



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:06 am BST

PDB ID : 3HVT  
Title : STRUCTURAL BASIS OF ASYMMETRY IN THE HUMAN IMMUNODEFICIENCY VIRUS TYPE 1 REVERSE TRANSCRIPTASE HETERO-DIMER  
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Deposited on : 1994-07-25  
Resolution : 2.90 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.

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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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

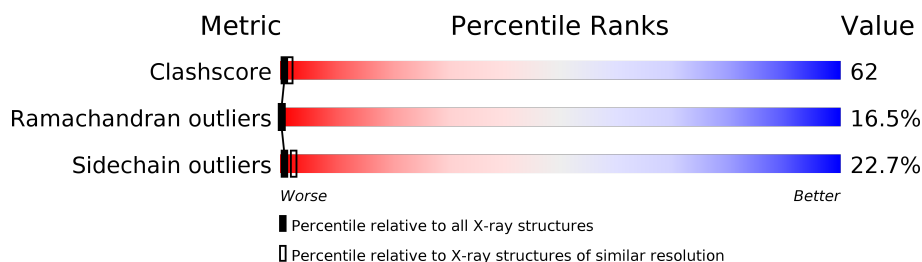
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	556	
2	B	428	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7426 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.

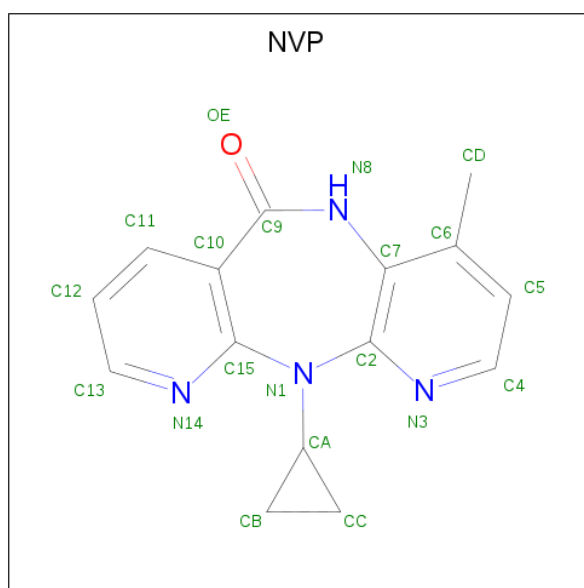
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4248	2744	709	787	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	398	Total	C	N	O	S	0	0	0
			3158	2050	523	579	6			

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O).



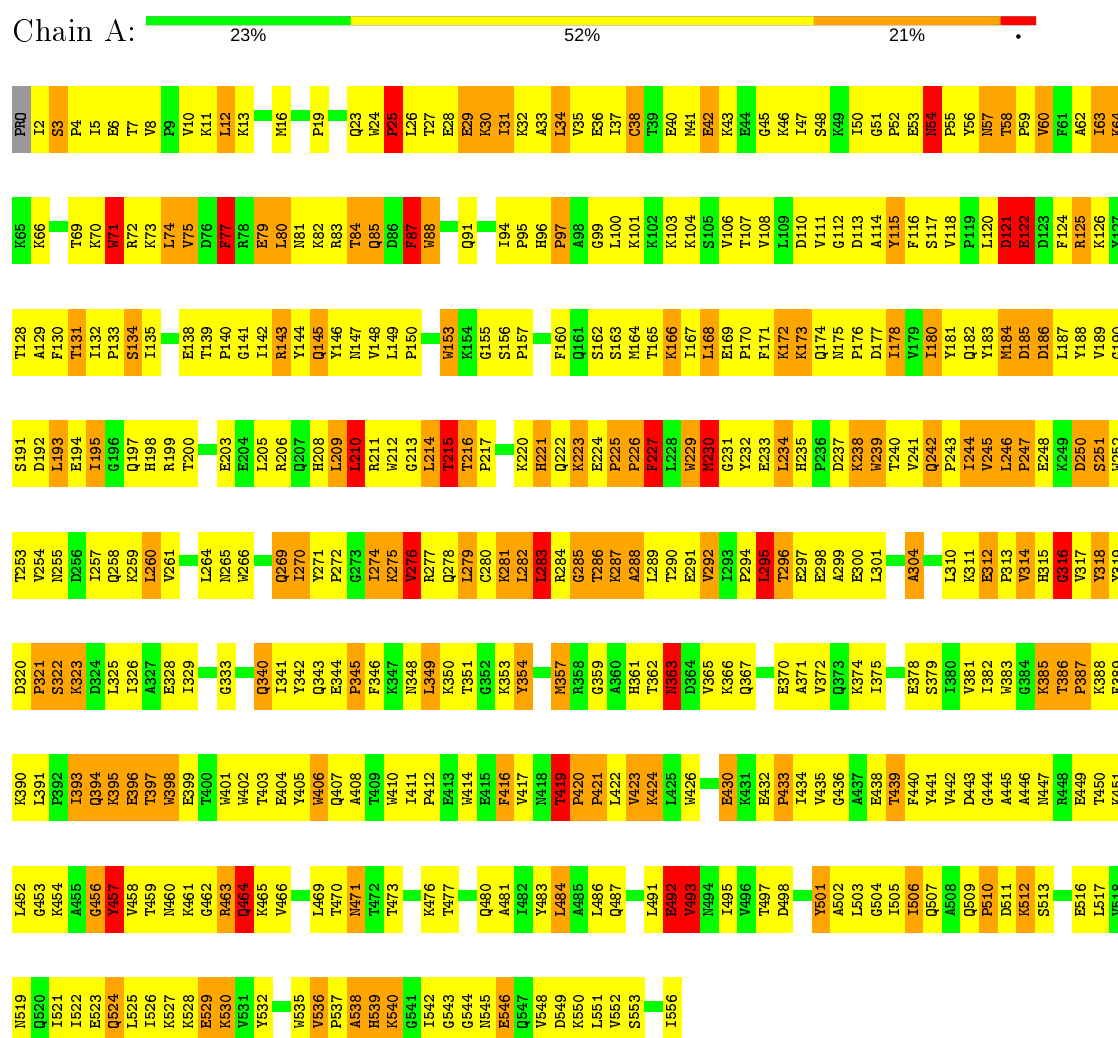
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

### 3 Residue-property plots

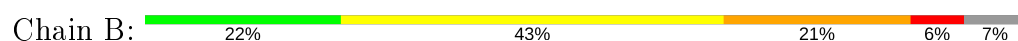
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P66)



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (SUBUNIT P51)



W398	V317	N255	I195	I132	I63	PRO
W401	P321	D256	G196	P133	K64	I2
W402	S322	I257	Q197	S134	K65	S3
T403	K323	Q258	H198	I135	K66	P4
E404	K323	K259	R199	N136	D67	I5
Y405	Q332	L260	T200	S68	S68	E6
W406	G333	V261	K201	T69	T69	T7
Q407	G334	G262	L202	P140	K70	V8
A408	Q334	K263	E203	G141	W71	P9
T409	Q336	L264	L205	I142	W71	P9
W410	Q337	N265	L205	R143	K72	V10
I411	K337	V266	R206	Y144	K73	K11
P412	P345	A267	Q207	Q145	L74	L12
E413	F346	S268	E208	Y146	K13	K13
W414	K347	Q269	L209	N147	D76	P14
E415	K347	I270	L210	V148	F77	G15
F416	K350	Y271	R211	L149	E79	M16
V417	K350	P272	W212	P150	E79	M16
M418	K354	G273	G213	Q151	L80	D17
T419	A355	V276	L214	G152	N81	D17
P420	R358	R277	T215	M153	K82	V21
L422	GLY	Q278	T216	K154	K82	K22
Y423	ALA	R279	D218	G155	T84	Q23
K424	HIS	K280	K219	T84	Q23	Q23
L425	THR	L282	H221	S156	P25	P25
W426	ASN	L283	K222	Q157	D86	L26
Y427	D364	R284	K223	A158	F87	T27
Q428	V365	G285	E224	I159	W88	E28
	K366	T286	P225	F160	E89	E29
	Q367	K287	PRO	Q161	V90	K30
	L368	A288	PHE	S162	Q91	I31
	T369	L289	LEU	G163	L92	K32
	E370	T290	TRP	M164	G93	A33
	A371	E291	MET	T165	I94	L34
	V372	V292	GLY	K166	P95	E36
	Q373	L293	TYR	I167	G99	I37
	K374	P294	GLU	L168	L100	C38
	I375	L295	LEU	E169	K101	T39
	T376	T296	HIS	P170	K102	E40
	T377	E297	PRO	F171	K103	M41
	E378	E298	ASP	K172	K104	E42
	S379	A299	LYS	Q174	S105	K43
	I380	E300	TRP	N175	S105	E44
	I382	L301	THR	D177	V108	G45
	W383	L303	GLN	I178	Y115	K46
	T386	A304	PRO	I180	F116	I47
	P387	E305	ILE	Y183	S117	S48
	K388	N306	VAL	M184	K49	K49
	F389	R307	LEU	D185	V118	I50
	K390	E308	PRO	D186	P119	G51
		I309	GLU	L187	L120	P52
			LYS	Y188	D121	E53
			D250	F124	E122	N54
			S251	Y189	D123	P55
			W252	V189	F124	Y56
			T253	G190	N57	N57
			T397	S191	R125	T58
			G316	D192	T128	P59
				L193	A129	V60
				T193	F130	F61
					T131	A62

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.60 Å   69.90 Å   105.50 Å 90.00°   106.40°   90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.266 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.76	1/4358 (0.0%)	1.06	15/5951 (0.3%)
2	B	0.81	0/3242	1.10	21/4411 (0.5%)
All	All	0.78	1/7600 (0.0%)	1.08	36/10362 (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
2	B	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ASP	CB-CG	5.37	1.63	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	GLY	C-N-CD	-9.27	100.21	120.60
2	B	419	THR	C-N-CD	-8.95	100.92	120.60
2	B	178	ILE	N-CA-C	-8.83	87.15	111.00
1	A	420	PRO	C-N-CD	-8.65	101.56	120.60
2	B	288	ALA	N-CA-C	8.18	133.10	111.00
2	B	104	LYS	N-CA-C	7.69	131.76	111.00
1	A	85	GLN	N-CA-C	7.43	131.05	111.00
2	B	277	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	B	345	PRO	N-CA-CB	7.22	111.97	103.30
1	A	313	PRO	N-CA-CB	7.16	111.89	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	198	HIS	N-CA-C	-6.98	92.16	111.00
2	B	422	LEU	CA-CB-CG	-6.91	99.40	115.30
1	A	231	GLY	N-CA-C	-6.72	96.29	113.10
2	B	74	LEU	N-CA-C	-6.44	93.60	111.00
2	B	321	PRO	N-CA-CB	6.26	110.81	103.30
1	A	230	MET	N-CA-C	-6.00	94.80	111.00
2	B	177	ASP	N-CA-C	5.96	127.09	111.00
1	A	45	GLY	N-CA-C	-5.86	98.46	113.10
1	A	251	SER	N-CA-C	-5.76	95.46	111.00
2	B	293	ILE	C-N-CD	-5.73	108.00	120.60
1	A	193	LEU	CA-CB-CG	5.72	128.47	115.30
1	A	316	GLY	N-CA-C	5.70	127.36	113.10
2	B	270	ILE	N-CA-C	-5.57	95.97	111.00
1	A	388	LYS	N-CA-C	-5.47	96.22	111.00
2	B	335	GLY	N-CA-C	-5.38	99.64	113.10
2	B	295	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	426	TRP	N-CA-C	-5.34	96.59	111.00
1	A	359	GLY	N-CA-C	5.32	126.41	113.10
2	B	187	LEU	CA-CB-CG	5.32	127.54	115.30
2	B	222	GLN	N-CA-C	5.29	125.28	111.00
1	A	274	ILE	N-CA-C	-5.24	96.85	111.00
2	B	315	HIS	N-CA-C	5.23	125.12	111.00
1	A	276	VAL	N-CA-C	5.10	124.76	111.00
1	A	456	GLY	N-CA-C	5.07	125.77	113.10
1	A	153	TRP	N-CA-C	-5.06	97.33	111.00
2	B	321	PRO	N-CA-C	-5.06	98.95	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	183	TYR	Sidechain
2	B	188	TYR	Sidechain
2	B	354	TYR	Sidechain
2	B	56	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4248	0	4052	553	4
2	B	3158	0	3082	380	1
3	A	20	0	14	3	0
All	All	7426	0	7148	905	4

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 62.

All (905) 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:A:441:TYR:HE2	2:B:286:THR:HG23	1.19	1.07
2:B:150:PRO:HD2	2:B:153:TRP:HE1	1.17	1.06
1:A:42:GLU:HA	1:A:46:LYS:HA	1.36	1.05
1:A:79:GLU:HG2	1:A:83:ARG:HH21	1.23	1.01
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.36	1.00
2:B:206:ARG:HG2	2:B:217:PRO:HG2	1.43	1.00
1:A:542:ILE:HG23	1:A:545:ASN:HB3	1.43	0.99
2:B:278:GLN:HB3	2:B:298:GLU:HB3	1.43	0.97
1:A:447:ASN:HB2	1:A:556:ILE:HG23	1.47	0.96
1:A:84:THR:O	1:A:87:PHE:HB2	1.66	0.94
2:B:223:LYS:O	2:B:225:PRO:HD3	1.67	0.94
1:A:441:TYR:CE2	2:B:286:THR:HG23	2.03	0.94
1:A:50:ILE:HG22	1:A:52:PRO:HD3	1.50	0.91
1:A:188:TYR:O	3:A:557:NVP:HCB1	1.71	0.90
2:B:7:THR:HG21	2:B:122:GLU:HB2	1.53	0.90
2:B:282:LEU:HD11	2:B:293:ILE:HD11	1.54	0.89
1:A:419:THR:HG22	1:A:420:PRO:HD3	1.52	0.89
2:B:135:ILE:H	2:B:135:ILE:HD12	1.38	0.89
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.54	0.89
1:A:278:GLN:HA	1:A:281:LYS:HB2	1.56	0.88
1:A:170:PRO:HA	1:A:173:LYS:HE3	1.54	0.87
2:B:34:LEU:HD23	2:B:132:ILE:HG23	1.55	0.87
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.15	0.87
2:B:154:LYS:HD3	2:B:184:MET:SD	2.15	0.86
1:A:242:GLN:HB3	1:A:243:PRO:HD3	1.56	0.86
2:B:293:ILE:HB	2:B:294:PRO:HA	1.57	0.86
2:B:45:GLY:O	2:B:47:ILE:HG12	1.76	0.85
1:A:115:TYR:O	1:A:149:LEU:HB2	1.76	0.85
1:A:542:ILE:HD11	2:B:283:LEU:HD12	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG21	1:A:77:PHE:HD2	1.42	0.85
2:B:254:VAL:HG23	2:B:283:LEU:HD22	1.57	0.85
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.57	0.84
1:A:522:ILE:HA	1:A:525:LEU:HD12	1.59	0.84
2:B:194:GLU:HB2	2:B:197:GLN:O	1.77	0.84
2:B:44:GLU:HB3	2:B:47:ILE:HD11	1.57	0.84
2:B:376:THR:O	2:B:380:ILE:HD12	1.75	0.84
2:B:60:VAL:HG22	2:B:75:VAL:HG23	1.60	0.83
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.60	0.83
1:A:170:PRO:HG2	1:A:208:HIS:CE1	2.13	0.83
1:A:180:ILE:HG22	1:A:189:VAL:HA	1.61	0.83
2:B:34:LEU:HD13	2:B:62:ALA:HB2	1.59	0.83
1:A:103:LYS:HD2	1:A:191:SER:HA	1.60	0.83
1:A:386:THR:HG22	1:A:387:PRO:HD2	1.61	0.83
1:A:458:VAL:HG22	1:A:464:GLN:HB3	1.61	0.82
1:A:59:PRO:O	1:A:75:VAL:HG12	1.80	0.82
1:A:34:LEU:HD23	1:A:60:VAL:HG12	1.61	0.82
2:B:277:ARG:HA	2:B:280:CYS:HB3	1.59	0.82
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.60	0.82
1:A:96:HIS:HD2	1:A:97:PRO:HD2	1.43	0.81
1:A:58:THR:HG21	1:A:77:PHE:CD2	2.14	0.81
1:A:536:VAL:CG2	1:A:542:ILE:HG12	2.09	0.81
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.62	0.81
2:B:150:PRO:HD2	2:B:153:TRP:NE1	1.95	0.81
1:A:517:LEU:O	1:A:521:ILE:HD13	1.82	0.80
2:B:254:VAL:HG11	2:B:288:ALA:HA	1.64	0.80
2:B:11:LYS:HE2	2:B:11:LYS:HA	1.64	0.80
1:A:536:VAL:HG23	2:B:258:GLN:HG3	1.63	0.79
1:A:170:PRO:HG2	1:A:208:HIS:HE1	1.47	0.79
2:B:5:ILE:O	2:B:6:GLU:HG3	1.83	0.79
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.65	0.79
2:B:292:VAL:HG12	2:B:293:ILE:HG12	1.64	0.79
2:B:65:LYS:HE3	2:B:72:ARG:CZ	2.13	0.78
1:A:229:TRP:HB3	1:A:232:TYR:HB2	1.65	0.78
1:A:166:LYS:HA	1:A:166:LYS:HE3	1.65	0.78
2:B:143:ARG:HB3	2:B:143:ARG:HH11	1.48	0.78
1:A:88:TRP:CE2	1:A:155:GLY:HA2	2.18	0.78
1:A:436:GLY:H	2:B:289:LEU:HD13	1.49	0.78
1:A:135:ILE:N	1:A:139:THR:HA	1.99	0.78
1:A:253:THR:HA	1:A:292:VAL:HA	1.63	0.78
1:A:546:GLU:O	1:A:549:ASP:HB3	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:O	1:A:382:ILE:HG12	1.83	0.77
1:A:247:PRO:HB2	1:A:252:TRP:HZ2	1.48	0.77
1:A:77:PHE:O	1:A:81:ASN:HB2	1.83	0.77
2:B:296:THR:HB	2:B:299:ALA:CB	2.15	0.77
1:A:184:MET:O	1:A:186:ASP:N	2.18	0.77
1:A:393:ILE:O	1:A:416:PHE:HB2	1.85	0.77
1:A:164:MET:HA	1:A:167:ILE:HD12	1.68	0.76
2:B:52:PRO:HD2	2:B:53:GLU:OE1	1.86	0.76
1:A:101:LYS:HG2	1:A:320:ASP:HB3	1.68	0.76
1:A:232:TYR:HB3	1:A:234:LEU:HD23	1.67	0.76
1:A:135:ILE:H	1:A:139:THR:HA	1.49	0.75
1:A:441:TYR:O	1:A:457:TYR:HA	1.85	0.75
2:B:31:ILE:O	2:B:35:VAL:HG23	1.87	0.75
2:B:147:ASN:HD22	2:B:147:ASN:N	1.85	0.75
1:A:164:MET:HG3	1:A:168:LEU:HD12	1.68	0.75
1:A:443:ASP:O	1:A:552:VAL:HG11	1.86	0.75
1:A:254:VAL:HG12	1:A:289:LEU:O	1.86	0.74
1:A:361:HIS:HB2	1:A:510:PRO:CB	2.17	0.74
2:B:13:LYS:HG2	2:B:14:PRO:N	2.01	0.74
2:B:7:THR:HG22	2:B:120:LEU:HD23	1.69	0.74
2:B:253:THR:O	2:B:256:ASP:HB2	1.88	0.74
2:B:74:LEU:CD2	2:B:411:ILE:HD11	2.18	0.73
2:B:197:GLN:HA	2:B:197:GLN:OE1	1.88	0.73
2:B:293:ILE:HG21	2:B:295:LEU:O	1.88	0.73
2:B:164:MET:SD	2:B:168:LEU:HD12	2.28	0.73
2:B:293:ILE:HB	2:B:294:PRO:CA	2.18	0.73
2:B:119:PRO:C	2:B:120:LEU:HD13	2.09	0.73
1:A:535:TRP:CZ2	1:A:537:PRO:HA	2.24	0.72
2:B:304:ALA:HA	2:B:307:ARG:HB3	1.70	0.72
1:A:258:GLN:NE2	1:A:283:LEU:HD21	2.04	0.72
1:A:87:PHE:O	2:B:55:PRO:HD3	1.89	0.72
1:A:269:GLN:HA	1:A:350:LYS:NZ	2.05	0.72
2:B:423:VAL:HG12	2:B:425:LEU:O	1.90	0.72
1:A:238:LYS:HB2	1:A:316:GLY:HA3	1.72	0.71
2:B:219:LYS:HG2	2:B:220:LYS:N	2.03	0.71
2:B:77:PHE:CE1	2:B:128:THR:HG22	2.24	0.71
1:A:124:PHE:O	1:A:126:LYS:HG2	1.90	0.71
1:A:165:THR:HG23	1:A:182:GLN:HE21	1.54	0.71
1:A:405:TYR:HE1	1:A:406:TRP:CZ3	2.08	0.71
1:A:483:TYR:HB2	1:A:521:ILE:HD11	1.72	0.71
1:A:480:GLN:HG2	1:A:517:LEU:HD23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.70	0.71
2:B:10:VAL:HA	2:B:88:TRP:CZ3	2.26	0.71
1:A:536:VAL:HG21	1:A:542:ILE:HG12	1.71	0.71
2:B:11:LYS:HZ1	2:B:12:LEU:HD21	1.54	0.70
1:A:208:HIS:O	1:A:212:TRP:HD1	1.74	0.70
1:A:503:LEU:HD12	1:A:504:GLY:N	2.06	0.70
1:A:77:PHE:CZ	1:A:150:PRO:HB2	2.26	0.70
2:B:271:TYR:HB3	2:B:272:PRO:HD2	1.73	0.70
1:A:258:GLN:HE22	1:A:283:LEU:HD21	1.56	0.70
1:A:57:ASN:ND2	1:A:58:THR:H	1.89	0.70
1:A:131:THR:HA	1:A:143:ARG:HG3	1.74	0.70
1:A:389:PHE:HB3	1:A:391:LEU:HD13	1.72	0.70
1:A:363:ASN:ND2	1:A:363:ASN:H	1.87	0.70
1:A:372:VAL:HG11	1:A:411:ILE:CD1	2.22	0.70
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.74	0.70
2:B:345:PRO:O	2:B:347:LYS:N	2.24	0.70
2:B:10:VAL:HG22	2:B:88:TRP:CZ2	2.27	0.70
1:A:435:VAL:HG12	2:B:289:LEU:HB2	1.73	0.69
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.73	0.69
1:A:361:HIS:HB2	1:A:510:PRO:HB2	1.73	0.69
2:B:372:VAL:O	2:B:376:THR:HG22	1.91	0.69
2:B:376:THR:OG1	2:B:386:THR:HG22	1.92	0.69
2:B:10:VAL:HA	2:B:88:TRP:CH2	2.26	0.69
2:B:45:GLY:O	2:B:47:ILE:N	2.25	0.69
1:A:247:PRO:HB2	1:A:252:TRP:CZ2	2.27	0.69
2:B:47:ILE:HG22	2:B:148:VAL:HG21	1.75	0.69
1:A:64:LYS:CB	1:A:72:ARG:H	2.06	0.69
1:A:245:VAL:HG22	1:A:247:PRO:HD3	1.73	0.69
1:A:56:TYR:O	1:A:57:ASN:HB2	1.93	0.69
1:A:193:LEU:HD22	1:A:197:GLN:HE21	1.58	0.69
1:A:235:HIS:HD2	1:A:237:ASP:HB2	1.57	0.68
1:A:440:PHE:HE2	1:A:457:TYR:CZ	2.11	0.68
1:A:165:THR:HG23	1:A:182:GLN:NE2	2.09	0.68
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.75	0.68
2:B:65:LYS:HA	2:B:407:GLN:HG2	1.75	0.68
2:B:48:SER:HA	2:B:145:GLN:O	1.93	0.67
2:B:57:ASN:ND2	2:B:143:ARG:HH12	1.91	0.67
1:A:435:VAL:HG12	2:B:289:LEU:CB	2.24	0.67
2:B:11:LYS:NZ	2:B:12:LEU:HD21	2.08	0.67
2:B:369:THR:HG22	2:B:370:GLU:HG3	1.76	0.67
1:A:433:PRO:HB3	1:A:532:TYR:CE2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD13	1:A:178:ILE:O	1.94	0.66
1:A:229:TRP:CE3	1:A:229:TRP:HA	2.30	0.66
1:A:513:SER:HB2	1:A:519:ASN:ND2	2.11	0.66
1:A:242:GLN:O	1:A:244:ILE:HG13	1.95	0.66
2:B:65:LYS:HG3	2:B:72:ARG:HD3	1.77	0.66
1:A:361:HIS:CG	1:A:511:ASP:O	2.49	0.66
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.76	0.66
1:A:124:PHE:O	1:A:126:LYS:N	2.29	0.66
1:A:261:VAL:HG11	1:A:280:CYS:HB3	1.77	0.66
2:B:282:LEU:HG	2:B:292:VAL:HG11	1.78	0.66
1:A:57:ASN:OD1	1:A:131:THR:HG22	1.95	0.65
1:A:164:MET:O	1:A:168:LEU:HD12	1.97	0.65
1:A:529:GLU:HG2	1:A:529:GLU:O	1.95	0.65
1:A:536:VAL:HG22	1:A:542:ILE:HG12	1.77	0.65
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.78	0.65
1:A:101:LYS:CG	1:A:320:ASP:HB3	2.26	0.65
2:B:286:THR:HG22	2:B:287:LYS:N	2.11	0.65
2:B:321:PRO:O	2:B:323:LYS:N	2.30	0.65
1:A:13:LYS:NZ	1:A:82:LYS:O	2.29	0.65
1:A:416:PHE:CD1	1:A:417:VAL:N	2.65	0.65
2:B:65:LYS:HG3	2:B:72:ARG:CD	2.27	0.65
2:B:118:VAL:HB	2:B:119:PRO:HD3	1.78	0.65
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.27	0.65
1:A:542:ILE:CD1	2:B:283:LEU:HD12	2.27	0.64
1:A:229:TRP:HA	1:A:229:TRP:HE3	1.63	0.64
1:A:242:GLN:CB	1:A:243:PRO:HD3	2.28	0.64
1:A:542:ILE:HG23	1:A:545:ASN:CB	2.25	0.64
1:A:33:ALA:HB2	1:A:71:TRP:HE3	1.62	0.64
2:B:198:HIS:O	2:B:202:ILE:HG12	1.98	0.64
1:A:357:MET:SD	1:A:357:MET:O	2.56	0.64
1:A:77:PHE:HZ	1:A:150:PRO:HB2	1.62	0.64
1:A:79:GLU:CG	1:A:83:ARG:HH21	2.05	0.64
2:B:28:GLU:HA	2:B:31:ILE:HG23	1.79	0.64
1:A:41:MET:HB3	1:A:48:SER:OG	1.97	0.64
2:B:200:THR:HG23	2:B:201:LYS:H	1.61	0.64
2:B:305:GLU:O	2:B:309:ILE:HG12	1.98	0.64
1:A:195:ILE:O	1:A:199:ARG:HG2	1.98	0.64
1:A:301:LEU:HA	1:A:304:ALA:HB3	1.79	0.63
1:A:391:LEU:O	1:A:416:PHE:HA	1.96	0.63
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.80	0.63
2:B:277:ARG:CA	2:B:280:CYS:HB3	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:O	1:A:36:GLU:HG2	1.97	0.63
1:A:539:HIS:O	1:A:542:ILE:HG22	1.98	0.63
2:B:332:GLN:HA	2:B:337:TRP:CD1	2.34	0.63
2:B:395:LYS:O	2:B:396:GLU:HB2	1.97	0.63
2:B:12:LEU:N	2:B:12:LEU:HD23	2.13	0.63
1:A:34:LEU:HD11	1:A:73:LYS:HB2	1.81	0.63
2:B:304:ALA:HA	2:B:307:ARG:CB	2.29	0.63
2:B:296:THR:HB	2:B:299:ALA:HB3	1.79	0.63
2:B:39:THR:O	2:B:43:LYS:HG2	1.98	0.63
1:A:132:ILE:HB	1:A:142:ILE:HB	1.81	0.62
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.34	0.62
2:B:280:CYS:SG	2:B:281:LYS:N	2.72	0.62
1:A:12:LEU:HA	1:A:84:THR:CG2	2.29	0.62
1:A:539:HIS:CG	1:A:540:LYS:N	2.68	0.62
2:B:368:LEU:HD23	2:B:393:ILE:HD12	1.81	0.62
1:A:131:THR:HB	1:A:143:ARG:HD2	1.81	0.62
1:A:175:ASN:OD1	1:A:175:ASN:N	2.32	0.62
1:A:245:VAL:HG22	1:A:246:LEU:H	1.65	0.62
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.99	0.62
2:B:108:VAL:HA	2:B:187:LEU:O	1.98	0.62
1:A:52:PRO:HA	1:A:143:ARG:HB3	1.81	0.62
2:B:116:PHE:O	2:B:119:PRO:HD2	1.98	0.62
1:A:165:THR:O	1:A:169:GLU:HG2	2.00	0.62
1:A:42:GLU:CA	1:A:46:LYS:HA	2.21	0.62
2:B:220:LYS:HB2	2:B:222:GLN:NE2	2.15	0.62
1:A:88:TRP:NE1	1:A:155:GLY:HA2	2.15	0.62
1:A:239:TRP:HH2	1:A:349:LEU:O	1.83	0.61
1:A:254:VAL:HG11	1:A:288:ALA:O	2.00	0.61
2:B:140:PRO:HG2	2:B:142:ILE:HD11	1.81	0.61
1:A:79:GLU:HG2	1:A:83:ARG:NH2	2.06	0.61
1:A:439:THR:HG21	2:B:288:ALA:H	1.64	0.61
1:A:501:TYR:HD1	1:A:502:ALA:N	1.99	0.61
2:B:125:ARG:HB3	2:B:146:TYR:O	2.00	0.61
2:B:286:THR:HG22	2:B:287:LYS:H	1.64	0.61
1:A:317:VAL:CB	1:A:349:LEU:HA	2.30	0.61
1:A:361:HIS:CE1	1:A:512:LYS:O	2.53	0.61
1:A:265:ASN:OD1	1:A:353:LYS:NZ	2.32	0.61
1:A:239:TRP:HZ3	1:A:317:VAL:CB	2.14	0.61
1:A:456:GLY:O	1:A:457:TYR:HB3	2.00	0.61
1:A:164:MET:O	1:A:164:MET:HG3	2.00	0.61
1:A:77:PHE:CD1	1:A:77:PHE:N	2.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TYR:HB2	2:B:374:LYS:HD2	1.82	0.61
2:B:3:SER:HB3	2:B:4:PRO:O	2.00	0.60
1:A:153:TRP:CZ3	1:A:155:GLY:HA3	2.37	0.60
1:A:258:GLN:NE2	1:A:283:LEU:HD11	2.16	0.60
1:A:296:THR:HG23	1:A:297:GLU:N	2.16	0.60
1:A:434:ILE:HG21	1:A:492:GLU:CG	2.31	0.60
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.83	0.60
1:A:52:PRO:CB	1:A:143:ARG:HB2	2.31	0.60
1:A:434:ILE:HD13	1:A:492:GLU:HG3	1.83	0.60
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.83	0.60
2:B:91:GLN:O	2:B:92:LEU:HB2	2.02	0.60
1:A:234:LEU:HB3	1:A:239:TRP:HB2	1.82	0.60
2:B:257:ILE:HA	2:B:260:LEU:HB3	1.82	0.60
1:A:443:ASP:HB2	1:A:548:VAL:HG13	1.84	0.60
2:B:123:ASP:H	2:B:125:ARG:NE	2.00	0.60
2:B:253:THR:HA	2:B:291:GLU:HA	1.84	0.60
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.83	0.60
1:A:19:PRO:HB3	1:A:79:GLU:HB3	1.82	0.60
2:B:252:TRP:CZ2	2:B:260:LEU:HD22	2.37	0.60
2:B:65:LYS:HE3	2:B:72:ARG:NE	2.17	0.59
1:A:144:TYR:O	1:A:145:GLN:HB3	2.01	0.59
1:A:171:PHE:O	1:A:173:LYS:N	2.34	0.59
1:A:235:HIS:CD2	1:A:237:ASP:HB2	2.35	0.59
1:A:300:GLU:O	1:A:304:ALA:HB2	2.02	0.59
1:A:457:TYR:C	1:A:457:TYR:CD1	2.75	0.59
1:A:12:LEU:HG	1:A:83:ARG:O	2.03	0.59
1:A:278:GLN:HA	1:A:281:LYS:CB	2.31	0.59
2:B:296:THR:HB	2:B:299:ALA:HB2	1.82	0.59
2:B:39:THR:HG23	2:B:40:GLU:OE2	2.01	0.59
2:B:86:ASP:O	2:B:89:GLU:HB3	2.02	0.59
1:A:12:LEU:HA	1:A:84:THR:HG23	1.84	0.59
2:B:128:THR:HG21	2:B:150:PRO:HG2	1.85	0.59
2:B:65:LYS:HD3	2:B:407:GLN:O	2.03	0.59
1:A:398:TRP:CE3	1:A:402:TRP:CD1	2.91	0.58
1:A:52:PRO:HB3	1:A:143:ARG:HB2	1.85	0.58
2:B:195:ILE:C	2:B:197:GLN:H	2.07	0.58
2:B:2:ILE:HD12	2:B:2:ILE:O	2.02	0.58
1:A:57:ASN:HD22	1:A:58:THR:H	1.48	0.58
2:B:266:TRP:HZ3	2:B:422:LEU:CD2	2.16	0.58
2:B:276:VAL:O	2:B:279:LEU:HB3	2.03	0.58
2:B:417:VAL:O	2:B:417:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:N	1:A:87:PHE:HE2	2.00	0.58
1:A:183:TYR:O	1:A:184:MET:HG2	2.03	0.58
1:A:210:LEU:O	1:A:210:LEU:HD23	2.03	0.58
1:A:176:PRO:O	1:A:177:ASP:HB2	2.03	0.58
1:A:271:TYR:O	1:A:274:ILE:HG12	2.04	0.58
2:B:219:LYS:HG2	2:B:220:LYS:H	1.67	0.58
1:A:31:ILE:HD11	1:A:133:PRO:HD2	1.86	0.58
1:A:8:VAL:O	1:A:10:VAL:HG13	2.05	0.57
2:B:40:GLU:O	2:B:44:GLU:HB2	2.04	0.57
1:A:31:ILE:O	1:A:35:VAL:HG23	2.04	0.57
1:A:362:THR:HG22	1:A:366:LYS:HB3	1.84	0.57
2:B:364:ASP:HA	2:B:367:GLN:HB2	1.85	0.57
2:B:43:LYS:C	2:B:45:GLY:H	2.05	0.57
2:B:66:LYS:H	2:B:407:GLN:NE2	2.02	0.57
1:A:10:VAL:HG12	1:A:88:TRP:CH2	2.39	0.57
1:A:171:PHE:C	1:A:173:LYS:H	2.08	0.57
2:B:378:GLU:O	2:B:382:ILE:HG13	2.05	0.57
1:A:465:LYS:HG2	1:A:466:VAL:N	2.18	0.57
1:A:69:THR:HG22	1:A:69:THR:O	2.04	0.57
1:A:461:LYS:O	1:A:463:ARG:N	2.37	0.57
2:B:425:LEU:O	2:B:426:TRP:HB3	2.05	0.57
1:A:167:ILE:HD13	1:A:214:LEU:HD11	1.85	0.57
1:A:366:LYS:O	1:A:370:GLU:HG3	2.05	0.57
2:B:260:LEU:HD21	2:B:279:LEU:HD11	1.84	0.57
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.40	0.57
1:A:296:THR:HG22	1:A:299:ALA:H	1.70	0.57
1:A:398:TRP:CH2	1:A:411:ILE:HG21	2.40	0.57
2:B:263:LYS:HG3	2:B:425:LEU:HB3	1.86	0.57
1:A:535:TRP:CH2	1:A:537:PRO:HA	2.40	0.57
2:B:270:ILE:O	2:B:271:TYR:CG	2.57	0.57
1:A:234:LEU:HD11	3:A:557:NVP:HCD1	1.85	0.57
1:A:5:ILE:HG22	1:A:6:GLU:N	2.20	0.57
1:A:203:GLU:HG2	1:A:206:ARG:HH22	1.70	0.57
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.86	0.57
1:A:95:PRO:HG2	1:A:181:TYR:CE2	2.40	0.57
2:B:183:TYR:CE2	2:B:380:ILE:HG12	2.39	0.57
2:B:278:GLN:HB3	2:B:298:GLU:CB	2.26	0.57
2:B:397:THR:HG22	2:B:397:THR:O	2.04	0.57
2:B:194:GLU:O	2:B:197:GLN:N	2.38	0.56
1:A:180:ILE:CG2	1:A:189:VAL:HG13	2.36	0.56
1:A:362:THR:CG2	1:A:366:LYS:HG3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:N	1:A:506:ILE:HD13	2.21	0.56
2:B:143:ARG:CB	2:B:143:ARG:HH11	2.17	0.56
1:A:47:ILE:O	1:A:47:ILE:HG22	2.05	0.56
1:A:75:VAL:O	1:A:75:VAL:HG23	2.05	0.56
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.41	0.56
2:B:389:PHE:O	2:B:415:GLU:N	2.37	0.56
1:A:276:VAL:HG12	1:A:280:CYS:SG	2.45	0.56
1:A:79:GLU:O	1:A:83:ARG:HG2	2.06	0.56
2:B:115:TYR:HE2	2:B:185:ASP:HA	1.70	0.56
2:B:163:SER:O	2:B:167:ILE:HG13	2.05	0.56
1:A:52:PRO:O	1:A:143:ARG:NH1	2.37	0.56
2:B:253:THR:HG22	2:B:256:ASP:H	1.68	0.56
1:A:116:PHE:O	1:A:148:VAL:HG11	2.05	0.56
1:A:5:ILE:HG22	1:A:6:GLU:H	1.71	0.56
2:B:116:PHE:O	2:B:118:VAL:N	2.39	0.56
2:B:7:THR:HG21	2:B:122:GLU:CB	2.32	0.56
1:A:483:TYR:HE1	1:A:524:GLN:HE22	1.53	0.56
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.88	0.56
2:B:282:LEU:HG	2:B:292:VAL:CG1	2.36	0.56
2:B:366:LYS:HZ2	2:B:405:TYR:HB3	1.71	0.56
1:A:12:LEU:O	1:A:13:LYS:C	2.43	0.56
1:A:122:GLU:HG3	1:A:125:ARG:NH1	2.21	0.56
2:B:191:SER:OG	2:B:198:HIS:HD2	1.87	0.56
2:B:267:ALA:O	2:B:269:GLN:N	2.40	0.55
1:A:52:PRO:HA	1:A:143:ARG:CB	2.36	0.55
1:A:398:TRP:CZ3	1:A:402:TRP:CD1	2.94	0.55
2:B:34:LEU:CD1	2:B:62:ALA:HB2	2.33	0.55
2:B:424:LYS:O	2:B:425:LEU:HB2	2.04	0.55
1:A:341:ILE:HD11	1:A:375:ILE:HG23	1.87	0.55
1:A:42:GLU:HA	1:A:46:LYS:CA	2.23	0.55
1:A:56:TYR:N	1:A:56:TYR:CD1	2.74	0.55
1:A:168:LEU:HD22	1:A:180:ILE:HD11	1.89	0.55
1:A:501:TYR:CD1	1:A:502:ALA:N	2.75	0.55
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.30	0.55
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.06	0.55
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.87	0.55
1:A:363:ASN:N	1:A:363:ASN:ND2	2.54	0.55
2:B:280:CYS:O	2:B:282:LEU:N	2.40	0.55
1:A:491:LEU:HB3	1:A:529:GLU:OE2	2.06	0.55
1:A:114:ALA:C	1:A:116:PHE:H	2.09	0.54
1:A:34:LEU:CD1	1:A:62:ALA:HB2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ALA:O	2:B:307:ARG:HB3	2.07	0.54
2:B:425:LEU:O	2:B:426:TRP:CB	2.54	0.54
1:A:74:LEU:HD12	1:A:75:VAL:N	2.22	0.54
1:A:193:LEU:HB2	1:A:198:HIS:CD2	2.42	0.54
1:A:441:TYR:CZ	1:A:544:GLY:HA3	2.42	0.54
1:A:56:TYR:O	1:A:143:ARG:NH2	2.41	0.54
1:A:10:VAL:HG12	1:A:88:TRP:HH2	1.72	0.54
2:B:46:LYS:HB3	2:B:148:VAL:HG13	1.89	0.54
2:B:300:GLU:OE1	2:B:303:LEU:HD22	2.08	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.43	0.54
1:A:168:LEU:O	1:A:172:LYS:HB2	2.07	0.54
1:A:183:TYR:C	1:A:184:MET:HG2	2.28	0.54
1:A:473:THR:HB	1:A:476:LYS:HE3	1.90	0.54
2:B:292:VAL:CG1	2:B:293:ILE:HG12	2.37	0.54
1:A:164:MET:CE	1:A:214:LEU:HD13	2.37	0.54
2:B:332:GLN:HA	2:B:337:TRP:NE1	2.23	0.54
2:B:39:THR:HG23	2:B:40:GLU:N	2.22	0.54
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.38	0.54
1:A:326:ILE:H	1:A:343:GLN:NE2	2.06	0.54
1:A:411:ILE:HG23	1:A:411:ILE:O	2.08	0.54
2:B:192:ASP:O	2:B:194:GLU:N	2.41	0.54
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.42	0.54
2:B:41:MET:O	2:B:47:ILE:HG13	2.07	0.54
1:A:108:VAL:HG13	1:A:108:VAL:O	2.07	0.53
1:A:280:CYS:O	1:A:283:LEU:HB3	2.08	0.53
2:B:100:LEU:HD12	2:B:100:LEU:O	2.08	0.53
2:B:85:GLN:OE1	2:B:89:GLU:HB2	2.08	0.53
1:A:53:GLU:O	1:A:54:ASN:HB2	2.08	0.53
1:A:193:LEU:HD22	1:A:197:GLN:HG3	1.90	0.53
1:A:232:TYR:HA	1:A:240:THR:O	2.08	0.53
1:A:58:THR:HG23	1:A:59:PRO:CD	2.38	0.53
2:B:270:ILE:O	2:B:271:TYR:CD1	2.61	0.53
2:B:206:ARG:CZ	2:B:219:LYS:H	2.22	0.53
1:A:254:VAL:O	1:A:258:GLN:HG2	2.08	0.53
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.90	0.53
1:A:405:TYR:HE1	1:A:406:TRP:CE3	2.27	0.53
1:A:503:LEU:HD13	1:A:507:GLN:OE1	2.08	0.53
2:B:254:VAL:HG12	2:B:290:THR:O	2.09	0.53
1:A:35:VAL:C	1:A:37:ILE:N	2.61	0.53
1:A:104:LYS:CB	1:A:192:ASP:HA	2.38	0.53
1:A:131:THR:HB	1:A:143:ARG:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:H	1:A:140:PRO:HD2	1.74	0.53
1:A:208:HIS:CD2	1:A:212:TRP:HE1	2.27	0.53
1:A:224:GLU:OE2	1:A:226:PRO:HD2	2.09	0.53
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.38	0.53
2:B:4:PRO:HG2	2:B:5:ILE:H	1.73	0.53
1:A:282:LEU:H	1:A:282:LEU:HD12	1.73	0.53
1:A:321:PRO:HG2	1:A:343:GLN:HG2	1.89	0.52
2:B:146:TYR:C	2:B:147:ASN:HD22	2.12	0.52
2:B:178:ILE:HG22	2:B:178:ILE:O	2.09	0.52
2:B:354:TYR:OH	2:B:367:GLN:HG3	2.08	0.52
1:A:10:VAL:HG22	1:A:121:ASP:OD2	2.09	0.52
2:B:366:LYS:HE3	2:B:404:GLU:HB2	1.91	0.52
1:A:35:VAL:C	1:A:37:ILE:H	2.11	0.52
1:A:10:VAL:O	1:A:10:VAL:HG23	2.08	0.52
1:A:424:LYS:C	1:A:426:TRP:H	2.13	0.52
1:A:441:TYR:CE1	1:A:544:GLY:HA3	2.44	0.52
1:A:282:LEU:O	1:A:284:ARG:N	2.42	0.52
1:A:411:ILE:HG13	1:A:412:PRO:HD2	1.91	0.52
1:A:10:VAL:CG1	1:A:88:TRP:HH2	2.22	0.52
2:B:129:ALA:O	2:B:130:PHE:HB3	2.10	0.52
2:B:47:ILE:CG2	2:B:148:VAL:HG21	2.39	0.52
2:B:252:TRP:HB2	2:B:294:PRO:HB3	1.91	0.52
1:A:33:ALA:CB	1:A:71:TRP:HE3	2.22	0.52
2:B:115:TYR:CE2	2:B:185:ASP:HA	2.45	0.52
2:B:115:TYR:O	2:B:149:LEU:HB2	2.09	0.52
1:A:184:MET:O	1:A:185:ASP:C	2.48	0.52
1:A:200:THR:O	1:A:203:GLU:HB2	2.10	0.52
1:A:354:TYR:CD2	1:A:371:ALA:HB2	2.43	0.52
1:A:10:VAL:HA	1:A:87:PHE:CE2	2.45	0.52
2:B:366:LYS:NZ	2:B:369:THR:HG21	2.25	0.52
2:B:88:TRP:CE2	2:B:92:LEU:HD13	2.45	0.52
1:A:203:GLU:HA	1:A:206:ARG:NH1	2.25	0.52
1:A:419:THR:CG2	1:A:420:PRO:HD3	2.34	0.52
1:A:210:LEU:HG	1:A:215:THR:HA	1.93	0.51
1:A:444:GLY:HA2	1:A:454:LYS:O	2.10	0.51
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.35	0.51
2:B:261:VAL:HG12	2:B:262:GLY:N	2.25	0.51
1:A:120:LEU:O	1:A:121:ASP:O	2.27	0.51
1:A:178:ILE:HA	1:A:191:SER:HB3	1.92	0.51
1:A:235:HIS:HD2	1:A:237:ASP:CB	2.22	0.51
1:A:287:LYS:O	1:A:288:ALA:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TRP:O	1:A:316:GLY:N	2.43	0.51
2:B:77:PHE:CZ	2:B:128:THR:HG22	2.45	0.51
1:A:35:VAL:O	1:A:37:ILE:N	2.43	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HG2	2.45	0.51
1:A:269:GLN:HA	1:A:350:LYS:HZ2	1.73	0.51
2:B:218:ASP:O	2:B:221:HIS:CE1	2.64	0.51
1:A:372:VAL:HG21	1:A:411:ILE:HD11	1.92	0.51
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.45	0.51
1:A:167:ILE:CD1	1:A:214:LEU:HD11	2.39	0.51
1:A:537:PRO:CG	2:B:262:GLY:HA2	2.40	0.51
1:A:97:PRO:O	1:A:99:GLY:N	2.44	0.51
1:A:282:LEU:N	1:A:282:LEU:HD12	2.26	0.51
2:B:135:ILE:H	2:B:135:ILE:CD1	2.16	0.51
2:B:140:PRO:O	2:B:141:GLY:C	2.48	0.51
2:B:147:ASN:ND2	2:B:147:ASN:N	2.56	0.51
2:B:302:GLU:HA	2:B:305:GLU:HB3	1.92	0.51
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.93	0.51
2:B:10:VAL:O	2:B:11:LYS:HE2	2.10	0.51
2:B:312:GLU:HB3	2:B:313:PRO:CD	2.39	0.51
2:B:33:ALA:O	2:B:36:GLU:N	2.42	0.51
1:A:80:LEU:HD22	1:A:153:TRP:HE1	1.75	0.50
2:B:93:GLY:O	2:B:95:PRO:HD3	2.11	0.50
1:A:194:GLU:O	1:A:195:ILE:C	2.50	0.50
2:B:36:GLU:HG2	2:B:40:GLU:OE1	2.10	0.50
1:A:166:LYS:HE3	1:A:166:LYS:CA	2.38	0.50
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.93	0.50
2:B:257:ILE:HG23	2:B:261:VAL:HG23	1.93	0.50
1:A:284:ARG:O	1:A:286:THR:N	2.44	0.50
1:A:379:SER:HA	1:A:383:TRP:CZ3	2.47	0.50
1:A:460:ASN:HB2	2:B:287:LYS:HG2	1.93	0.50
2:B:257:ILE:O	2:B:261:VAL:HB	2.12	0.50
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.58	0.50
1:A:103:LYS:HD2	1:A:190:GLY:O	2.11	0.50
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.92	0.50
2:B:285:GLY:O	2:B:286:THR:OG1	2.25	0.50
2:B:377:THR:HG1	2:B:410:TRP:HZ2	1.58	0.50
1:A:372:VAL:HG11	1:A:411:ILE:CG1	2.42	0.50
2:B:10:VAL:HG11	2:B:153:TRP:HH2	1.76	0.50
1:A:166:LYS:HA	1:A:166:LYS:CE	2.40	0.50
2:B:271:TYR:HB3	2:B:272:PRO:CD	2.39	0.50
1:A:108:VAL:HG21	1:A:188:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HB	1:A:276:VAL:HG11	1.93	0.50
2:B:263:LYS:HG3	2:B:425:LEU:CB	2.42	0.50
1:A:193:LEU:HB2	1:A:198:HIS:HD2	1.76	0.49
2:B:38:CYS:HG	2:B:132:ILE:HD11	1.77	0.49
2:B:366:LYS:NZ	2:B:405:TYR:H	2.10	0.49
1:A:134:SER:CB	1:A:141:GLY:H	2.25	0.49
1:A:38:CYS:O	1:A:41:MET:HB2	2.12	0.49
1:A:48:SER:HA	1:A:147:ASN:OD1	2.11	0.49
1:A:505:ILE:O	1:A:510:PRO:HD3	2.11	0.49
2:B:79:GLU:OE1	2:B:82:LYS:HE2	2.13	0.49
1:A:34:LEU:HD13	1:A:62:ALA:CB	2.36	0.49
1:A:539:HIS:CG	1:A:540:LYS:H	2.30	0.49
2:B:266:TRP:HZ3	2:B:422:LEU:HD23	1.77	0.49
2:B:46:LYS:HZ3	2:B:117:SER:HA	1.76	0.49
2:B:297:GLU:O	2:B:298:GLU:HB2	2.12	0.49
1:A:406:TRP:CD1	2:B:421:PRO:HD3	2.48	0.49
1:A:484:LEU:O	1:A:487:GLN:N	2.45	0.49
2:B:175:ASN:HD21	2:B:201:LYS:HE2	1.78	0.49
2:B:61:PHE:CE2	2:B:402:TRP:CZ2	3.00	0.49
2:B:80:LEU:O	2:B:84:THR:N	2.42	0.49
1:A:239:TRP:CD1	1:A:240:THR:N	2.80	0.49
1:A:361:HIS:NE2	1:A:512:LYS:O	2.46	0.49
2:B:46:LYS:O	2:B:48:SER:N	2.46	0.49
1:A:328:GLU:CB	1:A:341:ILE:HD12	2.42	0.49
1:A:386:THR:CG2	1:A:387:PRO:HD2	2.40	0.49
2:B:193:LEU:HD13	2:B:193:LEU:N	2.27	0.49
1:A:110:ASP:O	1:A:216:THR:HG22	2.12	0.49
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.47	0.49
2:B:270:ILE:HG12	2:B:346:PHE:CB	2.42	0.49
2:B:36:GLU:O	2:B:39:THR:HG22	2.11	0.49
1:A:361:HIS:HB2	1:A:510:PRO:HB3	1.95	0.49
1:A:362:THR:HG22	1:A:366:LYS:HG3	1.94	0.49
2:B:61:PHE:CE2	2:B:402:TRP:HZ2	2.30	0.49
1:A:31:ILE:CD1	1:A:133:PRO:HD2	2.43	0.48
2:B:390:LYS:HB3	2:B:417:VAL:HG11	1.95	0.48
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.94	0.48
2:B:193:LEU:H	2:B:193:LEU:HD22	1.79	0.48
1:A:543:GLY:HA3	2:B:283:LEU:O	2.13	0.48
2:B:3:SER:HB3	2:B:4:PRO:CA	2.42	0.48
2:B:22:LYS:O	2:B:23:GLN:HB2	2.12	0.48
1:A:543:GLY:CA	2:B:283:LEU:O	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:TYR:H	2:B:427:TYR:HD1	1.60	0.48
1:A:112:GLY:O	1:A:114:ALA:N	2.46	0.48
1:A:457:TYR:C	1:A:457:TYR:HD1	2.15	0.48
1:A:537:PRO:HG2	2:B:262:GLY:HA2	1.93	0.48
2:B:197:GLN:O	2:B:198:HIS:HB2	2.14	0.48
1:A:34:LEU:HD11	1:A:73:LYS:CB	2.44	0.48
1:A:372:VAL:HG11	1:A:411:ILE:HD11	1.94	0.48
1:A:391:LEU:HD22	1:A:414:TRP:HB2	1.96	0.48
2:B:254:VAL:HG13	2:B:255:ASN:H	1.78	0.48
1:A:276:VAL:CG1	1:A:276:VAL:O	2.61	0.48
1:A:363:ASN:O	1:A:367:GLN:N	2.43	0.48
1:A:440:PHE:CE2	1:A:457:TYR:CE1	3.01	0.48
2:B:153:TRP:CZ3	2:B:155:GLY:HA3	2.48	0.48
2:B:304:ALA:O	2:B:307:ARG:N	2.46	0.48
1:A:107:THR:N	1:A:189:VAL:O	2.47	0.48
1:A:405:TYR:CE1	1:A:406:TRP:CE3	3.01	0.48
2:B:173:LYS:C	2:B:173:LYS:HD3	2.33	0.48
2:B:277:ARG:O	2:B:280:CYS:HB3	2.13	0.48
2:B:306:ASN:O	2:B:309:ILE:HB	2.14	0.48
2:B:380:ILE:HD11	2:B:386:THR:CG2	2.43	0.48
1:A:443:ASP:C	1:A:552:VAL:HG11	2.33	0.48
1:A:458:VAL:HG22	1:A:464:GLN:CB	2.39	0.48
1:A:108:VAL:HA	1:A:187:LEU:O	2.14	0.48
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.96	0.48
1:A:546:GLU:O	1:A:550:LYS:HG2	2.13	0.48
2:B:63:ILE:CD1	2:B:74:LEU:HD12	2.44	0.48
1:A:103:LYS:CD	1:A:191:SER:HA	2.40	0.47
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.48	0.47
1:A:536:VAL:CG2	2:B:258:GLN:HE21	2.28	0.47
2:B:99:GLY:O	2:B:102:LYS:N	2.47	0.47
1:A:536:VAL:HG21	2:B:258:GLN:HE21	1.79	0.47
2:B:380:ILE:O	2:B:381:VAL:C	2.53	0.47
2:B:47:ILE:HG22	2:B:148:VAL:CG2	2.44	0.47
2:B:46:LYS:NZ	2:B:117:SER:HA	2.29	0.47
2:B:284:ARG:HD2	2:B:284:ARG:H	1.79	0.47
1:A:298:GLU:O	1:A:301:LEU:N	2.45	0.47
2:B:188:TYR:OH	2:B:410:TRP:CZ3	2.67	0.47
1:A:209:LEU:O	1:A:211:ARG:N	2.47	0.47
1:A:42:GLU:C	1:A:46:LYS:HG2	2.35	0.47
1:A:537:PRO:O	1:A:539:HIS:N	2.48	0.47
1:A:77:PHE:HZ	1:A:150:PRO:CB	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:HG3	1:A:84:THR:N	2.29	0.47
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.47
2:B:354:TYR:O	2:B:355:ALA:HB2	2.15	0.47
2:B:61:PHE:CZ	2:B:402:TRP:HZ2	2.33	0.47
1:A:114:ALA:O	1:A:116:PHE:N	2.48	0.47
1:A:3:SER:OG	1:A:5:ILE:HG13	2.15	0.47
1:A:483:TYR:HE1	1:A:524:GLN:NE2	2.13	0.47
2:B:21:VAL:HG12	2:B:22:LYS:H	1.80	0.47
1:A:318:TYR:HD1	1:A:318:TYR:O	1.97	0.47
1:A:354:TYR:HD2	1:A:371:ALA:HB2	1.78	0.47
1:A:42:GLU:O	1:A:46:LYS:HG2	2.14	0.47
1:A:502:ALA:O	1:A:506:ILE:HG12	2.14	0.47
2:B:302:GLU:HA	2:B:305:GLU:CB	2.45	0.47
2:B:84:THR:OG1	2:B:85:GLN:N	2.48	0.47
2:B:92:LEU:O	2:B:161:GLN:NE2	2.48	0.47
1:A:401:TRP:O	1:A:405:TYR:N	2.47	0.47
1:A:506:ILE:HD13	1:A:506:ILE:H	1.79	0.47
1:A:517:LEU:C	1:A:521:ILE:HD13	2.36	0.47
1:A:34:LEU:CD2	1:A:60:VAL:HG12	2.39	0.47
2:B:63:ILE:HD11	2:B:74:LEU:HD12	1.97	0.47
1:A:51:GLY:N	1:A:52:PRO:CD	2.78	0.47
2:B:143:ARG:NH1	2:B:143:ARG:CB	2.76	0.47
1:A:130:PHE:CE1	1:A:146:TYR:CE2	3.03	0.46
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.45	0.46
1:A:258:GLN:NE2	1:A:283:LEU:CD2	2.75	0.46
1:A:25:PRO:CG	1:A:133:PRO:HG2	2.45	0.46
1:A:257:ILE:HG23	1:A:279:LEU:HD23	1.97	0.46
1:A:440:PHE:CE2	1:A:457:TYR:CZ	2.98	0.46
1:A:129:ALA:HA	1:A:145:GLN:HA	1.98	0.46
1:A:183:TYR:O	1:A:186:ASP:HB2	2.15	0.46
2:B:12:LEU:CD2	2:B:124:PHE:HE2	2.28	0.46
2:B:201:LYS:O	2:B:204:GLU:HB3	2.15	0.46
2:B:206:ARG:HG2	2:B:217:PRO:CG	2.29	0.46
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.97	0.46
2:B:28:GLU:O	2:B:31:ILE:HG23	2.16	0.46
1:A:235:HIS:O	1:A:238:LYS:O	2.34	0.46
2:B:142:ILE:N	2:B:142:ILE:HD12	2.30	0.46
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.98	0.46
1:A:264:LEU:HD12	1:A:276:VAL:HG22	1.98	0.46
1:A:222:GLN:O	1:A:223:LYS:CB	2.63	0.46
1:A:242:GLN:CB	1:A:243:PRO:CD	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLN:O	1:A:395:LYS:C	2.53	0.46
2:B:388:LYS:HA	2:B:413:GLU:O	2.16	0.46
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.31	0.46
1:A:506:ILE:H	1:A:506:ILE:CD1	2.29	0.46
1:A:13:LYS:HG3	1:A:84:THR:CA	2.46	0.46
2:B:11:LYS:HZ1	2:B:124:PHE:HD2	1.64	0.46
1:A:460:ASN:HA	2:B:286:THR:HG21	1.98	0.46
2:B:369:THR:HG22	2:B:370:GLU:N	2.31	0.46
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.50	0.46
1:A:210:LEU:HA	1:A:213:GLY:O	2.16	0.46
1:A:421:PRO:O	1:A:423:VAL:N	2.49	0.46
1:A:312:GLU:C	1:A:314:VAL:H	2.19	0.46
1:A:29:GLU:C	1:A:71:TRP:HZ3	2.20	0.46
2:B:164:MET:SD	2:B:168:LEU:CD1	3.02	0.46
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.46
1:A:206:ARG:HB3	1:A:206:ARG:CZ	2.46	0.46
1:A:421:PRO:C	1:A:423:VAL:H	2.19	0.46
2:B:13:LYS:HB2	2:B:87:PHE:CG	2.51	0.46
2:B:153:TRP:CE3	2:B:155:GLY:HA3	2.50	0.46
1:A:460:ASN:HA	2:B:286:THR:CG2	2.45	0.46
2:B:293:ILE:HG22	2:B:295:LEU:HD12	1.97	0.46
1:A:180:ILE:HG21	1:A:189:VAL:HG22	1.97	0.45
1:A:326:ILE:N	1:A:343:GLN:HE22	2.14	0.45
1:A:329:ILE:CB	1:A:390:LYS:HB2	2.45	0.45
1:A:420:PRO:HA	1:A:421:PRO:HD2	1.46	0.45
2:B:191:SER:OG	2:B:198:HIS:CD2	2.67	0.45
2:B:252:TRP:CB	2:B:294:PRO:HB3	2.45	0.45
2:B:286:THR:CG2	2:B:287:LYS:N	2.79	0.45
2:B:401:TRP:CD1	2:B:401:TRP:N	2.83	0.45
2:B:66:LYS:N	2:B:407:GLN:NE2	2.64	0.45
2:B:43:LYS:C	2:B:45:GLY:N	2.70	0.45
2:B:91:GLN:O	2:B:92:LEU:CB	2.63	0.45
1:A:435:VAL:HG12	2:B:289:LEU:HB3	1.98	0.45
2:B:88:TRP:CD1	2:B:88:TRP:O	2.70	0.45
1:A:183:TYR:O	1:A:184:MET:O	2.33	0.45
1:A:285:GLY:O	1:A:287:LYS:N	2.50	0.45
1:A:101:LYS:HE3	1:A:322:SER:OG	2.17	0.45
1:A:41:MET:O	1:A:47:ILE:N	2.49	0.45
1:A:484:LEU:HD13	1:A:484:LEU:HA	1.63	0.45
1:A:538:ALA:O	1:A:539:HIS:HB3	2.16	0.45
2:B:11:LYS:NZ	2:B:12:LEU:CD2	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:THR:O	2:B:287:LYS:HB2	2.17	0.45
2:B:379:SER:O	2:B:383:TRP:N	2.50	0.45
1:A:374:LYS:O	1:A:378:GLU:HB2	2.15	0.45
1:A:406:TRP:CD1	1:A:406:TRP:C	2.90	0.45
1:A:412:PRO:HD3	2:B:401:TRP:HH2	1.82	0.45
1:A:442:VAL:CG2	1:A:495:ILE:HG23	2.46	0.45
1:A:438:GLU:OE2	1:A:461:LYS:HD3	2.17	0.45
2:B:116:PHE:CZ	2:B:151:GLN:CB	3.00	0.45
2:B:337:TRP:HH2	2:B:364:ASP:HB2	1.81	0.45
1:A:164:MET:SD	1:A:214:LEU:HD13	2.56	0.45
1:A:386:THR:HG21	1:A:412:PRO:HG2	1.97	0.45
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.99	0.45
1:A:443:ASP:HB2	1:A:548:VAL:CG1	2.47	0.45
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.45
1:A:200:THR:O	1:A:203:GLU:N	2.49	0.45
1:A:492:GLU:O	1:A:493:VAL:HG12	2.17	0.45
1:A:535:TRP:CG	1:A:536:VAL:N	2.85	0.45
1:A:548:VAL:O	1:A:549:ASP:C	2.53	0.45
1:A:100:LEU:HD21	3:A:557:NVP:C5	2.47	0.45
2:B:24:TRP:CZ3	2:B:25:PRO:O	2.70	0.45
1:A:170:PRO:C	1:A:174:GLN:HE21	2.20	0.45
1:A:430:GLU:O	1:A:532:TYR:HD1	2.00	0.45
2:B:150:PRO:HB2	2:B:153:TRP:CD1	2.52	0.45
2:B:22:LYS:O	2:B:23:GLN:CB	2.65	0.45
2:B:259:LYS:O	2:B:260:LEU:C	2.56	0.45
2:B:368:LEU:O	2:B:372:VAL:HG12	2.16	0.45
1:A:447:ASN:HD22	1:A:450:THR:H	1.65	0.44
1:A:33:ALA:HB1	1:A:71:TRP:HB3	1.99	0.44
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.99	0.44
1:A:341:ILE:O	1:A:349:LEU:HB2	2.16	0.44
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.85	0.44
2:B:23:GLN:HE22	2:B:26:LEU:HG	1.83	0.44
2:B:63:ILE:O	2:B:72:ARG:N	2.49	0.44
1:A:52:PRO:CA	1:A:143:ARG:HB2	2.48	0.44
1:A:160:PHE:C	1:A:162:SER:N	2.69	0.44
1:A:260:LEU:O	1:A:264:LEU:HG	2.17	0.44
1:A:492:GLU:HB3	1:A:493:VAL:H	1.51	0.44
1:A:505:ILE:HG22	1:A:506:ILE:HD13	1.98	0.44
1:A:80:LEU:HD22	1:A:153:TRP:NE1	2.32	0.44
1:A:13:LYS:HG3	1:A:84:THR:HA	1.99	0.44
2:B:21:VAL:HG12	2:B:22:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ILE:HB	2:B:295:LEU:H	1.82	0.44
1:A:125:ARG:CD	1:A:147:ASN:HA	2.44	0.44
1:A:318:TYR:O	1:A:319:TYR:HB2	2.17	0.44
1:A:432:GLU:HA	1:A:433:PRO:HD2	1.66	0.44
1:A:442:VAL:HG13	1:A:481:ALA:HB1	2.00	0.44
2:B:293:ILE:HG21	2:B:295:LEU:C	2.38	0.44
2:B:395:LYS:O	2:B:396:GLU:CB	2.62	0.44
1:A:163:SER:O	1:A:167:ILE:HG13	2.17	0.44
1:A:37:ILE:HG22	1:A:38:CYS:N	2.32	0.44
1:A:473:THR:CB	1:A:476:LYS:HE3	2.48	0.44
1:A:12:LEU:HD12	1:A:84:THR:HG23	2.00	0.44
2:B:217:PRO:O	2:B:219:LYS:O	2.36	0.44
2:B:254:VAL:HG13	2:B:255:ASN:N	2.32	0.44
1:A:160:PHE:O	1:A:162:SER:N	2.50	0.44
1:A:167:ILE:HD13	1:A:214:LEU:CD1	2.48	0.44
1:A:497:THR:O	1:A:536:VAL:HG12	2.18	0.44
1:A:289:LEU:O	1:A:291:GLU:N	2.51	0.44
1:A:321:PRO:O	1:A:322:SER:O	2.35	0.44
1:A:40:GLU:C	1:A:42:GLU:H	2.20	0.44
1:A:442:VAL:HG13	1:A:481:ALA:O	2.17	0.44
1:A:80:LEU:HD21	1:A:124:PHE:HZ	1.83	0.44
2:B:218:ASP:O	2:B:219:LYS:HB3	2.18	0.44
1:A:450:THR:HB	1:A:452:LEU:HG	1.99	0.44
2:B:286:THR:CG2	2:B:287:LYS:H	2.28	0.44
2:B:40:GLU:HG3	2:B:43:LYS:NZ	2.33	0.44
2:B:85:GLN:O	2:B:89:GLU:N	2.51	0.44
1:A:387:PRO:HG2	1:A:389:PHE:CE2	2.51	0.44
1:A:38:CYS:HA	1:A:41:MET:CG	2.48	0.44
1:A:60:VAL:HG21	1:A:131:THR:O	2.18	0.44
1:A:11:LYS:N	1:A:87:PHE:CE2	2.78	0.43
1:A:398:TRP:CH2	1:A:411:ILE:CG2	3.01	0.43
1:A:395:LYS:O	1:A:398:TRP:N	2.51	0.43
1:A:398:TRP:O	1:A:399:GLU:C	2.55	0.43
1:A:99:GLY:O	1:A:320:ASP:HB2	2.17	0.43
2:B:214:LEU:O	2:B:215:THR:C	2.56	0.43
2:B:220:LYS:HG2	2:B:220:LYS:H	1.54	0.43
2:B:51:GLY:HA2	2:B:52:PRO:HD3	1.66	0.43
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.40	0.43
2:B:85:GLN:O	2:B:86:ASP:C	2.53	0.43
1:A:47:ILE:HG23	1:A:148:VAL:HG21	1.99	0.43
1:A:548:VAL:HG13	1:A:549:ASP:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LEU:HD13	2:B:301:LEU:O	2.18	0.43
2:B:46:LYS:O	2:B:147:ASN:HB2	2.18	0.43
1:A:128:THR:O	1:A:145:GLN:HA	2.19	0.43
1:A:208:HIS:O	1:A:212:TRP:CD1	2.62	0.43
1:A:528:LYS:O	1:A:529:GLU:C	2.57	0.43
2:B:78:ARG:NH1	2:B:413:GLU:HA	2.33	0.43
1:A:203:GLU:HA	1:A:206:ARG:HH12	1.83	0.43
1:A:111:VAL:HG22	1:A:216:THR:HG23	2.00	0.43
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.86	0.43
1:A:357:MET:C	1:A:357:MET:SD	2.97	0.43
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.85	0.43
1:A:12:LEU:HA	1:A:84:THR:HG22	1.97	0.43
2:B:116:PHE:CZ	2:B:151:GLN:HB3	2.53	0.43
2:B:81:ASN:O	2:B:82:LYS:C	2.55	0.43
1:A:422:LEU:O	1:A:424:LYS:N	2.51	0.43
1:A:446:ALA:HA	1:A:452:LEU:O	2.19	0.43
1:A:77:PHE:CZ	1:A:150:PRO:CB	3.01	0.43
2:B:278:GLN:NE2	2:B:281:LYS:NZ	2.67	0.43
1:A:138:GLU:O	1:A:140:PRO:HD3	2.19	0.43
1:A:220:LYS:O	1:A:221:HIS:CB	2.66	0.43
1:A:275:LYS:HB3	1:A:275:LYS:HE3	1.64	0.43
1:A:340:GLN:HB2	1:A:348:ASN:ND2	2.33	0.43
1:A:329:ILE:HA	1:A:390:LYS:O	2.18	0.43
1:A:521:ILE:O	1:A:525:LEU:HG	2.19	0.43
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.19	0.43
2:B:149:LEU:HD21	2:B:159:ILE:CG2	2.48	0.43
2:B:263:LYS:O	2:B:267:ALA:N	2.49	0.43
1:A:503:LEU:HD12	1:A:504:GLY:H	1.80	0.43
1:A:5:ILE:CG2	1:A:6:GLU:H	2.31	0.43
1:A:138:GLU:O	1:A:140:PRO:CD	2.67	0.43
1:A:233:GLU:OE2	1:A:242:GLN:HG3	2.18	0.43
1:A:271:TYR:CD1	1:A:314:VAL:CB	3.01	0.43
1:A:328:GLU:O	1:A:389:PHE:HA	2.19	0.43
1:A:79:GLU:O	1:A:80:LEU:C	2.57	0.43
2:B:119:PRO:HG2	2:B:149:LEU:HD13	2.01	0.43
2:B:23:GLN:HE21	2:B:133:PRO:HG2	1.83	0.43
2:B:210:LEU:O	2:B:213:GLY:O	2.36	0.43
1:A:200:THR:HA	1:A:203:GLU:HG3	2.01	0.42
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.62	0.42
1:A:260:LEU:HD22	1:A:264:LEU:HG	2.00	0.42
1:A:353:LYS:HB2	1:A:353:LYS:HE3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD13	1:A:529:GLU:OE2	2.19	0.42
1:A:539:HIS:HA	1:A:545:ASN:OD1	2.19	0.42
2:B:207:GLN:O	2:B:211:ARG:HG3	2.20	0.42
2:B:28:GLU:O	2:B:29:GLU:C	2.57	0.42
1:A:525:LEU:O	1:A:527:LYS:N	2.52	0.42
2:B:206:ARG:CG	2:B:217:PRO:HG2	2.30	0.42
1:A:117:SER:OG	1:A:118:VAL:N	2.51	0.42
1:A:434:ILE:HG21	1:A:492:GLU:HG3	2.02	0.42
2:B:125:ARG:HD2	2:B:125:ARG:H	1.84	0.42
2:B:160:PHE:CD2	2:B:160:PHE:O	2.72	0.42
1:A:171:PHE:O	1:A:174:GLN:N	2.52	0.42
1:A:286:THR:O	1:A:288:ALA:N	2.52	0.42
1:A:362:THR:HG22	1:A:366:LYS:CB	2.48	0.42
1:A:424:LYS:C	1:A:426:TRP:N	2.72	0.42
2:B:101:LYS:O	2:B:104:LYS:HG2	2.20	0.42
2:B:122:GLU:O	2:B:123:ASP:CB	2.67	0.42
2:B:143:ARG:NH1	2:B:143:ARG:HB3	2.24	0.42
2:B:427:TYR:CD2	2:B:428:GLN:HG3	2.55	0.42
2:B:13:LYS:HA	2:B:87:PHE:CD2	2.55	0.42
2:B:13:LYS:HA	2:B:87:PHE:CE2	2.54	0.42
1:A:103:LYS:HA	1:A:192:ASP:OD1	2.18	0.42
1:A:258:GLN:HE21	1:A:283:LEU:HD11	1.84	0.42
1:A:521:ILE:O	1:A:521:ILE:HG22	2.20	0.42
2:B:208:HIS:HD2	2:B:211:ARG:NH2	2.17	0.42
2:B:46:LYS:HB3	2:B:148:VAL:CG1	2.48	0.42
1:A:270:ILE:HD12	1:A:315:HIS:HA	2.02	0.42
1:A:239:TRP:CZ3	1:A:317:VAL:CB	3.00	0.42
1:A:320:ASP:HA	1:A:321:PRO:HD3	1.84	0.42
2:B:50:ILE:HA	2:B:144:TYR:HA	2.02	0.42
2:B:192:ASP:O	2:B:194:GLU:HG2	2.20	0.42
2:B:268:SER:HA	2:B:271:TYR:HD2	1.84	0.42
2:B:286:THR:O	2:B:287:LYS:CB	2.67	0.42
1:A:132:ILE:HB	1:A:142:ILE:CB	2.49	0.42
1:A:294:PRO:C	1:A:295:LEU:O	2.57	0.42
1:A:389:PHE:HB2	1:A:414:TRP:HA	2.01	0.42
2:B:299:ALA:O	2:B:300:GLU:C	2.57	0.42
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.42
2:B:3:SER:HB3	2:B:4:PRO:HA	2.02	0.42
2:B:92:LEU:HD23	2:B:92:LEU:HA	1.97	0.42
1:A:16:MET:HG2	1:A:16:MET:H	1.57	0.42
1:A:322:SER:O	1:A:323:LYS:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:O	1:A:378:GLU:CB	2.68	0.42
1:A:506:ILE:O	1:A:509:GLN:N	2.49	0.42
2:B:116:PHE:CZ	2:B:151:GLN:HB2	2.55	0.42
2:B:205:LEU:HD12	2:B:205:LEU:O	2.19	0.42
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.34	0.42
2:B:397:THR:O	2:B:401:TRP:CD1	2.73	0.42
2:B:65:LYS:HG3	2:B:72:ARG:HD2	2.01	0.42
1:A:80:LEU:CD2	1:A:153:TRP:HE1	2.33	0.42
1:A:460:ASN:HB3	2:B:286:THR:HG22	2.02	0.42
1:A:527:LYS:HG3	1:A:527:LYS:O	2.20	0.42
2:B:172:LYS:O	2:B:176:PRO:HA	2.20	0.42
2:B:194:GLU:O	2:B:196:GLY:N	2.52	0.42
2:B:366:LYS:HZ3	2:B:369:THR:HG21	1.84	0.42
2:B:5:ILE:O	2:B:6:GLU:CG	2.63	0.42
1:A:171:PHE:HA	1:A:174:GLN:NE2	2.35	0.41
1:A:213:GLY:O	1:A:214:LEU:C	2.58	0.41
1:A:241:VAL:CG1	1:A:266:TRP:CD1	3.03	0.41
1:A:255:ASN:O	1:A:259:LYS:HG3	2.20	0.41
2:B:366:LYS:HA	2:B:366:LYS:HZ3	1.84	0.41
2:B:369:THR:CG2	2:B:370:GLU:N	2.83	0.41
1:A:296:THR:CG2	1:A:299:ALA:H	2.32	0.41
2:B:13:LYS:HE3	2:B:14:PRO:O	2.20	0.41
1:A:114:ALA:C	1:A:116:PHE:N	2.74	0.41
1:A:214:LEU:HD23	1:A:214:LEU:H	1.85	0.41
1:A:276:VAL:O	1:A:276:VAL:HG12	2.19	0.41
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.50	0.41
1:A:461:LYS:C	1:A:463:ARG:H	2.23	0.41
2:B:411:ILE:HA	2:B:412:PRO:HD2	1.92	0.41
1:A:385:LYS:HB3	1:A:385:LYS:HE3	1.80	0.41
1:A:106:VAL:HG12	1:A:190:GLY:HA3	2.02	0.41
1:A:350:LYS:HD3	1:A:351:THR:N	2.34	0.41
1:A:463:ARG:O	1:A:464:GLN:NE2	2.54	0.41
1:A:96:HIS:HD2	1:A:97:PRO:CD	2.25	0.41
2:B:206:ARG:HH21	2:B:218:ASP:HA	1.85	0.41
2:B:282:LEU:CG	2:B:292:VAL:HG11	2.48	0.41
2:B:301:LEU:O	2:B:302:GLU:HB2	2.20	0.41
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.86	0.41
1:A:276:VAL:O	1:A:277:ARG:C	2.58	0.41
1:A:38:CYS:HA	1:A:41:MET:HG2	2.03	0.41
1:A:12:LEU:HD12	1:A:84:THR:CG2	2.51	0.41
2:B:284:ARG:HD2	2:B:284:ARG:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
2:B:10:VAL:HG13	2:B:88:TRP:CE2	2.56	0.41
1:A:398:TRP:CE3	1:A:402:TRP:HD1	2.38	0.41
2:B:263:LYS:HA	2:B:263:LYS:HD3	1.72	0.41
2:B:49:LYS:O	2:B:145:GLN:N	2.53	0.41
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.01	0.41
1:A:398:TRP:CZ3	1:A:411:ILE:HG21	2.55	0.41
1:A:465:LYS:CG	1:A:466:VAL:N	2.84	0.41
1:A:492:GLU:O	1:A:493:VAL:CB	2.69	0.41
2:B:257:ILE:HG23	2:B:261:VAL:CG2	2.50	0.41
2:B:390:LYS:HB3	2:B:417:VAL:CG1	2.51	0.41
2:B:58:THR:HA	2:B:59:PRO:HD3	1.93	0.41
1:A:239:TRP:CG	1:A:240:THR:N	2.88	0.41
1:A:395:LYS:O	1:A:397:THR:N	2.54	0.41
1:A:451:LYS:O	1:A:470:THR:HA	2.21	0.41
1:A:5:ILE:CG2	1:A:6:GLU:N	2.83	0.41
1:A:79:GLU:HG3	1:A:83:ARG:HE	1.86	0.41
2:B:278:GLN:NE2	2:B:281:LYS:HZ2	2.18	0.41
2:B:418:ASN:OD1	2:B:418:ASN:N	2.54	0.41
2:B:425:LEU:HG	2:B:428:GLN:OXT	2.21	0.41
1:A:171:PHE:O	1:A:175:ASN:OD1	2.39	0.41
1:A:343:GLN:HB2	1:A:349:LEU:HD12	2.02	0.41
1:A:393:ILE:HG23	1:A:394:GLN:N	2.35	0.41
2:B:42:GLU:OE1	2:B:144:TYR:HE1	2.04	0.41
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.56	0.41
1:A:445:ALA:N	1:A:477:THR:OG1	2.54	0.41
1:A:548:VAL:CG1	1:A:549:ASP:N	2.84	0.41
2:B:293:ILE:CG2	2:B:295:LEU:N	2.84	0.41
2:B:395:LYS:HG3	2:B:416:PHE:CD2	2.56	0.41
1:A:206:ARG:NH1	1:A:206:ARG:HB3	2.36	0.40
1:A:64:LYS:CB	1:A:72:ARG:HD3	2.51	0.40
2:B:40:GLU:O	2:B:44:GLU:N	2.52	0.40
2:B:65:LYS:O	2:B:66:LYS:HB2	2.21	0.40
1:A:26:LEU:HB2	1:A:30:LYS:HB2	2.02	0.40
1:A:269:GLN:O	1:A:351:THR:HB	2.20	0.40
1:A:381:VAL:HG22	2:B:25:PRO:CB	2.52	0.40
1:A:63:ILE:O	1:A:71:TRP:CD1	2.74	0.40
1:A:80:LEU:O	1:A:81:ASN:C	2.60	0.40
2:B:13:LYS:HG2	2:B:14:PRO:CD	2.51	0.40
2:B:332:GLN:HA	2:B:337:TRP:CE2	2.56	0.40
1:A:247:PRO:O	1:A:247:PRO:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CD1	1:A:406:TRP:O	2.74	0.40
1:A:453:GLY:N	1:A:469:LEU:O	2.49	0.40
2:B:417:VAL:CG1	2:B:417:VAL:O	2.69	0.40
1:A:265:ASN:O	1:A:266:TRP:C	2.60	0.40
1:A:300:GLU:O	1:A:304:ALA:CB	2.68	0.40
1:A:365:VAL:HG22	1:A:393:ILE:HD11	2.03	0.40
2:B:156:SER:O	2:B:159:ILE:N	2.54	0.40
2:B:183:TYR:CD1	2:B:183:TYR:C	2.93	0.40
2:B:368:LEU:CD2	2:B:393:ILE:HD12	2.49	0.40
1:A:122:GLU:C	1:A:124:PHE:H	2.25	0.40
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.45	0.40
1:A:112:GLY:N	1:A:217:PRO:HD3	2.36	0.40
1:A:94:ILE:HD11	1:A:230:MET:HG2	2.03	0.40
2:B:166:LYS:HD2	2:B:166:LYS:HA	1.83	0.40
2:B:304:ALA:CA	2:B:307:ARG:HB3	2.45	0.40

All (4) 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:A:37:ILE:CG1	1:A:449:GLU:OE2[4_647]	1.87	0.33
1:A:37:ILE:CD1	1:A:449:GLU:OE2[4_647]	1.99	0.21
1:A:4:PRO:CB	2:B:211:ARG:NH2[4_646]	2.08	0.12
1:A:70:LYS:NZ	1:A:449:GLU:OE2[4_647]	2.09	0.11

## 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	553/556 (100%)	338 (61%)	125 (23%)	90 (16%)	<b>0</b> <b>0</b>
2	B	392/428 (92%)	264 (67%)	62 (16%)	66 (17%)	<b>0</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	945/984 (96%)	602 (64%)	187 (20%)	156 (16%)	<b>0</b> <b>0</b>

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	25	PRO
1	A	54	ASN
1	A	66	LYS
1	A	121	ASP
1	A	125	ARG
1	A	145	GLN
1	A	185	ASP
1	A	221	HIS
1	A	226	PRO
1	A	242	GLN
1	A	248	GLU
1	A	251	SER
1	A	276	VAL
1	A	286	THR
1	A	288	ALA
1	A	290	THR
1	A	311	LYS
1	A	321	PRO
1	A	322	SER
1	A	325	LEU
1	A	345	PRO
1	A	346	PHE
1	A	354	TYR
1	A	363	ASN
1	A	395	LYS
1	A	396	GLU
1	A	419	THR
1	A	421	PRO
1	A	424	LYS
1	A	457	TYR
1	A	471	ASN
1	A	492	GLU
1	A	538	ALA
2	B	4	PRO
2	B	6	GLU
2	B	21	VAL

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Mol	Chain	Res	Type
2	B	46	LYS
2	B	52	PRO
2	B	68	SER
2	B	104	LYS
2	B	117	SER
2	B	141	GLY
2	B	193	LEU
2	B	195	ILE
2	B	198	HIS
2	B	281	LYS
2	B	287	LYS
2	B	293	ILE
2	B	295	LEU
2	B	302	GLU
2	B	312	GLU
2	B	315	HIS
2	B	321	PRO
2	B	323	LYS
2	B	334	GLN
2	B	345	PRO
2	B	346	PHE
2	B	420	PRO
2	B	425	LEU
2	B	426	TRP
1	A	30	LYS
1	A	71	TRP
1	A	75	VAL
1	A	115	TYR
1	A	172	LYS
1	A	184	MET
1	A	195	ILE
1	A	210	LEU
1	A	214	LEU
1	A	223	LYS
1	A	247	PRO
1	A	283	LEU
1	A	285	GLY
1	A	295	LEU
1	A	310	LEU
1	A	316	GLY
1	A	323	LYS
1	A	462	GLY

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	512	LYS
1	A	516	GLU
1	A	540	LYS
2	B	23	GLN
2	B	47	ILE
2	B	66	LYS
2	B	92	LEU
2	B	116	PHE
2	B	177	ASP
2	B	212	TRP
2	B	218	ASP
2	B	280	CYS
2	B	317	VAL
2	B	322	SER
2	B	396	GLU
1	A	43	LYS
1	A	57	ASN
1	A	63	ILE
1	A	77	PHE
1	A	122	GLU
1	A	134	SER
1	A	215	THR
1	A	246	LEU
1	A	281	LYS
1	A	304	ALA
1	A	423	VAL
1	A	510	PRO
1	A	529	GLU
1	A	539	HIS
1	A	553	SER
2	B	45	GLY
2	B	91	GLN
2	B	105	SER
2	B	119	PRO
2	B	133	PRO
2	B	200	THR
2	B	251	SER
2	B	350	LYS
2	B	403	THR
1	A	27	THR
1	A	55	PRO

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Mol	Chain	Res	Type
1	A	87	PHE
1	A	186	ASP
1	A	287	LYS
1	A	312	GLU
1	A	433	PRO
1	A	464	GLN
2	B	184	MET
2	B	211	ARG
1	A	64	LYS
1	A	113	ASP
1	A	227	PHE
1	A	250	ASP
1	A	530	LYS
2	B	355	ALA
2	B	408	ALA
2	B	427	TYR
1	A	31	ILE
1	A	225	PRO
1	A	292	VAL
2	B	219	LYS
2	B	268	SER
2	B	276	VAL
2	B	423	VAL
1	A	333	GLY
1	A	526	ILE
2	B	25	PRO
2	B	271	TYR
2	B	9	PRO
2	B	261	VAL
2	B	273	GLY
2	B	152	GLY
2	B	421	PRO
2	B	262	GLY
1	A	314	VAL
2	B	294	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	422/496 (85%)	332 (79%)	90 (21%)	1	3
2	B	328/390 (84%)	248 (76%)	80 (24%)	0	2
All	All	750/886 (85%)	580 (77%)	170 (23%)	1	2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	7	THR
1	A	12	LEU
1	A	23	GLN
1	A	24	TRP
1	A	25	PRO
1	A	28	GLU
1	A	29	GLU
1	A	34	LEU
1	A	38	CYS
1	A	42	GLU
1	A	54	ASN
1	A	58	THR
1	A	60	VAL
1	A	71	TRP
1	A	74	LEU
1	A	77	PHE
1	A	79	GLU
1	A	80	LEU
1	A	84	THR
1	A	85	GLN
1	A	87	PHE
1	A	88	TRP
1	A	91	GLN
1	A	97	PRO
1	A	121	ASP
1	A	122	GLU
1	A	131	THR
1	A	143	ARG
1	A	166	LYS
1	A	168	LEU
1	A	173	LYS
1	A	178	ILE
1	A	180	ILE

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Mol	Chain	Res	Type
1	A	205	LEU
1	A	209	LEU
1	A	210	LEU
1	A	215	THR
1	A	216	THR
1	A	227	PHE
1	A	229	TRP
1	A	230	MET
1	A	234	LEU
1	A	238	LYS
1	A	239	TRP
1	A	244	ILE
1	A	245	VAL
1	A	260	LEU
1	A	269	GLN
1	A	270	ILE
1	A	275	LYS
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	295	LEU
1	A	296	THR
1	A	318	TYR
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	349	LEU
1	A	357	MET
1	A	363	ASN
1	A	385	LYS
1	A	386	THR
1	A	387	PRO
1	A	393	ILE
1	A	394	GLN
1	A	396	GLU
1	A	397	THR
1	A	398	TRP
1	A	406	TRP
1	A	416	PHE
1	A	419	THR
1	A	430	GLU
1	A	439	THR

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Mol	Chain	Res	Type
1	A	457	TYR
1	A	459	THR
1	A	463	ARG
1	A	464	GLN
1	A	471	ASN
1	A	484	LEU
1	A	492	GLU
1	A	493	VAL
1	A	501	TYR
1	A	506	ILE
1	A	523	GLU
1	A	524	GLN
1	A	536	VAL
1	A	546	GLU
2	B	2	ILE
2	B	5	ILE
2	B	12	LEU
2	B	16	MET
2	B	22	LYS
2	B	23	GLN
2	B	25	PRO
2	B	28	GLU
2	B	31	ILE
2	B	40	GLU
2	B	44	GLU
2	B	53	GLU
2	B	54	ASN
2	B	55	PRO
2	B	66	LYS
2	B	69	THR
2	B	70	LYS
2	B	82	LYS
2	B	86	ASP
2	B	91	GLN
2	B	108	VAL
2	B	119	PRO
2	B	120	LEU
2	B	121	ASP
2	B	125	ARG
2	B	128	THR
2	B	143	ARG
2	B	146	TYR

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Mol	Chain	Res	Type
2	B	147	ASN
2	B	153	TRP
2	B	159	ILE
2	B	165	THR
2	B	168	LEU
2	B	173	LYS
2	B	177	ASP
2	B	178	ILE
2	B	185	ASP
2	B	189	VAL
2	B	192	ASP
2	B	193	LEU
2	B	195	ILE
2	B	206	ARG
2	B	212	TRP
2	B	215	THR
2	B	216	THR
2	B	218	ASP
2	B	219	LYS
2	B	220	LYS
2	B	222	GLN
2	B	223	LYS
2	B	252	TRP
2	B	253	THR
2	B	255	ASN
2	B	265	ASN
2	B	278	GLN
2	B	279	LEU
2	B	280	CYS
2	B	284	ARG
2	B	289	LEU
2	B	291	GLU
2	B	293	ILE
2	B	295	LEU
2	B	301	LEU
2	B	303	LEU
2	B	337	TRP
2	B	354	TYR
2	B	366	LYS
2	B	367	GLN
2	B	369	THR
2	B	376	THR

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Mol	Chain	Res	Type
2	B	377	THR
2	B	401	TRP
2	B	414	TRP
2	B	418	ASN
2	B	420	PRO
2	B	423	VAL
2	B	424	LYS
2	B	425	LEU
2	B	427	TYR
2	B	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	96	HIS
1	A	174	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	258	GLN
1	A	340	GLN
1	A	343	GLN
1	A	363	ASN
1	A	373	GLN
1	A	428	GLN
1	A	447	ASN
1	A	487	GLN
1	A	524	GLN
2	B	54	ASN
2	B	57	ASN
2	B	147	ASN
2	B	198	HIS
2	B	222	GLN
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	373	GLN
2	B	407	GLN
2	B	428	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](#)

1 ligand 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$
3	NVP	A	557	-	15,23,23	1.23	1 (6%)	13,34,34	1.08	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NVP	A	557	-	-	0/0/6/6	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	NVP	OE-C9	-3.62	1.15	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	557	NVP	CD-C6-C7	2.69	122.64	120.03

There are no chirality outliers.

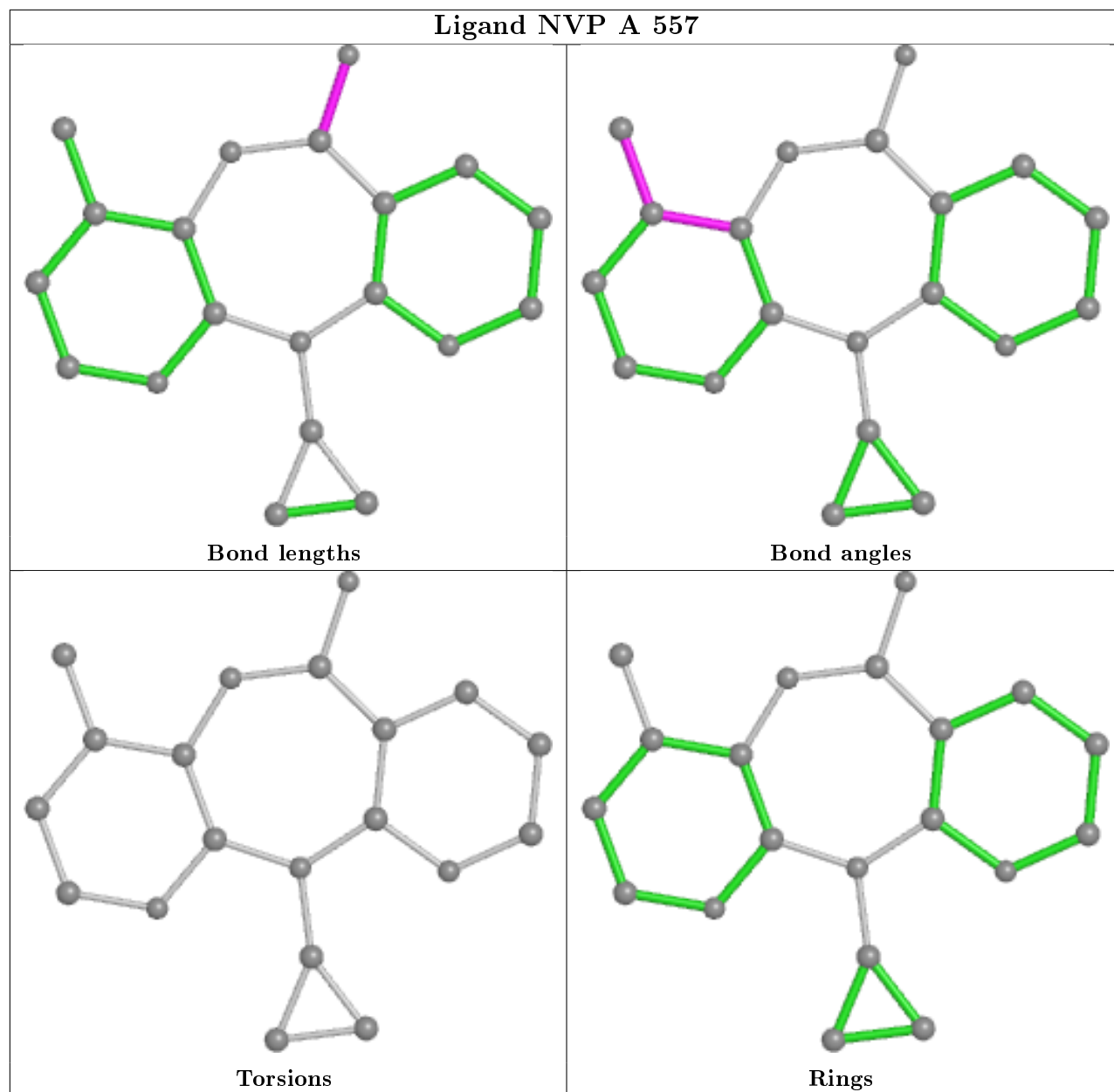
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	NVP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.