



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:04 PM GMT

PDB ID : 4GZZ  
Title : Crystal structures of bacterial RNA Polymerase paused elongation complexes  
Authors : Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.  
Deposited on : 2012-09-06  
Resolution : 4.29 Å(reported)

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

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

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

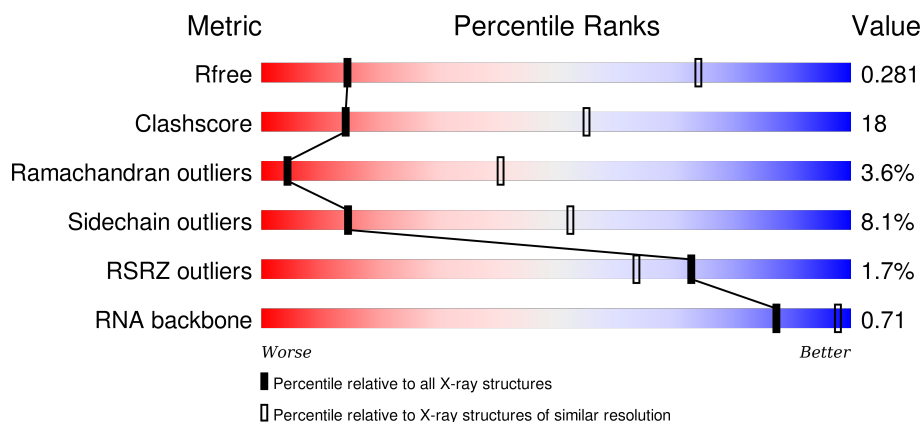
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.29 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)
RNA backbone	2183	1087 (5.60-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div> <div></div> <div>42%</div> <div>26%</div> <div>•</div> <div>29%</div> </div> </div>
1	B	315	<div> <div> <div></div> <div>48%</div> <div>22%</div> <div>•</div> <div>29%</div> </div> </div>
2	C	1119	<div> <div> <div></div> <div>54%</div> <div>38%</div> <div>5%</div> <div>•</div> </div> </div>
3	D	1534	<div> <div> <div>2%</div> <div>50%</div> <div>34%</div> <div>5%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	
5	N	13	
6	R	16	
7	T	22	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	D	1602	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8548	5412	1524	1588	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1358	Total	C	N	O	S	0	0	0
			10714	6780	1900	2001	33			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1526	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1527	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1528	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1529	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1530	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1531	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1532	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1533	HIS	-	EXPRESSION TAG	UNP Q8RQE8
D	1534	HIS	-	EXPRESSION TAG	UNP Q8RQE8

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	11	Total	C	N	O	P	0	0	0
			225	107	43	64	11			

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	9	Total	C	N	O	P	0	0	0
			191	85	31	66	9			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	22	Total	C	N	O	P	0	0	0
			447	213	81	131	22			

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

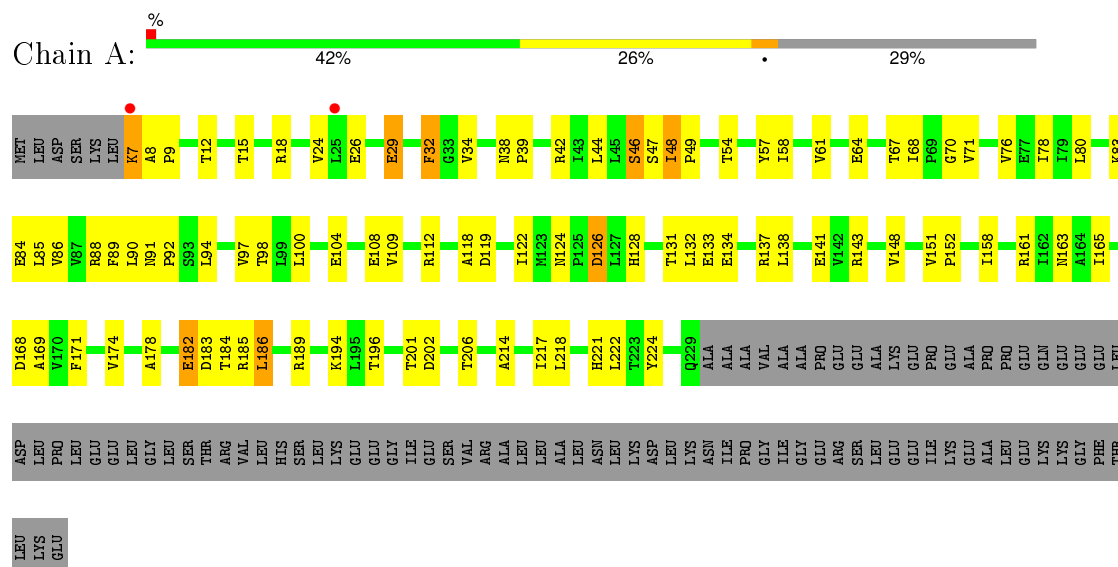
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

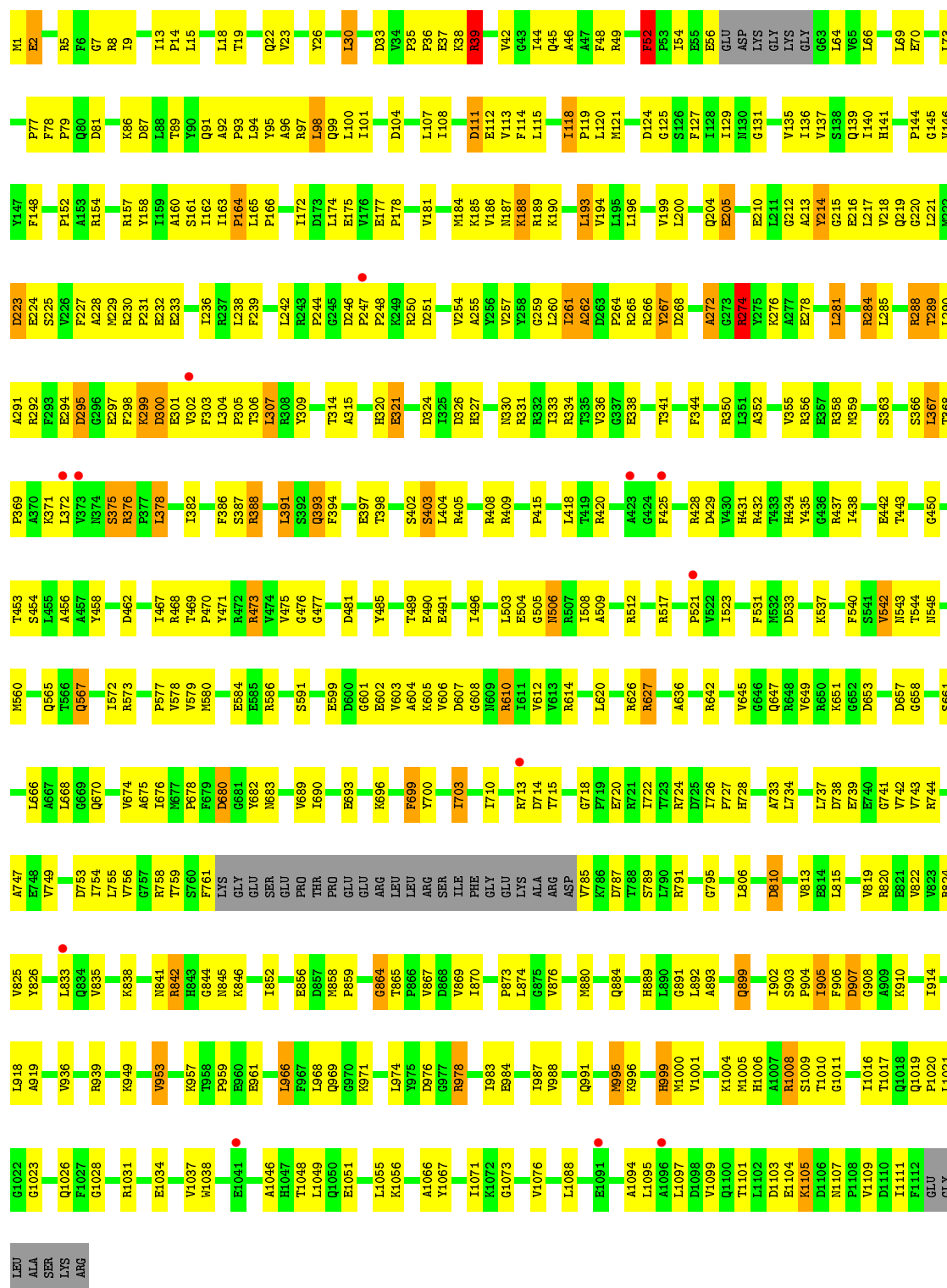
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

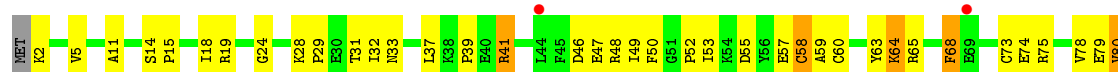
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA-directed RNA polymerase subunit alpha



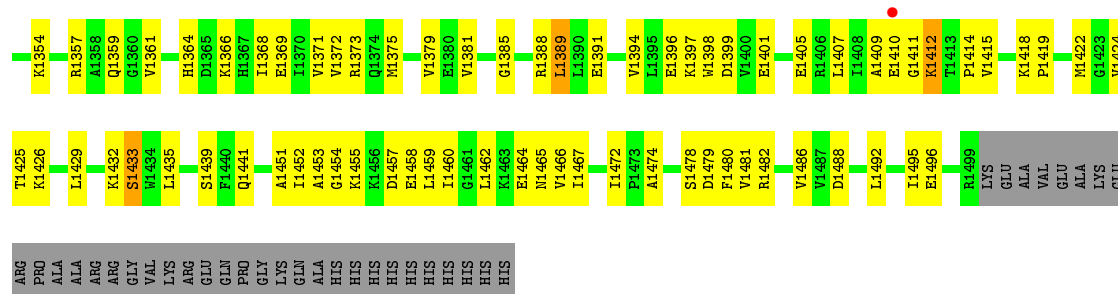


• Molecule 3: DNA-directed RNA polymerase subunit beta'

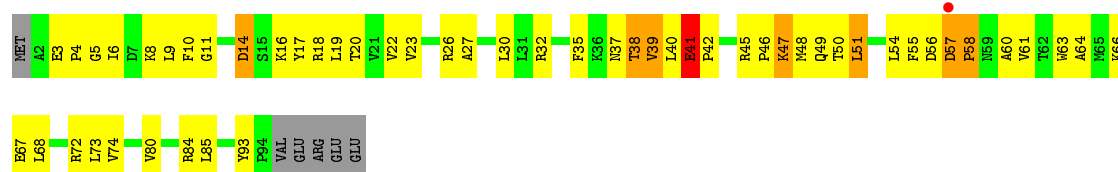








- Molecule 4: DNA-directed RNA polymerase subunit omega



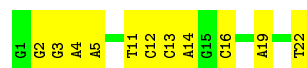
- Molecule 5: non-template DNA



- Molecule 6: RNA transcript



- Molecule 7: template DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.55Å 286.55Å 199.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.78 – 4.29 38.79 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-4.29) 87.8 (38.79-4.29)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 4.28Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.234 , 0.285 0.232 , 0.281	Depositor DCC
$R_{free}$ test set	1848 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	166.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 41308 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1791	0.47	0/2436
1	B	0.28	0/1791	0.47	0/2436
2	C	0.28	0/8711	0.51	0/11784
3	D	0.28	0/10897	0.50	1/14726 (0.0%)
4	E	0.29	0/768	0.55	0/1035
5	N	0.44	0/252	1.08	0/386
6	R	0.21	0/212	0.77	0/328
7	T	0.44	0/500	1.08	0/768
All	All	0.29	0/24922	0.53	1/33899 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	C-N-CD	5.17	139.25	128.40

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	65	0
1	B	1759	0	1805	50	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8548	0	8650	371	0
3	D	10714	0	10936	408	1
4	E	754	0	769	40	0
5	N	225	0	124	3	0
6	R	191	0	95	10	0
7	T	447	0	248	10	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	882	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (882) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:428:ARG:HH12	3:D:1086:LEU:HD21	1.24	0.98
2:C:610:ARG:HH11	2:C:610:ARG:HG3	1.27	0.96
2:C:846:LYS:NZ	6:R:29:U:OP1	1.99	0.96
1:B:188:GLN:O	3:D:646:LYS:NZ	2.00	0.94
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.34	0.92
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.57	0.87
3:D:808:THR:H	3:D:809:PRO:HD2	1.37	0.86
3:D:925:GLU:O	3:D:929:ARG:NH1	2.08	0.86
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.72	0.86
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.09	0.85
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.58	0.85
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.61	0.81
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.43	0.81
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.45	0.81
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.61	0.81
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.26	0.80
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.64	0.80
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.64	0.80
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.62	0.80
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.64	0.79
2:C:292:ARG:NH1	2:C:294:GLU:HB2	1.97	0.78
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.66	0.78
3:D:161:LEU:O	3:D:397:LYS:NZ	2.17	0.78
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.66	0.77
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.63	0.77
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.67	0.77
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.82	0.76
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.67	0.76
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.67	0.76
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	1.67	0.76
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.69	0.75
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.67	0.75
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.75
2:C:720:GLU:O	2:C:820:ARG:NH2	2.20	0.74
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.53	0.74
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.70	0.74
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.68	0.74
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.69	0.74
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.21	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.03	0.74
2:C:23:VAL:HA	2:C:121:MET:HE1	1.69	0.73
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.71	0.73
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.54	0.73
2:C:610:ARG:HH11	2:C:610:ARG:CG	2.02	0.73
2:C:1105:LYS:NZ	2:C:1107:ASN:HB2	2.03	0.73
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.71	0.73
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.71	0.72
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.72	0.72
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.54	0.72
2:C:670:GLN:NE2	2:C:699:PHE:O	2.22	0.72
2:C:290:LEU:HD11	2:C:301:GLU:H	1.55	0.72
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.55	0.72
2:C:224:GLU:O	2:C:228:ALA:N	2.21	0.72
3:D:1194:CYS:SG	3:D:1195:GLN:N	2.63	0.71
2:C:1048:THR:N	3:D:758:GLU:OE2	2.21	0.71
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.04	0.71
3:D:127:LEU:HG	3:D:152:LEU:HD12	1.72	0.70
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.87	0.70
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.74	0.70
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.25	0.70
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.74	0.69
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.72	0.69
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.74	0.69
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:701:LEU:HB3	3:D:713:ILE:HD11	1.74	0.69
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.75	0.69
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.74	0.69
2:C:579:VAL:O	2:C:842:ARG:NH2	2.26	0.69
1:A:58:ILE:HB	1:A:61:VAL:HB	1.74	0.68
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.75	0.68
1:A:104:GLU:HB3	1:A:137:ARG:HG3	1.74	0.68
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.76	0.68
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.74	0.68
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.58	0.68
3:D:346:ARG:NH1	3:D:347:VAL:O	2.27	0.68
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.76	0.68
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.75	0.68
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.26	0.68
2:C:22:GLN:NE2	2:C:136:ILE:O	2.25	0.68
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.75	0.68
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.74	0.67
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.09	0.67
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.74	0.67
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.43	0.67
2:C:292:ARG:HB3	2:C:299:LYS:HZ2	1.59	0.67
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.76	0.67
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.58	0.66
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.76	0.66
2:C:845:ASN:HB2	2:C:884:GLN:NE2	2.11	0.66
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.58	0.66
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.75	0.66
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.76	0.66
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.61	0.66
3:D:493:ARG:NH2	3:D:1389:LEU:O	2.27	0.66
2:C:30:LEU:HB3	2:C:44:ILE:HD12	1.78	0.66
2:C:115:LEU:HA	2:C:375:SER:HB2	1.78	0.65
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.78	0.65
2:C:265:ARG:HH11	2:C:267:TYR:HD1	1.45	0.65
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.61	0.65
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.29	0.65
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.79	0.65
2:C:184:MET:HE2	2:C:193:LEU:HD12	1.79	0.65
1:B:175:ARG:N	1:B:200:TRP:O	2.29	0.65
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.79	0.65
3:D:645:PRO:HG2	3:D:648:MET:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.29	0.65
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.78	0.65
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.62	0.64
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.80	0.64
3:D:1147:ARG:HE	3:D:1364:HIS:HE1	1.44	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.06	0.64
3:D:783:ARG:HH11	3:D:783:ARG:HG2	1.62	0.64
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.79	0.64
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.79	0.64
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.61	0.64
2:C:690:ILE:HG23	2:C:852:ILE:HG23	1.79	0.64
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.79	0.64
6:R:24:U:O4	7:T:19:DA:N1	2.31	0.64
2:C:668:LEU:O	2:C:995:MET:HB3	1.97	0.63
3:D:1213:ARG:HH22	4:E:11:GLY:HA2	1.63	0.63
3:D:950:GLY:N	3:D:953:ASP:OD2	2.30	0.63
3:D:414:ARG:HG3	3:D:433:GLY:H	1.63	0.63
3:D:362:GLU:O	3:D:364:GLY:N	2.22	0.63
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.81	0.63
6:R:24:U:H3	7:T:19:DA:H2	1.45	0.63
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.79	0.63
3:D:129:PHE:HB3	3:D:572:ARG:HG3	1.81	0.63
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.81	0.63
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.81	0.62
2:C:1009:SER:HA	3:D:625:TYR:HA	1.81	0.62
2:C:144:PRO:HB3	2:C:164:PRO:HA	1.82	0.62
2:C:658:GLY:N	2:C:661:SER:OG	2.32	0.62
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.81	0.62
2:C:264:PRO:HB2	2:C:289:THR:HG21	1.79	0.62
2:C:580:MET:HB2	2:C:584:GLU:OE2	1.99	0.62
3:D:163:TYR:O	3:D:165:LYS:N	2.29	0.62
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.81	0.62
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.65	0.62
3:D:1314:LYS:NZ	3:D:1316:GLY:HA3	2.14	0.62
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.35	0.62
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.62
3:D:501:ALA:O	3:D:505:SER:OG	2.15	0.61
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.81	0.61
3:D:115:LEU:HD21	3:D:468:LEU:HD22	1.81	0.61
3:D:1294:VAL:HG11	3:D:1319:VAL:HG11	1.82	0.61
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.98	0.61
2:C:505:GLY:O	2:C:506:ASN:ND2	2.31	0.61
3:D:1232:PRO:HB2	3:D:1361:VAL:HG11	1.81	0.61
2:C:873:PRO:HB3	3:D:949:ILE:HG12	1.81	0.61
2:C:165:LEU:HG	2:C:166:PRO:HA	1.82	0.61
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.81	0.61
2:C:599:GLU:OE2	2:C:651:LYS:HD2	2.01	0.61
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.82	0.60
3:D:1405:GLU:HA	3:D:1409:ALA:HB3	1.81	0.60
2:C:578:VAL:HG13	2:C:579:VAL:HG23	1.83	0.60
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.35	0.60
2:C:607:ASP:OD1	2:C:608:GLY:N	2.34	0.60
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.37	0.60
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.84	0.60
2:C:259:GLY:HA2	2:C:291:ALA:HB2	1.83	0.60
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.17	0.60
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.84	0.60
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.83	0.60
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.84	0.60
3:D:1394:VAL:HG21	3:D:1432:LYS:HZ1	1.66	0.60
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.84	0.60
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.83	0.60
2:C:759:THR:HG22	2:C:787:ASP:HA	1.84	0.60
3:D:1479:ASP:OD2	3:D:1482:ARG:NH2	2.34	0.60
3:D:184:GLU:HA	3:D:202:VAL:HA	1.82	0.60
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.83	0.60
2:C:978:ARG:HH11	2:C:978:ARG:CG	2.15	0.59
3:D:612:GLY:O	3:D:616:GLN:NE2	2.35	0.59
3:D:760:ARG:HD3	4:E:61:VAL:HG11	1.83	0.59
3:D:165:LYS:O	3:D:395:VAL:HG23	2.02	0.59
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.26	0.59
4:E:39:VAL:O	4:E:72:ARG:NH1	2.35	0.59
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.00	0.59
1:B:149:GLY:H	1:B:171:PHE:HB2	1.66	0.59
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.85	0.59
2:C:165:LEU:HD21	2:C:418:LEU:HD11	1.85	0.59
3:D:565:ILE:H	3:D:565:ILE:HD12	1.66	0.59
2:C:408:ARG:NH2	2:C:456:ALA:O	2.36	0.59
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.85	0.58
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.85	0.58
3:D:618:LEU:HD11	3:D:1467:ILE:HG12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:HZ2	2:C:299:LYS:HB3	1.67	0.58
1:A:80:LEU:HD21	2:C:573:ARG:NH1	2.12	0.58
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.06	0.58
2:C:443:THR:HG22	2:C:453:THR:HG22	1.85	0.58
3:D:647:ARG:NH1	3:D:724:GLN:OE1	2.36	0.58
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.85	0.58
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.84	0.58
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.04	0.58
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.85	0.58
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.85	0.58
2:C:216:GLU:O	2:C:218:VAL:N	2.37	0.58
2:C:38:LYS:HD2	2:C:39:ARG:NH1	2.18	0.58
3:D:58:CYS:SG	3:D:59:ALA:N	2.77	0.58
1:B:206:THR:HG22	1:B:207:PRO:HD2	1.84	0.58
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.86	0.58
4:E:14:ASP:N	4:E:14:ASP:OD1	2.30	0.58
3:D:1031:ASN:OD1	3:D:1033:GLN:NE2	2.36	0.57
2:C:18:LEU:HD21	2:C:542:VAL:HG11	1.86	0.57
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.86	0.57
3:D:520:LEU:HB3	3:D:525:ARG:HD3	1.85	0.57
2:C:473:ARG:HA	2:C:531:PHE:HA	1.85	0.57
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.86	0.57
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.36	0.57
3:D:783:ARG:HG2	3:D:783:ARG:NH1	2.20	0.57
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.86	0.57
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.40	0.57
3:D:1480:PHE:O	4:E:18:ARG:NH1	2.38	0.57
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.70	0.57
2:C:841:ASN:OD1	2:C:844:GLY:N	2.35	0.57
1:A:18:ARG:HH21	1:A:88:ARG:HD2	1.70	0.57
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.37	0.57
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.69	0.57
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.86	0.56
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	1.87	0.56
2:C:429:ASP:OD2	3:D:1079:LYS:HD3	2.05	0.56
3:D:1458:GLU:O	3:D:1460:ILE:N	2.37	0.56
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.47	0.56
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.86	0.56
1:A:143:ARG:HH12	1:A:158:ILE:HD12	1.69	0.56
1:B:174:VAL:HA	1:B:201:THR:HA	1.86	0.56
2:C:601:GLY:HA3	2:C:614:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:GLN:NE2	2:C:228:ALA:O	2.38	0.56
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.87	0.56
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.87	0.56
3:D:1131:SER:HB2	3:D:1133:ARG:NH2	2.21	0.56
2:C:845:ASN:HB2	2:C:884:GLN:HE22	1.71	0.56
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.87	0.56
2:C:689:VAL:HB	2:C:870:ILE:HB	1.86	0.56
3:D:180:LYS:NZ	3:D:388:HIS:HE1	2.03	0.56
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.87	0.56
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.36	0.56
2:C:437:ARG:HH11	2:C:437:ARG:HG3	1.70	0.56
2:C:324:ASP:O	2:C:330:ASN:ND2	2.39	0.56
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.88	0.56
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.87	0.56
2:C:756:VAL:O	2:C:789:SER:HB3	2.06	0.56
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.87	0.56
3:D:210:ARG:HH21	3:D:346:ARG:HD3	1.71	0.56
3:D:180:LYS:HZ1	3:D:388:HIS:HE1	1.54	0.56
2:C:145:GLY:H	2:C:163:ILE:HG23	1.71	0.55
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.42	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.88	0.55
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.88	0.55
2:C:91:GLN:HA	2:C:119:PRO:HA	1.88	0.55
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.41	0.55
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.72	0.55
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.40	0.55
2:C:5:ARG:HG2	2:C:902:ILE:HB	1.89	0.55
1:A:143:ARG:NH1	1:A:158:ILE:HD12	2.22	0.55
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.22	0.55
3:D:1236:LEU:HD23	3:D:1359:GLN:HG3	1.88	0.55
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.88	0.55
2:C:200:LEU:HD22	2:C:300:ASP:HB3	1.89	0.55
3:D:182:GLY:HA2	3:D:203:ALA:O	2.07	0.55
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.22	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.89	0.55
1:B:185:ARG:NH2	3:D:688:TRP:HB3	2.23	0.54
3:D:1128:VAL:HG23	3:D:1133:ARG:NH2	2.18	0.54
3:D:165:LYS:HD2	3:D:397:LYS:HG3	1.89	0.54
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.89	0.54
3:D:1107:VAL:O	3:D:1218:GLY:N	2.37	0.54
1:A:29:GLU:OE2	1:A:189:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.89	0.54
3:D:801:GLY:HA3	3:D:825:ALA:HA	1.88	0.54
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.08	0.54
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.23	0.54
2:C:292:ARG:HG3	2:C:292:ARG:NH1	2.23	0.54
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.22	0.54
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.71	0.54
2:C:46:ALA:HB1	2:C:266:ARG:NH1	2.23	0.54
3:D:764:LEU:HD23	3:D:766:ALA:H	1.71	0.54
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.54
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.41	0.54
2:C:398:THR:HG21	2:C:567:GLN:HA	1.89	0.54
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.90	0.54
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.73	0.54
3:D:1277:ILE:HG13	3:D:1301:LYS:NZ	2.23	0.54
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.88	0.54
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.90	0.54
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.42	0.54
3:D:842:VAL:HG12	3:D:865:THR:HB	1.90	0.54
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.90	0.54
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.89	0.54
3:D:800:LYS:HZ2	3:D:804:LEU:HD13	1.72	0.54
1:A:174:VAL:HA	1:A:201:THR:HG22	1.89	0.54
3:D:165:LYS:HB2	3:D:397:LYS:HB2	1.90	0.53
2:C:233:GLU:N	2:C:233:GLU:OE1	2.41	0.53
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.53
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.89	0.53
3:D:31:THR:OG1	3:D:32:ILE:N	2.39	0.53
2:C:1038:TRP:HB3	3:D:1227:GLN:HE21	1.73	0.53
2:C:274:ARG:HH12	2:C:284:ARG:CZ	2.21	0.53
2:C:580:MET:O	2:C:903:SER:N	2.35	0.53
3:D:626:SER:OG	3:D:627:GLY:N	2.42	0.53
3:D:361:VAL:HG13	3:D:365:ASP:HB2	1.91	0.53
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.73	0.53
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.08	0.53
3:D:1281:VAL:O	3:D:1315:ASP:HA	2.09	0.53
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.91	0.53
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.73	0.53
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.53
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.73	0.53
2:C:987:ILE:HA	3:D:948:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HD13	2:C:261:ILE:HG13	1.91	0.53
3:D:153:LEU:HD23	3:D:153:LEU:H	1.73	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.90	0.52
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.90	0.52
2:C:255:ALA:HB1	2:C:298:PHE:CE1	2.44	0.52
3:D:155:ASP:O	3:D:159:ARG:HG2	2.09	0.52
2:C:375:SER:OG	2:C:375:SER:O	2.24	0.52
3:D:664:LYS:NZ	3:D:693:GLU:OE2	2.41	0.52
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.52
2:C:48:PHE:O	2:C:52:PHE:HB2	2.10	0.52
1:B:163:ASN:OD1	1:B:163:ASN:N	2.43	0.52
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.39	0.52
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.24	0.52
4:E:54:LEU:HD23	4:E:58:PRO:HD2	1.89	0.52
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.45	0.52
2:C:404:LEU:HD22	2:C:591:SER:HB3	1.90	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.42	0.52
2:C:489:THR:HG23	2:C:490:GLU:HG3	1.92	0.52
4:E:17:TYR:O	4:E:20:THR:OG1	2.21	0.52
2:C:602:GLU:H	2:C:614:ARG:HB3	1.74	0.52
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.91	0.52
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.52
3:D:397:LYS:HD3	3:D:448:GLU:HB3	1.90	0.52
1:B:106:PRO:HG3	1:B:134:GLU:OE2	2.08	0.52
1:B:25:LEU:HD23	1:B:28:LEU:HD21	1.92	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.90	0.52
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.52
1:A:133:GLU:HG2	1:A:134:GLU:H	1.74	0.52
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.92	0.52
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.92	0.52
2:C:504:GLU:HG3	2:C:509:ALA:HB2	1.91	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.10	0.51
3:D:127:LEU:HD23	3:D:134:VAL:HB	1.91	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.39	0.51
3:D:925:GLU:OE1	4:E:6:ILE:N	2.44	0.51
3:D:19:ARG:NH1	3:D:19:ARG:HB2	2.25	0.51
2:C:1088:LEU:HD13	3:D:613:ARG:HG3	1.92	0.51
3:D:87:ARG:HB2	3:D:523:ASP:HB3	1.93	0.51
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.93	0.51
4:E:54:LEU:HA	4:E:58:PRO:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:ASP:OD2	2:C:125:GLY:N	2.44	0.51
2:C:338:GLU:HA	2:C:341:THR:HG22	1.93	0.51
2:C:540:PHE:HB3	2:C:544:THR:HB	1.92	0.51
2:C:186:VAL:O	2:C:188:LYS:N	2.43	0.51
1:B:58:ILE:HG23	1:B:140:MET:HB3	1.91	0.51
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.45	0.51
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.44	0.51
3:D:957:PRO:HG3	3:D:1007:VAL:HA	1.93	0.51
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.75	0.51
2:C:35:PRO:HD2	2:C:38:LYS:HG3	1.93	0.51
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.10	0.51
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.92	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.91	0.51
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.31	0.51
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.92	0.51
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.76	0.51
2:C:978:ARG:HH11	2:C:978:ARG:HG2	1.76	0.51
3:D:616:GLN:HG3	3:D:621:LYS:NZ	2.26	0.51
4:E:26:ARG:HH21	4:E:30:LEU:HD13	1.76	0.51
2:C:18:LEU:HB3	2:C:404:LEU:HD11	1.93	0.51
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.76	0.51
2:C:284:ARG:NH1	2:C:285:LEU:H	2.09	0.51
2:C:141:HIS:HB2	2:C:418:LEU:HD22	1.92	0.51
2:C:1095:LEU:HD23	3:D:101:HIS:HE2	1.74	0.51
2:C:46:ALA:HB1	2:C:266:ARG:HH12	1.76	0.50
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.76	0.50
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.50
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.41	0.50
2:C:610:ARG:HG3	2:C:610:ARG:NH1	2.08	0.50
3:D:415:VAL:HG21	3:D:421:LEU:HD21	1.92	0.50
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.47	0.50
3:D:695:ILE:HG13	3:D:696:HIS:H	1.76	0.50
3:D:728:LEU:HD21	3:D:736:PHE:HZ	1.75	0.50
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.93	0.50
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.46	0.50
2:C:38:LYS:NZ	2:C:38:LYS:HB3	2.27	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.94	0.50
2:C:680:ASP:H	3:D:943:THR:HG21	1.76	0.50
2:C:606:VAL:H	2:C:645:VAL:HG22	1.76	0.50
2:C:521:PRO:HG3	3:D:1068:LEU:HD21	1.94	0.50
2:C:1004:LYS:HD3	3:D:744:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:GLN:OE1	2:C:334:ARG:NH1	2.45	0.50
2:C:89:THR:HG22	2:C:129:ILE:HA	1.92	0.50
3:D:103:TRP:NE1	3:D:604:THR:OG1	2.41	0.50
2:C:636:ALA:HB3	2:C:703:ILE:HG13	1.93	0.50
1:B:176:ARG:NH2	3:D:888:GLU:OE2	2.45	0.50
2:C:1:MET:O	2:C:899:GLN:HA	2.12	0.50
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.93	0.50
3:D:1453:ALA:O	3:D:1455:LYS:N	2.44	0.50
3:D:1278:ASP:OD2	3:D:1278:ASP:N	2.40	0.50
3:D:690:ALA:O	3:D:694:VAL:HG13	2.12	0.50
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.45	0.49
1:B:184:THR:O	1:B:192:LEU:HB2	2.11	0.49
2:C:718:GLY:HA3	2:C:761:PHE:CD2	2.47	0.49
1:A:38:ASN:O	1:A:42:ARG:HG2	2.12	0.49
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.93	0.49
2:C:649:VAL:HG12	2:C:653:ASP:HB3	1.94	0.49
3:D:758:GLU:O	3:D:762:GLN:HG2	2.12	0.49
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.27	0.49
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.94	0.49
2:C:363:SER:H	2:C:371:LYS:HE3	1.77	0.49
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.93	0.49
2:C:175:GLU:OE1	2:C:190:LYS:NZ	2.41	0.49
3:D:191:LEU:HG	3:D:197:SER:HB2	1.94	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.92	0.49
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.12	0.49
3:D:628:ARG:HH12	7:T:16:DC:H2"	1.76	0.49
3:D:646:LYS:HB3	3:D:688:TRP:CH2	2.47	0.49
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.94	0.49
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.94	0.49
3:D:1008:PHE:HZ	3:D:1032:PRO:HA	1.78	0.49
3:D:126:VAL:HG13	3:D:132:TYR:HD2	1.78	0.49
1:B:24:VAL:HG11	1:B:194:LYS:NZ	2.27	0.49
2:C:292:ARG:CB	2:C:299:LYS:HZ2	2.25	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.94	0.49
3:D:116:LEU:O	3:D:118:LEU:HG	2.12	0.49
4:E:5:GLY:HA3	4:E:8:LYS:HE3	1.93	0.49
3:D:505:SER:OG	3:D:1453:ALA:HA	2.13	0.49
2:C:443:THR:CG2	2:C:453:THR:HG22	2.43	0.49
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.49
2:C:113:VAL:O	2:C:115:LEU:N	2.43	0.49
2:C:1103:ASP:OD2	2:C:1104:GLU:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.95	0.48
1:B:60:ASP:N	1:B:60:ASP:OD1	2.46	0.48
3:D:152:LEU:CD2	3:D:152:LEU:H	2.26	0.48
2:C:876:VAL:HG11	3:D:949:ILE:HG21	1.95	0.48
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.94	0.48
2:C:999:HIS:CE1	6:R:28:C:H4'	2.47	0.48
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.48	0.48
2:C:69:LEU:HD13	2:C:99:GLN:HG2	1.95	0.48
4:E:47:LYS:HB3	4:E:55:PHE:CE2	2.48	0.48
6:R:22:U:H2'	6:R:23:G:C8	2.48	0.48
2:C:292:ARG:NH2	2:C:294:GLU:OE1	2.46	0.48
3:D:615:ARG:NE	3:D:1439:SER:O	2.41	0.48
3:D:1041:LEU:H	3:D:1041:LEU:HD22	1.77	0.48
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.40	0.48
2:C:726:ILE:HD11	2:C:754:ILE:HG21	1.94	0.48
3:D:1495:ILE:HD12	4:E:84:ARG:HG2	1.94	0.48
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.78	0.48
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.28	0.48
3:D:1457:ASP:OD2	3:D:1464:GLU:OE2	2.31	0.48
2:C:185:LYS:HD2	2:C:190:LYS:HE2	1.95	0.48
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.78	0.48
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.96	0.48
3:D:719:VAL:O	3:D:721:VAL:HG23	2.14	0.48
3:D:152:LEU:HD23	3:D:152:LEU:H	1.78	0.48
3:D:970:LYS:HE3	3:D:974:ILE:HD11	1.96	0.48
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.47	0.48
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.78	0.48
3:D:207:PHE:O	3:D:390:PRO:HA	2.14	0.48
3:D:546:ARG:HA	3:D:549:ASN:HB2	1.96	0.48
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.96	0.48
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.96	0.48
3:D:433:GLY:HA3	3:D:447:VAL:O	2.13	0.48
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.78	0.48
3:D:832:ARG:O	3:D:834:THR:N	2.47	0.48
1:B:100:LEU:HD23	1:B:141:GLU:HB3	1.95	0.48
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.14	0.48
3:D:417:PRO:HG3	3:D:431:VAL:HA	1.96	0.48
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.49	0.48
3:D:704:ARG:HG2	3:D:736:PHE:O	2.14	0.47
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.96	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.48	0.47
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.96	0.47
3:D:1258:ARG:HH11	3:D:1258:ARG:HG3	1.78	0.47
4:E:51:LEU:HD23	4:E:51:LEU:H	1.78	0.47
3:D:47:GLU:HG2	3:D:52:PRO:HA	1.95	0.47
3:D:543:LEU:HG	3:D:600:LEU:HD12	1.96	0.47
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.15	0.47
2:C:19:THR:HG21	2:C:124:ASP:O	2.14	0.47
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.96	0.47
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.79	0.47
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.97	0.47
2:C:162:ILE:HB	2:C:172:ILE:HB	1.96	0.47
2:C:577:PRO:HB2	2:C:580:MET:HB3	1.97	0.47
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.96	0.47
2:C:274:ARG:NH1	2:C:284:ARG:HH22	2.10	0.47
3:D:1165:TYR:HB3	3:D:1207:TYR:CE1	2.42	0.47
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.29	0.47
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.49	0.47
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.49	0.47
2:C:971:LYS:HA	2:C:988:VAL:HA	1.95	0.47
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.95	0.47
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.14	0.47
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.49	0.47
3:D:1278:ASP:HA	3:D:1319:VAL:HG13	1.96	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.14	0.47
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.97	0.47
3:D:474:GLU:O	3:D:478:LEU:HB2	2.14	0.47
4:E:23:VAL:HG13	4:E:64:ALA:HB3	1.97	0.47
3:D:890:VAL:O	3:D:926:LYS:NZ	2.48	0.47
2:C:73:LEU:HB2	2:C:93:PRO:O	2.15	0.47
3:D:1315:ASP:N	3:D:1315:ASP:OD2	2.47	0.47
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.15	0.47
4:E:37:ASN:HB3	4:E:93:TYR:CZ	2.50	0.47
2:C:700:TYR:HB2	2:C:833:LEU:HB2	1.96	0.47
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.97	0.47
1:B:185:ARG:HH11	3:D:692:GLU:CD	2.18	0.47
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.45	0.47
3:D:46:ASP:OD2	3:D:48:ARG:HB3	2.15	0.47
1:A:83:LYS:HD3	1:A:168:ASP:HB2	1.96	0.47
3:D:853:VAL:HG11	3:D:860:LEU:HG	1.97	0.47
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.15	0.46
3:D:565:ILE:N	3:D:565:ILE:HD12	2.30	0.46
3:D:185:VAL:CG2	3:D:203:ALA:HB2	2.46	0.46
2:C:409:ARG:HA	2:C:454:SER:HA	1.95	0.46
3:D:82:LYS:C	3:D:84:ILE:H	2.18	0.46
3:D:989:TYR:O	3:D:993:LEU:HG	2.15	0.46
2:C:205:GLU:HG3	2:C:205:GLU:H	1.50	0.46
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.46
3:D:808:THR:H	3:D:809:PRO:CD	2.17	0.46
1:B:23:PHE:CD2	1:B:211:LEU:HD22	2.50	0.46
3:D:28:LYS:C	3:D:548:ILE:HG21	2.35	0.46
2:C:1051:GLU:OE1	3:D:752:SER:HB3	2.15	0.46
3:D:1272:ALA:O	3:D:1325:LEU:HD23	2.15	0.46
2:C:744:ARG:HH11	2:C:747:ALA:HB2	1.79	0.46
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.98	0.46
3:D:560:GLN:HG3	3:D:561:GLY:H	1.79	0.46
2:C:1073:GLY:HA3	3:D:659:LYS:HG2	1.97	0.46
2:C:475:VAL:O	2:C:477:GLY:N	2.48	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG11	1.98	0.46
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.15	0.46
1:B:11:PHE:CE1	1:B:23:PHE:HB3	2.51	0.46
2:C:260:LEU:HG	2:C:291:ALA:HB3	1.98	0.46
2:C:255:ALA:HB1	2:C:298:PHE:HE1	1.80	0.46
1:B:42:ARG:HH22	2:C:939:ARG:NH2	2.14	0.46
3:D:978:TYR:HB2	3:D:983:LEU:HD11	1.97	0.46
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.31	0.46
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.97	0.46
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.16	0.46
3:D:602:SER:O	3:D:606:ILE:HG12	2.15	0.46
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	1.97	0.46
3:D:65:ARG:HA	3:D:65:ARG:HD2	1.65	0.46
2:C:838:LYS:HE3	3:D:741:ASP:O	2.15	0.46
2:C:726:ILE:HD12	2:C:734:LEU:HD11	1.97	0.46
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.96	0.46
2:C:892:LEU:HD23	2:C:918:LEU:HD22	1.98	0.46
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.97	0.46
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.79	0.46
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.98	0.46
3:D:1018:ASN:HD21	3:D:1020:LEU:HB3	1.81	0.46
3:D:214:GLU:HB3	3:D:340:THR:OG1	2.15	0.46
3:D:1119:SER:HB2	3:D:1185:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:57:GLU:HG2	3:D:58:CYS:N	2.30	0.46
2:C:288:ARG:H	2:C:288:ARG:HD3	1.81	0.46
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.37	0.46
2:C:715:THR:OG1	2:C:718:GLY:O	2.34	0.46
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.98	0.46
3:D:352:ASN:ND2	3:D:371:ILE:HG12	2.30	0.46
2:C:260:LEU:O	2:C:262:ALA:N	2.45	0.45
2:C:358:ARG:HD3	2:C:372:LEU:HA	1.98	0.45
3:D:81:THR:HG22	3:D:82:LYS:H	1.81	0.45
2:C:15:LEU:O	2:C:586:ARG:NH2	2.49	0.45
2:C:957:LYS:HD3	2:C:961:GLU:HB3	1.98	0.45
1:B:186:LEU:O	1:B:188:GLN:NE2	2.50	0.45
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.30	0.45
3:D:1435:LEU:HB2	3:D:1464:GLU:HG3	1.98	0.45
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.33	0.45
3:D:1388:ARG:HD2	3:D:1388:ARG:N	2.31	0.45
3:D:63:TYR:HB3	3:D:68:PHE:CE1	2.51	0.45
3:D:709:HIS:ND1	3:D:1231:GLU:HG3	2.32	0.45
2:C:274:ARG:HG2	2:C:285:LEU:HB3	1.98	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.82	0.45
3:D:86:ARG:O	3:D:522:PRO:HD2	2.16	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.63	0.45
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.16	0.45
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.17	0.45
3:D:1310:ARG:NH1	3:D:1327:ARG:NH1	2.65	0.45
3:D:1371:VAL:O	3:D:1375:MET:HG3	2.16	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.98	0.45
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.97	0.45
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.99	0.45
2:C:431:HIS:N	2:C:434:HIS:HD2	2.15	0.45
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.17	0.45
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.99	0.45
2:C:196:LEU:HA	2:C:199:VAL:HG23	1.97	0.45
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.52	0.45
2:C:1109:VAL:HG22	3:D:2:LYS:HB2	1.99	0.45
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.99	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
3:D:496:LEU:HD21	3:D:1388:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.50	0.45
7:T:2:DG:H2"	7:T:3:DG:C8	2.52	0.45
3:D:41:ARG:HB3	3:D:41:ARG:HE	1.59	0.45
4:E:22:VAL:HG11	4:E:68:LEU:HD21	1.97	0.45
2:C:98:LEU:HD12	2:C:99:GLN:N	2.32	0.45
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.99	0.45
2:C:842:ARG:HB3	2:C:842:ARG:HH11	1.81	0.45
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.31	0.45
2:C:512:ARG:HD3	2:C:512:ARG:HA	1.77	0.45
3:D:527:MET:SD	3:D:537:THR:HB	2.57	0.45
3:D:1044:LEU:H	3:D:1044:LEU:HD23	1.82	0.45
2:C:281:LEU:H	2:C:281:LEU:HD13	1.82	0.45
3:D:53:ILE:HA	3:D:86:ARG:HH11	1.82	0.45
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.99	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.99	0.45
2:C:572:ILE:HG13	2:C:573:ARG:H	1.82	0.45
2:C:69:LEU:O	2:C:97:ARG:HB2	2.17	0.45
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.98	0.45
3:D:660:LYS:O	3:D:664:LYS:HG3	2.16	0.45
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.52	0.45
2:C:393:GLN:HG2	6:R:25:G:O2'	2.16	0.45
2:C:284:ARG:CG	2:C:301:GLU:HG2	2.47	0.44
2:C:77:PRO:HD2	2:C:91:GLN:O	2.16	0.44
2:C:1031:ARG:HB3	7:T:16:DC:OP1	2.17	0.44
2:C:431:HIS:CG	2:C:432:ARG:N	2.85	0.44
3:D:168:THR:HA	3:D:394:LEU:HB3	1.99	0.44
2:C:225:SER:O	2:C:229:MET:HB2	2.16	0.44
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.17	0.44
2:C:722:ILE:HA	2:C:758:ARG:HB3	1.99	0.44
3:D:1149:LEU:HD21	3:D:1166:LEU:HD11	1.99	0.44
2:C:974:LEU:HA	2:C:974:LEU:HD12	1.84	0.44
2:C:144:PRO:O	2:C:276:LYS:NZ	2.34	0.44
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.32	0.44
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.99	0.44
3:D:1435:LEU:HD23	3:D:1464:GLU:O	2.16	0.44
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.99	0.44
3:D:829:VAL:O	3:D:831:GLY:N	2.47	0.44
2:C:387:SER:OG	2:C:388:ARG:NH2	2.50	0.44
3:D:616:GLN:HG3	3:D:621:LYS:HZ3	1.83	0.44
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.00	0.44
1:B:201:THR:HG22	1:B:202:ASP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.18	0.44
2:C:397:GLU:HG2	2:C:403:SER:OG	2.18	0.44
2:C:675:ALA:HB2	2:C:867:VAL:HG21	1.99	0.44
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.99	0.44
2:C:724:ARG:HB2	2:C:741:GLY:H	1.83	0.44
3:D:808:THR:N	3:D:809:PRO:HD2	2.18	0.44
3:D:205:TYR:CD1	3:D:390:PRO:HG3	2.53	0.44
3:D:11:ALA:HA	3:D:1451:ALA:O	2.17	0.44
2:C:274:ARG:HH22	2:C:284:ARG:NH2	2.16	0.44
2:C:1017:THR:OG1	2:C:1019:GLN:HG2	2.17	0.44
4:E:47:LYS:HB3	4:E:55:PHE:HE2	1.83	0.44
2:C:468:ARG:NE	2:C:485:TYR:O	2.51	0.44
1:B:208:LEU:HA	1:B:208:LEU:HD13	1.86	0.44
2:C:295:ASP:C	2:C:297:GLU:H	2.20	0.44
3:D:1127:GLU:HB3	3:D:1133:ARG:CZ	2.48	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.99	0.44
3:D:825:ALA:HA	3:D:826:PRO:HD2	1.88	0.44
3:D:961:LYS:O	3:D:965:GLU:HB2	2.18	0.44
3:D:1314:LYS:HZ1	3:D:1316:GLY:HA3	1.83	0.43
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.51	0.43
2:C:468:ARG:HD3	2:C:485:TYR:HB3	1.99	0.43
2:C:108:ILE:HG13	2:C:366:SER:HB2	2.00	0.43
3:D:1466:VAL:HG22	3:D:1472:ILE:HG22	2.00	0.43
3:D:796:ARG:HB2	3:D:828:LYS:HG2	2.00	0.43
2:C:727:PRO:HG2	2:C:759:THR:HG21	1.99	0.43
2:C:64:LEU:HD13	2:C:359:MET:SD	2.58	0.43
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.54	0.43
2:C:1023:GLY:HA2	2:C:1026:GLN:O	2.19	0.43
2:C:842:ARG:HH11	2:C:842:ARG:CB	2.31	0.43
3:D:1314:LYS:HZ2	3:D:1316:GLY:HA3	1.81	0.43
3:D:1280:VAL:HG23	3:D:1282:ARG:HG3	2.00	0.43
1:A:122:ILE:HG22	1:A:124:ASN:H	1.84	0.43
2:C:250:ARG:O	2:C:254:VAL:HG23	2.18	0.43
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.43
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.19	0.43
3:D:58:CYS:HA	3:D:78:VAL:HG11	2.01	0.43
3:D:414:ARG:HG3	3:D:433:GLY:N	2.30	0.43
2:C:658:GLY:N	2:C:661:SER:HG	2.14	0.43
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.99	0.43
6:R:26:U:H2'	6:R:27:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:ILE:HA	2:C:14:PRO:HD3	1.90	0.43
1:B:186:LEU:O	1:B:188:GLN:N	2.52	0.43
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.76	0.43
2:C:1076:VAL:HB	3:D:752:SER:HA	2.00	0.43
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.49	0.43
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.49	0.43
2:C:146:VAL:HA	2:C:161:SER:O	2.18	0.43
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.52	0.43
4:E:38:THR:HG23	4:E:41:GLU:HG2	2.01	0.43
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.00	0.43
3:D:465:LEU:HD22	3:D:509:PRO:HB2	1.99	0.43
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.99	0.43
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.19	0.43
6:R:22:U:H2'	6:R:23:G:H8	1.82	0.43
2:C:700:TYR:HB3	2:C:996:LYS:HE3	2.00	0.43
3:D:1312:LEU:HD11	3:D:1327:ARG:HE	1.82	0.43
2:C:56:GLU:HB2	2:C:64:LEU:HB3	2.00	0.43
3:D:1381:VAL:HG23	3:D:1391:GLU:O	2.19	0.43
1:A:32:PHE:CE2	1:B:43:ILE:HG12	2.54	0.43
3:D:178:LEU:HD13	3:D:178:LEU:HA	1.83	0.43
3:D:1412:LYS:C	3:D:1414:PRO:HD3	2.39	0.43
1:B:59:GLU:HB3	1:B:137:ARG:NH1	2.31	0.43
3:D:1277:ILE:HG13	3:D:1301:LYS:HZ3	1.82	0.43
3:D:32:ILE:HG21	3:D:37:LEU:HD13	2.01	0.43
2:C:540:PHE:CE2	2:C:906:PHE:HE2	2.37	0.43
2:C:434:HIS:ND1	2:C:438:ILE:HD12	2.34	0.43
3:D:760:ARG:NH2	4:E:3:GLU:OE1	2.46	0.43
3:D:15:PRO:HB3	3:D:19:ARG:HH22	1.83	0.43
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.99	0.43
1:B:153:ALA:HB2	1:B:168:ASP:N	2.34	0.43
3:D:123:LEU:HG	3:D:152:LEU:HD21	2.00	0.42
3:D:148:GLU:OE2	3:D:153:LEU:HD22	2.18	0.42
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.54	0.42
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.52	0.42
3:D:462:GLN:O	3:D:466:LYS:HG3	2.19	0.42
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.35	0.42
2:C:542:VAL:HA	2:C:545:ASN:HB2	1.99	0.42
2:C:355:VAL:HG23	2:C:372:LEU:HB3	2.01	0.42
1:A:89:PHE:HB3	1:A:94:LEU:HD12	2.01	0.42
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:CZ	1:B:43:ILE:HG12	2.54	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	2.01	0.42
3:D:729:HIS:HE2	3:D:935:LYS:HD2	1.84	0.42
2:C:565:GLN:HG2	2:C:565:GLN:H	1.64	0.42
4:E:3:GLU:HB2	4:E:6:ILE:CG2	2.50	0.42
2:C:1016:ILE:HG13	2:C:1017:THR:HG22	2.00	0.42
3:D:1325:LEU:HD22	3:D:1325:LEU:H	1.84	0.42
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.48	0.42
3:D:176:ASP:HB3	3:D:177:ALA:H	1.55	0.42
2:C:603:VAL:HB	2:C:647:GLN:H	1.84	0.42
3:D:968:ASP:HA	3:D:971:LEU:HD23	2.01	0.42
1:B:20:TYR:HA	1:B:199:ILE:O	2.19	0.42
2:C:274:ARG:HB2	2:C:285:LEU:HD22	2.01	0.42
4:E:57:ASP:N	4:E:58:PRO:HD3	2.35	0.42
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.84	0.42
3:D:952:ASP:HA	3:D:1062:ARG:HH11	1.84	0.42
2:C:891:GLY:O	2:C:991:GLN:HG2	2.20	0.42
3:D:983:LEU:H	3:D:983:LEU:HG	1.60	0.42
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ2	1.79	0.42
2:C:1105:LYS:HD3	2:C:1105:LYS:H	1.84	0.42
3:D:57:GLU:HG3	3:D:64:LYS:HD2	2.02	0.42
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.01	0.42
1:A:143:ARG:NH1	1:A:158:ILE:HG21	2.35	0.42
1:A:57:TYR:CD2	1:A:161:ARG:HG3	2.54	0.42
2:C:442:GLU:OE2	2:C:543:ASN:ND2	2.43	0.42
1:A:24:VAL:HG22	1:A:196:THR:HG22	2.01	0.42
3:D:157:GLU:HA	3:D:160:GLU:HG2	2.01	0.42
2:C:425:PHE:H	2:C:428:ARG:HD2	1.84	0.42
2:C:1073:GLY:CA	3:D:659:LYS:HG2	2.50	0.42
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	2.02	0.42
3:D:462:GLN:HG2	3:D:466:LYS:HE3	2.02	0.42
3:D:206:ARG:HG2	3:D:392:SER:HB2	2.01	0.42
7:T:13:DC:H2"	7:T:14:DA:OP2	2.18	0.42
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.02	0.42
4:E:9:LEU:HD23	4:E:19:LEU:HD11	2.00	0.42
2:C:846:LYS:NZ	6:R:29:U:P	2.90	0.42
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	2.02	0.42
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.42
1:A:84:GLU:O	1:A:124:ASN:ND2	2.52	0.42
3:D:1301:LYS:HA	3:D:1301:LYS:HD3	1.94	0.42
3:D:807:ALA:HA	3:D:833:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:904:VAL:HB	3:D:905:PRO:HD2	2.02	0.42
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.55	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:466:LYS:HG2	3:D:510:GLU:HB3	2.02	0.42
5:N:7:DG:H2"	5:N:8:DA:C8	2.54	0.42
3:D:1462:LEU:O	3:D:1465:ASN:N	2.53	0.42
2:C:267:TYR:CB	2:C:272:ALA:HB3	2.50	0.42
2:C:148:PHE:CE2	2:C:309:TYR:HD2	2.38	0.42
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.40	0.42
3:D:841:TYR:HB3	3:D:843:PHE:CZ	2.55	0.42
3:D:1398:TRP:CE3	3:D:1398:TRP:HA	2.55	0.42
1:A:128:HIS:NE2	1:A:131:THR:HG23	2.35	0.42
2:C:216:GLU:C	2:C:218:VAL:H	2.22	0.42
3:D:568:ARG:HA	3:D:571:LYS:HG3	2.01	0.42
4:E:47:LYS:HA	4:E:54:LEU:HB3	2.01	0.42
2:C:810:ASP:HB2	2:C:813:VAL:HG13	2.02	0.42
2:C:889:HIS:O	2:C:918:LEU:HD21	2.20	0.42
7:T:3:DG:H2"	7:T:4:DA:C8	2.55	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.94	0.42
1:B:18:ARG:NH2	1:B:203:GLY:O	2.49	0.42
3:D:131:LYS:HG3	3:D:568:ARG:HG2	2.02	0.41
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.85	0.41
3:D:832:ARG:HA	3:D:832:ARG:HD2	1.74	0.41
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.50	0.41
3:D:1042:ARG:NH1	3:D:1073:SER:HB3	2.35	0.41
2:C:910:LYS:O	2:C:914:ILE:HG12	2.20	0.41
2:C:301:GLU:O	2:C:305:PRO:HD2	2.21	0.41
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.59	0.41
2:C:759:THR:HB	2:C:785:VAL:HG22	2.02	0.41
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.20	0.41
2:C:1038:TRP:HH2	3:D:1096:ARG:HA	1.85	0.41
2:C:9:ILE:HG12	2:C:907:ASP:OD2	2.19	0.41
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.01	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.20	0.41
2:C:473:ARG:NH1	2:C:473:ARG:HB2	2.35	0.41
2:C:118:ILE:HA	2:C:119:PRO:HD3	1.80	0.41
2:C:352:ALA:O	2:C:355:VAL:HG12	2.20	0.41
3:D:29:PRO:HB3	3:D:548:ILE:HB	2.01	0.41
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.41
4:E:80:VAL:HG11	4:E:85:LEU:HD23	2.01	0.41
2:C:181:VAL:HA	2:C:220:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:560:MET:HE3	2:C:846:LYS:HD3	2.02	0.41
2:C:1103:ASP:N	2:C:1107:ASN:O	2.53	0.41
2:C:334:ARG:HH11	2:C:418:LEU:CD1	2.34	0.41
1:A:90:LEU:HB3	1:A:119:ASP:HB3	2.03	0.41
3:D:357:GLU:OE2	3:D:386:HIS:ND1	2.37	0.41
2:C:1056:LYS:HB3	3:D:624:ASP:HB2	2.03	0.41
3:D:877:PRO:HA	3:D:880:ILE:HG22	2.02	0.41
1:A:183:ASP:N	1:A:183:ASP:OD1	2.53	0.41
2:C:327:HIS:CE1	2:C:489:THR:HA	2.56	0.41
3:D:32:ILE:HG22	3:D:33:ASN:O	2.20	0.41
2:C:724:ARG:HB2	2:C:741:GLY:N	2.36	0.41
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.36	0.41
2:C:36:PRO:HB2	2:C:70:GLU:CD	2.41	0.41
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	2.02	0.41
3:D:161:LEU:HD23	3:D:162:ARG:HG2	2.02	0.41
3:D:1412:LYS:HD3	3:D:1412:LYS:HA	1.47	0.41
2:C:969:GLN:HG2	3:D:952:ASP:OD2	2.21	0.41
3:D:1291:SER:HA	3:D:1302:GLU:OE2	2.20	0.41
1:A:67:THR:HB	2:C:627:ARG:HD3	2.02	0.41
3:D:426:LYS:HE2	3:D:426:LYS:HB3	1.90	0.41
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.56	0.41
2:C:1105:LYS:HZ3	2:C:1107:ASN:HB2	1.84	0.41
3:D:568:ARG:HA	3:D:568:ARG:HD2	1.97	0.41
3:D:764:LEU:O	3:D:768:ASN:ND2	2.45	0.41
1:B:11:PHE:HB2	1:B:25:LEU:HD12	2.02	0.41
4:E:41:GLU:HG3	4:E:41:GLU:H	1.56	0.41
2:C:749:VAL:HA	2:C:753:ASP:OD2	2.19	0.41
7:T:11:DT:H2''	7:T:12:DC:O5'	2.21	0.41
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.03	0.41
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.70	0.41
2:C:572:ILE:HG13	2:C:573:ARG:N	2.35	0.41
3:D:1290:LEU:HD21	3:D:1305:LEU:HD13	2.02	0.41
3:D:1142:ALA:HB1	3:D:1364:HIS:HA	2.03	0.41
3:D:31:THR:HG1	3:D:32:ILE:H	1.68	0.41
7:T:4:DA:H2''	7:T:5:DA:C8	2.56	0.41
1:A:151:VAL:HA	1:A:152:PRO:HD2	1.93	0.41
4:E:26:ARG:NH1	4:E:73:LEU:HD21	2.35	0.41
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.20	0.41
3:D:704:ARG:HG3	3:D:705:ALA:N	2.36	0.41
6:R:26:U:H2'	6:R:27:G:C8	2.56	0.41
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1492:LEU:O	3:D:1496:GLU:HB2	2.21	0.41
1:A:46:SER:OG	1:A:47:SER:N	2.52	0.41
1:A:141:GLU:N	1:A:141:GLU:OE1	2.53	0.41
2:C:177:GLU:HG2	2:C:178:PRO:HD2	2.03	0.41
2:C:214:TYR:HD1	2:C:215:GLY:H	1.69	0.41
2:C:137:VAL:HG23	2:C:391:LEU:HD23	2.02	0.41
1:B:77:GLU:OE2	3:D:867:ARG:NH1	2.54	0.41
5:N:3:DA:H2"	5:N:4:DA:C8	2.56	0.41
3:D:1407:LEU:HA	3:D:1407:LEU:HD23	1.91	0.41
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	2.03	0.41
1:B:56:VAL:HG23	1:B:167:VAL:HG21	2.02	0.41
3:D:1197:ARG:HH21	3:D:1198:TYR:HE2	1.69	0.41
2:C:1071:ILE:HA	2:C:1071:ILE:HD13	1.90	0.41
2:C:73:LEU:HD22	2:C:94:LEU:HA	2.03	0.41
2:C:378:LEU:O	2:C:382:ILE:HG12	2.21	0.40
3:D:108:VAL:HB	3:D:109:PRO:HD3	2.02	0.40
2:C:682:TYR:HA	3:D:633:VAL:HG11	2.02	0.40
3:D:470:LEU:H	3:D:470:LEU:HG	1.69	0.40
2:C:219:GLN:O	2:C:223:ASP:OD2	2.38	0.40
3:D:629:SER:OG	3:D:630:VAL:N	2.55	0.40
2:C:257:VAL:O	2:C:264:PRO:HD3	2.21	0.40
3:D:465:LEU:HD13	3:D:509:PRO:O	2.22	0.40
1:A:26:GLU:OE2	1:A:185:ARG:HB2	2.21	0.40
3:D:983:LEU:CD1	3:D:988:ARG:HB2	2.44	0.40
1:A:42:ARG:HE	2:C:856:GLU:HB2	1.84	0.40
3:D:834:THR:HB	3:D:838:ARG:HD2	2.04	0.40
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.40
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.20	0.40
3:D:1310:ARG:HH11	3:D:1327:ARG:NH1	2.20	0.40
5:N:6:DA:H2"	5:N:7:DG:C8	2.56	0.40
1:A:100:LEU:HD22	1:A:141:GLU:HG3	2.02	0.40
1:A:214:ALA:HA	1:A:217:ILE:HD12	2.03	0.40
1:A:86:VAL:HG21	1:A:202:ASP:HB2	2.04	0.40
2:C:184:MET:O	2:C:190:LYS:HA	2.21	0.40
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.52	0.40
3:D:801:GLY:HA3	3:D:826:PRO:HD2	2.04	0.40
2:C:442:GLU:HG2	2:C:454:SER:CB	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:NH1	3:D:1297:GLU:OE2[3_455]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/315 (70%)	186 (84%)	29 (13%)	6 (3%)	6	47
1	B	221/315 (70%)	193 (87%)	25 (11%)	3 (1%)	14	59
2	C	1077/1119 (96%)	897 (83%)	144 (13%)	36 (3%)	5	43
3	D	1352/1534 (88%)	1097 (81%)	198 (15%)	57 (4%)	3	35
4	E	91/99 (92%)	73 (80%)	13 (14%)	5 (6%)	2	30
All	All	2962/3382 (88%)	2446 (83%)	409 (14%)	107 (4%)	4	40

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA
2	C	217	LEU
2	C	262	ALA
3	D	117	ASP
3	D	165	LYS
3	D	176	ASP
3	D	363	ALA
3	D	705	ALA
3	D	808	THR
3	D	823	LEU
3	D	1067	VAL

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Mol	Chain	Res	Type
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1433	SER
3	D	1454	GLY
3	D	1459	LEU
1	A	29	GLU
2	C	96	ALA
2	C	114	PHE
2	C	248	PRO
2	C	320	HIS
2	C	476	GLY
2	C	517	ARG
2	C	984	GLU
3	D	55	ASP
3	D	82	LYS
3	D	137	PRO
3	D	594	PRO
3	D	824	ASN
3	D	1205	TYR
1	A	48	ILE
1	B	125	PRO
2	C	231	PRO
2	C	244	PRO
2	C	274	ARG
2	C	367	LEU
2	C	542	VAL
2	C	815	LEU
3	D	164	GLY
3	D	200	ASP
3	D	345	TYR
3	D	374	GLU
3	D	417	PRO
3	D	560	GLN
3	D	616	GLN
3	D	806	PHE
3	D	830	ALA
3	D	844	ALA
3	D	1128	VAL
3	D	1284	GLU
3	D	1287	GLU

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Mol	Chain	Res	Type
3	D	1302	GLU
4	E	4	PRO
4	E	42	PRO
4	E	50	THR
1	A	186	LEU
2	C	33	ASP
2	C	187	ASN
2	C	188	LYS
2	C	315	ALA
2	C	864	GLY
3	D	406	ASP
3	D	425	GLY
3	D	832	ARG
3	D	1129	THR
3	D	1269	LYS
3	D	1385	GLY
2	C	39	ARG
2	C	369	PRO
2	C	680	ASP
2	C	795	GLY
3	D	410	SER
3	D	522	PRO
3	D	722	GLU
3	D	1317	ASP
2	C	272	ALA
2	C	999	HIS
3	D	146	PRO
3	D	601	ARG
3	D	735	ALA
3	D	1197	ARG
4	E	58	PRO
1	B	187	GLY
2	C	905	ILE
3	D	182	GLY
3	D	1032	PRO
2	C	52	PHE
2	C	152	PRO
2	C	983	ILE
3	D	109	PRO
3	D	1155	VAL
3	D	1411	GLY
1	B	158	ILE

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Mol	Chain	Res	Type
3	D	208	PRO
3	D	1306	PRO
2	C	376	ARG
4	E	41	GLU
1	A	109	VAL
2	C	261	ILE
3	D	809	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/273 (72%)	188 (96%)	8 (4%)	37	72
1	B	196/273 (72%)	189 (96%)	7 (4%)	42	76
2	C	912/941 (97%)	837 (92%)	75 (8%)	14	51
3	D	1147/1289 (89%)	1044 (91%)	103 (9%)	12	47
4	E	82/88 (93%)	70 (85%)	12 (15%)	4	26
All	All	2533/2864 (88%)	2328 (92%)	205 (8%)	15	52

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	32	PHE
1	A	46	SER
1	A	126	ASP
1	A	165	ILE
1	A	182	GLU
1	B	26	GLU
1	B	63	HIS
1	B	112	ARG
1	B	201	THR

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Mol	Chain	Res	Type
1	B	205	VAL
1	B	206	THR
1	B	208	LEU
2	C	8	ARG
2	C	26	TYR
2	C	30	LEU
2	C	39	ARG
2	C	49	ARG
2	C	52	PHE
2	C	81	ASP
2	C	98	LEU
2	C	104	ASP
2	C	118	ILE
2	C	127	PHE
2	C	135	VAL
2	C	154	ARG
2	C	157	ARG
2	C	189	ARG
2	C	193	LEU
2	C	205	GLU
2	C	214	TYR
2	C	223	ASP
2	C	232	GLU
2	C	267	TYR
2	C	268	ASP
2	C	274	ARG
2	C	281	LEU
2	C	284	ARG
2	C	288	ARG
2	C	289	THR
2	C	295	ASP
2	C	299	LYS
2	C	300	ASP
2	C	303	PHE
2	C	306	THR
2	C	307	LEU
2	C	321	GLU
2	C	350	ARG
2	C	367	LEU
2	C	375	SER
2	C	376	ARG
2	C	378	LEU

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Mol	Chain	Res	Type
2	C	388	ARG
2	C	391	LEU
2	C	393	GLN
2	C	394	PHE
2	C	402	SER
2	C	403	SER
2	C	405	ARG
2	C	420	ARG
2	C	473	ARG
2	C	481	ASP
2	C	506	ASN
2	C	567	GLN
2	C	610	ARG
2	C	620	LEU
2	C	626	ARG
2	C	627	ARG
2	C	699	PHE
2	C	703	ILE
2	C	728	HIS
2	C	810	ASP
2	C	835	VAL
2	C	842	ARG
2	C	865	THR
2	C	880	MET
2	C	899	GLN
2	C	907	ASP
2	C	953	VAL
2	C	966	LEU
2	C	978	ARG
2	C	995	MET
2	C	1000	MET
2	C	1001	VAL
2	C	1008	ARG
2	C	1021	LEU
2	C	1099	VAL
2	C	1105	LYS
3	D	5	VAL
3	D	41	ARG
3	D	58	CYS
3	D	60	CYS
3	D	64	LYS
3	D	68	PHE

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Mol	Chain	Res	Type
3	D	73	CYS
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	85	VAL
3	D	87	ARG
3	D	107	ASP
3	D	124	GLU
3	D	127	LEU
3	D	142	LEU
3	D	149	LYS
3	D	150	ARG
3	D	152	LEU
3	D	153	LEU
3	D	161	LEU
3	D	166	GLN
3	D	176	ASP
3	D	178	LEU
3	D	186	VAL
3	D	340	THR
3	D	347	VAL
3	D	372	ASP
3	D	382	GLU
3	D	400	VAL
3	D	435	VAL
3	D	449	SER
3	D	468	LEU
3	D	483	HIS
3	D	494	LYS
3	D	507	ASN
3	D	520	LEU
3	D	527	MET
3	D	550	ARG
3	D	642	CYS
3	D	686	GLU
3	D	724	GLN
3	D	734	GLU
3	D	754	PHE
3	D	783	ARG
3	D	800	LYS
3	D	804	LEU

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Mol	Chain	Res	Type
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	892	ASP
3	D	902	LEU
3	D	932	ASP
3	D	935	LYS
3	D	971	LEU
3	D	983	LEU
3	D	991	GLN
3	D	1001	GLU
3	D	1012	GLU
3	D	1013	GLU
3	D	1029	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1070	TYR
3	D	1083	ASP
3	D	1094	LEU
3	D	1106	VAL
3	D	1109	GLU
3	D	1115	THR
3	D	1151	ARG
3	D	1162	GLU
3	D	1195	GLN
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1235	GLN
3	D	1262	LEU
3	D	1278	ASP
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1314	LYS
3	D	1315	ASP

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Mol	Chain	Res	Type
3	D	1318	TYR
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1389	LEU
3	D	1410	GLU
3	D	1412	LYS
3	D	1424	VAL
3	D	1433	SER
3	D	1441	GLN
3	D	1478	SER
3	D	1488	ASP
4	E	14	ASP
4	E	32	ARG
4	E	35	PHE
4	E	38	THR
4	E	39	VAL
4	E	41	GLU
4	E	47	LYS
4	E	49	GLN
4	E	51	LEU
4	E	56	ASP
4	E	57	ASP
4	E	74	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	B	156	HIS
2	C	141	HIS
2	C	406	HIS
2	C	431	HIS
2	C	434	HIS
2	C	609	ASN
2	C	884	GLN
3	D	388	HIS
3	D	462	GLN
3	D	1031	ASN
3	D	1033	GLN
3	D	1227	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/16 (50%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	223/315 (70%)	-0.11	2 (0%) 85 80	52, 116, 169, 205	0
1	B	223/315 (70%)	-0.12	1 (0%) 93 90	53, 107, 163, 198	0
2	C	1083/1119 (96%)	-0.13	12 (1%) 82 76	34, 108, 177, 264	0
3	D	1358/1534 (88%)	-0.01	35 (2%) 59 49	31, 110, 196, 250	0
4	E	93/99 (93%)	0.05	1 (1%) 82 76	65, 121, 179, 228	0
5	N	11/13 (84%)	0.35	1 (9%) 11 9	340, 362, 386, 405	0
6	R	9/16 (56%)	-0.21	0 100 100	201, 206, 235, 243	0
7	T	22/22 (100%)	-0.09	0 100 100	219, 336, 388, 406	0
All	All	3022/3433 (88%)	-0.07	52 (1%) 73 63	31, 111, 192, 406	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	368	VAL	6.0
3	D	1311	LEU	5.1
3	D	1279	GLY	4.8
3	D	1276	GLU	4.4
2	C	372	LEU	4.3
3	D	1321	ALA	4.1
3	D	1303	TYR	4.0
3	D	1299	PHE	3.9
3	D	367	ILE	3.8
3	D	393	ILE	3.5
3	D	802	ALA	3.5
2	C	373	VAL	3.5
1	A	7	LYS	3.5
3	D	355	VAL	3.4
3	D	1269	LYS	3.2
3	D	1278	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	1322	GLY	3.2
3	D	1327	ARG	3.0
3	D	191	LEU	2.9
3	D	949	ILE	2.9
3	D	1410	GLU	2.7
4	E	57	ASP	2.7
2	C	425	PHE	2.6
3	D	1290	LEU	2.6
5	N	13	DC	2.6
3	D	1298	GLY	2.5
3	D	44	LEU	2.5
3	D	69	GLU	2.5
3	D	1312	LEU	2.5
3	D	1310	ARG	2.4
3	D	810	GLU	2.4
1	A	25	LEU	2.4
2	C	302	VAL	2.3
3	D	164	GLY	2.3
3	D	1263	PHE	2.3
3	D	777	PRO	2.3
3	D	677	LEU	2.3
2	C	833	LEU	2.3
3	D	1328	GLY	2.3
2	C	423	ALA	2.2
2	C	521	PRO	2.2
3	D	769	LEU	2.2
3	D	720	LEU	2.2
3	D	455	ARG	2.2
2	C	247	PRO	2.2
3	D	1305	LEU	2.2
2	C	1041	GLU	2.2
2	C	713	ARG	2.1
2	C	1091	GLU	2.1
3	D	1288	GLU	2.1
2	C	1096	ALA	2.1
1	B	225	PHE	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
8	ZN	D	1602	1/1	0.98	0.29	2.20	70,70,70,70	0
8	ZN	D	1601	1/1	0.92	0.12	-1.39	70,70,70,70	0
9	MG	D	1603	1/1	0.93	0.22	-	70,70,70,70	0

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

There are no such residues in this entry.