



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:36 PM EDT

PDB ID : 4W1Y  
Title : Crystal structure of Escherichia coli Tryptophanase in 'semi-holo' form  
Authors : Goldgur, Y.  
Deposited on : 2014-08-13  
Resolution : 3.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

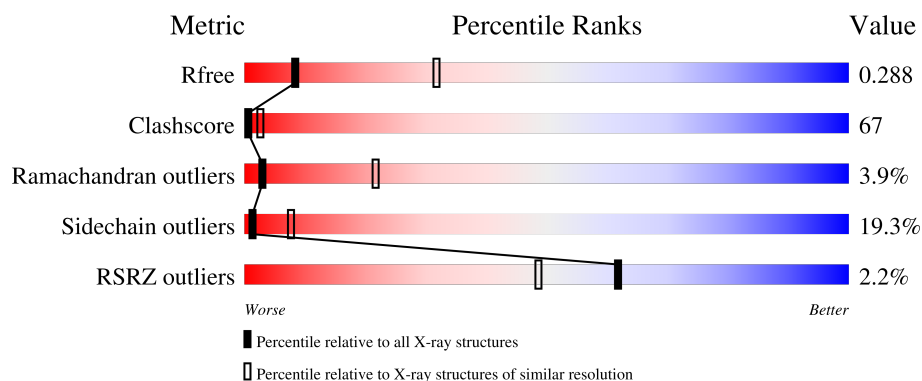
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	467	
2	B	467	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6957 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	P	S	0	0	0
			3428	2181	575	650	1	21			

- Molecule 2 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	433	Total	C	N	O	S	0	0	0
			3412	2175	575	641	21			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

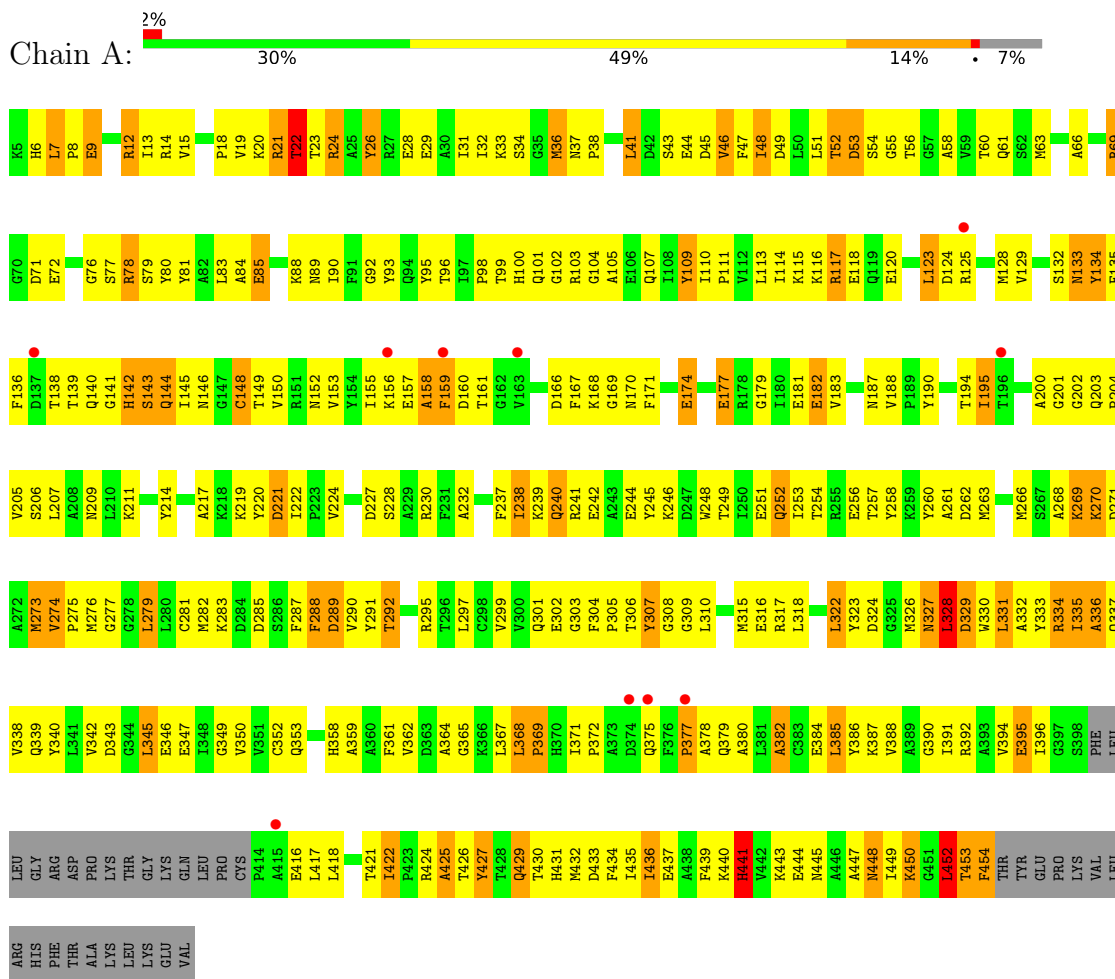
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	65	Total 65	O 65	0	0

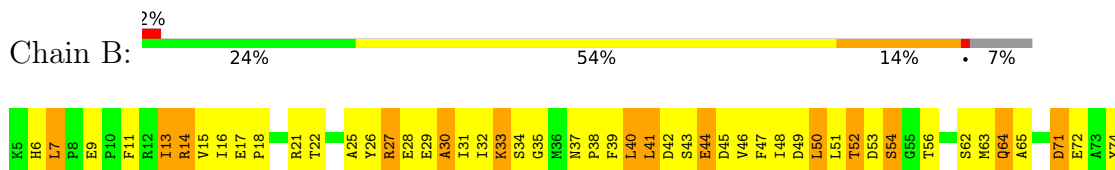
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Tryptophanase



#### • Molecule 2: Tryptophanase



T465	PRO	V330	A268	S206	GLN	S75
A466	LYS	L331	K269	L207	GLY	
K467	THR	A332	K270	A208	HIS	S79
L468	GLY	Y333	D271	N209	SER	Y80
K469	LYS	R334	A272	L210	GLN	Y81
E470	GLN	I335	M273	K211	ILE	A82
V471	LEU	A336	V274	A212	ASN	L83
	PRO	Q337	F275	M213	GLY	A84
	C413	V338	M276	Y214	CYS	E85
	P414	Q339	G277	S215	T149	S86
	A415	Y340	G278	I216	T149	V87
	E416	L341	L279	A217	V153	K88
	L417		L280		Y154	K89
L418	Q353		C281	Y220		I90
R419	Q354		M282	D221	E157	F91
L420	A355		K283	I222	A158	G92
T421	G356		D284	P223	F159	Y93
I422	G357		D285	V224	D160	Q94
P423	H358		S286	V225	T161	Y95
R424	A359		F287	M226	G162	T96
A425	A360		F288	D227	V163	Y98
T426	F361		D289	A229	R164	T99
Y427	D362		V290	R230	D166	H100
T428	D363		Y291	F231	F167	G101
Q429	A364		T292	A232	K168	G102
T430			E293	E233	G169	R103
H431	L367		C294	E234	N170	
M432	L368		R295	N234	F171	E106
D433			T296	A235	D172	Q107
F434	I371		L297	Y236	L173	I108
I435	P372		C298		E174	I109
I436			V299	K239		I110
E437	Q375		V300	Q240		P111
A438	F376		Q301	R241	E177	V112
F439	P377		E302	E242	G179	L113
K440	A378		GLY	A243	I180	I114
H441	D379		PHE	E244	E181	K115
V442	A380		PRO	Y245	E182	K116
K443	L381		THR	K286	D247	R117
E444	A382		TYR	W248	GLY	E118
M445	C383		GLY	T249	G184	Q119
A446	E384		G309	I250		E120
A447			L310	E251	M187	
M448	K387		E311	Q252	V188	L123
I449	V388			I253	P189	D124
K450	A389		A314	T254	Y190	R125
G451			M315	R255	I191	S126
L452	R392		E316	E256		K127
T453	A393		R317	T257	T194	M128
F454	V394		L318	Y258	I195	V129
T455	E395		A319	K259	T196	
Y456	I396		V320		S197	
E457	G397			Y260	N198	S132
S458	S398		Y323	A261	S199	N133
K459	PHE		D324	D262	A200	Y134
V460	LEU		G395	M263	G201	PHE
L461	LEU		H326	L264	Q202	PHE
R462	GLY		N327	A265	Q203	ASP
H463	ARG		L328	M266	P204	THR
F464	ASP		D329	S267	V205	THR

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.97Å 109.97Å 238.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 29.06 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-3.20) 94.9 (29.06-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.214 , 0.290 0.212 , 0.288	Depositor DCC
$R_{free}$ test set	1207 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: LLP, SO4

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	1.02	2/3473 (0.1%)	1.12	11/4692 (0.2%)
2	B	1.09	4/3478 (0.1%)	1.20	16/4694 (0.3%)
All	All	1.05	6/6951 (0.1%)	1.16	27/9386 (0.3%)

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	1
2	B	0	2
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	GLU	CG-CD	6.80	1.62	1.51
2	B	281	CYS	CB-SG	-6.40	1.71	1.82
1	A	427	TYR	CD1-CE1	6.06	1.48	1.39
2	B	154	TYR	CD2-CE2	-5.92	1.30	1.39
2	B	74	TYR	CE1-CZ	5.05	1.45	1.38
2	B	154	TYR	CD1-CE1	-5.04	1.31	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	MET	CB-CG-SD	-7.79	89.05	112.40
2	B	14	ARG	NE-CZ-NH1	-7.49	116.56	120.30
2	B	418	LEU	CA-CB-CG	7.07	131.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	LEU	CB-CG-CD2	-6.96	99.17	111.00
2	B	282	MET	CG-SD-CE	6.80	111.08	100.20
1	A	53	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	255	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	452	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	46	VAL	CB-CA-C	-5.93	100.14	111.40
1	A	69	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	A	7	LEU	CB-CG-CD2	-5.73	101.27	111.00
1	A	273	MET	CG-SD-CE	5.69	109.30	100.20
2	B	269	LYS	CD-CE-NZ	5.54	124.44	111.70
2	B	317	ARG	NE-CZ-NH1	-5.53	117.53	120.30
2	B	424	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	B	71	ASP	N-CA-C	-5.49	96.17	111.00
2	B	278	GLY	N-CA-C	-5.48	99.40	113.10
1	A	48	ILE	N-CA-C	-5.47	96.23	111.00
2	B	40	LEU	CB-CG-CD1	5.47	120.29	111.00
1	A	53	ASP	CB-CG-OD1	-5.36	113.47	118.30
2	B	71	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	22	THR	N-CA-C	5.22	125.10	111.00
2	B	324	ASP	CB-CG-OD2	5.20	122.97	118.30
2	B	210	LEU	CA-CB-CG	-5.07	103.63	115.30
1	A	299	VAL	CB-CA-C	-5.04	101.82	111.40
1	A	279	LEU	CA-CB-CG	-5.01	103.78	115.30
2	B	230	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	THR	Peptide
2	B	162	GLY	Peptide
2	B	309	GLY	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	3428	0	3371	418	0
2	B	3412	0	3395	515	1
3	B	10	0	0	1	0
4	A	42	0	0	28	0
4	B	65	0	0	40	0
All	All	6957	0	6766	916	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 67.

All (916) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:THR:CG2	2:B:27:ARG:HH11	1.02	1.58
2:B:22:THR:CG2	2:B:27:ARG:HG3	1.39	1.52
2:B:450:LYS:HB2	2:B:470:GLU:CD	1.31	1.46
2:B:375:GLN:HE21	2:B:471:VAL:CG1	1.26	1.46
1:A:170:ASN:CB	1:A:209:ASN:ND2	1.79	1.45
2:B:22:THR:HG21	2:B:27:ARG:CG	1.57	1.35
2:B:375:GLN:HG2	2:B:471:VAL:CG2	1.55	1.34
2:B:451:GLY:O	2:B:470:GLU:HA	1.19	1.34
2:B:455:THR:HG23	4:B:645:HOH:O	1.17	1.32
2:B:375:GLN:NE2	2:B:471:VAL:CG1	1.93	1.29
1:A:200:ALA:CB	1:A:203:GLN:HG2	1.63	1.26
2:B:450:LYS:HB2	2:B:470:GLU:OE1	1.26	1.26
1:A:170:ASN:HB3	1:A:209:ASN:ND2	0.93	1.25
2:B:353:GLN:OE1	2:B:417:LEU:HD21	1.24	1.25
2:B:161:THR:CG2	2:B:354:GLN:OE1	1.85	1.24
1:A:60:THR:OG1	1:A:63:MET:HG3	1.33	1.23
2:B:377:PRO:HD2	2:B:416:GLU:OE2	1.39	1.22
2:B:22:THR:HG22	2:B:27:ARG:NH1	0.89	1.21
2:B:170:ASN:HB3	2:B:209:ASN:OD1	1.39	1.20
2:B:31:ILE:CD1	2:B:383:CYS:HB3	1.72	1.19
1:A:450:LYS:HD3	1:A:450:LYS:N	1.46	1.19
1:A:445:ASN:O	1:A:449:ILE:HG13	1.42	1.18
2:B:198:ASN:HB3	4:B:627:HOH:O	1.42	1.18
1:A:262:ASP:HB3	1:A:287:PHE:CE2	1.78	1.18
1:A:200:ALA:HB1	1:A:203:GLN:CG	1.73	1.17
2:B:22:THR:CG2	2:B:27:ARG:NH1	1.74	1.17
2:B:353:GLN:O	2:B:354:GLN:HG2	1.46	1.15
2:B:450:LYS:CB	2:B:470:GLU:CD	2.17	1.12
2:B:389:ALA:HB1	2:B:434:PHE:CE2	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:CB	1:A:209:ASN:HD22	1.47	1.12
2:B:451:GLY:O	2:B:470:GLU:CA	1.98	1.10
2:B:389:ALA:HB1	2:B:434:PHE:HE2	0.95	1.10
2:B:251:GLU:HG3	2:B:326:MET:CE	1.81	1.10
2:B:245:TYR:O	2:B:247:ASP:N	1.86	1.09
1:A:36:MET:HA	1:A:36:MET:HE2	1.34	1.09
2:B:372:PRO:HD2	2:B:375:GLN:HB2	1.33	1.09
2:B:134:TYR:CD1	2:B:199:SER:HB3	1.88	1.08
2:B:375:GLN:HG2	2:B:471:VAL:HG21	1.29	1.08
2:B:43:SER:O	2:B:44:GLU:CB	1.96	1.07
2:B:381:LEU:HG	4:B:620:HOH:O	1.55	1.07
2:B:9:GLU:HG3	2:B:333:TYR:CE1	1.90	1.06
2:B:327:ASN:ND2	2:B:330:TRP:H	1.51	1.06
2:B:39:PHE:CE2	2:B:51:LEU:HD21	1.91	1.05
2:B:363:ASP:OD1	4:B:628:HOH:O	1.74	1.05
2:B:9:GLU:HG3	2:B:333:TYR:CZ	1.90	1.04
1:A:204:PRO:HG3	1:A:237:PHE:CD2	1.91	1.04
1:A:170:ASN:CG	1:A:209:ASN:HD22	1.63	1.02
2:B:251:GLU:HG3	2:B:326:MET:HE3	1.41	1.02
2:B:375:GLN:CD	2:B:471:VAL:HB	1.79	1.02
2:B:38:PRO:O	2:B:41:LEU:HB2	1.60	1.01
2:B:199:SER:O	4:B:623:HOH:O	1.77	1.01
2:B:379:GLN:HG2	2:B:395:GLU:OE1	1.61	1.00
2:B:375:GLN:HE21	2:B:471:VAL:HG11	0.85	1.00
1:A:38:PRO:O	1:A:41:LEU:HB2	1.60	0.99
2:B:31:ILE:HD11	2:B:383:CYS:HB3	1.44	0.99
2:B:375:GLN:NE2	2:B:471:VAL:CB	2.25	0.99
2:B:450:LYS:HB2	2:B:470:GLU:OE2	1.63	0.99
1:A:159:PHE:O	1:A:353:GLN:NE2	1.95	0.99
2:B:43:SER:O	2:B:44:GLU:HB3	1.15	0.98
2:B:361:PHE:HB2	4:B:624:HOH:O	1.61	0.98
2:B:164:ARG:HG3	4:B:657:HOH:O	1.61	0.98
2:B:450:LYS:CB	2:B:470:GLU:OE2	2.10	0.98
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.29	0.98
1:A:202:GLY:HA3	4:A:536:HOH:O	1.62	0.98
2:B:353:GLN:OE1	2:B:417:LEU:CD2	2.12	0.97
1:A:450:LYS:HD3	1:A:450:LYS:H	1.23	0.97
1:A:32:ILE:HA	1:A:36:MET:HE1	1.44	0.97
1:A:60:THR:HG1	1:A:63:MET:HG3	1.27	0.97
2:B:452:LEU:HA	2:B:469:LYS:O	1.65	0.97
2:B:198:ASN:N	2:B:198:ASN:OD1	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HD11	4:A:524:HOH:O	1.64	0.97
2:B:133:ASN:N	2:B:133:ASN:HD22	1.61	0.97
2:B:450:LYS:CD	2:B:470:GLU:OE2	2.13	0.96
1:A:36:MET:HA	1:A:36:MET:CE	1.94	0.96
2:B:296:THR:O	2:B:299:VAL:HG22	1.66	0.95
1:A:307:TYR:HD1	1:A:309:GLY:H	1.14	0.94
2:B:22:THR:HG22	2:B:27:ARG:CZ	1.98	0.94
1:A:133:ASN:HD22	1:A:133:ASN:H	1.11	0.94
2:B:375:GLN:CG	2:B:471:VAL:HG21	1.97	0.94
1:A:262:ASP:CB	1:A:287:PHE:CE2	2.50	0.94
2:B:40:LEU:HD11	2:B:465:THR:HA	1.48	0.94
1:A:432:MET:HE2	1:A:432:MET:HA	1.47	0.94
2:B:22:THR:O	2:B:27:ARG:NH1	2.01	0.94
1:A:141:GLY:O	1:A:145:ILE:HB	1.67	0.94
2:B:467:LYS:HB2	4:B:647:HOH:O	1.68	0.94
1:A:429:GLN:O	1:A:432:MET:HB2	1.66	0.93
2:B:375:GLN:CG	2:B:471:VAL:CG2	2.47	0.93
1:A:200:ALA:HB1	1:A:203:GLN:HG2	0.94	0.93
2:B:375:GLN:NE2	2:B:471:VAL:HB	1.82	0.93
1:A:32:ILE:HA	1:A:36:MET:CE	2.00	0.92
2:B:22:THR:HG23	2:B:27:ARG:HG3	1.51	0.92
2:B:240:GLN:HB2	4:B:632:HOH:O	1.69	0.92
1:A:166:ASP:HB2	4:A:528:HOH:O	1.68	0.92
2:B:389:ALA:CB	2:B:434:PHE:HE2	1.81	0.92
2:B:117:ARG:HH21	2:B:222:ILE:HD13	1.35	0.92
1:A:450:LYS:N	1:A:450:LYS:CD	2.29	0.92
2:B:450:LYS:CB	2:B:470:GLU:OE1	2.18	0.91
2:B:375:GLN:HG2	2:B:471:VAL:CB	1.99	0.91
1:A:391:ILE:HD13	1:A:435:ILE:HG23	1.53	0.91
1:A:135:PHE:CE2	1:A:150:VAL:HB	2.07	0.90
2:B:154:TYR:HD2	2:B:154:TYR:H	0.92	0.90
2:B:6:HIS:CD2	2:B:429:GLN:HB2	2.07	0.90
2:B:375:GLN:NE2	2:B:471:VAL:HG11	1.70	0.89
2:B:22:THR:HG21	2:B:27:ARG:HG3	0.90	0.89
2:B:171:PHE:HB2	2:B:209:ASN:HD21	1.37	0.89
2:B:368:LEU:HB3	2:B:371:ILE:CD1	2.02	0.89
2:B:22:THR:HG22	2:B:27:ARG:HH12	1.32	0.89
2:B:375:GLN:NE2	2:B:471:VAL:HG12	1.84	0.88
2:B:451:GLY:O	2:B:470:GLU:HG2	1.73	0.88
1:A:143:SER:O	1:A:148:CYS:O	1.92	0.87
1:A:249:THR:O	1:A:253:ILE:HD12	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:O	1:A:368:LEU:C	2.12	0.87
2:B:378:ALA:CB	2:B:395:GLU:HG3	2.05	0.87
1:A:432:MET:HA	1:A:432:MET:CE	2.05	0.87
2:B:22:THR:HG21	2:B:27:ARG:CD	2.05	0.87
2:B:202:GLY:CA	2:B:358:HIS:CD2	2.58	0.87
2:B:22:THR:CG2	2:B:27:ARG:CG	2.30	0.86
2:B:251:GLU:CG	2:B:326:MET:CE	2.54	0.86
2:B:450:LYS:HD2	2:B:470:GLU:OE2	1.74	0.86
1:A:433:ASP:HA	1:A:436:ILE:HD12	1.56	0.86
1:A:170:ASN:CB	1:A:209:ASN:HD21	1.66	0.86
2:B:331:LEU:O	2:B:335:ILE:HG13	1.75	0.86
2:B:271:ASP:OD1	2:B:424:ARG:NH2	2.08	0.86
1:A:15:VAL:HB	2:B:15:VAL:HB	1.57	0.85
1:A:331:LEU:O	1:A:335:ILE:HG12	1.75	0.85
2:B:22:THR:HG21	2:B:27:ARG:HH11	1.33	0.85
2:B:327:ASN:HD21	2:B:330:TRP:H	1.22	0.85
2:B:230:ARG:HH11	2:B:230:ARG:CG	1.89	0.85
2:B:395:GLU:HB3	4:B:637:HOH:O	1.76	0.85
1:A:372:PRO:O	1:A:375:GLN:O	1.94	0.84
2:B:161:THR:HG23	2:B:354:GLN:OE1	1.77	0.84
2:B:22:THR:CB	2:B:27:ARG:HH11	1.89	0.84
2:B:31:ILE:HD11	2:B:383:CYS:CB	2.07	0.84
2:B:251:GLU:CG	2:B:326:MET:HE3	2.07	0.84
1:A:60:THR:OG1	1:A:63:MET:CG	2.21	0.84
1:A:327:ASN:ND2	1:A:330:TRP:H	1.75	0.84
2:B:353:GLN:O	2:B:354:GLN:CG	2.26	0.83
2:B:202:GLY:HA2	2:B:358:HIS:CD2	2.13	0.83
2:B:368:LEU:O	2:B:371:ILE:HD12	1.79	0.82
2:B:161:THR:HG22	2:B:354:GLN:OE1	1.77	0.82
1:A:9:GLU:OE2	1:A:333:TYR:CE1	2.33	0.82
1:A:19:VAL:HG12	2:B:11:PHE:HA	1.62	0.82
1:A:54:SER:HB2	1:A:270:LLP:HE3	1.60	0.82
2:B:354:GLN:NE2	4:B:653:HOH:O	2.12	0.82
1:A:289:ASP:HB3	4:A:537:HOH:O	1.80	0.81
1:A:114:ILE:HG21	1:A:125:ARG:HH12	1.44	0.81
1:A:345:LEU:HD23	1:A:436:ILE:HG23	1.62	0.81
2:B:196:THR:CG2	2:B:203:GLN:O	2.29	0.81
2:B:161:THR:HG21	2:B:354:GLN:OE1	1.81	0.81
2:B:453:THR:N	2:B:469:LYS:O	2.14	0.81
2:B:170:ASN:CB	2:B:209:ASN:OD1	2.26	0.81
1:A:422:ILE:O	1:A:422:ILE:HG22	1.77	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ARG:HG2	2:B:117:ARG:HH11	1.46	0.80
2:B:375:GLN:CG	2:B:471:VAL:HB	2.11	0.79
2:B:381:LEU:CG	4:B:620:HOH:O	2.20	0.79
2:B:31:ILE:HG13	4:B:659:HOH:O	1.82	0.79
2:B:196:THR:HG23	2:B:203:GLN:O	1.82	0.79
1:A:200:ALA:O	1:A:203:GLN:NE2	2.16	0.78
2:B:361:PHE:CD1	2:B:419:ARG:HB2	2.18	0.78
2:B:368:LEU:HB3	2:B:371:ILE:HD13	1.62	0.78
1:A:54:SER:O	1:A:56:THR:HG23	1.84	0.78
2:B:31:ILE:CD1	2:B:383:CYS:CB	2.58	0.78
2:B:209:ASN:C	2:B:209:ASN:HD22	1.85	0.78
2:B:21:ARG:NH2	2:B:47:PHE:CZ	2.51	0.78
1:A:268:ALA:O	1:A:274:VAL:HG23	1.84	0.78
1:A:431:HIS:O	1:A:435:ILE:HG13	1.82	0.77
2:B:456:TYR:HB3	4:B:647:HOH:O	1.84	0.77
2:B:236:TYR:CD2	2:B:335:ILE:HD12	2.18	0.77
1:A:251:GLU:HG2	1:A:326:MET:HE1	1.66	0.77
1:A:449:ILE:C	1:A:450:LYS:HD3	2.05	0.77
2:B:154:TYR:HD2	2:B:154:TYR:N	1.76	0.77
2:B:40:LEU:CD1	2:B:465:THR:HA	2.15	0.77
1:A:365:GLY:O	1:A:368:LEU:O	2.03	0.77
2:B:167:PHE:HB3	2:B:170:ASN:HD21	1.49	0.76
1:A:169:GLY:O	1:A:205:VAL:HG22	1.84	0.76
2:B:31:ILE:HD11	2:B:383:CYS:SG	2.24	0.76
1:A:161:THR:HG23	1:A:353:GLN:NE2	2.01	0.76
1:A:200:ALA:CB	1:A:203:GLN:CG	2.49	0.76
1:A:350:VAL:HG22	1:A:367:LEU:HD13	1.67	0.75
1:A:117:ARG:HH11	1:A:117:ARG:CG	1.98	0.75
1:A:161:THR:HG22	1:A:353:GLN:CD	2.05	0.75
2:B:375:GLN:CG	2:B:471:VAL:CB	2.64	0.75
2:B:50:LEU:HD12	2:B:420:LEU:HD23	1.69	0.75
2:B:180:ILE:O	2:B:184:GLY:HA2	1.86	0.75
2:B:224:VAL:CG1	2:B:261:ALA:HA	2.16	0.75
1:A:135:PHE:CZ	1:A:150:VAL:CG1	2.69	0.75
1:A:161:THR:HG22	1:A:353:GLN:HA	1.67	0.75
1:A:454:PHE:CE2	4:A:529:HOH:O	2.39	0.75
2:B:133:ASN:HD22	2:B:133:ASN:H	1.31	0.75
2:B:154:TYR:N	2:B:154:TYR:CD2	2.46	0.75
1:A:454:PHE:HE2	4:A:529:HOH:O	1.69	0.75
2:B:375:GLN:HE21	2:B:471:VAL:CB	1.96	0.75
1:A:433:ASP:HA	1:A:436:ILE:CD1	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:HD12	2:B:383:CYS:HB3	1.69	0.74
1:A:9:GLU:OE1	2:B:428:THR:HG21	1.87	0.74
2:B:389:ALA:CB	2:B:434:PHE:CE2	2.64	0.74
1:A:133:ASN:H	1:A:133:ASN:ND2	1.83	0.74
2:B:337:GLN:O	2:B:337:GLN:HG2	1.86	0.74
2:B:381:LEU:CD1	4:B:620:HOH:O	2.35	0.74
2:B:451:GLY:O	2:B:470:GLU:CB	2.35	0.74
2:B:368:LEU:HD13	4:B:630:HOH:O	1.87	0.74
1:A:28:GLU:O	1:A:32:ILE:HG12	1.88	0.73
2:B:117:ARG:HH11	2:B:117:ARG:CG	2.00	0.73
2:B:375:GLN:HG2	2:B:471:VAL:HG23	1.63	0.73
1:A:6:HIS:ND1	1:A:429:GLN:HB2	2.03	0.73
1:A:449:ILE:HA	1:A:450:LYS:HD3	1.69	0.73
1:A:60:THR:HG1	1:A:63:MET:CG	1.99	0.73
1:A:238:ILE:HG23	1:A:242:GLU:HB3	1.71	0.73
2:B:108:ILE:HD11	2:B:298:CYS:SG	2.28	0.73
2:B:460:VAL:O	4:B:601:HOH:O	2.06	0.73
2:B:161:THR:CG2	2:B:354:GLN:CD	2.58	0.72
2:B:419:ARG:HG2	2:B:420:LEU:N	2.04	0.72
2:B:451:GLY:O	2:B:470:GLU:CG	2.37	0.72
1:A:6:HIS:CE1	1:A:337:GLN:HG3	2.25	0.72
1:A:41:LEU:HD21	1:A:386:TYR:CD2	2.25	0.71
2:B:99:THR:OG1	2:B:278:GLY:HA3	1.90	0.71
1:A:20:LYS:HD3	4:A:532:HOH:O	1.89	0.71
1:A:55:GLY:N	1:A:269:LYS:HB3	2.04	0.71
2:B:133:ASN:N	2:B:133:ASN:ND2	2.37	0.71
2:B:422:ILE:HG23	2:B:423:PRO:HD2	1.72	0.71
1:A:32:ILE:HD13	1:A:36:MET:HE1	1.71	0.71
2:B:214:TYR:HB2	2:B:260:TYR:HB3	1.72	0.71
2:B:196:THR:CG2	2:B:203:GLN:C	2.59	0.71
1:A:249:THR:OG1	1:A:252:GLN:HB2	1.91	0.71
2:B:372:PRO:O	2:B:375:GLN:O	2.09	0.71
1:A:204:PRO:HG3	1:A:237:PHE:HD2	1.56	0.71
2:B:9:GLU:HG3	2:B:333:TYR:OH	1.91	0.71
2:B:189:PRO:HB2	2:B:190:TYR:CD1	2.26	0.71
1:A:72:GLU:HA	4:A:538:HOH:O	1.90	0.70
1:A:98:PRO:O	1:A:308:GLY:HA3	1.91	0.70
2:B:22:THR:CB	2:B:27:ARG:NH1	2.52	0.70
2:B:181:GLU:C	2:B:183:VAL:H	1.94	0.70
2:B:251:GLU:HG3	2:B:326:MET:HE1	1.71	0.70
2:B:251:GLU:CG	2:B:326:MET:HE1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:HD21	1:A:194:THR:H	1.39	0.70
1:A:251:GLU:CG	1:A:326:MET:HE1	2.22	0.69
2:B:6:HIS:CE1	2:B:337:GLN:HG3	2.26	0.69
2:B:445:ASN:O	2:B:447:ALA:N	2.25	0.69
1:A:450:LYS:H	1:A:450:LYS:CD	1.97	0.69
2:B:262:ASP:HB3	2:B:287:PHE:CE2	2.28	0.69
2:B:361:PHE:CE1	2:B:419:ARG:HD3	2.27	0.69
1:A:55:GLY:H	1:A:269:LYS:HB3	1.58	0.69
2:B:50:LEU:HD13	2:B:421:THR:H	1.57	0.69
2:B:378:ALA:HB3	2:B:395:GLU:HG3	1.73	0.69
1:A:124:ASP:HB3	1:A:187:ASN:HD21	1.56	0.69
2:B:327:ASN:ND2	2:B:330:TRP:N	2.36	0.69
1:A:135:PHE:CZ	1:A:150:VAL:HG12	2.29	0.68
1:A:171:PHE:N	1:A:209:ASN:HD21	1.90	0.68
1:A:371:ILE:CG2	1:A:377:PRO:HB3	2.22	0.68
1:A:214:TYR:HB2	1:A:260:TYR:HB3	1.76	0.68
1:A:9:GLU:OE2	1:A:333:TYR:HE1	1.74	0.68
2:B:110:ILE:O	2:B:114:ILE:HG13	1.94	0.68
1:A:254:THR:HA	4:A:527:HOH:O	1.93	0.68
2:B:22:THR:C	2:B:27:ARG:HH12	1.95	0.68
2:B:354:GLN:CD	4:B:653:HOH:O	2.30	0.68
2:B:452:LEU:CA	2:B:469:LYS:O	2.41	0.68
1:A:161:THR:CG2	1:A:353:GLN:CD	2.62	0.68
2:B:6:HIS:HB2	2:B:340:TYR:CD1	2.28	0.68
2:B:375:GLN:HG2	2:B:471:VAL:HB	1.71	0.68
1:A:8:PRO:HG2	2:B:21:ARG:NH2	2.09	0.68
1:A:327:ASN:ND2	1:A:327:ASN:C	2.47	0.68
1:A:31:ILE:O	1:A:36:MET:HE2	1.93	0.67
1:A:449:ILE:CA	1:A:450:LYS:HD3	2.23	0.67
2:B:28:GLU:O	2:B:29:GLU:C	2.33	0.67
2:B:80:TYR:N	2:B:315:MET:HE3	2.09	0.67
1:A:171:PHE:H	1:A:209:ASN:HD21	1.43	0.67
2:B:202:GLY:HA3	2:B:358:HIS:CD2	2.28	0.67
1:A:93:TYR:CE2	1:A:283:LYS:HB2	2.30	0.67
2:B:240:GLN:HG2	2:B:241:ARG:HG3	1.74	0.67
1:A:9:GLU:CG	2:B:431:HIS:CE1	2.78	0.66
1:A:384:GLU:O	1:A:388:VAL:HG12	1.95	0.66
2:B:181:GLU:C	2:B:183:VAL:N	2.44	0.66
2:B:445:ASN:C	2:B:447:ALA:H	1.98	0.66
1:A:248:TRP:CD1	4:A:517:HOH:O	2.47	0.66
2:B:21:ARG:HH21	2:B:47:PHE:HZ	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:O	1:A:239:LYS:C	2.31	0.66
1:A:385:LEU:HD11	1:A:439:PHE:CE1	2.30	0.66
1:A:327:ASN:HD21	1:A:330:TRP:H	1.43	0.66
1:A:274:VAL:HG12	1:A:317:ARG:HE	1.61	0.66
1:A:445:ASN:HD22	1:A:449:ILE:CG1	2.09	0.66
1:A:214:TYR:HD2	1:A:260:TYR:HD1	1.43	0.66
2:B:110:ILE:HB	2:B:111:PRO:HD3	1.77	0.66
2:B:117:ARG:NH2	2:B:222:ILE:HD13	2.08	0.66
2:B:179:GLY:HA2	2:B:182:GLU:OE2	1.96	0.66
1:A:251:GLU:HG3	1:A:326:MET:HE3	1.79	0.65
1:A:449:ILE:HA	1:A:450:LYS:CD	2.26	0.65
1:A:251:GLU:CG	1:A:326:MET:CE	2.74	0.65
1:A:336:ALA:O	1:A:339:GLN:HB3	1.95	0.65
1:A:20:LYS:HB2	4:A:512:HOH:O	1.95	0.65
2:B:378:ALA:HB3	2:B:395:GLU:CG	2.25	0.65
1:A:103:ARG:O	1:A:107:GLN:HG3	1.96	0.65
2:B:43:SER:C	2:B:45:ASP:H	1.99	0.65
1:A:46:VAL:HG12	1:A:47:PHE:N	2.11	0.65
2:B:6:HIS:HE1	2:B:337:GLN:HG3	1.61	0.65
1:A:24:ARG:CZ	4:A:511:HOH:O	2.44	0.65
2:B:230:ARG:HH11	2:B:230:ARG:HG2	1.61	0.65
2:B:239:LYS:HB2	2:B:253:ILE:CD1	2.27	0.65
2:B:199:SER:OG	4:B:623:HOH:O	2.14	0.64
1:A:135:PHE:CE2	1:A:150:VAL:CB	2.81	0.64
1:A:135:PHE:CE2	1:A:150:VAL:CG1	2.80	0.64
1:A:327:ASN:C	1:A:327:ASN:HD22	2.01	0.64
2:B:230:ARG:HH11	2:B:230:ARG:HG3	1.62	0.64
2:B:379:GLN:HB2	2:B:452:LEU:HD12	1.79	0.64
2:B:39:PHE:CD2	2:B:51:LEU:HD21	2.33	0.64
1:A:88:LYS:O	1:A:92:GLY:HA2	1.97	0.64
2:B:224:VAL:HG12	2:B:261:ALA:HA	1.79	0.64
1:A:90:ILE:HD11	1:A:323:TYR:CE2	2.33	0.64
1:A:170:ASN:HB3	1:A:209:ASN:HD21	0.82	0.64
1:A:83:LEU:HD23	1:A:315:MET:HG2	1.78	0.64
2:B:21:ARG:NE	2:B:47:PHE:CE1	2.66	0.64
2:B:428:THR:O	2:B:432:MET:HG2	1.98	0.64
2:B:216:ILE:HG22	2:B:216:ILE:O	1.97	0.63
2:B:330:TRP:HH2	2:B:424:ARG:HB3	1.64	0.63
1:A:46:VAL:CG1	1:A:47:PHE:N	2.62	0.63
1:A:262:ASP:HB3	1:A:287:PHE:CD2	2.29	0.63
2:B:37:ASN:ND2	2:B:463:HIS:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:SER:HB2	2:B:323:TYR:CE1	2.33	0.63
2:B:443:LYS:HG2	2:B:443:LYS:O	1.98	0.63
1:A:36:MET:CE	1:A:36:MET:CA	2.73	0.63
1:A:432:MET:CE	1:A:432:MET:CA	2.75	0.63
2:B:201:GLY:O	2:B:356:GLY:HA3	1.97	0.63
2:B:245:TYR:O	2:B:246:LYS:C	2.37	0.63
1:A:32:ILE:CA	1:A:36:MET:HE1	2.24	0.63
2:B:327:ASN:HD22	2:B:330:TRP:H	1.41	0.63
2:B:375:GLN:HA	2:B:452:LEU:O	1.98	0.63
1:A:345:LEU:CD2	1:A:436:ILE:HG23	2.29	0.63
1:A:352:CYS:CB	1:A:361:PHE:O	2.47	0.63
2:B:245:TYR:C	2:B:247:ASP:N	2.52	0.63
2:B:384:GLU:O	2:B:388:VAL:HG23	1.99	0.62
1:A:289:ASP:O	1:A:292:THR:HB	1.98	0.62
2:B:93:TYR:HB3	2:B:282:MET:O	1.98	0.62
1:A:288:PHE:CD1	1:A:288:PHE:C	2.73	0.62
1:A:380:ALA:N	1:A:452:LEU:HD11	2.14	0.62
2:B:327:ASN:HD21	2:B:330:TRP:N	1.95	0.62
2:B:372:PRO:CD	2:B:375:GLN:OE1	2.47	0.62
2:B:384:GLU:OE1	2:B:387:LYS:HE2	1.99	0.62
2:B:224:VAL:HG12	2:B:261:ALA:CB	2.29	0.62
1:A:251:GLU:HG2	1:A:326:MET:CE	2.30	0.62
1:A:41:LEU:HD21	1:A:386:TYR:CE2	2.35	0.62
1:A:115:LYS:O	1:A:116:LYS:C	2.34	0.62
1:A:437:GLU:OE1	1:A:437:GLU:HA	2.00	0.62
2:B:17:GLU:O	2:B:17:GLU:HG2	1.98	0.62
1:A:28:GLU:OE2	1:A:387:LYS:HD3	2.00	0.62
2:B:195:ILE:HG23	2:B:234:ASN:CG	2.20	0.62
2:B:167:PHE:O	2:B:170:ASN:ND2	2.33	0.61
2:B:372:PRO:HD2	2:B:375:GLN:CB	2.22	0.61
1:A:228:SER:HB2	1:A:266:MET:HB2	1.82	0.61
2:B:48:ILE:HD11	2:B:431:HIS:HD2	1.65	0.61
2:B:354:GLN:O	4:B:624:HOH:O	2.16	0.61
2:B:230:ARG:HG3	2:B:358:HIS:CE1	2.36	0.61
2:B:207:LEU:HD13	2:B:245:TYR:CZ	2.35	0.61
1:A:227:ASP:OD1	1:A:270:LLP:H2'2	2.00	0.61
1:A:287:PHE:HA	4:A:537:HOH:O	2.00	0.61
2:B:103:ARG:O	2:B:107:GLN:HG3	2.01	0.61
2:B:32:ILE:O	2:B:35:GLY:N	2.34	0.61
1:A:132:SER:HB3	1:A:135:PHE:CE2	2.37	0.60
2:B:88:LYS:O	2:B:92:GLY:HA2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:HD22	2:B:330:TRP:HB3	1.66	0.60
2:B:196:THR:HG23	2:B:203:GLN:C	2.20	0.60
2:B:291:TYR:CZ	2:B:295:ARG:HD2	2.36	0.60
2:B:441:HIS:N	2:B:441:HIS:ND1	2.49	0.60
1:A:99:THR:HG21	1:A:105:ALA:N	2.17	0.60
1:A:29:GLU:OE2	1:A:29:GLU:HA	2.01	0.60
1:A:76:GLY:N	1:A:306:THR:HG21	2.16	0.60
1:A:220:TYR:N	1:A:220:TYR:CD1	2.68	0.60
1:A:143:SER:OG	1:A:190:TYR:OH	2.18	0.60
1:A:333:TYR:C	1:A:333:TYR:CD2	2.75	0.60
2:B:355:ALA:N	4:B:619:HOH:O	2.34	0.60
1:A:102:GLY:N	1:A:270:LLP:OP2	2.34	0.60
1:A:379:GLN:OE1	1:A:395:GLU:HG2	2.02	0.60
2:B:245:TYR:C	2:B:247:ASP:H	2.05	0.60
2:B:361:PHE:CE1	2:B:419:ARG:HB2	2.35	0.60
1:A:269:LYS:HD3	1:A:276:MET:HA	1.82	0.60
2:B:51:LEU:HD23	2:B:392:ARG:HD3	1.84	0.60
1:A:303:GLY:HA3	1:A:307:TYR:HE1	1.66	0.59
2:B:254:THR:O	2:B:258:TYR:HD2	1.85	0.59
1:A:200:ALA:HB3	1:A:203:GLN:HG2	1.76	0.59
2:B:378:ALA:CB	2:B:395:GLU:CG	2.80	0.59
1:A:268:ALA:HB1	1:A:274:VAL:HG21	1.84	0.59
1:A:135:PHE:CZ	1:A:150:VAL:HG11	2.36	0.59
2:B:40:LEU:CD1	2:B:464:PHE:O	2.50	0.59
2:B:217:ALA:O	2:B:221:ASP:N	2.36	0.59
2:B:232:ALA:HB1	2:B:331:LEU:HD21	1.84	0.59
2:B:211:LYS:HD3	2:B:260:TYR:OH	2.03	0.59
1:A:21:ARG:NH1	1:A:47:PHE:CE1	2.71	0.59
1:A:132:SER:OG	1:A:134:TYR:O	2.10	0.59
1:A:445:ASN:HD22	1:A:449:ILE:HG13	1.68	0.59
2:B:239:LYS:HD2	2:B:248:TRP:O	2.03	0.59
2:B:171:PHE:CD1	2:B:213:MET:HG3	2.37	0.59
2:B:214:TYR:HD1	2:B:224:VAL:HG21	1.67	0.59
1:A:161:THR:CG2	1:A:353:GLN:NE2	2.66	0.58
1:A:170:ASN:CA	1:A:209:ASN:ND2	2.62	0.58
2:B:51:LEU:HD23	2:B:392:ARG:CD	2.33	0.58
2:B:189:PRO:HB2	2:B:190:TYR:HD1	1.66	0.58
1:A:114:ILE:HG21	1:A:125:ARG:NH1	2.18	0.58
1:A:195:ILE:O	1:A:195:ILE:HG12	2.02	0.58
2:B:195:ILE:CD1	2:B:226:MET:SD	2.91	0.58
1:A:352:CYS:HB3	1:A:361:PHE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ILE:HB	2:B:111:PRO:CD	2.32	0.58
2:B:450:LYS:CG	2:B:470:GLU:OE2	2.51	0.58
2:B:318:LEU:HD12	2:B:318:LEU:O	2.04	0.57
1:A:24:ARG:HD3	4:A:511:HOH:O	2.04	0.57
2:B:166:ASP:HB3	2:B:241:ARG:HD3	1.86	0.57
2:B:116:LYS:HE2	2:B:120:GLU:OE2	2.04	0.57
2:B:268:ALA:O	2:B:272:ALA:HB3	2.05	0.57
2:B:449:ILE:HG22	4:B:630:HOH:O	2.04	0.57
2:B:220:TYR:N	2:B:220:TYR:CD1	2.72	0.57
1:A:107:GLN:HG2	1:A:142:HIS:CE1	2.39	0.57
1:A:432:MET:HE2	1:A:432:MET:CA	2.27	0.57
1:A:90:ILE:HD11	1:A:323:TYR:CD2	2.40	0.57
1:A:96:THR:O	1:A:96:THR:HG22	2.04	0.56
2:B:39:PHE:HE2	2:B:51:LEU:HD21	1.60	0.56
2:B:161:THR:HG21	2:B:354:GLN:CD	2.24	0.56
2:B:171:PHE:N	2:B:209:ASN:OD1	2.37	0.56
2:B:181:GLU:O	2:B:183:VAL:N	2.38	0.56
2:B:194:THR:HG21	2:B:198:ASN:ND2	2.20	0.56
2:B:170:ASN:N	2:B:170:ASN:HD22	2.03	0.56
2:B:182:GLU:O	2:B:182:GLU:HG2	2.04	0.56
1:A:183:VAL:HG12	1:A:183:VAL:O	2.04	0.56
1:A:445:ASN:O	1:A:445:ASN:ND2	2.38	0.56
2:B:124:ASP:OD1	2:B:124:ASP:C	2.42	0.56
2:B:189:PRO:O	2:B:223:PRO:HD2	2.05	0.56
1:A:34:SER:HB3	1:A:41:LEU:HD12	1.86	0.56
1:A:429:GLN:O	1:A:432:MET:CB	2.49	0.56
2:B:80:TYR:C	2:B:80:TYR:CD2	2.78	0.56
1:A:58:ALA:HB3	1:A:425:ALA:HB3	1.87	0.56
1:A:251:GLU:HG3	1:A:326:MET:CE	2.35	0.56
2:B:165:TYR:HB3	2:B:168:LYS:HD3	1.87	0.56
1:A:168:LYS:HB3	1:A:203:GLN:HG3	1.88	0.56
1:A:343:ASP:O	1:A:347:GLU:HG3	2.06	0.56
1:A:285:ASP:C	1:A:287:PHE:H	2.08	0.56
1:A:380:ALA:H	1:A:452:LEU:HD11	1.70	0.56
2:B:9:GLU:CG	2:B:333:TYR:OH	2.53	0.56
2:B:86:SER:HA	4:B:664:HOH:O	2.05	0.56
2:B:378:ALA:HB3	2:B:395:GLU:CD	2.27	0.56
2:B:228:SER:HB3	2:B:231:PHE:HB3	1.88	0.56
2:B:467:LYS:HB3	4:B:643:HOH:O	2.06	0.56
2:B:9:GLU:HA	2:B:333:TYR:CE1	2.41	0.55
1:A:9:GLU:HG2	2:B:431:HIS:CE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.87	0.55
2:B:195:ILE:HD11	2:B:226:MET:SD	2.45	0.55
2:B:316:GLU:O	2:B:319:ALA:HB3	2.06	0.55
2:B:438:ALA:O	2:B:442:VAL:HG23	2.06	0.55
2:B:445:ASN:N	4:B:629:HOH:O	2.38	0.55
1:A:8:PRO:HG2	2:B:21:ARG:HH22	1.70	0.55
1:A:327:ASN:HD21	1:A:329:ASP:HB2	1.71	0.55
2:B:182:GLU:O	2:B:182:GLU:CG	2.54	0.55
2:B:330:TRP:CH2	2:B:424:ARG:HB3	2.41	0.55
2:B:90:ILE:HG22	2:B:91:PHE:CD2	2.42	0.55
2:B:230:ARG:CG	2:B:230:ARG:NH1	2.61	0.55
1:A:128:MET:SD	1:A:148:CYS:HB2	2.47	0.55
1:A:183:VAL:O	1:A:183:VAL:CG1	2.54	0.55
1:A:79:SER:OG	1:A:316:GLU:HG2	2.07	0.55
1:A:358:HIS:ND1	4:A:536:HOH:O	2.33	0.55
2:B:383:CYS:O	2:B:387:LYS:CG	2.55	0.55
1:A:188:VAL:HG11	1:A:222:ILE:HD13	1.87	0.55
1:A:331:LEU:O	1:A:335:ILE:CG1	2.50	0.55
2:B:202:GLY:CA	2:B:358:HIS:HD2	2.13	0.55
2:B:340:TYR:C	2:B:340:TYR:CD2	2.80	0.55
1:A:76:GLY:H	1:A:306:THR:HG21	1.72	0.55
2:B:95:TYR:O	2:B:281:CYS:HA	2.07	0.55
1:A:371:ILE:HG22	1:A:377:PRO:HB3	1.89	0.54
1:A:307:TYR:HD1	1:A:308:GLY:N	2.05	0.54
2:B:81:TYR:O	2:B:85:GLU:HB2	2.07	0.54
2:B:463:HIS:HB2	4:B:665:HOH:O	2.08	0.54
1:A:7:LEU:HD12	1:A:336:ALA:HB2	1.90	0.54
1:A:93:TYR:HD1	1:A:93:TYR:N	2.05	0.54
1:A:365:GLY:O	1:A:369:PRO:N	2.41	0.54
2:B:251:GLU:OE2	2:B:251:GLU:N	2.41	0.54
1:A:124:ASP:HB3	1:A:187:ASN:ND2	2.23	0.54
1:A:364:ALA:HB1	1:A:377:PRO:O	2.08	0.54
2:B:290:VAL:HG23	4:B:650:HOH:O	2.08	0.54
2:B:108:ILE:CD1	2:B:298:CYS:SG	2.94	0.54
1:A:270:LLP:HD3	1:A:270:LLP:N	2.23	0.54
2:B:339:GLN:O	2:B:340:TYR:C	2.44	0.54
2:B:334:ARG:O	2:B:334:ARG:HD3	2.08	0.54
1:A:217:ALA:O	1:A:221:ASP:HA	2.08	0.53
2:B:161:THR:HG23	2:B:354:GLN:NE2	2.24	0.53
1:A:107:GLN:HG2	1:A:142:HIS:NE2	2.23	0.53
1:A:204:PRO:CG	1:A:237:PHE:CD2	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:HB3	1:A:287:PHE:HE2	1.59	0.53
1:A:93:TYR:HB3	1:A:282:MET:O	2.08	0.53
1:A:307:TYR:HD1	1:A:309:GLY:N	1.94	0.53
2:B:6:HIS:NE2	2:B:429:GLN:HB2	2.23	0.53
2:B:230:ARG:NH1	4:B:616:HOH:O	2.39	0.53
2:B:327:ASN:ND2	2:B:327:ASN:C	2.61	0.53
2:B:376:PHE:HZ	2:B:454:PHE:CE1	2.26	0.53
1:A:224:VAL:HG12	1:A:261:ALA:CB	2.39	0.53
2:B:201:GLY:O	2:B:356:GLY:CA	2.57	0.53
2:B:17:GLU:O	2:B:17:GLU:CG	2.56	0.53
1:A:220:TYR:HD1	1:A:220:TYR:H	1.56	0.53
2:B:117:ARG:O	2:B:119:GLN:N	2.42	0.53
2:B:161:THR:HG23	2:B:354:GLN:CD	2.26	0.53
2:B:422:ILE:CG2	2:B:423:PRO:HD2	2.39	0.53
2:B:134:TYR:CE1	2:B:199:SER:HB3	2.41	0.53
2:B:372:PRO:HD3	2:B:375:GLN:OE1	2.07	0.53
2:B:383:CYS:O	2:B:387:LYS:HG2	2.08	0.53
1:A:9:GLU:HG3	2:B:431:HIS:CE1	2.44	0.53
1:A:394:VAL:HG22	1:A:395:GLU:H	1.74	0.53
2:B:230:ARG:NH1	2:B:358:HIS:ND1	2.57	0.53
1:A:93:TYR:N	1:A:93:TYR:CD1	2.77	0.53
1:A:88:LYS:O	1:A:92:GLY:N	2.40	0.52
1:A:166:ASP:O	1:A:241:ARG:NH1	2.41	0.52
1:A:361:PHE:N	1:A:361:PHE:CD2	2.77	0.52
2:B:384:GLU:HA	2:B:387:LYS:HG3	1.90	0.52
1:A:135:PHE:CE1	1:A:150:VAL:HG11	2.44	0.52
1:A:230:ARG:HA	1:A:271:ASP:CG	2.30	0.52
2:B:102:GLY:HA3	2:B:267:SER:HB2	1.91	0.52
2:B:460:VAL:HG22	2:B:461:LEU:HG	1.91	0.52
1:A:9:GLU:CG	2:B:431:HIS:HE1	2.22	0.52
2:B:368:LEU:O	2:B:371:ILE:CD1	2.56	0.52
2:B:117:ARG:CG	2:B:117:ARG:NH1	2.69	0.52
2:B:195:ILE:CG2	2:B:234:ASN:CB	2.88	0.52
2:B:42:ASP:O	2:B:45:ASP:HB2	2.09	0.52
2:B:84:ALA:CB	2:B:96:THR:HB	2.39	0.52
2:B:133:ASN:H	2:B:133:ASN:ND2	2.05	0.52
1:A:93:TYR:CG	1:A:283:LYS:HA	2.45	0.52
1:A:270:LLP:N	1:A:270:LLP:CD	2.72	0.52
1:A:282:MET:SD	1:A:282:MET:N	2.83	0.52
1:A:371:ILE:HG21	1:A:377:PRO:HB3	1.91	0.52
1:A:21:ARG:NH1	1:A:47:PHE:CD1	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:HB1	1:A:274:VAL:CG2	2.39	0.52
2:B:196:THR:HG22	2:B:197:SER:N	2.25	0.52
1:A:93:TYR:CD2	1:A:283:LYS:CA	2.93	0.52
1:A:327:ASN:ND2	1:A:330:TRP:HB3	2.25	0.52
1:A:375:GLN:O	1:A:377:PRO:HD3	2.10	0.52
1:A:391:ILE:CD1	1:A:435:ILE:HG23	2.34	0.52
1:A:76:GLY:H	1:A:306:THR:CG2	2.23	0.51
2:B:334:ARG:C	2:B:334:ARG:CD	2.77	0.51
2:B:452:LEU:HA	2:B:470:GLU:HA	1.91	0.51
1:A:100:HIS:ND1	1:A:302:GLU:OE1	2.34	0.51
2:B:432:MET:HA	2:B:435:ILE:HD13	1.92	0.51
1:A:80:TYR:CD2	1:A:80:TYR:C	2.82	0.51
2:B:251:GLU:HG2	2:B:326:MET:HE1	1.92	0.51
1:A:138:THR:O	1:A:142:HIS:HB2	2.11	0.51
2:B:118:GLU:CD	2:B:125:ARG:HH21	2.12	0.51
1:A:37:ASN:OD1	1:A:37:ASN:C	2.48	0.51
1:A:93:TYR:OH	1:A:258:TYR:O	2.17	0.51
1:A:340:TYR:CZ	1:A:429:GLN:NE2	2.79	0.51
2:B:263:MET:HB2	2:B:282:MET:HG3	1.91	0.51
2:B:361:PHE:CE1	2:B:419:ARG:CD	2.94	0.51
2:B:431:HIS:O	2:B:435:ILE:HD12	2.11	0.51
1:A:269:LYS:C	1:A:270:LLP:HD3	2.31	0.51
1:A:340:TYR:OH	1:A:433:ASP:OD1	2.22	0.51
2:B:168:LYS:HB3	2:B:203:GLN:HB3	1.92	0.51
1:A:24:ARG:NE	4:A:520:HOH:O	1.91	0.51
1:A:117:ARG:CG	1:A:117:ARG:NH1	2.67	0.51
2:B:47:PHE:CD2	2:B:48:ILE:HG13	2.46	0.51
2:B:86:SER:HB2	2:B:323:TYR:HE1	1.72	0.51
2:B:311:GLU:O	2:B:314:ALA:HB3	2.11	0.51
1:A:159:PHE:C	1:A:353:GLN:NE2	2.63	0.51
1:A:214:TYR:CD2	1:A:260:TYR:HA	2.46	0.51
1:A:254:THR:HG23	4:A:527:HOH:O	2.09	0.51
2:B:160:ASP:OD2	2:B:163:VAL:CG2	2.59	0.51
1:A:88:LYS:O	1:A:92:GLY:CA	2.58	0.51
2:B:63:MET:HE1	2:B:273:MET:O	2.11	0.51
1:A:170:ASN:CA	1:A:209:ASN:HD21	2.22	0.50
2:B:93:TYR:CE1	2:B:283:LYS:HG3	2.45	0.50
2:B:134:TYR:CG	2:B:199:SER:HB3	2.44	0.50
2:B:195:ILE:HD12	2:B:226:MET:SD	2.51	0.50
2:B:220:TYR:O	2:B:221:ASP:C	2.48	0.50
2:B:394:VAL:HG22	2:B:396:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:HE	1:A:14:ARG:HA	1.75	0.50
1:A:179:GLY:HA2	1:A:182:GLU:OE2	2.11	0.50
1:A:217:ALA:O	1:A:221:ASP:CA	2.59	0.50
2:B:196:THR:H	2:B:230:ARG:HB2	1.76	0.50
2:B:285:ASP:C	2:B:287:PHE:N	2.65	0.50
2:B:450:LYS:HD3	2:B:470:GLU:OE2	2.05	0.50
2:B:9:GLU:HA	2:B:333:TYR:CD1	2.47	0.50
1:A:425:ALA:O	2:B:13:ILE:HB	2.11	0.50
2:B:22:THR:HG21	2:B:27:ARG:HD3	1.90	0.50
2:B:117:ARG:C	2:B:119:GLN:N	2.65	0.50
2:B:367:LEU:HD11	2:B:443:LYS:HB2	1.94	0.50
1:A:77:SER:H	1:A:306:THR:CG2	2.25	0.50
2:B:230:ARG:HG3	2:B:358:HIS:HE1	1.76	0.50
2:B:242:GLU:CD	2:B:245:TYR:HE1	2.15	0.50
1:A:8:PRO:CG	2:B:21:ARG:HH22	2.25	0.50
1:A:38:PRO:HG2	1:A:382:ALA:HB1	1.93	0.50
1:A:214:TYR:CB	1:A:260:TYR:HB3	2.42	0.50
2:B:51:LEU:HB2	2:B:392:ARG:HD2	1.92	0.50
1:A:104:GLY:O	1:A:105:ALA:C	2.50	0.50
2:B:194:THR:HG21	2:B:198:ASN:CG	2.32	0.50
1:A:34:SER:HB3	1:A:41:LEU:CD1	2.42	0.49
2:B:97:ILE:O	2:B:97:ILE:HG22	2.11	0.49
1:A:83:LEU:CD2	1:A:315:MET:HG2	2.42	0.49
1:A:93:TYR:CD2	1:A:283:LYS:HA	2.47	0.49
2:B:361:PHE:CE1	2:B:419:ARG:CB	2.95	0.49
1:A:359:ALA:HB3	1:A:361:PHE:HE2	1.76	0.49
1:A:434:PHE:O	1:A:437:GLU:HB3	2.13	0.49
2:B:161:THR:HG23	2:B:354:GLN:HE22	1.77	0.49
2:B:220:TYR:N	2:B:220:TYR:HD1	2.09	0.49
1:A:9:GLU:HA	1:A:333:TYR:CD1	2.46	0.49
1:A:153:VAL:HG23	1:A:153:VAL:O	2.12	0.49
1:A:346:GLU:O	1:A:349:GLY:N	2.43	0.49
2:B:269:LYS:HA	2:B:274:VAL:O	2.12	0.49
1:A:110:ILE:N	1:A:111:PRO:HD2	2.27	0.49
1:A:242:GLU:HG2	1:A:245:TYR:CD2	2.48	0.49
2:B:117:ARG:O	2:B:118:GLU:C	2.50	0.49
1:A:251:GLU:O	1:A:254:THR:HB	2.12	0.49
2:B:126:SER:OG	2:B:127:LYS:HE2	2.13	0.49
2:B:191:ILE:HD12	2:B:222:ILE:HG21	1.93	0.49
1:A:365:GLY:O	1:A:369:PRO:CA	2.61	0.49
2:B:110:ILE:HD12	4:B:658:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ASN:ND2	2:B:330:TRP:HB3	2.27	0.49
1:A:31:ILE:HG23	1:A:32:ILE:N	2.27	0.49
1:A:47:PHE:CD2	1:A:48:ILE:HG13	2.47	0.49
2:B:132:SER:O	2:B:133:ASN:C	2.49	0.49
2:B:361:PHE:HA	4:B:633:HOH:O	2.12	0.49
1:A:114:ILE:CG2	1:A:125:ARG:HH12	2.20	0.49
2:B:95:TYR:HB2	2:B:282:MET:HB2	1.95	0.49
2:B:358:HIS:CE1	4:B:616:HOH:O	2.65	0.49
1:A:52:THR:OG1	1:A:53:ASP:N	2.44	0.49
1:A:118:GLU:HA	1:A:123:LEU:H	1.78	0.49
1:A:340:TYR:CD2	1:A:340:TYR:C	2.85	0.49
1:A:368:LEU:HB2	1:A:371:ILE:HD13	1.94	0.49
2:B:168:LYS:HB3	2:B:203:GLN:HG3	1.94	0.49
1:A:134:TYR:HA	1:A:152:ASN:OD1	2.12	0.48
2:B:216:ILE:O	2:B:216:ILE:CG2	2.60	0.48
2:B:378:ALA:HB1	2:B:395:GLU:HG3	1.88	0.48
2:B:453:THR:HG22	2:B:469:LYS:HG3	1.94	0.48
2:B:358:HIS:O	2:B:421:THR:HG22	2.13	0.48
1:A:95:TYR:O	1:A:281:CYS:HA	2.14	0.48
1:A:109:TYR:CD1	1:A:109:TYR:C	2.87	0.48
1:A:263:MET:HB2	1:A:281:CYS:O	2.14	0.48
1:A:333:TYR:O	1:A:334:ARG:C	2.48	0.48
1:A:340:TYR:OH	1:A:429:GLN:NE2	2.39	0.48
1:A:424:ARG:O	1:A:426:THR:N	2.46	0.48
2:B:468:LEU:HD12	2:B:468:LEU:N	2.28	0.48
1:A:13:ILE:HD13	2:B:13:ILE:HD13	1.96	0.48
1:A:335:ILE:O	1:A:336:ALA:C	2.50	0.48
2:B:83:LEU:HD11	2:B:318:LEU:HG	1.96	0.48
2:B:107:GLN:HA	4:B:658:HOH:O	2.13	0.48
1:A:365:GLY:O	1:A:369:PRO:HA	2.14	0.48
2:B:106:GLU:O	2:B:107:GLN:C	2.50	0.48
1:A:18:PRO:HA	2:B:11:PHE:HB3	1.96	0.48
1:A:307:TYR:HB2	1:A:310:LEU:O	2.13	0.48
2:B:360:ALA:HB3	2:B:420:LEU:HB2	1.95	0.48
1:A:55:GLY:H	1:A:269:LYS:CB	2.26	0.48
1:A:89:ASN:OD1	1:A:89:ASN:N	2.45	0.48
1:A:90:ILE:CG1	1:A:323:TYR:CE2	2.97	0.48
1:A:369:PRO:HA	4:A:515:HOH:O	2.13	0.48
1:A:240:GLN:HG3	1:A:241:ARG:HG3	1.95	0.48
1:A:327:ASN:HD22	1:A:330:TRP:HB3	1.78	0.48
2:B:439:PHE:HA	2:B:442:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PRO:HD2	4:A:526:HOH:O	2.14	0.47
2:B:230:ARG:CG	4:B:616:HOH:O	2.62	0.47
2:B:288:PHE:CD1	2:B:288:PHE:C	2.87	0.47
2:B:396:ILE:HG22	2:B:396:ILE:O	2.14	0.47
1:A:24:ARG:H	1:A:24:ARG:HG2	1.37	0.47
1:A:77:SER:O	1:A:80:TYR:HB3	2.15	0.47
2:B:28:GLU:HA	2:B:31:ILE:HG22	1.96	0.47
2:B:64:GLN:O	2:B:65:ALA:C	2.53	0.47
2:B:224:VAL:HG12	2:B:261:ALA:CA	2.42	0.47
2:B:239:LYS:CD	2:B:248:TRP:O	2.61	0.47
1:A:9:GLU:OE2	1:A:333:TYR:CZ	2.68	0.47
2:B:209:ASN:C	2:B:209:ASN:ND2	2.59	0.47
1:A:84:ALA:HA	1:A:96:THR:HG21	1.97	0.47
1:A:149:THR:HG22	1:A:150:VAL:N	2.30	0.47
1:A:167:PHE:O	1:A:170:ASN:ND2	2.48	0.47
1:A:248:TRP:CD1	1:A:248:TRP:N	2.83	0.47
1:A:449:ILE:HG22	1:A:450:LYS:N	2.29	0.47
2:B:32:ILE:HG22	2:B:33:LYS:N	2.30	0.47
2:B:427:TYR:HB3	2:B:431:HIS:CB	2.44	0.47
1:A:36:MET:HE2	1:A:36:MET:CA	2.23	0.47
2:B:174:GLU:O	2:B:177:GLU:HB2	2.14	0.47
2:B:439:PHE:HA	2:B:442:VAL:HG23	1.97	0.47
1:A:268:ALA:CB	1:A:274:VAL:HG21	2.44	0.47
2:B:432:MET:HA	2:B:435:ILE:CD1	2.44	0.47
1:A:90:ILE:HG13	1:A:323:TYR:CE2	2.50	0.46
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.54	0.46
1:A:144:GLN:OE1	1:A:149:THR:HG23	2.15	0.46
1:A:290:VAL:HG12	1:A:291:TYR:N	2.30	0.46
2:B:90:ILE:HD11	2:B:323:TYR:CD2	2.50	0.46
1:A:24:ARG:NE	4:A:511:HOH:O	2.46	0.46
1:A:338:VAL:HB	4:A:514:HOH:O	2.16	0.46
2:B:80:TYR:H	2:B:315:MET:CE	2.28	0.46
2:B:123:LEU:HD23	2:B:123:LEU:C	2.35	0.46
2:B:262:ASP:CB	2:B:287:PHE:CE2	2.97	0.46
2:B:361:PHE:CE1	2:B:419:ARG:CG	2.98	0.46
1:A:32:ILE:CA	1:A:36:MET:CE	2.84	0.46
2:B:6:HIS:HB2	2:B:340:TYR:CE1	2.51	0.46
2:B:230:ARG:HA	2:B:271:ASP:OD2	2.15	0.46
2:B:353:GLN:C	2:B:354:GLN:HG2	2.29	0.46
1:A:24:ARG:NH1	4:A:511:HOH:O	2.47	0.46
1:A:114:ILE:CG2	1:A:125:ARG:NH1	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.09	0.46
1:A:135:PHE:CE2	1:A:150:VAL:HG11	2.50	0.46
1:A:171:PHE:H	1:A:209:ASN:ND2	2.09	0.46
1:A:219:LYS:C	1:A:221:ASP:H	2.19	0.46
2:B:249:THR:HG23	2:B:252:GLN:OE1	2.16	0.46
2:B:330:TRP:O	2:B:333:TYR:HB3	2.14	0.46
1:A:248:TRP:HB2	1:A:253:ILE:HD11	1.98	0.46
1:A:285:ASP:C	1:A:287:PHE:N	2.69	0.46
2:B:22:THR:C	2:B:27:ARG:NH1	2.62	0.46
2:B:242:GLU:HB3	2:B:245:TYR:HD1	1.81	0.46
2:B:264:LEU:C	2:B:264:LEU:HD12	2.36	0.46
2:B:341:LEU:HD13	2:B:432:MET:SD	2.56	0.46
2:B:54:SER:O	2:B:56:THR:HG23	2.16	0.46
2:B:93:TYR:N	2:B:93:TYR:CD1	2.83	0.46
2:B:80:TYR:N	2:B:315:MET:CE	2.77	0.46
2:B:230:ARG:HA	2:B:271:ASP:CG	2.36	0.46
2:B:381:LEU:HD23	2:B:418:LEU:HG	1.98	0.46
1:A:361:PHE:N	1:A:361:PHE:HD2	2.12	0.46
2:B:50:LEU:HD12	2:B:420:LEU:CD2	2.44	0.46
2:B:93:TYR:N	2:B:93:TYR:HD1	2.14	0.46
2:B:436:ILE:O	2:B:439:PHE:HB2	2.15	0.46
1:A:24:ARG:CD	4:A:511:HOH:O	2.61	0.45
1:A:26:TYR:OH	1:A:45:ASP:OD1	2.23	0.45
1:A:38:PRO:HD3	1:A:379:GLN:HE22	1.81	0.45
1:A:307:TYR:O	1:A:308:GLY:C	2.54	0.45
1:A:429:GLN:O	1:A:432:MET:N	2.49	0.45
2:B:123:LEU:HD23	2:B:124:ASP:N	2.31	0.45
2:B:427:TYR:HB3	2:B:431:HIS:HB2	1.98	0.45
1:A:26:TYR:CD1	1:A:26:TYR:C	2.88	0.45
2:B:376:PHE:HA	2:B:377:PRO:HD3	1.83	0.45
2:B:367:LEU:O	2:B:368:LEU:HD23	2.16	0.45
1:A:224:VAL:O	1:A:261:ALA:HB1	2.17	0.45
2:B:440:LYS:O	2:B:441:HIS:C	2.55	0.45
1:A:101:GLN:OE1	1:A:103:ARG:HD2	2.17	0.45
1:A:149:THR:HG22	1:A:150:VAL:H	1.81	0.45
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.74	0.45
1:A:371:ILE:HG22	1:A:377:PRO:CG	2.47	0.45
2:B:239:LYS:HB2	2:B:253:ILE:HD11	1.98	0.45
1:A:159:PHE:N	1:A:159:PHE:CD1	2.85	0.45
2:B:40:LEU:HD12	2:B:464:PHE:O	2.16	0.45
2:B:80:TYR:H	2:B:315:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:THR:CG2	2:B:197:SER:N	2.79	0.45
1:A:427:TYR:HB3	1:A:431:HIS:ND1	2.32	0.45
1:A:19:VAL:HG12	2:B:11:PHE:CA	2.41	0.45
1:A:72:GLU:CA	4:A:538:HOH:O	2.59	0.45
1:A:246:LYS:O	1:A:246:LYS:HG2	2.17	0.45
1:A:448:ASN:ND2	1:A:448:ASN:H	2.15	0.45
2:B:22:THR:CG2	2:B:27:ARG:CZ	2.77	0.45
2:B:160:ASP:OD2	2:B:163:VAL:HG23	2.17	0.45
2:B:214:TYR:CD1	2:B:224:VAL:HG21	2.49	0.45
2:B:226:MET:HG2	2:B:258:TYR:CE1	2.52	0.45
1:A:55:GLY:CA	1:A:269:LYS:HB3	2.47	0.45
1:A:69:ARG:O	1:A:316:GLU:HG3	2.17	0.45
1:A:95:TYR:HB2	1:A:282:MET:HB2	1.99	0.45
1:A:271:ASP:O	1:A:273:MET:HG2	2.16	0.45
2:B:328:LEU:O	2:B:329:ASP:C	2.55	0.45
2:B:383:CYS:O	2:B:387:LYS:HG3	2.16	0.45
2:B:450:LYS:HB3	2:B:470:GLU:OE2	2.10	0.45
1:A:395:GLU:O	1:A:396:ILE:C	2.55	0.44
2:B:118:GLU:OE2	2:B:125:ARG:NH2	2.49	0.44
2:B:207:LEU:HD13	2:B:245:TYR:CE2	2.52	0.44
2:B:256:GLU:HA	2:B:259:LYS:HE3	1.99	0.44
1:A:21:ARG:HG3	4:A:534:HOH:O	2.17	0.44
1:A:136:PHE:HD2	1:A:138:THR:OG1	1.99	0.44
2:B:413:CYS:SG	2:B:413:CYS:O	2.75	0.44
1:A:155:ILE:O	1:A:158:ALA:HB2	2.18	0.44
1:A:394:VAL:O	1:A:418:LEU:HD12	2.17	0.44
2:B:230:ARG:HD3	2:B:424:ARG:HH22	1.82	0.44
1:A:248:TRP:HB2	1:A:253:ILE:CD1	2.48	0.44
2:B:452:LEU:HB3	2:B:468:LEU:HB3	1.98	0.44
2:B:7:LEU:HD12	2:B:336:ALA:HB2	1.98	0.44
2:B:93:TYR:CG	2:B:283:LYS:HA	2.53	0.44
2:B:317:ARG:O	2:B:320:VAL:N	2.37	0.44
2:B:83:LEU:CD1	2:B:318:LEU:HG	2.47	0.44
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.59	0.44
2:B:230:ARG:HG3	4:B:616:HOH:O	2.17	0.44
2:B:375:GLN:CD	2:B:471:VAL:CB	2.59	0.44
1:A:200:ALA:CB	1:A:203:GLN:CB	2.96	0.44
1:A:436:ILE:H	1:A:436:ILE:HG13	1.72	0.44
2:B:6:HIS:HE1	2:B:337:GLN:CG	2.30	0.44
2:B:133:ASN:ND2	2:B:134:TYR:H	2.16	0.44
2:B:368:LEU:HB3	2:B:371:ILE:HD11	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LYS:HB2	1:A:33:LYS:HE3	1.74	0.44
1:A:288:PHE:O	1:A:289:ASP:C	2.56	0.44
2:B:117:ARG:NE	2:B:188:VAL:O	2.51	0.44
2:B:169:GLY:O	2:B:205:VAL:HG22	2.18	0.44
2:B:171:PHE:CG	2:B:213:MET:HG3	2.53	0.44
2:B:211:LYS:HD3	2:B:260:TYR:CZ	2.53	0.44
1:A:6:HIS:CE1	1:A:429:GLN:HA	2.53	0.44
1:A:188:VAL:CG1	1:A:222:ILE:HD13	2.48	0.44
1:A:232:ALA:HB1	1:A:331:LEU:HD21	2.00	0.44
2:B:116:LYS:O	2:B:120:GLU:HG3	2.18	0.44
1:A:167:PHE:HE2	1:A:238:ILE:HG12	1.82	0.43
2:B:274:VAL:HA	2:B:275:PRO:HD3	1.73	0.43
2:B:339:GLN:O	2:B:341:LEU:N	2.51	0.43
2:B:379:GLN:O	2:B:382:ALA:HB3	2.18	0.43
2:B:384:GLU:OE1	2:B:387:LYS:CE	2.64	0.43
2:B:445:ASN:OD1	2:B:448:ASN:OD1	2.36	0.43
1:A:13:ILE:HG23	2:B:13:ILE:HG23	2.00	0.43
1:A:124:ASP:CB	1:A:187:ASN:HD21	2.28	0.43
1:A:329:ASP:O	1:A:332:ALA:HB3	2.17	0.43
1:A:340:TYR:CD2	1:A:340:TYR:O	2.71	0.43
2:B:50:LEU:CD1	2:B:421:THR:H	2.28	0.43
2:B:359:ALA:CB	2:B:419:ARG:HD2	2.48	0.43
2:B:445:ASN:C	2:B:447:ALA:N	2.59	0.43
1:A:129:VAL:O	1:A:188:VAL:HA	2.19	0.43
2:B:440:LYS:O	2:B:443:LYS:N	2.51	0.43
1:A:46:VAL:HG11	1:A:49:ASP:HB2	1.99	0.43
1:A:371:ILE:HG22	1:A:377:PRO:CB	2.49	0.43
1:A:251:GLU:HB2	4:A:533:HOH:O	2.18	0.43
1:A:307:TYR:CD1	1:A:308:GLY:N	2.86	0.43
1:A:437:GLU:OE1	1:A:437:GLU:CA	2.56	0.43
1:A:181:GLU:O	1:A:183:VAL:N	2.51	0.43
1:A:291:TYR:O	1:A:292:THR:C	2.56	0.43
1:A:315:MET:O	1:A:316:GLU:C	2.57	0.43
2:B:26:TYR:C	2:B:28:GLU:H	2.22	0.43
2:B:196:THR:HG22	2:B:203:GLN:O	2.17	0.43
2:B:225:VAL:HA	2:B:263:MET:O	2.19	0.43
2:B:287:PHE:HA	4:B:650:HOH:O	2.17	0.43
2:B:297:LEU:HD12	2:B:297:LEU:HA	1.55	0.43
2:B:334:ARG:O	2:B:338:VAL:HG23	2.18	0.43
2:B:453:THR:HB	2:B:471:VAL:HG22	2.00	0.43
1:A:7:LEU:HD12	1:A:336:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:CYS:HB2	1:A:361:PHE:O	2.16	0.43
2:B:181:GLU:O	2:B:182:GLU:C	2.53	0.43
2:B:437:GLU:HA	2:B:437:GLU:OE1	2.18	0.43
1:A:251:GLU:HG3	4:A:533:HOH:O	2.17	0.43
2:B:102:GLY:CA	2:B:267:SER:HB2	2.49	0.43
2:B:233:GLU:O	2:B:234:ASN:C	2.57	0.43
2:B:279:LEU:HD23	2:B:279:LEU:HA	1.76	0.43
2:B:285:ASP:C	2:B:287:PHE:H	2.22	0.43
1:A:71:ASP:HB2	1:A:78:ARG:HD3	2.00	0.42
1:A:133:ASN:ND2	1:A:133:ASN:N	2.52	0.42
1:A:245:TYR:HD1	1:A:248:TRP:CE2	2.37	0.42
2:B:372:PRO:CD	2:B:375:GLN:HB2	2.23	0.42
1:A:346:GLU:HA	1:A:346:GLU:OE1	2.19	0.42
2:B:16:ILE:O	2:B:16:ILE:HG13	2.19	0.42
2:B:72:GLU:HG3	4:B:611:HOH:O	2.19	0.42
1:A:371:ILE:HG22	1:A:377:PRO:HG3	2.02	0.42
2:B:177:GLU:HA	2:B:177:GLU:OE1	2.19	0.42
2:B:361:PHE:CZ	2:B:419:ARG:HD3	2.53	0.42
1:A:13:ILE:CD1	2:B:13:ILE:HD13	2.50	0.42
1:A:110:ILE:HB	1:A:111:PRO:CD	2.50	0.42
2:B:327:ASN:HD21	2:B:329:ASP:HB2	1.85	0.42
1:A:38:PRO:O	1:A:41:LEU:N	2.49	0.42
1:A:159:PHE:C	1:A:353:GLN:HE22	2.23	0.42
2:B:48:ILE:HD11	2:B:431:HIS:CD2	2.49	0.42
2:B:198:ASN:CB	4:B:627:HOH:O	2.25	0.42
2:B:197:SER:O	2:B:202:GLY:HA2	2.20	0.42
1:A:98:PRO:HD2	1:A:305:PRO:O	2.19	0.42
2:B:79:SER:O	2:B:80:TYR:C	2.58	0.42
2:B:242:GLU:O	2:B:243:ALA:C	2.58	0.42
1:A:77:SER:H	1:A:306:THR:HG23	1.84	0.42
1:A:90:ILE:CD1	1:A:323:TYR:CE2	3.01	0.42
1:A:100:HIS:O	1:A:277:GLY:CA	2.67	0.42
1:A:136:PHE:O	1:A:140:GLN:HG2	2.18	0.42
1:A:237:PHE:O	1:A:238:ILE:C	2.58	0.42
1:A:339:GLN:O	1:A:342:VAL:N	2.52	0.42
1:A:424:ARG:O	1:A:425:ALA:C	2.55	0.42
2:B:110:ILE:N	2:B:111:PRO:HD2	2.34	0.42
2:B:354:GLN:HB3	4:B:619:HOH:O	2.19	0.42
1:A:60:THR:O	1:A:61:GLN:C	2.58	0.42
2:B:165:TYR:HD1	2:B:166:ASP:H	1.68	0.42
1:A:328:LEU:O	1:A:329:ASP:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:GLY:O	2:B:356:GLY:C	2.58	0.42
2:B:436:ILE:O	2:B:439:PHE:N	2.53	0.42
1:A:93:TYR:CD2	1:A:283:LYS:N	2.88	0.41
1:A:12:ARG:NH1	2:B:49:ASP:HB2	2.35	0.41
1:A:368:LEU:HA	1:A:369:PRO:HD3	1.54	0.41
2:B:195:ILE:HG23	2:B:234:ASN:CB	2.50	0.41
2:B:260:TYR:CD2	2:B:260:TYR:N	2.87	0.41
2:B:418:LEU:C	2:B:418:LEU:HD13	2.41	0.41
1:A:214:TYR:CD2	1:A:260:TYR:HD1	2.30	0.41
1:A:268:ALA:O	1:A:274:VAL:CG2	2.63	0.41
2:B:99:THR:OG1	2:B:278:GLY:CA	2.64	0.41
2:B:372:PRO:HD2	2:B:375:GLN:OE1	2.19	0.41
1:A:26:TYR:CD1	1:A:26:TYR:O	2.73	0.41
1:A:440:LYS:O	1:A:441:HIS:C	2.58	0.41
2:B:375:GLN:HG3	2:B:471:VAL:HG21	1.92	0.41
2:B:429:GLN:O	2:B:430:THR:C	2.57	0.41
2:B:168:LYS:HB3	2:B:203:GLN:CB	2.50	0.41
2:B:429:GLN:O	2:B:432:MET:N	2.54	0.41
1:A:107:GLN:HB2	1:A:301:GLN:OE1	2.20	0.41
1:A:279:LEU:HA	1:A:279:LEU:HD23	1.43	0.41
1:A:328:LEU:HB3	1:A:329:ASP:H	1.59	0.41
1:A:453:THR:HB	4:A:508:HOH:O	2.20	0.41
2:B:188:VAL:HA	2:B:189:PRO:HD3	1.76	0.41
2:B:215:SER:C	2:B:217:ALA:H	2.24	0.41
1:A:12:ARG:NH2	2:B:46:VAL:O	2.54	0.41
1:A:128:MET:HG3	1:A:148:CYS:HB2	2.02	0.41
1:A:201:GLY:HA2	1:A:361:PHE:CE2	2.56	0.41
1:A:369:PRO:C	1:A:371:ILE:H	2.24	0.41
1:A:384:GLU:O	1:A:385:LEU:C	2.58	0.41
1:A:386:TYR:HA	1:A:391:ILE:O	2.21	0.41
2:B:21:ARG:HD3	2:B:21:ARG:HA	1.97	0.41
2:B:28:GLU:C	2:B:30:ALA:N	2.66	0.41
2:B:50:LEU:HD22	2:B:50:LEU:HA	1.61	0.41
3:B:501:SO4:O1	4:B:602:HOH:O	2.22	0.41
1:A:81:TYR:O	1:A:85:GLU:HB2	2.21	0.41
1:A:155:ILE:O	1:A:156:LYS:C	2.59	0.41
1:A:318:LEU:HD12	1:A:322:LEU:HG	2.02	0.41
2:B:128:MET:HA	2:B:187:ASN:HB3	2.03	0.41
2:B:364:ALA:O	2:B:368:LEU:N	2.54	0.41
1:A:21:ARG:O	1:A:22:THR:HG23	2.21	0.40
1:A:143:SER:C	1:A:148:CYS:O	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:HA	1:A:177:GLU:HB2	2.03	0.40
2:B:97:ILE:HG21	2:B:97:ILE:HD13	1.56	0.40
2:B:112:VAL:HG11	2:B:290:VAL:HG13	2.03	0.40
2:B:168:LYS:HB3	2:B:203:GLN:CG	2.51	0.40
2:B:172:ASP:O	2:B:173:LEU:C	2.58	0.40
2:B:359:ALA:HB1	2:B:419:ARG:HD2	2.03	0.40
1:A:47:PHE:HB3	1:A:390:GLY:O	2.22	0.40
1:A:253:ILE:O	1:A:257:THR:OG1	2.29	0.40
1:A:254:THR:O	1:A:257:THR:HB	2.21	0.40
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.65	0.40
2:B:395:GLU:CB	4:B:637:HOH:O	2.50	0.40
2:B:457:GLU:HA	2:B:458:PRO:HD3	1.97	0.40
1:A:38:PRO:O	1:A:41:LEU:CB	2.50	0.40
1:A:71:ASP:OD1	1:A:78:ARG:N	2.54	0.40
2:B:51:LEU:HD23	2:B:392:ARG:HD2	2.01	0.40
2:B:196:THR:HG21	2:B:203:GLN:C	2.41	0.40
1:A:63:MET:O	1:A:66:ALA:HB3	2.21	0.40
1:A:304:PHE:HA	1:A:305:PRO:HD3	1.82	0.40
2:B:26:TYR:O	2:B:28:GLU:N	2.55	0.40
2:B:52:THR:OG1	2:B:53:ASP:N	2.53	0.40
2:B:120:GLU:HG3	2:B:120:GLU:H	1.52	0.40
2:B:157:GLU:O	2:B:158:ALA:C	2.60	0.40
2:B:364:ALA:O	2:B:368:LEU:HB2	2.22	0.40
1:A:269:LYS:HD2	1:A:275:PRO:O	2.22	0.40
2:B:33:LYS:C	2:B:35:GLY:H	2.25	0.40
2:B:458:PRO:HD2	2:B:462:ARG:HA	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ARG:NH1	2:B:301:GLN:O[8_665]	2.16	0.04

## 5.3 Torsion angles [i](#)

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

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/467 (92%)	331 (77%)	81 (19%)	18 (4%)	3	20
2	B	425/467 (91%)	327 (77%)	83 (20%)	15 (4%)	3	24
All	All	855/934 (92%)	658 (77%)	164 (19%)	33 (4%)	3	22

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
2	B	246	LYS
1	A	157	GLU
1	A	238	ILE
2	B	243	ALA
2	B	425	ALA
2	B	446	ALA
1	A	158	ALA
1	A	182	GLU
1	A	329	ASP
1	A	378	ALA
1	A	425	ALA
1	A	443	LYS
2	B	340	TYR
1	A	324	ASP
1	A	336	ALA
1	A	447	ALA
2	B	27	ARG
2	B	30	ALA
1	A	221	ASP
1	A	322	LEU
1	A	369	PRO
1	A	382	ALA
1	A	441	HIS
2	B	25	ALA
2	B	75	SER
2	B	103	ARG
2	B	118	GLU
2	B	244	GLU
2	B	414	PRO
2	B	216	ILE
1	A	377	PRO
2	B	204	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/385 (92%)	286 (80%)	70 (20%)	1	7
2	B	358/386 (93%)	290 (81%)	68 (19%)	1	8
All	All	714/771 (93%)	576 (81%)	138 (19%)	1	8

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	12	ARG
1	A	21	ARG
1	A	22	THR
1	A	23	THR
1	A	24	ARG
1	A	26	TYR
1	A	36	MET
1	A	41	LEU
1	A	43	SER
1	A	44	GLU
1	A	51	LEU
1	A	52	THR
1	A	78	ARG
1	A	85	GLU
1	A	109	TYR
1	A	117	ARG
1	A	120	GLU
1	A	123	LEU
1	A	133	ASN
1	A	134	TYR
1	A	139	THR
1	A	142	HIS
1	A	143	SER
1	A	144	GLN
1	A	146	ASN
1	A	148	CYS

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Mol	Chain	Res	Type
1	A	159	PHE
1	A	160	ASP
1	A	174	GLU
1	A	177	GLU
1	A	195	ILE
1	A	206	SER
1	A	207	LEU
1	A	211	LYS
1	A	240	GLN
1	A	244	GLU
1	A	252	GLN
1	A	269	LYS
1	A	274	VAL
1	A	288	PHE
1	A	289	ASP
1	A	292	THR
1	A	295	ARG
1	A	297	LEU
1	A	307	TYR
1	A	327	ASN
1	A	328	LEU
1	A	331	LEU
1	A	334	ARG
1	A	335	ILE
1	A	345	LEU
1	A	362	VAL
1	A	368	LEU
1	A	385	LEU
1	A	392	ARG
1	A	395	GLU
1	A	416	GLU
1	A	417	LEU
1	A	421	THR
1	A	422	ILE
1	A	429	GLN
1	A	430	THR
1	A	436	ILE
1	A	441	HIS
1	A	444	GLU
1	A	448	ASN
1	A	450	LYS
1	A	452	LEU

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Mol	Chain	Res	Type
1	A	454	PHE
2	B	13	ILE
2	B	14	ARG
2	B	18	PRO
2	B	33	LYS
2	B	34	SER
2	B	41	LEU
2	B	44	GLU
2	B	50	LEU
2	B	52	THR
2	B	54	SER
2	B	62	SER
2	B	64	GLN
2	B	71	ASP
2	B	100	HIS
2	B	109	TYR
2	B	117	ARG
2	B	120	GLU
2	B	123	LEU
2	B	127	LYS
2	B	129	VAL
2	B	133	ASN
2	B	153	VAL
2	B	154	TYR
2	B	165	TYR
2	B	168	LYS
2	B	191	ILE
2	B	194	THR
2	B	198	ASN
2	B	207	LEU
2	B	209	ASN
2	B	211	LYS
2	B	215	SER
2	B	220	TYR
2	B	222	ILE
2	B	228	SER
2	B	230	ARG
2	B	239	LYS
2	B	240	GLN
2	B	246	LYS
2	B	252	GLN
2	B	263	MET

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Mol	Chain	Res	Type
2	B	264	LEU
2	B	267	SER
2	B	269	LYS
2	B	273	MET
2	B	276	MET
2	B	283	LYS
2	B	288	PHE
2	B	293	GLU
2	B	300	VAL
2	B	301	GLN
2	B	302	GLU
2	B	324	ASP
2	B	327	ASN
2	B	328	LEU
2	B	331	LEU
2	B	334	ARG
2	B	371	ILE
2	B	394	VAL
2	B	398	SER
2	B	417	LEU
2	B	418	LEU
2	B	421	THR
2	B	440	LYS
2	B	441	HIS
2	B	443	LYS
2	B	448	ASN
2	B	459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	119	GLN
1	A	133	ASN
1	A	144	GLN
1	A	146	ASN
1	A	187	ASN
1	A	198	ASN
1	A	209	ASN
1	A	327	ASN
1	A	358	HIS
1	A	445	ASN

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Mol	Chain	Res	Type
1	A	448	ASN
2	B	6	HIS
2	B	64	GLN
2	B	101	GLN
2	B	133	ASN
2	B	170	ASN
2	B	327	ASN
2	B	375	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	LLP	A	270	1	23,24,25	2.17	6 (26%)	25,32,34	2.43	7 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	270	1	-	4/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	LLP	O3-C3	-6.59	1.21	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	LLP	C4-C4'	3.71	1.53	1.46
1	A	270	LLP	C2-N1	2.99	1.39	1.33
1	A	270	LLP	C6-N1	2.81	1.40	1.34
1	A	270	LLP	C4'-NZ	2.63	1.36	1.27
1	A	270	LLP	CE-NZ	2.30	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LLP	OP4-C5'-C5	7.15	122.98	109.35
1	A	270	LLP	C4-C3-C2	6.41	124.16	120.19
1	A	270	LLP	CE-NZ-C4'	-3.67	107.62	118.90
1	A	270	LLP	OP3-P-OP1	3.06	122.68	110.68
1	A	270	LLP	C3-C2-N1	-2.44	117.62	120.77
1	A	270	LLP	CD-CG-CB	2.18	121.33	113.62
1	A	270	LLP	OP3-P-OP4	-2.08	101.19	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	270	LLP	C4-C5-C5'-OP4
1	A	270	LLP	C6-C5-C5'-OP4
1	A	270	LLP	C4-C4'-NZ-CE
1	A	270	LLP	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	270	LLP	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	B	500	-	4,4,4	0.14	0	6,6,6	0.60	0
3	SO4	B	501	-	4,4,4	0.17	0	6,6,6	0.20	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	434/467 (92%)	-0.32	10 (2%) 60 47	50, 82, 120, 126	0
2	B	433/467 (92%)	-0.27	9 (2%) 63 49	48, 82, 129, 170	0
All	All	867/934 (92%)	-0.29	19 (2%) 62 48	48, 82, 121, 170	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	VAL	5.9
2	B	414	PRO	4.6
2	B	413	CYS	3.8
1	A	415	ALA	3.2
2	B	398	SER	3.1
2	B	463	HIS	3.1
2	B	301	GLN	2.7
1	A	377	PRO	2.7
1	A	375	GLN	2.6
2	B	459	LYS	2.6
1	A	196	THR	2.5
1	A	374	ASP	2.5
1	A	159	PHE	2.4
1	A	163	VAL	2.3
2	B	456	TYR	2.2
1	A	125	ARG	2.2
1	A	137	ASP	2.2
1	A	156	LYS	2.2
2	B	467	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	A	270	24/25	0.97	0.18	63,73,78,80	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	501	5/5	0.81	0.26	184,184,184,185	0
3	SO4	B	500	5/5	0.92	0.15	110,110,111,112	0

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

There are no such residues in this entry.