



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:03 PM GMT

PDB ID : 4WHB  
Title : Crystal structure of phenylurea hydrolase B  
Authors : Sugrue, E.; Carr, P.D.; Khurana, J.L.; Jackson, C.J.  
Deposited on : 2014-09-21  
Resolution : 2.96 Å(reported)

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

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

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

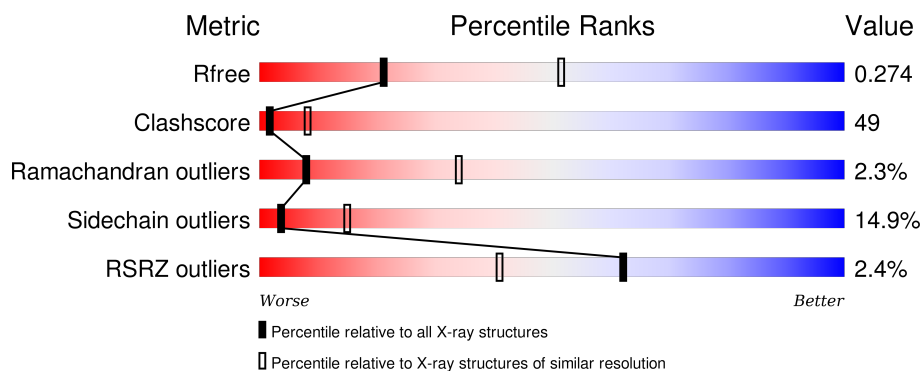
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	461	<div> <div>2%</div> <div>39%</div> <div>50%</div> <div>10%</div> <div>.</div> </div>
1	B	461	<div> <div>46%</div> <div>43%</div> <div>10%</div> <div>.</div> </div>
1	C	461	<div> <div>2%</div> <div>45%</div> <div>46%</div> <div>8%</div> <div>.</div> </div>
1	D	461	<div> <div>2%</div> <div>40%</div> <div>46%</div> <div>12%</div> <div>.</div> </div>
1	E	461	<div> <div>2%</div> <div>41%</div> <div>48%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	461	<div><div></div><div>6%</div><div>37%</div><div>53%</div><div>8%</div><div></div></div>
1	G	461	<div><div></div><div>4%</div><div>42%</div><div>46%</div><div>10%</div><div></div></div>
1	H	461	<div><div></div><div>3%</div><div>34%</div><div>52%</div><div>13%</div><div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 55405 atoms, of which 27459 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 Phenylurea hydrolase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	459	Total	C	H	N	O	S	0	0	0
			6918	2190	3430	618	670	10			
1	A	459	Total	C	H	N	O	S	0	0	0
			6915	2190	3427	618	670	10			
1	B	459	Total	C	H	N	O	S	0	2	0
			6944	2196	3445	622	671	10			
1	C	459	Total	C	H	N	O	S	0	2	0
			6941	2196	3442	622	671	10			
1	D	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			
1	F	459	Total	C	H	N	O	S	0	0	0
			6916	2190	3428	618	670	10			
1	G	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			
1	H	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	4	Total	O	0	0
			4	4		
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		

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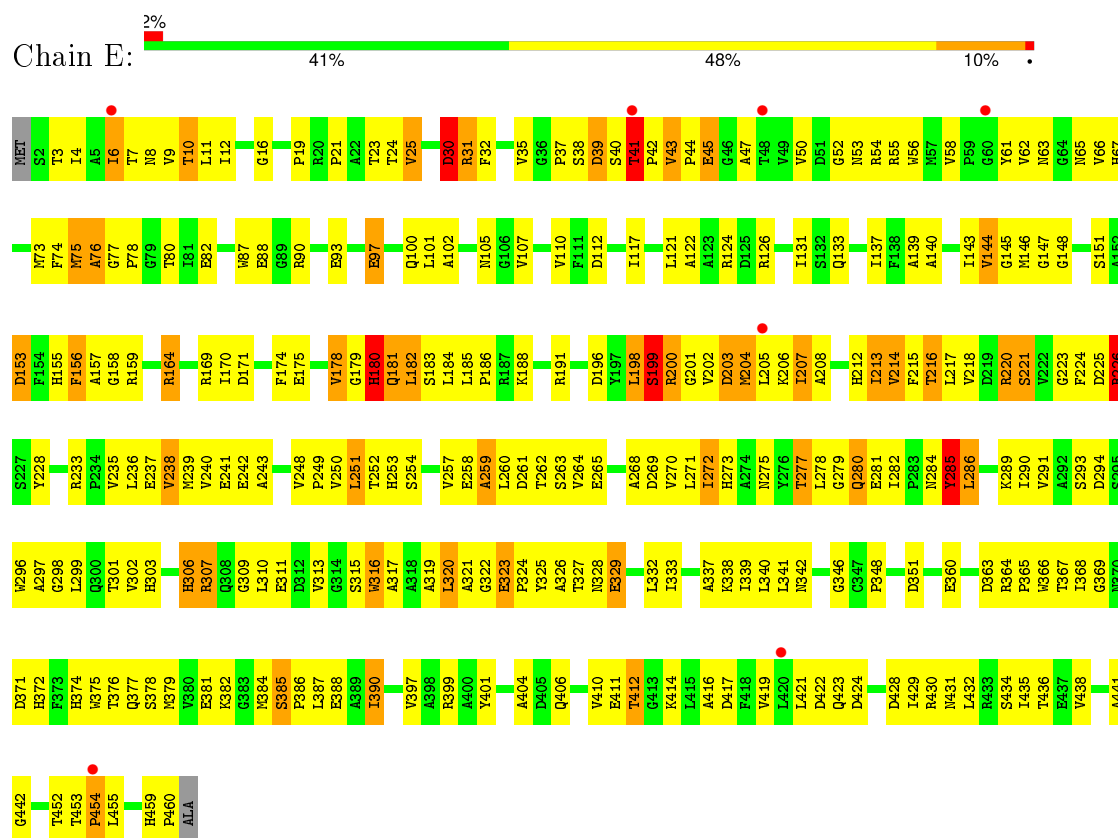
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	O 2	0	0
3	F	3	Total 3	O 3	0	0
3	G	1	Total 1	O 1	0	0
3	H	3	Total 3	O 3	0	0

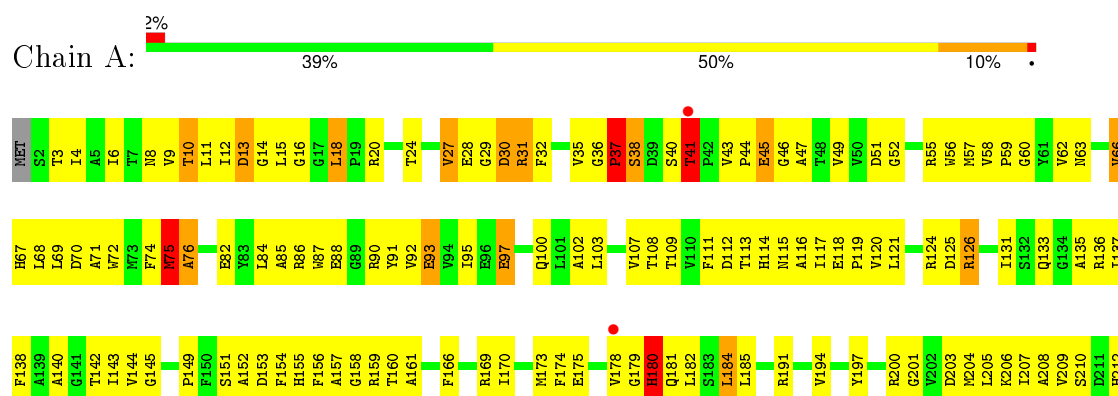
### 3 Residue-property plots

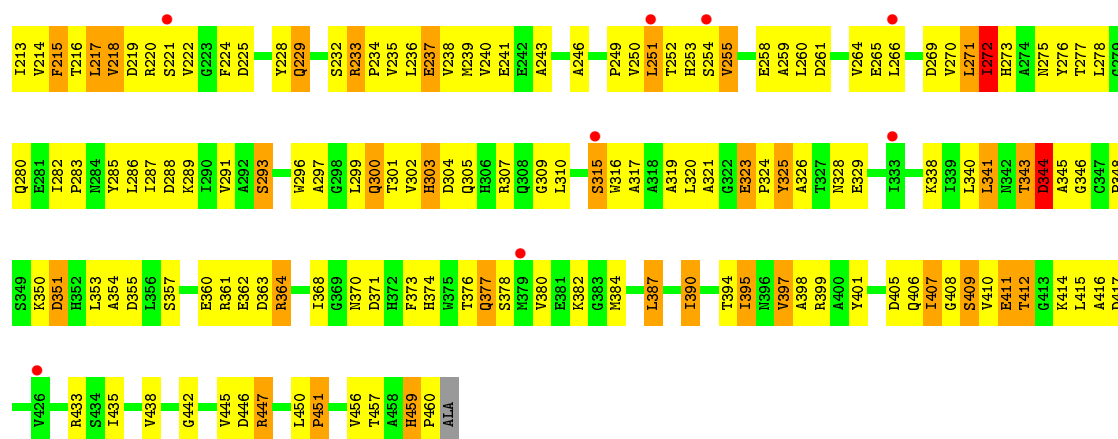
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

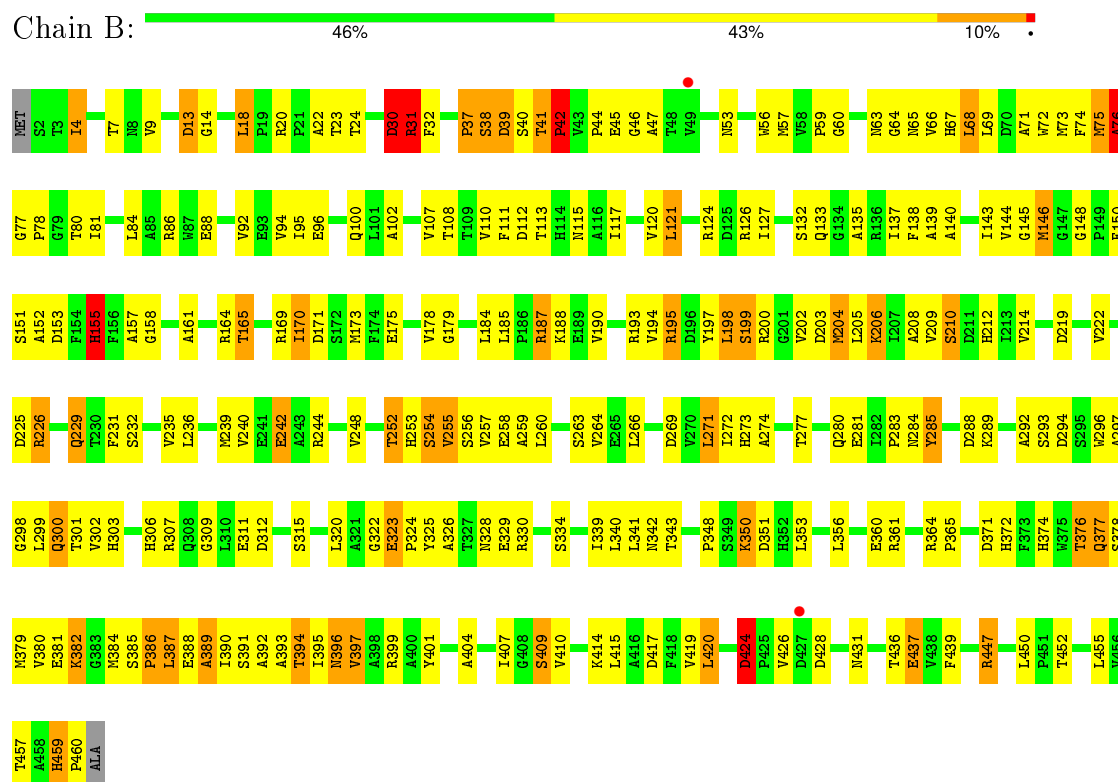


#### • Molecule 1: Phenylurea hydrolase B

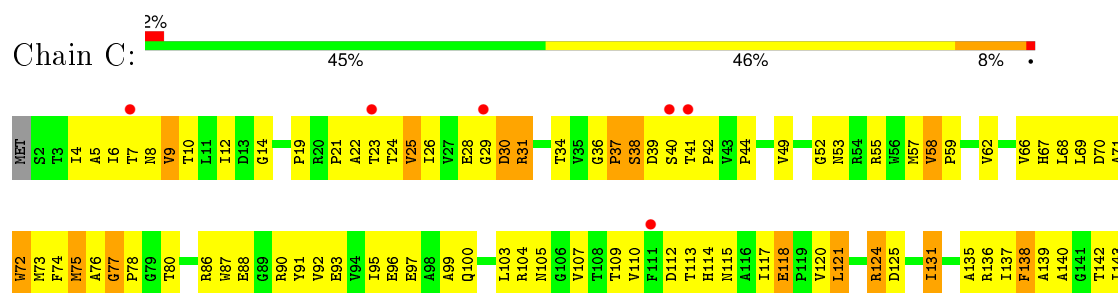


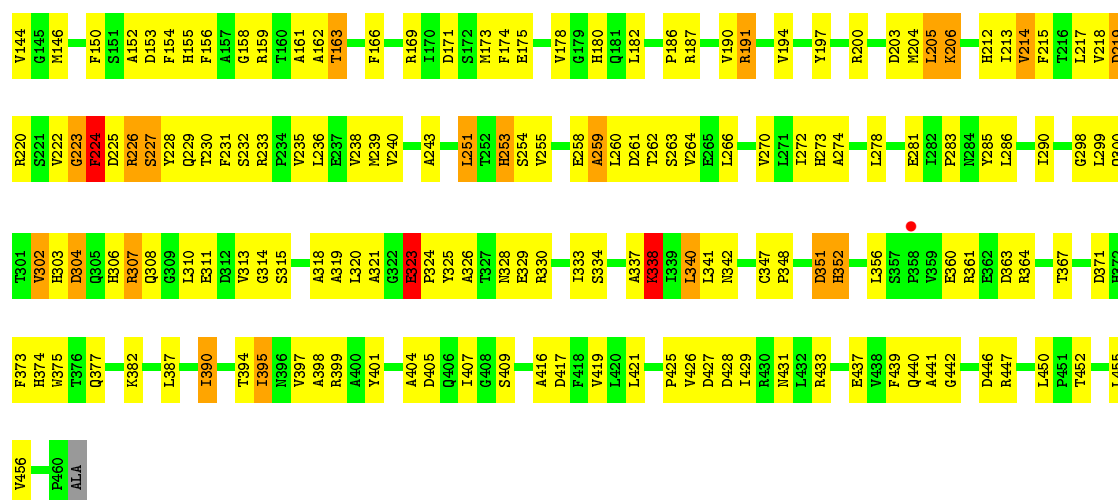


### • Molecule 1: Phenylurea hydrolase B

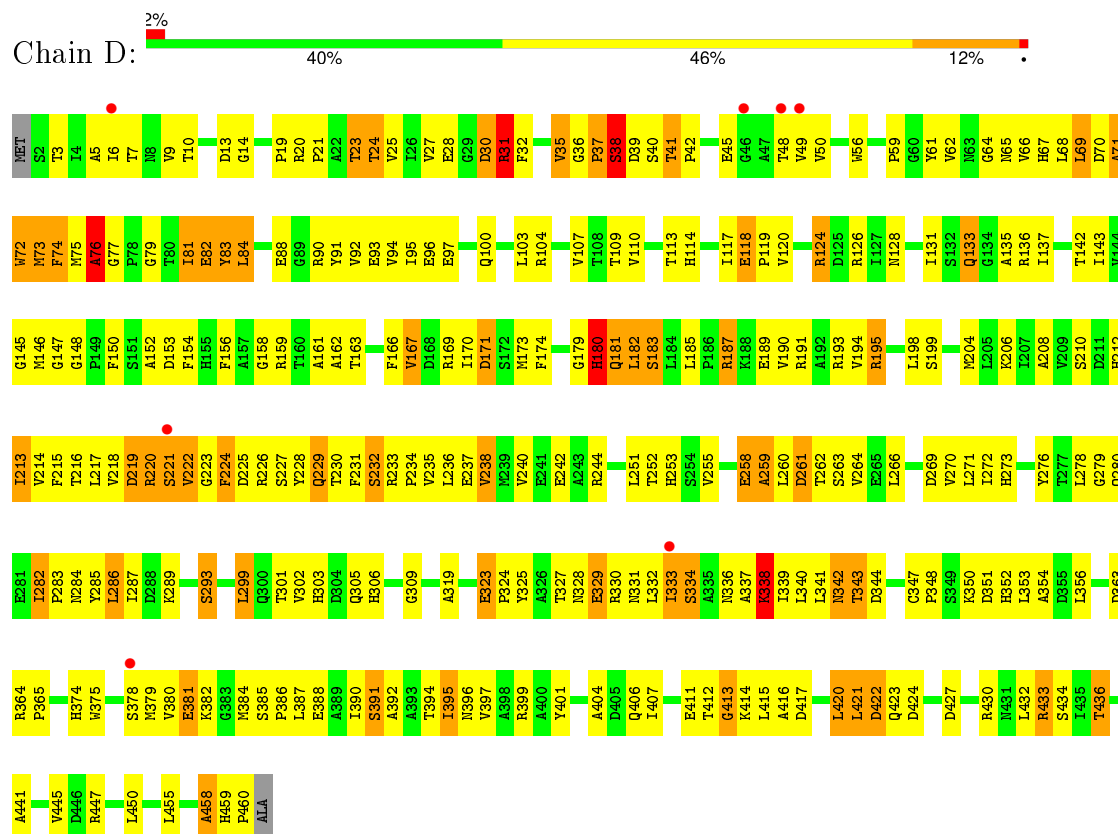


### • Molecule 1: Phenylurea hydrolase B

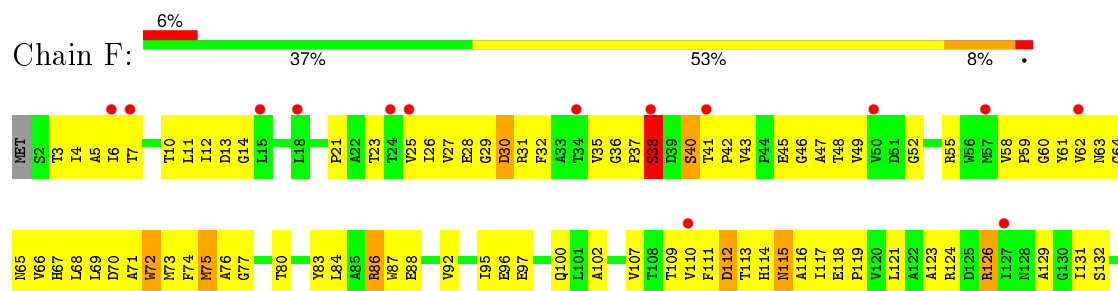




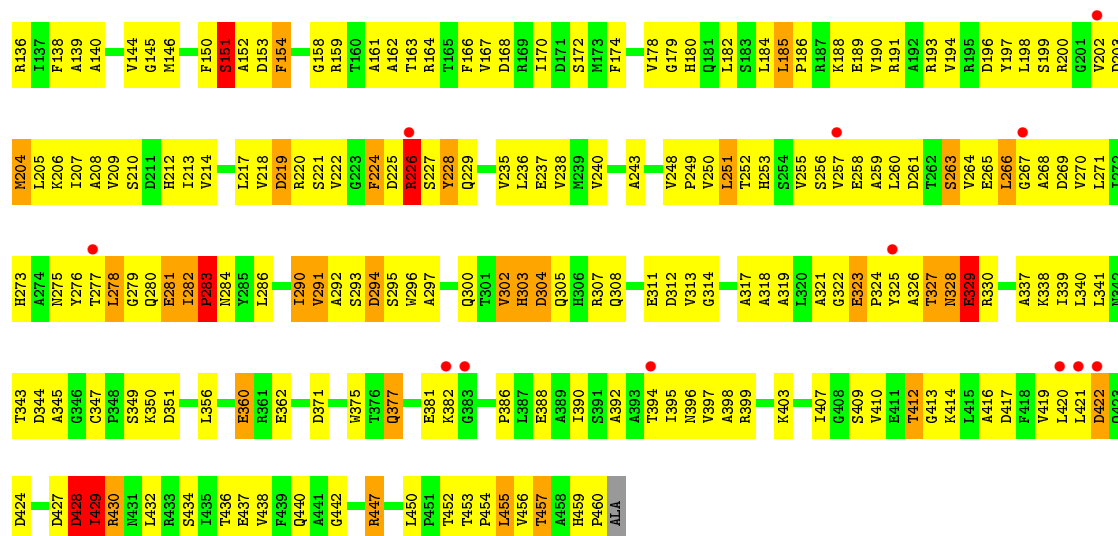
• Molecule 1: Phenylurea hydrolase B



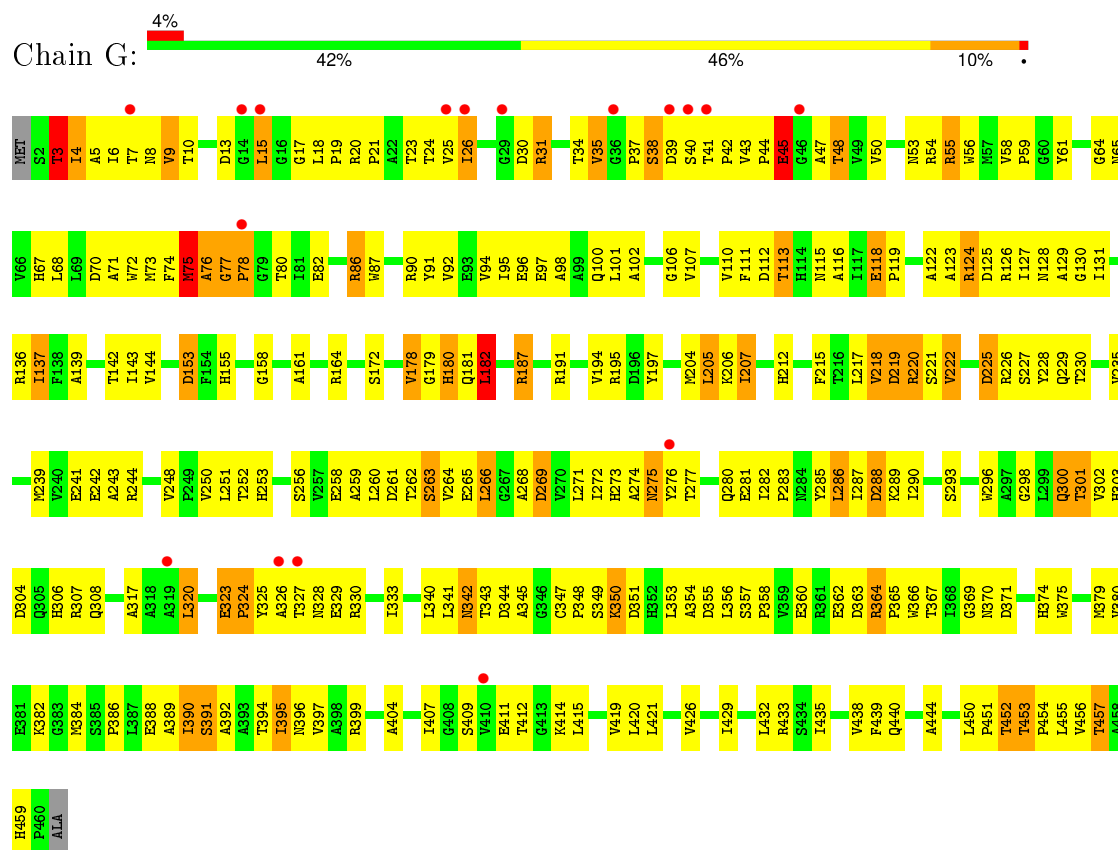
• Molecule 1: Phenylurea hydrolase B



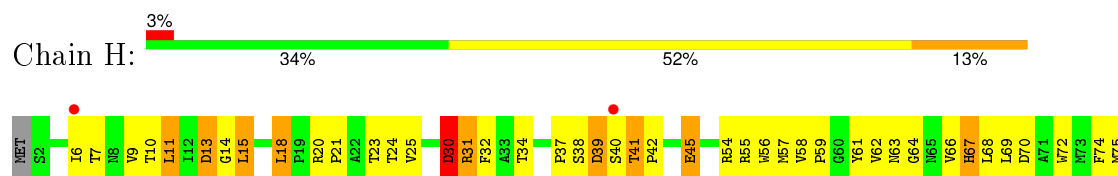




### • Molecule 1: Phenylurea hydrolase B



### • Molecule 1: Phenylurea hydrolase B



V426	D427	D428	I429	R430	M431	L432	R433	S434	T435	V436	E437	V438	F439	Q440	A441	G442	A443	A444	V445	D446	R447	P451	T452	T453	P454	L455	V456	T457	A458	H459	P460	ALA																											
S357	F358	V359	E360	R361	E362	D363	R364	F365	P366	T367	I368	D371	H372		W375	G376	Q377	S378	R379	V380	E381	K382	G383	N384	S385	F386	L387	E388	A389	I390	S391	A392	A393	T394	I395	N396	V397	K403	A404	D405	Q406	I407	G408	T412	G413	K414	L415	A416	D417	F418	V419	L420	Q423	D424	P425				
P283	N284	Y285	L286	R287		I290	V291	A292	S293	D294	S295	T296	A297		H303	D304	Q305	H306		I310	E311	D312	V313	A317	A318	A319	L320	A321	G322	E323	P324	Y325	A326	T327	N328	E329	R330	L331	I332	I333	S334	A335	N336	A337	K338	I339	L340	L341	N342	T343	D344		K350	D351	H352	L353	L356		
L217	V218	D219	R220	S221		F224	D225	R226	S227	Y228	Q229	T230	F231	S232	R233	P234	V235	L236	E237	V238	M239	V240	E241	E242	A243		G247	V248	P249	V250	L251	T252	H253	S254	V255	A256	V257	E258	A259	L260	D261	T262	S263	V264	E265	L266		D269	V270	L271	I272	H273	A274	N275	Y276	T277	L278		I282
A76	G77	P78		I81	E82		R86	W87		V92	E93	V94	I95	E96	E97	Q100	L101	A102	L103	R104		V107	T108	T109	V110	F111	D112	T113		I117	E118	P119	V120	L121	A122	A123	R124	D125	L126	I127		I131		G134	A135	R136	I137	F138	A139	A140	G141	T142	I143	V144	G145	M146	G147	G148	
P149	F150	S151	A152	D153	F154	H155	F156	A157		R164	T165	F166	V167	D168	R169	I170	M173	F174	E175	A176	G177	V178	G179	H180	Q181	L182		L185	P186		E189	V190	R191	A192	R193	V194	R195	D196	Y197	L198	I199	R200	G201	V202	D203	N204	L205	K206	I207	A208	V209	S210	D211	D212	I213	V214	F215	T216	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.37Å 100.53Å 238.55Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	39.59 – 2.96 39.59 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.59-2.96) 89.7 (39.59-2.96)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.252 , 0.309 0.241 , 0.274	Depositor DCC
$R_{free}$ test set	3585 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	1.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	1 of 75111 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	55405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8842e-03.*

<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

### 5.1 Standard geometry

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

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	0.69	1/3560 (0.0%)	0.85	7/4857 (0.1%)
1	B	0.83	1/3576 (0.0%)	0.93	9/4878 (0.2%)
1	C	0.69	1/3576 (0.0%)	0.83	2/4878 (0.0%)
1	D	0.79	1/3560 (0.0%)	0.90	2/4857 (0.0%)
1	E	0.79	1/3560 (0.0%)	0.84	2/4857 (0.0%)
1	F	0.71	2/3560 (0.1%)	0.83	2/4857 (0.0%)
1	G	0.75	2/3560 (0.1%)	0.85	5/4857 (0.1%)
1	H	0.68	0/3560	0.84	0/4857
All	All	0.74	9/28512 (0.0%)	0.86	29/38898 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	5
1	D	0	7
1	E	0	4
1	F	0	3
1	G	0	7
1	H	0	1
All	All	0	39

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	181	GLN	CD-OE1	6.14	1.37	1.24
1	G	300	GLN	CD-OE1	5.73	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	229	GLN	CD-OE1	5.53	1.36	1.24
1	F	72	TRP	CB-CG	-5.44	1.40	1.50
1	D	229	GLN	CD-OE1	5.33	1.35	1.24
1	B	42	PRO	N-CD	5.13	1.55	1.47
1	G	78	PRO	N-CD	5.12	1.55	1.47
1	F	377	GLN	CD-OE1	5.06	1.35	1.24
1	A	229	GLN	CD-OE1	5.03	1.35	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	F	283	PRO	CA-N-CD	-7.30	101.29	111.50
1	A	76	ALA	N-CA-C	-7.27	91.37	111.00
1	B	13	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	42	PRO	CA-N-CD	-6.51	102.39	111.50
1	A	41	THR	N-CA-C	6.33	128.09	111.00
1	B	18	LEU	C-N-CD	6.17	141.36	128.40
1	A	215	PHE	N-CA-C	6.12	127.53	111.00
1	A	351	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	86	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	D	329	GLU	OE1-CD-OE2	-5.87	116.26	123.30
1	B	424	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	86	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	272	ILE	N-CA-C	-5.69	95.64	111.00
1	C	304	ASP	CB-CG-OD2	5.63	123.37	118.30
1	G	77	GLY	C-N-CD	5.63	140.22	128.40
1	E	43	VAL	C-N-CD	5.58	140.11	128.40
1	G	187	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	76	ALA	C-N-CA	5.51	133.86	122.30
1	G	182	LEU	CA-CB-CG	5.48	127.90	115.30
1	F	86	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	C	340	LEU	CA-CB-CG	5.42	127.75	115.30
1	D	344	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	126	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	351	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	180	HIS	N-CA-C	-5.30	96.68	111.00
1	G	75	MET	N-CA-C	-5.21	96.94	111.00
1	B	155	HIS	CB-CA-C	5.19	120.78	110.40
1	A	233	ARG	NE-CZ-NH1	5.15	122.87	120.30

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	LEU	Peptide
1	A	293	SER	Peptide
1	A	344	ASP	Peptide
1	A	37	PRO	Peptide
1	A	38	SER	Peptide
1	A	75	MET	Peptide
1	B	30	ASP	Peptide
1	B	38	SER	Peptide
1	B	386	PRO	Peptide
1	B	407	ILE	Peptide
1	B	409	SER	Peptide
1	B	76	ALA	Peptide
1	C	138	PHE	Peptide
1	C	227	SER	Peptide
1	C	315	SER	Peptide
1	C	38	SER	Peptide
1	C	77	GLY	Peptide
1	D	180	HIS	Peptide
1	D	38	SER	Peptide
1	D	41	THR	Peptide
1	D	42	PRO	Peptide
1	D	458	ALA	Peptide
1	D	69	LEU	Peptide
1	D	76	ALA	Peptide
1	E	30	ASP	Peptide
1	E	39	ASP	Peptide
1	E	41	THR	Peptide
1	E	6	ILE	Peptide
1	F	284	ASN	Peptide
1	F	38	SER	Peptide
1	F	75	MET	Peptide
1	G	218	VAL	Peptide
1	G	222	VAL	Peptide
1	G	3	THR	Peptide
1	G	30	ASP	Peptide
1	G	39	ASP	Peptide
1	G	75	MET	Peptide
1	G	76	ALA	Peptide
1	H	218	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3488	3427	3427	386	1
1	B	3499	3445	3437	299	0
1	C	3499	3442	3437	271	1
1	D	3488	3429	3429	369	5
1	E	3488	3430	3429	317	0
1	F	3488	3428	3428	382	1
1	G	3488	3429	3429	257	5
1	H	3488	3429	3429	427	1
2	A	1	0	0	0	0
3	A	3	0	0	2	0
3	B	3	0	0	0	0
3	D	2	0	0	2	0
3	E	4	0	0	0	0
3	F	3	0	0	1	0
3	G	1	0	0	1	0
3	H	3	0	0	1	0
All	All	27946	27459	27445	2687	7

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 49.

All (2687) 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:H:6:ILE:HB	1:H:25:VAL:CG1	1.25	1.64
1:B:391:SER:CB	1:B:394:THR:HB	1.15	1.63
1:A:251:LEU:HD12	1:A:270:VAL:CB	1.46	1.45
1:E:224:PHE:CD1	1:E:278:LEU:HD11	1.51	1.43
1:F:322:GLY:HA2	1:F:326:ALA:CB	1.48	1.42
1:H:6:ILE:CB	1:H:25:VAL:CG1	1.99	1.39
1:C:227:SER:OG	1:C:228:TYR:HA	1.25	1.36
1:A:251:LEU:CD1	1:A:270:VAL:HB	1.55	1.36
1:F:72:TRP:O	1:F:76:ALA:CB	1.75	1.32
1:F:97:GLU:OE1	1:F:456:VAL:CG1	1.76	1.32
1:A:287:ILE:O	1:A:291:VAL:HG23	1.29	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:THR:O	1:F:455:LEU:CD2	1.81	1.27
1:B:391:SER:CB	1:B:394:THR:CB	2.11	1.26
1:D:70:ASP:O	1:D:72:TRP:N	1.69	1.26
1:B:389:ALA:O	1:B:392:ALA:CB	1.82	1.26
1:C:6:ILE:HG22	1:C:25:VAL:O	1.10	1.23
1:F:72:TRP:O	1:F:76:ALA:HB2	1.10	1.23
1:B:391:SER:HB3	1:B:394:THR:CB	1.68	1.22
1:C:6:ILE:HG21	1:C:25:VAL:CG2	1.67	1.22
1:D:7:THR:HA	1:D:24:THR:CG2	1.68	1.21
1:A:251:LEU:HD12	1:A:270:VAL:CG1	1.69	1.21
1:H:423:GLN:NE2	3:H:501:HOH:O	1.62	1.18
1:H:206:LYS:HE3	1:H:272:ILE:HG21	1.24	1.18
1:A:251:LEU:CD1	1:A:270:VAL:CB	2.13	1.18
1:F:322:GLY:O	1:F:323:GLU:HB2	1.40	1.18
1:F:453:THR:O	1:F:455:LEU:HD23	1.40	1.18
1:E:429:ILE:O	1:E:432:LEU:HD12	1.44	1.18
1:H:145:GLY:CA	1:H:179:GLY:HA2	1.73	1.17
1:H:204:MET:HA	1:H:248:VAL:CG1	1.72	1.17
1:B:389:ALA:O	1:B:392:ALA:HB1	1.39	1.17
1:B:301:THR:HG21	1:B:379:MET:HE2	1.20	1.15
1:H:253:HIS:CD2	1:H:273:HIS:CE1	2.33	1.15
1:H:253:HIS:CD2	1:H:273:HIS:NE2	2.13	1.15
1:F:217:LEU:CD1	1:F:226:ARG:HH22	1.59	1.15
1:C:323:GLU:CB	1:C:324:PRO:HD2	1.76	1.15
1:C:6:ILE:O	1:C:24:THR:HG23	1.43	1.15
1:G:68:LEU:HB3	1:G:95:ILE:HG23	1.27	1.15
1:B:301:THR:HG21	1:B:379:MET:CE	1.76	1.15
1:F:323:GLU:HB3	1:F:324:PRO:HD3	1.28	1.15
1:F:3:THR:HB	1:F:28:GLU:OE2	1.47	1.14
1:B:299:LEU:HD23	1:B:329:GLU:HB3	1.26	1.14
1:H:204:MET:HA	1:H:248:VAL:HG12	1.23	1.13
1:H:6:ILE:CB	1:H:25:VAL:HG13	1.70	1.13
1:D:219:ASP:HB3	1:D:222:VAL:HG11	1.31	1.13
1:A:75:MET:CE	1:A:212:HIS:HE1	1.63	1.12
1:A:459:HIS:HB2	1:A:460:PRO:HA	1.26	1.12
1:H:206:LYS:CE	1:H:272:ILE:HG21	1.78	1.12
1:A:75:MET:CE	1:A:212:HIS:CE1	2.30	1.12
1:H:6:ILE:CB	1:H:25:VAL:HG12	1.70	1.11
1:H:145:GLY:HA2	1:H:179:GLY:HA2	1.22	1.11
1:H:255:VAL:O	1:H:278:LEU:HD12	1.51	1.11
1:F:275:ASN:O	1:F:325:TYR:HD1	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:VAL:HB	1:H:278:LEU:HD11	1.12	1.10
1:D:32:PHE:HE2	1:D:412:THR:N	1.47	1.10
1:H:146:MET:HE2	1:H:208:ALA:HB2	1.23	1.10
1:F:322:GLY:CA	1:F:326:ALA:HB2	1.81	1.09
1:F:264:VAL:CG1	1:F:293:SER:HB2	1.79	1.09
1:H:6:ILE:HD12	1:H:25:VAL:HG11	1.25	1.09
1:E:153:ASP:HB3	1:E:212:HIS:HB3	1.29	1.09
1:E:235:VAL:O	1:E:239:MET:HG3	1.52	1.09
1:A:251:LEU:CD1	1:A:270:VAL:CG1	2.28	1.08
1:C:304:ASP:HA	1:C:307:ARG:HG2	1.09	1.08
1:D:333:ILE:HD13	1:D:334:SER:N	1.68	1.08
1:D:332:LEU:O	1:D:337:ALA:HB2	1.52	1.08
1:E:224:PHE:CE1	1:E:278:LEU:HD11	1.88	1.07
1:F:323:GLU:HB3	1:F:324:PRO:CD	1.80	1.07
1:C:224:PHE:HE1	1:C:325:TYR:OH	1.32	1.07
1:H:278:LEU:HA	1:H:325:TYR:OH	1.50	1.07
1:H:356:LEU:HB2	1:H:360:GLU:HG3	1.35	1.07
1:C:6:ILE:CG2	1:C:25:VAL:O	2.03	1.07
1:F:325:TYR:O	1:F:329:GLU:OE2	1.73	1.07
1:H:6:ILE:HB	1:H:25:VAL:HG12	1.10	1.06
1:D:84:LEU:HD23	1:D:91:TYR:OH	1.55	1.06
1:G:97:GLU:O	1:G:101:LEU:HD12	1.55	1.06
1:G:124:ARG:NH1	1:G:125:ASP:OD1	1.88	1.06
1:A:13:ASP:O	1:A:410:VAL:HG23	1.52	1.06
1:F:97:GLU:OE1	1:F:456:VAL:HG12	1.55	1.06
1:A:235:VAL:O	1:A:238:VAL:HG12	1.54	1.06
1:E:224:PHE:CD1	1:E:278:LEU:CD1	2.39	1.05
1:F:97:GLU:OE1	1:F:456:VAL:HG11	1.52	1.05
1:A:194:VAL:HG21	1:A:239:MET:CE	1.86	1.05
1:H:77:GLY:O	1:H:155:HIS:CD2	2.09	1.05
1:H:405:ASP:OD1	1:H:406:GLN:NE2	1.89	1.05
1:F:279:GLY:HA2	1:F:324:PRO:HG2	1.33	1.05
1:C:260:LEU:O	1:C:264:VAL:HG23	1.56	1.05
1:D:7:THR:CA	1:D:24:THR:HG23	1.86	1.04
1:D:70:ASP:CG	1:D:72:TRP:O	1.96	1.04
1:F:427:ASP:O	1:F:428:ASP:HB2	1.57	1.04
1:F:97:GLU:CD	1:F:456:VAL:HG12	1.78	1.03
1:D:32:PHE:CE2	1:D:412:THR:N	2.24	1.03
1:C:258:GLU:O	1:C:259:ALA:HB3	1.58	1.03
1:D:70:ASP:OD2	1:D:73:MET:CB	2.07	1.02
1:A:210:SER:OG	1:A:254:SER:HA	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASP:OD2	1:D:73:MET:HB2	1.59	1.02
1:C:323:GLU:CB	1:C:324:PRO:CD	2.36	1.02
1:F:322:GLY:CA	1:F:326:ALA:CB	2.38	1.02
1:C:6:ILE:HG21	1:C:25:VAL:HG23	1.03	1.02
1:E:323:GLU:HB3	1:E:324:PRO:HD2	1.41	1.01
1:E:236:LEU:O	1:E:240:VAL:HG23	1.60	1.01
1:H:381:GLU:O	1:H:382:LYS:NZ	1.91	1.01
1:D:6:ILE:HA	1:D:50:VAL:CG1	1.91	1.01
1:G:262:THR:O	1:G:266:LEU:HD21	1.60	1.01
1:C:227:SER:OG	1:C:228:TYR:CA	2.08	1.00
1:D:70:ASP:O	1:D:72:TRP:O	1.78	1.00
1:H:255:VAL:HB	1:H:278:LEU:CD1	1.89	1.00
1:H:145:GLY:HA2	1:H:179:GLY:CA	1.91	1.00
1:A:240:VAL:HG21	1:A:266:LEU:HG	1.39	1.00
1:B:391:SER:HB2	1:B:394:THR:CB	1.83	1.00
1:B:391:SER:HB2	1:B:394:THR:HB	1.01	1.00
1:F:73:MET:HA	1:F:76:ALA:HB1	1.39	1.00
1:D:6:ILE:O	1:D:24:THR:HG22	1.61	1.00
1:H:76:ALA:HB3	1:H:77:GLY:HA2	1.44	1.00
1:D:381:GLU:N	1:D:381:GLU:OE2	1.95	0.99
1:B:391:SER:HB3	1:B:394:THR:HB	1.00	0.99
1:H:6:ILE:CG2	1:H:25:VAL:HG12	1.91	0.99
1:H:225:ASP:OD2	1:H:226:ARG:NH2	1.94	0.99
1:A:253:HIS:ND1	1:A:273:HIS:ND1	2.10	0.99
1:E:214:VAL:HG13	1:E:215:PHE:HD1	1.23	0.99
1:B:22:ALA:O	1:B:37:PRO:HB3	1.61	0.99
1:A:251:LEU:HD11	1:A:270:VAL:HG11	1.43	0.99
1:A:251:LEU:CD1	1:A:270:VAL:HG11	1.92	0.99
1:H:145:GLY:N	1:H:179:GLY:HA2	1.77	0.99
1:F:253:HIS:CE1	1:F:273:HIS:CD2	2.51	0.99
1:G:6:ILE:HG12	1:G:9:VAL:HG22	1.41	0.99
1:A:13:ASP:HA	1:A:410:VAL:HG21	1.45	0.98
1:E:226:ARG:HD2	1:E:228:TYR:HE2	1.24	0.98
1:H:253:HIS:HD2	1:H:273:HIS:CE1	1.72	0.98
1:E:252:THR:HG22	1:E:271:LEU:HA	1.44	0.98
1:A:67:HIS:HE1	1:A:344:ASP:OD1	1.46	0.98
1:F:257:VAL:HG23	1:F:277:THR:CG2	1.94	0.98
1:F:113:THR:HG23	1:F:206:LYS:HD3	1.42	0.98
1:H:6:ILE:HB	1:H:25:VAL:HG13	1.00	0.98
1:C:323:GLU:HB3	1:C:324:PRO:HD2	1.41	0.97
1:A:275:ASN:OD1	1:A:276:TYR:N	1.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:GLY:H	1:H:179:GLY:CA	1.77	0.97
1:D:70:ASP:O	1:D:71:ALA:C	2.02	0.97
1:C:323:GLU:HB2	1:C:324:PRO:HD2	1.47	0.97
1:A:271:LEU:CD1	1:A:296:TRP:O	2.12	0.96
1:F:264:VAL:HG13	1:F:293:SER:HB2	1.45	0.96
1:H:253:HIS:CD2	1:H:273:HIS:HE2	1.74	0.96
1:B:390:ILE:C	1:B:392:ALA:HB3	1.84	0.96
1:G:68:LEU:CB	1:G:95:ILE:HG23	1.95	0.96
1:F:264:VAL:CG1	1:F:293:SER:CB	2.42	0.96
1:C:272:ILE:HG22	1:C:273:HIS:CD2	2.01	0.96
1:A:271:LEU:HD12	1:A:296:TRP:O	1.62	0.96
1:D:190:VAL:O	1:D:194:VAL:HG23	1.66	0.96
1:C:6:ILE:CG2	1:C:25:VAL:HG23	1.94	0.96
1:H:31:ARG:NH1	1:H:415:LEU:HD11	1.79	0.96
1:H:322:GLY:HA2	1:H:326:ALA:HB2	1.48	0.96
1:B:409:SER:HB2	1:B:410:VAL:HA	1.47	0.96
1:B:307:ARG:HH21	1:B:322:GLY:HA2	1.29	0.96
1:A:4:ILE:O	1:A:27:VAL:HG23	1.66	0.96
1:D:32:PHE:CZ	1:D:414:LYS:HB2	2.00	0.95
1:A:240:VAL:HG21	1:A:266:LEU:CG	1.94	0.95
1:F:217:LEU:HD12	1:F:226:ARG:HH22	1.28	0.95
1:H:206:LYS:HE3	1:H:272:ILE:CG2	1.96	0.95
1:D:25:VAL:HG12	1:D:35:VAL:HG12	1.48	0.95
1:A:350:LYS:O	1:A:354:ALA:N	1.99	0.95
1:D:301:THR:OG1	1:D:379:MET:CE	2.14	0.95
1:D:350:LYS:HE3	1:D:460:PRO:HB3	1.45	0.95
1:G:68:LEU:HB3	1:G:95:ILE:CG2	1.97	0.95
1:B:389:ALA:C	1:B:392:ALA:CB	2.35	0.94
1:A:40:SER:O	1:A:41:THR:HG22	1.65	0.94
1:F:322:GLY:HA2	1:F:326:ALA:HB2	0.96	0.94
1:F:453:THR:O	1:F:455:LEU:HD21	1.66	0.94
1:C:6:ILE:CG2	1:C:25:VAL:H	1.78	0.94
1:H:253:HIS:NE2	1:H:273:HIS:NE2	2.13	0.94
1:H:107:VAL:HG23	1:H:372:HIS:CE1	2.02	0.94
1:D:421:LEU:HB3	1:D:434:SER:O	1.66	0.94
1:C:304:ASP:HA	1:C:307:ARG:CG	1.98	0.94
1:F:322:GLY:HA2	1:F:326:ALA:HB3	1.47	0.94
1:E:233:ARG:NH2	1:E:265:GLU:OE1	2.00	0.94
1:E:253:HIS:ND1	1:E:273:HIS:CD2	2.35	0.94
1:F:217:LEU:CD1	1:F:226:ARG:NH2	2.30	0.94
1:C:144:VAL:HA	1:C:178:VAL:HG11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ASP:OD1	1:G:289:LYS:NZ	2.01	0.93
1:F:61:TYR:HB2	1:F:107:VAL:HG12	1.48	0.93
1:F:113:THR:CG2	1:F:206:LYS:HD3	1.99	0.93
1:H:146:MET:CE	1:H:208:ALA:HB2	1.98	0.93
1:H:145:GLY:CA	1:H:179:GLY:CA	2.47	0.93
1:E:423:GLN:OE1	1:E:431:ASN:OD1	1.86	0.93
1:A:206:LYS:NZ	3:A:603:HOH:O	1.98	0.93
1:B:388:GLU:O	1:B:390:ILE:N	2.02	0.92
1:E:321:ALA:O	1:E:326:ALA:HB2	1.69	0.92
1:G:262:THR:O	1:G:266:LEU:CD2	2.16	0.92
1:C:6:ILE:HG23	1:C:25:VAL:H	1.34	0.92
1:F:217:LEU:HD13	1:F:226:ARG:HH22	1.35	0.92
1:H:343:THR:HG23	1:H:375:TRP:HD1	1.35	0.92
1:H:225:ASP:HB2	1:H:226:ARG:HE	1.34	0.92
1:B:391:SER:N	1:B:392:ALA:HB3	1.83	0.92
1:A:67:HIS:HA	1:A:112:ASP:OD1	1.69	0.92
1:H:439:PHE:CZ	1:H:444:ALA:HB2	2.04	0.92
1:A:251:LEU:HD12	1:A:270:VAL:HB	0.93	0.92
1:G:272:ILE:HG23	1:G:342:ASN:OD1	1.68	0.92
1:C:259:ALA:O	1:C:263:SER:OG	1.85	0.92
1:A:206:LYS:HE3	1:A:272:ILE:HD11	1.49	0.92
1:H:142:THR:HG22	1:H:143:ILE:O	1.70	0.91
1:H:6:ILE:CD1	1:H:25:VAL:HG11	1.99	0.91
1:C:227:SER:HG	1:C:228:TYR:HA	1.23	0.91
1:H:203:ASP:O	1:H:248:VAL:HG13	1.68	0.91
1:F:217:LEU:HD13	1:F:226:ARG:NH2	1.84	0.91
1:B:299:LEU:CD2	1:B:329:GLU:HB3	1.99	0.91
1:A:235:VAL:O	1:A:238:VAL:CG1	2.18	0.91
1:A:75:MET:HE1	1:A:212:HIS:HE1	1.34	0.90
1:B:225:ASP:OD1	1:B:226:ARG:N	2.03	0.90
1:D:328:ASN:O	1:D:331:ASN:N	2.02	0.90
1:B:388:GLU:OE1	1:B:388:GLU:N	2.04	0.90
1:F:97:GLU:CD	1:F:456:VAL:CG1	2.38	0.90
1:D:219:ASP:HB3	1:D:222:VAL:CG1	2.01	0.90
1:F:253:HIS:ND1	1:F:273:HIS:HD2	1.69	0.90
1:E:253:HIS:ND1	1:E:273:HIS:HD2	1.67	0.90
1:D:32:PHE:HE2	1:D:412:THR:H	0.90	0.90
1:A:236:LEU:HB3	1:A:266:LEU:HD22	1.54	0.90
1:D:279:GLY:H	1:D:325:TYR:HE1	1.19	0.90
1:F:275:ASN:O	1:F:325:TYR:CD1	2.23	0.89
1:D:411:GLU:O	1:D:412:THR:HB	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:LEU:HD13	1:H:95:ILE:CG2	2.02	0.89
1:A:209:VAL:HG21	1:A:252:THR:OG1	1.72	0.89
1:A:194:VAL:HG21	1:A:239:MET:HE3	1.52	0.89
1:E:181:GLN:O	1:E:184:LEU:N	2.05	0.89
1:H:34:THR:HG22	1:H:41:THR:HG21	1.53	0.89
1:D:7:THR:HA	1:D:24:THR:HG23	0.90	0.89
1:G:65:ASN:OD1	1:G:113:THR:OG1	1.89	0.89
1:A:350:LYS:HA	1:A:353:LEU:HB2	1.54	0.89
1:A:459:HIS:CB	1:A:460:PRO:HA	2.01	0.89
1:H:225:ASP:HB2	1:H:226:ARG:NE	1.87	0.89
1:A:191:ARG:HD2	1:A:238:VAL:CG2	2.02	0.89
1:H:6:ILE:CG1	1:H:25:VAL:HG13	2.02	0.89
1:A:75:MET:HE2	1:A:212:HIS:CE1	2.08	0.89
1:A:13:ASP:HA	1:A:410:VAL:CG2	2.02	0.89
1:E:220:ARG:O	1:E:221:SER:OG	1.89	0.89
1:H:6:ILE:CG1	1:H:25:VAL:CG1	2.50	0.89
1:F:257:VAL:HG23	1:F:277:THR:HG23	1.53	0.89
1:D:6:ILE:C	1:D:24:THR:HG22	1.93	0.88
1:A:71:ALA:O	1:A:74:PHE:HB2	1.74	0.88
1:A:348:PRO:HG3	1:A:364:ARG:HH12	1.37	0.88
1:H:360:GLU:OE1	1:H:361:ARG:NE	2.07	0.88
1:G:360:GLU:O	1:G:364:ARG:HG3	1.72	0.88
1:B:72:TRP:O	1:B:76:ALA:HB2	1.73	0.88
1:D:219:ASP:CB	1:D:222:VAL:HG11	2.02	0.88
1:F:158:GLY:HA2	1:F:161:ALA:HB3	1.56	0.88
1:D:387:LEU:O	1:D:391:SER:N	2.05	0.88
1:F:253:HIS:ND1	1:F:273:HIS:CD2	2.42	0.88
1:H:323:GLU:HB3	1:H:324:PRO:HD3	1.54	0.88
1:D:148:GLY:O	1:D:154:PHE:HD2	1.56	0.88
1:C:113:THR:HB	1:C:206:LYS:HD2	1.56	0.88
1:G:92:VAL:O	1:G:96:GLU:HG3	1.72	0.88
1:C:78:PRO:O	1:C:352:HIS:NE2	2.06	0.88
1:D:258:GLU:O	1:D:260:LEU:N	2.07	0.88
1:D:68:LEU:CD1	1:D:95:ILE:HG23	2.04	0.87
1:B:69:LEU:HD13	1:B:95:ILE:CG1	2.04	0.87
1:B:296:TRP:HZ3	1:B:396:ASN:HB3	1.39	0.87
1:H:206:LYS:NZ	1:H:272:ILE:HG21	1.88	0.87
1:H:72:TRP:CZ3	1:H:75:MET:HE1	2.09	0.87
1:G:126:ARG:HA	1:G:131:ILE:HD12	1.57	0.87
1:F:277:THR:N	1:F:325:TYR:HE1	1.71	0.87
1:D:303:HIS:HB2	1:D:306:HIS:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASP:OD1	1:A:71:ALA:N	2.08	0.87
1:A:287:ILE:C	1:A:291:VAL:HG23	1.94	0.87
1:C:254:SER:OG	1:C:260:LEU:CD1	2.22	0.87
1:H:145:GLY:N	1:H:179:GLY:CA	2.35	0.87
1:H:353:LEU:O	1:H:360:GLU:OE2	1.91	0.87
1:H:70:ASP:O	1:H:74:PHE:CE1	2.28	0.87
1:H:313:VAL:HG11	1:H:357:SER:CB	2.03	0.86
1:A:240:VAL:HG21	1:A:266:LEU:CD1	2.03	0.86
1:F:114:HIS:O	1:F:115:ASN:ND2	2.08	0.86
1:E:378:SER:O	1:E:382:LYS:HG2	1.75	0.86
1:H:66:VAL:O	1:H:67:HIS:HD2	1.58	0.86
1:F:251:LEU:CD2	1:F:270:VAL:HB	2.04	0.86
1:D:30:ASP:OD1	1:D:31:ARG:N	2.08	0.86
1:A:250:VAL:H	1:A:269:ASP:HB2	1.40	0.86
1:C:6:ILE:HG22	1:C:25:VAL:C	1.95	0.86
1:B:66:VAL:HG21	1:B:110:VAL:HG21	1.55	0.86
1:A:30:ASP:OD1	1:A:31:ARG:N	2.08	0.86
1:G:97:GLU:OE2	1:G:457:THR:OG1	1.93	0.86
1:F:159:ARG:HD2	1:F:167:VAL:HG11	1.58	0.86
1:D:233:ARG:NH1	1:D:237:GLU:OE1	2.09	0.86
1:F:68:LEU:HD13	1:F:95:ILE:HG23	1.57	0.86
1:H:202:VAL:O	1:H:204:MET:N	2.07	0.86
1:A:253:HIS:ND1	1:A:273:HIS:CE1	2.43	0.85
1:D:279:GLY:N	1:D:325:TYR:HE1	1.74	0.85
1:G:275:ASN:O	1:G:328:ASN:ND2	2.08	0.85
1:G:260:LEU:O	1:G:264:VAL:HG23	1.76	0.85
1:A:13:ASP:C	1:A:410:VAL:HG23	1.95	0.85
1:E:282:ILE:HG13	1:E:328:ASN:HD21	1.41	0.85
1:B:252:THR:HG21	1:B:263:SER:HB3	1.59	0.85
1:F:73:MET:CA	1:F:76:ALA:HB1	2.06	0.85
1:F:66:VAL:HG21	1:F:110:VAL:HG11	1.58	0.85
1:D:388:GLU:HA	1:D:391:SER:OG	1.77	0.85
1:F:75:MET:N	1:F:76:ALA:HB3	1.92	0.84
1:E:153:ASP:HA	1:E:212:HIS:O	1.77	0.84
1:C:323:GLU:HB3	1:C:324:PRO:CD	2.02	0.84
1:A:235:VAL:C	1:A:238:VAL:HG12	1.97	0.84
1:A:175:GLU:OE1	1:A:181:GLN:OE1	1.95	0.84
1:A:215:PHE:H	1:A:216:THR:HB	1.43	0.84
1:B:112:ASP:O	1:B:140:ALA:CB	2.25	0.84
1:B:153:ASP:O	1:B:212:HIS:ND1	2.09	0.84
1:D:301:THR:OG1	1:D:379:MET:HE3	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:VAL:HB	1:F:278:LEU:CD2	2.08	0.83
1:D:32:PHE:HZ	1:D:414:LYS:HB2	1.42	0.83
1:H:72:TRP:CE3	1:H:75:MET:CE	2.61	0.83
1:H:68:LEU:HD13	1:H:95:ILE:HG23	1.60	0.83
1:C:30:ASP:OD1	1:C:31:ARG:N	2.10	0.83
1:B:395:ILE:O	1:B:399[B]:ARG:N	2.12	0.83
1:F:322:GLY:O	1:F:323:GLU:CB	2.23	0.83
1:A:237:GLU:HA	1:A:266:LEU:HD11	1.58	0.83
1:A:446:ASP:O	1:A:450:LEU:HD13	1.78	0.83
1:F:61:TYR:OH	1:F:432:LEU:HD22	1.78	0.83
1:H:66:VAL:C	1:H:67:HIS:HD2	1.82	0.83
1:A:86:ARG:NH2	1:F:88:GLU:O	2.12	0.83
1:H:313:VAL:HG11	1:H:357:SER:HB3	1.61	0.83
1:D:31:ARG:NH2	1:D:406:GLN:OE1	2.11	0.83
1:D:38:SER:OG	3:D:501:HOH:O	1.64	0.83
1:C:254:SER:OG	1:C:260:LEU:HD12	1.79	0.83
1:E:226:ARG:HD2	1:E:228:TYR:CE2	2.12	0.83
1:H:282:ILE:HG13	1:H:328:ASN:OD1	1.78	0.83
1:B:301:THR:CG2	1:B:379:MET:CE	2.57	0.82
1:F:251:LEU:HD22	1:F:270:VAL:HB	1.58	0.82
1:H:323:GLU:HB3	1:H:324:PRO:CD	2.09	0.82
1:H:207:ILE:HD11	1:H:239:MET:SD	2.19	0.82
1:F:66:VAL:HG21	1:F:110:VAL:CG1	2.09	0.82
1:H:275:ASN:OD1	1:H:329:GLU:HG3	1.79	0.82
1:B:385:SER:HB3	1:B:387:LEU:O	1.79	0.82
1:F:281:GLU:OE1	1:F:281:GLU:N	2.12	0.82
1:E:261:ASP:O	1:E:265:GLU:HG3	1.80	0.82
1:A:271:LEU:CD1	1:A:297:ALA:HA	2.09	0.82
1:F:253:HIS:HE1	1:F:273:HIS:NE2	1.77	0.82
1:H:313:VAL:HG21	1:H:357:SER:OG	1.80	0.82
1:H:220:ARG:O	1:H:221:SER:OG	1.95	0.82
1:E:372:HIS:O	1:E:376:THR:HG23	1.79	0.82
1:G:97:GLU:O	1:G:101:LEU:CD1	2.28	0.82
1:F:428:ASP:OD2	1:F:430:ARG:CD	2.27	0.82
1:A:210:SER:HG	1:A:254:SER:HA	1.43	0.82
1:G:4:ILE:HD12	1:G:5:ALA:N	1.95	0.82
1:D:6:ILE:O	1:D:24:THR:CG2	2.27	0.82
1:A:12:ILE:HD12	1:A:56:TRP:HD1	1.42	0.82
1:B:113:THR:HA	1:B:140:ALA:CB	2.10	0.81
1:H:23:THR:HG22	1:H:37:PRO:HG3	1.62	0.81
1:F:253:HIS:CE1	1:F:273:HIS:NE2	2.48	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:ILE:HG21	1:H:146:MET:HE2	1.62	0.81
1:H:72:TRP:CZ3	1:H:75:MET:CE	2.63	0.81
1:A:251:LEU:HD13	1:A:270:VAL:HB	1.63	0.81
1:F:454:PRO:C	1:F:455:LEU:HD23	2.01	0.81
1:B:14:GLY:O	1:B:391:SER:OG	1.98	0.81
1:F:96:GLU:OE2	1:F:126:ARG:NH1	2.14	0.81
1:D:215:PHE:O	1:D:218:VAL:HG13	1.80	0.81
1:B:253:HIS:CD2	1:B:273:HIS:NE2	2.49	0.81
1:B:244:ARG:NH2	1:B:269:ASP:OD1	2.14	0.81
1:A:12:ILE:HD12	1:A:56:TRP:CD1	2.16	0.81
1:E:153:ASP:CB	1:E:212:HIS:HB3	2.10	0.81
1:C:307:ARG:NH2	1:C:311:GLU:OE2	2.14	0.81
1:E:214:VAL:HG13	1:E:215:PHE:CD1	2.14	0.81
1:B:73:MET:O	1:B:77:GLY:HA2	1.80	0.81
1:A:67:HIS:CE1	1:A:344:ASP:OD1	2.32	0.80
1:B:296:TRP:CZ3	1:B:396:ASN:HB3	2.17	0.80
1:A:445:VAL:O	1:A:447:ARG:NH1	2.12	0.80
1:D:217:LEU:HD13	1:D:226:ARG:NH1	1.95	0.80
1:H:204:MET:CA	1:H:248:VAL:CG1	2.56	0.80
1:H:357:SER:O	1:H:360:GLU:N	2.14	0.80
1:A:233:ARG:NH1	1:A:265:GLU:OE1	2.14	0.80
1:D:191:ARG:NH1	1:D:242:GLU:OE2	2.14	0.80
1:F:72:TRP:O	1:F:76:ALA:HB1	1.81	0.80
1:D:70:ASP:OD2	1:D:73:MET:HB3	1.80	0.80
1:B:307:ARG:NH2	1:B:322:GLY:CA	2.45	0.80
1:B:307:ARG:NH2	1:B:322:GLY:HA2	1.97	0.80
1:D:301:THR:HG21	1:D:378:SER:CB	2.12	0.80
1:D:220:ARG:HG3	1:D:220:ARG:HH11	1.47	0.79
1:G:275:ASN:ND2	1:G:276:TYR:HD1	1.81	0.79
1:E:364:ARG:NH1	1:E:367:THR:OG1	2.16	0.79
1:E:53:ASN:O	1:E:55:ARG:NH1	2.14	0.79
1:A:191:ARG:CZ	1:A:238:VAL:HG22	2.12	0.79
1:E:124:ARG:NH1	1:E:203:ASP:OD1	2.15	0.79
1:D:272:ILE:O	1:D:273:HIS:HB2	1.83	0.79
1:H:252:THR:O	1:H:272:ILE:HB	1.82	0.79
1:H:278:LEU:CA	1:H:325:TYR:OH	2.31	0.78
1:B:395:ILE:O	1:B:399[A]:ARG:N	2.12	0.78
1:E:257:VAL:HG22	1:E:277:THR:HG22	1.65	0.78
1:E:385:SER:O	1:E:388:GLU:N	2.16	0.78
1:H:342:ASN:O	1:H:375:TRP:NE1	2.16	0.78
1:E:179:GLY:C	1:E:180:HIS:ND1	2.37	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:HIS:NE2	1:B:377:GLN:HG2	1.97	0.78
1:E:224:PHE:CE1	1:E:278:LEU:CD1	2.65	0.78
1:B:69:LEU:HD13	1:B:95:ILE:HG12	1.66	0.78
1:G:296:TRP:HZ3	1:G:396:ASN:HD22	1.32	0.78
1:C:258:GLU:O	1:C:259:ALA:CB	2.27	0.78
1:D:7:THR:CA	1:D:24:THR:CG2	2.54	0.78
1:H:204:MET:HB2	1:H:249:PRO:HG2	1.65	0.78
1:D:222:VAL:HG22	1:D:223:GLY:N	1.97	0.78
1:H:66:VAL:C	1:H:67:HIS:CD2	2.57	0.78
1:D:337:ALA:O	1:D:338:LYS:HD3	1.83	0.78
1:D:68:LEU:HD13	1:D:95:ILE:HG23	1.64	0.78
1:C:217:LEU:HD23	1:C:224:PHE:HB3	1.66	0.77
1:H:143:ILE:HG21	1:H:146:MET:CE	2.13	0.77
1:A:206:LYS:HE3	1:A:272:ILE:CD1	2.14	0.77
1:A:91:TYR:O	1:A:95:ILE:HG13	1.85	0.77
1:D:75:MET:HG2	1:D:215:PHE:CE1	2.18	0.77
1:H:225:ASP:C	1:H:226:ARG:HG2	2.05	0.77
1:A:215:PHE:N	1:A:216:THR:HB	2.00	0.77
1:A:409:SER:OG	1:A:414:LYS:NZ	2.17	0.77
1:D:387:LEU:O	1:D:390:ILE:HB	1.85	0.77
1:E:323:GLU:HB3	1:E:324:PRO:CD	2.14	0.77
1:B:394:THR:HG22	1:B:395:ILE:N	1.98	0.77
1:B:307:ARG:HH21	1:B:322:GLY:CA	1.97	0.77
1:G:204:MET:HA	1:G:248:VAL:HB	1.65	0.77
1:F:428:ASP:OD2	1:F:430:ARG:HD2	1.85	0.77
1:G:91:TYR:O	1:G:95:ILE:HG13	1.85	0.76
1:E:257:VAL:HG22	1:E:277:THR:CG2	2.15	0.76
1:D:350:LYS:HD3	1:D:458:ALA:O	1.85	0.76
1:B:210:SER:HB2	1:B:255:VAL:CG2	2.15	0.76
1:H:406:GLN:HB2	1:H:415:LEU:HD13	1.67	0.76
1:A:66:VAL:HA	1:A:345:ALA:HB3	1.68	0.76
1:C:62:VAL:HG13	1:C:109:THR:HB	1.66	0.76
1:G:102:ALA:HB1	1:G:107:VAL:HB	1.65	0.76
1:H:30:ASP:H	1:H:442:GLY:HA3	1.49	0.76
1:G:266:LEU:H	1:G:266:LEU:HD22	1.51	0.76
1:G:250:VAL:CG1	1:G:268:ALA:HA	2.15	0.76
1:B:385:SER:C	1:B:387:LEU:O	2.24	0.76
1:D:279:GLY:N	1:D:325:TYR:CE1	2.53	0.76
1:F:255:VAL:O	1:F:278:LEU:HD23	1.86	0.76
1:H:260:LEU:HD12	1:H:271:LEU:HD23	1.68	0.76
1:D:303:HIS:HB2	1:D:306:HIS:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:CB	1:A:259:ALA:HB1	2.14	0.76
1:A:240:VAL:CG2	1:A:266:LEU:HG	2.16	0.76
1:E:225:ASP:O	1:E:226:ARG:HB3	1.86	0.76
1:G:64:GLY:HA2	1:G:111:PHE:HD2	1.51	0.76
1:F:273:HIS:ND1	1:F:276:TYR:CD2	2.53	0.75
1:H:41:THR:H	1:H:42:PRO:HA	1.50	0.75
1:B:391:SER:HB2	1:B:395:ILE:H	1.51	0.75
1:D:301:THR:CG2	1:D:378:SER:CB	2.64	0.75
1:D:301:THR:HG21	1:D:378:SER:HB2	1.66	0.75
1:D:386:PRO:O	1:D:390:ILE:HG13	1.86	0.75
1:E:264:VAL:CG1	1:E:293:SER:CB	2.64	0.75
1:F:429:ILE:HD11	1:F:432:LEU:HD11	1.66	0.75
1:G:357:SER:OG	1:G:360:GLU:HG3	1.85	0.75
1:G:323:GLU:HB2	1:G:324:PRO:CD	2.16	0.75
1:G:275:ASN:ND2	1:G:276:TYR:CD1	2.55	0.75
1:E:224:PHE:CG	1:E:278:LEU:CD1	2.70	0.75
1:F:74:PHE:O	1:F:154:PHE:HB3	1.85	0.75
1:F:65:ASN:OD1	1:F:113:THR:HB	1.86	0.75
1:A:125:ASP:HB2	1:A:126:ARG:HH12	1.52	0.75
1:D:32:PHE:CD2	1:D:412:THR:HA	2.22	0.75
1:A:158:GLY:HA2	1:A:161:ALA:HB3	1.69	0.75
1:E:224:PHE:CG	1:E:278:LEU:HD11	2.19	0.75
1:D:251:LEU:HD22	1:D:270:VAL:HB	1.67	0.75
1:A:75:MET:SD	1:A:215:PHE:CD2	2.79	0.75
1:B:395:ILE:HG13	1:B:396:ASN:OD1	1.87	0.74
1:D:113:THR:HB	1:D:206:LYS:HD2	1.69	0.74
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.51	0.74
1:B:399[B]:ARG:HG3	1:B:399[B]:ARG:HH11	1.53	0.74
1:H:251:LEU:HD22	1:H:270:VAL:HB	1.67	0.74
1:F:225:ASP:O	1:F:226:ARG:HB2	1.84	0.74
1:E:43:VAL:HG22	1:E:45:GLU:H	1.52	0.74
1:F:136:ARG:NH2	1:F:417:ASP:OD2	2.20	0.74
1:G:24:THR:HB	1:G:41:THR:HG21	1.69	0.74
1:H:343:THR:HG23	1:H:375:TRP:CD1	2.20	0.74
1:E:279:GLY:N	1:E:325:TYR:CE1	2.55	0.74
1:H:210:SER:OG	1:H:255:VAL:HG22	1.86	0.74
1:H:214:VAL:O	1:H:217:LEU:HB3	1.88	0.74
1:E:217:LEU:HD11	1:E:223:GLY:O	1.87	0.74
1:D:30:ASP:HB2	1:D:441:ALA:O	1.86	0.74
1:E:24:THR:HG21	1:E:40:SER:HB2	1.69	0.74
1:H:6:ILE:CD1	1:H:25:VAL:CG1	2.65	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:VAL:HG12	1:D:35:VAL:CG1	2.18	0.74
1:D:385:SER:HB3	1:D:388:GLU:HG2	1.68	0.74
1:G:250:VAL:HG13	1:G:268:ALA:HA	1.68	0.74
1:G:3:THR:HG23	1:G:47:ALA:HA	1.67	0.74
1:H:260:LEU:HD12	1:H:271:LEU:CD2	2.16	0.74
1:D:217:LEU:HD13	1:D:226:ARG:HH12	1.52	0.74
1:B:40:SER:O	1:B:41:THR:OG1	2.05	0.74
1:D:25:VAL:CG1	1:D:35:VAL:HG12	2.17	0.74
1:D:278:LEU:HA	1:D:325:TYR:CE1	2.23	0.74
1:G:129:ALA:HB3	1:G:131:ILE:HG13	1.69	0.74
1:D:187:ARG:NH1	1:D:187:ARG:HB3	2.02	0.74
1:B:391:SER:CA	1:B:394:THR:HB	2.16	0.74
1:C:6:ILE:CG2	1:C:25:VAL:N	2.51	0.74
1:E:157:ALA:O	1:E:159:ARG:N	2.20	0.74
1:D:84:LEU:HD23	1:D:91:TYR:CZ	2.23	0.73
1:H:107:VAL:CG2	1:H:372:HIS:CE1	2.70	0.73
1:D:328:ASN:O	1:D:331:ASN:HB2	1.87	0.73
1:D:436:THR:O	1:D:447:ARG:NH2	2.21	0.73
1:H:6:ILE:HD12	1:H:25:VAL:CG1	2.10	0.73
1:B:395:ILE:HD12	1:B:399[B]:ARG:NH1	2.02	0.73
1:E:207:ILE:HD12	1:E:239:MET:SD	2.28	0.73
1:D:84:LEU:HD22	1:D:170:ILE:CG2	2.17	0.73
1:D:7:THR:HG22	1:D:24:THR:HG21	1.69	0.73
1:C:12:ILE:HG12	1:C:19:PRO:HB3	1.70	0.73
1:D:350:LYS:HE3	1:D:460:PRO:CB	2.17	0.73
1:A:438:VAL:HG23	1:A:447:ARG:HD3	1.69	0.73
1:B:92:VAL:O	1:B:96:GLU:HG3	1.89	0.73
1:H:191:ARG:NH1	1:H:241:GLU:OE2	2.22	0.73
1:C:387:LEU:HD21	1:C:426:VAL:HG22	1.69	0.73
1:C:6:ILE:O	1:C:24:THR:CG2	2.32	0.73
1:H:136:ARG:HH12	1:H:417:ASP:HB3	1.52	0.73
1:F:66:VAL:CG2	1:F:110:VAL:CG1	2.67	0.73
1:A:271:LEU:HD11	1:A:296:TRP:O	1.89	0.73
1:G:6:ILE:HD11	1:G:9:VAL:CG1	2.18	0.73
1:F:278:LEU:H	1:F:325:TYR:HE1	1.36	0.73
1:D:70:ASP:OD1	1:D:72:TRP:O	2.04	0.73
1:F:264:VAL:HG11	1:F:293:SER:HB3	1.71	0.73
1:E:277:THR:CB	1:E:280:GLN:O	2.37	0.73
1:F:97:GLU:OE2	1:F:456:VAL:HG12	1.89	0.72
1:A:11:LEU:HD21	1:A:13:ASP:HB3	1.70	0.72
1:E:423:GLN:CD	1:E:431:ASN:OD1	2.27	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:THR:OG1	1:G:263:SER:OG	2.05	0.72
1:E:148:GLY:N	1:E:175:GLU:OE2	2.21	0.72
1:A:282:ILE:HG23	1:A:328:ASN:HD21	1.52	0.72
1:C:254:SER:OG	1:C:260:LEU:HD13	1.89	0.72
1:F:126:ARG:NH1	1:F:132:SER:OG	2.22	0.72
1:B:112:ASP:O	1:B:140:ALA:HB3	1.87	0.72
1:H:175:GLU:O	1:H:178:VAL:HG22	1.88	0.72
1:A:203:ASP:OD1	3:A:602:HOH:O	2.08	0.72
1:D:142:THR:OG1	1:D:174:PHE:O	2.06	0.72
1:A:191:ARG:CD	1:A:238:VAL:CG2	2.68	0.72
1:F:207:ILE:HG22	1:F:251:LEU:O	1.89	0.72
1:A:38:SER:OG	1:A:41:THR:N	2.23	0.72
1:A:254:SER:HB2	1:A:259:ALA:CB	2.19	0.72
1:A:254:SER:HB2	1:A:259:ALA:HB1	1.69	0.72
1:C:272:ILE:HG22	1:C:273:HIS:HD2	1.53	0.72
1:E:284:ASN:O	1:E:285:TYR:CD2	2.42	0.72
1:C:6:ILE:CG2	1:C:25:VAL:CG2	2.60	0.72
1:E:179:GLY:O	1:E:180:HIS:ND1	2.23	0.72
1:C:28:GLU:O	1:C:30:ASP:O	2.08	0.72
1:B:253:HIS:NE2	1:B:273:HIS:NE2	2.37	0.72
1:C:319:ALA:HB1	1:C:323:GLU:OE1	1.88	0.72
1:H:72:TRP:CE3	1:H:75:MET:HE2	2.23	0.72
1:B:69:LEU:HD13	1:B:95:ILE:HG13	1.70	0.72
1:D:333:ILE:HD13	1:D:334:SER:H	1.55	0.71
1:C:224:PHE:CE1	1:C:325:TYR:OH	2.18	0.71
1:F:182:LEU:HA	1:F:185:LEU:HD12	1.72	0.71
1:E:66:VAL:O	1:E:67:HIS:HD2	1.73	0.71
1:B:389:ALA:C	1:B:392:ALA:HB2	2.11	0.71
1:A:12:ILE:CD1	1:A:56:TRP:CD1	2.72	0.71
1:B:195:ARG:HG2	1:B:242:GLU:HG3	1.70	0.71
1:D:158:GLY:HA2	1:D:161:ALA:HB3	1.72	0.71
1:D:32:PHE:HE1	1:D:415:LEU:O	1.73	0.71
1:C:59:PRO:HB3	1:C:409:SER:HA	1.73	0.71
1:E:204:MET:HA	1:E:248:VAL:HB	1.73	0.71
1:B:391:SER:HA	1:B:394:THR:N	2.05	0.71
1:D:114:HIS:ND1	1:D:143:ILE:HG13	2.05	0.71
1:A:194:VAL:HG21	1:A:239:MET:HE1	1.70	0.71
1:F:113:THR:HG21	1:F:206:LYS:NZ	2.06	0.71
1:F:67:HIS:N	1:F:345:ALA:O	2.22	0.71
1:A:113:THR:HB	1:A:206:LYS:HG3	1.71	0.71
1:F:266:LEU:HD12	1:F:266:LEU:H	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:ARG:O	1:G:221:SER:OG	2.06	0.71
1:E:275:ASN:HB3	1:E:299:LEU:HD12	1.71	0.71
1:H:272:ILE:HG22	1:H:273:HIS:ND1	2.05	0.71
1:G:95:ILE:O	1:G:98:ALA:HB3	1.90	0.71
1:D:231:PHE:HB2	1:D:236:LEU:HD13	1.72	0.71
1:H:357:SER:O	1:H:360:GLU:CB	2.39	0.71
1:B:41:THR:H	1:B:42:PRO:HA	1.56	0.71
1:A:13:ASP:CA	1:A:410:VAL:HG23	2.20	0.71
1:H:31:ARG:NH1	1:H:415:LEU:CD1	2.54	0.71
1:F:281:GLU:C	1:F:283:PRO:HB3	2.10	0.71
1:G:4:ILE:HD12	1:G:5:ALA:H	1.54	0.71
1:A:409:SER:C	1:A:414:LYS:HZ1	1.94	0.70
1:D:195:ARG:HH11	1:D:195:ARG:HG3	1.56	0.70
1:B:178:VAL:HG12	1:B:179:GLY:H	1.56	0.70
1:G:6:ILE:O	1:G:24:THR:HG23	1.92	0.70
1:H:431:ASN:O	1:H:434:SER:OG	2.09	0.70
1:F:277:THR:CG2	1:F:280:GLN:O	2.40	0.70
1:F:279:GLY:CA	1:F:324:PRO:HG2	2.19	0.70
1:D:6:ILE:HA	1:D:50:VAL:HG11	1.71	0.70
1:F:313:VAL:HG21	1:F:360:GLU:OE2	1.91	0.70
1:F:277:THR:HG21	1:F:280:GLN:O	1.91	0.70
1:H:293:SER:HB2	1:H:295:SER:OG	1.92	0.70
1:H:277:THR:HG21	1:H:282:ILE:HG12	1.74	0.70
1:C:158:GLY:HA2	1:C:161:ALA:HB3	1.72	0.70
1:F:277:THR:HG22	1:F:280:GLN:HB2	1.74	0.70
1:F:277:THR:N	1:F:325:TYR:CE1	2.58	0.70
1:H:416:ALA:HB3	1:H:442:GLY:H	1.55	0.70
1:C:78:PRO:O	1:C:352:HIS:CD2	2.45	0.70
1:G:323:GLU:HB2	1:G:324:PRO:HD3	1.73	0.70
1:C:395:ILE:O	1:C:399[B]:ARG:HG2	1.92	0.70
1:E:277:THR:OG1	1:E:280:GLN:O	2.08	0.70
1:G:390:ILE:HG22	1:G:429:ILE:HD11	1.73	0.70
1:F:455:LEU:HD23	1:F:455:LEU:N	2.06	0.70
1:E:428:ASP:HB3	1:E:431:ASN:HD22	1.56	0.70
1:A:13:ASP:CA	1:A:410:VAL:CG2	2.69	0.70
1:C:235:VAL:O	1:C:239:MET:HG3	1.92	0.70
1:D:9:VAL:HG22	1:D:23:THR:O	1.91	0.70
1:E:38:SER:OG	1:E:39:ASP:N	2.22	0.70
1:G:343:THR:HG21	1:G:371:ASP:HB2	1.74	0.70
1:B:385:SER:O	1:B:387:LEU:O	2.09	0.69
1:E:282:ILE:HG13	1:E:328:ASN:ND2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:HB3	1:A:266:LEU:CD2	2.22	0.69
1:H:232:SER:OG	1:H:235:VAL:HG23	1.92	0.69
1:D:133:GLN:OE1	1:D:450:LEU:HD21	1.92	0.69
1:B:340:LEU:CD1	1:B:397:VAL:HA	2.22	0.69
1:F:224:PHE:CE2	1:F:278:LEU:CD1	2.75	0.69
1:A:303:HIS:HB2	1:A:374:HIS:CE1	2.26	0.69
1:G:127:ILE:O	1:G:130:GLY:N	2.20	0.69
1:F:264:VAL:HG12	1:F:293:SER:HB2	1.72	0.69
1:H:328:ASN:HA	1:H:331:ASN:HB2	1.74	0.69
1:H:151:SER:OG	1:H:152:ALA:N	2.24	0.69
1:G:6:ILE:HG12	1:G:9:VAL:CG2	2.20	0.69
1:G:272:ILE:CG2	1:G:342:ASN:OD1	2.38	0.69
1:A:240:VAL:HG21	1:A:266:LEU:HD11	1.74	0.69
1:A:74:PHE:CZ	1:A:84:LEU:HD11	2.27	0.69
1:G:142:THR:HG22	1:G:197:TYR:OH	1.92	0.69
1:A:275:ASN:CG	1:A:276:TYR:H	1.95	0.69
1:H:185:LEU:HD13	1:H:193:ARG:NH2	2.08	0.69
1:F:264:VAL:CG1	1:F:293:SER:HB3	2.23	0.69
1:A:29:GLY:O	1:A:30:ASP:HB3	1.91	0.69
1:G:251:LEU:HD23	1:G:272:ILE:HD11	1.72	0.69
1:E:238:VAL:O	1:E:242:GLU:OE1	2.11	0.69
1:G:307:ARG:HG3	1:G:308:GLN:HG3	1.75	0.69
1:B:399[B]:ARG:HG3	1:B:399[B]:ARG:NH1	2.08	0.69
1:A:75:MET:HE3	1:A:212:HIS:CE1	2.26	0.69
1:A:210:SER:OG	1:A:254:SER:CA	2.36	0.69
1:A:44:PRO:HB2	1:A:45:GLU:HG3	1.75	0.69
1:E:75:MET:CE	1:E:316:TRP:CH2	2.76	0.69
1:H:6:ILE:O	1:H:24:THR:HG23	1.93	0.69
1:B:341:LEU:HD12	1:B:393:ALA:HB2	1.75	0.69
1:A:288:ASP:HA	1:A:291:VAL:HB	1.74	0.69
1:B:69:LEU:CD1	1:B:95:ILE:HG13	2.23	0.69
1:G:67:HIS:HA	1:G:112:ASP:OD1	1.93	0.69
1:A:66:VAL:HG11	1:A:368:ILE:HD11	1.73	0.68
1:D:301:THR:CG2	1:D:378:SER:HB3	2.21	0.68
1:E:65:ASN:O	1:E:66:VAL:HG23	1.93	0.68
1:H:407:ILE:HG22	1:H:408:GLY:N	2.08	0.68
1:A:14:GLY:O	1:A:15:LEU:HD23	1.93	0.68
1:H:255:VAL:C	1:H:278:LEU:HD12	2.12	0.68
1:C:364:ARG:NH1	1:C:367:THR:OG1	2.26	0.68
1:E:264:VAL:CG1	1:E:293:SER:HB2	2.22	0.68
1:A:363:ASP:OD1	1:A:370:ASN:OD1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ARG:NH1	1:E:238:VAL:HG22	2.08	0.68
1:F:268:ALA:O	1:F:295:SER:OG	2.11	0.68
1:G:273:HIS:NE2	3:G:501:HOH:O	2.26	0.68
1:A:207:ILE:HG22	1:A:252:THR:HA	1.74	0.68
1:A:261:ASP:OD1	1:A:289:LYS:NZ	2.21	0.68
1:H:64:GLY:HA3	1:H:340:LEU:CD2	2.23	0.68
1:D:261:ASP:HB2	1:D:286:LEU:HD11	1.75	0.68
1:B:121:LEU:HD22	1:B:124:ARG:HH21	1.57	0.68
1:F:322:GLY:CA	1:F:326:ALA:HB3	2.18	0.68
1:C:323:GLU:HB2	1:C:324:PRO:CD	2.13	0.68
1:H:357:SER:O	1:H:360:GLU:HB2	1.93	0.68
1:F:129:ALA:HB1	1:H:92:VAL:HG11	1.75	0.68
1:F:75:MET:H	1:F:76:ALA:HB3	1.56	0.68
1:A:3:THR:O	1:A:47:ALA:HB1	1.93	0.68
1:G:179:GLY:O	1:G:182:LEU:HD12	1.93	0.68
1:B:111:PHE:HD2	1:B:204:MET:CE	2.06	0.68
1:B:390:ILE:CA	1:B:392:ALA:HB3	2.23	0.68
1:B:112:ASP:O	1:B:140:ALA:HB2	1.94	0.68
1:F:40:SER:OG	1:F:42:PRO:HA	1.94	0.68
1:F:66:VAL:O	1:F:112:ASP:HA	1.94	0.68
1:C:30:ASP:CG	1:C:31:ARG:H	1.97	0.68
1:D:59:PRO:HG2	1:D:394:THR:HG21	1.74	0.68
1:F:278:LEU:N	1:F:325:TYR:CE1	2.56	0.68
1:A:282:ILE:HG23	1:A:328:ASN:ND2	2.08	0.68
1:G:256:SER:OG	1:G:258:GLU:O	2.01	0.68
1:H:260:LEU:CD1	1:H:271:LEU:CD2	2.72	0.67
1:D:38:SER:OG	1:D:39:ASP:N	2.27	0.67
1:D:84:LEU:HD22	1:D:170:ILE:HG21	1.74	0.67
1:D:68:LEU:HD12	1:D:95:ILE:HG23	1.75	0.67
1:F:62:VAL:HA	1:F:109:THR:O	1.94	0.67
1:F:73:MET:CA	1:F:76:ALA:CB	2.72	0.67
1:A:181:GLN:O	1:A:184:LEU:HD12	1.94	0.67
1:E:323:GLU:CB	1:E:324:PRO:HD2	2.22	0.67
1:H:229:GLN:OE1	1:H:233:ARG:NH2	2.27	0.67
1:D:208:ALA:HB1	1:D:253:HIS:HD2	1.59	0.67
1:A:350:LYS:O	1:A:353:LEU:N	2.28	0.67
1:B:66:VAL:CG2	1:B:110:VAL:HG21	2.25	0.67
1:H:406:GLN:CB	1:H:415:LEU:CD1	2.73	0.67
1:A:406:GLN:O	1:A:407:ILE:HG23	1.93	0.67
1:C:4:ILE:HG22	1:C:5:ALA:N	2.09	0.67
1:H:217:LEU:HD13	1:H:226:ARG:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:GLY:O	1:F:30:ASP:HB2	1.94	0.67
1:F:292:ALA:O	3:F:502:HOH:O	2.12	0.67
1:F:45:GLU:HG2	1:F:46:GLY:H	1.60	0.67
1:G:370:ASN:OD1	1:G:433:ARG:NH2	2.22	0.67
1:F:214:VAL:O	1:F:218:VAL:HG23	1.95	0.67
1:A:209:VAL:CG2	1:A:252:THR:OG1	2.42	0.67
1:G:127:ILE:HD12	1:G:136:ARG:HA	1.77	0.67
1:B:143:ILE:HG12	1:B:206:LYS:HD2	1.77	0.67
1:E:399:ARG:HA	1:E:404:ALA:HB2	1.76	0.67
1:C:217:LEU:HD23	1:C:224:PHE:CB	2.25	0.67
1:D:189:GLU:HB3	1:D:193:ARG:NH1	2.10	0.67
1:A:178:VAL:HA	1:A:182:LEU:HD11	1.77	0.66
1:A:111:PHE:HA	1:A:138:PHE:O	1.95	0.66
1:F:73:MET:C	1:F:76:ALA:HB3	2.15	0.66
1:D:5:ALA:O	1:D:50:VAL:HG12	1.95	0.66
1:G:6:ILE:HG22	1:G:25:VAL:O	1.94	0.66
1:B:96:GLU:OE1	1:B:132:SER:HB2	1.95	0.66
1:F:307:ARG:NH2	1:F:311:GLU:OE2	2.27	0.66
1:D:341:LEU:H	1:D:397:VAL:HG12	1.61	0.66
1:H:59:PRO:HG2	1:H:394:THR:HG21	1.78	0.66
1:A:191:ARG:NE	1:A:238:VAL:HG22	2.09	0.66
1:A:179:GLY:O	1:A:180:HIS:ND1	2.26	0.66
1:C:77:GLY:O	1:C:155:HIS:ND1	2.28	0.66
1:C:124:ARG:HB2	1:C:137:ILE:HB	1.76	0.66
1:A:208:ALA:HA	1:A:253:HIS:HB3	1.77	0.66
1:E:279:GLY:H	1:E:325:TYR:HE1	1.40	0.66
1:D:340:LEU:HD12	1:D:397:VAL:HG12	1.76	0.66
1:A:126:ARG:HG2	1:A:126:ARG:NH1	2.09	0.66
1:G:358:PRO:O	1:G:362:GLU:HG3	1.95	0.66
1:F:419:VAL:HG13	1:F:438:VAL:HG22	1.77	0.66
1:D:76:ALA:HB3	1:D:77:GLY:HA2	1.76	0.66
1:C:38:SER:OG	1:C:40:SER:O	2.12	0.66
1:H:206:LYS:HZ2	1:H:272:ILE:HG21	1.61	0.66
1:G:127:ILE:HG13	1:G:128:ASN:N	2.10	0.66
1:C:254:SER:HG	1:C:260:LEU:HD13	1.61	0.66
1:A:287:ILE:O	1:A:291:VAL:CG2	2.25	0.66
1:E:226:ARG:CA	1:E:226:ARG:HH11	2.08	0.66
1:G:356:LEU:HD22	1:G:360:GLU:OE1	1.95	0.66
1:A:145:GLY:H	1:A:179:GLY:HA2	1.60	0.66
1:E:319:ALA:O	1:E:325:TYR:HD2	1.79	0.66
1:D:6:ILE:CA	1:D:50:VAL:HG11	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ALA:HA	1:H:262:THR:HB	1.78	0.66
1:C:337:ALA:O	1:C:338:LYS:HB2	1.96	0.66
1:D:70:ASP:O	1:D:72:TRP:C	2.33	0.65
1:F:251:LEU:HD23	1:F:270:VAL:HB	1.78	0.65
1:H:407:ILE:HG22	1:H:408:GLY:H	1.60	0.65
1:D:56:TRP:HZ3	1:D:422:ASP:O	1.77	0.65
1:A:282:ILE:CG2	1:A:328:ASN:HD21	2.09	0.65
1:G:123:ALA:O	1:G:127:ILE:HG23	1.96	0.65
1:D:301:THR:CG2	1:D:378:SER:HB2	2.26	0.65
1:E:196:ASP:O	1:E:199:SER:HB3	1.96	0.65
1:G:277:THR:OG1	1:G:280:GLN:O	2.11	0.65
1:A:62:VAL:HG13	1:A:109:THR:HB	1.77	0.65
1:A:275:ASN:CG	1:A:276:TYR:N	2.50	0.65
1:F:340:LEU:HD22	1:F:397:VAL:HA	1.78	0.65
1:D:328:ASN:OD1	1:D:329:GLU:N	2.29	0.65
1:E:226:ARG:NH1	1:E:226:ARG:HB2	2.12	0.65
1:H:322:GLY:HA2	1:H:326:ALA:CB	2.23	0.65
1:A:88:GLU:OE1	1:A:169:ARG:NH1	2.28	0.65
1:B:391:SER:CA	1:B:394:THR:H	2.10	0.65
1:F:87:TRP:CH2	1:F:455:LEU:O	2.49	0.65
1:D:412:THR:O	1:D:414:LYS:N	2.26	0.65
1:H:356:LEU:HB2	1:H:360:GLU:CG	2.21	0.65
1:C:259:ALA:O	1:C:263:SER:N	2.30	0.65
1:E:145:GLY:CA	1:E:179:GLY:HA2	2.26	0.65
1:H:34:THR:HG22	1:H:41:THR:CG2	2.26	0.65
1:E:324:PRO:O	1:E:325:TYR:C	2.32	0.65
1:D:32:PHE:CE2	1:D:412:THR:CA	2.80	0.65
1:H:378:SER:O	1:H:380:VAL:O	2.14	0.65
1:F:178:VAL:HG12	1:F:179:GLY:H	1.59	0.65
1:C:26:ILE:CD1	1:C:41:THR:OG1	2.44	0.65
1:B:384:MET:HE2	1:B:389:ALA:HA	1.79	0.65
1:A:275:ASN:O	1:A:328:ASN:ND2	2.28	0.65
1:E:217:LEU:HD23	1:E:217:LEU:O	1.96	0.65
1:G:326:ALA:HA	1:G:329:GLU:OE1	1.96	0.65
1:C:74:PHE:HA	1:C:80:THR:OG1	1.97	0.65
1:B:395:ILE:HD12	1:B:399[B]:ARG:CZ	2.26	0.65
1:F:323:GLU:CB	1:F:324:PRO:CD	2.69	0.65
1:H:204:MET:CA	1:H:248:VAL:HG12	2.14	0.65
1:E:207:ILE:HD11	1:E:236:LEU:HD23	1.79	0.65
1:F:166:PHE:CE1	1:F:170:ILE:HD11	2.32	0.65
1:B:144:VAL:HG22	1:B:178:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:ALA:HA	1:H:204:MET:HG2	1.79	0.64
1:D:62:VAL:HG13	1:D:109:THR:HB	1.79	0.64
1:C:4:ILE:HG22	1:C:5:ALA:H	1.62	0.64
1:H:6:ILE:CG2	1:H:9:VAL:HG21	2.28	0.64
1:D:301:THR:HG23	1:D:382:LYS:NZ	2.13	0.64
1:G:421:LEU:HD11	1:G:432:LEU:HD23	1.79	0.64
1:A:224:PHE:CD2	1:A:278:LEU:HD22	2.32	0.64
1:C:103:LEU:HD12	1:C:107:VAL:O	1.97	0.64
1:B:301:THR:CG2	1:B:379:MET:HE3	2.26	0.64
1:D:231:PHE:HB2	1:D:236:LEU:CD1	2.27	0.64
1:A:178:VAL:HG12	1:A:179:GLY:N	2.12	0.64
1:H:96:GLU:OE2	1:H:126:ARG:NH2	2.30	0.64
1:F:308:GLN:O	1:F:312:ASP:N	2.31	0.64
1:D:195:ARG:HD2	1:D:242:GLU:OE1	1.98	0.64
1:E:257:VAL:CG2	1:E:277:THR:HG22	2.27	0.64
1:H:39:ASP:N	1:H:39:ASP:OD1	2.29	0.64
1:G:253:HIS:ND1	1:G:273:HIS:HD2	1.96	0.64
1:G:274:ALA:HB3	1:G:298:GLY:O	1.98	0.64
1:B:340:LEU:HD11	1:B:397:VAL:HA	1.79	0.64
1:G:9:VAL:O	1:G:23:THR:HG22	1.98	0.64
1:F:282:ILE:HG22	1:F:286:LEU:HB3	1.80	0.64
1:B:111:PHE:HD2	1:B:204:MET:HE1	1.61	0.64
1:D:65:ASN:OD1	1:D:66:VAL:N	2.30	0.64
1:F:70:ASP:OD1	1:F:71:ALA:N	2.30	0.64
1:B:74:PHE:CZ	1:B:84:LEU:HD21	2.33	0.64
1:F:279:GLY:O	1:F:280:GLN:OE1	2.14	0.64
1:H:67:HIS:CD2	1:H:67:HIS:N	2.64	0.64
1:G:6:ILE:HD11	1:G:9:VAL:HG13	1.79	0.64
1:F:63:ASN:ND2	1:F:371:ASP:OD2	2.30	0.64
1:F:257:VAL:HG23	1:F:277:THR:HG21	1.77	0.64
1:D:75:MET:O	1:D:76:ALA:C	2.35	0.64
1:F:268:ALA:O	1:F:295:SER:CB	2.45	0.64
1:D:70:ASP:O	1:D:72:TRP:CA	2.46	0.63
1:H:180:HIS:O	1:H:182:LEU:N	2.30	0.63
1:B:299:LEU:HD23	1:B:329:GLU:CB	2.16	0.63
1:G:390:ILE:HG22	1:G:429:ILE:CD1	2.28	0.63
1:A:238:VAL:O	1:A:241:GLU:HG2	1.98	0.63
1:G:262:THR:O	1:G:266:LEU:HD22	1.98	0.63
1:E:226:ARG:CB	1:E:226:ARG:HH11	2.10	0.63
1:C:178:VAL:O	1:C:182:LEU:HG	1.97	0.63
1:G:391:SER:O	1:G:396:ASN:OD1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:MET:HG2	1:F:73:MET:O	1.99	0.63
1:A:153:ASP:HB3	1:A:212:HIS:HB3	1.79	0.63
1:A:237:GLU:HA	1:A:266:LEU:CD1	2.28	0.63
1:D:171:ASP:OD1	1:D:171:ASP:N	2.28	0.63
1:B:259:ALA:O	1:B:263:SER:OG	2.14	0.63
1:H:332:LEU:HD22	1:H:337:ALA:HB2	1.81	0.63
1:F:290:ILE:HG23	1:F:291:VAL:N	2.14	0.63
1:F:395:ILE:HA	1:F:398:ALA:HB3	1.79	0.63
1:E:419:VAL:HG23	1:E:438:VAL:HG22	1.79	0.63
1:D:6:ILE:C	1:D:24:THR:CG2	2.66	0.63
1:B:31:ARG:NH1	1:B:415:LEU:N	2.46	0.63
1:F:14:GLY:HA2	1:F:390:ILE:HD13	1.80	0.63
1:F:74:PHE:CD1	1:F:80:THR:HG23	2.33	0.63
1:A:348:PRO:HG3	1:A:364:ARG:NH1	2.12	0.63
1:D:32:PHE:CD2	1:D:412:THR:CA	2.81	0.63
1:C:254:SER:HG	1:C:260:LEU:CD1	2.12	0.63
1:E:290:ILE:HA	1:E:293:SER:OG	1.98	0.63
1:E:75:MET:CE	1:E:316:TRP:CZ3	2.81	0.63
1:F:311:GLU:HG2	1:F:318:ALA:HB1	1.80	0.63
1:G:94:VAL:HG13	1:G:456:VAL:HG23	1.81	0.63
1:H:6:ILE:CD1	1:H:57:MET:SD	2.87	0.63
1:A:251:LEU:HD11	1:A:270:VAL:CG1	2.12	0.63
1:A:251:LEU:CD1	1:A:270:VAL:CG2	2.76	0.63
1:C:26:ILE:HD12	1:C:34:THR:OG1	1.99	0.63
1:F:118:GLU:CG	1:F:119:PRO:HD3	2.29	0.63
1:C:69:LEU:HB2	1:C:115:ASN:OD1	1.98	0.63
1:G:13:ASP:O	1:G:409:SER:OG	2.12	0.63
1:D:459:HIS:O	1:D:459:HIS:ND1	2.31	0.63
1:E:175:GLU:O	1:E:178:VAL:N	2.22	0.63
1:C:251:LEU:N	1:C:251:LEU:HD12	2.14	0.63
1:A:250:VAL:N	1:A:269:ASP:HB2	2.14	0.63
1:F:97:GLU:OE2	1:F:456:VAL:CG1	2.46	0.63
1:D:333:ILE:C	1:D:333:ILE:HD13	2.16	0.63
1:D:350:LYS:CD	1:D:458:ALA:O	2.46	0.63
1:B:253:HIS:CD2	1:B:273:HIS:CE1	2.87	0.63
1:E:277:THR:HB	1:E:280:GLN:O	1.98	0.63
1:D:96:GLU:O	1:D:100:GLN:N	2.32	0.63
1:H:7:THR:HA	1:H:24:THR:HG23	1.80	0.62
1:F:279:GLY:HA2	1:F:324:PRO:CG	2.20	0.62
1:F:328:ASN:O	1:F:329:GLU:C	2.35	0.62
1:D:301:THR:OG1	1:D:379:MET:HE2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:O	1:C:416:ALA:HB2	1.98	0.62
1:H:87:TRP:HB3	1:H:94:VAL:HG21	1.80	0.62
1:G:127:ILE:HD13	1:G:137:ILE:HG12	1.81	0.62
1:A:191:ARG:NE	1:A:238:VAL:CG2	2.61	0.62
1:D:67:HIS:CG	1:D:71:ALA:HB3	2.35	0.62
1:F:178:VAL:HG12	1:F:179:GLY:N	2.15	0.62
1:A:224:PHE:HB3	1:A:278:LEU:HD13	1.79	0.62
1:A:250:VAL:H	1:A:269:ASP:CB	2.11	0.62
1:A:275:ASN:OD1	1:A:276:TYR:CD2	2.53	0.62
1:H:153:ASP:O	1:H:212:HIS:ND1	2.33	0.62
1:H:253:HIS:HE2	1:H:273:HIS:HE2	1.42	0.62
1:A:75:MET:SD	1:A:215:PHE:HD2	2.22	0.62
1:F:428:ASP:CG	1:F:430:ARG:HD2	2.19	0.62
1:B:307:ARG:NH2	1:B:322:GLY:HA3	2.13	0.62
1:A:179:GLY:C	1:A:180:HIS:O	2.28	0.62
1:D:195:ARG:HE	1:D:242:GLU:HB3	1.64	0.62
1:F:313:VAL:CG2	1:F:360:GLU:OE2	2.47	0.62
1:G:181:GLN:O	1:G:182:LEU:HD12	2.00	0.62
1:E:25:VAL:HB	1:E:35:VAL:HG12	1.81	0.62
1:D:124:ARG:O	1:D:128:ASN:ND2	2.28	0.62
1:F:153:ASP:OD2	1:F:180:HIS:NE2	2.32	0.62
1:D:273:HIS:NE2	3:D:502:HOH:O	2.30	0.62
1:D:222:VAL:CG2	1:D:223:GLY:N	2.62	0.62
1:D:56:TRP:CZ3	1:D:422:ASP:O	2.53	0.62
1:F:72:TRP:C	1:F:76:ALA:CB	2.64	0.62
1:A:115:ASN:OD1	1:A:116:ALA:N	2.32	0.62
1:D:339:ILE:HG22	1:D:340:LEU:N	2.15	0.62
1:H:406:GLN:HB2	1:H:415:LEU:CD1	2.29	0.62
1:C:113:THR:HB	1:C:206:LYS:CD	2.28	0.62
1:D:350:LYS:CE	1:D:460:PRO:HB3	2.26	0.62
1:G:286:LEU:O	1:G:288:ASP:N	2.33	0.62
1:F:75:MET:CE	1:F:212:HIS:HE1	2.13	0.62
1:B:151:SER:OG	1:B:152:ALA:O	2.10	0.62
1:H:164:ARG:HA	1:H:167:VAL:HB	1.80	0.62
1:F:255:VAL:HA	1:F:276:TYR:O	2.00	0.62
1:C:10:THR:HA	1:C:21:PRO:HA	1.81	0.62
1:A:72:TRP:O	1:A:76:ALA:HA	2.00	0.61
1:H:149:PRO:O	1:H:155:HIS:N	2.33	0.61
1:E:226:ARG:CD	1:E:228:TYR:HE2	2.07	0.61
1:G:26:ILE:HD11	1:G:42:PRO:O	2.00	0.61
1:E:264:VAL:HG12	1:E:293:SER:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:GLN:O	1:D:309:GLY:N	2.32	0.61
1:F:227:SER:O	1:F:228:TYR:O	2.17	0.61
1:H:303:HIS:ND1	1:H:306:HIS:HB2	2.15	0.61
1:B:341:LEU:CD1	1:B:393:ALA:HB2	2.31	0.61
1:B:380:VAL:HG13	1:B:384:MET:O	2.00	0.61
1:B:385:SER:CB	1:B:387:LEU:O	2.47	0.61
1:A:191:ARG:HD2	1:A:238:VAL:HG21	1.82	0.61
1:H:406:GLN:HB3	1:H:415:LEU:CD1	2.30	0.61
1:H:217:LEU:HD13	1:H:226:ARG:CG	2.31	0.61
1:H:240:VAL:O	1:H:241:GLU:HB3	2.00	0.61
1:B:178:VAL:HG21	1:B:197:TYR:CG	2.34	0.61
1:H:6:ILE:CG2	1:H:25:VAL:CG1	2.61	0.61
1:A:236:LEU:O	1:A:240:VAL:HG23	1.99	0.61
1:C:66:VAL:HG21	1:C:110:VAL:HB	1.83	0.61
1:C:219:ASP:OD1	1:C:222:VAL:N	2.33	0.61
1:B:396:ASN:OD1	1:B:396:ASN:N	2.33	0.61
1:E:226:ARG:HA	1:E:226:ARG:HH11	1.63	0.61
1:B:195:ARG:O	1:B:199:SER:OG	2.18	0.61
1:A:235:VAL:HA	1:A:238:VAL:CG1	2.30	0.61
1:C:121:LEU:HD21	1:C:124:ARG:NH2	2.15	0.61
1:E:169:ARG:NH2	1:D:351:ASP:OD2	2.34	0.61
1:A:253:HIS:CE1	1:A:273:HIS:CE1	2.87	0.61
1:D:136:ARG:CZ	1:D:415:LEU:HD13	2.31	0.61
1:A:180:HIS:O	1:A:181:GLN:HB2	1.99	0.61
1:A:125:ASP:HB2	1:A:126:ARG:NH1	2.14	0.61
1:C:302:VAL:HA	1:C:374:HIS:HE1	1.65	0.61
1:B:44:PRO:HD2	1:B:47:ALA:HB2	1.82	0.61
1:C:6:ILE:HG21	1:C:25:VAL:HG22	1.75	0.61
1:H:253:HIS:CD2	1:H:273:HIS:HE1	2.15	0.61
1:A:235:VAL:CA	1:A:238:VAL:HG12	2.30	0.61
1:A:254:SER:HB3	1:A:259:ALA:HB1	1.81	0.61
1:H:340:LEU:HD21	1:H:397:VAL:HG13	1.81	0.61
1:D:387:LEU:HA	1:D:390:ILE:HB	1.82	0.61
1:F:324:PRO:O	1:F:328:ASN:HB3	2.00	0.61
1:D:6:ILE:CG1	1:D:50:VAL:HG11	2.30	0.61
1:E:272:ILE:HG22	1:E:273:HIS:CE1	2.36	0.61
1:E:178:VAL:HG22	1:E:182:LEU:HD11	1.83	0.61
1:G:386:PRO:O	1:G:390:ILE:HG23	2.00	0.61
1:G:389:ALA:O	1:G:392:ALA:HB3	2.01	0.61
1:E:309:GLY:O	1:E:313:VAL:HG23	2.01	0.61
1:E:217:LEU:C	1:E:217:LEU:HD23	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:HG21	1:D:378:SER:HB3	1.80	0.61
1:G:286:LEU:C	1:G:288:ASP:N	2.52	0.61
1:H:240:VAL:HG12	1:H:241:GLU:N	2.16	0.61
1:G:178:VAL:HG12	1:G:179:GLY:H	1.65	0.61
1:H:170:ILE:HA	1:H:173:MET:HE2	1.83	0.61
1:C:142:THR:OG1	1:C:174:PHE:O	2.16	0.61
1:B:372:HIS:O	1:B:376:THR:OG1	2.17	0.61
1:A:206:LYS:CE	1:A:272:ILE:CD1	2.79	0.61
1:E:38:SER:HG	1:E:39:ASP:H	1.49	0.61
1:C:72:TRP:O	1:C:75:MET:O	2.19	0.61
1:F:304:ASP:OD1	1:F:381:GLU:CD	2.39	0.61
1:D:153:ASP:O	1:D:212:HIS:ND1	2.29	0.60
1:E:329:GLU:O	1:E:333:ILE:HG13	2.00	0.60
1:B:393:ALA:O	1:B:397:VAL:HG23	2.01	0.60
1:F:150:PHE:HB2	1:F:167:VAL:HG13	1.84	0.60
1:G:68:LEU:HD11	1:G:137:ILE:HG21	1.83	0.60
1:C:307:ARG:HG3	1:C:308:GLN:N	2.16	0.60
1:C:236:LEU:HD13	1:C:266:LEU:HD11	1.84	0.60
1:C:58:VAL:HG23	1:C:419:VAL:HB	1.82	0.60
1:D:282:ILE:HB	1:D:287:ILE:CD1	2.32	0.60
1:B:424:ASP:O	1:B:431:ASN:OD1	2.19	0.60
1:A:100:GLN:OE1	1:A:451:PRO:CB	2.49	0.60
1:C:214:VAL:O	1:C:217:LEU:N	2.26	0.60
1:H:356:LEU:CB	1:H:360:GLU:HG3	2.20	0.60
1:H:63:ASN:HA	1:H:341:LEU:HD23	1.83	0.60
1:G:102:ALA:O	1:G:107:VAL:N	2.34	0.60
1:D:97:GLU:HA	1:D:100:GLN:HE21	1.66	0.60
1:G:362:GLU:O	1:G:363:ASP:HB2	2.01	0.60
1:B:389:ALA:O	1:B:392:ALA:HB3	1.94	0.60
1:B:399[B]:ARG:HA	1:B:404:ALA:HB2	1.83	0.60
1:F:255:VAL:HB	1:F:278:LEU:HD23	1.83	0.60
1:F:87:TRP:CZ2	1:F:455:LEU:O	2.54	0.60
1:A:238:VAL:HG13	1:A:239:MET:N	2.17	0.60
1:D:180:HIS:O	1:D:181:GLN:HB3	2.01	0.60
1:H:178:VAL:HG11	1:H:197:TYR:CG	2.36	0.60
1:E:185:LEU:HD12	1:E:186:PRO:HD2	1.83	0.60
1:E:153:ASP:CA	1:E:212:HIS:O	2.49	0.60
1:B:197:TYR:O	1:B:200:ARG:HB2	2.01	0.60
1:F:23:THR:HA	1:F:37:PRO:HA	1.83	0.60
1:F:323:GLU:O	1:F:327:THR:OG1	2.18	0.60
1:H:208:ALA:HA	1:H:253:HIS:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:VAL:O	1:G:23:THR:CG2	2.50	0.60
1:F:166:PHE:CZ	1:F:170:ILE:HD11	2.37	0.60
1:B:139:ALA:N	1:B:203:ASP:OD2	2.35	0.60
1:B:391:SER:N	1:B:394:THR:H	2.00	0.60
1:G:6:ILE:HD13	1:G:9:VAL:HG21	1.82	0.60
1:E:264:VAL:HG12	1:E:293:SER:HB2	1.84	0.60
1:E:214:VAL:HG22	1:E:215:PHE:CD1	2.37	0.60
1:B:31:ARG:HH11	1:B:415:LEU:N	2.00	0.60
1:E:206:LYS:HE2	1:E:253:HIS:HB2	1.84	0.60
1:A:296:TRP:CE3	1:A:338:LYS:HB3	2.36	0.59
1:H:41:THR:N	1:H:42:PRO:HA	2.16	0.59
1:E:75:MET:HE3	1:E:316:TRP:CZ3	2.37	0.59
1:G:56:TRP:O	1:G:420:LEU:HA	2.02	0.59
1:F:277:THR:HB	1:F:280:GLN:O	2.03	0.59
1:A:75:MET:SD	1:A:215:PHE:CE2	2.95	0.59
1:D:411:GLU:O	1:D:412:THR:CB	2.46	0.59
1:H:68:LEU:CD1	1:H:95:ILE:HG23	2.32	0.59
1:D:420:LEU:O	1:D:436:THR:OG1	2.19	0.59
1:H:202:VAL:O	1:H:203:ASP:C	2.39	0.59
1:A:45:GLU:C	1:A:47:ALA:H	2.05	0.59
1:D:244:ARG:NH2	1:D:269:ASP:OD2	2.32	0.59
1:B:397:VAL:O	1:B:401:TYR:HD1	1.85	0.59
1:D:136:ARG:NH2	1:D:417:ASP:OD2	2.34	0.59
1:A:3:THR:HA	1:A:28:GLU:HA	1.84	0.59
1:A:206:LYS:CE	1:A:272:ILE:HD11	2.29	0.59
1:B:96:GLU:OE1	1:B:132:SER:CB	2.50	0.59
1:D:252:THR:HG22	1:D:271:LEU:HA	1.84	0.59
1:H:207:ILE:CD1	1:H:239:MET:SD	2.90	0.59
1:G:282:ILE:HG13	1:G:328:ASN:OD1	2.02	0.59
1:F:35:VAL:HG12	1:F:36:GLY:H	1.68	0.59
1:C:136:ARG:NH2	1:C:417:ASP:OD2	2.34	0.59
1:F:235:VAL:HA	1:F:238:VAL:HB	1.83	0.59
1:E:429:ILE:HG13	1:E:432:LEU:CD1	2.32	0.59
1:H:100:GLN:HG2	1:H:134:GLY:HA2	1.83	0.59
1:F:204:MET:HA	1:F:248:VAL:HB	1.84	0.59
1:B:254:SER:OG	1:B:271:LEU:CD2	2.51	0.59
1:B:254:SER:OG	1:B:271:LEU:HD21	2.02	0.59
1:D:195:ARG:HG3	1:D:195:ARG:NH1	2.17	0.59
1:B:303:HIS:HB2	1:B:306:HIS:H	1.67	0.59
1:C:399[B]:ARG:HD3	1:C:404:ALA:CB	2.33	0.59
1:H:169:ARG:O	1:H:173:MET:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:428:ASP:OD2	1:H:430:ARG:NH1	2.36	0.59
1:C:299:LEU:O	1:C:375:TRP:NE1	2.31	0.59
1:B:391:SER:N	1:B:392:ALA:CB	2.62	0.59
1:B:102:ALA:HB1	1:B:107:VAL:HB	1.84	0.59
1:B:289:LYS:O	1:B:293:SER:N	2.30	0.59
1:D:187:ARG:HH11	1:D:187:ARG:HB3	1.66	0.59
1:D:232:SER:HB2	1:D:234:PRO:HD2	1.83	0.59
1:E:214:VAL:CG1	1:E:215:PHE:HD1	2.09	0.59
1:A:363:ASP:OD2	1:A:374:HIS:ND1	2.35	0.59
1:D:289:LYS:O	1:D:293:SER:HB2	2.03	0.59
1:C:397:VAL:O	1:C:401:TYR:HD1	1.86	0.59
1:C:318:ALA:O	1:C:319:ALA:C	2.41	0.58
1:H:150:PHE:HA	1:H:155:HIS:O	2.02	0.58
1:G:259:ALA:HA	1:G:262:THR:HB	1.84	0.58
1:A:409:SER:CB	1:A:414:LYS:NZ	2.65	0.58
1:H:6:ILE:HG22	1:H:9:VAL:HG22	1.84	0.58
1:F:322:GLY:O	1:F:323:GLU:OE1	2.20	0.58
1:G:388:GLU:HA	1:G:391:SER:OG	2.04	0.58
1:A:409:SER:CB	1:A:414:LYS:HZ3	2.15	0.58
1:F:269:ASP:O	1:F:296:TRP:HB2	2.03	0.58
1:B:436:THR:O	1:B:447:ARG:NH2	2.36	0.58
1:B:391:SER:HB3	1:B:394:THR:OG1	2.03	0.58
1:A:179:GLY:O	1:A:180:HIS:O	2.20	0.58
1:G:326:ALA:HA	1:G:329:GLU:HB2	1.84	0.58
1:F:64:GLY:HA3	1:F:341:LEU:O	2.04	0.58
1:D:6:ILE:HA	1:D:50:VAL:HG13	1.84	0.58
1:H:213:ILE:O	1:H:213:ILE:HG22	2.01	0.58
1:F:226:ARG:CB	1:F:226:ARG:HH11	2.16	0.58
1:G:217:LEU:HB2	1:G:219:ASP:HB2	1.86	0.58
1:D:100:GLN:HG2	1:D:450:LEU:HD22	1.86	0.58
1:A:240:VAL:CG2	1:A:266:LEU:CG	2.77	0.58
1:E:290:ILE:O	1:E:293:SER:OG	2.19	0.58
1:F:258:GLU:C	1:F:260:LEU:H	2.07	0.58
1:B:117:ILE:HA	1:B:120:VAL:HG12	1.85	0.58
1:F:38:SER:HB2	1:F:40:SER:N	2.17	0.58
1:F:45:GLU:CG	1:F:46:GLY:H	2.16	0.58
1:E:279:GLY:N	1:E:325:TYR:HE1	1.97	0.58
1:H:206:LYS:HE3	1:H:272:ILE:CB	2.34	0.58
1:D:301:THR:HG22	1:D:302:VAL:N	2.18	0.58
1:G:122:ALA:O	1:G:126:ARG:HG3	2.04	0.58
1:B:66:VAL:CG2	1:B:110:VAL:CG2	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:MET:CE	1:F:212:HIS:CE1	2.86	0.58
1:G:258:GLU:O	1:G:259:ALA:HB3	2.04	0.58
1:G:286:LEU:C	1:G:288:ASP:H	2.06	0.58
1:D:195:ARG:NH2	1:D:242:GLU:O	2.28	0.58
1:D:104:ARG:O	1:D:447:ARG:HD3	2.03	0.58
1:D:49:VAL:HG23	1:D:49:VAL:O	2.02	0.58
1:E:10:THR:HA	1:E:21:PRO:HA	1.85	0.58
1:B:73:MET:HA	1:B:76:ALA:CB	2.34	0.58
1:D:68:LEU:HD13	1:D:95:ILE:CG2	2.34	0.58
1:B:41:THR:N	1:B:42:PRO:HA	2.17	0.58
1:D:10:THR:HA	1:D:21:PRO:HA	1.85	0.58
1:C:240:VAL:O	1:C:243:ALA:HB3	2.03	0.58
1:E:74:PHE:HA	1:E:80:THR:OG1	2.04	0.58
1:G:380:VAL:HA	1:G:384:MET:HB2	1.84	0.58
1:D:75:MET:O	1:D:76:ALA:O	2.21	0.58
1:D:214:VAL:O	1:D:217:LEU:HB3	2.04	0.58
1:G:388:GLU:O	1:G:391:SER:OG	2.22	0.58
1:G:363:ASP:O	1:G:374:HIS:CE1	2.56	0.58
1:F:290:ILE:CD1	1:F:337:ALA:HA	2.34	0.58
1:F:375:TRP:HH2	1:F:392:ALA:HB1	1.69	0.58
1:C:9:VAL:HG13	1:C:52:GLY:HA3	1.86	0.58
1:F:113:THR:HG21	1:F:206:LYS:HD3	1.85	0.58
1:F:126:ARG:NH1	1:F:132:SER:HG	2.01	0.58
1:E:303:HIS:HB2	1:E:306:HIS:H	1.67	0.58
1:B:190:VAL:O	1:B:194:VAL:HG23	2.04	0.58
1:B:187:ARG:HB3	1:B:235:VAL:HG22	1.85	0.58
1:A:11:LEU:HD11	1:A:410:VAL:HG11	1.86	0.57
1:B:258:GLU:O	1:B:259:ALA:HB3	2.03	0.57
1:D:79:GLY:HA2	1:D:82:GLU:OE1	2.04	0.57
1:E:224:PHE:CG	1:E:278:LEU:HD12	2.37	0.57
1:H:145:GLY:H	1:H:179:GLY:HA3	1.64	0.57
1:B:273:HIS:HB3	1:B:300:GLN:HE21	1.69	0.57
1:G:94:VAL:HG22	1:G:455:LEU:HD22	1.84	0.57
1:A:250:VAL:O	1:A:270:VAL:N	2.36	0.57
1:H:231:PHE:HB2	1:H:236:LEU:HD21	1.84	0.57
1:F:429:ILE:HG13	1:F:429:ILE:O	2.04	0.57
1:A:66:VAL:HG11	1:A:368:ILE:CD1	2.34	0.57
1:G:67:HIS:N	1:G:345:ALA:O	2.31	0.57
1:A:97:GLU:OE2	1:A:451:PRO:HG3	2.05	0.57
1:B:60:GLY:HA2	1:B:419:VAL:HG23	1.86	0.57
1:E:23:THR:HG22	1:E:37:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:ILE:HD11	1:G:137:ILE:H	1.69	0.57
1:A:213:ILE:HG23	1:A:216:THR:HG21	1.87	0.57
1:E:213:ILE:CG2	1:E:216:THR:HG22	2.34	0.57
1:B:240:VAL:O	1:B:244:ARG:HG2	2.04	0.57
1:B:391:SER:CA	1:B:394:THR:N	2.68	0.57
1:D:146:MET:O	1:D:179:GLY:HA3	2.04	0.57
1:F:30:ASP:O	1:F:416:ALA:CB	2.52	0.57
1:F:111:PHE:CE1	1:F:138:PHE:HD2	2.22	0.57
1:H:6:ILE:HG21	1:H:25:VAL:HG12	1.85	0.57
1:B:389:ALA:C	1:B:392:ALA:HB3	2.21	0.57
1:H:225:ASP:CB	1:H:226:ARG:HE	2.13	0.57
1:D:117:ILE:HA	1:D:120:VAL:HG12	1.86	0.57
1:C:351:ASP:OD2	1:H:166:PHE:HB2	2.04	0.57
1:D:32:PHE:HD2	1:D:412:THR:HA	1.67	0.57
1:H:356:LEU:HD12	1:H:360:GLU:HG3	1.86	0.57
1:E:225:ASP:O	1:E:226:ARG:CB	2.53	0.57
1:A:343:THR:OG1	1:A:345:ALA:HB2	2.05	0.57
1:E:301:THR:HG21	1:E:379:MET:SD	2.45	0.57
1:H:240:VAL:O	1:H:241:GLU:CB	2.53	0.57
1:A:51:ASP:O	1:A:55:ARG:NH2	2.37	0.57
1:F:319:ALA:O	1:F:322:GLY:O	2.23	0.57
1:H:201:GLY:C	1:H:202:VAL:HG22	2.25	0.57
1:A:411:GLU:CB	1:A:414:LYS:HE2	2.35	0.57
1:B:203:ASP:HB2	1:B:204:MET:HG3	1.85	0.57
1:E:419:VAL:HG22	1:E:435:ILE:HG23	1.85	0.57
1:C:219:ASP:OD1	1:C:223:GLY:N	2.37	0.57
1:E:77:GLY:N	1:E:78:PRO:CD	2.68	0.57
1:E:78:PRO:HA	1:E:155:HIS:CE1	2.40	0.57
1:G:58:VAL:O	1:G:419:VAL:N	2.33	0.57
1:G:9:VAL:N	1:G:23:THR:O	2.37	0.57
1:B:69:LEU:CD1	1:B:95:ILE:CG1	2.80	0.57
1:D:217:LEU:HD22	1:D:226:ARG:HG2	1.87	0.57
1:B:210:SER:HB2	1:B:255:VAL:HG23	1.86	0.57
1:F:330:ARG:HG2	1:F:382:LYS:HD2	1.87	0.57
1:D:220:ARG:O	1:D:221:SER:OG	2.21	0.57
1:G:6:ILE:CG1	1:G:9:VAL:HG22	2.26	0.57
1:H:61:TYR:CE1	1:H:432:LEU:HD23	2.39	0.57
1:B:63:ASN:HB3	1:B:110:VAL:HG23	1.86	0.57
1:A:32:PHE:HD2	1:A:411:GLU:O	1.88	0.57
1:H:202:VAL:O	1:H:202:VAL:HG23	2.04	0.56
1:D:217:LEU:HD11	1:D:225:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:THR:HA	1:H:136:ARG:HB2	1.86	0.56
1:A:406:GLN:O	1:A:415:LEU:HB2	2.05	0.56
1:C:67:HIS:CE1	1:C:114:HIS:CB	2.88	0.56
1:E:278:LEU:CA	1:E:325:TYR:HE1	2.19	0.56
1:F:205:LEU:HD13	1:F:243:ALA:HB2	1.86	0.56
1:H:326:ALA:HA	1:H:329:GLU:OE2	2.05	0.56
1:G:218:VAL:HB	1:G:219:ASP:HA	1.87	0.56
1:H:122:ALA:O	1:H:126:ARG:HD2	2.04	0.56
1:G:9:VAL:O	1:G:23:THR:O	2.24	0.56
1:E:19:PRO:O	1:E:21:PRO:HD3	2.04	0.56
1:C:162:ALA:HB1	1:H:82:GLU:OE1	2.04	0.56
1:A:219:ASP:HB3	1:A:222:VAL:HB	1.87	0.56
1:E:205:LEU:HD13	1:E:243:ALA:HB2	1.87	0.56
1:B:73:MET:HA	1:B:76:ALA:HB3	1.87	0.56
1:E:284:ASN:O	1:E:285:TYR:CB	2.51	0.56
1:B:257:VAL:CG2	1:B:277:THR:OG1	2.53	0.56
1:F:277:THR:O	1:F:277:THR:HG22	2.04	0.56
1:H:189:GLU:O	1:H:193:ARG:NH2	2.39	0.56
1:D:38:SER:OG	1:D:40:SER:O	2.24	0.56
1:A:125:ASP:CB	1:A:126:ARG:HH12	2.17	0.56
1:F:304:ASP:OD1	1:F:381:GLU:OE1	2.24	0.56
1:F:6:ILE:HD11	1:F:420:LEU:HD21	1.87	0.56
1:H:11:LEU:HB2	1:H:57:MET:HB2	1.88	0.56
1:A:209:VAL:HG23	1:A:253:HIS:H	1.71	0.56
1:A:251:LEU:HD12	1:A:270:VAL:HG12	1.81	0.56
1:H:260:LEU:O	1:H:264:VAL:HG23	2.04	0.56
1:F:3:THR:CB	1:F:28:GLU:OE2	2.39	0.56
1:F:65:ASN:OD1	1:F:113:THR:CB	2.53	0.56
1:C:326:ALA:O	1:C:329:GLU:N	2.39	0.56
1:E:23:THR:HA	1:E:37:PRO:HA	1.87	0.56
1:F:277:THR:CB	1:F:280:GLN:O	2.54	0.56
1:F:154:PHE:CD1	1:F:154:PHE:N	2.73	0.56
1:F:73:MET:C	1:F:76:ALA:CB	2.73	0.56
1:F:453:THR:C	1:F:455:LEU:HD23	2.24	0.56
1:H:146:MET:SD	1:H:212:HIS:HB2	2.45	0.56
1:G:127:ILE:CD1	1:G:136:ARG:HA	2.36	0.56
1:A:240:VAL:CG2	1:A:266:LEU:HD11	2.35	0.56
1:F:256:SER:HB2	1:F:258:GLU:O	2.06	0.56
1:E:198:LEU:O	1:E:201:GLY:N	2.24	0.56
1:G:453:THR:O	1:G:453:THR:OG1	2.24	0.56
1:C:286:LEU:O	1:C:290:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ILE:HG22	1:H:9:VAL:CG2	2.36	0.56
1:E:307:ARG:HB2	1:E:321:ALA:HB1	1.87	0.56
1:F:204:MET:CE	1:F:251:LEU:HD11	2.35	0.56
1:H:68:LEU:HB3	1:H:95:ILE:HG23	1.87	0.56
1:D:191:ARG:HH21	1:D:238:VAL:HG22	1.69	0.56
1:G:317:ALA:O	1:G:320:LEU:HG	2.06	0.56
1:G:341:LEU:HG	1:G:375:TRP:CD2	2.41	0.56
1:A:253:HIS:CE1	1:A:273:HIS:ND1	2.72	0.56
1:D:195:ARG:CD	1:D:242:GLU:OE1	2.54	0.56
1:F:41:THR:OG1	1:F:42:PRO:O	2.23	0.56
1:B:73:MET:O	1:B:76:ALA:N	2.33	0.56
1:G:323:GLU:CB	1:G:324:PRO:CD	2.84	0.56
1:G:323:GLU:CB	1:G:324:PRO:HD3	2.34	0.56
1:G:340:LEU:HG	1:G:397:VAL:HG22	1.87	0.56
1:F:263:SER:O	1:F:266:LEU:HD12	2.07	0.56
1:H:255:VAL:CB	1:H:278:LEU:CD1	2.75	0.55
1:F:204:MET:HE3	1:F:251:LEU:HD11	1.87	0.55
1:F:185:LEU:HD23	1:F:186:PRO:HD2	1.88	0.55
1:H:303:HIS:NE2	1:H:305:GLN:HB2	2.20	0.55
1:B:379:MET:O	1:B:382:LYS:HB2	2.05	0.55
1:F:264:VAL:HG13	1:F:293:SER:CB	2.22	0.55
1:H:352:HIS:O	1:H:356:LEU:HG	2.06	0.55
1:E:226:ARG:HB2	1:E:226:ARG:HH11	1.67	0.55
1:G:6:ILE:HD11	1:G:9:VAL:HG11	1.86	0.55
1:H:323:GLU:CB	1:H:324:PRO:CD	2.83	0.55
1:B:409:SER:HB3	1:B:414:LYS:HE3	1.89	0.55
1:C:78:PRO:HG2	1:C:352:HIS:CE1	2.40	0.55
1:B:133:GLN:HG2	1:B:450:LEU:HD11	1.88	0.55
1:F:38:SER:HB2	1:F:40:SER:O	2.05	0.55
1:F:60:GLY:HA2	1:F:419:VAL:HG23	1.87	0.55
1:D:124:ARG:HB2	1:D:137:ILE:HB	1.88	0.55
1:C:114:HIS:CE1	1:C:143:ILE:H	2.24	0.55
1:E:153:ASP:HB3	1:E:212:HIS:CB	2.19	0.55
1:E:153:ASP:OD1	1:E:212:HIS:O	2.24	0.55
1:A:91:TYR:CE2	1:A:173:MET:HE1	2.42	0.55
1:B:96:GLU:O	1:B:100:GLN:NE2	2.39	0.55
1:C:21:PRO:O	1:C:22:ALA:HB3	2.05	0.55
1:D:14:GLY:O	1:D:395:ILE:HD11	2.06	0.55
1:C:112:ASP:O	1:C:139:ALA:HA	2.06	0.55
1:G:100:GLN:OE1	1:G:451:PRO:HA	2.06	0.55
1:H:6:ILE:HG13	1:H:25:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143:ILE:CG2	1:H:146:MET:HE2	2.34	0.55
1:H:208:ALA:HA	1:H:253:HIS:HB3	1.87	0.55
1:E:429:ILE:CD1	1:E:432:LEU:HD11	2.37	0.55
1:E:252:THR:HG21	1:E:271:LEU:HD22	1.87	0.55
1:A:3:THR:HA	1:A:27:VAL:O	2.07	0.55
1:E:144:VAL:HA	1:E:178:VAL:HG13	1.89	0.55
1:H:41:THR:HG22	1:H:41:THR:O	2.06	0.55
1:E:453:THR:HG23	1:E:453:THR:O	2.06	0.55
1:C:373:PHE:HB3	1:C:433:ARG:HE	1.70	0.55
1:A:395:ILE:HA	1:A:398:ALA:HB3	1.89	0.55
1:F:317:ALA:C	1:F:319:ALA:H	2.08	0.55
1:A:325:TYR:CD1	1:A:325:TYR:N	2.74	0.55
1:D:6:ILE:CB	1:D:50:VAL:HG11	2.36	0.55
1:D:222:VAL:HG22	1:D:223:GLY:H	1.70	0.55
1:A:343:THR:HG21	1:A:371:ASP:OD2	2.06	0.55
1:C:390:ILE:O	1:C:394:THR:HG23	2.06	0.55
1:G:253:HIS:ND1	1:G:273:HIS:CD2	2.74	0.55
1:H:100:GLN:OE1	1:H:452:THR:OG1	2.24	0.55
1:C:205:LEU:O	1:C:251:LEU:HD12	2.06	0.55
1:D:422:ASP:OD1	1:D:422:ASP:N	2.36	0.55
1:H:10:THR:HG23	1:H:21:PRO:HA	1.89	0.55
1:D:412:THR:C	1:D:414:LYS:H	2.08	0.55
1:E:213:ILE:O	1:E:213:ILE:HG22	2.05	0.55
1:H:322:GLY:O	1:H:323:GLU:HG3	2.07	0.55
1:B:73:MET:O	1:B:76:ALA:HB3	2.07	0.55
1:C:26:ILE:HD12	1:C:41:THR:OG1	2.07	0.55
1:B:81:ILE:HG12	1:B:150:PHE:HE1	1.72	0.55
1:G:205:LEU:HD22	1:G:243:ALA:HB2	1.88	0.55
1:G:19:PRO:HG3	1:G:426:VAL:HG21	1.88	0.55
1:C:92:VAL:O	1:C:96:GLU:HG3	2.07	0.55
1:H:6:ILE:HG21	1:H:9:VAL:HG21	1.88	0.55
1:B:399[A]:ARG:HA	1:B:404:ALA:HB2	1.88	0.55
1:E:324:PRO:O	1:E:326:ALA:N	2.40	0.55
1:D:76:ALA:CB	1:D:77:GLY:CA	2.85	0.55
1:C:318:ALA:O	1:C:320:LEU:N	2.39	0.55
1:D:220:ARG:NH1	1:D:220:ARG:HG3	2.19	0.55
1:H:387:LEU:O	1:H:391:SER:OG	2.21	0.55
1:H:361:ARG:O	1:H:362:GLU:C	2.45	0.55
1:A:32:PHE:CD2	1:A:411:GLU:O	2.60	0.55
1:E:66:VAL:O	1:E:67:HIS:CD2	2.58	0.55
1:C:222:VAL:HG22	1:C:222:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:VAL:HG23	1:G:419:VAL:HB	1.88	0.55
1:H:435:ILE:CG2	1:H:438:VAL:HG23	2.37	0.55
1:F:321:ALA:O	1:F:326:ALA:HB2	2.07	0.55
1:F:198:LEU:HA	1:F:202:VAL:HG22	1.89	0.55
1:A:303:HIS:HB2	1:A:374:HIS:HE1	1.69	0.55
1:F:111:PHE:CE1	1:F:138:PHE:CD2	2.95	0.55
1:B:330:ARG:O	1:B:334:SER:OG	2.24	0.55
1:B:386:PRO:HB2	1:B:426:VAL:HG13	1.87	0.55
1:H:287:ILE:O	1:H:291:VAL:HG23	2.07	0.55
1:F:273:HIS:O	1:F:276:TYR:HB2	2.08	0.54
1:E:429:ILE:HG23	1:E:430:ARG:N	2.22	0.54
1:E:233:ARG:HA	1:E:236:LEU:HD12	1.87	0.54
1:A:194:VAL:CG2	1:A:239:MET:HE1	2.37	0.54
1:G:324:PRO:O	1:G:328:ASN:CB	2.55	0.54
1:D:189:GLU:HB3	1:D:193:ARG:HH11	1.71	0.54
1:H:379:MET:O	1:H:384:MET:N	2.37	0.54
1:A:92:VAL:HG12	1:C:131:ILE:HD11	1.89	0.54
1:F:75:MET:N	1:F:76:ALA:CB	2.68	0.54
1:F:75:MET:HB3	1:F:76:ALA:HB2	1.89	0.54
1:H:153:ASP:OD1	1:H:213:ILE:HG13	2.07	0.54
1:H:360:GLU:HG2	1:H:361:ARG:N	2.21	0.54
1:A:235:VAL:O	1:A:239:MET:HG3	2.07	0.54
1:A:144:VAL:HG22	1:A:178:VAL:HG11	1.88	0.54
1:G:391:SER:C	1:G:396:ASN:OD1	2.46	0.54
1:G:153:ASP:O	1:G:212:HIS:ND1	2.40	0.54
1:H:6:ILE:CG2	1:H:9:VAL:CG2	2.85	0.54
1:E:214:VAL:O	1:E:217:LEU:O	2.24	0.54
1:C:124:ARG:NH1	1:C:125:ASP:OD1	2.41	0.54
1:A:149:PRO:O	1:A:154:PHE:HB3	2.07	0.54
1:H:317:ALA:O	1:H:318:ALA:C	2.44	0.54
1:A:151:SER:OG	1:A:159:ARG:NH1	2.40	0.54
1:G:45:GLU:N	1:G:45:GLU:OE1	2.39	0.54
1:D:76:ALA:HB3	1:D:77:GLY:CA	2.37	0.54
1:C:273:HIS:HA	1:C:300:GLN:HE21	1.72	0.54
1:D:301:THR:HG23	1:D:382:LYS:HZ3	1.71	0.54
1:D:182:LEU:HB3	1:D:231:PHE:CE2	2.42	0.54
1:C:117:ILE:HD13	1:C:200:ARG:HD3	1.88	0.54
1:C:75:MET:O	1:C:76:ALA:HB3	2.08	0.54
1:G:158:GLY:HA2	1:G:161:ALA:HB3	1.89	0.54
1:H:6:ILE:HD13	1:H:57:MET:SD	2.48	0.54
1:F:209:VAL:HB	1:F:253:HIS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:296:TRP:CD2	1:H:338:LYS:HB3	2.42	0.54
1:E:264:VAL:HG11	1:E:293:SER:OG	2.07	0.54
1:E:284:ASN:O	1:E:285:TYR:CG	2.61	0.54
1:E:9:VAL:O	1:E:23:THR:OG1	2.18	0.54
1:E:76:ALA:N	1:E:77:GLY:HA2	2.22	0.54
1:C:70:ASP:OD2	1:C:73:MET:HB2	2.06	0.54
1:H:457:THR:HA	1:H:459:HIS:CD2	2.42	0.54
1:D:75:MET:HE2	1:D:212:HIS:CE1	2.43	0.54
1:C:74:PHE:N	1:C:74:PHE:CD1	2.73	0.54
1:H:435:ILE:HG21	1:H:438:VAL:HG23	1.90	0.54
1:B:231:PHE:HB2	1:B:236:LEU:HD13	1.90	0.54
1:E:340:LEU:HD11	1:E:397:VAL:HA	1.89	0.54
1:A:74:PHE:C	1:A:76:ALA:N	2.59	0.54
1:F:126:ARG:HH11	1:F:132:SER:HG	1.55	0.54
1:F:268:ALA:O	1:F:295:SER:HB3	2.06	0.54
1:C:117:ILE:O	1:C:121:LEU:HB2	2.08	0.54
1:D:404:ALA:O	1:D:414:LYS:NZ	2.38	0.54
1:D:227:SER:C	1:D:228:TYR:HD1	2.12	0.54
1:E:307:ARG:NH2	1:E:311:GLU:OE1	2.41	0.54
1:C:254:SER:HB2	1:C:259:ALA:HB1	1.90	0.54
1:F:290:ILE:HG23	1:F:291:VAL:H	1.73	0.54
1:B:190:VAL:HG11	1:B:239:MET:HE3	1.89	0.54
1:E:102:ALA:HB1	1:E:107:VAL:HB	1.91	0.54
1:F:4:ILE:HG22	1:F:48:THR:HB	1.90	0.54
1:C:163:THR:HB	1:C:166:PHE:HB3	1.89	0.54
1:D:72:TRP:O	1:D:73:MET:HB3	2.07	0.53
1:D:75:MET:CE	1:D:212:HIS:CE1	2.91	0.53
1:D:224:PHE:HE1	1:D:325:TYR:HH	1.54	0.53
1:B:38:SER:OG	1:B:39:ASP:N	2.40	0.53
1:D:97:GLU:HA	1:D:100:GLN:NE2	2.23	0.53
1:D:208:ALA:CB	1:D:253:HIS:HD2	2.21	0.53
1:H:424:ASP:OD1	1:H:426:VAL:N	2.38	0.53
1:H:453:THR:HG22	1:H:454:PRO:HD2	1.90	0.53
1:E:87:TRP:CZ2	1:E:455:LEU:O	2.61	0.53
1:H:436:THR:OG1	1:H:437:GLU:N	2.40	0.53
1:F:220:ARG:NH2	1:F:314:GLY:O	2.41	0.53
1:D:206:LYS:HG3	1:D:251:LEU:HB2	1.90	0.53
1:H:231:PHE:CE2	1:H:239:MET:HE3	2.43	0.53
1:A:194:VAL:CG2	1:A:239:MET:CE	2.75	0.53
1:H:439:PHE:CE1	1:H:444:ALA:HB2	2.42	0.53
1:E:40:SER:OG	1:E:42:PRO:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:SER:OG	1:E:39:ASP:OD1	2.25	0.53
1:G:407:ILE:HG23	1:G:415:LEU:HD12	1.90	0.53
1:C:217:LEU:CD2	1:C:224:PHE:CB	2.86	0.53
1:B:303:HIS:CD2	1:B:377:GLN:HG2	2.43	0.53
1:G:15:LEU:HA	1:G:395:ILE:HD11	1.90	0.53
1:G:15:LEU:HD11	1:G:411:GLU:OE2	2.08	0.53
1:H:10:THR:O	1:H:56:TRP:HA	2.07	0.53
1:F:5:ALA:HA	1:F:26:ILE:HA	1.90	0.53
1:G:10:THR:O	1:G:10:THR:HG23	2.07	0.53
1:F:75:MET:HE1	1:F:212:HIS:CE1	2.43	0.53
1:H:77:GLY:O	1:H:155:HIS:CG	2.60	0.53
1:A:346:GLY:O	1:A:368:ILE:N	2.41	0.53
1:H:86:ARG:HG2	1:H:87:TRP:CE2	2.43	0.53
1:A:100:GLN:OE1	1:A:451:PRO:HB2	2.07	0.53
1:F:6:ILE:N	1:F:25:VAL:O	2.42	0.53
1:D:13:ASP:OD1	1:D:14:GLY:N	2.42	0.53
1:F:273:HIS:ND1	1:F:276:TYR:CE2	2.76	0.53
1:D:182:LEU:HB3	1:D:231:PHE:HE2	1.74	0.53
1:D:38:SER:HB3	1:D:41:THR:HG22	1.89	0.53
1:F:290:ILE:HD12	1:F:337:ALA:HA	1.91	0.53
1:F:7:THR:O	1:F:52:GLY:HA3	2.08	0.53
1:B:391:SER:OG	1:B:391:SER:O	2.24	0.53
1:D:339:ILE:HD13	1:D:384:MET:HE3	1.91	0.53
1:H:68:LEU:CB	1:H:95:ILE:HG23	2.39	0.53
1:E:75:MET:CE	1:E:316:TRP:HH2	2.20	0.53
1:D:252:THR:HG21	1:D:263:SER:HB3	1.90	0.53
1:E:76:ALA:HB3	1:E:77:GLY:HA2	1.91	0.53
1:D:343:THR:OG1	1:D:343:THR:O	2.26	0.53
1:D:283:PRO:HB2	1:D:285:TYR:CD2	2.44	0.53
1:H:30:ASP:O	1:H:31:ARG:CB	2.56	0.53
1:A:37:PRO:HB2	1:A:38:SER:O	2.08	0.53
1:B:365:PRO:HG3	1:B:374:HIS:CE1	2.44	0.53
1:H:103:LEU:HD21	1:H:445:VAL:HG21	1.90	0.53
1:E:224:PHE:CD2	1:E:325:TYR:OH	2.48	0.53
1:A:283:PRO:O	1:A:287:ILE:HD12	2.09	0.53
1:D:380:VAL:HG13	1:D:384:MET:O	2.09	0.53
1:B:22:ALA:O	1:B:37:PRO:CB	2.47	0.53
1:F:206:LYS:HB2	1:F:251:LEU:HD12	1.90	0.53
1:B:138:PHE:HA	1:B:203:ASP:OD2	2.08	0.53
1:C:117:ILE:HG13	1:C:121:LEU:HD12	1.90	0.53
1:G:94:VAL:HG13	1:G:456:VAL:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:TRP:O	1:G:75:MET:HE2	2.09	0.53
1:A:287:ILE:HG22	1:A:291:VAL:HG21	1.90	0.53
1:H:253:HIS:HD2	1:H:273:HIS:HE1	1.48	0.53
1:G:124:ARG:HG3	1:G:125:ASP:N	2.23	0.53
1:D:412:THR:HG22	1:D:413:GLY:N	2.23	0.53
1:H:31:ARG:HH11	1:H:415:LEU:CD1	2.20	0.53
1:G:6:ILE:CG2	1:G:25:VAL:H	2.21	0.53
1:H:64:GLY:HA2	1:H:111:PHE:HD2	1.73	0.53
1:D:278:LEU:HA	1:D:325:TYR:HE1	1.71	0.53
1:B:76:ALA:H	1:B:77:GLY:HA2	1.73	0.53
1:H:96:GLU:HG2	1:H:127:ILE:HD11	1.89	0.53
1:D:351:ASP:O	1:D:354:ALA:N	2.42	0.53
1:H:45:GLU:O	1:H:45:GLU:HG3	2.09	0.53
1:G:324:PRO:O	1:G:328:ASN:HB3	2.09	0.53
1:A:14:GLY:HA3	1:A:59:PRO:HG2	1.91	0.53
1:C:41:THR:HB	1:C:42:PRO:O	2.09	0.53
1:A:299:LEU:HD22	1:A:329:GLU:HB2	1.91	0.53
1:B:348:PRO:HG2	1:B:353:LEU:HD21	1.90	0.53
1:A:373:PHE:O	1:A:377:GLN:HG2	2.08	0.53
1:G:71:ALA:O	1:G:74:PHE:HB2	2.09	0.53
1:F:277:THR:O	1:F:278:LEU:HB2	2.09	0.52
1:F:70:ASP:OD1	1:F:72:TRP:N	2.42	0.52
1:G:252:THR:HG21	1:G:271:LEU:HD22	1.91	0.52
1:H:61:TYR:CD2	1:H:372:HIS:NE2	2.78	0.52
1:B:68:LEU:HB3	1:B:95:ILE:HG23	1.91	0.52
1:F:45:GLU:HG2	1:F:46:GLY:N	2.24	0.52
1:C:41:THR:HB	1:C:42:PRO:C	2.29	0.52
1:F:395:ILE:O	1:F:399:ARG:N	2.29	0.52
1:H:56:TRP:CZ2	1:H:424:ASP:HB2	2.44	0.52
1:E:296:TRP:CE3	1:E:338:LYS:HB3	2.44	0.52
1:C:91:TYR:HE2	1:C:173:MET:HE1	1.75	0.52
1:F:205:LEU:O	1:F:250:VAL:HA	2.08	0.52
1:D:303:HIS:HB3	1:D:306:HIS:H	1.74	0.52
1:C:86:ARG:HA	1:H:86:ARG:HB2	1.90	0.52
1:B:257:VAL:HG23	1:B:277:THR:OG1	2.09	0.52
1:H:20:ARG:HB3	1:H:23:THR:HG21	1.92	0.52
1:B:340:LEU:HD12	1:B:397:VAL:HA	1.91	0.52
1:E:278:LEU:HA	1:E:325:TYR:CE1	2.43	0.52
1:C:25:VAL:HG21	1:C:57:MET:CE	2.40	0.52
1:H:30:ASP:N	1:H:442:GLY:HA3	2.20	0.52
1:E:264:VAL:HG11	1:E:293:SER:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:HIS:NE2	1:F:377:GLN:OE1	2.43	0.52
1:H:194:VAL:O	1:H:198:LEU:HD13	2.10	0.52
1:F:427:ASP:O	1:F:428:ASP:CB	2.41	0.52
1:C:28:GLU:O	1:C:29:GLY:C	2.47	0.52
1:H:453:THR:O	1:H:455:LEU:N	2.40	0.52
1:E:411:GLU:HB3	1:E:414:LYS:HD2	1.90	0.52
1:A:63:ASN:HA	1:A:341:LEU:CD2	2.39	0.52
1:E:323:GLU:CB	1:E:324:PRO:CD	2.83	0.52
1:D:341:LEU:H	1:D:397:VAL:CG1	2.23	0.52
1:D:32:PHE:CE1	1:D:415:LEU:O	2.59	0.52
1:F:117:ILE:HG21	1:F:200:ARG:HD2	1.91	0.52
1:F:140:ALA:HB2	1:F:204:MET:HE2	1.90	0.52
1:D:278:LEU:CA	1:D:325:TYR:HE1	2.23	0.52
1:E:286:LEU:O	1:E:290:ILE:HG13	2.10	0.52
1:H:235:VAL:O	1:H:238:VAL:HG12	2.10	0.52
1:D:10:THR:HB	1:D:56:TRP:CD1	2.44	0.52
1:E:73:MET:O	1:E:76:ALA:HB3	2.08	0.52
1:A:124:ARG:NH2	1:A:201:GLY:O	2.38	0.52
1:H:224:PHE:CD1	1:H:224:PHE:N	2.76	0.52
1:H:186:PRO:HG2	1:H:189:GLU:HG3	1.91	0.52
1:H:206:LYS:HA	1:H:251:LEU:HB2	1.90	0.52
1:E:207:ILE:CD1	1:E:236:LEU:HD23	2.39	0.52
1:D:36:GLY:HA3	1:D:41:THR:CG2	2.39	0.52
1:E:385:SER:O	1:E:387:LEU:N	2.43	0.52
1:A:69:LEU:HD11	1:A:91:TYR:HB3	1.92	0.52
1:B:206:LYS:HE3	1:B:272:ILE:HG13	1.90	0.52
1:C:70:ASP:CG	1:C:71:ALA:H	2.13	0.52
1:E:87:TRP:CH2	1:E:455:LEU:O	2.63	0.52
1:B:315:SER:OG	1:B:360:GLU:OE2	2.25	0.52
1:F:270:VAL:HG22	1:F:340:LEU:HD11	1.90	0.52
1:D:350:LYS:HD2	1:D:459:HIS:HA	1.92	0.52
1:B:292:ALA:O	1:B:294:ASP:OD1	2.28	0.52
1:E:252:THR:CG2	1:E:271:LEU:HA	2.29	0.52
1:D:181:GLN:CG	1:D:182:LEU:H	2.23	0.52
1:E:45:GLU:C	1:E:47:ALA:N	2.61	0.52
1:H:232:SER:OG	1:H:235:VAL:CG2	2.57	0.52
1:H:232:SER:HG	1:H:235:VAL:HG23	1.73	0.52
1:G:303:HIS:O	1:G:307:ARG:HB3	2.10	0.52
1:C:298:GLY:HA3	1:C:342:ASN:ND2	2.24	0.52
1:D:103:LEU:HD21	1:D:445:VAL:HG21	1.92	0.52
1:F:59:PRO:CG	1:F:394:THR:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ASP:O	1:C:450:LEU:HD12	2.09	0.52
1:E:307:ARG:CZ	1:E:311:GLU:OE1	2.58	0.52
1:A:235:VAL:HA	1:A:238:VAL:HG12	1.90	0.52
1:A:66:VAL:HA	1:A:345:ALA:CB	2.39	0.52
1:D:252:THR:HG21	1:D:263:SER:CB	2.39	0.52
1:B:135:ALA:O	1:B:137:ILE:HG13	2.09	0.52
1:H:32:PHE:N	1:H:414:LYS:O	2.31	0.52
1:G:348:PRO:HG2	1:G:353:LEU:HG	1.92	0.52
1:F:300:GLN:OE1	1:F:344:ASP:OD1	2.28	0.52
1:A:276:TYR:CE1	1:A:320:LEU:HD22	2.45	0.52
1:D:222:VAL:CG2	1:D:223:GLY:H	2.23	0.52
1:A:213:ILE:HG23	1:A:216:THR:CG2	2.40	0.52
1:B:30:ASP:O	1:B:31:ARG:O	2.28	0.52
1:C:144:VAL:HG13	1:C:178:VAL:HG13	1.91	0.52
1:D:148:GLY:HA3	1:D:171:ASP:HB3	1.92	0.52
1:E:226:ARG:CD	1:E:228:TYR:CE2	2.89	0.51
1:A:271:LEU:HD13	1:A:297:ALA:HA	1.90	0.51
1:H:107:VAL:HG23	1:H:372:HIS:HE1	1.66	0.51
1:G:129:ALA:HB3	1:G:131:ILE:CG1	2.37	0.51
1:B:143:ILE:HG22	1:B:208:ALA:HB2	1.92	0.51
1:B:56:TRP:O	1:B:420:LEU:HA	2.09	0.51
1:C:255:VAL:O	1:C:278:LEU:HG	2.10	0.51
1:B:64:GLY:CA	1:B:397:VAL:HG11	2.40	0.51
1:F:70:ASP:O	1:F:74:PHE:CE2	2.63	0.51
1:F:225:ASP:O	1:F:226:ARG:CB	2.55	0.51
1:H:255:VAL:C	1:H:278:LEU:CD1	2.79	0.51
1:E:329:GLU:OE1	1:E:382:LYS:HE3	2.11	0.51
1:D:181:GLN:HG2	1:D:182:LEU:H	1.75	0.51
1:D:36:GLY:CA	1:D:41:THR:HG21	2.41	0.51
1:C:97:GLU:OE1	1:C:456:VAL:HG12	2.09	0.51
1:B:301:THR:OG1	1:B:378:SER:OG	2.10	0.51
1:A:287:ILE:O	1:A:291:VAL:N	2.39	0.51
1:D:143:ILE:HG23	1:D:206:LYS:HB3	1.91	0.51
1:H:285:TYR:CE1	1:H:286:LEU:HD12	2.45	0.51
1:D:220:ARG:C	1:D:222:VAL:HG12	2.30	0.51
1:H:31:ARG:HH11	1:H:415:LEU:HG	1.75	0.51
1:E:252:THR:HG21	1:E:263:SER:HB3	1.92	0.51
1:B:77:GLY:HA3	1:B:155:HIS:CB	2.41	0.51
1:G:143:ILE:HG12	1:G:206:LYS:HD3	1.91	0.51
1:C:105:ASN:OD1	1:C:373:PHE:CE2	2.63	0.51
1:B:127:ILE:HD12	1:B:137:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:SER:O	1:H:266:LEU:N	2.42	0.51
1:F:257:VAL:CG2	1:F:277:THR:HG21	2.39	0.51
1:F:209:VAL:HG11	1:F:259:ALA:O	2.10	0.51
1:D:341:LEU:HA	1:D:375:TRP:CZ2	2.46	0.51
1:B:113:THR:HA	1:B:140:ALA:HB2	1.91	0.51
1:D:37:PRO:O	1:D:39:ASP:O	2.28	0.51
1:F:341:LEU:HA	1:F:375:TRP:CZ2	2.45	0.51
1:C:153:ASP:HB3	1:C:212:HIS:HB3	1.91	0.51
1:A:151:SER:HA	1:A:156:PHE:HD1	1.75	0.51
1:D:227:SER:O	1:D:228:TYR:HD1	1.92	0.51
1:F:303:HIS:NE2	1:F:377:GLN:CD	2.64	0.51
1:D:90:ARG:NH2	1:D:93:GLU:OE2	2.44	0.51
1:A:204:MET:HB3	1:A:249:PRO:HG2	1.92	0.51
1:B:391:SER:HB2	1:B:394:THR:CG2	2.38	0.51
1:A:209:VAL:N	1:A:253:HIS:O	2.43	0.51
1:H:67:HIS:HA	1:H:112:ASP:OD1	2.10	0.51
1:F:118:GLU:HG2	1:F:119:PRO:HD3	1.92	0.51
1:B:117:ILE:HD13	1:B:200:ARG:HD2	1.92	0.51
1:C:26:ILE:HD11	1:C:41:THR:OG1	2.09	0.51
1:F:409:SER:OG	1:F:414:LYS:HE3	2.10	0.51
1:A:310:LEU:HD22	1:A:360:GLU:HG2	1.93	0.51
1:A:68:LEU:HD11	1:A:137:ILE:HD12	1.92	0.51
1:E:419:VAL:CG2	1:E:435:ILE:HG23	2.41	0.51
1:F:388:GLU:OE1	1:F:388:GLU:N	2.44	0.51
1:E:213:ILE:HG21	1:E:216:THR:CG2	2.40	0.51
1:E:140:ALA:HB2	1:E:204:MET:HG2	1.91	0.51
1:H:333:ILE:HG21	1:H:384:MET:HG3	1.93	0.51
1:F:409:SER:O	1:F:414:LYS:HD2	2.11	0.51
1:D:118:GLU:HB2	1:D:119:PRO:HD3	1.93	0.51
1:E:259:ALA:O	1:E:262:THR:N	2.44	0.51
1:E:272:ILE:HG22	1:E:273:HIS:ND1	2.26	0.51
1:F:356:LEU:HD23	1:F:360:GLU:OE1	2.11	0.51
1:C:143:ILE:HB	1:C:146:MET:HG3	1.93	0.51
1:A:302:VAL:HB	1:A:321:ALA:HA	1.92	0.51
1:E:121:LEU:HD11	1:E:202:VAL:HG12	1.92	0.51
1:G:68:LEU:CB	1:G:95:ILE:CG2	2.70	0.51
1:H:77:GLY:O	1:H:155:HIS:NE2	2.43	0.51
1:E:180:HIS:CG	1:E:181:GLN:H	2.28	0.51
1:D:181:GLN:C	1:D:183:SER:H	2.14	0.51
1:B:100:GLN:HG2	1:B:450:LEU:HD11	1.93	0.51
1:E:284:ASN:OD1	1:E:285:TYR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:GLY:HA3	1:E:342:ASN:ND2	2.26	0.51
1:E:258:GLU:O	1:E:260:LEU:N	2.44	0.51
1:B:391:SER:H	1:B:393:ALA:N	2.08	0.51
1:D:218:VAL:O	1:D:218:VAL:HG23	2.11	0.51
1:H:152:ALA:HB1	1:H:213:ILE:HG12	1.93	0.51
1:E:213:ILE:CG2	1:E:216:THR:HB	2.41	0.51
1:B:155:HIS:CD2	1:B:155:HIS:C	2.84	0.51
1:H:328:ASN:HD22	1:H:328:ASN:C	2.13	0.51
1:F:261:ASP:HB2	1:F:286:LEU:HD11	1.93	0.51
1:C:399[B]:ARG:HH11	1:C:404:ALA:HB1	1.75	0.51
1:G:144:VAL:HG11	1:G:239:MET:HE1	1.93	0.51
1:E:117:ILE:HG23	1:E:121:LEU:HD13	1.93	0.51
1:A:258:GLU:C	1:A:260:LEU:H	2.15	0.51
1:C:226:ARG:HG2	1:C:228:TYR:CZ	2.46	0.50
1:A:288:ASP:HA	1:A:291:VAL:CB	2.40	0.50
1:F:61:TYR:HH	1:F:432:LEU:HD22	1.73	0.50
1:F:203:ASP:C	1:F:204:MET:HG3	2.31	0.50
1:D:301:THR:CG2	1:D:302:VAL:N	2.73	0.50
1:H:70:ASP:O	1:H:74:PHE:CD1	2.64	0.50
1:C:204:MET:HB2	1:C:251:LEU:HD11	1.93	0.50
1:F:144:VAL:HA	1:F:178:VAL:HG11	1.92	0.50
1:C:186:PRO:O	1:C:190:VAL:HG23	2.11	0.50
1:A:221:SER:OG	1:G:44:PRO:HB3	2.11	0.50
1:A:70:ASP:CG	1:A:71:ALA:H	2.08	0.50
1:A:191:ARG:HD2	1:A:238:VAL:HG23	1.89	0.50
1:F:113:THR:HG21	1:F:206:LYS:HZ3	1.76	0.50
1:B:146:MET:SD	1:B:212:HIS:CD2	3.05	0.50
1:D:36:GLY:HA3	1:D:41:THR:HG23	1.92	0.50
1:E:55:ARG:HG2	1:E:422:ASP:OD1	2.11	0.50
1:E:385:SER:OG	1:E:388:GLU:CD	2.49	0.50
1:B:203:ASP:O	1:B:248:VAL:HB	2.12	0.50
1:F:25:VAL:HG22	1:F:35:VAL:HG13	1.93	0.50
1:D:92:VAL:HG22	1:D:119:PRO:HA	1.93	0.50
1:C:191:ARG:HB2	1:C:238:VAL:CG1	2.40	0.50
1:C:421:LEU:CD1	1:C:425:PRO:HG3	2.40	0.50
1:D:150:PHE:O	1:D:159:ARG:HG2	2.11	0.50
1:E:332:LEU:O	1:E:337:ALA:HB3	2.11	0.50
1:C:7:THR:O	1:C:8:ASN:OD1	2.29	0.50
1:D:222:VAL:HG22	1:D:223:GLY:O	2.11	0.50
1:H:340:LEU:CD2	1:H:397:VAL:HG13	2.41	0.50
1:G:452:THR:O	1:G:454:PRO:HD3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:LEU:HD21	1:H:104:ARG:HH21	1.77	0.50
1:D:430:ARG:O	1:D:433:ARG:HB2	2.12	0.50
1:B:280:GLN:H	1:B:280:GLN:CD	2.13	0.50
1:H:6:ILE:HG21	1:H:25:VAL:CG1	2.41	0.50
1:C:6:ILE:CG2	1:C:25:VAL:CA	2.89	0.50
1:H:182:LEU:HD12	1:H:231:PHE:HZ	1.75	0.50
1:A:235:VAL:HA	1:A:238:VAL:HG11	1.93	0.50
1:D:276:TYR:CD1	1:D:325:TYR:HB3	2.47	0.50
1:D:148:GLY:O	1:D:154:PHE:CD2	2.48	0.50
1:F:118:GLU:HG3	1:F:119:PRO:HD3	1.93	0.50
1:H:240:VAL:HG12	1:H:241:GLU:H	1.76	0.50
1:G:421:LEU:HD13	1:G:432:LEU:HA	1.92	0.50
1:C:104:ARG:HG2	1:C:447:ARG:NH1	2.26	0.50
1:F:153:ASP:HB3	1:F:212:HIS:HB3	1.94	0.50
1:H:360:GLU:CG	1:H:361:ARG:N	2.75	0.50
1:H:30:ASP:O	1:H:31:ARG:HB2	2.12	0.50
1:G:37:PRO:HA	1:G:41:THR:HG23	1.94	0.50
1:G:61:TYR:HB2	1:G:107:VAL:HA	1.93	0.50
1:C:394:THR:OG1	1:C:395:ILE:N	2.44	0.50
1:G:90:ARG:HD3	1:G:455:LEU:HD21	1.94	0.50
1:F:35:VAL:HG23	1:F:412:THR:HG22	1.94	0.50
1:B:356:LEU:O	1:B:361:ARG:NH1	2.44	0.50
1:C:171:ASP:O	1:C:175:GLU:HG3	2.11	0.50
1:B:7:THR:HA	1:B:24:THR:HG23	1.92	0.50
1:F:224:PHE:CD1	1:F:224:PHE:N	2.80	0.50
1:D:412:THR:CG2	1:D:413:GLY:N	2.75	0.50
1:E:252:THR:HG21	1:E:271:LEU:CD2	2.42	0.50
1:B:273:HIS:ND1	1:B:273:HIS:O	2.44	0.50
1:E:285:TYR:CD1	1:E:285:TYR:C	2.84	0.50
1:C:96:GLU:O	1:C:100:GLN:HG3	2.10	0.50
1:A:251:LEU:HD11	1:A:270:VAL:CB	2.30	0.50
1:B:68:LEU:CB	1:B:95:ILE:HG23	2.42	0.50
1:D:180:HIS:O	1:D:181:GLN:CB	2.60	0.50
1:C:417:ASP:HA	1:C:439:PHE:O	2.12	0.50
1:H:456:VAL:HG13	1:H:457:THR:H	1.76	0.50
1:D:70:ASP:OD2	1:D:72:TRP:O	2.29	0.50
1:D:328:ASN:O	1:D:331:ASN:CB	2.58	0.50
1:D:387:LEU:O	1:D:390:ILE:CB	2.58	0.50
1:F:282:ILE:HB	1:F:283:PRO:HA	1.94	0.50
1:E:45:GLU:O	1:E:47:ALA:HB2	2.11	0.50
1:H:317:ALA:O	1:H:320:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:ASP:OD1	1:G:269:ASP:N	2.43	0.50
1:D:206:LYS:HE3	1:D:272:ILE:HG13	1.93	0.50
1:F:428:ASP:OD2	1:F:430:ARG:HD3	2.09	0.50
1:H:429:ILE:HG13	1:H:432:LEU:HD13	1.93	0.50
1:D:276:TYR:HD1	1:D:325:TYR:HB3	1.77	0.50
1:B:67:HIS:HA	1:B:112:ASP:OD1	2.12	0.50
1:E:371:ASP:OD1	1:E:372:HIS:ND1	2.42	0.50
1:H:435:ILE:HG21	1:H:438:VAL:CG2	2.42	0.50
1:C:131:ILE:N	1:C:131:ILE:HD13	2.26	0.50
1:H:97:GLU:OE1	1:H:451:PRO:HB2	2.12	0.50
1:D:6:ILE:CA	1:D:50:VAL:CG1	2.74	0.49
1:E:429:ILE:C	1:E:431:ASN:H	2.14	0.49
1:B:153:ASP:CB	1:B:212:HIS:HB3	2.42	0.49
1:F:356:LEU:HD23	1:F:360:GLU:CD	2.33	0.49
1:G:303:HIS:HB2	1:G:306:HIS:HB2	1.94	0.49
1:G:303:HIS:HB2	1:G:306:HIS:CB	2.42	0.49
1:G:344:ASP:O	1:G:345:ALA:HB2	2.11	0.49
1:D:56:TRP:CZ2	1:D:424:ASP:HB2	2.47	0.49
1:B:84:LEU:HD12	1:B:150:PHE:CZ	2.47	0.49
1:C:274:ALA:HB3	1:C:298:GLY:O	2.12	0.49
1:H:455:LEU:HD12	1:H:456:VAL:H	1.76	0.49
1:G:367:THR:HG22	1:G:369:GLY:H	1.77	0.49
1:F:146:MET:SD	1:F:212:HIS:CD2	3.04	0.49
1:A:459:HIS:CB	1:A:460:PRO:CA	2.85	0.49
1:B:165:THR:O	1:B:169:ARG:HB2	2.11	0.49
1:A:217:LEU:HG	1:A:225:ASP:H	1.78	0.49
1:B:384:MET:CE	1:B:389:ALA:HA	2.42	0.49
1:G:127:ILE:CG1	1:G:128:ASN:N	2.74	0.49
1:D:32:PHE:CD2	1:D:412:THR:N	2.73	0.49
1:E:217:LEU:HD21	1:E:223:GLY:O	2.13	0.49
1:C:14:GLY:O	1:C:395:ILE:HD11	2.12	0.49
1:B:143:ILE:HG23	1:B:206:LYS:HB3	1.95	0.49
1:G:379:MET:HB3	1:G:384:MET:SD	2.52	0.49
1:D:337:ALA:O	1:D:338:LYS:HB2	2.12	0.49
1:C:253:HIS:HD1	1:C:273:HIS:CE1	2.29	0.49
1:H:368:ILE:HA	1:H:371:ASP:HB2	1.94	0.49
1:E:145:GLY:C	1:E:179:GLY:HA2	2.33	0.49
1:B:66:VAL:HG22	1:B:110:VAL:CG2	2.43	0.49
1:D:237:GLU:HA	1:D:240:VAL:HG22	1.95	0.49
1:A:409:SER:O	1:A:414:LYS:NZ	2.35	0.49
1:G:111:PHE:CE2	1:G:397:VAL:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ARG:O	1:H:237:GLU:HG3	2.12	0.49
1:F:263:SER:HA	1:F:266:LEU:CD1	2.42	0.49
1:F:302:VAL:HG12	1:F:303:HIS:H	1.77	0.49
1:F:10:THR:HA	1:F:21:PRO:HA	1.95	0.49
1:B:260:LEU:O	1:B:264:VAL:HG23	2.11	0.49
1:H:182:LEU:HD13	1:H:239:MET:CE	2.41	0.49
1:E:61:TYR:OH	1:E:432:LEU:HB3	2.13	0.49
1:A:27:VAL:HG12	1:A:31:ARG:O	2.13	0.49
1:H:341:LEU:HD12	1:H:375:TRP:CE3	2.48	0.49
1:D:148:GLY:C	1:D:154:PHE:HD2	2.14	0.49
1:A:91:TYR:HE2	1:A:173:MET:HE1	1.78	0.49
1:H:23:THR:CG2	1:H:37:PRO:HG3	2.40	0.49
1:A:252:THR:HG22	1:A:270:VAL:O	2.12	0.49
1:F:428:ASP:CG	1:F:430:ARG:CD	2.79	0.49
1:G:6:ILE:CD1	1:G:9:VAL:HG11	2.43	0.49
1:F:121:LEU:HD22	1:F:124:ARG:HE	1.77	0.49
1:B:256:SER:OG	1:B:258:GLU:O	2.28	0.49
1:B:153:ASP:HA	1:B:212:HIS:O	2.12	0.49
1:E:293:SER:O	1:E:294:ASP:HB3	2.12	0.49
1:H:175:GLU:O	1:H:178:VAL:CG2	2.60	0.49
1:A:315:SER:O	1:A:316:TRP:HB3	2.13	0.49
1:C:377:GLN:HA	1:C:429:ILE:HG21	1.95	0.49
1:B:66:VAL:HG22	1:B:110:VAL:HG22	1.94	0.49
1:H:277:THR:CG2	1:H:282:ILE:HG12	2.42	0.49
1:D:282:ILE:HB	1:D:287:ILE:HD11	1.94	0.49
1:B:111:PHE:CD2	1:B:204:MET:HE1	2.44	0.49
1:D:152:ALA:O	1:D:153:ASP:HB2	2.12	0.49
1:D:6:ILE:HG23	1:D:50:VAL:CG1	2.42	0.49
1:G:68:LEU:HB2	1:G:95:ILE:HG23	1.91	0.49
1:A:74:PHE:C	1:A:76:ALA:H	2.16	0.49
1:F:282:ILE:HD12	1:F:282:ILE:H	1.78	0.49
1:F:109:THR:OG1	1:F:136:ARG:NH2	2.46	0.49
1:D:208:ALA:HA	1:D:253:HIS:HB3	1.95	0.49
1:C:205:LEU:O	1:C:251:LEU:CD1	2.60	0.49
1:B:209:VAL:HG13	1:B:236:LEU:HD21	1.93	0.49
1:H:55:ARG:HD3	1:H:420:LEU:CD1	2.43	0.49
1:H:253:HIS:NE2	1:H:273:HIS:CE1	2.69	0.49
1:E:212:HIS:O	1:E:213:ILE:CG1	2.61	0.49
1:H:75:MET:SD	1:H:215:PHE:CE2	3.06	0.49
1:A:254:SER:CB	1:A:259:ALA:CB	2.84	0.49
1:A:346:GLY:O	1:A:368:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:HG3	1:A:28:GLU:O	2.12	0.49
1:F:68:LEU:CD1	1:F:95:ILE:HG23	2.37	0.49
1:A:145:GLY:N	1:A:179:GLY:HA2	2.26	0.49
1:A:445:VAL:C	1:A:447:ARG:HH12	2.09	0.49
1:A:140:ALA:O	1:A:197:TYR:OH	2.24	0.49
1:B:340:LEU:HG	1:B:397:VAL:HG13	1.95	0.49
1:B:145:GLY:H	1:B:179:GLY:HA2	1.78	0.49
1:B:395:ILE:CD1	1:B:399[B]:ARG:NH2	2.75	0.48
1:F:325:TYR:O	1:F:329:GLU:CD	2.48	0.48
1:A:282:ILE:HG23	1:A:328:ASN:OD1	2.13	0.48
1:H:283:PRO:HD2	1:H:286:LEU:HD13	1.95	0.48
1:H:155:HIS:HE1	1:H:157:ALA:HB3	1.77	0.48
1:G:6:ILE:CD1	1:G:9:VAL:CG2	2.91	0.48
1:C:206:LYS:HZ1	1:C:253:HIS:HB2	1.78	0.48
1:D:303:HIS:CB	1:D:306:HIS:H	2.26	0.48
1:B:365:PRO:HG3	1:B:374:HIS:NE2	2.28	0.48
1:E:286:LEU:HA	1:E:289:LYS:HB3	1.94	0.48
1:A:126:ARG:CG	1:A:126:ARG:HH11	2.22	0.48
1:G:112:ASP:OD2	1:G:115:ASN:ND2	2.37	0.48
1:C:428:ASP:HB3	1:C:431:ASN:ND2	2.28	0.48
1:A:117:ILE:HD13	1:A:200:ARG:HE	1.78	0.48
1:A:251:LEU:HA	1:A:270:VAL:HB	1.95	0.48
1:E:40:SER:O	1:E:41:THR:OG1	2.29	0.48
1:D:20:ARG:O	1:D:23:THR:CG2	2.61	0.48
1:A:82:GLU:OE2	1:F:162:ALA:HB1	2.14	0.48
1:C:303:HIS:CE1	1:C:306:HIS:HB2	2.48	0.48
1:G:76:ALA:HB1	1:G:77:GLY:C	2.33	0.48
1:H:231:PHE:CE2	1:H:239:MET:CE	2.95	0.48
1:B:254:SER:O	1:B:273:HIS:CE1	2.66	0.48
1:G:142:THR:OG1	1:G:143:ILE:N	2.46	0.48
1:F:145:GLY:HA2	1:F:179:GLY:O	2.13	0.48
1:H:350:LYS:HB3	1:H:459:HIS:CE1	2.48	0.48
1:D:156:PHE:O	1:D:159:ARG:HG3	2.12	0.48
1:B:309:GLY:O	1:B:312:ASP:HB2	2.13	0.48
1:B:387:LEU:CB	1:B:388:GLU:HA	2.43	0.48
1:B:399[B]:ARG:CG	1:B:399[B]:ARG:HH11	2.25	0.48
1:E:341:LEU:HD13	1:E:375:TRP:CE3	2.49	0.48
1:A:374:HIS:CD2	1:A:374:HIS:C	2.87	0.48
1:G:207:ILE:HD12	1:G:239:MET:SD	2.54	0.48
1:F:30:ASP:O	1:F:416:ALA:N	2.44	0.48
1:F:210:SER:HA	1:F:229:GLN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:HIS:CE1	1:C:114:HIS:HB3	2.47	0.48
1:A:149:PRO:HA	1:A:154:PHE:CD2	2.48	0.48
1:F:303:HIS:CE1	1:F:377:GLN:HG2	2.48	0.48
1:B:165:THR:HG21	1:G:354:ALA:HB3	1.95	0.48
1:A:288:ASP:HA	1:A:291:VAL:CG2	2.43	0.48
1:H:75:MET:SD	1:H:215:PHE:HE2	2.36	0.48
1:G:37:PRO:HA	1:G:41:THR:CG2	2.44	0.48
1:H:275:ASN:OD1	1:H:329:GLU:CG	2.58	0.48
1:C:4:ILE:CG2	1:C:5:ALA:H	2.25	0.48
1:C:4:ILE:CG2	1:C:5:ALA:N	2.75	0.48
1:G:325:TYR:O	1:G:329:GLU:N	2.44	0.48
1:D:259:ALA:CA	1:D:262:THR:HG22	2.44	0.48
1:A:456:VAL:O	1:A:456:VAL:HG12	2.13	0.48
1:H:356:LEU:CD1	1:H:360:GLU:HG3	2.43	0.48
1:A:13:ASP:C	1:A:410:VAL:CG2	2.74	0.48
1:A:235:VAL:O	1:A:238:VAL:HG13	2.11	0.48
1:E:263:SER:HB3	1:E:271:LEU:HD22	1.96	0.48
1:C:281:GLU:HB2	1:C:328:ASN:OD1	2.14	0.48
1:D:136:ARG:CZ	1:D:415:LEU:CD1	2.92	0.48
1:E:148:GLY:HA3	1:E:171:ASP:OD1	2.14	0.48
1:E:379:MET:HB3	1:E:384:MET:HG3	1.95	0.48
1:F:260:LEU:HA	1:F:263:SER:OG	2.13	0.48
1:D:97:GLU:OE1	1:D:455:LEU:HB2	2.14	0.48
1:C:146:MET:SD	1:C:212:HIS:HB2	2.54	0.48
1:H:333:ILE:CD1	1:H:379:MET:SD	3.02	0.48
1:C:310:LEU:O	1:C:314:GLY:N	2.31	0.48
1:H:386:PRO:O	1:H:389:ALA:N	2.47	0.48
1:H:251:LEU:HD13	1:H:272:ILE:HD11	1.96	0.48
1:G:6:ILE:CG1	1:G:9:VAL:CG2	2.90	0.48
1:D:181:GLN:CG	1:D:185:LEU:HD11	2.44	0.48
1:A:182:LEU:HD22	1:A:185:LEU:HD12	1.96	0.48
1:C:367:THR:O	1:C:371:ASP:HB3	2.14	0.48
1:C:117:ILE:CG1	1:C:121:LEU:HD12	2.44	0.48
1:H:87:TRP:HB3	1:H:94:VAL:CG2	2.42	0.48
1:B:236:LEU:HD23	1:B:266:LEU:HD11	1.95	0.48
1:F:168:ASP:O	1:F:172:SER:OG	2.26	0.48
1:B:108:THR:HG21	1:B:417:ASP:HB3	1.96	0.48
1:E:7:THR:O	1:E:52:GLY:HA3	2.14	0.48
1:H:13:ASP:N	1:H:13:ASP:OD1	2.24	0.48
1:F:257:VAL:HG21	1:F:280:GLN:HB3	1.96	0.48
1:D:339:ILE:CG2	1:D:340:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:290:ILE:HA	1:H:293:SER:OG	2.13	0.48
1:B:326:ALA:HA	1:B:329:GLU:HG3	1.96	0.48
1:F:113:THR:HG21	1:F:206:LYS:HZ2	1.79	0.48
1:F:112:ASP:OD2	1:F:115:ASN:ND2	2.47	0.48
1:H:425:PRO:CB	1:H:432:LEU:HD12	2.44	0.48
1:A:182:LEU:CD2	1:A:185:LEU:HD12	2.43	0.48
1:C:62:VAL:HG21	1:C:407:ILE:HG22	1.95	0.48
1:F:45:GLU:C	1:F:47:ALA:N	2.64	0.48
1:E:306:HIS:O	1:E:310:LEU:N	2.27	0.48
1:B:187:ARG:HA	1:B:190:VAL:CG2	2.44	0.48
1:D:103:LEU:HD12	1:D:107:VAL:O	2.14	0.48
1:A:316:TRP:CG	1:A:317:ALA:N	2.81	0.48
1:F:27:VAL:HG11	1:F:442:GLY:HA3	1.96	0.48
1:C:53:ASN:O	1:C:55:ARG:HG3	2.14	0.48
1:E:429:ILE:O	1:E:432:LEU:CD1	2.38	0.48
1:G:286:LEU:O	1:G:287:ILE:C	2.51	0.48
1:A:272:ILE:HD12	1:A:272:ILE:H	1.78	0.48
1:D:68:LEU:CD1	1:D:95:ILE:CG2	2.84	0.48
1:E:257:VAL:HG22	1:E:277:THR:HG21	1.95	0.48
1:H:110:VAL:N	1:H:136:ARG:O	2.41	0.48
1:G:144:VAL:HG13	1:G:178:VAL:CG1	2.44	0.48
1:D:252:THR:HG21	1:D:263:SER:OG	2.13	0.48
1:F:52:GLY:O	1:F:55:ARG:HB2	2.14	0.48
1:A:416:ALA:HB3	1:A:442:GLY:N	2.28	0.48
1:C:330:ARG:O	1:C:334:SER:N	2.43	0.48
1:F:224:PHE:N	1:F:224:PHE:HD1	2.12	0.47
1:F:255:VAL:CA	1:F:276:TYR:O	2.62	0.47
1:F:75:MET:H	1:F:76:ALA:CB	2.24	0.47
1:D:153:ASP:HA	1:D:212:HIS:HB3	1.96	0.47
1:D:152:ALA:HB1	1:D:213:ILE:HG12	1.95	0.47
1:H:269:ASP:O	1:H:296:TRP:HB2	2.14	0.47
1:E:213:ILE:HG23	1:E:216:THR:HB	1.96	0.47
1:C:262:THR:HG22	1:C:262:THR:O	2.12	0.47
1:E:214:VAL:HG22	1:E:215:PHE:CE1	2.48	0.47
1:A:414:LYS:HE3	1:A:414:LYS:HB2	1.67	0.47
1:E:12:ILE:HB	1:E:58:VAL:HG12	1.96	0.47
1:E:212:HIS:O	1:E:213:ILE:HG13	2.14	0.47
1:H:62:VAL:HG13	1:H:109:THR:HB	1.96	0.47
1:D:264:VAL:HG11	1:D:289:LYS:HG2	1.95	0.47
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.75	0.47
1:G:350:LYS:HA	1:G:350:LYS:HD2	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:NH2	1:A:417:ASP:OD2	2.35	0.47
1:D:3:THR:HA	1:D:27:VAL:O	2.13	0.47
1:B:94:VAL:HG23	1:B:455:LEU:HD23	1.95	0.47
1:A:118:GLU:HB2	1:A:119:PRO:HD3	1.95	0.47
1:H:198:LEU:O	1:H:201:GLY:HA2	2.14	0.47
1:A:191:ARG:CD	1:A:238:VAL:HG22	2.42	0.47
1:G:6:ILE:CD1	1:G:9:VAL:CG1	2.91	0.47
1:A:112:ASP:OD2	1:A:115:ASN:HB2	2.14	0.47
1:A:111:PHE:HD1	1:A:138:PHE:HB2	1.79	0.47
1:C:341:LEU:HD13	1:C:375:TRP:CD2	2.48	0.47
1:A:218:VAL:HG13	1:A:219:ASP:HB2	1.95	0.47
1:G:38:SER:C	1:G:40:SER:H	2.17	0.47
1:H:447:ARG:HH11	1:H:447:ARG:HB3	1.79	0.47
1:H:260:LEU:HD11	1:H:271:LEU:HD22	1.96	0.47
1:A:153:ASP:CB	1:A:212:HIS:HB3	2.44	0.47
1:G:144:VAL:HB	1:G:207:ILE:HA	1.95	0.47
1:E:77:GLY:O	1:E:78:PRO:C	2.48	0.47
1:E:198:LEU:O	1:E:200:ARG:N	2.48	0.47
1:C:191:ARG:HB2	1:C:238:VAL:HG11	1.95	0.47
1:G:365:PRO:HG2	1:G:366:TRP:CE3	2.49	0.47
1:D:352:HIS:O	1:D:356:LEU:HD13	2.13	0.47
1:A:275:ASN:O	1:A:277:THR:HG23	2.14	0.47
1:A:75:MET:HE1	1:A:212:HIS:CE1	2.21	0.47
1:G:395:ILE:O	1:G:399:ARG:HG3	2.14	0.47
1:C:67:HIS:HE1	1:C:114:HIS:HB2	1.80	0.47
1:F:58:VAL:HB	1:F:59:PRO:HD2	1.97	0.47
1:H:330:ARG:O	1:H:334:SER:OG	2.22	0.47
1:D:83:TYR:C	1:D:83:TYR:CD1	2.88	0.47
1:H:11:LEU:HB3	1:H:23:THR:OG1	2.15	0.47
1:A:207:ILE:CG2	1:A:252:THR:HA	2.44	0.47
1:E:324:PRO:O	1:E:327:THR:N	2.48	0.47
1:F:277:THR:CG2	1:F:280:GLN:HB2	2.43	0.47
1:A:277:THR:OG1	1:A:280:GLN:O	2.11	0.47
1:H:180:HIS:C	1:H:182:LEU:N	2.68	0.47
1:C:319:ALA:O	1:C:323:GLU:HG3	2.15	0.47
1:E:213:ILE:CG2	1:E:216:THR:CG2	2.92	0.47
1:C:270:VAL:HG12	1:C:272:ILE:HG12	1.97	0.47
1:A:447:ARG:HB2	1:A:447:ARG:CZ	2.44	0.47
1:B:343:THR:OG1	1:B:371:ASP:HB2	2.14	0.47
1:F:236:LEU:HB3	1:F:266:LEU:HD21	1.97	0.47
1:E:315:SER:O	1:E:317:ALA:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:MET:HE3	1:E:316:TRP:CH2	2.50	0.47
1:G:399:ARG:HG2	1:G:404:ALA:HB2	1.96	0.47
1:C:341:LEU:HD12	1:C:342:ASN:N	2.30	0.47
1:C:330:ARG:HA	1:C:333:ILE:HB	1.96	0.47
1:G:191:ARG:NH2	1:G:241:GLU:OE1	2.37	0.47
1:F:31:ARG:HD3	1:F:413:GLY:HA2	1.97	0.47
1:A:340:LEU:HD11	1:A:397:VAL:HA	1.97	0.47
1:B:391:SER:H	1:B:394:THR:H	1.62	0.47
1:D:339:ILE:HD13	1:D:384:MET:CE	2.44	0.47
1:H:230:THR:HB	1:H:231:PHE:HD1	1.78	0.47
1:C:318:ALA:O	1:C:321:ALA:N	2.31	0.47
1:H:210:SER:CB	1:H:255:VAL:HG22	2.43	0.47
1:F:429:ILE:HG13	1:F:432:LEU:CD1	2.45	0.47
1:G:6:ILE:CD1	1:G:9:VAL:HG21	2.44	0.47
1:A:38:SER:OG	1:A:40:SER:N	2.48	0.47
1:E:181:GLN:O	1:E:182:LEU:C	2.52	0.47
1:E:178:VAL:CG2	1:E:182:LEU:HD11	2.44	0.47
1:D:303:HIS:HE1	1:D:363:ASP:OD2	1.97	0.47
1:D:236:LEU:HB3	1:D:266:LEU:HD11	1.97	0.47
1:B:112:ASP:OD2	1:B:115:ASN:HB2	2.15	0.47
1:B:113:THR:HA	1:B:140:ALA:HB3	1.93	0.47
1:A:68:LEU:HB3	1:A:95:ILE:HG23	1.97	0.47
1:H:191:ARG:HB2	1:H:238:VAL:HG22	1.95	0.47
1:B:178:VAL:HG12	1:B:179:GLY:N	2.27	0.47
1:F:45:GLU:CG	1:F:46:GLY:N	2.78	0.47
1:A:224:PHE:CB	1:A:278:LEU:HD13	2.45	0.47
1:B:428:ASP:HB3	1:B:431:ASN:OD1	2.15	0.47
1:F:271:LEU:HG	1:F:296:TRP:O	2.15	0.47
1:C:213:ILE:O	1:C:213:ILE:HG13	2.15	0.47
1:H:459:HIS:ND1	1:H:459:HIS:O	2.47	0.47
1:F:59:PRO:HG2	1:F:394:THR:HG21	1.95	0.47
1:A:155:HIS:CE1	1:A:157:ALA:O	2.67	0.47
1:G:17:GLY:O	1:G:18:LEU:C	2.53	0.47
1:B:158:GLY:HA2	1:B:161:ALA:HB3	1.96	0.47
1:H:38:SER:HB3	1:H:40:SER:O	2.15	0.47
1:F:13:ASP:OD1	1:F:13:ASP:N	2.45	0.47
1:G:31:ARG:CB	1:G:414:LYS:O	2.63	0.47
1:E:251:LEU:HD22	1:E:270:VAL:HB	1.95	0.47
1:F:208:ALA:HA	1:F:253:HIS:HB3	1.97	0.47
1:D:73:MET:HE2	1:D:74:PHE:HE1	1.79	0.47
1:H:145:GLY:N	1:H:179:GLY:HA3	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LEU:C	1:D:337:ALA:HB2	2.31	0.47
1:B:32:PHE:HE2	1:B:409:SER:HB2	1.80	0.47
1:E:333:ILE:HG12	1:E:339:ILE:HD11	1.97	0.47
1:E:386:PRO:O	1:E:390:ILE:HB	2.14	0.47
1:H:233:ARG:NH2	1:H:262:THR:OG1	2.43	0.47
1:G:194:VAL:O	1:G:197:TYR:HB3	2.15	0.47
1:H:14:GLY:HA3	1:H:59:PRO:HG3	1.96	0.47
1:D:19:PRO:O	1:D:21:PRO:HD3	2.15	0.47
1:B:81:ILE:HG12	1:B:150:PHE:CE1	2.50	0.47
1:C:447:ARG:HA	1:C:450:LEU:HD13	1.96	0.47
1:E:97:GLU:OE2	1:E:454:PRO:HA	2.15	0.47
1:G:70:ASP:OD2	1:G:73:MET:HB3	2.15	0.47
1:H:76:ALA:HB3	1:H:78:PRO:HD3	1.97	0.47
1:H:406:GLN:O	1:H:415:LEU:HD13	2.14	0.47
1:E:214:VAL:CG1	1:E:215:PHE:CD1	2.90	0.47
1:F:198:LEU:HD21	1:F:205:LEU:HD12	1.97	0.47
1:H:102:ALA:HB1	1:H:107:VAL:HB	1.95	0.47
1:F:290:ILE:HG23	1:F:291:VAL:HG22	1.97	0.47
1:F:421:LEU:HA	1:F:434:SER:O	2.15	0.47
1:F:151:SER:HB2	1:F:152:ALA:O	2.15	0.47
1:A:320:LEU:HA	1:A:325:TYR:HD2	1.80	0.47
1:H:207:ILE:HG22	1:H:251:LEU:O	2.15	0.47
1:F:429:ILE:HG13	1:F:432:LEU:HD12	1.96	0.47
1:E:333:ILE:CD1	1:E:382:LYS:HB2	2.45	0.47
1:D:240:VAL:O	1:D:244:ARG:HG2	2.15	0.47
1:E:16:GLY:HA2	1:E:387:LEU:HG	1.97	0.47
1:B:38:SER:HB3	1:B:40:SER:O	2.14	0.47
1:E:122:ALA:O	1:E:126:ARG:HG3	2.15	0.47
1:E:88:GLU:OE1	1:E:169:ARG:NH1	2.45	0.47
1:C:138:PHE:O	1:C:203:ASP:HB2	2.15	0.47
1:D:341:LEU:HB3	1:D:397:VAL:HG11	1.97	0.46
1:H:31:ARG:HH11	1:H:415:LEU:CG	2.27	0.46
1:F:297:ALA:O	1:F:340:LEU:HG	2.15	0.46
1:H:74:PHE:N	1:H:74:PHE:CD1	2.83	0.46
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.79	0.46
1:A:32:PHE:HB2	1:A:412:THR:HA	1.97	0.46
1:E:62:VAL:O	1:E:397:VAL:HG21	2.15	0.46
1:A:9:VAL:HG22	1:A:52:GLY:HA3	1.97	0.46
1:A:207:ILE:O	1:A:253:HIS:N	2.48	0.46
1:E:226:ARG:NH1	1:E:226:ARG:CB	2.76	0.46
1:C:70:ASP:CG	1:C:71:ALA:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG11	1:B:57:MET:HB2	1.97	0.46
1:B:394:THR:HG22	1:B:395:ILE:H	1.76	0.46
1:F:74:PHE:O	1:F:154:PHE:CB	2.62	0.46
1:H:209:VAL:O	1:H:230:THR:N	2.38	0.46
1:E:153:ASP:O	1:E:212:HIS:ND1	2.49	0.46
1:D:88:GLU:HA	1:D:91:TYR:CE1	2.50	0.46
1:A:11:LEU:HD23	1:A:11:LEU:C	2.36	0.46
1:E:217:LEU:HD13	1:E:225:ASP:O	2.15	0.46
1:H:439:PHE:CE2	1:H:444:ALA:HB2	2.46	0.46
1:F:92:VAL:HG22	1:F:119:PRO:HA	1.97	0.46
1:G:330:ARG:O	1:G:333:ILE:N	2.48	0.46
1:E:100:GLN:CG	1:E:133:GLN:O	2.63	0.46
1:B:4:ILE:HD12	1:B:439:PHE:HE2	1.80	0.46
1:F:317:ALA:O	1:F:319:ALA:N	2.47	0.46
1:A:283:PRO:HD2	1:A:286:LEU:HB2	1.97	0.46
1:D:330:ARG:O	1:D:333:ILE:HD13	2.14	0.46
1:G:252:THR:HG21	1:G:263:SER:OG	2.16	0.46
1:F:112:ASP:O	1:F:139:ALA:HA	2.15	0.46
1:F:198:LEU:HD13	1:F:248:VAL:HG21	1.98	0.46
1:B:72:TRP:HD1	1:B:364:ARG:HH22	1.64	0.46
1:B:273:HIS:HB3	1:B:300:GLN:NE2	2.29	0.46
1:G:64:GLY:HA2	1:G:111:PHE:CD2	2.39	0.46
1:C:68:LEU:HB2	1:C:95:ILE:HG23	1.98	0.46
1:E:250:VAL:HG22	1:E:268:ALA:HA	1.97	0.46
1:A:102:ALA:HB1	1:A:107:VAL:HB	1.98	0.46
1:H:117:ILE:HA	1:H:120:VAL:HG12	1.97	0.46
1:F:257:VAL:CG2	1:F:277:THR:CG2	2.81	0.46
1:E:377:GLN:HA	1:E:429:ILE:HG21	1.96	0.46
1:D:88:GLU:OE1	1:D:169:ARG:NH1	2.48	0.46
1:H:64:GLY:HA2	1:H:111:PHE:CD2	2.50	0.46
1:A:14:GLY:CA	1:A:59:PRO:HG2	2.45	0.46
1:E:126:ARG:O	1:E:131:ILE:HG22	2.15	0.46
1:G:363:ASP:O	1:G:374:HIS:ND1	2.48	0.46
1:D:259:ALA:HA	1:D:262:THR:HG22	1.96	0.46
1:A:214:VAL:O	1:A:217:LEU:HB2	2.15	0.46
1:A:243:ALA:HA	1:A:246:ALA:HB3	1.96	0.46
1:H:177:GLY:O	1:H:193:ARG:HD2	2.15	0.46
1:C:144:VAL:HG11	1:C:239:MET:HE2	1.98	0.46
1:B:253:HIS:NE2	1:B:273:HIS:CE1	2.83	0.46
1:C:66:VAL:O	1:C:112:ASP:HA	2.16	0.46
1:D:262:THR:HG23	1:D:263:SER:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:379:MET:HB3	1:H:384:MET:HB2	1.98	0.46
1:C:166:PHE:HB2	1:H:351:ASP:OD2	2.16	0.46
1:E:105:ASN:OD1	1:E:369:GLY:HA2	2.16	0.46
1:C:156:PHE:H	1:C:215:PHE:HE2	1.63	0.46
1:G:226:ARG:HD2	1:G:228:TYR:CE2	2.51	0.46
1:D:75:MET:HG2	1:D:215:PHE:CZ	2.51	0.46
1:E:259:ALA:O	1:E:263:SER:N	2.46	0.46
1:B:271:LEU:HD22	1:B:274:ALA:HB2	1.98	0.46
1:F:30:ASP:O	1:F:416:ALA:HB2	2.16	0.46
1:B:297:ALA:O	1:B:339:ILE:HA	2.16	0.46
1:C:304:ASP:N	1:C:304:ASP:OD1	2.48	0.46
1:D:330:ARG:O	1:D:333:ILE:CD1	2.64	0.46
1:F:66:VAL:HG22	1:F:110:VAL:CG1	2.44	0.46
1:H:322:GLY:O	1:H:323:GLU:CB	2.63	0.46
1:E:290:ILE:CA	1:E:293:SER:OG	2.64	0.46
1:B:169:ARG:NH2	1:G:351:ASP:OD2	2.49	0.46
1:D:3:THR:HG22	1:D:28:GLU:HA	1.98	0.46
1:B:320:LEU:HD23	1:B:325:TYR:CE2	2.51	0.46
1:F:74:PHE:HA	1:F:80:THR:OG1	2.16	0.46
1:A:282:ILE:HD11	1:A:287:ILE:HG13	1.98	0.46
1:D:147:GLY:HA3	1:D:180:HIS:CE1	2.51	0.46
1:E:77:GLY:N	1:E:78:PRO:HD3	2.30	0.46
1:C:447:ARG:NH1	1:C:447:ARG:HB3	2.31	0.46
1:E:459:HIS:HA	1:E:460:PRO:HA	1.62	0.46
1:A:142:THR:HB	1:A:174:PHE:O	2.16	0.46
1:F:403:LYS:HB3	1:F:407:ILE:HD12	1.97	0.46
1:H:271:LEU:HB3	1:H:274:ALA:HB2	1.98	0.46
1:H:145:GLY:CA	1:H:179:GLY:HA3	2.44	0.46
1:A:232:SER:HB2	1:A:234:PRO:HD2	1.97	0.46
1:H:439:PHE:CE1	1:H:444:ALA:CB	2.99	0.46
1:E:378:SER:O	1:E:382:LYS:CG	2.57	0.46
1:C:140:ALA:HA	1:C:204:MET:HG2	1.98	0.46
1:C:326:ALA:HA	1:C:329:GLU:HB2	1.97	0.46
1:B:190:VAL:HG11	1:B:239:MET:CE	2.45	0.46
1:C:91:TYR:CE2	1:C:173:MET:HE1	2.51	0.46
1:E:170:ILE:HG23	1:E:174:PHE:HE1	1.81	0.46
1:F:74:PHE:C	1:F:154:PHE:HB3	2.36	0.45
1:D:215:PHE:C	1:D:218:VAL:HG13	2.36	0.45
1:H:296:TRP:CE3	1:H:338:LYS:HB3	2.51	0.45
1:E:429:ILE:O	1:E:431:ASN:N	2.50	0.45
1:D:219:ASP:C	1:D:222:VAL:CG1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:N	1:A:27:VAL:O	2.48	0.45
1:B:153:ASP:HA	1:B:212:HIS:HB3	1.98	0.45
1:G:218:VAL:N	1:G:219:ASP:HB2	2.31	0.45
1:C:360:GLU:O	1:C:364:ARG:HB2	2.15	0.45
1:F:422:ASP:CG	1:F:434:SER:HB3	2.36	0.45
1:H:243:ALA:O	1:H:247:GLY:N	2.48	0.45
1:A:35:VAL:HG12	1:A:36:GLY:H	1.80	0.45
1:B:387:LEU:HA	1:B:388:GLU:C	2.36	0.45
1:A:275:ASN:OD1	1:A:276:TYR:CG	2.69	0.45
1:H:208:ALA:HA	1:H:253:HIS:HB2	1.97	0.45
1:E:213:ILE:HG22	1:E:216:THR:HG22	1.96	0.45
1:C:206:LYS:HE2	1:C:272:ILE:HG21	1.97	0.45
1:A:438:VAL:CG2	1:A:447:ARG:HD3	2.43	0.45
1:A:447:ARG:NH1	1:A:447:ARG:N	2.64	0.45
1:A:166:PHE:O	1:A:170:ILE:HG12	2.16	0.45
1:F:38:SER:HB2	1:F:40:SER:H	1.82	0.45
1:C:219:ASP:OD1	1:C:222:VAL:HG12	2.16	0.45
1:C:281:GLU:HA	1:C:328:ASN:HD21	1.82	0.45
1:H:447:ARG:HH11	1:H:447:ARG:CB	2.29	0.45
1:H:344:ASP:O	1:H:366:TRP:HD1	1.99	0.45
1:E:322:GLY:O	1:E:323:GLU:HB2	2.16	0.45
1:H:260:LEU:CD1	1:H:271:LEU:HD23	2.39	0.45
1:F:226:ARG:CB	1:F:226:ARG:NH1	2.79	0.45
1:G:227:SER:OG	1:G:256:SER:HB3	2.16	0.45
1:F:198:LEU:HD11	1:F:205:LEU:HD12	1.97	0.45
1:C:253:HIS:ND1	1:C:273:HIS:ND1	2.55	0.45
1:E:148:GLY:O	1:E:151:SER:OG	2.28	0.45
1:D:236:LEU:O	1:D:240:VAL:HG13	2.16	0.45
1:F:267:GLY:C	1:F:295:SER:OG	2.54	0.45
1:C:115:ASN:ND2	1:C:120:VAL:HB	2.31	0.45
1:G:187:ARG:HB3	1:G:235:VAL:HG22	1.98	0.45
1:G:281:GLU:O	1:G:283:PRO:HD3	2.16	0.45
1:B:391:SER:HB2	1:B:395:ILE:N	2.27	0.45
1:F:74:PHE:N	1:F:76:ALA:HB3	2.32	0.45
1:A:282:ILE:HG23	1:A:328:ASN:CG	2.36	0.45
1:H:231:PHE:HB2	1:H:236:LEU:CD2	2.47	0.45
1:C:217:LEU:CD2	1:C:224:PHE:HB2	2.46	0.45
1:H:361:ARG:O	1:H:364:ARG:N	2.49	0.45
1:G:261:ASP:O	1:G:265:GLU:CG	2.64	0.45
1:D:387:LEU:C	1:D:390:ILE:HB	2.37	0.45
1:F:258:GLU:O	1:F:260:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:LEU:C	1:B:200:ARG:H	2.20	0.45
1:C:219:ASP:CG	1:C:222:VAL:HG12	2.36	0.45
1:A:100:GLN:NE2	1:A:133:GLN:O	2.47	0.45
1:A:140:ALA:HB2	1:A:204:MET:HG2	1.99	0.45
1:B:171:ASP:O	1:B:175:GLU:HG3	2.16	0.45
1:A:207:ILE:O	1:A:207:ILE:HG23	2.15	0.45
1:F:276:TYR:HA	1:F:325:TYR:CD1	2.52	0.45
1:C:25:VAL:HG21	1:C:57:MET:SD	2.56	0.45
1:H:270:VAL:HA	1:H:296:TRP:O	2.17	0.45
1:G:124:ARG:O	1:G:127:ILE:HG12	2.16	0.45
1:A:67:HIS:O	1:A:346:GLY:HA2	2.16	0.45
1:A:271:LEU:HD11	1:A:296:TRP:C	2.36	0.45
1:H:341:LEU:HD21	1:H:372:HIS:HB3	1.98	0.45
1:D:179:GLY:H	1:D:182:LEU:HG	1.81	0.45
1:F:307:ARG:O	1:F:311:GLU:HG3	2.16	0.45
1:F:269:ASP:O	1:F:296:TRP:N	2.47	0.45
1:A:260:LEU:O	1:A:264:VAL:N	2.45	0.45
1:E:11:LEU:HD11	1:E:410:VAL:HG21	1.98	0.45
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.83	0.45
1:G:35:VAL:HG12	1:G:412:THR:HG23	1.99	0.45
1:D:341:LEU:HD13	1:D:375:TRP:CE3	2.52	0.45
1:H:278:LEU:HA	1:H:325:TYR:HH	1.72	0.45
1:A:180:HIS:HE1	1:A:181:GLN:OE1	1.99	0.45
1:H:220:ARG:O	1:H:221:SER:CB	2.65	0.45
1:G:43:VAL:HG13	1:G:47:ALA:HB3	1.98	0.45
1:B:144:VAL:HG13	1:B:178:VAL:HG12	1.98	0.45
1:E:78:PRO:HA	1:E:155:HIS:HE1	1.78	0.45
1:E:77:GLY:HA3	1:E:155:HIS:ND1	2.32	0.45
1:F:237:GLU:HA	1:F:240:VAL:HB	1.99	0.45
1:C:88:GLU:OE2	1:C:169:ARG:NH1	2.49	0.45
1:D:220:ARG:NH1	1:D:220:ARG:CG	2.79	0.45
1:A:11:LEU:O	1:A:11:LEU:HD23	2.17	0.45
1:D:387:LEU:CA	1:D:390:ILE:HB	2.46	0.45
1:G:129:ALA:CB	1:G:131:ILE:HG13	2.44	0.45
1:B:65:ASN:O	1:B:66:VAL:HG13	2.16	0.45
1:F:341:LEU:HD13	1:F:375:TRP:CE3	2.52	0.45
1:H:135:ALA:O	1:H:137:ILE:HG13	2.16	0.45
1:D:392:ALA:HA	1:D:396:ASN:CG	2.37	0.45
1:G:53:ASN:O	1:G:55:ARG:NE	2.50	0.45
1:A:380:VAL:HA	1:A:384:MET:HB3	1.99	0.45
1:B:380:VAL:C	1:B:382:LYS:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:MET:HE2	1:F:73:MET:HB3	1.75	0.45
1:F:226:ARG:HB3	1:F:226:ARG:NH1	2.32	0.45
1:A:70:ASP:CG	1:A:71:ALA:N	2.70	0.45
1:F:61:TYR:OH	1:F:432:LEU:CD2	2.57	0.45
1:D:37:PRO:O	1:D:39:ASP:C	2.55	0.45
1:C:70:ASP:OD2	1:C:73:MET:CB	2.65	0.45
1:C:154:PHE:O	1:C:215:PHE:HD2	2.00	0.45
1:B:185:LEU:HD13	1:B:193:ARG:HH12	1.82	0.45
1:F:410:VAL:HG12	1:F:410:VAL:O	2.16	0.45
1:H:361:ARG:HA	1:H:364:ARG:HB2	1.98	0.45
1:F:63:ASN:CG	1:F:66:VAL:CG1	2.85	0.45
1:H:322:GLY:CA	1:H:326:ALA:HB2	2.32	0.45
1:C:30:ASP:HB2	1:C:441:ALA:O	2.17	0.45
1:A:321:ALA:O	1:A:326:ALA:HB2	2.17	0.45
1:A:120:VAL:HG13	1:A:121:LEU:HD23	1.99	0.45
1:G:263:SER:O	1:G:266:LEU:HD23	2.17	0.45
1:G:6:ILE:HG23	1:G:25:VAL:H	1.82	0.45
1:F:65:ASN:O	1:F:343:THR:O	2.35	0.45
1:A:170:ILE:O	1:A:173:MET:HB2	2.17	0.45
1:F:109:THR:OG1	1:F:136:ARG:NE	2.50	0.45
1:H:197:TYR:HE2	1:H:205:LEU:HD11	1.82	0.45
1:B:74:PHE:CD1	1:B:80:THR:HG23	2.52	0.45
1:C:153:ASP:CB	1:C:212:HIS:HB3	2.47	0.45
1:B:88:GLU:O	1:G:86:ARG:NH2	2.50	0.45
1:A:319:ALA:O	1:A:323:GLU:HB2	2.17	0.45
1:H:327:THR:HB	1:H:330:ARG:HH11	1.81	0.45
1:F:339:ILE:O	1:F:396:ASN:HB3	2.16	0.45
1:A:378:SER:O	1:A:382:LYS:HE2	2.17	0.45
1:E:281:GLU:O	1:E:282:ILE:C	2.54	0.44
1:H:201:GLY:O	1:H:202:VAL:HG22	2.17	0.44
1:E:181:GLN:C	1:E:183:SER:N	2.68	0.44
1:E:220:ARG:O	1:E:221:SER:CB	2.64	0.44
1:A:191:ARG:CD	1:A:238:VAL:HG21	2.42	0.44
1:A:254:SER:HB2	1:A:259:ALA:HB3	1.96	0.44
1:H:214:VAL:O	1:H:217:LEU:N	2.45	0.44
1:D:302:VAL:HA	1:D:374:HIS:HE1	1.83	0.44
1:G:286:LEU:O	1:G:289:LYS:N	2.51	0.44
1:D:20:ARG:O	1:D:23:THR:HG22	2.16	0.44
1:E:75:MET:HE2	1:E:316:TRP:HH2	1.81	0.44
1:D:261:ASP:O	1:D:264:VAL:HB	2.17	0.44
1:H:456:VAL:HG13	1:H:457:THR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HD12	1:B:137:ILE:CD1	2.47	0.44
1:A:250:VAL:N	1:A:269:ASP:OD2	2.50	0.44
1:H:285:TYR:HE1	1:H:286:LEU:HD12	1.82	0.44
1:H:297:ALA:N	1:H:338:LYS:O	2.47	0.44
1:E:423:GLN:CB	1:E:431:ASN:OD1	2.65	0.44
1:H:147:GLY:O	1:H:154:PHE:CD2	2.70	0.44
1:H:155:HIS:CE1	1:H:157:ALA:HB3	2.52	0.44
1:D:382:LYS:N	1:D:382:LYS:CD	2.80	0.44
1:H:425:PRO:HB3	1:H:432:LEU:HD12	1.99	0.44
1:B:65:ASN:O	1:B:66:VAL:CG1	2.65	0.44
1:G:217:LEU:CB	1:G:219:ASP:HB2	2.46	0.44
1:D:48:THR:HG22	1:D:49:VAL:N	2.33	0.44
1:C:67:HIS:ND1	1:C:114:HIS:HB3	2.32	0.44
1:C:100:GLN:OE1	1:C:452:THR:HG23	2.18	0.44
1:A:220:ARG:O	1:A:221:SER:HB3	2.18	0.44
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.77	0.44
1:B:298:GLY:HA3	1:B:342:ASN:ND2	2.32	0.44
1:B:378:SER:O	1:B:381:GLU:HB2	2.18	0.44
1:E:326:ALA:C	1:E:328:ASN:H	2.20	0.44
1:F:224:PHE:CE2	1:F:278:LEU:HD12	2.52	0.44
1:A:324:PRO:O	1:A:328:ASN:HB2	2.18	0.44
1:D:153:ASP:CB	1:D:212:HIS:HB3	2.48	0.44
1:F:226:ARG:HB2	1:F:226:ARG:HH11	1.83	0.44
1:E:147:GLY:HA2	1:E:175:GLU:HG2	1.98	0.44
1:E:66:VAL:C	1:E:67:HIS:CD2	2.90	0.44
1:C:59:PRO:HG2	1:C:394:THR:HG21	2.00	0.44
1:B:204:MET:HA	1:B:248:VAL:HB	1.99	0.44
1:H:118:GLU:HB3	1:H:119:PRO:HD3	1.98	0.44
1:E:307:ARG:C	1:E:307:ARG:CD	2.86	0.44
1:F:224:PHE:CZ	1:F:278:LEU:CD1	3.01	0.44
1:D:72:TRP:O	1:D:73:MET:CB	2.66	0.44
1:D:73:MET:HE2	1:D:74:PHE:CE1	2.53	0.44
1:H:255:VAL:O	1:H:278:LEU:CD1	2.43	0.44
1:C:253:HIS:CD2	1:C:253:HIS:O	2.70	0.44
1:B:153:ASP:HB3	1:B:212:HIS:HB3	1.99	0.44
1:D:234:PRO:O	1:D:238:VAL:HG23	2.18	0.44
1:B:164:ARG:N	1:G:355:ASP:OD2	2.49	0.44
1:C:281:GLU:HA	1:C:328:ASN:ND2	2.33	0.44
1:E:100:GLN:HG2	1:E:133:GLN:O	2.17	0.44
1:D:61:TYR:OH	1:D:432:LEU:HD22	2.18	0.44
1:D:323:GLU:HB3	1:D:324:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:HIS:HA	1:B:460:PRO:HA	1.70	0.44
1:F:80:THR:HG22	1:F:84:LEU:HD12	1.98	0.44
1:E:429:ILE:HD12	1:E:432:LEU:HD11	1.98	0.44
1:A:114:HIS:CG	1:A:143:ILE:HG13	2.53	0.44
1:G:260:LEU:HD21	1:G:290:ILE:HD11	1.99	0.44
1:A:178:VAL:CG1	1:A:179:GLY:N	2.79	0.44
1:C:117:ILE:HG23	1:C:118:GLU:H	1.81	0.44
1:A:92:VAL:CG1	1:C:131:ILE:HD11	2.48	0.44
1:H:456:VAL:HG22	1:H:457:THR:HG23	2.00	0.44
1:C:446:ASP:O	1:C:450:LEU:CD1	2.66	0.44
1:A:397:VAL:O	1:A:401:TYR:HD2	2.01	0.44
1:B:59:PRO:HG2	1:B:394:THR:OG1	2.18	0.44
1:D:330:ARG:HA	1:D:333:ILE:HD12	2.00	0.44
1:C:217:LEU:HD21	1:C:225:ASP:H	1.81	0.44
1:F:121:LEU:HA	1:F:124:ARG:HB3	1.99	0.44
1:B:365:PRO:O	1:B:371:ASP:HA	2.18	0.44
1:C:26:ILE:CD1	1:C:34:THR:OG1	2.64	0.44
1:C:87:TRP:CZ3	1:C:455:LEU:HG	2.52	0.44
1:H:120:VAL:O	1:H:123:ALA:N	2.46	0.44
1:A:305:GLN:O	1:A:309:GLY:N	2.43	0.44
1:C:150:PHE:O	1:C:159:ARG:HB3	2.17	0.44
1:A:103:LEU:HD13	1:A:135:ALA:HA	1.99	0.44
1:A:251:LEU:CD1	1:A:270:VAL:HG21	2.47	0.44
1:H:193:ARG:HB2	1:H:193:ARG:CZ	2.47	0.44
1:H:286:LEU:O	1:H:290:ILE:HG13	2.18	0.44
1:G:110:VAL:O	1:G:137:ILE:HA	2.17	0.44
1:C:273:HIS:N	1:C:273:HIS:CD2	2.86	0.44
1:B:155:HIS:CD2	1:B:157:ALA:O	2.71	0.44
1:E:297:ALA:O	1:E:339:ILE:HA	2.17	0.44
1:E:301:THR:HG22	1:E:329:GLU:OE1	2.18	0.44
1:C:30:ASP:CG	1:C:31:ARG:N	2.65	0.44
1:D:187:ARG:CZ	1:D:187:ARG:HB3	2.48	0.44
1:C:398:ALA:O	1:C:399[B]:ARG:C	2.54	0.44
1:F:305:GLN:O	1:F:308:GLN:N	2.48	0.44
1:C:341:LEU:HD13	1:C:375:TRP:CE3	2.53	0.44
1:A:92:VAL:HG13	1:A:93:GLU:N	2.33	0.44
1:F:221:SER:HA	1:F:222:VAL:HA	1.72	0.44
1:F:447:ARG:CZ	1:F:447:ARG:HB2	2.47	0.44
1:B:391:SER:N	1:B:392:ALA:CA	2.81	0.44
1:E:429:ILE:C	1:E:431:ASN:N	2.71	0.44
1:E:236:LEU:O	1:E:240:VAL:CG2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ASN:O	1:F:66:VAL:CG1	2.66	0.44
1:B:32:PHE:CZ	1:B:410:VAL:HG22	2.53	0.44
1:F:150:PHE:HE2	1:F:170:ILE:HD12	1.83	0.44
1:F:186:PRO:O	1:F:190:VAL:HG23	2.17	0.44
1:C:112:ASP:O	1:C:140:ALA:N	2.50	0.44
1:C:137:ILE:HG22	1:C:139:ALA:HB2	1.98	0.44
1:F:228:TYR:O	1:F:229:GLN:HG3	2.18	0.44
1:C:97:GLU:OE2	1:C:455:LEU:N	2.30	0.44
1:C:283:PRO:HG2	1:C:285:TYR:HE1	1.83	0.44
1:C:283:PRO:HG2	1:C:285:TYR:CE1	2.53	0.44
1:H:440:GLN:O	1:H:443:ALA:O	2.35	0.44
1:E:278:LEU:HA	1:E:325:TYR:HE1	1.82	0.43
1:D:170:ILE:O	1:D:173:MET:HB3	2.18	0.43
1:H:342:ASN:O	1:H:375:TRP:CD1	2.69	0.43
1:C:399[B]:ARG:NH1	1:C:404:ALA:HB1	2.32	0.43
1:E:131:ILE:HD11	1:B:124:ARG:HH22	1.82	0.43
1:D:56:TRP:CZ3	1:D:423:GLN:HA	2.53	0.43
1:B:170:ILE:O	1:B:173:MET:HB2	2.18	0.43
1:C:302:VAL:O	1:C:382:LYS:NZ	2.34	0.43
1:C:152:ALA:HB1	1:C:213:ILE:HG22	1.99	0.43
1:E:32:PHE:CE2	1:E:410:VAL:HA	2.52	0.43
1:D:67:HIS:HD2	1:D:114:HIS:O	2.01	0.43
1:A:300:GLN:OE1	1:A:344:ASP:HB2	2.19	0.43
1:B:32:PHE:CE2	1:B:409:SER:HB2	2.53	0.43
1:C:416:ALA:HB3	1:C:442:GLY:N	2.33	0.43
1:E:63:ASN:ND2	1:E:371:ASP:OD2	2.51	0.43
1:G:304:ASP:HA	1:G:307:ARG:HD2	2.00	0.43
1:B:283:PRO:O	1:B:285:TYR:N	2.51	0.43
1:E:4:ILE:HD12	1:E:442:GLY:O	2.18	0.43
1:F:97:GLU:OE2	1:F:457:THR:OG1	2.31	0.43
1:E:429:ILE:CG2	1:E:430:ARG:N	2.80	0.43
1:H:359:VAL:O	1:H:360:GLU:C	2.56	0.43
1:A:236:LEU:O	1:A:266:LEU:HD21	2.18	0.43
1:G:8:ASN:N	1:G:24:THR:OG1	2.44	0.43
1:F:63:ASN:OD1	1:F:66:VAL:HG13	2.17	0.43
1:D:278:LEU:CA	1:D:325:TYR:CE1	2.96	0.43
1:F:282:ILE:N	1:F:283:PRO:HB3	2.33	0.43
1:G:178:VAL:HG21	1:G:197:TYR:CG	2.53	0.43
1:B:138:PHE:CA	1:B:203:ASP:OD2	2.66	0.43
1:B:84:LEU:HD13	1:B:170:ILE:HG21	2.00	0.43
1:G:395:ILE:H	1:G:395:ILE:HG13	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ASP:OD2	1:C:223:GLY:N	2.51	0.43
1:D:283:PRO:HB2	1:D:285:TYR:HD2	1.83	0.43
1:C:104:ARG:CG	1:C:447:ARG:NH1	2.81	0.43
1:B:165:THR:HG22	1:G:355:ASP:OD1	2.19	0.43
1:H:13:ASP:HB2	1:H:15:LEU:H	1.84	0.43
1:B:71:ALA:O	1:B:75:MET:HB3	2.18	0.43
1:H:6:ILE:O	1:H:24:THR:CG2	2.63	0.43
1:A:287:ILE:HG22	1:A:291:VAL:CG2	2.48	0.43
1:D:75:MET:SD	1:D:215:PHE:CZ	3.12	0.43
1:H:203:ASP:C	1:H:248:VAL:HG13	2.33	0.43
1:D:330:ARG:O	1:D:334:SER:OG	2.29	0.43
1:A:235:VAL:O	1:A:239:MET:CG	2.65	0.43
1:E:181:GLN:O	1:E:183:SER:N	2.51	0.43
1:F:92:VAL:HG13	1:F:123:ALA:HB2	1.99	0.43
1:F:252:THR:HG23	1:F:268:ALA:CB	2.48	0.43
1:H:306:HIS:HD2	1:H:365:PRO:HG3	1.83	0.43
1:H:333:ILE:HD11	1:H:379:MET:SD	2.59	0.43
1:A:149:PRO:HA	1:A:154:PHE:HD2	1.82	0.43
1:A:317:ALA:O	1:A:319:ALA:N	2.44	0.43
1:F:116:ALA:HB2	1:F:174:PHE:CE1	2.53	0.43
1:G:118:GLU:HG3	1:G:118:GLU:H	1.42	0.43
1:E:324:PRO:HA	1:E:327:THR:HB	2.01	0.43
1:D:74:PHE:CD1	1:D:74:PHE:N	2.85	0.43
1:H:260:LEU:HD23	1:H:286:LEU:HD23	2.00	0.43
1:A:72:TRP:O	1:A:76:ALA:CB	2.66	0.43
1:F:264:VAL:HG12	1:F:293:SER:CB	2.37	0.43
1:F:428:ASP:CG	1:F:430:ARG:CG	2.87	0.43
1:F:429:ILE:CD1	1:F:432:LEU:HD11	2.42	0.43
1:C:206:LYS:HZ1	1:C:253:HIS:CB	2.32	0.43
1:E:143:ILE:HG23	1:E:206:LYS:HG2	2.00	0.43
1:B:258:GLU:O	1:B:259:ALA:CB	2.67	0.43
1:D:259:ALA:O	1:D:262:THR:HG22	2.19	0.43
1:G:195:ARG:NE	1:G:242:GLU:OE1	2.26	0.43
1:H:339:ILE:O	1:H:396:ASN:HB3	2.19	0.43
1:H:180:HIS:C	1:H:182:LEU:H	2.22	0.43
1:A:191:ARG:NE	1:A:238:VAL:HG21	2.33	0.43
1:H:76:ALA:CB	1:H:77:GLY:HA2	2.21	0.43
1:E:387:LEU:O	1:E:390:ILE:HG22	2.18	0.43
1:G:215:PHE:HA	1:G:218:VAL:HA	2.01	0.43
1:F:290:ILE:CG2	1:F:291:VAL:N	2.81	0.43
1:C:153:ASP:H	1:C:213:ILE:HG22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ALA:C	1:A:154:PHE:H	2.20	0.43
1:E:411:GLU:HG2	1:E:412:THR:H	1.83	0.43
1:C:93:GLU:O	1:C:97:GLU:HB2	2.18	0.43
1:G:435:ILE:HG21	1:G:438:VAL:HG23	1.99	0.43
1:A:355:ASP:OD2	1:F:164:ARG:HG2	2.19	0.43
1:A:6:ILE:O	1:A:24:THR:HG23	2.18	0.43
1:D:220:ARG:O	1:D:221:SER:CB	2.66	0.43
1:F:293:SER:O	1:F:294:ASP:HB2	2.18	0.43
1:A:238:VAL:CG1	1:A:239:MET:N	2.81	0.43
1:A:210:SER:HA	1:A:229:GLN:HA	2.00	0.43
1:G:261:ASP:O	1:G:265:GLU:HG2	2.18	0.43
1:D:167:VAL:O	1:D:171:ASP:OD1	2.37	0.43
1:H:232:SER:O	1:H:233:ARG:C	2.56	0.43
1:F:32:PHE:CE2	1:F:416:ALA:HA	2.54	0.43
1:D:64:GLY:O	1:D:401:TYR:OH	2.34	0.43
1:B:380:VAL:HA	1:B:384:MET:HB3	2.01	0.43
1:F:69:LEU:HA	1:F:69:LEU:HD23	1.77	0.43
1:D:75:MET:HE3	1:D:212:HIS:CE1	2.53	0.43
1:A:13:ASP:N	1:A:13:ASP:OD1	2.41	0.43
1:D:224:PHE:HE1	1:D:325:TYR:OH	2.02	0.43
1:D:416:ALA:O	1:D:441:ALA:N	2.52	0.43
1:G:4:ILE:HB	1:G:48:THR:OG1	2.18	0.43
1:B:41:THR:H	1:B:42:PRO:CA	2.29	0.43
1:E:75:MET:CE	1:E:316:TRP:HZ3	2.30	0.43
1:D:66:VAL:CG2	1:D:110:VAL:CG1	2.96	0.43
1:G:87:TRP:HB3	1:G:94:VAL:HG21	2.00	0.43
1:C:219:ASP:CG	1:C:222:VAL:CG1	2.87	0.43
1:H:391:SER:O	1:H:395:ILE:HD12	2.19	0.43
1:A:151:SER:HA	1:A:159:ARG:HD2	2.01	0.43
1:G:31:ARG:HB2	1:G:414:LYS:O	2.19	0.43
1:H:58:VAL:HG23	1:H:419:VAL:HB	2.01	0.43
1:C:227:SER:OG	1:C:228:TYR:N	2.52	0.43
1:G:124:ARG:HB2	1:G:137:ILE:HG13	2.00	0.43
1:E:261:ASP:O	1:E:265:GLU:CG	2.56	0.43
1:H:149:PRO:HA	1:H:154:PHE:HB3	2.01	0.43
1:F:203:ASP:O	1:F:249:PRO:HD2	2.19	0.43
1:F:63:ASN:CG	1:F:66:VAL:HG13	2.39	0.43
1:B:76:ALA:N	1:B:77:GLY:CA	2.82	0.43
1:H:303:HIS:CE1	1:H:306:HIS:HB2	2.52	0.43
1:C:114:HIS:ND1	1:C:143:ILE:HG13	2.34	0.43
1:A:357:SER:OG	1:A:360:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:THR:HA	1:G:412:THR:HG22	2.01	0.43
1:F:131:ILE:HD13	1:H:93:GLU:OE1	2.19	0.43
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.89	0.43
1:A:277:THR:CG2	1:A:282:ILE:HG22	2.49	0.43
1:C:307:ARG:NH2	1:C:311:GLU:CD	2.72	0.43
1:H:382:LYS:HA	1:H:382:LYS:HD3	1.73	0.43
1:G:256:SER:C	1:G:258:GLU:O	2.57	0.43
1:F:67:HIS:ND1	1:F:114:HIS:HB3	2.34	0.43
1:D:36:GLY:HA2	1:D:41:THR:HG21	2.00	0.43
1:D:158:GLY:O	1:D:162:ALA:N	2.52	0.43
1:A:303:HIS:O	1:A:307:ARG:HB2	2.18	0.43
1:E:317:ALA:O	1:E:320:LEU:N	2.51	0.43
1:C:302:VAL:HA	1:C:374:HIS:CE1	2.50	0.43
1:H:97:GLU:HG3	1:H:455:LEU:HB3	2.00	0.43
1:G:365:PRO:HG2	1:G:366:TRP:CZ3	2.54	0.43
1:G:195:ARG:HD3	1:G:195:ARG:O	2.19	0.43
1:A:353:LEU:HD21	1:A:364:ARG:NH1	2.34	0.42
1:C:416:ALA:O	1:C:441:ALA:N	2.52	0.42
1:D:195:ARG:HD2	1:D:242:GLU:CD	2.40	0.42
1:E:320:LEU:HD23	1:E:320:LEU:N	2.34	0.42
1:H:103:LEU:HD22	1:H:134:GLY:O	2.19	0.42
1:G:15:LEU:HA	1:G:395:ILE:CD1	2.48	0.42
1:D:103:LEU:CD2	1:D:445:VAL:HG21	2.49	0.42
1:G:76:ALA:HA	1:G:77:GLY:O	2.18	0.42
1:H:120:VAL:HG13	1:H:121:LEU:N	2.33	0.42
1:E:56:TRP:NE1	1:E:424:ASP:OD1	2.52	0.42
1:A:43:VAL:HG11	1:A:49:VAL:HG22	2.02	0.42
1:H:338:LYS:HA	1:H:338:LYS:HD2	1.65	0.42
1:A:180:HIS:O	1:A:182:LEU:N	2.46	0.42
1:E:365:PRO:HD2	1:E:366:TRP:CE3	2.54	0.42
1:E:43:VAL:O	1:E:43:VAL:HG13	2.18	0.42
1:C:231:PHE:HB2	1:C:236:LEU:HD21	2.01	0.42
1:H:317:ALA:C	1:H:319:ALA:N	2.71	0.42
1:D:103:LEU:HA	1:D:107:VAL:O	2.19	0.42
1:F:152:ALA:O	1:F:153:ASP:HB2	2.19	0.42
1:F:217:LEU:HD12	1:F:226:ARG:NH2	2.10	0.42
1:H:275:ASN:CG	1:H:329:GLU:HG3	2.36	0.42
1:H:111:PHE:CE2	1:H:397:VAL:HG12	2.54	0.42
1:D:9:VAL:CG2	1:D:23:THR:O	2.64	0.42
1:E:75:MET:HE1	1:E:316:TRP:CZ3	2.53	0.42
1:D:282:ILE:HG22	1:D:286:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ASN:HA	1:D:287:ILE:HB	2.00	0.42
1:G:94:VAL:CG1	1:G:456:VAL:CG2	2.97	0.42
1:C:401:TYR:CD1	1:C:401:TYR:N	2.88	0.42
1:E:76:ALA:HB3	1:E:77:GLY:CA	2.49	0.42
1:E:452:THR:OG1	1:E:453:THR:N	2.52	0.42
1:H:142:THR:HG22	1:H:143:ILE:N	2.34	0.42
1:H:182:LEU:HD12	1:H:231:PHE:CZ	2.54	0.42
1:A:72:TRP:O	1:A:76:ALA:CA	2.67	0.42
1:E:214:VAL:CG2	1:E:215:PHE:CE1	3.03	0.42
1:G:286:LEU:HA	1:G:286:LEU:HD12	1.90	0.42
1:B:229:GLN:CD	1:B:259:ALA:HB2	2.40	0.42
1:B:40:SER:C	1:B:41:THR:HG1	2.12	0.42
1:E:204:MET:HB2	1:E:249:PRO:O	2.19	0.42
1:F:227:SER:O	1:F:228:TYR:C	2.58	0.42
1:B:437:GLU:HA	1:B:447:ARG:HH21	1.84	0.42
1:C:104:ARG:HG2	1:C:447:ARG:HH12	1.84	0.42
1:B:185:LEU:HG	1:B:185:LEU:H	1.62	0.42
1:E:421:LEU:HB3	1:E:434:SER:OG	2.19	0.42
1:C:356:LEU:O	1:C:361:ARG:NE	2.52	0.42
1:C:227:SER:CB	1:C:228:TYR:HA	2.36	0.42
1:D:109:THR:HG23	1:D:136:ARG:HB2	2.02	0.42
1:D:166:PHE:CE1	1:D:170:ILE:HG13	2.55	0.42
1:A:232:SER:OG	1:A:235:VAL:HG23	2.19	0.42
1:H:343:THR:OG1	1:H:371:ASP:OD1	2.36	0.42
1:A:180:HIS:ND1	1:A:180:HIS:C	2.72	0.42
1:A:12:ILE:HG21	1:A:390:ILE:HD13	2.01	0.42
1:H:96:GLU:O	1:H:100:GLN:HG3	2.19	0.42
1:F:14:GLY:HA2	1:F:390:ILE:CD1	2.47	0.42
1:H:317:ALA:O	1:H:319:ALA:N	2.52	0.42
1:H:392:ALA:HA	1:H:396:ASN:HB2	2.00	0.42
1:D:74:PHE:O	1:D:75:MET:CB	2.68	0.42
1:A:350:LYS:CB	1:A:459:HIS:NE2	2.82	0.42
1:F:102:ALA:HB1	1:F:107:VAL:CG2	2.49	0.42
1:F:163:THR:O	1:F:166:PHE:N	2.52	0.42
1:B:302:VAL:HG12	1:B:306:HIS:HB3	2.01	0.42
1:H:92:VAL:O	1:H:96:GLU:HG3	2.19	0.42
1:D:252:THR:CG2	1:D:263:SER:OG	2.68	0.42
1:B:323:GLU:HB3	1:B:324:PRO:CD	2.49	0.42
1:E:416:ALA:O	1:E:441:ALA:N	2.53	0.42
1:A:250:VAL:HB	1:A:269:ASP:H	1.84	0.42
1:A:286:LEU:O	1:A:289:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:LEU:O	1:D:375:TRP:NE1	2.43	0.42
1:B:326:ALA:C	1:B:328:ASN:H	2.22	0.42
1:A:236:LEU:C	1:A:266:LEU:HD21	2.40	0.42
1:A:126:ARG:N	1:A:126:ARG:HH11	2.18	0.42
1:G:304:ASP:O	1:G:307:ARG:HG2	2.20	0.42
1:F:420:LEU:HD12	1:F:437:GLU:HB2	2.02	0.42
1:G:100:GLN:OE1	1:G:450:LEU:HG	2.19	0.42
1:A:373:PHE:HB3	1:A:433:ARG:HH21	1.84	0.42
1:E:3:THR:HG21	1:E:44:PRO:HG2	2.01	0.42
1:E:6:ILE:HD13	1:E:50:VAL:HB	2.01	0.42
1:H:143:ILE:HG21	1:H:146:MET:HE3	1.98	0.42
1:H:182:LEU:HB3	1:H:231:PHE:HE2	1.85	0.42
1:H:30:ASP:O	1:H:31:ARG:CG	2.68	0.42
1:A:178:VAL:HA	1:A:182:LEU:CD1	2.48	0.42
1:G:239:MET:HE2	1:G:239:MET:HB3	1.85	0.42
1:C:373:PHE:CD2	1:C:433:ARG:HG2	2.54	0.42
1:F:4:ILE:CG2	1:F:48:THR:HB	2.49	0.42
1:H:224:PHE:O	1:H:224:PHE:HD1	2.03	0.42
1:G:76:ALA:HB1	1:G:77:GLY:CA	2.49	0.42
1:H:138:PHE:CE2	1:H:403:LYS:HG3	2.55	0.42
1:F:459:HIS:HA	1:F:460:PRO:HA	1.65	0.42
1:E:90:ARG:NE	1:E:93:GLU:OE1	2.42	0.42
1:H:152:ALA:O	1:H:153:ASP:HB2	2.20	0.42
1:E:351:ASP:OD2	1:D:169:ARG:NH2	2.53	0.42
1:A:180:HIS:C	1:A:182:LEU:N	2.74	0.42
1:F:123:ALA:O	1:F:126:ARG:HB2	2.20	0.42
1:G:320:LEU:HA	1:G:325:TYR:CE1	2.55	0.42
1:H:459:HIS:HA	1:H:460:PRO:HA	1.85	0.42
1:F:12:ILE:O	1:F:58:VAL:HA	2.20	0.42
1:C:447:ARG:HH11	1:C:447:ARG:HB3	1.85	0.42
1:H:386:PRO:O	1:H:390:ILE:HD12	2.20	0.42
1:A:9:VAL:HG12	1:A:10:THR:N	2.34	0.42
1:B:350:LYS:HD3	1:B:459:HIS:HB3	2.01	0.42
1:D:364:ARG:HA	1:D:365:PRO:HD2	1.95	0.42
1:G:301:THR:HG22	1:G:302:VAL:H	1.85	0.42
1:F:75:MET:HE1	1:F:212:HIS:HE1	1.80	0.42
1:H:230:THR:HB	1:H:231:PHE:CD1	2.55	0.42
1:H:361:ARG:O	1:H:363:ASP:N	2.53	0.42
1:H:406:GLN:CB	1:H:415:LEU:HD13	2.34	0.42
1:F:428:ASP:O	1:F:429:ILE:HG22	2.19	0.42
1:G:258:GLU:O	1:G:259:ALA:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ILE:HD11	1:F:197:TYR:CE1	2.55	0.42
1:E:143:ILE:HD13	1:E:206:LYS:HE2	2.02	0.42
1:E:364:ARG:HA	1:E:365:PRO:HD3	1.83	0.42
1:H:197:TYR:CE2	1:H:205:LEU:HD11	2.55	0.42
1:H:387:LEU:HD13	1:H:426:VAL:HG21	2.02	0.42
1:G:59:PRO:HG2	1:G:394:THR:HG21	2.02	0.42
1:A:60:GLY:HA3	1:A:108:THR:OG1	2.19	0.42
1:E:146:MET:SD	1:E:212:HIS:HB2	2.60	0.41
1:C:259:ALA:HA	1:C:262:THR:HB	2.02	0.41
1:H:340:LEU:O	1:H:375:TRP:CZ2	2.73	0.41
1:E:208:ALA:HA	1:E:253:HIS:HB3	2.02	0.41
1:D:145:GLY:HA2	1:D:231:PHE:HZ	1.85	0.41
1:E:341:LEU:HA	1:E:375:TRP:CZ2	2.55	0.41
1:G:111:PHE:HE2	1:G:397:VAL:CG1	2.33	0.41
1:D:81:ILE:HD11	1:D:158:GLY:HA3	2.01	0.41
1:E:191:ARG:HB2	1:E:238:VAL:CG1	2.49	0.41
1:C:21:PRO:O	1:C:22:ALA:CB	2.68	0.41
1:F:296:TRP:CE3	1:F:338:LYS:HB3	2.55	0.41
1:A:140:ALA:HB2	1:A:204:MET:CG	2.50	0.41
1:C:36:GLY:HA2	1:C:37:PRO:HD3	1.78	0.41
1:C:6:ILE:HG22	1:C:25:VAL:CA	2.49	0.41
1:D:337:ALA:O	1:D:338:LYS:CB	2.67	0.41
1:D:378:SER:O	1:D:382:LYS:HG2	2.20	0.41
1:G:282:ILE:CG1	1:G:328:ASN:OD1	2.68	0.41
1:A:179:GLY:O	1:A:180:HIS:C	2.59	0.41
1:B:117:ILE:HD11	1:B:202:VAL:HG13	2.01	0.41
1:G:87:TRP:CE3	1:G:455:LEU:HD23	2.54	0.41
1:C:340:LEU:HD23	1:C:341:LEU:N	2.35	0.41
1:A:35:VAL:HG12	1:A:36:GLY:N	2.35	0.41
1:F:100:GLN:HB3	1:F:450:LEU:HG	2.03	0.41
1:H:69:LEU:HA	1:H:69:LEU:HD23	1.79	0.41
1:E:54:ARG:O	1:E:54:ARG:HG2	2.19	0.41
1:F:213:ILE:HG22	1:F:213:ILE:O	2.19	0.41
1:B:389:ALA:O	1:B:392:ALA:HB2	1.95	0.41
1:C:227:SER:CB	1:C:228:TYR:CA	2.97	0.41
1:D:74:PHE:C	1:D:76:ALA:N	2.73	0.41
1:D:219:ASP:CG	1:D:222:VAL:HG11	2.39	0.41
1:D:109:THR:HG21	1:D:407:ILE:HD13	2.01	0.41
1:H:380:VAL:O	1:H:381:GLU:CB	2.68	0.41
1:C:206:LYS:NZ	1:C:253:HIS:CB	2.84	0.41
1:D:378:SER:HB3	1:D:382:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HA	1:D:276:TYR:O	2.21	0.41
1:D:387:LEU:O	1:D:390:ILE:CA	2.69	0.41
1:E:367:THR:O	1:E:371:ASP:HB3	2.21	0.41
1:E:286:LEU:O	1:E:286:LEU:HD23	2.20	0.41
1:D:104:ARG:HB2	1:D:447:ARG:HG3	2.02	0.41
1:C:399[B]:ARG:HH11	1:C:404:ALA:CB	2.33	0.41
1:F:386:PRO:O	1:F:390:ILE:HG13	2.20	0.41
1:D:103:LEU:HD13	1:D:135:ALA:HB2	2.03	0.41
1:G:38:SER:C	1:G:40:SER:N	2.73	0.41
1:D:348:PRO:CG	1:D:353:LEU:HD21	2.49	0.41
1:D:347:CYS:HA	1:D:348:PRO:HD2	1.83	0.41
1:H:121:LEU:HD22	1:H:124:ARG:NH1	2.35	0.41
1:A:87:TRP:O	1:A:90:ARG:HB2	2.20	0.41
1:D:270:VAL:HG13	1:D:340:LEU:HD21	2.03	0.41
1:F:121:LEU:HD11	1:F:202:VAL:HG12	2.03	0.41
1:F:194:VAL:O	1:F:197:TYR:HB3	2.20	0.41
1:H:74:PHE:HD1	1:H:74:PHE:N	2.16	0.41
1:A:180:HIS:HD1	1:A:180:HIS:C	2.24	0.41
1:D:187:ARG:NH1	1:D:234:PRO:HB2	2.35	0.41
1:G:111:PHE:HE2	1:G:397:VAL:HG12	1.86	0.41
1:B:450:LEU:HA	1:B:450:LEU:HD12	1.91	0.41
1:C:398:ALA:HB1	1:C:404:ALA:N	2.35	0.41
1:E:77:GLY:H	1:E:78:PRO:HD3	1.85	0.41
1:E:97:GLU:O	1:E:101:LEU:HD12	2.20	0.41
1:C:194:VAL:O	1:C:197:TYR:N	2.53	0.41
1:C:405:ASP:N	1:C:405:ASP:OD1	2.42	0.41
1:H:258:GLU:C	1:H:260:LEU:H	2.24	0.41
1:B:299:LEU:HD13	1:B:339:ILE:HG23	2.01	0.41
1:A:350:LYS:CA	1:A:353:LEU:HB2	2.37	0.41
1:H:255:VAL:HG23	1:H:256:SER:N	2.35	0.41
1:F:61:TYR:CZ	1:F:432:LEU:HD22	2.54	0.41
1:F:251:LEU:HD22	1:F:270:VAL:CB	2.41	0.41
1:D:36:GLY:CA	1:D:41:THR:CG2	2.98	0.41
1:E:30:ASP:O	1:E:31:ARG:C	2.59	0.41
1:B:205:LEU:HA	1:B:205:LEU:HD12	1.89	0.41
1:H:218:VAL:O	1:H:218:VAL:CG2	2.69	0.41
1:A:394:THR:HB	1:A:408:GLY:O	2.20	0.41
1:B:395:ILE:HD13	1:B:399[B]:ARG:NH2	2.35	0.41
1:H:152:ALA:CB	1:H:213:ILE:HG12	2.50	0.41
1:G:8:ASN:H	1:G:24:THR:HG1	1.65	0.41
1:C:206:LYS:NZ	1:C:253:HIS:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ILE:HG12	1:E:206:LYS:HD3	2.03	0.41
1:B:229:GLN:OE1	1:B:259:ALA:HB2	2.20	0.41
1:G:219:ASP:O	1:G:220:ARG:HB2	2.20	0.41
1:G:15:LEU:HD12	1:G:409:SER:OG	2.20	0.41
1:B:165:THR:HG23	1:G:351:ASP:HB3	2.02	0.41
1:A:350:LYS:HB2	1:A:459:HIS:NE2	2.36	0.41
1:F:194:VAL:O	1:F:198:LEU:HG	2.21	0.41
1:E:372:HIS:O	1:E:375:TRP:HB3	2.20	0.41
1:G:5:ALA:HB1	1:G:26:ILE:HG12	2.03	0.41
1:F:356:LEU:CD2	1:F:360:GLU:CD	2.89	0.41
1:C:121:LEU:HD21	1:C:124:ARG:CZ	2.50	0.41
1:H:332:LEU:HD22	1:H:337:ALA:CB	2.48	0.41
1:B:44:PRO:C	1:B:46:GLY:H	2.24	0.41
1:G:116:ALA:O	1:G:119:PRO:HD2	2.20	0.41
1:H:18:LEU:HD22	1:H:18:LEU:HA	1.62	0.41
1:B:395:ILE:HD12	1:B:399[B]:ARG:NH2	2.35	0.41
1:D:272:ILE:HG23	1:D:342:ASN:OD1	2.20	0.41
1:D:74:PHE:O	1:D:75:MET:HB2	2.20	0.41
1:G:124:ARG:CB	1:G:137:ILE:HG13	2.51	0.41
1:D:91:TYR:O	1:D:94:VAL:N	2.53	0.41
1:A:191:ARG:HH22	1:A:239:MET:HE3	1.86	0.41
1:H:111:PHE:HE2	1:H:397:VAL:CG1	2.33	0.41
1:G:261:ASP:OD1	1:G:289:LYS:CE	2.69	0.41
1:B:256:SER:O	1:B:258:GLU:O	2.38	0.41
1:A:175:GLU:O	1:A:178:VAL:O	2.38	0.41
1:D:38:SER:CB	1:D:40:SER:O	2.69	0.41
1:D:235:VAL:HA	1:D:238:VAL:HB	2.02	0.41
1:B:144:VAL:O	1:B:208:ALA:HB3	2.21	0.41
1:F:38:SER:HB2	1:F:40:SER:C	2.41	0.41
1:C:74:PHE:N	1:C:74:PHE:HD1	2.17	0.41
1:A:255:VAL:CG1	1:A:278:LEU:HG	2.51	0.41
1:G:341:LEU:HG	1:G:375:TRP:CE3	2.56	0.41
1:D:319:ALA:O	1:D:323:GLU:HG3	2.21	0.41
1:A:18:LEU:H	1:A:18:LEU:HD12	1.86	0.41
1:A:251:LEU:HD11	1:A:270:VAL:HG21	2.02	0.41
1:D:75:MET:CG	1:D:215:PHE:CE1	2.98	0.41
1:H:66:VAL:O	1:H:67:HIS:CD2	2.50	0.41
1:H:75:MET:O	1:H:76:ALA:C	2.59	0.41
1:G:256:SER:O	1:G:258:GLU:O	2.38	0.41
1:A:114:HIS:O	1:A:115:ASN:HB2	2.20	0.41
1:B:31:ARG:HH11	1:B:414:LYS:C	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:SER:HA	1:E:381:GLU:HB3	2.03	0.41
1:F:281:GLU:O	1:F:283:PRO:HB3	2.20	0.41
1:E:348:PRO:HG2	1:E:364:ARG:HH12	1.86	0.41
1:B:306:HIS:NE2	1:B:365:PRO:HD3	2.36	0.41
1:F:185:LEU:HD22	1:F:189:GLU:HB2	2.03	0.41
1:D:450:LEU:HD23	1:D:450:LEU:HA	1.84	0.41
1:C:261:ASP:OD1	1:C:286:LEU:HD13	2.21	0.41
1:G:10:THR:HA	1:G:21:PRO:HA	2.02	0.41
1:F:100:GLN:OE1	1:F:452:THR:HG22	2.20	0.41
1:B:219:ASP:O	1:B:222:VAL:O	2.38	0.41
1:A:131:ILE:HA	1:A:131:ILE:HD12	1.94	0.41
1:A:20:ARG:HA	1:A:20:ARG:HD3	1.85	0.41
1:H:11:LEU:HD13	1:H:57:MET:HB3	2.03	0.41
1:H:252:THR:CG2	1:H:271:LEU:HA	2.50	0.41
1:A:353:LEU:HA	1:A:353:LEU:HD23	1.89	0.41
1:C:326:ALA:HB1	1:C:382:LYS:HE3	2.02	0.41
1:C:232:SER:O	1:C:236:LEU:HG	2.21	0.41
1:E:74:PHE:N	1:E:74:PHE:CD1	2.87	0.41
1:E:397:VAL:O	1:E:401:TYR:HD2	2.04	0.41
1:A:456:VAL:O	1:A:456:VAL:CG1	2.68	0.41
1:A:382:LYS:HD3	1:A:382:LYS:HA	1.82	0.41
1:E:164:ARG:HD3	1:E:164:ARG:HA	1.76	0.41
1:B:385:SER:CA	1:B:387:LEU:O	2.69	0.40
1:F:83:TYR:O	1:F:87:TRP:HD1	2.04	0.40
1:D:71:ALA:O	1:D:74:PHE:N	2.55	0.40
1:H:182:LEU:CD2	1:H:193:ARG:NH1	2.84	0.40
1:H:206:LYS:NZ	1:H:272:ILE:CG2	2.73	0.40
1:H:260:LEU:CD1	1:H:271:LEU:HD22	2.49	0.40
1:F:428:ASP:HB3	1:F:430:ARG:HG3	2.02	0.40
1:A:66:VAL:CG1	1:A:368:ILE:CD1	2.98	0.40
1:G:129:ALA:HB3	1:G:131:ILE:CD1	2.51	0.40
1:E:339:ILE:HG21	1:E:379:MET:CE	2.52	0.40
1:E:156:PHE:HA	1:E:157:ALA:C	2.42	0.40
1:D:282:ILE:HB	1:D:287:ILE:HD12	2.01	0.40
1:B:148:GLY:O	1:B:151:SER:OG	2.39	0.40
1:C:219:ASP:CG	1:C:223:GLY:N	2.74	0.40
1:F:11:LEU:HB2	1:F:23:THR:HG21	2.03	0.40
1:E:416:ALA:HB3	1:E:442:GLY:HA2	2.03	0.40
1:B:75:MET:CG	1:B:75:MET:O	2.69	0.40
1:E:363:ASP:OD2	1:E:374:HIS:ND1	2.52	0.40
1:A:16:GLY:O	1:A:387:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLY:HA2	1:E:368:ILE:HD12	2.03	0.40
1:H:112:ASP:O	1:H:140:ALA:HB3	2.21	0.40
1:A:235:VAL:CA	1:A:238:VAL:CG1	2.94	0.40
1:A:271:LEU:HD12	1:A:297:ALA:HA	1.98	0.40
1:E:124:ARG:HG3	1:E:137:ILE:O	2.21	0.40
1:G:181:GLN:O	1:G:182:LEU:CG	2.69	0.40
1:G:350:LYS:HD2	1:G:353:LEU:HD12	2.02	0.40
1:D:353:LEU:O	1:D:356:LEU:HB2	2.20	0.40
1:C:99:ALA:HB1	1:C:135:ALA:H	1.86	0.40
1:E:213:ILE:HG21	1:E:216:THR:HG22	2.03	0.40
1:B:409:SER:CB	1:B:410:VAL:HA	2.32	0.40
1:G:61:TYR:HD2	1:G:106:GLY:C	2.25	0.40
1:B:178:VAL:CG2	1:B:197:TYR:HB2	2.52	0.40
1:E:191:ARG:HB2	1:E:238:VAL:HG13	2.03	0.40
1:E:315:SER:O	1:E:316:TRP:CD1	2.74	0.40
1:C:10:THR:HB	1:C:21:PRO:HB3	2.03	0.40
1:E:73:MET:O	1:E:76:ALA:CB	2.70	0.40
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.72	0.40
1:C:347:CYS:HA	1:C:348:PRO:HD3	1.94	0.40
1:A:71:ALA:O	1:A:74:PHE:CB	2.58	0.40
1:A:191:ARG:NH1	1:A:238:VAL:HG22	2.35	0.40
1:B:77:GLY:C	1:B:155:HIS:HD1	2.25	0.40
1:B:73:MET:O	1:B:76:ALA:CB	2.70	0.40
1:B:77:GLY:N	1:B:78:PRO:CD	2.84	0.40
1:F:150:PHE:HE2	1:F:170:ILE:CD1	2.34	0.40
1:F:236:LEU:HB3	1:F:266:LEU:CD2	2.50	0.40
1:E:315:SER:C	1:E:317:ALA:H	2.24	0.40
1:E:313:VAL:HG11	1:E:360:GLU:OE1	2.22	0.40
1:B:88:GLU:OE1	1:B:169:ARG:NH1	2.53	0.40
1:E:112:ASP:HB3	1:E:139:ALA:HA	2.03	0.40
1:F:69:LEU:O	1:F:70:ASP:HB3	2.20	0.40
1:A:71:ALA:O	1:A:75:MET:N	2.47	0.40
1:H:360:GLU:OE2	1:H:361:ARG:CZ	2.70	0.40
1:H:341:LEU:HA	1:H:375:TRP:CH2	2.56	0.40
1:B:65:ASN:C	1:B:66:VAL:HG13	2.42	0.40
1:G:244:ARG:HH22	1:G:250:VAL:HG12	1.87	0.40
1:H:233:ARG:HH22	1:H:262:THR:HG1	1.65	0.40
1:H:178:VAL:HG11	1:H:197:TYR:CD1	2.56	0.40
1:E:284:ASN:O	1:E:285:TYR:HB3	2.18	0.40
1:E:140:ALA:HB2	1:E:204:MET:CG	2.52	0.40
1:G:181:GLN:CG	1:G:182:LEU:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:VAL:CG2	1:C:419:VAL:HB	2.51	0.40
1:F:420:LEU:HA	1:F:420:LEU:HD23	1.92	0.40
1:A:117:ILE:HG13	1:A:121:LEU:HG	2.04	0.40
1:B:323:GLU:O	1:B:325:TYR:N	2.54	0.40
1:H:227:SER:OG	1:H:228:TYR:N	2.55	0.40
1:G:439:PHE:CZ	1:G:444:ALA:HB2	2.56	0.40
1:F:193:ARG:HA	1:F:196:ASP:HB3	2.02	0.40
1:A:205:LEU:HA	1:A:205:LEU:HD12	1.93	0.40

All (7) 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:D:226:ARG:HE	1:G:180:HIS:HE2[1_455]	0.67	0.93
1:D:226:ARG:HE	1:G:180:HIS:NE2[1_455]	1.26	0.34
1:A:261:ASP:OD2	1:C:187:ARG:HH21[1_655]	1.42	0.18
1:F:219:ASP:OD2	1:H:164:ARG:NH2[1_655]	2.12	0.08
1:D:187:ARG:NH2	1:G:258:GLU:OE2[1_455]	2.13	0.07
1:D:226:ARG:NE	1:G:180:HIS:NE2[1_455]	2.18	0.02
1:D:229:GLN:H	1:G:229:GLN:O[1_455]	1.60	0.00

## 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	457/461 (99%)	391 (86%)	57 (12%)	9 (2%)	9	38
1	B	459/461 (100%)	420 (92%)	32 (7%)	7 (2%)	13	47
1	C	459/461 (100%)	415 (90%)	35 (8%)	9 (2%)	9	38
1	D	457/461 (99%)	410 (90%)	33 (7%)	14 (3%)	5	25
1	E	457/461 (99%)	412 (90%)	31 (7%)	14 (3%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	457/461 (99%)	402 (88%)	45 (10%)	10 (2%)	8	35
1	G	457/461 (99%)	407 (89%)	40 (9%)	10 (2%)	8	35
1	H	457/461 (99%)	401 (88%)	46 (10%)	10 (2%)	8	35
All	All	3660/3688 (99%)	3258 (89%)	319 (9%)	83 (2%)	8	34

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	323	GLU
1	A	41	THR
1	A	255	VAL
1	B	31	ARG
1	B	41	THR
1	B	394	THR
1	C	323	GLU
1	D	37	PRO
1	D	71	ALA
1	D	73	MET
1	D	76	ALA
1	F	30	ASP
1	F	228	TYR
1	F	283	PRO
1	F	323	GLU
1	F	429	ILE
1	G	323	GLU
1	H	203	ASP
1	H	323	GLU
1	H	360	GLU
1	E	76	ALA
1	E	158	GLY
1	E	221	SER
1	C	31	ARG
1	C	223	GLY
1	C	338	LYS
1	F	77	GLY
1	F	226	ARG
1	F	428	ASP
1	G	31	ARG
1	G	45	GLU
1	G	225	ASP
1	H	31	ARG

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Mol	Chain	Res	Type
1	E	180	HIS
1	A	228	TYR
1	B	37	PRO
1	B	389	ALA
1	C	259	ALA
1	D	338	LYS
1	F	329	GLU
1	G	139	ALA
1	E	41	THR
1	E	182	LEU
1	E	226	ARG
1	E	259	ALA
1	E	285	TYR
1	A	37	PRO
1	A	75	MET
1	D	45	GLU
1	D	181	GLN
1	D	258	GLU
1	F	151	SER
1	G	3	THR
1	G	153	ASP
1	H	30	ASP
1	H	181	GLN
1	H	456	VAL
1	A	85	ALA
1	B	42	PRO
1	B	323	GLU
1	C	219	ASP
1	C	224	PHE
1	D	31	ARG
1	D	259	ALA
1	H	41	THR
1	E	199	SER
1	E	213	ILE
1	E	316	TRP
1	A	30	ASP
1	C	44	PRO
1	G	182	LEU
1	G	452	THR
1	E	454	PRO
1	A	323	GLU
1	D	323	GLU

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Mol	Chain	Res	Type
1	G	178	VAL
1	D	222	VAL
1	C	37	PRO
1	D	167	VAL
1	D	413	GLY
1	H	78	PRO
1	A	46	GLY
1	H	255	VAL

### 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	367/368 (100%)	313 (85%)	54 (15%)	4	15
1	B	368/368 (100%)	313 (85%)	55 (15%)	4	15
1	C	368/368 (100%)	327 (89%)	41 (11%)	8	27
1	D	367/368 (100%)	307 (84%)	60 (16%)	3	12
1	E	367/368 (100%)	315 (86%)	52 (14%)	4	17
1	F	367/368 (100%)	315 (86%)	52 (14%)	4	17
1	G	367/368 (100%)	308 (84%)	59 (16%)	3	12
1	H	367/368 (100%)	302 (82%)	65 (18%)	2	10
All	All	2938/2944 (100%)	2500 (85%)	438 (15%)	4	15

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	ASN
1	E	10	THR
1	E	25	VAL
1	E	30	ASP
1	E	31	ARG
1	E	41	THR
1	E	45	GLU

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Mol	Chain	Res	Type
1	E	75	MET
1	E	82	GLU
1	E	97	GLU
1	E	110	VAL
1	E	144	VAL
1	E	153	ASP
1	E	156	PHE
1	E	164	ARG
1	E	178	VAL
1	E	180	HIS
1	E	188	LYS
1	E	198	LEU
1	E	199	SER
1	E	200	ARG
1	E	203	ASP
1	E	204	MET
1	E	207	ILE
1	E	214	VAL
1	E	216	THR
1	E	218	VAL
1	E	220	ARG
1	E	226	ARG
1	E	237	GLU
1	E	238	VAL
1	E	241	GLU
1	E	251	LEU
1	E	254	SER
1	E	269	ASP
1	E	272	ILE
1	E	277	THR
1	E	280	GLN
1	E	285	TYR
1	E	286	LEU
1	E	291	VAL
1	E	302	VAL
1	E	306	HIS
1	E	307	ARG
1	E	320	LEU
1	E	329	GLU
1	E	385	SER
1	E	390	ILE
1	E	406	GLN

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Mol	Chain	Res	Type
1	E	412	THR
1	E	417	ASP
1	E	436	THR
1	A	8	ASN
1	A	10	THR
1	A	13	ASP
1	A	18	LEU
1	A	27	VAL
1	A	31	ARG
1	A	45	GLU
1	A	57	MET
1	A	58	VAL
1	A	66	VAL
1	A	75	MET
1	A	93	GLU
1	A	97	GLU
1	A	126	ARG
1	A	160	THR
1	A	180	HIS
1	A	184	LEU
1	A	218	VAL
1	A	237	GLU
1	A	251	LEU
1	A	271	LEU
1	A	272	ILE
1	A	285	TYR
1	A	293	SER
1	A	300	GLN
1	A	301	THR
1	A	303	HIS
1	A	304	ASP
1	A	315	SER
1	A	325	TYR
1	A	341	LEU
1	A	343	THR
1	A	344	ASP
1	A	351	ASP
1	A	361	ARG
1	A	362	GLU
1	A	364	ARG
1	A	376	THR
1	A	377	GLN

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Mol	Chain	Res	Type
1	A	387	LEU
1	A	390	ILE
1	A	395	ILE
1	A	397	VAL
1	A	399	ARG
1	A	405	ASP
1	A	407	ILE
1	A	409	SER
1	A	411	GLU
1	A	412	THR
1	A	435	ILE
1	A	447	ARG
1	A	451	PRO
1	A	457	THR
1	A	459	HIS
1	B	4	ILE
1	B	13	ASP
1	B	18	LEU
1	B	20	ARG
1	B	23	THR
1	B	30	ASP
1	B	31	ARG
1	B	39	ASP
1	B	45	GLU
1	B	53	ASN
1	B	68	LEU
1	B	75	MET
1	B	121	LEU
1	B	146	MET
1	B	155	HIS
1	B	165	THR
1	B	170	ILE
1	B	184	LEU
1	B	187	ARG
1	B	188	LYS
1	B	195	ARG
1	B	198	LEU
1	B	199	SER
1	B	204	MET
1	B	206	LYS
1	B	210	SER
1	B	214	VAL

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Mol	Chain	Res	Type
1	B	226	ARG
1	B	229	GLN
1	B	232	SER
1	B	242	GLU
1	B	252	THR
1	B	254	SER
1	B	255	VAL
1	B	271	LEU
1	B	281	GLU
1	B	284	ASN
1	B	285	TYR
1	B	288	ASP
1	B	300	GLN
1	B	311	GLU
1	B	350	LYS
1	B	376	THR
1	B	377	GLN
1	B	382	LYS
1	B	387	LEU
1	B	396	ASN
1	B	397	VAL
1	B	420	LEU
1	B	424	ASP
1	B	437	GLU
1	B	447	ARG
1	B	452	THR
1	B	457	THR
1	B	459	HIS
1	C	9	VAL
1	C	23	THR
1	C	25	VAL
1	C	30	ASP
1	C	39	ASP
1	C	49	VAL
1	C	58	VAL
1	C	72	TRP
1	C	75	MET
1	C	90	ARG
1	C	118	GLU
1	C	121	LEU
1	C	124	ARG
1	C	131	ILE

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Mol	Chain	Res	Type
1	C	163	THR
1	C	180	HIS
1	C	191	ARG
1	C	205	LEU
1	C	206	LYS
1	C	214	VAL
1	C	218	VAL
1	C	220	ARG
1	C	224	PHE
1	C	226	ARG
1	C	230	THR
1	C	233	ARG
1	C	251	LEU
1	C	253	HIS
1	C	302	VAL
1	C	307	ARG
1	C	313	VAL
1	C	323	GLU
1	C	338	LYS
1	C	351	ASP
1	C	352	HIS
1	C	363	ASP
1	C	390	ILE
1	C	395	ILE
1	C	427	ASP
1	C	437	GLU
1	C	440	GLN
1	D	23	THR
1	D	24	THR
1	D	30	ASP
1	D	31	ARG
1	D	35	VAL
1	D	38	SER
1	D	72	TRP
1	D	74	PHE
1	D	81	ILE
1	D	82	GLU
1	D	83	TYR
1	D	84	LEU
1	D	118	GLU
1	D	124	ARG
1	D	126	ARG

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Mol	Chain	Res	Type
1	D	131	ILE
1	D	133	GLN
1	D	163	THR
1	D	171	ASP
1	D	180	HIS
1	D	182	LEU
1	D	183	SER
1	D	187	ARG
1	D	195	ARG
1	D	198	LEU
1	D	199	SER
1	D	204	MET
1	D	210	SER
1	D	213	ILE
1	D	216	THR
1	D	219	ASP
1	D	220	ARG
1	D	221	SER
1	D	224	PHE
1	D	230	THR
1	D	232	SER
1	D	238	VAL
1	D	261	ASP
1	D	280	GLN
1	D	282	ILE
1	D	286	LEU
1	D	293	SER
1	D	299	LEU
1	D	327	THR
1	D	333	ILE
1	D	334	SER
1	D	336	ASN
1	D	338	LYS
1	D	342	ASN
1	D	343	THR
1	D	381	GLU
1	D	391	SER
1	D	395	ILE
1	D	399	ARG
1	D	420	LEU
1	D	421	LEU
1	D	422	ASP

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Mol	Chain	Res	Type
1	D	427	ASP
1	D	433	ARG
1	D	436	THR
1	F	38	SER
1	F	40	SER
1	F	43	VAL
1	F	49	VAL
1	F	86	ARG
1	F	112	ASP
1	F	115	ASN
1	F	126	ARG
1	F	151	SER
1	F	154	PHE
1	F	184	LEU
1	F	185	LEU
1	F	188	LYS
1	F	191	ARG
1	F	199	SER
1	F	204	MET
1	F	219	ASP
1	F	224	PHE
1	F	226	ARG
1	F	251	LEU
1	F	263	SER
1	F	265	GLU
1	F	266	LEU
1	F	278	LEU
1	F	281	GLU
1	F	282	ILE
1	F	290	ILE
1	F	291	VAL
1	F	294	ASP
1	F	302	VAL
1	F	303	HIS
1	F	304	ASP
1	F	327	THR
1	F	328	ASN
1	F	329	GLU
1	F	347	CYS
1	F	349	SER
1	F	350	LYS
1	F	351	ASP

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Mol	Chain	Res	Type
1	F	360	GLU
1	F	362	GLU
1	F	412	THR
1	F	422	ASP
1	F	424	ASP
1	F	428	ASP
1	F	429	ILE
1	F	430	ARG
1	F	436	THR
1	F	440	GLN
1	F	447	ARG
1	F	455	LEU
1	F	457	THR
1	G	4	ILE
1	G	7	THR
1	G	9	VAL
1	G	15	LEU
1	G	20	ARG
1	G	26	ILE
1	G	35	VAL
1	G	38	SER
1	G	45	GLU
1	G	48	THR
1	G	50	VAL
1	G	54	ARG
1	G	55	ARG
1	G	75	MET
1	G	78	PRO
1	G	80	THR
1	G	82	GLU
1	G	113	THR
1	G	118	GLU
1	G	124	ARG
1	G	137	ILE
1	G	155	HIS
1	G	164	ARG
1	G	172	SER
1	G	180	HIS
1	G	182	LEU
1	G	205	LEU
1	G	207	ILE
1	G	219	ASP

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Mol	Chain	Res	Type
1	G	220	ARG
1	G	222	VAL
1	G	225	ASP
1	G	230	THR
1	G	263	SER
1	G	266	LEU
1	G	269	ASP
1	G	275	ASN
1	G	285	TYR
1	G	286	LEU
1	G	288	ASP
1	G	293	SER
1	G	300	GLN
1	G	301	THR
1	G	320	LEU
1	G	324	PRO
1	G	327	THR
1	G	342	ASN
1	G	347	CYS
1	G	349	SER
1	G	350	LYS
1	G	364	ARG
1	G	382	LYS
1	G	390	ILE
1	G	391	SER
1	G	395	ILE
1	G	440	GLN
1	G	453	THR
1	G	457	THR
1	G	459	HIS
1	H	11	LEU
1	H	13	ASP
1	H	15	LEU
1	H	18	LEU
1	H	30	ASP
1	H	39	ASP
1	H	45	GLU
1	H	54	ARG
1	H	67	HIS
1	H	101	LEU
1	H	113	THR
1	H	118	GLU

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Mol	Chain	Res	Type
1	H	126	ARG
1	H	151	SER
1	H	180	HIS
1	H	181	GLN
1	H	195	ARG
1	H	199	SER
1	H	200	ARG
1	H	204	MET
1	H	216	THR
1	H	217	LEU
1	H	218	VAL
1	H	220	ARG
1	H	224	PHE
1	H	226	ARG
1	H	229	GLN
1	H	233	ARG
1	H	256	SER
1	H	261	ASP
1	H	271	LEU
1	H	273	HIS
1	H	275	ASN
1	H	285	TYR
1	H	286	LEU
1	H	295	SER
1	H	306	HIS
1	H	310	LEU
1	H	312	ASP
1	H	327	THR
1	H	328	ASN
1	H	330	ARG
1	H	331	ASN
1	H	333	ILE
1	H	338	LYS
1	H	340	LEU
1	H	353	LEU
1	H	357	SER
1	H	361	ARG
1	H	377	GLN
1	H	378	SER
1	H	380	VAL
1	H	381	GLU
1	H	382	LYS

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Mol	Chain	Res	Type
1	H	385	SER
1	H	395	ILE
1	H	406	GLN
1	H	412	THR
1	H	432	LEU
1	H	436	THR
1	H	445	VAL
1	H	447	ARG
1	H	452	THR
1	H	453	THR
1	H	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	273	HIS
1	E	352	HIS
1	A	212	HIS
1	A	370	ASN
1	F	212	HIS
1	F	253	HIS
1	G	273	HIS
1	H	100	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](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	459/461 (99%)	0.17	10 (2%) 65 44	19, 40, 57, 93	0
1	B	459/461 (99%)	-0.08	2 (0%) 93 83	9, 26, 44, 70	0
1	C	459/461 (99%)	0.13	7 (1%) 76 57	16, 38, 60, 77	0
1	D	459/461 (99%)	-0.11	7 (1%) 76 57	10, 27, 48, 80	0
1	E	459/461 (99%)	0.05	7 (1%) 76 57	9, 32, 55, 80	0
1	F	459/461 (99%)	0.41	26 (5%) 27 15	23, 47, 68, 87	0
1	G	459/461 (99%)	0.12	17 (3%) 45 27	12, 34, 64, 92	0
1	H	459/461 (99%)	0.29	12 (2%) 59 38	22, 43, 58, 78	0
All	All	3672/3688 (99%)	0.12	88 (2%) 62 41	9, 37, 60, 93	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	THR	6.0
1	F	62	VAL	5.6
1	F	6	ILE	5.2
1	D	49	VAL	5.0
1	F	421	LEU	4.7
1	G	39	ASP	4.6
1	D	46	GLY	4.2
1	H	435	ILE	3.9
1	A	221	SER	3.8
1	G	15	LEU	3.7
1	A	251	LEU	3.5
1	H	429	ILE	3.5
1	F	394	THR	3.5
1	E	60	GLY	3.5
1	E	6	ILE	3.4
1	F	127	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	257	VAL	3.3
1	E	454	PRO	3.2
1	E	420	LEU	3.2
1	F	34	THR	3.1
1	F	38	SER	3.1
1	C	40	SER	3.1
1	F	18	LEU	3.0
1	G	14	GLY	3.0
1	E	41	THR	2.9
1	F	41	THR	2.9
1	F	267	GLY	2.9
1	H	383	GLY	2.9
1	H	270	VAL	2.8
1	A	254	SER	2.8
1	F	15	LEU	2.8
1	G	46	GLY	2.8
1	G	29	GLY	2.7
1	C	23	THR	2.7
1	F	24	THR	2.7
1	E	48	THR	2.7
1	A	41	THR	2.7
1	B	427	ASP	2.7
1	G	319	ALA	2.6
1	H	40	SER	2.6
1	F	325	TYR	2.6
1	G	78	PRO	2.5
1	F	422	ASP	2.5
1	F	25	VAL	2.5
1	F	50	VAL	2.5
1	G	7	THR	2.5
1	G	40	SER	2.5
1	F	57	MET	2.5
1	F	382	LYS	2.4
1	F	383	GLY	2.4
1	G	326	ALA	2.4
1	A	266	LEU	2.4
1	F	7	THR	2.4
1	G	276	TYR	2.3
1	G	410	VAL	2.3
1	H	131	ILE	2.3
1	G	41	THR	2.3
1	F	420	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	333	ILE	2.2
1	G	26	ILE	2.2
1	H	390	ILE	2.2
1	H	337	ALA	2.2
1	A	178	VAL	2.2
1	F	277	THR	2.2
1	A	426	VAL	2.2
1	F	110	VAL	2.2
1	H	432	LEU	2.2
1	D	48	THR	2.2
1	F	226	ARG	2.2
1	C	7	THR	2.2
1	D	221	SER	2.1
1	G	36	GLY	2.1
1	H	336	ASN	2.1
1	G	25	VAL	2.1
1	A	379	MET	2.1
1	E	205	LEU	2.1
1	H	6	ILE	2.1
1	C	358	PRO	2.1
1	C	29	GLY	2.0
1	C	111	PHE	2.0
1	D	378	SER	2.0
1	H	81	ILE	2.0
1	G	327	THR	2.0
1	F	202	VAL	2.0
1	A	315	SER	2.0
1	D	333	ILE	2.0
1	B	49	VAL	2.0
1	D	6	ILE	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 ⓘ

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
2	ZN	A	501	1/1	0.98	0.05	-2.51	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.