	905	26/26	0.94	0.28	1.10	68,73,76,77	0
3	DAT	F	906	26/26	0.94	0.26	0.94	62,69,70,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.