



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 AM GMT

PDB ID : 2QKY  
Title : complex structure of dipeptidyl peptidase IV and a oxadiazolyl ketone  
Authors : Kim, K.-H.; Hong, S.Y.; Koo, K.D.; Lee, C.-S.; Kim, G.T.; Han, H.O.  
Deposited on : 2007-07-12  
Resolution : 3.10 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

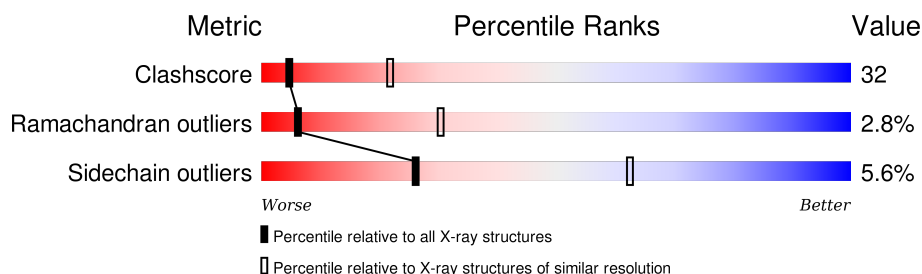
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>44%</div> <div>51%</div> <div>5%</div> </div>
1	B	728	<div> <div>46%</div> <div>49%</div> <div>.</div> </div>
1	C	728	<div> <div>46%</div> <div>49%</div> <div>5%</div> </div>
1	D	728	<div> <div>47%</div> <div>48%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24275 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.

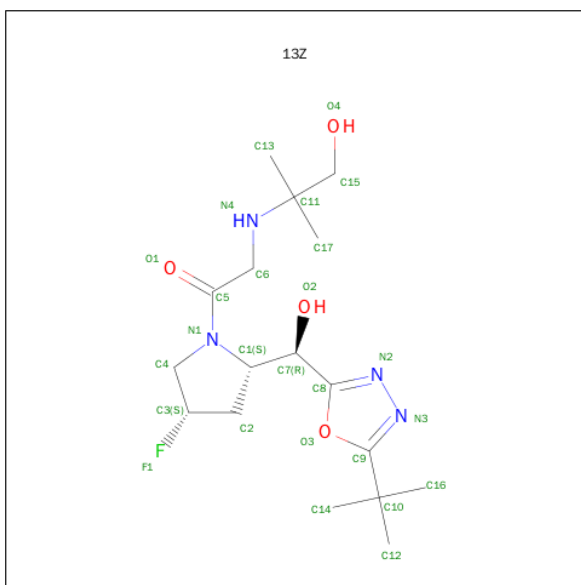
- Molecule 1 is a protein called Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	C	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	D	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	-	EXPRESSION TAG	UNP P27487
B	39	THR	-	EXPRESSION TAG	UNP P27487
C	39	THR	-	EXPRESSION TAG	UNP P27487
D	39	THR	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 2-[(2-{(2S,4S)-2-[(R)-(5-TERT-BUTYL-1,3,4-OXADIAZOL-2-YL)(HYDROXY)METHYL]-4-FLUOROPYRROLIDIN-1-YL}-2-OXOETHYL)AMINO]-2-METHYLPAN-1-OL (three-letter code: 13Z) (formula: C<sub>17</sub>H<sub>29</sub>FN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			26	17	1	4	4		
2	B	1	Total	C	F	N	O	0	0
			26	17	1	4	4		
2	C	1	Total	C	F	N	O	0	0
			26	17	1	4	4		
2	D	1	Total	C	F	N	O	0	0
			26	17	1	4	4		

- Molecule 3 is water.

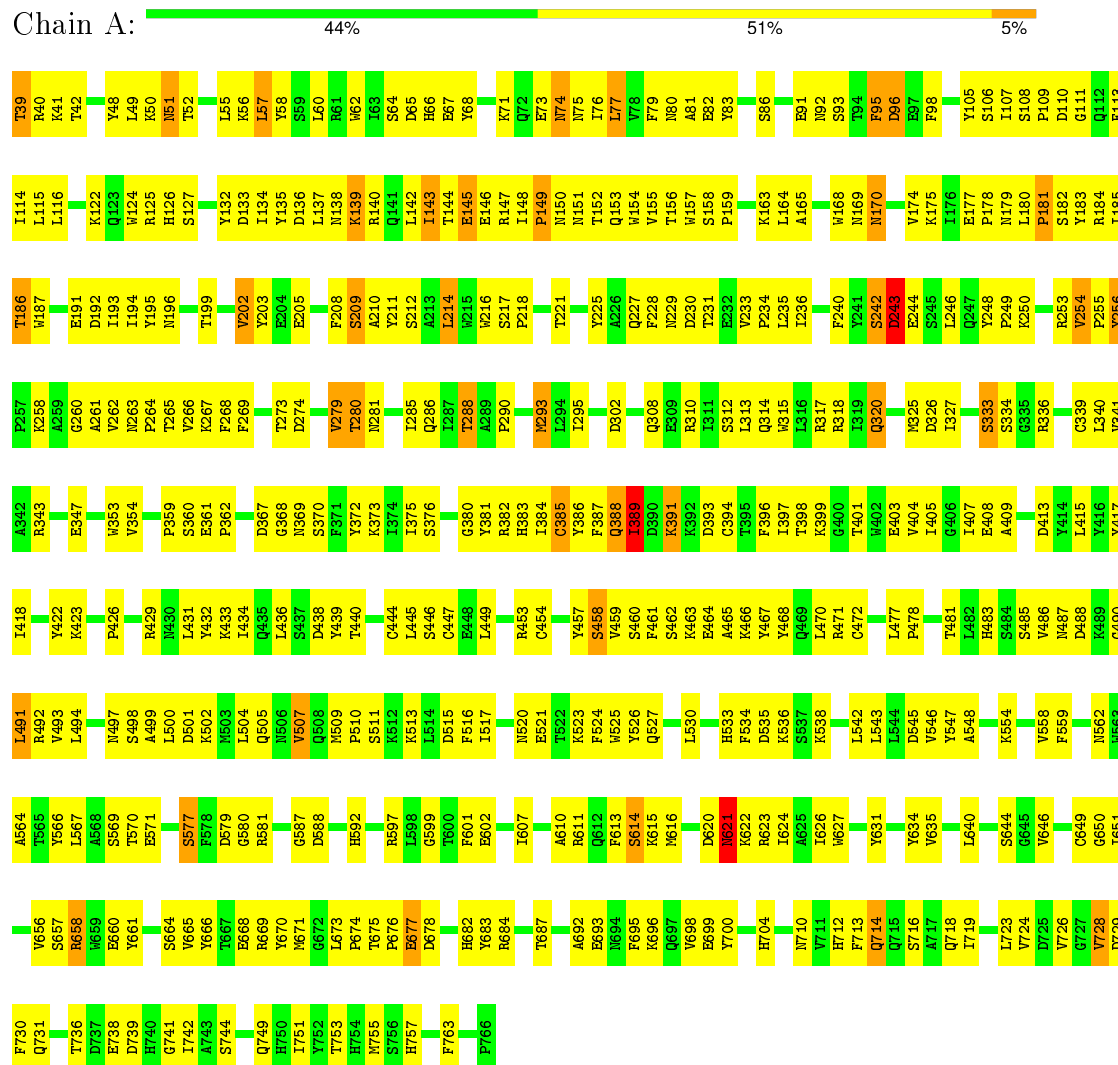
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	72	Total	O	0	0
			72	72		
3	C	66	Total	O	0	0
			66	66		
3	D	92	Total	O	0	0
			92	92		

### 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.

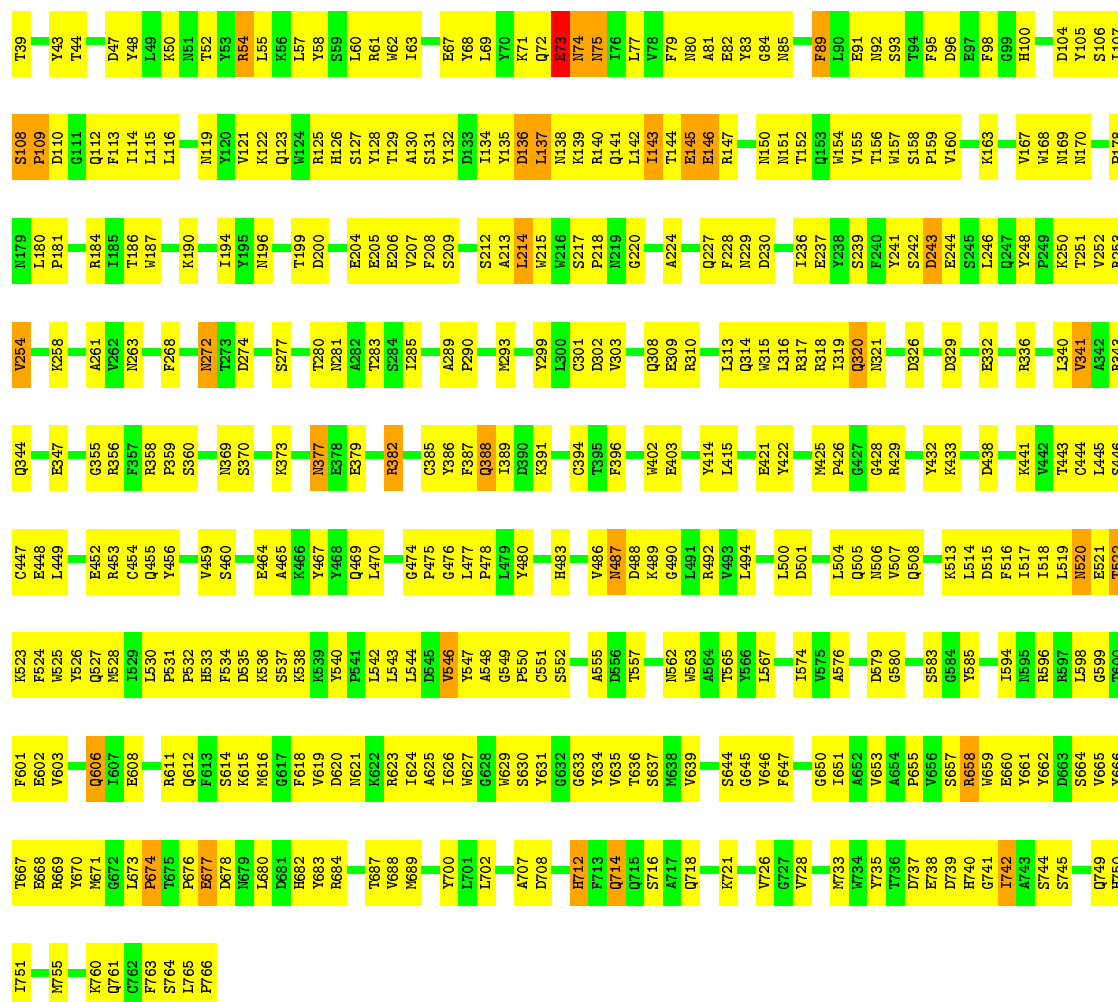
Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)



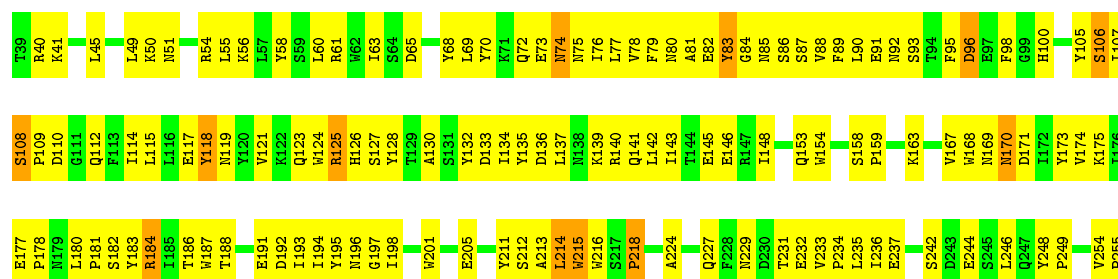
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

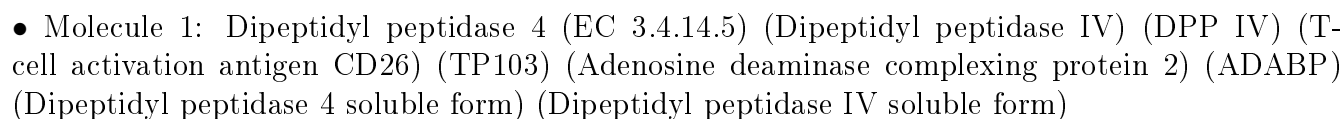
Chain B:  46% 49%



- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

Chain C:  46% 49% 5%





R597	L504	K399	D331	Y248	W174	P109	T39
L598	Q505	E403	E332	P249	K175	D110	R40
F601	M506	E403	S333		I176	G111	
E602		L405	S334	R253	E177	Q112	D47
		G406	G335	P254	P178	F113	Y48
		L407	K336	P255	M179	I114	L49
D605	R513		M337	Y256	P257	L115	K50
Q606	L514			Z258	P181	L116	N51
R611	D515	Y414	V341	K258		E117	T52
Q612	F516	L415	A342	A259	R184	Y118	Y53
F613	Y517		R343		I185	M119	R54
S614	M520	Y422	Q344	T265	T186	Y120	L55
K615	E521	K423	R345	V266			K56
	T522	G424	L346	K267			L57
K523		G427	E347	F268	E191	W124	Y58
				F269	D192	R125	S59
D620			T351	V270		H126	L60
K622	Y526	K433		Z271	Y185		R61
R623	Q527	L434	V354	M272	M196	T129	M62
I624			G355	T273	G197	A130	I63
L530	L530	V442	R356	D274	T198		S64
I626	P631		F357	S278	T199	D133	D65
R627	P532	L445	R358	T279	D200	I134	H66
G628	B533		P359	W201	Y135	E67	
M629		E448	S360	T280		D136	Y68
S630	P641	L449	E361		E205	L137	
Y631		K450	P362	S284	E206	N138	Q72
G632	L544	P451	R363	T285	V207	K139	E73
G633	F645		H364	Q286	F208	R140	N74
Y634	Y546	Q455	T365		S209	Q141	N75
B635	F547	Y456	L366	P290			I76
A548			D367		S212	I143	L77
T636	Y459		G368	M293	L214		V78
	P650	S460	N369	L300	Q215	E146	F79
L640	C551	F461	S370	C301	N216	I148	N80
G642	S552	K462	F371		S217	P149	A81
S643		E464	Y372	A306	P218	M150	E82
	T557	L465	K374	K307	N219	N151	Y83
F647		K466	L375	Q308	G220		G84
K648	L561		S376	P309	T221	W154	N85
C649	M562			R310	F222	S56	S87
G650	W563	G474	G380		L223	Y155	S87
		P475	V381	L313	A224	T156	V88
P655	F566	G476	R382	Q314		M157	F89
S567	L567		H383	W315	Q227	P159	L90
		T481	L384	K316	F228	V160	E91
B658	B571	H482	C385	R317	M229	G161	N92
M589	M572	H483	V386	R318		H162	
E600	L573	S484	F387	L319	L235	K163	F95
Y661		S485	Q388	Q320	T236	L164	F98
Y662	S577	K487	L389	N321	E237	A165	G99
D663			M390	Y322		V166	H100
S664	B581		K391	S323	F240	V167	S101
V665		L491	K392	S324	T241	W168	
F666	Y585	R492	D392	S325	S242	M169	I102
T667	Q566	L494	C394	D326	D243	N170	Y105
E668						D171	
R669	L594		L397	D329	L246	I172	S106
		D501	T397	Y320	C247	K172	I107
							S108

P766	D678 M679 L680 D681 H682 Y683 R684 M685  M689  V688 E699  I703 H704  D708 W709 M710 V711 H712 F713 Q714 Q715  I719 S720 K721  V724  A732 M733 W734  D737 E738 D739 H740 G741 I742 A743 S744 S745  Q749 H750 Y752  M755  I759 K760 Q761 C762 F763 S764 I765
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.18 Å   106.11 Å   132.05 Å 76.30°   78.62°   80.11°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	86.7 (20.00-3.10)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
13Z

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	0.56	0/6137	0.76	0/8346
1	B	0.56	0/6137	0.75	2/8346 (0.0%)
1	C	0.56	0/6137	0.73	2/8346 (0.0%)
1	D	0.56	0/6137	0.75	0/8346
All	All	0.56	0/24548	0.75	4/33384 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	214	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	415	LEU	N-CA-C	-5.60	95.89	111.00
1	C	388	GLN	N-CA-C	-5.33	96.60	111.00
1	B	388	GLN	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	700	TYR	Sidechain
1	B	128	TYR	Sidechain
1	C	83	TYR	Sidechain
1	D	752	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5965	0	5686	385	0
1	B	5965	0	5686	389	0
1	C	5965	0	5686	364	0
1	D	5965	0	5686	383	0
2	A	26	0	28	2	0
2	B	26	0	28	2	0
2	C	26	0	28	1	0
2	D	26	0	28	3	0
3	A	81	0	0	2	0
3	B	72	0	0	5	0
3	C	66	0	0	2	0
3	D	92	0	0	9	0
All	All	24275	0	22856	1490	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 32.

All (1490) 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:D:173:TYR:HE2	1:D:184:ARG:HG2	1.07	1.12
1:D:173:TYR:CE2	1:D:184:ARG:HG2	1.89	1.06
1:A:253:ARG:HH21	1:B:253:ARG:NH1	1.55	1.05
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.41	1.03
1:A:154:TRP:CZ3	1:A:214:LEU:HD21	1.95	1.02
1:A:429:ARG:HG2	1:A:429:ARG:HH11	1.31	0.95
1:D:180:LEU:HB2	1:D:181:PRO:HD2	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.49	0.94
1:D:481:THR:HG1	1:D:483:HIS:HE2	1.07	0.93
1:D:143:ILE:HG23	1:D:179:ASN:OD1	1.67	0.93
1:A:286:GLN:HE21	1:A:288:THR:HG23	1.34	0.92
1:B:54:ARG:H	1:B:54:ARG:CD	1.83	0.92
1:A:154:TRP:HZ3	1:A:214:LEU:HD21	1.30	0.91
1:D:75:ASN:HD22	1:D:92:ASN:ND2	1.68	0.90
1:A:65:ASP:OD1	1:A:464:GLU:N	2.04	0.90
1:A:693:GLU:HG3	1:A:696:LYS:NZ	1.86	0.90
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.55	0.89
1:B:518:ILE:O	1:B:519:LEU:HD23	1.74	0.88
1:D:134:ILE:HD11	1:D:157:TRP:CH2	2.09	0.87
1:A:253:ARG:HH21	1:B:253:ARG:HH11	1.16	0.87
1:C:98:PHE:HE2	1:C:100:HIS:HB2	1.39	0.86
1:C:621:ASN:HD22	1:C:622:LYS:H	1.22	0.86
1:A:295:ILE:HD11	1:A:317:ARG:HH21	1.38	0.86
1:A:382:ARG:H	1:A:403:GLU:HG2	1.39	0.85
1:C:621:ASN:ND2	1:C:622:LYS:HG3	1.92	0.84
1:D:114:ILE:HG22	1:D:137:LEU:HD21	1.59	0.84
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.44	0.83
1:C:354:VAL:CG1	1:C:359:PRO:HG3	2.08	0.82
1:D:293:MET:HE2	1:D:317:ARG:HG3	1.60	0.82
1:D:621:ASN:HA	1:D:624:ILE:HD11	1.62	0.82
1:B:84:GLY:HA3	1:B:492:ARG:NH1	1.95	0.81
1:B:109:PRO:HG2	1:B:158:SER:O	1.81	0.81
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.62	0.81
1:B:433:LYS:HD3	1:B:445:LEU:HD11	1.62	0.80
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.63	0.80
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.82	0.80
1:C:369:ASN:C	1:C:389:ILE:HG23	2.01	0.80
1:B:765:LEU:HB2	1:B:766:PRO:C	2.02	0.80
1:A:718:GLN:NE2	1:B:244:GLU:HA	1.96	0.80
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.83	0.79
1:D:134:ILE:HD11	1:D:157:TRP:HH2	1.47	0.79
1:D:549:GLY:O	1:D:552:SER:HB3	1.83	0.79
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.18	0.79
1:B:139:LYS:O	1:B:141:GLN:HG3	1.82	0.78
1:C:622:LYS:O	1:C:623:ARG:HG3	1.83	0.78
1:B:75:ASN:O	1:B:77:LEU:HD13	1.83	0.78
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.18	0.77
1:D:336:ARG:HG3	1:D:337:TRP:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HD11	1:A:317:ARG:NH2	1.99	0.77
1:D:272:ASN:HD22	1:D:272:ASN:C	1.88	0.77
1:C:119:ASN:O	1:C:130:ALA:HA	1.84	0.77
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.20	0.77
1:D:143:ILE:HG13	3:D:822:HOH:O	1.84	0.77
1:C:722:ALA:O	1:C:726:VAL:HG22	1.85	0.76
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.21	0.76
1:A:405:ILE:HG13	1:A:429:ARG:HD3	1.67	0.76
1:D:387:PHE:CE1	1:D:394:CYS:HB3	2.21	0.76
1:C:651:ILE:CD1	1:C:755:MET:HE2	2.15	0.76
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.68	0.76
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.01	0.76
1:C:651:ILE:HD13	1:C:755:MET:HE2	1.66	0.76
1:D:134:ILE:HD13	1:D:178:PRO:HB3	1.68	0.75
1:C:658:ARG:NH2	1:C:684:ARG:HD3	2.01	0.75
1:D:110:ASP:O	1:D:112:GLN:N	2.19	0.75
1:D:765:LEU:HB2	1:D:766:PRO:O	1.87	0.75
1:B:54:ARG:H	1:B:54:ARG:HD3	1.50	0.75
1:C:631:TYR:O	1:C:634:TYR:HB3	1.87	0.75
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.20	0.74
1:B:71:LYS:HE3	1:B:105:TYR:HE1	1.51	0.74
1:C:542:LEU:HD23	1:C:542:LEU:C	2.06	0.74
1:D:47:ASP:OD2	1:D:52:THR:HG21	1.87	0.74
1:B:134:ILE:HB	1:B:143:ILE:HD12	1.69	0.74
1:A:214:LEU:HD23	1:A:214:LEU:O	1.88	0.74
1:D:310:ARG:HG3	1:D:329:ASP:OD1	1.87	0.73
1:D:598:LEU:HD22	1:D:631:TYR:OH	1.87	0.73
1:A:50:LYS:O	1:A:51:ASN:HB2	1.86	0.73
1:D:571:GLU:CD	1:D:760:LYS:HD3	2.08	0.73
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.23	0.73
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.69	0.73
1:A:159:PRO:HG3	1:A:217:SER:O	1.87	0.73
1:A:55:LEU:HD12	1:A:500:LEU:HD22	1.69	0.73
1:C:621:ASN:HD22	1:C:622:LYS:N	1.85	0.73
1:D:369:ASN:O	1:D:389:ILE:HG23	1.89	0.73
1:C:354:VAL:HG12	1:C:359:PRO:HG3	1.71	0.73
1:C:121:VAL:O	1:C:128:TYR:HB2	1.89	0.73
1:A:397:ILE:HD12	1:A:434:ILE:HG21	1.70	0.73
1:D:235:LEU:HD23	1:D:255:PRO:HA	1.71	0.73
1:D:133:ASP:CG	1:D:147:ARG:HH21	1.91	0.73
1:B:329:ASP:OD1	1:B:343:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ASN:O	1:B:389:ILE:HG23	1.88	0.73
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.69	0.72
1:B:123:GLN:HB3	1:B:127:SER:OG	1.89	0.72
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.24	0.72
1:C:114:ILE:HG22	1:C:137:LEU:HD21	1.71	0.72
1:C:79:PHE:CE1	1:C:86:SER:HB3	2.25	0.72
1:A:150:ASN:O	1:A:151:ASN:HB2	1.90	0.72
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.70	0.72
1:D:135:TYR:OH	1:D:140:ARG:HG2	1.90	0.71
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:D:293:MET:CE	1:D:317:ARG:HG3	2.20	0.71
1:D:272:ASN:HD22	1:D:273:THR:N	1.87	0.71
1:B:487:ASN:HD22	1:B:489:LYS:H	1.38	0.71
1:D:158:SER:CB	1:D:163:LYS:HB2	2.19	0.71
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.55	0.71
1:A:376:SER:HA	1:A:381:TYR:O	1.89	0.71
1:A:415:LEU:HB2	1:A:436:LEU:HD21	1.71	0.71
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.09	0.71
1:C:146:GLU:OE1	1:C:181:PRO:HB3	1.90	0.71
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.71	0.71
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.71	0.71
1:A:134:ILE:HD11	1:A:164:LEU:HD11	1.72	0.71
1:C:516:PHE:CD2	1:C:523:LYS:HB2	2.26	0.71
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.73	0.71
1:D:272:ASN:ND2	1:D:274:ASP:H	1.88	0.71
1:C:137:LEU:O	1:C:140:ARG:HD2	1.90	0.71
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.89	0.70
1:C:420:ASN:HD22	1:C:426:PRO:HA	1.56	0.70
1:C:458:SER:HB3	1:C:471:ARG:HB3	1.71	0.70
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.73	0.70
1:C:596:ARG:O	1:C:597:ARG:HD2	1.91	0.70
1:B:603:VAL:HG22	1:B:635:VAL:HG13	1.73	0.70
1:B:519:LEU:O	1:B:522:THR:N	2.24	0.70
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.72	0.70
1:C:65:ASP:OD1	1:C:464:GLU:N	2.24	0.70
1:C:55:LEU:CD1	1:C:561:LEU:HD12	2.21	0.70
1:A:429:ARG:HG2	1:A:429:ARG:NH1	2.06	0.70
1:D:134:ILE:CG2	1:D:143:ILE:HD12	2.21	0.70
1:B:93:SER:HA	1:B:96:ASP:OD1	1.92	0.69
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.27	0.69
1:D:138:ASN:OD1	1:D:139:LYS:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:O	1:C:139:LYS:HG3	1.91	0.69
1:A:693:GLU:HG3	1:A:696:LYS:HZ1	1.57	0.69
1:C:258:LYS:NZ	1:C:712:HIS:HD2	1.91	0.69
1:D:40:ARG:HB3	1:D:506:ASN:O	1.93	0.69
1:A:286:GLN:NE2	1:A:288:THR:HG23	2.05	0.69
1:C:658:ARG:HE	1:C:687:THR:HG21	1.56	0.69
1:B:674:PRO:O	1:B:680:LEU:HD13	1.93	0.69
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.23	0.69
1:A:477:LEU:HD13	1:A:500:LEU:HD23	1.74	0.69
1:A:258:LYS:NZ	1:A:712:HIS:CD2	2.61	0.69
1:D:95:PHE:CE1	1:D:116:LEU:HD11	2.28	0.69
1:A:248:TYR:CE2	1:B:258:LYS:HD2	2.28	0.69
1:C:633:GLY:HA3	1:C:655:PRO:HB3	1.73	0.69
1:B:487:ASN:ND2	1:B:489:LYS:H	1.90	0.68
1:B:602:GLU:OE2	1:B:602:GLU:N	2.26	0.68
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.09	0.68
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.23	0.68
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.75	0.68
1:A:127:SER:HB3	1:A:211:TYR:CG	2.28	0.68
1:C:365:THR:O	1:C:368:GLY:N	2.26	0.68
1:C:369:ASN:O	1:C:389:ILE:HG23	1.93	0.68
1:C:654:ALA:HA	1:C:704:HIS:ND1	2.09	0.68
1:D:235:LEU:HD23	1:D:255:PRO:CA	2.24	0.68
1:B:388:GLN:HG2	1:B:391:LYS:HE3	1.76	0.68
1:C:258:LYS:HD2	1:D:248:TYR:CE2	2.28	0.68
1:A:459:VAL:HG22	1:A:460:SER:H	1.58	0.68
1:D:195:TYR:O	1:D:227:GLN:HA	1.94	0.68
1:D:62:TRP:CE3	1:D:462:SER:HB3	2.29	0.68
1:B:667:THR:O	1:B:671:MET:HB2	1.93	0.68
1:A:621:ASN:HA	1:A:624:ILE:HD11	1.77	0.67
1:B:702:LEU:HD21	1:B:716:SER:HB3	1.76	0.67
1:B:745:SER:O	1:B:749:GLN:HG3	1.94	0.67
1:D:134:ILE:HG23	1:D:143:ILE:HD12	1.76	0.67
1:C:542:LEU:HD23	1:C:543:LEU:N	2.08	0.67
1:C:458:SER:CB	1:C:471:ARG:HD3	2.23	0.67
1:A:244:GLU:HA	1:B:718:GLN:NE2	2.10	0.67
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.09	0.67
1:B:516:PHE:HE2	1:B:518:ILE:HD11	1.59	0.67
1:A:263:ASN:ND2	1:A:318:ARG:CZ	2.58	0.67
1:C:720:SER:O	1:C:724:VAL:HG23	1.95	0.67
1:B:534:PHE:HE1	1:B:574:ILE:HD11	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.30	0.67
1:D:108:SER:HB3	1:D:157:TRP:CE2	2.30	0.67
1:C:244:GLU:HG3	1:D:689:MET:HE3	1.76	0.67
1:C:117:GLU:HB2	1:C:132:TYR:CE2	2.30	0.67
1:D:319:ILE:O	1:D:321:ASN:N	2.28	0.67
1:D:139:LYS:HG2	1:D:141:GLN:HB2	1.77	0.67
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.30	0.67
1:B:635:VAL:O	1:B:639:VAL:HG23	1.95	0.67
1:A:502:LYS:O	1:A:505:GLN:HG2	1.95	0.67
1:C:507:VAL:HG13	1:C:509:MET:HG2	1.76	0.67
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.77	0.67
1:D:214:LEU:HD12	1:D:223:LEU:HD11	1.77	0.66
1:D:763:PHE:HB2	1:D:765:LEU:HD21	1.77	0.66
1:C:93:SER:O	1:C:96:ASP:HB2	1.95	0.66
1:B:483:HIS:HD1	1:B:490:GLY:HA2	1.60	0.66
1:C:74:ASN:O	1:C:92:ASN:HA	1.95	0.66
1:D:745:SER:O	1:D:749:GLN:HG3	1.94	0.66
1:D:125:ARG:NH2	1:D:205:GLU:OE2	2.27	0.66
1:C:761:GLN:NE2	1:C:762:CYS:HA	2.11	0.66
1:B:242:SER:CB	1:B:246:LEU:HD23	2.25	0.66
1:C:235:LEU:HD23	1:C:255:PRO:HA	1.77	0.66
1:D:492:ARG:HB3	1:D:492:ARG:NH1	2.11	0.66
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.11	0.66
1:A:175:LYS:CG	1:A:182:SER:HB3	2.23	0.66
1:B:518:ILE:CD1	1:B:523:LYS:HB3	2.25	0.66
1:A:263:ASN:HD22	1:A:318:ARG:CZ	2.09	0.65
1:C:72:GLN:O	1:C:75:ASN:HB2	1.97	0.65
1:A:156:THR:HG23	1:A:165:ALA:HB3	1.78	0.65
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.31	0.65
1:A:240:PHE:HB3	1:A:250:LYS:HG3	1.77	0.65
1:C:702:LEU:HD11	1:C:716:SER:OG	1.95	0.65
1:B:242:SER:HB3	1:B:246:LEU:HD23	1.79	0.65
1:B:644:SER:O	1:B:646:VAL:HG23	1.97	0.65
1:B:514:LEU:HD22	1:B:557:THR:HG22	1.78	0.65
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.32	0.65
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.31	0.65
1:C:65:ASP:OD2	1:C:464:GLU:HB2	1.96	0.65
1:A:64:SER:O	1:A:463:LYS:HG2	1.97	0.65
1:D:365:THR:O	1:D:368:GLY:N	2.24	0.65
1:C:513:LYS:O	1:C:527:GLN:HA	1.96	0.65
1:C:458:SER:HB3	1:C:471:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:VAL:HG22	1:C:508:GLN:N	2.12	0.65
1:C:125:ARG:HG2	1:C:126:HIS:CE1	2.32	0.65
1:C:114:ILE:CG2	1:C:137:LEU:HD21	2.26	0.64
1:D:397:ILE:HD12	1:D:434:ILE:HD13	1.77	0.64
1:A:511:SER:OG	1:A:530:LEU:HB2	1.96	0.64
1:C:535:ASP:OD1	1:C:538:LYS:HE2	1.96	0.64
1:D:57:LEU:HD12	1:D:57:LEU:H	1.62	0.64
1:A:218:PRO:HB2	1:A:308:GLN:CD	2.18	0.64
1:A:381:TYR:CE2	1:A:401:THR:HA	2.32	0.64
1:C:581:ARG:HB2	1:C:605:ASP:OD2	1.97	0.64
1:A:459:VAL:HG22	1:A:460:SER:N	2.11	0.64
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.31	0.64
1:D:146:GLU:HB2	1:D:179:ASN:O	1.96	0.64
1:C:244:GLU:HG3	1:D:689:MET:CE	2.27	0.64
1:D:571:GLU:O	1:D:573:ILE:HG13	1.97	0.64
1:C:745:SER:O	1:C:749:GLN:HG3	1.98	0.64
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.95	0.64
1:C:75:ASN:HD21	1:C:92:ASN:ND2	1.95	0.64
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.79	0.64
1:C:127:SER:HB3	1:C:211:TYR:CD1	2.33	0.64
1:D:159:PRO:HG3	1:D:217:SER:O	1.97	0.64
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.78	0.64
1:C:258:LYS:HZ1	1:C:712:HIS:HD2	1.45	0.64
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.27	0.64
1:D:515:ASP:OD2	1:D:516:PHE:N	2.30	0.64
1:A:260:GLY:HA3	1:A:674:PRO:HG3	1.79	0.63
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.80	0.63
1:D:492:ARG:HB3	1:D:492:ARG:HH11	1.63	0.63
1:B:446:SER:O	1:B:449:LEU:HG	1.98	0.63
1:C:90:LEU:HD21	1:C:95:PHE:HE2	1.63	0.63
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.34	0.63
1:A:58:TYR:CE2	1:A:494:LEU:HD13	2.33	0.63
1:C:336:ARG:HH11	1:C:336:ARG:HG3	1.64	0.63
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.81	0.63
1:B:130:ALA:HB3	1:B:132:TYR:CE1	2.33	0.63
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.79	0.63
1:C:127:SER:HB3	1:C:211:TYR:CG	2.34	0.63
1:B:426:PRO:HG3	1:B:525:TRP:CD1	2.33	0.63
1:D:173:TYR:HE2	1:D:184:ARG:CG	1.98	0.63
1:D:217:SER:HB2	1:D:222:PHE:HB2	1.80	0.63
1:C:702:LEU:HD21	1:C:716:SER:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:NH1	1:C:54:ARG:HG2	2.11	0.63
1:B:71:LYS:HE3	1:B:105:TYR:CE1	2.31	0.63
1:A:192:ASP:O	1:A:193:ILE:HD13	1.99	0.63
1:C:383:HIS:HB3	1:C:398:THR:OG1	1.97	0.63
1:C:354:VAL:HG11	1:C:359:PRO:HG3	1.80	0.62
1:D:370:SER:HB2	1:D:387:PHE:O	2.00	0.62
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.34	0.62
1:C:170:ASN:HD22	1:C:170:ASN:N	1.97	0.62
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.00	0.62
1:B:54:ARG:N	1:B:54:ARG:CD	2.60	0.62
1:C:135:TYR:CD1	1:C:141:GLN:O	2.52	0.62
1:B:513:LYS:NZ	1:B:515:ASP:HB2	2.14	0.62
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.82	0.62
1:D:75:ASN:HD22	1:D:92:ASN:HD22	1.45	0.62
1:A:62:TRP:CG	1:A:462:SER:HA	2.34	0.62
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.34	0.62
1:D:596:ARG:O	1:D:597:ARG:HD2	2.00	0.62
1:A:673:LEU:HB2	1:A:678:ASP:OD2	2.00	0.62
1:A:168:TRP:O	1:A:169:ASN:HB2	1.99	0.62
1:C:376:SER:HA	1:C:382:ARG:HA	1.82	0.62
1:D:75:ASN:ND2	1:D:92:ASN:ND2	2.44	0.62
1:A:461:PHE:CE2	1:A:468:TYR:HB3	2.35	0.62
1:C:118:TYR:O	1:C:130:ALA:HB1	1.99	0.62
1:A:693:GLU:HG3	1:A:696:LYS:HZ2	1.62	0.61
1:D:40:ARG:HH11	1:D:40:ARG:HG3	1.65	0.61
1:B:75:ASN:HD22	1:B:92:ASN:ND2	1.98	0.61
1:D:336:ARG:HG3	1:D:337:TRP:N	2.14	0.61
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.47	0.61
1:B:145:GLU:O	1:B:146:GLU:C	2.38	0.61
1:C:492:ARG:HH11	1:C:492:ARG:HB3	1.65	0.61
1:C:550:PRO:HD3	1:C:631:TYR:CE2	2.35	0.61
1:C:73:GLU:O	1:C:75:ASN:N	2.34	0.61
1:A:675:THR:HB	1:A:676:PRO:HD2	1.81	0.61
1:B:486:VAL:HG13	1:B:487:ASN:N	2.15	0.61
1:D:133:ASP:OD2	1:D:147:ARG:NH2	2.32	0.61
1:A:453:ARG:HG2	1:A:454:CYS:SG	2.41	0.61
1:B:268:PHE:CE2	1:B:313:LEU:HD21	2.35	0.61
1:D:433:LYS:HB2	1:D:445:LEU:HD11	1.81	0.61
1:A:81:ALA:O	1:A:491:LEU:HD13	2.01	0.61
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.35	0.61
1:B:528:MET:HG2	1:B:576:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:OD1	1:B:93:SER:N	2.33	0.61
1:A:76:ILE:HD11	1:A:105:TYR:CE1	2.36	0.61
1:C:658:ARG:HH22	1:C:684:ARG:HD3	1.66	0.61
1:B:658:ARG:HH22	1:B:684:ARG:HD3	1.66	0.61
1:A:71:LYS:HG3	1:A:76:ILE:HG12	1.83	0.61
1:C:455:GLN:HB2	1:C:475:PRO:HD3	1.82	0.61
1:D:136:ASP:OD1	1:D:138:ASN:HB3	2.00	0.61
1:B:414:TYR:CD2	1:B:433:LYS:HG2	2.36	0.61
1:D:167:VAL:HA	1:D:171:ASP:O	2.01	0.61
1:C:541:PRO:HB2	1:C:763:PHE:CE2	2.36	0.61
1:A:253:ARG:NH2	1:B:253:ARG:HH11	1.94	0.61
1:D:235:LEU:HD21	1:D:255:PRO:HG3	1.82	0.61
1:B:741:GLY:O	1:B:742:ILE:C	2.39	0.61
1:D:414:TYR:CE2	1:D:433:LYS:HE3	2.36	0.61
1:A:730:PHE:HD1	1:A:731:GLN:O	1.84	0.61
1:C:218:PRO:HB2	1:C:308:GLN:NE2	2.16	0.60
1:B:75:ASN:ND2	1:B:92:ASN:ND2	2.49	0.60
1:A:138:ASN:C	1:A:140:ARG:H	2.03	0.60
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.01	0.60
1:A:403:GLU:OE2	1:A:587:GLY:N	2.34	0.60
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.32	0.60
1:D:751:ILE:HG23	1:D:752:TYR:N	2.16	0.60
1:D:241:TYR:O	1:D:246:LEU:HD23	2.01	0.60
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.16	0.60
1:A:95:PHE:CB	1:A:98:PHE:HB2	2.31	0.60
1:A:438:ASP:O	1:A:440:THR:N	2.35	0.60
1:D:208:PHE:HE1	1:D:300:LEU:O	1.84	0.60
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.37	0.60
1:C:134:ILE:HD13	1:C:178:PRO:HB3	1.83	0.60
1:D:134:ILE:HG21	1:D:178:PRO:HB2	1.81	0.60
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.31	0.60
1:B:106:SER:HG	1:B:157:TRP:HE1	1.50	0.60
1:B:150:ASN:O	1:B:151:ASN:HB2	2.02	0.60
1:B:152:THR:HG23	1:B:167:VAL:O	2.01	0.60
1:C:105:TYR:O	1:C:106:SER:HB2	2.02	0.60
1:C:258:LYS:NZ	1:C:712:HIS:CD2	2.70	0.60
1:D:765:LEU:HB2	1:D:766:PRO:C	2.22	0.60
1:C:82:GLU:HG2	1:C:83:TYR:CZ	2.37	0.60
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.83	0.60
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.83	0.60
1:A:248:TYR:CZ	1:B:258:LYS:HD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:N	1:A:92:ASN:HB3	2.17	0.60
1:B:122:LYS:HG2	1:B:123:GLN:N	2.16	0.60
1:B:199:THR:HA	1:B:228:PHE:CE2	2.37	0.60
1:D:110:ASP:C	1:D:112:GLN:H	2.05	0.59
1:C:73:GLU:C	1:C:75:ASN:H	2.06	0.59
1:D:272:ASN:ND2	1:D:272:ASN:C	2.55	0.59
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.37	0.59
1:B:159:PRO:O	1:B:160:VAL:HG23	2.02	0.59
1:A:631:TYR:O	1:A:634:TYR:HB3	2.01	0.59
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.37	0.59
1:A:42:THR:HB	1:A:569:SER:OG	2.03	0.59
1:A:432:TYR:CE2	1:A:444:CYS:HB2	2.38	0.59
1:C:658:ARG:HE	1:C:687:THR:CG2	2.15	0.59
1:B:52:THR:O	1:B:54:ARG:NH1	2.31	0.59
1:C:49:LEU:CD2	1:C:749:GLN:HA	2.31	0.59
1:D:235:LEU:CD2	1:D:255:PRO:HG3	2.32	0.59
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.99	0.59
1:B:206:GLU:OE1	2:B:767:13Z:H15	2.02	0.59
1:C:720:SER:HB2	1:C:730:PHE:HZ	1.67	0.59
1:C:580:GLY:O	1:C:583:SER:OG	2.20	0.59
1:A:148:ILE:HD12	1:A:148:ILE:H	1.67	0.59
1:A:611:ARG:O	1:A:614:SER:HB3	2.03	0.59
1:A:227:GLN:O	1:A:266:VAL:HA	2.01	0.59
1:D:708:ASP:OD2	1:D:740:HIS:HA	2.02	0.59
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.82	0.59
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.38	0.59
1:A:286:GLN:HE21	1:A:288:THR:CG2	2.11	0.59
1:D:614:SER:HB2	1:D:621:ASN:OD1	2.03	0.59
1:D:602:GLU:OE2	1:D:602:GLU:N	2.32	0.59
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.36	0.59
1:D:487:ASN:HD22	1:D:487:ASN:H	1.49	0.59
1:B:555:ALA:HB3	1:B:579:ASP:OD2	2.02	0.59
1:A:57:LEU:HD12	1:A:57:LEU:N	2.17	0.59
1:A:293:MET:HE3	1:A:315:TRP:O	2.01	0.59
1:A:644:SER:HB2	1:A:646:VAL:HG23	1.85	0.59
1:D:316:LEU:HD21	1:D:320:GLN:HG2	1.85	0.59
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.38	0.59
1:C:621:ASN:ND2	1:C:622:LYS:H	1.98	0.59
1:D:370:SER:HG	1:D:386:TYR:HE1	1.49	0.59
1:C:634:TYR:HD1	1:C:656:VAL:O	1.85	0.59
1:C:597:ARG:HH12	1:C:682:HIS:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.85	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.03	0.59
1:B:611:ARG:O	1:B:615:LYS:HG2	2.03	0.59
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.83	0.59
1:B:765:LEU:H	1:B:765:LEU:HD22	1.68	0.59
1:D:664:SER:HB2	1:D:668:GLU:OE2	2.02	0.59
1:B:355:GLY:HA2	1:B:382:ARG:HH12	1.68	0.59
1:C:174:VAL:O	1:C:183:TYR:HD2	1.84	0.58
1:D:743:ALA:O	1:D:744:SER:C	2.39	0.58
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.03	0.58
1:C:658:ARG:HB2	1:C:687:THR:CG2	2.29	0.58
1:D:118:TYR:O	1:D:130:ALA:HB1	2.02	0.58
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.85	0.58
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.85	0.58
1:C:58:TYR:HD2	1:C:58:TYR:O	1.86	0.58
1:D:486:VAL:HG13	1:D:487:ASN:N	2.19	0.58
1:A:472:CYS:O	1:A:478:PRO:HA	2.04	0.58
1:A:369:ASN:C	1:A:389:ILE:HG23	2.23	0.58
1:D:513:LYS:O	1:D:527:GLN:HA	2.02	0.58
1:A:524:PHE:HD2	1:A:580:GLY:HA2	1.69	0.58
1:B:208:PHE:O	1:B:209:SER:HB2	2.03	0.58
1:D:633:GLY:C	1:D:655:PRO:HB3	2.24	0.58
1:D:422:TYR:CE2	1:D:423:LYS:HE2	2.39	0.58
1:A:468:TYR:CE2	1:A:483:HIS:HB2	2.38	0.58
1:B:135:TYR:CE2	1:B:140:ARG:HA	2.37	0.58
1:D:113:PHE:CD2	1:D:113:PHE:N	2.71	0.58
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.18	0.58
1:D:114:ILE:HG22	1:D:137:LEU:CD2	2.31	0.58
1:B:122:LYS:CG	1:B:123:GLN:N	2.67	0.58
1:D:74:ASN:C	1:D:92:ASN:HB3	2.24	0.58
1:C:325:MET:HE3	1:C:371:PHE:CE2	2.38	0.58
1:D:191:GLU:O	1:D:192:ASP:HB2	2.03	0.58
1:B:54:ARG:H	1:B:54:ARG:HD2	1.65	0.58
1:C:516:PHE:HD2	1:C:523:LYS:HB2	1.66	0.58
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.85	0.58
1:A:260:GLY:HA3	1:A:674:PRO:CG	2.34	0.58
1:C:621:ASN:HD21	1:C:622:LYS:HG3	1.68	0.57
1:A:75:ASN:OD1	1:A:91:GLU:HA	2.03	0.57
1:B:125:ARG:NH2	1:B:205:GLU:OE2	2.37	0.57
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.04	0.57
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:751:ILE:O	1:C:755:MET:HG3	2.03	0.57
1:D:765:LEU:N	1:D:765:LEU:HD22	2.20	0.57
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.39	0.57
1:B:751:ILE:O	1:B:755:MET:HG3	2.04	0.57
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.39	0.57
1:C:644:SER:HB2	1:C:646:VAL:HG23	1.85	0.57
1:D:455:GLN:NE2	1:D:475:PRO:HG3	2.19	0.57
1:A:458:SER:HB3	1:A:471:ARG:HD3	1.85	0.57
1:B:113:PHE:CD1	1:B:136:ASP:HA	2.40	0.57
1:A:415:LEU:HD23	1:A:415:LEU:C	2.25	0.57
1:C:77:LEU:HD22	1:C:87:SER:O	2.05	0.57
1:D:314:GLN:NE2	1:D:362:PRO:HD3	2.20	0.57
1:B:443:THR:HG22	1:B:445:LEU:HD23	1.86	0.57
1:D:374:ILE:CD1	1:D:404:VAL:HG12	2.35	0.57
1:D:266:VAL:O	1:D:267:LYS:HG2	2.04	0.57
1:D:336:ARG:CG	1:D:337:TRP:N	2.68	0.57
1:C:63:ILE:HG21	1:C:69:LEU:HG	1.84	0.57
1:C:56:LYS:HD3	1:C:495:GLU:OE1	2.05	0.57
1:C:236:ILE:HD12	1:C:237:GLU:H	1.67	0.57
1:B:272:ASN:C	1:B:272:ASN:HD22	2.08	0.57
1:B:459:VAL:HG22	1:B:460:SER:N	2.18	0.57
1:B:301:CYS:O	1:B:358:ARG:NH1	2.37	0.57
1:C:621:ASN:HD22	1:C:621:ASN:N	2.01	0.57
1:A:524:PHE:CD2	1:A:580:GLY:HA2	2.40	0.57
1:C:387:PHE:CE1	1:C:394:CYS:HB3	2.39	0.57
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.86	0.57
1:D:180:LEU:HB2	1:D:181:PRO:CD	2.30	0.57
1:D:516:PHE:CD2	1:D:523:LYS:HB2	2.38	0.57
1:D:544:LEU:HD21	1:D:606:GLN:HG3	1.87	0.57
1:A:175:LYS:HG3	1:A:182:SER:CB	2.25	0.57
1:D:75:ASN:ND2	1:D:92:ASN:HD22	2.01	0.57
1:D:658:ARG:O	1:D:661:TYR:HB2	2.04	0.57
1:B:146:GLU:OE1	1:B:181:PRO:HB3	2.05	0.57
1:B:464:GLU:O	1:B:465:ALA:HB3	2.04	0.56
1:A:143:ILE:HD13	1:A:178:PRO:HB2	1.87	0.56
1:C:545:ASP:OD1	1:C:554:LYS:NZ	2.35	0.56
1:C:620:ASP:OD2	1:C:623:ARG:HD3	2.05	0.56
1:A:163:LYS:NZ	1:A:273:THR:OG1	2.37	0.56
1:C:41:LYS:HG3	1:C:507:VAL:HG23	1.87	0.56
1:A:293:MET:HG2	1:A:315:TRP:CB	2.36	0.56
1:A:580:GLY:O	1:A:581:ARG:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:SER:HB3	1:C:719:ILE:HD11	1.86	0.56
1:A:433:LYS:HD3	1:A:445:LEU:HD21	1.87	0.56
1:C:397:ILE:HD12	1:C:434:ILE:HD13	1.88	0.56
1:D:124:TRP:HA	1:D:124:TRP:CE3	2.41	0.56
1:B:61:ARG:NH1	1:B:105:TYR:CE2	2.73	0.56
1:B:242:SER:OG	1:B:243:ASP:N	2.38	0.56
1:A:736:THR:HG22	1:B:721:LYS:HD3	1.86	0.56
1:B:54:ARG:N	1:B:54:ARG:HD3	2.20	0.56
1:B:535:ASP:O	1:B:537:SER:N	2.38	0.56
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.87	0.56
1:B:63:ILE:HG21	1:B:69:LEU:HG	1.86	0.56
1:B:57:LEU:HA	1:B:480:TYR:CZ	2.41	0.56
1:B:487:ASN:HD22	1:B:489:LYS:N	2.03	0.56
1:D:236:ILE:HG23	1:D:254:VAL:HG13	1.88	0.56
1:B:119:ASN:O	1:B:121:VAL:HG23	2.06	0.56
1:A:116:LEU:O	1:A:132:TYR:HA	2.06	0.56
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.05	0.56
1:D:765:LEU:H	1:D:766:PRO:HA	1.70	0.56
1:D:253:ARG:HB2	1:D:253:ARG:HH11	1.71	0.56
1:D:422:TYR:CE2	1:D:423:LYS:HG3	2.41	0.56
1:C:459:VAL:HG22	1:C:460:SER:N	2.20	0.56
1:C:711:VAL:HG12	1:C:715:GLN:HG3	1.87	0.56
1:D:169:ASN:HD22	1:D:169:ASN:N	2.03	0.56
1:D:310:ARG:HH11	1:D:310:ARG:HG3	1.71	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.24	0.56
1:A:724:VAL:HG22	1:B:750:HIS:CD2	2.41	0.56
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.87	0.56
1:D:376:SER:OG	1:D:380:GLY:HA2	2.05	0.56
1:C:621:ASN:ND2	1:C:622:LYS:N	2.54	0.56
1:A:242:SER:OG	1:A:243:ASP:N	2.39	0.56
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.41	0.56
1:D:114:ILE:CG2	1:D:137:LEU:HD21	2.34	0.55
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.41	0.55
1:A:422:TYR:CZ	1:A:423:LYS:HE3	2.41	0.55
1:A:184:ARG:HD3	1:A:186:THR:O	2.07	0.55
1:A:148:ILE:HD12	1:A:148:ILE:N	2.21	0.55
1:D:484:SER:HB3	1:D:487:ASN:HD21	1.71	0.55
1:D:267:LYS:HD2	1:D:286:GLN:HE22	1.71	0.55
1:D:146:GLU:OE1	1:D:181:PRO:HA	2.06	0.55
1:B:518:ILE:HD13	1:B:523:LYS:HB3	1.87	0.55
1:A:325:MET:CE	1:A:362:PRO:HG3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ARG:HG2	1:C:615:LYS:NZ	2.20	0.55
1:C:55:LEU:HD11	1:C:561:LEU:HD12	1.87	0.55
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.88	0.55
1:D:67:GLU:OE1	1:D:78:VAL:HG21	2.06	0.55
1:D:765:LEU:N	1:D:766:PRO:HA	2.21	0.55
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.87	0.55
1:A:263:ASN:HD22	1:A:318:ARG:NH1	2.03	0.55
1:D:124:TRP:HA	1:D:124:TRP:HE3	1.71	0.55
1:D:241:TYR:O	1:D:242:SER:HB3	2.07	0.55
1:A:280:THR:HG22	1:A:281:ASN:H	1.71	0.55
1:B:379:GLU:HG3	3:B:809:HOH:O	2.06	0.55
1:C:258:LYS:HZ3	1:C:712:HIS:CD2	2.25	0.55
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.75	0.55
1:C:486:VAL:HG13	1:C:487:ASN:H	1.71	0.55
1:C:377:ASN:OD1	1:C:379:GLU:N	2.39	0.55
1:B:168:TRP:O	1:B:169:ASN:HB2	2.07	0.55
1:B:658:ARG:HD2	1:B:661:TYR:CZ	2.42	0.55
1:C:542:LEU:CD2	1:C:542:LEU:C	2.73	0.55
1:D:40:ARG:HD2	1:D:506:ASN:HA	1.88	0.55
1:A:458:SER:CB	1:A:471:ARG:HD3	2.37	0.55
1:B:657:SER:HB2	1:B:689:MET:SD	2.47	0.55
1:A:408:GLU:HG3	1:A:418:ILE:HG13	1.88	0.55
1:D:47:ASP:HA	1:D:52:THR:CG2	2.38	0.54
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.36	0.54
1:C:507:VAL:HG22	1:C:508:GLN:H	1.73	0.54
1:C:75:ASN:ND2	1:C:92:ASN:CG	2.60	0.54
1:D:741:GLY:O	1:D:742:ILE:C	2.45	0.54
1:B:538:LYS:O	1:B:618:PHE:HA	2.05	0.54
1:B:115:LEU:HD21	1:B:132:TYR:CD2	2.41	0.54
1:C:372:TYR:OH	1:C:436:LEU:HD22	2.07	0.54
1:A:360:SER:O	1:A:373:LYS:NZ	2.37	0.54
1:D:174:VAL:HG23	1:D:185:ILE:CG1	2.38	0.54
1:C:732:ALA:HB1	1:D:734:TRP:CZ3	2.42	0.54
1:D:158:SER:OG	1:D:163:LYS:HB2	2.07	0.54
1:B:75:ASN:HB3	1:B:92:ASN:N	2.22	0.54
1:A:158:SER:HA	1:A:216:TRP:CE2	2.43	0.54
1:A:142:LEU:O	1:A:144:THR:HG23	2.08	0.54
1:C:420:ASN:HD22	1:C:426:PRO:CA	2.20	0.54
1:B:627:TRP:HA	1:B:651:ILE:O	2.08	0.54
1:D:611:ARG:O	1:D:615:LYS:HG2	2.06	0.54
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	1:A:343:ARG:N	2.38	0.54
1:A:154:TRP:CH2	1:A:156:THR:HB	2.43	0.54
1:C:651:ILE:HD12	1:C:755:MET:HE2	1.89	0.54
1:C:195:TYR:HB3	1:C:198:ILE:O	2.07	0.54
1:A:242:SER:O	1:A:243:ASP:O	2.26	0.54
1:C:370:SER:HA	1:C:387:PHE:O	2.08	0.54
1:B:218:PRO:HB2	1:B:308:GLN:HE22	1.72	0.54
1:C:167:VAL:HA	1:C:171:ASP:O	2.08	0.54
1:A:108:SER:O	1:A:111:GLY:N	2.39	0.54
1:A:154:TRP:CZ3	1:A:214:LEU:CD2	2.82	0.54
1:B:136:ASP:O	1:B:138:ASN:N	2.40	0.54
1:B:134:ILE:CB	1:B:143:ILE:HD12	2.37	0.54
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.42	0.54
1:A:142:LEU:O	1:A:143:ILE:C	2.45	0.54
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.06	0.54
1:C:58:TYR:O	1:C:58:TYR:CD2	2.60	0.54
1:D:74:ASN:O	1:D:92:ASN:HB3	2.08	0.54
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.05	0.54
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.90	0.54
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.28	0.54
1:D:657:SER:HB2	1:D:689:MET:SD	2.48	0.54
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.90	0.54
1:D:384:ILE:HG23	1:D:407:ILE:HD11	1.90	0.54
1:A:736:THR:CG2	1:B:721:LYS:HD3	2.37	0.54
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.43	0.54
1:B:75:ASN:HB3	1:B:92:ASN:H	1.73	0.53
1:C:651:ILE:HG21	1:C:755:MET:CE	2.39	0.53
1:C:357:PHE:O	1:C:669:ARG:NH1	2.41	0.53
1:C:491:LEU:O	1:C:492:ARG:HB3	2.08	0.53
1:B:272:ASN:ND2	1:B:274:ASP:H	2.07	0.53
1:D:346:ILE:CG2	1:D:347:GLU:N	2.71	0.53
1:A:634:TYR:HD1	1:A:656:VAL:O	1.90	0.53
1:C:520:ASN:O	1:C:521:GLU:HB2	2.07	0.53
1:B:631:TYR:O	1:B:634:TYR:HB3	2.09	0.53
1:D:760:LYS:HD2	1:D:766:PRO:O	2.08	0.53
1:A:397:ILE:CD1	1:A:434:ILE:HG21	2.37	0.53
1:D:321:ASN:HA	1:D:354:VAL:HG23	1.91	0.53
1:C:195:TYR:O	1:C:227:GLN:HA	2.09	0.53
1:D:65:ASP:OD2	1:D:466:LYS:HD2	2.08	0.53
1:B:74:ASN:HB3	1:B:92:ASN:HB2	1.91	0.53
1:D:629:TRP:O	1:D:630:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:PRO:O	1:C:680:LEU:HD13	2.09	0.53
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.09	0.53
1:C:621:ASN:N	1:C:621:ASN:ND2	2.55	0.53
1:A:170:ASN:OD1	1:A:194:ILE:O	2.26	0.53
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.39	0.53
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.08	0.53
1:B:708:ASP:OD2	1:B:740:HIS:HA	2.09	0.53
1:B:60:LEU:HD12	1:B:60:LEU:C	2.29	0.53
1:D:81:ALA:O	1:D:491:LEU:HD13	2.09	0.53
1:C:661:TYR:HB2	1:C:715:GLN:NE2	2.24	0.53
1:D:482:LEU:HD13	1:D:494:LEU:HD11	1.91	0.53
1:A:370:SER:HA	1:A:387:PHE:O	2.09	0.53
1:B:658:ARG:NH2	1:B:684:ARG:HD3	2.23	0.53
1:C:127:SER:O	1:C:128:TYR:HB3	2.08	0.53
1:A:74:ASN:C	1:A:92:ASN:HB3	2.29	0.53
1:A:724:VAL:HA	1:B:750:HIS:HD2	1.74	0.53
1:A:515:ASP:OD1	1:A:516:PHE:N	2.38	0.53
1:C:316:LEU:HD12	1:C:323:SER:HB3	1.90	0.53
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.09	0.53
1:D:360:SER:O	1:D:373:LYS:NZ	2.38	0.53
1:A:545:ASP:OD1	1:A:554:LYS:NZ	2.42	0.53
1:C:334:SER:OG	1:C:336:ARG:HG2	2.09	0.53
1:D:129:THR:O	1:D:130:ALA:HB2	2.09	0.53
1:C:266:VAL:HG22	1:C:267:LYS:N	2.23	0.53
1:D:77:LEU:N	1:D:77:LEU:HD12	2.24	0.52
1:D:199:THR:HA	1:D:228:PHE:CE2	2.45	0.52
1:C:110:ASP:OD2	1:C:112:GLN:HB2	2.10	0.52
1:B:293:MET:CE	1:B:317:ARG:HG3	2.39	0.52
1:D:73:GLU:N	1:D:73:GLU:CD	2.62	0.52
1:B:428:GLY:O	1:B:429:ARG:HG2	2.09	0.52
1:D:487:ASN:H	1:D:487:ASN:ND2	2.07	0.52
1:B:516:PHE:CE2	1:B:518:ILE:HD11	2.43	0.52
1:B:763:PHE:HB2	1:B:765:LEU:HD21	1.90	0.52
1:A:235:LEU:HD23	1:A:255:PRO:CA	2.39	0.52
1:C:73:GLU:C	1:C:75:ASN:N	2.63	0.52
1:A:385:CYS:HB3	1:A:387:PHE:HE2	1.74	0.52
1:B:664:SER:O	1:B:668:GLU:HB2	2.09	0.52
1:B:237:GLU:HA	1:B:252:VAL:O	2.09	0.52
1:B:765:LEU:HD22	1:B:765:LEU:N	2.25	0.52
1:D:640:LEU:HD22	1:D:698:VAL:HG21	1.91	0.52
1:B:155:VAL:HG12	1:B:156:THR:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:TYR:O	1:D:242:SER:CB	2.57	0.52
1:A:354:VAL:CG1	1:A:359:PRO:HG3	2.39	0.52
1:C:324:VAL:HG22	1:C:346:ILE:HG12	1.90	0.52
1:A:49:LEU:HD13	1:A:749:GLN:HA	1.92	0.52
1:A:684:ARG:HG3	1:A:684:ARG:HH11	1.74	0.52
1:C:170:ASN:O	1:C:196:ASN:HB2	2.10	0.52
1:A:610:ALA:O	1:A:613:PHE:N	2.42	0.52
1:A:431:LEU:CD2	1:A:445:LEU:HD12	2.39	0.52
1:A:445:LEU:HD22	1:A:488:ASP:OD1	2.08	0.52
1:C:312:SER:O	1:C:313:LEU:HD12	2.09	0.52
1:C:300:LEU:HD13	1:C:315:TRP:CH2	2.44	0.52
1:A:39:THR:HG23	1:A:40:ARG:H	1.72	0.52
1:A:208:PHE:O	1:A:209:SER:C	2.48	0.52
1:D:541:PRO:HG2	1:D:573:ILE:HA	1.91	0.52
1:A:621:ASN:HD22	1:A:621:ASN:N	2.08	0.52
1:A:333:SER:OG	1:A:334:SER:N	2.41	0.52
1:C:80:ASN:O	1:C:84:GLY:N	2.39	0.52
1:D:218:PRO:HB2	1:D:308:GLN:OE1	2.09	0.52
1:B:459:VAL:CG2	1:B:460:SER:N	2.73	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:D:301:CYS:SG	1:D:359:PRO:HD2	2.50	0.52
1:A:517:ILE:O	1:A:517:ILE:HG13	2.09	0.52
1:C:191:GLU:O	1:C:193:ILE:HG12	2.09	0.52
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.44	0.52
1:C:224:ALA:HA	1:C:270:VAL:HA	1.91	0.52
1:D:703:ILE:HG23	1:D:733:MET:O	2.09	0.52
1:A:486:VAL:HG13	1:A:487:ASN:N	2.25	0.52
1:C:60:LEU:HD12	1:C:60:LEU:C	2.30	0.52
1:A:718:GLN:HE22	1:B:244:GLU:HA	1.72	0.52
1:B:429:ARG:HG3	1:B:456:TYR:CE1	2.45	0.52
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.45	0.52
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.23	0.51
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.45	0.51
1:D:268:PHE:CE2	1:D:313:LEU:HD21	2.45	0.51
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.45	0.51
1:C:589:LYS:HB3	3:C:782:HOH:O	2.10	0.51
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.91	0.51
1:C:733:MET:HG3	1:C:735:TYR:CE1	2.45	0.51
1:D:236:ILE:HG12	1:D:712:HIS:ND1	2.25	0.51
1:C:535:ASP:C	1:C:537:SER:H	2.14	0.51
1:B:208:PHE:CD1	1:B:208:PHE:N	2.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:VAL:CG2	1:C:267:LYS:N	2.72	0.51
1:B:629:TRP:O	1:B:630:SER:HB3	2.10	0.51
1:C:173:TYR:HA	1:C:183:TYR:O	2.10	0.51
1:B:459:VAL:HG23	1:B:469:GLN:O	2.10	0.51
1:A:742:ILE:HG22	1:A:742:ILE:O	2.10	0.51
1:B:134:ILE:CG2	1:B:143:ILE:HD12	2.41	0.51
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.92	0.51
1:B:57:LEU:HA	1:B:480:TYR:CE1	2.45	0.51
1:D:174:VAL:HG23	1:D:185:ILE:HD11	1.93	0.51
1:A:177:GLU:HB2	1:A:180:LEU:CG	2.40	0.51
1:D:134:ILE:HD13	1:D:178:PRO:CB	2.38	0.51
1:D:343:ARG:O	1:D:345:HIS:ND1	2.43	0.51
1:D:343:ARG:HA	1:D:389:ILE:O	2.11	0.51
1:C:184:ARG:HB3	1:C:187:TRP:CZ2	2.46	0.51
1:C:336:ARG:CG	1:C:336:ARG:HH11	2.22	0.51
1:B:108:SER:HB3	1:B:157:TRP:CE3	2.44	0.51
1:A:382:ARG:N	1:A:403:GLU:HG2	2.17	0.51
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.92	0.51
1:B:552:SER:O	1:B:583:SER:HB2	2.09	0.51
1:C:148:ILE:HD12	1:C:148:ILE:H	1.76	0.51
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.41	0.51
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.46	0.51
1:D:146:GLU:HG3	1:D:181:PRO:N	2.26	0.51
1:D:163:LYS:NZ	1:D:273:THR:OG1	2.44	0.51
1:C:596:ARG:C	1:C:597:ARG:HD2	2.31	0.51
1:B:242:SER:HB2	1:B:246:LEU:HD23	1.93	0.51
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.59	0.51
1:B:115:LEU:HD11	1:B:132:TYR:HB3	1.93	0.51
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.46	0.51
1:D:331:ASP:HB3	1:D:334:SER:OG	2.10	0.51
1:D:272:ASN:HD21	1:D:274:ASP:H	1.59	0.51
1:C:180:LEU:HB3	1:C:181:PRO:HD2	1.91	0.51
1:B:217:SER:O	1:B:220:GLY:N	2.37	0.51
1:A:146:GLU:HB2	1:A:179:ASN:O	2.11	0.51
1:D:60:LEU:C	1:D:60:LEU:HD12	2.31	0.51
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.93	0.51
1:B:534:PHE:CE1	1:B:574:ILE:HD11	2.43	0.51
1:C:236:ILE:HD12	1:C:237:GLU:N	2.25	0.51
1:A:139:LYS:HE2	1:D:333:SER:OG	2.11	0.51
1:D:415:LEU:C	1:D:415:LEU:HD23	2.31	0.51
1:B:673:LEU:O	1:B:678:ASP:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ALA:HB2	1:A:461:PHE:CD1	2.46	0.50
1:C:508:GLN:O	1:C:532:PRO:HG2	2.11	0.50
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.11	0.50
1:C:231:THR:HG22	1:C:232:GLU:HG3	1.93	0.50
1:C:168:TRP:O	1:C:169:ASN:HB2	2.12	0.50
1:B:360:SER:O	1:B:373:LYS:HE2	2.11	0.50
1:D:341:VAL:O	1:D:344:GLN:HB2	2.11	0.50
1:B:105:TYR:HD2	1:B:107:ILE:HD12	1.75	0.50
1:A:530:LEU:HD13	1:A:534:PHE:CD2	2.46	0.50
1:D:474:GLY:HA2	1:D:476:GLY:O	2.11	0.50
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.26	0.50
1:C:736:THR:HB	1:D:721:LYS:HB2	1.93	0.50
1:D:272:ASN:ND2	1:D:274:ASP:N	2.59	0.50
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.25	0.50
1:A:313:LEU:O	1:A:325:MET:HA	2.10	0.50
1:B:547:TYR:HD1	1:B:549:GLY:H	1.54	0.50
1:C:761:GLN:NE2	1:C:762:CYS:CA	2.74	0.50
1:A:383:HIS:CD2	1:A:399:LYS:HA	2.46	0.50
1:C:195:TYR:CD1	1:C:195:TYR:N	2.79	0.50
1:A:558:VAL:HG12	1:A:559:PHE:N	2.26	0.50
1:B:135:TYR:C	1:B:135:TYR:CD2	2.85	0.50
1:C:258:LYS:HD2	1:D:248:TYR:CD2	2.46	0.50
1:D:649:CYS:HA	1:D:699:GLU:O	2.11	0.50
1:A:692:ALA:O	1:A:695:PHE:HB2	2.11	0.50
1:D:709:ASP:O	1:D:712:HIS:CE1	2.65	0.50
1:A:607:ILE:O	1:A:610:ALA:HB3	2.11	0.50
1:B:207:VAL:HG12	1:B:208:PHE:HD1	1.76	0.50
1:D:243:ASP:HB3	3:D:796:HOH:O	2.11	0.50
1:D:175:LYS:HD3	1:D:178:PRO:HA	1.93	0.50
1:A:76:ILE:CD1	1:A:105:TYR:CZ	2.95	0.50
1:A:542:LEU:C	1:A:542:LEU:HD23	2.32	0.50
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.47	0.50
1:B:614:SER:HA	1:B:619:VAL:HB	1.92	0.50
1:A:93:SER:O	1:A:96:ASP:HB2	2.11	0.50
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.92	0.50
1:C:518:ILE:O	1:C:519:LEU:HD23	2.11	0.50
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.94	0.50
1:A:676:PRO:HG2	1:A:677:GLU:H	1.77	0.50
1:A:71:LYS:HG3	1:A:76:ILE:CG1	2.42	0.50
1:B:341:VAL:O	1:B:344:GLN:HB2	2.11	0.50
1:C:701:LEU:HD13	1:C:731:GLN:CB	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:TYR:HE1	1:B:549:GLY:HA3	1.77	0.49
1:A:664:SER:O	1:A:668:GLU:HG3	2.12	0.49
1:D:236:ILE:CG2	1:D:254:VAL:HG13	2.42	0.49
1:B:377:ASN:OD1	1:B:379:GLU:N	2.44	0.49
1:D:681:ASP:HB3	3:D:852:HOH:O	2.12	0.49
1:A:429:ARG:NH1	1:A:429:ARG:CG	2.70	0.49
1:C:68:TYR:CE1	1:C:79:PHE:CD2	3.01	0.49
1:D:214:LEU:CD1	1:D:223:LEU:HD11	2.41	0.49
1:D:751:ILE:CG2	1:D:752:TYR:N	2.75	0.49
1:B:316:LEU:CD2	1:B:320:GLN:HG2	2.42	0.49
1:C:385:CYS:HA	1:C:396:PHE:HA	1.93	0.49
1:C:61:ARG:O	1:C:63:ILE:HG23	2.12	0.49
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.33	0.49
1:B:535:ASP:C	1:B:537:SER:H	2.16	0.49
1:C:316:LEU:CD1	1:C:323:SER:HB3	2.42	0.49
1:D:98:PHE:HE1	1:D:142:LEU:HD21	1.76	0.49
1:C:408:GLU:N	1:C:416:TYR:O	2.39	0.49
1:C:512:LYS:HD3	3:C:818:HOH:O	2.12	0.49
1:B:134:ILE:O	1:B:142:LEU:HD12	2.12	0.49
1:B:73:GLU:O	1:B:75:ASN:ND2	2.46	0.49
1:C:175:LYS:NZ	1:C:180:LEU:O	2.46	0.49
1:B:388:GLN:HG2	1:B:391:LYS:CE	2.42	0.49
1:B:534:PHE:HA	1:B:540:TYR:OH	2.12	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.49
1:B:199:THR:HA	1:B:228:PHE:CD2	2.47	0.49
1:B:60:LEU:O	1:B:60:LEU:HD12	2.12	0.49
1:A:588:ASP:O	1:A:592:HIS:HB2	2.12	0.49
1:B:486:VAL:CG1	1:B:487:ASN:N	2.75	0.49
1:C:728:VAL:HG22	1:C:728:VAL:O	2.12	0.49
1:D:370:SER:OG	1:D:386:TYR:HE1	1.95	0.49
1:C:597:ARG:HA	1:C:682:HIS:CD2	2.47	0.49
1:A:613:PHE:O	1:A:615:LYS:N	2.46	0.49
1:B:542:LEU:HD23	1:B:543:LEU:N	2.28	0.49
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.94	0.49
1:A:175:LYS:HD2	3:A:812:HOH:O	2.12	0.49
1:D:631:TYR:HB2	2:D:767:13Z:F1	2.03	0.49
1:A:142:LEU:O	1:A:143:ILE:O	2.31	0.49
1:D:159:PRO:HD3	1:D:216:TRP:CG	2.47	0.49
1:B:636:THR:HG21	1:B:651:ILE:O	2.13	0.49
1:D:51:ASN:O	1:D:54:ARG:HD3	2.13	0.49
1:A:716:SER:O	1:A:719:ILE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:HB3	1:D:180:LEU:O	2.13	0.49
1:C:345:HIS:HE1	1:C:389:ILE:O	1.95	0.49
1:C:471:ARG:HH11	1:C:471:ARG:HG3	1.77	0.49
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.27	0.49
1:B:438:ASP:HB3	1:B:441:LYS:HG3	1.95	0.49
1:C:755:MET:O	1:C:759:ILE:HG12	2.12	0.49
1:D:257:PRO:O	1:D:663:ASP:HA	2.12	0.49
1:A:626:ILE:O	1:A:626:ILE:HG23	2.12	0.49
1:B:184:ARG:HD3	1:B:186:THR:O	2.12	0.49
1:B:241:TYR:O	1:B:242:SER:HB3	2.13	0.49
1:A:225:TYR:CZ	1:A:269:PHE:HB2	2.48	0.49
1:D:562:ASN:HB2	3:D:845:HOH:O	2.13	0.49
1:B:289:ALA:HB2	1:B:315:TRP:CZ3	2.48	0.49
1:D:704:HIS:NE2	1:D:711:VAL:O	2.45	0.49
1:C:454:CYS:HA	1:C:474:GLY:O	2.13	0.49
1:C:61:ARG:O	1:C:68:TYR:HA	2.12	0.48
1:C:654:ALA:HA	1:C:704:HIS:CE1	2.47	0.48
1:A:242:SER:HB3	1:A:246:LEU:HD22	1.94	0.48
1:C:300:LEU:HD13	1:C:315:TRP:CZ3	2.48	0.48
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.42	0.48
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.95	0.48
1:B:208:PHE:N	1:B:208:PHE:HD1	2.11	0.48
1:B:169:ASN:N	1:B:169:ASN:HD22	2.10	0.48
1:A:199:THR:HG21	1:A:208:PHE:HD2	1.78	0.48
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.48
1:B:80:ASN:OD1	1:B:82:GLU:N	2.46	0.48
1:C:249:PRO:HD3	1:D:714:GLN:NE2	2.27	0.48
1:D:108:SER:HB3	1:D:157:TRP:CZ2	2.48	0.48
1:A:138:ASN:O	1:A:140:ARG:HG2	2.12	0.48
1:A:478:PRO:HB2	1:A:497:ASN:HD21	1.77	0.48
1:D:169:ASN:O	1:D:170:ASN:HB2	2.12	0.48
1:C:374:ILE:HD11	1:C:404:VAL:HG12	1.95	0.48
1:D:620:ASP:OD2	1:D:623:ARG:HD3	2.12	0.48
1:A:60:LEU:O	1:A:60:LEU:HD12	2.13	0.48
1:B:156:THR:HG21	1:B:214:LEU:CD1	2.43	0.48
1:A:73:GLU:C	1:A:75:ASN:H	2.15	0.48
1:A:347:GLU:OE1	1:A:373:LYS:HE3	2.13	0.48
1:D:501:ASP:O	1:D:505:GLN:HG2	2.14	0.48
1:D:224:ALA:CB	1:D:270:VAL:HG22	2.44	0.48
1:B:89:PHE:CD1	1:B:89:PHE:C	2.87	0.48
1:D:175:LYS:HE3	1:D:180:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:HA3	1:B:492:ARG:HH12	1.71	0.48
1:A:498:SER:O	1:A:501:ASP:HB3	2.13	0.48
1:B:513:LYS:HZ3	1:B:515:ASP:HB2	1.79	0.48
1:B:207:VAL:HG12	1:B:208:PHE:CD1	2.49	0.48
1:D:382:ARG:HD2	1:D:403:GLU:OE2	2.13	0.48
1:C:486:VAL:HG13	1:C:487:ASN:N	2.28	0.48
1:B:657:SER:O	1:B:688:VAL:HG23	2.13	0.48
1:C:301:CYS:SG	1:C:316:LEU:HB2	2.54	0.48
1:A:558:VAL:CG1	1:A:559:PHE:N	2.77	0.48
1:B:370:SER:HB2	1:B:387:PHE:O	2.13	0.48
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.48
1:B:666:TYR:C	1:B:666:TYR:CD1	2.86	0.48
1:C:73:GLU:O	1:C:75:ASN:ND2	2.43	0.48
1:A:367:ASP:OD1	1:A:369:ASN:N	2.43	0.48
1:A:48:TYR:CD2	1:A:49:LEU:HD23	2.48	0.48
1:A:481:THR:HG22	1:A:493:VAL:HG22	1.96	0.48
1:C:472:CYS:O	1:C:478:PRO:HA	2.14	0.48
1:D:293:MET:HG3	1:D:315:TRP:HB2	1.95	0.48
1:D:259:ALA:HB3	1:D:660:GLU:HA	1.96	0.48
1:B:733:MET:HG3	1:B:735:TYR:CE2	2.49	0.48
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.94	0.48
1:B:562:ASN:HB2	3:B:830:HOH:O	2.14	0.48
1:C:553:GLN:HA	1:C:579:ASP:OD1	2.14	0.48
1:C:675:THR:HB	1:C:676:PRO:HD2	1.95	0.48
1:D:581:ARG:HB2	1:D:605:ASP:OD2	2.14	0.48
1:D:68:TYR:CD1	1:D:68:TYR:O	2.66	0.48
1:B:644:SER:O	1:B:646:VAL:N	2.47	0.48
1:C:135:TYR:HD1	1:C:142:LEU:HD13	1.78	0.48
1:A:334:SER:C	1:A:336:ARG:H	2.16	0.48
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.48
1:B:422:TYR:CD1	1:B:447:CYS:SG	3.07	0.48
1:C:45:LEU:HD13	1:C:566:TYR:CD2	2.48	0.48
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.95	0.48
1:B:55:LEU:HD11	1:B:478:PRO:HD2	1.96	0.48
1:C:107:ILE:CD1	1:C:114:ILE:HD12	2.44	0.48
1:B:170:ASN:O	1:B:196:ASN:HB2	2.14	0.48
1:D:341:VAL:HG13	1:D:342:ALA:N	2.28	0.48
1:D:755:MET:O	1:D:759:ILE:HG12	2.14	0.48
1:D:219:ASN:OD1	1:D:219:ASN:C	2.53	0.48
1:C:233:VAL:HG12	1:C:234:PRO:O	2.14	0.47
1:C:627:TRP:HB2	1:C:651:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:PHE:CD2	1:D:523:LYS:HD3	2.49	0.47
1:C:308:GLN:HA	1:C:308:GLN:OE1	2.14	0.47
1:A:615:LYS:O	1:A:616:MET:C	2.52	0.47
1:D:99:GLY:O	1:D:100:HIS:CG	2.67	0.47
1:A:154:TRP:CZ3	1:A:156:THR:CG2	2.98	0.47
1:D:75:ASN:OD1	1:D:77:LEU:HD11	2.14	0.47
1:B:445:LEU:HD23	1:B:445:LEU:N	2.29	0.47
1:B:487:ASN:C	1:B:487:ASN:HD22	2.17	0.47
1:B:763:PHE:HB2	1:B:765:LEU:CD2	2.44	0.47
1:B:113:PHE:CD2	1:B:178:PRO:HG2	2.48	0.47
1:C:107:ILE:HG22	1:C:108:SER:O	2.14	0.47
1:A:150:ASN:O	1:A:151:ASN:CB	2.59	0.47
1:B:500:LEU:HG	1:B:504:LEU:HD12	1.96	0.47
1:A:67:GLU:HA	1:A:79:PHE:O	2.14	0.47
1:A:546:VAL:HG12	1:A:627:TRP:O	2.13	0.47
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.47
1:C:74:ASN:C	1:C:92:ASN:HB3	2.35	0.47
1:A:468:TYR:O	1:A:483:HIS:N	2.36	0.47
1:C:75:ASN:HD21	1:C:92:ASN:CG	2.18	0.47
1:B:319:ILE:O	1:B:321:ASN:N	2.43	0.47
1:C:309:GLU:HB3	1:C:330:TYR:HB3	1.96	0.47
1:A:753:THR:O	1:A:757:HIS:CD2	2.67	0.47
1:B:136:ASP:HB3	1:B:139:LYS:HG2	1.96	0.47
1:C:510:PRO:HB2	1:C:530:LEU:O	2.14	0.47
1:D:156:THR:HG23	1:D:165:ALA:O	2.15	0.47
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.49	0.47
1:B:369:ASN:C	1:B:389:ILE:HG23	2.34	0.47
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.79	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.50	0.47
1:D:487:ASN:N	1:D:487:ASN:HD22	2.09	0.47
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.97	0.47
1:B:477:LEU:HD12	1:B:501:ASP:HB2	1.97	0.47
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.48	0.47
1:B:454:CYS:HA	1:B:474:GLY:O	2.15	0.47
1:B:39:THR:HG22	1:B:39:THR:O	2.13	0.47
1:D:173:TYR:CD2	1:D:184:ARG:HA	2.50	0.47
1:D:293:MET:HE3	1:D:324:VAL:HG23	1.97	0.47
1:C:369:ASN:HA	1:C:389:ILE:CG2	2.44	0.47
1:C:50:LYS:HE3	1:C:749:GLN:OE1	2.15	0.47
1:A:51:ASN:O	1:A:52:THR:C	2.51	0.47
1:B:206:GLU:OE2	1:B:666:TYR:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:PRO:HD3	1:C:216:TRP:HB2	1.95	0.47
1:D:484:SER:HB2	1:D:491:LEU:HD21	1.96	0.47
1:B:57:LEU:HB3	1:B:480:TYR:OH	2.15	0.47
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.14	0.47
1:C:124:TRP:HA	1:C:124:TRP:CE3	2.50	0.47
1:A:465:ALA:O	1:A:485:SER:OG	2.21	0.47
1:D:520:ASN:C	1:D:522:THR:H	2.16	0.47
1:A:509:MET:HE3	1:A:510:PRO:HD2	1.97	0.47
1:C:319:ILE:HG13	1:C:319:ILE:O	2.15	0.47
1:D:356:ARG:HD3	1:D:551:CYS:SG	2.54	0.47
1:A:499:ALA:O	1:A:500:LEU:C	2.53	0.47
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.50	0.47
1:D:154:TRP:NE1	1:D:212:SER:HB2	2.30	0.47
1:C:482:LEU:C	1:C:483:HIS:CD2	2.87	0.47
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.49	0.47
1:D:571:GLU:O	1:D:572:ASN:C	2.53	0.47
1:A:135:TYR:OH	1:A:140:ARG:NE	2.48	0.47
1:D:208:PHE:O	1:D:209:SER:HB3	2.14	0.47
1:A:634:TYR:CD1	1:A:656:VAL:O	2.68	0.47
1:A:122:LYS:NZ	1:A:124:TRP:O	2.31	0.47
1:B:453:ARG:HG2	1:B:454:CYS:SG	2.55	0.47
1:A:154:TRP:CZ3	1:A:156:THR:HB	2.50	0.47
1:D:306:ALA:HB3	1:D:310:ARG:O	2.15	0.47
1:A:404:VAL:HG13	1:A:417:TYR:HD1	1.80	0.47
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.30	0.47
1:B:620:ASP:O	1:B:621:ASN:C	2.53	0.47
1:A:751:ILE:HG12	1:A:751:ILE:O	2.15	0.47
1:B:285:ILE:HG21	1:B:336:ARG:HA	1.95	0.46
1:B:519:LEU:O	1:B:522:THR:HG23	2.15	0.46
1:D:764:SER:OG	1:D:764:SER:O	2.32	0.46
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.62	0.46
1:A:543:LEU:HD11	1:A:627:TRP:HD1	1.80	0.46
1:A:651:ILE:CD1	1:A:755:MET:HE2	2.45	0.46
1:D:320:GLN:OE1	1:D:669:ARG:HD3	2.15	0.46
1:A:279:VAL:HG12	1:A:280:THR:OG1	2.15	0.46
1:C:411:THR:OG1	1:C:414:TYR:N	2.47	0.46
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.46
1:D:463:LYS:HB3	1:D:464:GLU:OE2	2.14	0.46
1:B:105:TYR:HD2	1:B:107:ILE:CD1	2.29	0.46
1:C:375:ILE:O	1:C:382:ARG:HA	2.16	0.46
1:C:310:ARG:NH1	1:C:368:GLY:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:O	1:C:492:ARG:NH2	2.47	0.46
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.46	0.46
1:A:314:GLN:HG2	1:A:325:MET:HB2	1.97	0.46
1:B:263:ASN:ND2	1:B:318:ARG:CZ	2.78	0.46
1:C:374:ILE:HD11	1:C:404:VAL:CG1	2.45	0.46
1:D:530:LEU:HA	1:D:531:PRO:HD3	1.81	0.46
1:C:701:LEU:CD1	1:C:731:GLN:HB2	2.37	0.46
1:C:118:TYR:N	1:C:118:TYR:CD1	2.83	0.46
1:B:105:TYR:CD2	1:B:107:ILE:CD1	2.99	0.46
1:C:69:LEU:HD23	1:C:78:VAL:HA	1.96	0.46
1:B:187:TRP:CH2	1:B:281:ASN:OD1	2.69	0.46
1:C:105:TYR:HA	1:C:115:LEU:O	2.16	0.46
1:A:631:TYR:HB2	2:A:767:13Z:F1	2.05	0.46
1:D:374:ILE:HD11	1:D:404:VAL:HG12	1.97	0.46
1:A:664:SER:OG	1:A:665:VAL:N	2.48	0.46
1:D:586:GLN:HB2	3:D:843:HOH:O	2.15	0.46
1:D:72:GLN:NE2	1:D:77:LEU:HD22	2.30	0.46
1:B:519:LEU:O	1:B:521:GLU:N	2.49	0.46
1:A:542:LEU:O	1:A:624:ILE:HA	2.15	0.46
1:B:170:ASN:OD1	1:B:170:ASN:N	2.48	0.46
1:B:508:GLN:HB3	1:B:532:PRO:HG2	1.97	0.46
1:B:107:ILE:HA	1:B:114:ILE:HA	1.98	0.46
1:A:712:HIS:C	1:A:714:GLN:N	2.67	0.46
1:D:55:LEU:CD2	1:D:561:LEU:HD12	2.46	0.46
1:B:550:PRO:O	1:B:551:CYS:HB3	2.16	0.46
1:B:527:GLN:HG3	1:B:527:GLN:O	2.16	0.46
1:C:621:ASN:H	1:C:621:ASN:ND2	2.14	0.46
1:A:157:TRP:O	1:A:216:TRP:NE1	2.49	0.46
1:C:216:TRP:HZ3	1:C:273:THR:HG21	1.80	0.46
1:B:500:LEU:HG	1:B:504:LEU:CD1	2.46	0.46
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.15	0.46
1:C:201:TRP:CH2	1:C:205:GLU:HG2	2.51	0.46
1:A:230:ASP:O	1:A:233:VAL:HB	2.16	0.46
1:D:307:THR:OG1	1:D:310:ARG:N	2.49	0.46
1:A:68:TYR:CE1	1:A:79:PHE:CB	2.98	0.46
1:B:115:LEU:HB2	1:B:157:TRP:HZ2	1.81	0.46
1:B:317:ARG:O	1:B:319:ILE:N	2.48	0.46
1:C:530:LEU:HD13	1:C:534:PHE:CD2	2.51	0.46
1:A:312:SER:HA	1:A:326:ASP:O	2.15	0.46
1:D:80:ASN:OD1	1:D:83:TYR:N	2.49	0.46
1:D:532:PRO:O	1:D:533:HIS:C	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:TRP:N	1:C:215:TRP:CE3	2.84	0.46
1:D:709:ASP:OD1	1:D:709:ASP:N	2.48	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.50	0.46
1:A:325:MET:HE1	1:A:362:PRO:HG3	1.97	0.46
1:A:728:VAL:HG23	1:A:729:ASP:O	2.15	0.46
1:B:317:ARG:O	1:B:318:ARG:C	2.54	0.46
1:D:224:ALA:HB2	1:D:270:VAL:HG22	1.98	0.46
1:B:532:PRO:O	1:B:533:HIS:HB2	2.15	0.46
1:A:77:LEU:HD23	1:A:77:LEU:N	2.31	0.46
1:D:253:ARG:NH1	1:D:253:ARG:CB	2.79	0.46
1:B:246:LEU:HD11	1:B:248:TYR:O	2.15	0.46
1:A:228:PHE:HA	1:A:265:THR:O	2.16	0.46
1:C:109:PRO:HG2	1:C:158:SER:O	2.16	0.46
1:D:173:TYR:CE2	1:D:184:ARG:CG	2.80	0.45
1:D:139:LYS:HG2	1:D:141:GLN:CB	2.46	0.45
1:D:47:ASP:HA	1:D:52:THR:HG23	1.99	0.45
1:A:610:ALA:O	1:A:611:ARG:C	2.53	0.45
1:A:742:ILE:HD13	1:A:751:ILE:HD12	1.97	0.45
1:B:43:TYR:CD2	1:B:565:THR:CG2	2.99	0.45
1:B:598:LEU:O	1:B:682:HIS:NE2	2.44	0.45
1:B:633:GLY:C	1:B:655:PRO:HB3	2.36	0.45
1:B:81:ALA:HB3	1:B:467:TYR:CE2	2.50	0.45
1:B:237:GLU:CG	1:B:253:ARG:HG2	2.46	0.45
1:C:244:GLU:OE2	1:D:658:ARG:NH2	2.48	0.45
1:A:381:TYR:CE2	1:A:401:THR:CA	2.98	0.45
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.16	0.45
1:A:533:HIS:O	1:A:534:PHE:C	2.55	0.45
1:A:208:PHE:O	1:A:210:ALA:N	2.49	0.45
1:D:597:ARG:HA	1:D:682:HIS:CD2	2.51	0.45
1:D:414:TYR:CD2	1:D:433:LYS:CG	3.00	0.45
1:A:256:TYR:O	1:B:248:TYR:OH	2.28	0.45
1:D:57:LEU:N	1:D:57:LEU:HD12	2.28	0.45
1:A:314:GLN:HE22	1:A:361:GLU:HA	1.80	0.45
1:B:422:TYR:CE1	1:B:447:CYS:HB3	2.51	0.45
1:D:76:ILE:O	1:D:89:PHE:N	2.49	0.45
1:B:52:THR:HG22	3:B:816:HOH:O	2.16	0.45
1:C:507:VAL:CG2	1:C:508:GLN:N	2.79	0.45
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.99	0.45
1:A:676:PRO:HG2	1:A:677:GLU:N	2.31	0.45
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.51	0.45
1:A:60:LEU:C	1:A:60:LEU:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:PHE:HA	1:C:371:PHE:CB	2.47	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.16	0.45
1:D:331:ASP:O	1:D:335:GLY:N	2.37	0.45
1:B:250:LYS:HG2	1:B:251:THR:N	2.31	0.45
1:A:114:ILE:HG22	1:A:137:LEU:HG	1.99	0.45
1:D:95:PHE:CD1	1:D:116:LEU:HD11	2.52	0.45
1:A:290:PRO:HD3	1:A:326:ASP:OD2	2.17	0.45
1:B:516:PHE:HA	1:B:526:TYR:HD2	1.82	0.45
1:D:763:PHE:O	1:D:764:SER:C	2.55	0.45
1:D:343:ARG:NE	1:D:389:ILE:HD12	2.32	0.45
1:A:138:ASN:C	1:A:140:ARG:N	2.70	0.45
1:A:113:PHE:CE1	1:A:143:ILE:HD11	2.52	0.45
1:A:49:LEU:HB3	1:A:749:GLN:HG2	1.98	0.45
1:A:738:GLU:OE2	1:A:744:SER:OG	2.34	0.45
1:D:459:VAL:CG1	1:D:461:PHE:HE1	2.30	0.45
1:D:164:LEU:HA	1:D:164:LEU:HD23	1.80	0.45
1:A:233:VAL:HG22	1:A:262:VAL:O	2.17	0.45
1:C:367:ASP:OD1	1:C:369:ASN:N	2.50	0.45
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.97	0.45
1:B:58:TYR:CE2	1:B:494:LEU:HB3	2.52	0.45
1:A:76:ILE:HD11	1:A:105:TYR:CZ	2.51	0.45
1:B:547:TYR:CE1	1:B:549:GLY:HA3	2.50	0.45
1:C:558:VAL:HG12	1:C:559:PHE:N	2.32	0.45
1:A:426:PRO:HD2	1:A:525:TRP:CE2	2.52	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:B:627:TRP:O	1:B:627:TRP:CG	2.69	0.45
1:B:742:ILE:HD12	1:B:751:ILE:HD12	1.99	0.45
1:A:490:GLY:O	1:A:491:LEU:C	2.55	0.45
1:D:422:TYR:CD2	1:D:423:LYS:HG3	2.52	0.45
1:C:611:ARG:HG2	1:C:615:LYS:HZ2	1.80	0.45
1:A:285:ILE:HG23	1:A:336:ARG:HE	1.82	0.45
1:B:215:TRP:CH2	1:B:303:VAL:HG21	2.52	0.45
1:B:662:TYR:CE2	2:B:767:13Z:H4	2.52	0.44
1:C:581:ARG:CZ	1:C:601:PHE:CD1	3.00	0.44
1:B:316:LEU:HD21	1:B:320:GLN:HB3	1.99	0.44
1:B:535:ASP:OD2	1:B:535:ASP:C	2.54	0.44
1:C:148:ILE:HD12	1:C:148:ILE:N	2.31	0.44
1:D:60:LEU:O	1:D:60:LEU:HD12	2.16	0.44
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.17	0.44
1:A:620:ASP:OD2	1:A:623:ARG:CD	2.64	0.44
1:A:562:ASN:OD1	1:A:564:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:VAL:HG12	1:D:161:GLY:N	2.32	0.44
1:A:202:VAL:CG1	1:A:203:TYR:N	2.80	0.44
1:C:602:GLU:N	1:C:602:GLU:OE2	2.48	0.44
1:D:39:THR:HB	3:D:768:HOH:O	2.16	0.44
1:A:288:THR:HG22	3:A:815:HOH:O	2.16	0.44
1:C:175:LYS:HG3	1:C:182:SER:HA	2.00	0.44
1:C:300:LEU:HA	1:C:300:LEU:HD12	1.86	0.44
1:D:451:PRO:HA	3:D:859:HOH:O	2.16	0.44
1:C:544:LEU:HD12	1:C:576:ALA:O	2.17	0.44
1:C:272:ASN:OD1	1:C:274:ASP:N	2.50	0.44
1:B:113:PHE:CE1	1:B:136:ASP:HA	2.52	0.44
1:C:747:ALA:O	1:C:751:ILE:HG22	2.17	0.44
1:D:662:TYR:CE2	2:D:767:13Z:H4	2.52	0.44
1:A:417:TYR:CE2	1:A:432:TYR:HB2	2.51	0.44
1:C:364:PHE:HA	1:C:371:PHE:HB3	2.00	0.44
1:C:257:PRO:HG2	1:C:664:SER:OG	2.17	0.44
1:D:72:GLN:O	1:D:74:ASN:N	2.50	0.44
1:D:137:LEU:N	1:D:137:LEU:CD2	2.79	0.44
1:D:740:HIS:NE2	2:D:767:13Z:N2	2.66	0.44
1:D:258:LYS:NZ	1:D:712:HIS:HD2	2.16	0.44
1:D:636:THR:HG22	1:D:640:LEU:HD12	2.00	0.44
1:C:137:LEU:O	1:C:140:ARG:CD	2.62	0.44
1:B:662:TYR:HB3	1:B:667:THR:OG1	2.18	0.44
1:B:513:LYS:HZ2	1:B:515:ASP:HB2	1.81	0.44
1:D:63:ILE:HG22	1:D:67:GLU:O	2.16	0.44
1:B:73:GLU:O	1:B:74:ASN:HB2	2.17	0.44
1:D:594:ILE:CG2	1:D:601:PHE:HB2	2.47	0.44
1:A:477:LEU:HD22	1:A:500:LEU:HD23	1.98	0.44
1:A:372:TYR:CD2	1:A:415:LEU:HD12	2.52	0.44
1:A:64:SER:C	1:A:463:LYS:HG2	2.38	0.44
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.16	0.44
1:A:723:LEU:HD22	1:A:728:VAL:HG11	1.99	0.44
1:C:302:ASP:OD1	1:C:303:VAL:N	2.51	0.44
1:C:317:ARG:O	1:C:318:ARG:C	2.55	0.44
1:B:136:ASP:O	1:B:137:LEU:C	2.56	0.44
1:A:477:LEU:CD1	1:A:500:LEU:HD23	2.44	0.44
1:D:102:ILE:HD13	1:D:116:LEU:HD22	2.00	0.44
1:C:630:SER:O	1:C:655:PRO:HA	2.18	0.44
1:C:310:ARG:HH21	1:C:343:ARG:HH12	1.66	0.44
1:B:115:LEU:CG	1:B:132:TYR:HD2	2.31	0.44
1:B:268:PHE:CD2	1:B:313:LEU:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PHE:O	1:D:209:SER:CB	2.66	0.44
1:B:85:ASN:N	1:B:85:ASN:OD1	2.50	0.44
1:C:272:ASN:OD1	1:C:272:ASN:C	2.56	0.44
1:A:82:GLU:OE1	1:A:467:TYR:CE1	2.70	0.44
1:D:112:GLN:HB3	1:D:113:PHE:CE2	2.52	0.44
1:A:235:LEU:HD21	1:A:255:PRO:HG3	2.00	0.44
1:B:115:LEU:HB2	1:B:157:TRP:CZ2	2.51	0.44
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.17	0.44
1:C:487:ASN:O	1:C:488:ASP:C	2.55	0.44
1:C:312:SER:C	1:C:313:LEU:HD12	2.37	0.44
1:C:124:TRP:HA	1:C:124:TRP:HE3	1.82	0.44
1:B:428:GLY:C	1:B:429:ARG:HG2	2.38	0.44
1:D:266:VAL:HG22	1:D:267:LYS:N	2.33	0.44
1:C:418:ILE:HA	1:C:430:ASN:O	2.18	0.44
1:A:125:ARG:NH2	1:A:205:GLU:OE2	2.51	0.44
1:D:761:GLN:HB3	1:D:761:GLN:HE21	1.57	0.44
1:C:658:ARG:HH22	1:C:684:ARG:CD	2.30	0.44
1:C:107:ILE:HD11	1:C:114:ILE:HD12	1.99	0.44
1:C:75:ASN:OD1	1:C:92:ASN:OD1	2.36	0.44
1:A:730:PHE:CD1	1:A:731:GLN:O	2.68	0.44
1:B:546:VAL:HB	1:B:606:GLN:OE1	2.18	0.44
1:A:280:THR:HG22	1:A:281:ASN:N	2.33	0.44
1:D:76:ILE:O	1:D:89:PHE:HB3	2.18	0.44
1:B:200:ASP:OD2	1:B:230:ASP:OD2	2.36	0.44
1:D:73:GLU:CD	1:D:73:GLU:H	2.20	0.43
1:C:751:ILE:HG23	1:C:752:TYR:N	2.33	0.43
1:A:79:PHE:CE1	1:A:86:SER:HB3	2.52	0.43
1:A:658:ARG:CB	1:A:687:THR:HG22	2.48	0.43
1:A:267:LYS:HB3	1:A:269:PHE:CE1	2.53	0.43
1:C:608:GLU:O	1:C:612:GLN:HG3	2.17	0.43
1:D:68:TYR:C	1:D:68:TYR:CD1	2.91	0.43
1:A:738:GLU:CD	1:A:744:SER:OG	2.56	0.43
1:D:715:GLN:O	1:D:719:ILE:HG13	2.18	0.43
1:B:487:ASN:HD22	1:B:488:ASP:N	2.17	0.43
1:D:631:TYR:O	1:D:634:TYR:HB3	2.18	0.43
1:C:175:LYS:HG3	1:C:182:SER:CA	2.48	0.43
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.83	0.43
1:D:546:VAL:HG21	1:D:606:GLN:HG2	2.00	0.43
1:B:543:LEU:HD12	1:B:625:ALA:O	2.18	0.43
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.17	0.43
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ILE:CG2	1:D:179:ASN:OD1	2.53	0.43
1:B:658:ARG:CB	1:B:687:THR:HG22	2.42	0.43
1:D:640:LEU:CD2	1:D:698:VAL:HG21	2.48	0.43
1:C:331:ASP:HB3	1:C:334:SER:HB3	2.00	0.43
1:B:131:SER:C	1:B:132:TYR:CD1	2.92	0.43
1:C:662:TYR:CE2	2:C:767:13Z:H4	2.53	0.43
1:C:40:ARG:NH1	1:C:505:GLN:O	2.48	0.43
1:B:520:ASN:O	1:B:521:GLU:HB2	2.18	0.43
1:A:98:PHE:HE1	1:A:142:LEU:HD11	1.83	0.43
1:A:244:GLU:HA	1:B:718:GLN:HE22	1.82	0.43
1:A:170:ASN:N	1:A:170:ASN:HD22	2.15	0.43
1:D:199:THR:CG2	1:D:208:PHE:CD2	3.02	0.43
1:C:224:ALA:HB2	1:C:270:VAL:HG13	1.99	0.43
1:D:174:VAL:CG2	1:D:185:ILE:HD11	2.47	0.43
1:A:554:LYS:H	1:A:579:ASP:CG	2.21	0.43
1:D:520:ASN:O	1:D:522:THR:N	2.52	0.43
1:C:413:ASP:C	1:C:414:TYR:CD1	2.92	0.43
1:A:623:ARG:NH2	1:A:763:PHE:O	2.45	0.43
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.53	0.43
1:B:516:PHE:HA	1:B:526:TYR:CD2	2.54	0.43
1:D:310:ARG:NH1	1:D:310:ARG:HG3	2.33	0.43
1:D:662:TYR:HE1	1:D:710:ASN:OD1	2.02	0.43
1:C:114:ILE:HG22	1:C:137:LEU:CD2	2.46	0.43
1:A:113:PHE:CD1	1:A:136:ASP:HA	2.53	0.43
1:C:471:ARG:NH1	1:C:471:ARG:HG3	2.34	0.43
1:D:120:TYR:HA	1:D:130:ALA:HB2	1.99	0.43
1:A:486:VAL:CG1	1:A:487:ASN:N	2.82	0.43
1:C:76:ILE:O	1:C:89:PHE:N	2.45	0.43
1:D:195:TYR:HB3	1:D:198:ILE:O	2.18	0.43
1:C:600:THR:OG1	1:C:601:PHE:N	2.51	0.43
1:A:547:TYR:CE1	2:A:767:13Z:H14A	2.53	0.43
1:D:170:ASN:O	1:D:196:ASN:HB2	2.18	0.43
1:C:457:TYR:CE1	1:C:472:CYS:HB2	2.52	0.43
1:D:149:PRO:HB2	1:D:168:TRP:NE1	2.33	0.43
1:B:680:LEU:O	1:B:683:TYR:HB2	2.18	0.43
1:A:55:LEU:CD1	1:A:500:LEU:HD22	2.46	0.43
1:A:666:TYR:O	1:A:669:ARG:HB3	2.19	0.43
1:C:661:TYR:CB	1:C:715:GLN:NE2	2.81	0.43
1:C:611:ARG:O	1:C:614:SER:HB3	2.19	0.43
1:D:162:HIS:HD2	1:D:176:ILE:O	2.01	0.43
1:A:138:ASN:O	1:A:140:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.53	0.43
1:A:148:ILE:HG22	1:A:152:THR:OG1	2.18	0.43
1:A:446:SER:HB2	1:A:457:TYR:CD2	2.54	0.43
1:B:272:ASN:HD22	1:B:274:ASP:H	1.64	0.43
1:D:58:TYR:CE2	1:D:494:LEU:HB3	2.53	0.43
1:C:88:VAL:HG11	1:C:91:GLU:OE2	2.19	0.43
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.53	0.43
1:C:756:SER:O	1:C:760:LYS:HG3	2.19	0.43
1:B:104:ASP:OD1	1:B:105:TYR:N	2.50	0.43
1:D:253:ARG:CB	1:D:253:ARG:HH11	2.31	0.43
1:C:75:ASN:ND2	1:C:92:ASN:ND2	2.63	0.43
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.34	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HD12	2.00	0.43
1:B:624:ILE:HG22	1:B:647:PHE:CD1	2.54	0.43
1:A:80:ASN:OD1	1:A:80:ASN:C	2.57	0.43
1:B:73:GLU:OE2	1:B:73:GLU:N	2.52	0.43
1:B:644:SER:C	1:B:646:VAL:H	2.21	0.43
1:A:76:ILE:HD13	1:A:105:TYR:CZ	2.54	0.43
1:C:171:ASP:OD2	1:C:186:THR:OG1	2.35	0.43
1:B:190:LYS:HA	3:B:811:HOH:O	2.18	0.43
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.88	0.43
1:A:380:GLY:O	1:A:587:GLY:HA2	2.19	0.42
1:C:369:ASN:HA	1:C:389:ILE:HG21	2.01	0.42
1:C:627:TRP:CE3	1:C:755:MET:HE3	2.54	0.42
1:C:742:ILE:HG21	1:C:751:ILE:HD12	2.00	0.42
1:C:127:SER:CB	1:C:211:TYR:CG	3.02	0.42
1:B:651:ILE:HG21	1:B:755:MET:CE	2.48	0.42
1:B:154:TRP:CG	1:B:155:VAL:N	2.87	0.42
1:B:199:THR:HG22	1:B:228:PHE:CE2	2.54	0.42
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.01	0.42
1:B:546:VAL:CG2	1:B:547:TYR:N	2.82	0.42
1:B:637:SER:HB3	1:B:688:VAL:HG11	2.01	0.42
1:A:516:PHE:CE2	1:A:523:LYS:HE3	2.53	0.42
1:A:139:LYS:HB2	1:D:334:SER:HB3	2.00	0.42
1:C:573:ILE:HD11	1:C:765:LEU:CD1	2.49	0.42
1:C:598:LEU:HD21	1:C:670:TYR:HB3	2.00	0.42
1:B:608:GLU:O	1:B:612:GLN:HG2	2.19	0.42
1:A:310:ARG:NH1	1:A:368:GLY:O	2.52	0.42
1:A:174:VAL:HG23	1:A:185:ILE:CG1	2.48	0.42
1:B:676:PRO:HD2	1:B:677:GLU:OE2	2.18	0.42
1:D:135:TYR:HA	3:D:822:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.44	0.42
1:A:712:HIS:O	1:A:713:PHE:C	2.57	0.42
1:D:201:TRP:CH2	1:D:205:GLU:HG2	2.53	0.42
1:C:235:LEU:HD21	1:C:255:PRO:HG3	2.00	0.42
1:B:150:ASN:O	1:B:151:ASN:CB	2.64	0.42
1:A:581:ARG:NH1	1:A:601:PHE:CD1	2.88	0.42
1:C:123:GLN:HB3	1:C:124:TRP:H	1.69	0.42
1:B:765:LEU:H	1:B:765:LEU:CD2	2.29	0.42
1:C:692:ALA:HB1	1:C:726:VAL:HG21	2.00	0.42
1:C:376:SER:OG	1:C:380:GLY:HA2	2.19	0.42
1:A:613:PHE:C	1:A:615:LYS:N	2.72	0.42
1:B:358:ARG:O	1:B:359:PRO:C	2.58	0.42
1:C:482:LEU:HD12	1:C:482:LEU:HA	1.66	0.42
1:A:310:ARG:HD3	1:A:327:ILE:CG2	2.49	0.42
1:B:44:THR:O	1:B:47:ASP:HB2	2.19	0.42
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.01	0.42
1:A:158:SER:HA	1:A:216:TRP:CD2	2.54	0.42
1:B:310:ARG:NH1	1:B:329:ASP:OD2	2.52	0.42
1:C:55:LEU:HD11	1:C:561:LEU:CD1	2.50	0.42
1:A:459:VAL:CG2	1:A:460:SER:N	2.80	0.42
1:B:115:LEU:HG	1:B:132:TYR:HD2	1.84	0.42
1:C:649:CYS:CB	1:C:699:GLU:HB2	2.48	0.42
1:D:142:LEU:HA	1:D:142:LEU:HD12	1.73	0.42
1:C:360:SER:OG	1:C:374:ILE:O	2.32	0.42
1:D:514:LEU:HD12	1:D:526:TYR:O	2.19	0.42
1:B:204:GLU:O	1:B:204:GLU:HG2	2.20	0.42
1:D:157:TRP:CE3	1:D:164:LEU:HD23	2.54	0.42
1:D:75:ASN:HB3	1:D:92:ASN:H	1.83	0.42
1:C:621:ASN:HA	1:C:624:ILE:HD11	2.01	0.42
1:D:594:ILE:HD12	1:D:598:LEU:HD23	2.00	0.42
1:A:459:VAL:CG2	1:A:460:SER:H	2.29	0.42
1:B:514:LEU:CD2	1:B:557:THR:HG22	2.48	0.42
1:D:383:HIS:CE1	1:D:399:LYS:HA	2.55	0.42
1:D:384:ILE:CG1	1:D:404:VAL:HG11	2.50	0.42
1:B:464:GLU:O	1:B:465:ALA:CB	2.67	0.42
1:C:519:LEU:HD21	1:C:612:GLN:HE22	1.82	0.42
1:C:249:PRO:HG3	1:D:714:GLN:NE2	2.34	0.42
1:B:194:ILE:HD13	1:B:229:ASN:HA	2.01	0.42
1:C:242:SER:HB3	1:C:246:LEU:HD23	2.02	0.42
1:A:526:TYR:CD1	1:A:526:TYR:C	2.92	0.42
1:C:234:PRO:HB2	1:D:248:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:GLU:OE1	1:C:742:ILE:HA	2.20	0.42
1:D:739:ASP:HB2	1:D:740:HIS:H	1.58	0.42
1:B:651:ILE:HG21	1:B:755:MET:HE3	2.02	0.42
1:A:75:ASN:CA	1:A:92:ASN:HB3	2.48	0.42
1:A:293:MET:HE2	1:A:315:TRP:HB2	2.02	0.42
1:D:374:ILE:HD13	1:D:404:VAL:HG12	2.02	0.42
1:D:301:CYS:O	1:D:358:ARG:NH1	2.53	0.42
1:B:517:ILE:HD12	1:B:612:GLN:HG3	2.01	0.42
1:D:229:ASN:HB3	1:D:265:THR:OG1	2.20	0.42
1:B:519:LEU:O	1:B:520:ASN:C	2.58	0.42
1:A:240:PHE:CE2	1:A:242:SER:HA	2.54	0.42
1:A:266:VAL:HG22	1:A:267:LYS:N	2.34	0.42
1:A:422:TYR:OH	1:A:423:LYS:HE3	2.20	0.42
1:B:317:ARG:C	1:B:319:ILE:N	2.72	0.42
1:A:125:ARG:HH21	1:A:710:ASN:HD21	1.66	0.42
1:D:526:TYR:HB2	1:D:577:SER:O	2.19	0.42
1:D:146:GLU:HG3	1:D:180:LEU:C	2.40	0.42
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.42
1:A:60:LEU:HD22	1:A:68:TYR:CD2	2.55	0.42
1:A:110:ASP:OD2	1:A:111:GLY:N	2.53	0.42
1:C:705:GLY:O	1:C:708:ASP:HB2	2.20	0.42
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.55	0.42
1:D:449:LEU:HD23	1:D:449:LEU:HA	1.73	0.42
1:B:110:ASP:OD2	1:B:112:GLN:HB2	2.20	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.20	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.85	0.42
1:B:168:TRP:CZ2	1:B:169:ASN:OD1	2.73	0.42
1:D:323:SER:OG	1:D:347:GLU:HB3	2.20	0.42
1:B:474:GLY:HA2	1:B:476:GLY:O	2.20	0.42
1:D:361:GLU:OE2	1:D:363:HIS:NE2	2.50	0.42
1:C:562:ASN:O	1:C:565:THR:N	2.52	0.42
1:B:50:LYS:HA	1:B:50:LYS:HD3	1.82	0.42
1:D:634:TYR:HD1	1:D:656:VAL:O	2.02	0.42
1:B:236:ILE:HG23	1:B:254:VAL:HG13	2.02	0.42
1:A:192:ASP:HA	1:A:195:TYR:OH	2.19	0.42
1:B:546:VAL:HA	3:B:826:HOH:O	2.20	0.42
1:B:535:ASP:C	1:B:537:SER:N	2.72	0.42
1:C:256:TYR:CD1	1:C:256:TYR:C	2.93	0.42
1:A:620:ASP:C	1:A:620:ASP:OD1	2.58	0.42
1:A:599:GLY:N	1:A:602:GLU:OE1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.42
1:C:188:THR:HB	1:C:194:ILE:HG21	2.02	0.42
1:B:385:CYS:HA	1:B:396:PHE:HA	2.02	0.42
1:C:433:LYS:O	1:C:433:LYS:HG3	2.19	0.42
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.02	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:742:ILE:CD1	1:B:751:ILE:HD12	2.50	0.41
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.50	0.41
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.20	0.41
1:C:468:TYR:O	1:C:482:LEU:HD12	2.20	0.41
1:C:263:ASN:HD21	1:C:664:SER:HB2	1.84	0.41
1:C:551:CYS:HB2	1:C:591:MET:SD	2.59	0.41
1:C:714:GLN:NE2	1:D:249:PRO:HD3	2.35	0.41
1:C:446:SER:HA	1:C:449:LEU:HG	2.02	0.41
1:C:547:TYR:O	1:C:549:GLY:N	2.53	0.41
1:B:433:LYS:HB2	1:B:445:LEU:HD21	2.02	0.41
1:D:167:VAL:HG13	1:D:171:ASP:O	2.20	0.41
1:B:425:MET:HA	1:B:426:PRO:HD2	1.90	0.41
1:B:629:TRP:HA	1:B:653:VAL:O	2.20	0.41
1:D:51:ASN:OD1	1:D:54:ARG:HD2	2.20	0.41
1:C:510:PRO:CB	1:C:530:LEU:O	2.68	0.41
1:A:620:ASP:OD2	1:A:623:ARG:HD2	2.20	0.41
1:A:535:ASP:OD1	1:A:538:LYS:HE2	2.20	0.41
1:B:707:ALA:HB2	1:B:737:ASP:HA	2.02	0.41
1:C:477:LEU:CD1	1:C:501:ASP:HB2	2.50	0.41
1:B:136:ASP:CB	1:B:139:LYS:HG2	2.51	0.41
1:C:177:GLU:HB2	1:C:180:LEU:HD12	2.01	0.41
1:A:248:TYR:CD2	1:B:258:LYS:HD2	2.54	0.41
1:C:336:ARG:NH1	1:C:336:ARG:CG	2.82	0.41
1:D:596:ARG:NH2	1:D:679:ASN:HB2	2.35	0.41
1:A:148:ILE:HA	1:A:149:PRO:HD2	1.79	0.41
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.56	0.41
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.90	0.41
1:A:500:LEU:O	1:A:501:ASP:C	2.59	0.41
1:D:195:TYR:CE2	1:D:200:ASP:HA	2.56	0.41
1:D:434:ILE:HG13	1:D:442:VAL:HG22	2.02	0.41
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.20	0.41
1:A:543:LEU:HD23	1:A:567:LEU:HD13	2.03	0.41
1:A:446:SER:HA	1:A:449:LEU:HD12	2.02	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.03	0.41
1:D:482:LEU:HD12	1:D:482:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:VAL:CG1	1:D:161:GLY:N	2.84	0.41
1:D:105:TYR:HD2	1:D:107:ILE:HD12	1.86	0.41
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.41
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.41
1:D:330:TYR:HD1	1:D:337:TRP:CE2	2.38	0.41
1:D:475:PRO:HD3	1:D:557:THR:HB	2.01	0.41
1:A:375:ILE:HD11	1:A:396:PHE:CZ	2.55	0.41
1:B:340:LEU:HA	1:B:340:LEU:HD23	1.88	0.41
1:D:240:PHE:CE1	1:D:737:ASP:HB3	2.55	0.41
1:B:187:TRP:CZ3	1:B:281:ASN:OD1	2.73	0.41
1:A:673:LEU:HD23	1:A:674:PRO:HD2	2.02	0.41
1:D:374:ILE:CD1	1:D:406:GLY:HA2	2.50	0.41
1:B:293:MET:HE1	1:B:317:ARG:HG3	2.02	0.41
1:B:347:GLU:OE1	1:B:373:LYS:NZ	2.52	0.41
1:A:124:TRP:HE3	1:A:124:TRP:HA	1.84	0.41
1:A:620:ASP:O	1:A:622:LYS:N	2.54	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.93	0.41
1:D:258:LYS:O	1:D:259:ALA:C	2.59	0.41
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.83	0.41
1:D:125:ARG:HG2	1:D:126:HIS:CD2	2.56	0.41
1:A:383:HIS:HA	1:A:404:VAL:HG23	2.03	0.41
1:A:457:TYR:CE1	1:A:472:CYS:HB2	2.56	0.41
1:D:422:TYR:C	1:D:424:GLY:H	2.24	0.41
1:D:629:TRP:O	1:D:630:SER:CB	2.69	0.41
1:D:520:ASN:C	1:D:522:THR:N	2.74	0.41
1:D:107:ILE:N	1:D:107:ILE:HD12	2.35	0.41
1:D:206:GLU:CD	1:D:666:TYR:HB2	2.41	0.41
1:B:563:TRP:CZ3	1:B:567:LEU:HD11	2.55	0.41
1:B:660:GLU:OE2	1:B:684:ARG:NE	2.53	0.41
1:B:135:TYR:O	1:B:137:LEU:N	2.54	0.41
1:C:175:LYS:HG3	1:C:182:SER:HB3	2.02	0.41
1:B:738:GLU:OE2	1:B:744:SER:HB2	2.21	0.41
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.20	0.41
1:A:227:GLN:N	1:A:267:LYS:O	2.54	0.41
1:C:397:ILE:HG13	1:C:397:ILE:O	2.20	0.41
1:C:293:MET:HG2	1:C:315:TRP:CB	2.51	0.41
1:D:256:TYR:HA	1:D:257:PRO:HD3	1.92	0.41
1:C:568:ALA:HA	1:C:573:ILE:O	2.21	0.41
1:A:353:TRP:CZ2	1:A:670:TYR:HE1	2.38	0.41
1:C:622:LYS:C	1:C:623:ARG:HG3	2.41	0.41
1:D:624:ILE:O	1:D:647:PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:PHE:CZ	1:D:394:CYS:SG	3.14	0.41
1:A:415:LEU:CD2	1:A:415:LEU:C	2.89	0.41
1:B:599:GLY:N	1:B:602:GLU:OE1	2.46	0.41
1:B:644:SER:C	1:B:646:VAL:N	2.74	0.41
1:D:154:TRP:O	1:D:166:TYR:HA	2.21	0.41
1:A:343:ARG:HG2	1:A:389:ILE:HD12	2.02	0.41
1:A:640:LEU:HB3	1:A:698:VAL:HG21	2.02	0.41
1:A:132:TYR:CZ	1:A:155:VAL:HG12	2.56	0.41
1:C:192:ASP:HA	1:C:195:TYR:OH	2.21	0.41
1:A:387:PHE:CE2	1:A:394:CYS:CB	3.04	0.41
1:A:513:LYS:HE2	1:A:515:ASP:CB	2.51	0.41
1:D:732:ALA:O	1:D:733:MET:HB2	2.20	0.41
1:C:248:TYR:O	1:C:249:PRO:C	2.59	0.41
1:D:581:ARG:NE	1:D:605:ASP:OD2	2.49	0.41
1:C:188:THR:O	1:C:194:ILE:CG2	2.69	0.41
1:D:105:TYR:CD2	1:D:107:ILE:CD1	3.03	0.41
1:B:524:PHE:CD2	1:B:580:GLY:HA2	2.56	0.41
1:B:67:GLU:HA	1:B:79:PHE:O	2.20	0.41
1:D:563:TRP:CZ3	1:D:567:LEU:HD11	2.56	0.41
1:B:506:ASN:CG	1:B:506:ASN:O	2.59	0.41
1:D:146:GLU:HB3	1:D:180:LEU:C	2.42	0.41
1:C:82:GLU:HG2	1:C:83:TYR:CE1	2.56	0.41
1:B:308:GLN:C	1:B:309:GLU:HG3	2.41	0.41
1:D:148:ILE:O	1:D:149:PRO:C	2.59	0.41
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.21	0.41
1:D:136:ASP:N	3:D:822:HOH:O	2.54	0.40
1:D:623:ARG:HB3	1:D:763:PHE:CD1	2.56	0.40
1:D:258:LYS:NZ	1:D:661:TYR:O	2.52	0.40
1:B:659:TRP:O	1:B:667:THR:HG21	2.21	0.40
1:A:341:VAL:C	1:A:343:ARG:H	2.24	0.40
1:B:739:ASP:HB2	1:B:740:HIS:H	1.74	0.40
1:A:180:LEU:O	1:A:181:PRO:O	2.39	0.40
1:C:169:ASN:HD22	1:C:169:ASN:N	2.19	0.40
1:D:51:ASN:O	1:D:54:ARG:CD	2.69	0.40
1:B:501:ASP:O	1:B:505:GLN:HG2	2.21	0.40
1:B:594:ILE:CG2	1:B:601:PHE:HB2	2.51	0.40
1:C:197:GLY:C	1:C:213:ALA:HB3	2.42	0.40
1:D:72:GLN:O	1:D:73:GLU:C	2.58	0.40
1:B:760:LYS:HD2	1:B:766:PRO:O	2.22	0.40
1:A:158:SER:HB2	1:A:159:PRO:HD2	2.04	0.40
1:A:372:TYR:CZ	1:A:386:TYR:CE1	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:CB	1:A:246:LEU:HD22	2.50	0.40
1:B:446:SER:HA	1:B:449:LEU:HG	2.01	0.40
1:C:540:TYR:C	1:C:541:PRO:O	2.55	0.40
1:D:427:GLY:O	1:D:557:THR:HG23	2.21	0.40
1:B:289:ALA:HB2	1:B:315:TRP:CE3	2.55	0.40
1:D:627:TRP:CZ3	1:D:755:MET:HE1	2.56	0.40
1:B:550:PRO:O	1:B:551:CYS:CB	2.69	0.40
1:A:107:ILE:HA	1:A:114:ILE:HA	2.02	0.40
1:A:82:GLU:O	1:A:492:ARG:NH2	2.54	0.40
1:D:148:ILE:O	1:D:149:PRO:O	2.38	0.40
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.22	0.40
1:D:720:SER:O	1:D:724:VAL:HG23	2.21	0.40
1:A:302:ASP:C	1:A:302:ASP:OD1	2.59	0.40
1:B:433:LYS:HE2	1:B:488:ASP:OD1	2.21	0.40
1:C:369:ASN:CA	1:C:389:ILE:HG23	2.51	0.40
1:C:70:TYR:HB3	1:C:79:PHE:HE2	1.87	0.40
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.93	0.40
1:B:480:TYR:CD1	1:B:480:TYR:N	2.90	0.40
1:B:629:TRP:O	1:B:630:SER:CB	2.66	0.40
1:A:739:ASP:C	1:A:741:GLY:H	2.23	0.40
1:B:356:ARG:HD3	1:B:585:TYR:HE1	1.85	0.40
1:B:144:THR:O	1:B:147:ARG:HD2	2.21	0.40
1:D:504:LEU:HD22	1:D:509:MET:CE	2.52	0.40
1:A:671:MET:SD	1:A:682:HIS:HD2	2.44	0.40
1:C:741:GLY:O	1:C:742:ILE:C	2.59	0.40
1:D:110:ASP:C	1:D:112:GLN:N	2.71	0.40
1:D:90:LEU:HA	1:D:90:LEU:HD12	1.89	0.40
1:C:633:GLY:CA	1:C:655:PRO:HB3	2.46	0.40
1:B:744:SER:O	1:B:745:SER:C	2.59	0.40
1:C:761:GLN:NE2	1:C:762:CYS:N	2.69	0.40
1:C:325:MET:CE	1:C:371:PHE:CE2	3.03	0.40
1:B:82:GLU:OE1	1:B:82:GLU:HA	2.22	0.40
1:C:558:VAL:CG1	1:C:559:PHE:N	2.85	0.40
1:A:602:GLU:N	1:A:602:GLU:OE2	2.50	0.40
1:D:87:SER:O	1:D:88:VAL:C	2.59	0.40
1:C:753:THR:O	1:C:757:HIS:CD2	2.75	0.40
1:D:77:LEU:N	1:D:77:LEU:CD1	2.84	0.40
1:B:658:ARG:HE	1:B:687:THR:HG21	1.87	0.40
1:D:383:HIS:HB3	1:D:398:THR:OG1	2.20	0.40
1:B:199:THR:HG23	1:B:213:ALA:HB2	2.03	0.40
1:C:657:SER:HB3	1:C:719:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:HB	1:B:129:THR:OG1	2.22	0.40
1:A:126:HIS:CD2	1:A:209:SER:C	2.95	0.40
1:A:83:TYR:C	1:A:492:ARG:NH2	2.75	0.40
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.01	0.40
1:C:743:ALA:O	1:C:744:SER:C	2.60	0.40
1:D:50:LYS:HD3	1:D:50:LYS:HA	1.80	0.40
1:D:642:SER:O	1:D:643:GLY:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/728 (100%)	593 (82%)	112 (15%)	21 (3%)	6	29
1	B	726/728 (100%)	622 (86%)	84 (12%)	20 (3%)	6	30
1	C	726/728 (100%)	620 (85%)	86 (12%)	20 (3%)	6	30
1	D	726/728 (100%)	634 (87%)	73 (10%)	19 (3%)	7	32
All	All	2904/2912 (100%)	2469 (85%)	355 (12%)	80 (3%)	6	30

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	320	GLN
1	A	439	TYR
1	B	137	LEU
1	B	320	GLN
1	B	520	ASN
1	B	712	HIS
1	C	74	ASN

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Mol	Chain	Res	Type
1	C	106	SER
1	C	143	ILE
1	C	548	ALA
1	D	88	VAL
1	D	111	GLY
1	D	320	GLN
1	A	139	LYS
1	A	143	ILE
1	A	181	PRO
1	A	209	SER
1	A	261	ALA
1	A	389	ILE
1	A	614	SER
1	A	621	ASN
1	B	73	GLU
1	B	146	GLU
1	B	280	THR
1	B	536	LYS
1	B	764	SER
1	C	712	HIS
1	D	138	ASN
1	D	764	SER
1	A	231	THR
1	A	242	SER
1	A	577	SER
1	B	377	ASN
1	B	616	MET
1	C	583	SER
1	C	668	GLU
1	D	149	PRO
1	D	366	LEU
1	D	521	GLU
1	D	710	ASN
1	D	712	HIS
1	A	51	ASN
1	A	74	ASN
1	A	149	PRO
1	A	333	SER
1	A	491	LEU
1	B	261	ALA
1	C	366	LEU
1	C	536	LYS

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Mol	Chain	Res	Type
1	C	695	PHE
1	D	178	PRO
1	D	423	LYS
1	D	683	TYR
1	A	191	GLU
1	A	447	CYS
1	B	136	ASP
1	B	143	ILE
1	B	548	ALA
1	C	51	ASN
1	C	218	PRO
1	C	259	ALA
1	C	320	GLN
1	C	664	SER
1	C	667	THR
1	C	715	GLN
1	C	737	ASP
1	D	130	ALA
1	D	714	GLN
1	B	645	GLY
1	B	714	GLN
1	D	143	ILE
1	D	280	THR
1	B	109	PRO
1	B	674	PRO
1	B	742	ILE
1	D	742	ILE
1	C	355	GLY
1	C	541	PRO
1	D	181	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	653/653 (100%)	610 (93%)	43 (7%)	21 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	653/653 (100%)	624 (96%)	29 (4%)	35	71
1	C	653/653 (100%)	616 (94%)	37 (6%)	25	62
1	D	653/653 (100%)	616 (94%)	37 (6%)	25	62
All	All	2612/2612 (100%)	2466 (94%)	146 (6%)	26	62

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	57	LEU
1	A	77	LEU
1	A	95	PHE
1	A	96	ASP
1	A	106	SER
1	A	109	PRO
1	A	133	ASP
1	A	145	GLU
1	A	147	ARG
1	A	170	ASN
1	A	186	THR
1	A	202	VAL
1	A	214	LEU
1	A	243	ASP
1	A	254	VAL
1	A	256	TYR
1	A	279	VAL
1	A	280	THR
1	A	288	THR
1	A	293	MET
1	A	339	CYS
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	391	LYS
1	A	393	ASP
1	A	413	ASP
1	A	458	SER
1	A	507	VAL
1	A	536	LYS
1	A	566	TYR
1	A	570	THR

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Mol	Chain	Res	Type
1	A	577	SER
1	A	597	ARG
1	A	621	ASN
1	A	657	SER
1	A	658	ARG
1	A	677	GLU
1	A	683	TYR
1	A	704	HIS
1	A	714	GLN
1	A	728	VAL
1	B	54	ARG
1	B	72	GLN
1	B	73	GLU
1	B	74	ASN
1	B	75	ASN
1	B	89	PHE
1	B	91	GLU
1	B	108	SER
1	B	145	GLU
1	B	214	LEU
1	B	239	SER
1	B	243	ASP
1	B	254	VAL
1	B	272	ASN
1	B	277	SER
1	B	283	THR
1	B	332	GLU
1	B	341	VAL
1	B	382	ARG
1	B	448	GLU
1	B	452	GLU
1	B	487	ASN
1	B	522	THR
1	B	546	VAL
1	B	606	GLN
1	B	658	ARG
1	B	677	GLU
1	B	700	TYR
1	B	761	GLN
1	C	96	ASP
1	C	108	SER
1	C	118	TYR

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Mol	Chain	Res	Type
1	C	125	ARG
1	C	133	ASP
1	C	145	GLU
1	C	170	ASN
1	C	184	ARG
1	C	214	LEU
1	C	215	TRP
1	C	254	VAL
1	C	256	TYR
1	C	293	MET
1	C	301	CYS
1	C	319	ILE
1	C	326	ASP
1	C	329	ASP
1	C	333	SER
1	C	336	ARG
1	C	382	ARG
1	C	385	CYS
1	C	388	GLN
1	C	401	THR
1	C	448	GLU
1	C	472	CYS
1	C	492	ARG
1	C	539	LYS
1	C	546	VAL
1	C	566	TYR
1	C	583	SER
1	C	621	ASN
1	C	627	TRP
1	C	658	ARG
1	C	663	ASP
1	C	728	VAL
1	C	761	GLN
1	C	764	SER
1	D	52	THR
1	D	55	LEU
1	D	57	LEU
1	D	63	ILE
1	D	80	ASN
1	D	85	ASN
1	D	113	PHE
1	D	121	VAL

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Mol	Chain	Res	Type
1	D	125	ARG
1	D	137	LEU
1	D	138	ASN
1	D	151	ASN
1	D	156	THR
1	D	158	SER
1	D	169	ASN
1	D	180	LEU
1	D	184	ARG
1	D	191	GLU
1	D	214	LEU
1	D	221	THR
1	D	254	VAL
1	D	256	TYR
1	D	272	ASN
1	D	278	SER
1	D	284	SER
1	D	351	THR
1	D	385	CYS
1	D	393	ASP
1	D	448	GLU
1	D	487	ASN
1	D	492	ARG
1	D	566	TYR
1	D	606	GLN
1	D	677	GLU
1	D	681	ASP
1	D	685	ASN
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	123	GLN
1	A	126	HIS
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	286	GLN
1	A	314	GLN

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Mol	Chain	Res	Type
1	A	345	HIS
1	A	388	GLN
1	A	505	GLN
1	A	572	ASN
1	A	595	ASN
1	A	621	ASN
1	A	712	HIS
1	A	731	GLN
1	A	757	HIS
1	B	51	ASN
1	B	66	HIS
1	B	74	ASN
1	B	75	ASN
1	B	123	GLN
1	B	169	ASN
1	B	272	ASN
1	B	281	ASN
1	B	314	GLN
1	B	435	GLN
1	B	487	ASN
1	B	506	ASN
1	B	712	HIS
1	B	731	GLN
1	B	748	HIS
1	B	761	GLN
1	C	75	ASN
1	C	103	ASN
1	C	123	GLN
1	C	126	HIS
1	C	138	ASN
1	C	169	ASN
1	C	170	ASN
1	C	345	HIS
1	C	572	ASN
1	C	621	ASN
1	C	712	HIS
1	C	731	GLN
1	C	757	HIS
1	D	72	GLN
1	D	74	ASN
1	D	92	ASN
1	D	123	GLN

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Mol	Chain	Res	Type
1	D	150	ASN
1	D	169	ASN
1	D	227	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	435	GLN
1	D	455	GLN
1	D	487	ASN
1	D	506	ASN
1	D	595	ASN
1	D	685	ASN
1	D	712	HIS
1	D	714	GLN
1	D	731	GLN
1	D	761	GLN

### 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](#)

4 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
2	13Z	A	767	1	22,27,27	1.68	6 (27%)	24,41,41	2.36	4 (16%)
2	13Z	B	767	1	22,27,27	1.48	4 (18%)	24,41,41	2.24	4 (16%)
2	13Z	C	767	1	22,27,27	1.73	3 (13%)	24,41,41	1.96	2 (8%)
2	13Z	D	767	1	22,27,27	1.44	5 (22%)	24,41,41	2.23	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	13Z	A	767	1	-	0/20/39/39	0/1/2/2
2	13Z	B	767	1	-	0/20/39/39	0/1/2/2
2	13Z	C	767	1	-	0/20/39/39	0/1/2/2
2	13Z	D	767	1	-	0/20/39/39	0/1/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	767	13Z	F1-C3	-2.99	1.33	1.41
2	D	767	13Z	C8-N2	-2.94	1.30	1.33
2	A	767	13Z	F1-C3	-2.83	1.34	1.41
2	D	767	13Z	F1-C3	-2.78	1.34	1.41
2	B	767	13Z	F1-C3	-2.69	1.34	1.41
2	B	767	13Z	C8-N2	-2.42	1.30	1.33
2	A	767	13Z	C8-N2	-2.27	1.30	1.33
2	D	767	13Z	C9-N3	-2.24	1.31	1.33
2	D	767	13Z	C5-N1	2.04	1.40	1.35
2	A	767	13Z	C1-N1	2.13	1.50	1.47
2	A	767	13Z	C5-N1	2.55	1.41	1.35
2	B	767	13Z	C5-N1	2.66	1.41	1.35
2	C	767	13Z	C5-N1	2.74	1.42	1.35
2	D	767	13Z	C7-C1	3.50	1.58	1.54
2	A	767	13Z	C11-N4	3.88	1.53	1.49
2	A	767	13Z	C7-C1	4.13	1.58	1.54
2	B	767	13Z	C7-C1	4.14	1.59	1.54
2	C	767	13Z	C7-C1	5.90	1.60	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	767	13Z	O2-C7-C8	-2.33	104.54	109.78
2	D	767	13Z	O2-C7-C8	-2.07	105.13	109.78
2	A	767	13Z	C2-C1-N1	2.02	104.77	101.68
2	B	767	13Z	C6-N4-C11	2.45	122.69	117.68
2	A	767	13Z	C6-N4-C11	2.46	122.72	117.68
2	C	767	13Z	C8-C7-C1	2.93	115.56	110.06
2	A	767	13Z	C8-C7-C1	3.35	116.36	110.06
2	B	767	13Z	C8-C7-C1	4.14	117.83	110.06
2	D	767	13Z	C8-C7-C1	4.20	117.96	110.06
2	C	767	13Z	C10-C9-N3	7.95	129.30	120.53
2	D	767	13Z	C10-C9-N3	8.87	130.31	120.53
2	B	767	13Z	C10-C9-N3	8.96	130.41	120.53
2	A	767	13Z	C10-C9-N3	9.70	131.23	120.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	13Z	2	0
2	B	767	13Z	2	0
2	C	767	13Z	1	0
2	D	767	13Z	3	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.