



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:42 AM GMT

PDB ID : 2IC3  
Title : Crystal Structure of K103N/Y181C Mutant HIV-1 Reverse Transcriptase (RT)  
in Complex with Nonnucleoside Inhibitor HBY 097  
Authors : Das, K.; Arnold, E.  
Deposited on : 2006-09-12  
Resolution : 3.00 Å(reported)

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

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

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

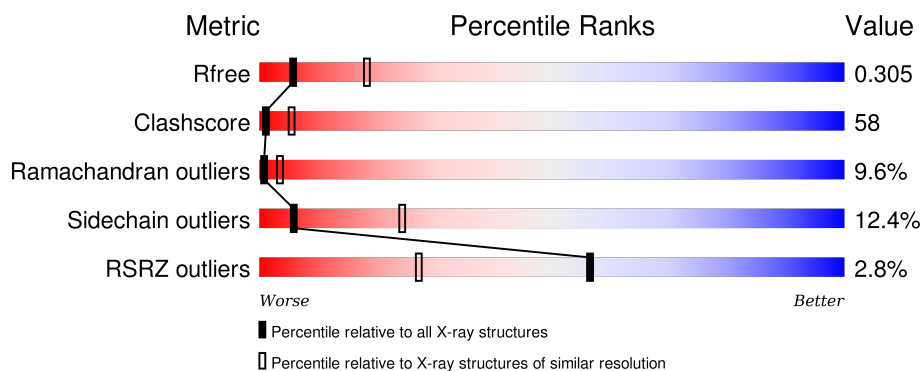
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	447	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8002 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 Reverse transcriptase/ribonuclease H (p66 RT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	4	0	0
			4501	2912	749	832	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	ENGINEERED	UNP P03366
A	181	CYS	TYR	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase/ribonuclease H (p51 RT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	12	0	0
			3476	2258	575	636	7			

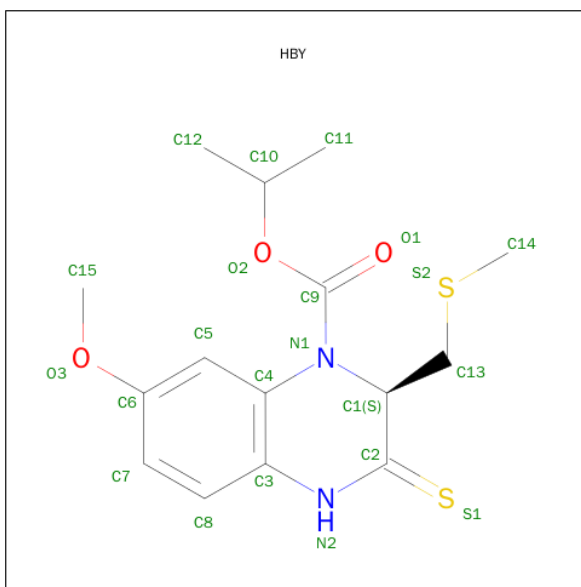
There are 3 discrepancies between the modelled and reference sequences:

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B	103	ASN	LYS	ENGINEERED	UNP P03366
B	181	CYS	TYR	ENGINEERED	UNP P03366
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is (S)-4-ISOPROPOXYCARBONYL-6-METHOXY-3-METHYLTHIOMETHYL-3,4-DIHYDROQUINOXALIN-2(1H)-THIONE (three-letter code: HBY) (formula: C<sub>15</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			22	15	2	3	2		

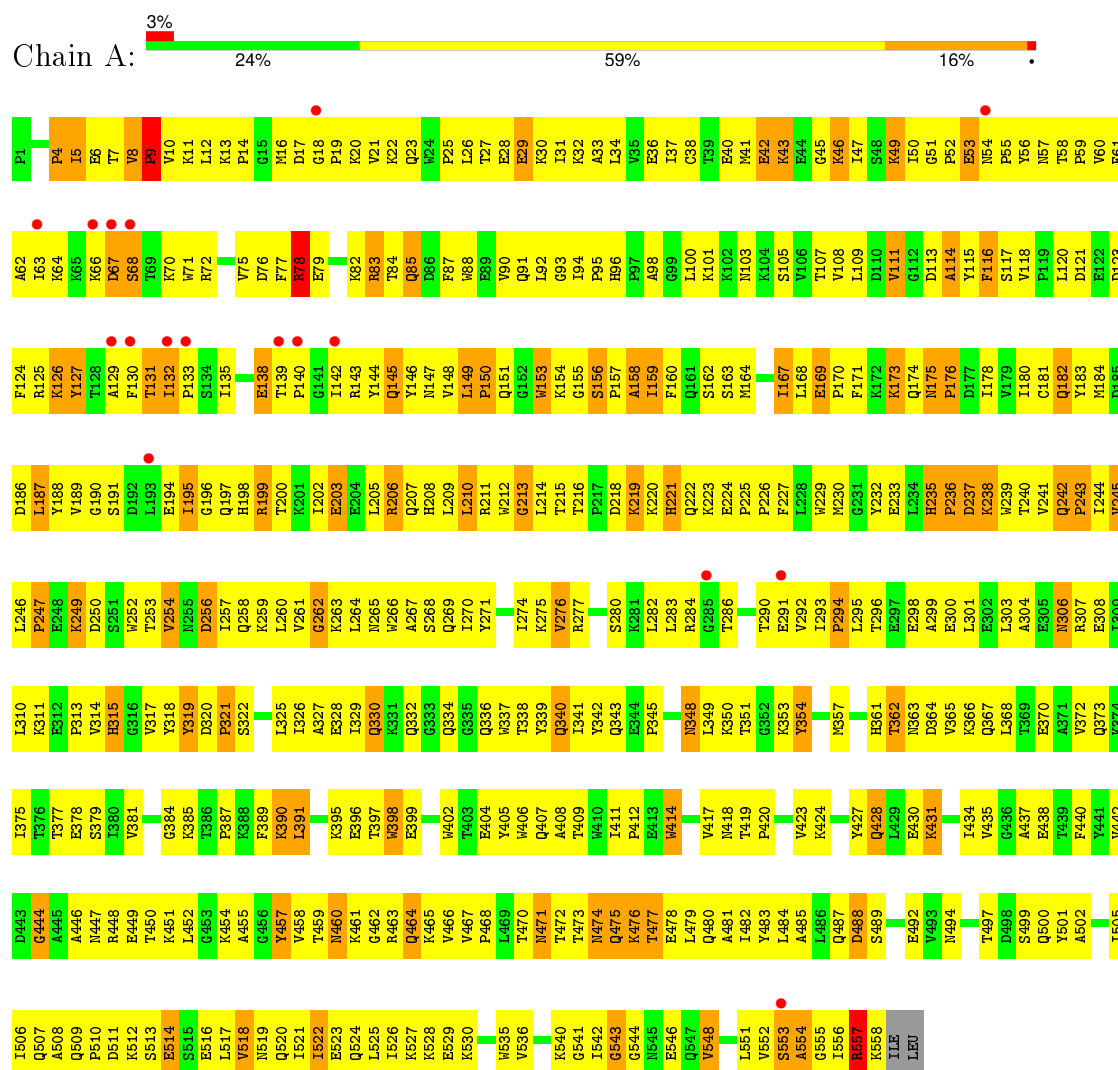
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Reverse transcriptase/ribonuclease H (p66 RT)



E404	Y405	T409	W410	I411	P412	F416	V417	N418	T419	P420	P421	L422	V423	K424	L425	W426	Y427	GLN	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE	TYR	THR	ASP	GLY	ALA	ALA	ASN																						
Q332	G333	Q334	G335	Q336	V337	T338	Y339	Q340	T341	Y342	Q343	E344	F345	K346	K347	N348	L349	K350	K353	Y354	A355	R356	K357	R358	G359	N363	D364	V365	K366	T369	E370	Q373	K374	I375	T376	T377	E378	S379	I380	V381	G384	K385	T386	I388	Q389	K394	K395	W398	E399	T400	W401	W402	T403						
Q141	I142	R143	Y144	Q145	R146	N147	Y148	L149	P150	Q151	G152	W153	K154	G155	S156	P157	A158	E159	F160	Q161	S162	S163	L164	T165	K166	I167	L168	E169	P170	K173	Q174	M175	P176	D177	I178	Y179	I180	C181	Q182	Y183	M184	D185	D186	L187	S191	D192	L193	E194	I195	Q196	Q197	H198	R199	T200	K201	I202	L203	E203	
E204	L205	Q206	Q207	E208	L209	L210	L214	T215	T216	P217	D218	K219	R220	Q221	Q222	K223	E224	P225	P226	F227	S228	L229	W229	W230	G231	Y232	E233	L234	E235	P236	D237	K238	W239	T240	V241	Q242	P243	I244	V245	L246	P247	E248	K249	D250	S251	W252	T253	V254	N255	D256	I257	Q258	K259	L260	V261	G262	K263	L264	N265
W266	Q269	I270	Y271	T274	K275	W276	R277	Q278	L279	S280	K281	L282	L283	R284	G285	T286	K287	A288	L289	T290	E291	W292	T293	P294	L295	T296	E297	E300	L301	E302	L303	A304	E305	N306	R307	E308	I309	L310	K311	E312	P313	V314	H315	G316	V317	V318	V319	D320	P321	L325	L326	T329	Q330	L331					

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.21Å 67.61Å 103.58Å 90.00° 108.39° 90.00°	Depositor
Resolution (Å)	19.90 – 3.00 32.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	86.9 (19.90-3.00) 85.2 (32.20-2.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.257 , 0.310 0.258 , 0.305	Depositor DCC
$R_{free}$ test set	1274 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 89.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27966 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.55	0/4618	0.85	3/6279 (0.0%)
2	B	0.66	0/3576	0.95	12/4867 (0.2%)
All	All	0.60	0/8194	0.89	15/11146 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
All	All	0	5

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	359	GLY	N-CA-C	-7.50	94.35	113.10
2	B	249	LYS	N-CA-C	6.98	129.85	111.00
2	B	226	PRO	N-CA-C	6.90	130.03	112.10
2	B	228	LEU	N-CA-C	5.98	127.15	111.00
2	B	426	TRP	N-CA-C	5.63	126.20	111.00
2	B	225	PRO	C-N-CD	-5.46	108.58	120.60
1	A	428	GLN	N-CA-C	-5.45	96.30	111.00
2	B	425	LEU	CA-CB-CG	-5.44	102.79	115.30
2	B	141	GLY	N-CA-C	-5.35	99.72	113.10
2	B	325	LEU	CA-CB-CG	5.34	127.58	115.30
2	B	252	TRP	CA-CB-CG	5.29	123.76	113.70
1	A	390	LYS	N-CA-C	-5.18	97.02	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	TRP	CB-CA-C	-5.13	100.14	110.40
1	A	412	PRO	N-CA-C	-5.12	98.79	112.10
2	B	363	ASN	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	TYR	Sidechain
1	A	339	TYR	Sidechain
1	A	354	TYR	Sidechain
2	B	318	TYR	Sidechain
2	B	339	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4501	0	4533	610	0
2	B	3476	0	3477	338	3
3	A	1	0	0	0	0
4	A	22	0	20	5	0
5	A	2	0	0	0	0
All	All	8002	0	8030	935	3

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 58.

All (935) 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:13:LYS:HB3	2:B:14:PRO:HD2	1.23	1.09
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.13	1.08
2:B:174:GLN:O	2:B:176:PRO:HD3	1.53	1.07
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HG22	1:A:451:LYS:H	1.19	1.06
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.34	1.06
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.38	1.05
1:A:452:LEU:HD22	1:A:470:THR:HA	1.38	1.05
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.36	1.03
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.41	1.02
1:A:206:ARG:HH12	1:A:219:LYS:HG2	1.25	1.01
1:A:111:VAL:HG21	1:A:187:LEU:HD13	1.43	1.00
1:A:472:THR:HG21	1:A:477:THR:HG23	1.42	1.00
1:A:540:LYS:HB3	1:A:542:ILE:HD11	1.41	0.98
1:A:460:ASN:HD22	1:A:461:LYS:N	1.60	0.98
1:A:418:ASN:O	1:A:420:PRO:HD3	1.65	0.96
1:A:460:ASN:HD22	1:A:461:LYS:H	1.03	0.96
1:A:197:GLN:O	1:A:200:THR:HB	1.66	0.95
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.48	0.95
1:A:257:ILE:HD11	1:A:282:LEU:HD13	1.48	0.94
2:B:57:ASN:HB2	2:B:143:ARG:HH12	1.31	0.94
1:A:249:LYS:HE3	1:A:250:ASP:H	1.33	0.94
1:A:451:LYS:O	1:A:471:ASN:HA	1.65	0.93
2:B:182:GLN:HB2	2:B:187:LEU:HD23	1.48	0.93
2:B:314:VAL:HG12	2:B:315:HIS:H	1.33	0.92
1:A:241:VAL:HG11	1:A:266:TRP:HE1	1.31	0.92
2:B:332:GLN:NE2	2:B:424:LYS:O	2.03	0.92
2:B:249:LYS:HB2	2:B:252:TRP:NE1	1.83	0.92
2:B:164:MET:HE3	2:B:187:LEU:HD21	1.51	0.92
1:A:327:ALA:HB2	1:A:341:ILE:HG13	1.52	0.91
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.06	0.91
1:A:125:ARG:HE	1:A:147:ASN:HA	1.36	0.90
1:A:100:LEU:HD11	4:A:562:HBY:H121	1.55	0.89
1:A:58:THR:HG22	1:A:76:ASP:O	1.71	0.89
1:A:84:THR:OG1	1:A:154:LYS:HD2	1.73	0.88
2:B:2:ILE:HG13	2:B:162:SER:OG	1.73	0.88
1:A:510:PRO:HG2	1:A:522:ILE:HD11	1.56	0.88
1:A:58:THR:HG21	1:A:77:PHE:HA	1.54	0.88
2:B:395:LYS:HE2	2:B:395:LYS:H	1.36	0.87
1:A:120:LEU:HD21	1:A:149:LEU:HD23	1.55	0.87
1:A:10:VAL:HG12	1:A:11:LYS:N	1.90	0.87
2:B:13:LYS:HB3	2:B:14:PRO:CD	2.05	0.87
2:B:107:THR:HG23	2:B:232:TYR:CE1	2.09	0.86
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.74	0.86
1:A:148:VAL:O	1:A:150:PRO:HD3	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:O	1:A:203:GLU:HB2	1.75	0.85
1:A:198:HIS:CD2	1:A:202:ILE:HD11	2.11	0.85
1:A:317:VAL:HG12	1:A:318:TYR:H	1.42	0.85
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.58	0.85
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.59	0.85
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.56	0.84
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.57	0.84
1:A:257:ILE:HD11	1:A:282:LEU:CD1	2.07	0.84
2:B:115:TYR:HE1	2:B:185:ASP:OD1	1.59	0.84
2:B:395:LYS:CE	2:B:395:LYS:H	1.91	0.83
1:A:7:THR:O	1:A:9:PRO:HD3	1.77	0.83
1:A:483:TYR:O	1:A:487:GLN:HG3	1.79	0.83
1:A:12:LEU:HB3	1:A:83:ARG:O	1.77	0.83
2:B:314:VAL:HG12	2:B:315:HIS:N	1.93	0.83
1:A:434:ILE:HB	1:A:494:ASN:ND2	1.94	0.82
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.10	0.81
1:A:84:THR:HG21	1:A:153:TRP:NE1	1.93	0.81
1:A:275:LYS:HB3	1:A:336:GLN:OE1	1.78	0.81
2:B:88:TRP:C	2:B:90:VAL:H	1.80	0.81
2:B:106:VAL:HG21	2:B:236:PRO:HG2	1.63	0.81
1:A:472:THR:HG22	1:A:473:THR:N	1.96	0.80
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.63	0.80
1:A:125:ARG:NE	1:A:147:ASN:HA	1.96	0.80
1:A:361:HIS:CE1	1:A:513:SER:HG	1.99	0.80
2:B:354:TYR:HD2	2:B:374:LYS:HD3	1.47	0.80
1:A:90:VAL:HG11	1:A:184:MET:HE1	1.63	0.80
1:A:4:PRO:HG2	1:A:5:ILE:H	1.47	0.80
1:A:96:HIS:HD2	1:A:98:ALA:H	1.29	0.79
1:A:368:LEU:O	1:A:372:VAL:HG23	1.81	0.79
1:A:440:PHE:HZ	1:A:463:ARG:NH2	1.81	0.78
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.65	0.78
1:A:175:ASN:HD22	1:A:175:ASN:N	1.81	0.78
1:A:551:LEU:O	1:A:551:LEU:HG	1.83	0.78
1:A:482:ILE:HD11	1:A:497:THR:HG21	1.64	0.78
2:B:356:ARG:HG2	2:B:357:MET:H	1.48	0.78
2:B:106:VAL:CG2	2:B:236:PRO:HG2	2.13	0.78
2:B:49:LYS:HD3	2:B:144:TYR:CE1	2.19	0.78
2:B:65:LYS:HD2	2:B:72:ARG:HG3	1.66	0.77
1:A:292:VAL:HG22	1:A:294:PRO:HD3	1.66	0.77
1:A:276:VAL:O	1:A:276:VAL:HG12	1.85	0.77
1:A:120:LEU:CD2	1:A:149:LEU:HD23	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:C	2:B:89:GLU:H	1.88	0.77
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.46	0.77
1:A:205:LEU:O	1:A:209:LEU:HD12	1.84	0.77
1:A:28:GLU:OE1	1:A:135:ILE:HG12	1.85	0.76
1:A:241:VAL:HG22	1:A:243:PRO:HD2	1.65	0.76
1:A:450:THR:HG22	1:A:451:LYS:N	1.98	0.76
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.16	0.75
1:A:434:ILE:CB	1:A:494:ASN:HD21	1.98	0.75
2:B:50:ILE:HD12	2:B:143:ARG:HH21	1.51	0.75
2:B:281:LYS:HA	2:B:284:ARG:HD3	1.69	0.75
1:A:362:THR:CG2	1:A:363:ASN:N	2.49	0.75
1:A:458:VAL:HG12	1:A:464:GLN:CG	2.17	0.75
1:A:75:VAL:HG12	1:A:76:ASP:H	1.50	0.75
1:A:446:ALA:O	1:A:474:ASN:ND2	2.20	0.75
1:A:36:GLU:O	1:A:40:GLU:HG2	1.86	0.75
1:A:88:TRP:NE1	2:B:143:ARG:HD3	2.01	0.74
1:A:93:GLY:HA3	2:B:137:ASN:ND2	2.02	0.74
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.18	0.74
1:A:435:VAL:CG2	2:B:290:THR:HG21	2.17	0.74
1:A:171:PHE:HB2	1:A:208:HIS:ND1	2.02	0.74
2:B:57:ASN:HB2	2:B:143:ARG:NH1	2.03	0.74
1:A:12:LEU:HD21	1:A:124:PHE:HE1	1.53	0.74
1:A:517:LEU:O	1:A:520:GLN:N	2.20	0.74
1:A:440:PHE:HE1	1:A:489:SER:HB3	1.51	0.74
2:B:131:THR:OG1	2:B:143:ARG:HD2	1.88	0.74
2:B:314:VAL:CG1	2:B:315:HIS:H	1.99	0.74
1:A:452:LEU:CD2	1:A:470:THR:HA	2.18	0.74
1:A:12:LEU:HD22	1:A:84:THR:HA	1.70	0.74
2:B:258:GLN:O	2:B:261:VAL:HG23	1.88	0.74
1:A:63:ILE:HG13	1:A:63:ILE:O	1.88	0.74
1:A:29:GLU:HG3	1:A:30:LYS:H	1.53	0.73
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.68	0.73
2:B:174:GLN:O	2:B:176:PRO:CD	2.36	0.73
1:A:472:THR:CG2	1:A:473:THR:H	2.01	0.73
1:A:330:GLN:OE1	1:A:340:GLN:NE2	2.20	0.73
1:A:277:ARG:O	1:A:280:SER:HB2	1.87	0.73
1:A:173:LYS:HA	1:A:173:LYS:HE3	1.70	0.73
1:A:218:ASP:C	1:A:220:LYS:H	1.91	0.73
2:B:237:ASP:OD1	2:B:238:LYS:HG2	1.89	0.73
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.70	0.72
1:A:195:ILE:HD13	1:A:223:LYS:NZ	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:HB	1:A:476:LYS:HB3	1.71	0.72
2:B:30:LYS:HE3	2:B:403:THR:HG21	1.70	0.72
2:B:233:GLU:OE2	2:B:235:HIS:NE2	2.20	0.72
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.90	0.72
1:A:138:GLU:HG3	1:A:139:THR:H	1.55	0.72
1:A:450:THR:CG2	1:A:451:LYS:H	2.01	0.72
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.72	0.72
1:A:341:ILE:O	1:A:349:LEU:HD12	1.90	0.72
1:A:319:TYR:O	1:A:321:PRO:HD3	1.90	0.71
1:A:242:GLN:H	1:A:243:PRO:HD3	1.54	0.71
1:A:116:PHE:O	1:A:148:VAL:HG11	1.90	0.71
1:A:317:VAL:HG23	1:A:348:ASN:O	1.91	0.71
2:B:277:ARG:HG3	2:B:277:ARG:HH11	1.55	0.70
1:A:17:ASP:OD1	1:A:56:TYR:HE2	1.73	0.70
1:A:291:GLU:OE2	1:A:292:VAL:HG12	1.91	0.70
1:A:252:TRP:HZ3	1:A:295:LEU:HD22	1.55	0.70
2:B:88:TRP:N	2:B:88:TRP:CE3	2.59	0.70
1:A:458:VAL:HG12	1:A:464:GLN:HG3	1.72	0.70
1:A:472:THR:CG2	1:A:473:THR:N	2.53	0.70
1:A:472:THR:HG23	1:A:476:LYS:HG2	1.73	0.70
1:A:362:THR:HG23	1:A:363:ASN:H	1.56	0.70
2:B:41:MET:HB3	2:B:47:ILE:HG12	1.74	0.70
2:B:249:LYS:HB2	2:B:252:TRP:CD1	2.27	0.70
2:B:104:LYS:HD2	2:B:192:ASP:O	1.91	0.70
2:B:50:ILE:HD11	2:B:143:ARG:HB3	1.74	0.70
1:A:10:VAL:CG1	1:A:11:LYS:N	2.55	0.70
1:A:238:LYS:HD3	1:A:315:HIS:CE1	2.26	0.70
1:A:90:VAL:HG11	1:A:184:MET:CE	2.21	0.70
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.74	0.69
2:B:336:GLN:HE22	2:B:426:TRP:HZ2	1.39	0.69
1:A:261:VAL:HG23	1:A:262:GLY:H	1.56	0.69
1:A:45:GLY:O	1:A:47:ILE:N	2.25	0.69
1:A:430:GLU:HG3	1:A:530:LYS:HD2	1.74	0.69
2:B:87:PHE:C	2:B:89:GLU:N	2.44	0.69
2:B:209:LEU:HD22	2:B:214:LEU:HD13	1.73	0.69
2:B:13:LYS:HE3	2:B:85:GLN:HB2	1.75	0.69
2:B:150:PRO:HD2	2:B:153:TRP:HE3	1.58	0.69
1:A:116:PHE:O	1:A:148:VAL:HG21	1.93	0.69
1:A:241:VAL:CG2	1:A:243:PRO:HD2	2.23	0.69
1:A:107:THR:HG21	1:A:222:GLN:OE1	1.93	0.68
1:A:446:ALA:H	1:A:474:ASN:ND2	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:ILE:HG22	2:B:412:PRO:O	1.93	0.68
1:A:440:PHE:CZ	1:A:463:ARG:NH2	2.61	0.68
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.75	0.68
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.29	0.68
1:A:19:PRO:HB3	1:A:79:GLU:HG3	1.75	0.68
1:A:414:TRP:H	1:A:414:TRP:HE3	1.42	0.68
2:B:17:ASP:O	2:B:83:ARG:HD3	1.93	0.68
1:A:332:GLN:NE2	1:A:338:THR:HB	2.09	0.68
2:B:21:VAL:O	2:B:57:ASN:ND2	2.26	0.67
1:A:449:GLU:O	1:A:449:GLU:HG2	1.93	0.67
1:A:202:ILE:HG21	1:A:222:GLN:OE1	1.94	0.67
2:B:50:ILE:CD1	2:B:143:ARG:HH21	2.07	0.67
1:A:472:THR:CG2	1:A:477:THR:HG23	2.22	0.67
1:A:170:PRO:O	1:A:173:LYS:HB2	1.95	0.67
1:A:246:LEU:HD12	1:A:247:PRO:HD2	1.75	0.67
1:A:254:VAL:O	1:A:258:GLN:HG3	1.94	0.67
1:A:101:LYS:NZ	2:B:138:GLU:OE1	2.27	0.67
1:A:470:THR:C	1:A:471:ASN:HD22	1.99	0.67
1:A:408:ALA:HB3	2:B:393:ILE:HD13	1.75	0.67
2:B:418:ASN:O	2:B:419:THR:OG1	2.12	0.67
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.24	0.66
1:A:459:THR:HG22	1:A:463:ARG:H	1.60	0.66
2:B:107:THR:HG23	2:B:232:TYR:HE1	1.60	0.66
1:A:16:MET:SD	1:A:83:ARG:HA	2.34	0.66
1:A:484:LEU:O	1:A:487:GLN:HB2	1.96	0.66
1:A:22:LYS:HG3	1:A:23:GLN:H	1.60	0.66
1:A:31:ILE:HD12	1:A:133:PRO:HD2	1.77	0.66
1:A:10:VAL:HG12	1:A:11:LYS:H	1.60	0.66
2:B:252:TRP:CH2	2:B:260:LEU:HD22	2.31	0.66
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.31	0.66
1:A:175:ASN:N	1:A:175:ASN:ND2	2.42	0.66
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.31	0.66
1:A:12:LEU:HD21	1:A:124:PHE:CE1	2.31	0.66
1:A:252:TRP:CZ3	1:A:295:LEU:HD22	2.31	0.65
2:B:175:ASN:OD1	2:B:201:LYS:HD2	1.97	0.65
1:A:21:VAL:HG11	1:A:78:ARG:HH21	1.61	0.65
1:A:249:LYS:CE	1:A:250:ASP:H	2.07	0.65
1:A:379:SER:OG	1:A:387:PRO:HD3	1.96	0.65
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.76	0.65
1:A:38:CYS:SG	1:A:144:TYR:HE2	2.20	0.65
2:B:13:LYS:HB2	2:B:16:MET:CG	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:THR:HG23	1:A:476:LYS:CG	2.26	0.65
1:A:460:ASN:ND2	1:A:461:LYS:N	2.41	0.65
1:A:10:VAL:CG1	1:A:11:LYS:H	2.10	0.65
1:A:54:ASN:HD21	1:A:129:ALA:CB	2.09	0.65
1:A:58:THR:CG2	1:A:77:PHE:HA	2.25	0.65
1:A:194:GLU:HG2	1:A:196:GLY:H	1.62	0.65
1:A:520:GLN:O	1:A:523:GLU:HB2	1.97	0.65
2:B:150:PRO:HD2	2:B:153:TRP:CE3	2.32	0.65
1:A:438:GLU:HG2	1:A:459:THR:OG1	1.97	0.64
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.32	0.64
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.28	0.64
2:B:87:PHE:O	2:B:89:GLU:N	2.30	0.64
1:A:451:LYS:O	1:A:471:ASN:CA	2.43	0.64
1:A:242:GLN:H	1:A:243:PRO:CD	2.11	0.64
1:A:57:ASN:OD1	1:A:131:THR:HB	1.98	0.64
2:B:241:VAL:O	2:B:243:PRO:HD3	1.98	0.64
1:A:465:LYS:HG2	1:A:466:VAL:N	2.11	0.64
1:A:460:ASN:ND2	1:A:461:LYS:H	1.86	0.64
1:A:237:ASP:O	1:A:237:ASP:CG	2.35	0.64
1:A:459:THR:HG22	1:A:463:ARG:N	2.11	0.64
1:A:178:ILE:HD11	1:A:189:VAL:HG12	1.80	0.64
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.32	0.64
1:A:206:ARG:NH1	1:A:219:LYS:HG2	2.05	0.64
1:A:481:ALA:O	1:A:482:ILE:C	2.36	0.64
2:B:253:THR:OG1	2:B:256:ASP:OD1	2.16	0.64
1:A:5:ILE:HG22	1:A:6:GLU:N	2.11	0.64
2:B:44:GLU:OE2	2:B:46:LYS:HE3	1.98	0.64
1:A:541:GLY:HA2	1:A:546:GLU:HB2	1.79	0.64
1:A:236:PRO:O	1:A:238:LYS:N	2.29	0.64
1:A:221:HIS:C	1:A:222:GLN:HG3	2.16	0.64
2:B:80:LEU:HD12	2:B:80:LEU:O	1.97	0.64
1:A:475:GLN:O	1:A:477:THR:N	2.31	0.63
2:B:88:TRP:C	2:B:90:VAL:N	2.51	0.63
1:A:157:PRO:HB3	1:A:184:MET:HE2	1.80	0.63
2:B:97:PRO:HG2	2:B:181:CYS:HB3	1.80	0.63
1:A:139:THR:CB	1:A:140:PRO:HD3	2.27	0.63
1:A:95:PRO:HD2	1:A:229:TRP:HH2	1.64	0.63
1:A:50:ILE:HD12	1:A:143:ARG:HD2	1.80	0.63
2:B:316:GLY:C	2:B:318:TYR:H	2.01	0.63
1:A:215:THR:HG22	1:A:216:THR:N	2.13	0.63
2:B:244:ILE:HG13	2:B:244:ILE:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:THR:HB	1:A:476:LYS:CB	2.29	0.63
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.28	0.63
1:A:38:CYS:HG	1:A:144:TYR:HE2	1.46	0.63
2:B:12:LEU:HD22	2:B:83:ARG:O	1.99	0.62
2:B:249:LYS:HB2	2:B:252:TRP:HE1	1.65	0.62
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.34	0.62
2:B:395:LYS:HE2	2:B:395:LYS:N	2.13	0.62
2:B:339:TYR:C	2:B:340:GLN:OE1	2.38	0.62
2:B:87:PHE:HB2	2:B:88:TRP:CZ3	2.35	0.62
1:A:132:ILE:HG22	1:A:142:ILE:HB	1.81	0.62
1:A:195:ILE:HG13	1:A:199:ARG:HE	1.64	0.62
1:A:75:VAL:HG12	1:A:76:ASP:N	2.15	0.62
1:A:480:GLN:HE21	1:A:517:LEU:HD22	1.64	0.62
1:A:257:ILE:O	1:A:260:LEU:HB3	1.99	0.62
2:B:149:LEU:HB3	2:B:156:SER:HB2	1.80	0.62
1:A:19:PRO:HB3	1:A:79:GLU:O	2.00	0.62
1:A:174:GLN:C	1:A:176:PRO:HD3	2.19	0.62
2:B:115:TYR:CE1	2:B:185:ASP:OD1	2.49	0.62
2:B:111:VAL:HG12	2:B:214:LEU:HD21	1.81	0.62
1:A:50:ILE:HD11	1:A:144:TYR:C	2.20	0.62
2:B:103:ASN:HD22	2:B:103:ASN:H	1.48	0.62
2:B:18:GLY:CA	2:B:127:TYR:HD1	2.12	0.62
2:B:167:ILE:O	2:B:170:PRO:HD2	2.00	0.62
2:B:332:GLN:OE1	2:B:338:THR:OG1	2.06	0.62
2:B:244:ILE:HD11	2:B:271:TYR:HE2	1.65	0.62
2:B:157:PRO:O	2:B:161:GLN:N	2.31	0.62
1:A:260:LEU:HD11	1:A:303:LEU:HD11	1.81	0.61
2:B:248:GLU:O	2:B:249:LYS:CG	2.48	0.61
1:A:225:PRO:HB3	1:A:227:PHE:CE1	2.34	0.61
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.35	0.61
1:A:198:HIS:O	1:A:202:ILE:HG13	2.00	0.61
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.26	0.61
1:A:30:LYS:O	1:A:33:ALA:HB3	2.00	0.61
1:A:53:GLU:O	1:A:55:PRO:HD3	2.01	0.61
1:A:155:GLY:O	1:A:158:ALA:HB3	2.01	0.61
1:A:190:GLY:HA3	4:A:562:HBY:H143	1.83	0.61
2:B:296:THR:HG22	2:B:297:GLU:N	2.14	0.61
2:B:4:PRO:O	2:B:6:GLU:HG3	2.01	0.61
1:A:452:LEU:HD23	1:A:471:ASN:H	1.65	0.61
1:A:472:THR:HG22	1:A:473:THR:H	1.60	0.61
1:A:480:GLN:O	1:A:483:TYR:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:HB3	1:A:512:LYS:NZ	2.16	0.61
2:B:195:ILE:CG2	2:B:199:ARG:HE	2.14	0.61
1:A:419:THR:HG22	1:A:419:THR:O	2.01	0.61
1:A:120:LEU:HD11	1:A:150:PRO:HD3	1.83	0.60
2:B:78:ARG:O	2:B:81:ASN:HB2	2.01	0.60
1:A:78:ARG:HD3	1:A:79:GLU:H	1.66	0.60
1:A:434:ILE:CG2	1:A:437:ALA:HB2	2.32	0.60
1:A:437:ALA:HB3	1:A:494:ASN:ND2	2.17	0.60
1:A:291:GLU:HG3	1:A:292:VAL:H	1.67	0.60
1:A:32:LYS:O	1:A:36:GLU:HG3	2.00	0.60
1:A:511:ASP:HA	1:A:522:ILE:HG21	1.84	0.60
1:A:501:TYR:O	1:A:505:ILE:HG12	2.02	0.60
1:A:246:LEU:HD11	1:A:260:LEU:HD12	1.83	0.60
1:A:257:ILE:HG22	1:A:258:GLN:N	2.17	0.60
1:A:283:LEU:O	1:A:286:THR:HG22	2.02	0.60
2:B:376:THR:HG23	2:B:386:THR:HG22	1.83	0.60
1:A:38:CYS:SG	1:A:144:TYR:CE2	2.94	0.60
2:B:301:LEU:O	2:B:305:GLU:HG3	2.02	0.60
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.83	0.59
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.34	0.59
1:A:197:GLN:HA	1:A:200:THR:OG1	2.02	0.59
2:B:260:LEU:HD21	2:B:279:LEU:HD21	1.83	0.59
2:B:311:LYS:O	2:B:312:GLU:HG3	2.02	0.59
2:B:10:VAL:HG12	2:B:11:LYS:N	2.16	0.59
1:A:199:ARG:HD2	1:A:221:HIS:CE1	2.37	0.59
1:A:241:VAL:HG11	1:A:266:TRP:NE1	2.10	0.59
1:A:101:LYS:N	1:A:101:LYS:HD2	2.17	0.59
1:A:398:TRP:CD1	1:A:398:TRP:C	2.75	0.59
1:A:306:ASN:HD22	1:A:307:ARG:H	1.50	0.59
2:B:139:THR:HG22	2:B:141:GLY:H	1.68	0.59
2:B:118:VAL:HG11	2:B:149:LEU:HD11	1.84	0.59
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.37	0.58
2:B:110:ASP:HB2	2:B:186:ASP:OD2	2.03	0.58
1:A:524:GLN:O	1:A:528:LYS:HG2	2.02	0.58
2:B:249:LYS:CB	2:B:252:TRP:CD1	2.87	0.58
1:A:108:VAL:HG21	1:A:227:PHE:CE2	2.38	0.58
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.38	0.58
2:B:366:LYS:HB2	2:B:405:TYR:CE2	2.39	0.58
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.03	0.58
2:B:348:ASN:N	2:B:348:ASN:OD1	2.37	0.58
1:A:21:VAL:HG21	1:A:78:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:O	1:A:159:ILE:HG22	2.03	0.57
1:A:362:THR:HG22	1:A:363:ASN:N	2.19	0.57
2:B:398:TRP:O	2:B:402:TRP:HB3	2.04	0.57
2:B:326:ILE:HB	2:B:342:TYR:CE1	2.38	0.57
1:A:220:LYS:HG3	1:A:221:HIS:O	2.04	0.57
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.86	0.57
1:A:21:VAL:O	1:A:21:VAL:HG13	2.03	0.57
1:A:459:THR:HG23	1:A:461:LYS:N	2.19	0.57
1:A:90:VAL:HG21	1:A:157:PRO:HB2	1.86	0.57
2:B:164:MET:O	2:B:165:THR:C	2.43	0.57
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.85	0.57
1:A:404:GLU:OE1	1:A:428:GLN:NE2	2.35	0.57
1:A:190:GLY:HA3	4:A:562:HBY:C14	2.35	0.57
1:A:458:VAL:HG22	1:A:548:VAL:HG13	1.85	0.57
1:A:306:ASN:HD22	1:A:306:ASN:N	2.01	0.57
1:A:4:PRO:CG	1:A:5:ILE:H	2.14	0.57
2:B:395:LYS:HB3	2:B:416:PHE:CE2	2.40	0.57
1:A:138:GLU:OE1	1:A:138:GLU:HA	2.04	0.57
1:A:430:GLU:HG3	1:A:530:LYS:CD	2.34	0.57
1:A:306:ASN:ND2	1:A:306:ASN:N	2.52	0.57
2:B:317:VAL:HG12	2:B:317:VAL:O	2.05	0.57
1:A:196:GLY:O	1:A:199:ARG:HG2	2.05	0.56
2:B:100:LEU:CD2	2:B:381:VAL:HG13	2.36	0.56
2:B:30:LYS:HE3	2:B:403:THR:CG2	2.35	0.56
1:A:236:PRO:C	1:A:238:LYS:H	2.09	0.56
1:A:115:TYR:O	1:A:149:LEU:HB2	2.05	0.56
1:A:249:LYS:HE3	1:A:250:ASP:N	2.14	0.56
2:B:18:GLY:CA	2:B:127:TYR:CD1	2.88	0.56
1:A:357:MET:C	1:A:357:MET:SD	2.83	0.56
1:A:107:THR:HG22	1:A:108:VAL:N	2.21	0.56
1:A:511:ASP:OD2	1:A:512:LYS:N	2.38	0.56
2:B:87:PHE:O	2:B:90:VAL:HG13	2.05	0.56
2:B:419:THR:HG22	2:B:421:PRO:HD3	1.87	0.56
1:A:238:LYS:HD3	1:A:315:HIS:HE1	1.68	0.56
1:A:542:ILE:HD12	1:A:542:ILE:N	2.21	0.56
1:A:232:TYR:HE2	1:A:269:GLN:NE2	2.04	0.56
1:A:266:TRP:O	1:A:269:GLN:HG2	2.05	0.56
1:A:480:GLN:HE21	1:A:517:LEU:CD2	2.19	0.56
1:A:260:LEU:HD11	1:A:303:LEU:CD1	2.36	0.56
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.87	0.56
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:HD23	2:B:210:LEU:O	2.05	0.56
2:B:78:ARG:O	2:B:81:ASN:N	2.39	0.56
1:A:470:THR:O	1:A:471:ASN:ND2	2.30	0.56
1:A:457:TYR:CE1	1:A:465:LYS:HB3	2.41	0.56
1:A:94:ILE:O	1:A:95:PRO:C	2.42	0.56
1:A:340:GLN:CB	1:A:351:THR:HG22	2.36	0.56
1:A:326:ILE:O	1:A:341:ILE:HA	2.05	0.55
1:A:328:GLU:HA	1:A:390:LYS:O	2.05	0.55
1:A:157:PRO:HB3	1:A:184:MET:CE	2.35	0.55
2:B:52:PRO:C	2:B:54:ASN:H	2.08	0.55
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.88	0.55
2:B:282:LEU:HD21	2:B:296:THR:OG1	2.06	0.55
1:A:225:PRO:HA	1:A:226:PRO:C	2.26	0.55
1:A:223:LYS:HB2	1:A:225:PRO:HD3	1.89	0.55
2:B:260:LEU:HD11	2:B:264:LEU:HD11	1.88	0.55
1:A:125:ARG:C	1:A:127:TYR:H	2.08	0.55
2:B:200:THR:O	2:B:204:GLU:N	2.34	0.55
1:A:232:TYR:CE2	1:A:269:GLN:NE2	2.73	0.55
2:B:30:LYS:HD3	2:B:62:ALA:O	2.07	0.55
2:B:401:TRP:O	2:B:403:THR:N	2.39	0.55
2:B:274:ILE:HG22	2:B:275:LYS:N	2.21	0.55
1:A:208:HIS:CD2	1:A:212:TRP:HD1	2.25	0.55
2:B:195:ILE:O	2:B:197:GLN:N	2.38	0.55
2:B:366:LYS:HB2	2:B:405:TYR:CD2	2.41	0.55
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.42	0.55
1:A:350:LYS:HE2	1:A:378:GLU:OE1	2.07	0.55
2:B:332:GLN:O	2:B:333:GLY:C	2.45	0.55
1:A:215:THR:CG2	1:A:216:THR:N	2.70	0.55
2:B:266:TRP:HZ2	2:B:427:TYR:CE2	2.23	0.55
1:A:8:VAL:CG2	1:A:159:ILE:HG23	2.37	0.55
1:A:293:ILE:HG23	1:A:293:ILE:O	2.07	0.55
1:A:291:GLU:HG3	1:A:292:VAL:N	2.21	0.55
1:A:449:GLU:CG	1:A:449:GLU:O	2.56	0.54
2:B:164:MET:O	2:B:167:ILE:N	2.34	0.54
1:A:398:TRP:CD1	1:A:402:TRP:HD1	2.24	0.54
2:B:85:GLN:O	2:B:85:GLN:HG3	2.07	0.54
2:B:257:ILE:O	2:B:260:LEU:HB3	2.07	0.54
2:B:306:ASN:HA	2:B:309:ILE:HD12	1.89	0.54
2:B:202:ILE:O	2:B:205:LEU:HB3	2.07	0.54
1:A:507:GLN:C	1:A:509:GLN:H	2.09	0.54
1:A:60:VAL:HG13	1:A:130:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:GLU:OE2	1:A:499:SER:HB2	2.07	0.54
1:A:291:GLU:CG	1:A:292:VAL:H	2.20	0.54
1:A:459:THR:CG2	1:A:463:ARG:H	2.21	0.54
1:A:259:LYS:O	1:A:263:LYS:HG3	2.08	0.54
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.95	0.54
1:A:477:THR:O	1:A:480:GLN:N	2.33	0.54
1:A:203:GLU:HA	1:A:203:GLU:OE1	2.06	0.54
2:B:334:GLN:C	2:B:336:GLN:H	2.10	0.54
1:A:337:TRP:HB2	1:A:354:TYR:HB3	1.90	0.54
1:A:437:ALA:HB3	1:A:494:ASN:HD22	1.73	0.54
2:B:217:PRO:O	2:B:219:LYS:N	2.38	0.54
1:A:242:GLN:N	1:A:243:PRO:CD	2.71	0.54
2:B:276:VAL:HG22	2:B:280:SER:OG	2.08	0.54
1:A:174:GLN:HB2	1:A:175:ASN:ND2	2.23	0.53
2:B:234:LEU:C	2:B:236:PRO:HD3	2.28	0.53
1:A:5:ILE:HG22	1:A:6:GLU:O	2.08	0.53
1:A:64:LYS:CB	1:A:71:TRP:HA	2.37	0.53
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.39	0.53
1:A:261:VAL:HG23	1:A:262:GLY:N	2.23	0.53
2:B:161:GLN:HA	2:B:161:GLN:HE21	1.73	0.53
1:A:17:ASP:OD1	1:A:56:TYR:CE2	2.58	0.53
2:B:393:ILE:HG23	2:B:398:TRP:HB2	1.91	0.53
2:B:100:LEU:HD23	2:B:100:LEU:O	2.09	0.53
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.72	0.53
2:B:99:GLY:O	2:B:102:LYS:HB2	2.09	0.53
2:B:233:GLU:CD	2:B:235:HIS:HE2	2.11	0.53
1:A:153:TRP:CG	1:A:154:LYS:N	2.76	0.53
1:A:116:PHE:HD2	1:A:148:VAL:CG2	2.22	0.53
1:A:242:GLN:O	1:A:244:ILE:N	2.35	0.53
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.43	0.53
1:A:60:VAL:HG12	1:A:75:VAL:CG2	2.25	0.53
1:A:276:VAL:CG1	1:A:276:VAL:O	2.57	0.53
2:B:111:VAL:CG1	2:B:214:LEU:HD21	2.39	0.53
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.44	0.53
2:B:340:GLN:NE2	2:B:427:TYR:CG	2.77	0.52
1:A:406:TRP:HZ3	1:A:407:GLN:HG3	1.74	0.52
1:A:114:ALA:O	1:A:117:SER:N	2.33	0.52
1:A:60:VAL:O	1:A:61:PHE:HD1	1.91	0.52
2:B:316:GLY:C	2:B:318:TYR:N	2.63	0.52
2:B:302:GLU:HA	2:B:305:GLU:OE2	2.10	0.52
1:A:233:GLU:O	1:A:239:TRP:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:CG2	1:A:6:GLU:N	2.72	0.52
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.45	0.52
1:A:191:SER:OG	1:A:198:HIS:ND1	2.41	0.52
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.39	0.52
2:B:164:MET:CE	2:B:187:LEU:HD21	2.32	0.52
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.39	0.52
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.44	0.52
1:A:557:ARG:HH11	1:A:557:ARG:HG2	1.75	0.52
2:B:106:VAL:HG23	2:B:236:PRO:HG2	1.91	0.52
1:A:295:LEU:HD21	1:A:300:GLU:HG3	1.92	0.52
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.39	0.52
1:A:20:LYS:HG2	1:A:55:PRO:O	2.09	0.52
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.45	0.52
1:A:517:LEU:O	1:A:519:ASN:N	2.43	0.52
1:A:240:THR:OG1	1:A:241:VAL:N	2.41	0.52
1:A:126:LYS:C	1:A:127:TYR:CD1	2.83	0.52
1:A:156:SER:N	1:A:157:PRO:CD	2.73	0.52
1:A:23:GLN:O	1:A:25:PRO:HD3	2.10	0.52
1:A:207:GLN:O	1:A:210:LEU:HB3	2.09	0.52
1:A:479:LEU:O	1:A:521:ILE:HD11	2.09	0.51
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.91	0.51
1:A:186:ASP:CB	1:A:188:TYR:HE1	2.22	0.51
2:B:395:LYS:O	2:B:399:GLU:HG3	2.10	0.51
1:A:390:LYS:O	1:A:391:LEU:HD23	2.10	0.51
2:B:65:LYS:HG3	2:B:72:ARG:CB	2.39	0.51
1:A:557:ARG:NH1	1:A:557:ARG:HG2	2.24	0.51
1:A:457:TYR:HE2	1:A:488:ASP:OD1	1.92	0.51
2:B:183:TYR:CE2	2:B:380:ILE:HD13	2.45	0.51
1:A:84:THR:CG2	1:A:153:TRP:HE1	2.05	0.51
1:A:111:VAL:O	1:A:111:VAL:HG12	2.09	0.51
1:A:406:TRP:CZ3	1:A:407:GLN:CG	2.93	0.51
1:A:257:ILE:CG2	1:A:258:GLN:N	2.74	0.51
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.93	0.51
2:B:274:ILE:CG2	2:B:275:LYS:N	2.73	0.51
1:A:164:MET:HG2	1:A:182:GLN:OE1	2.10	0.51
2:B:149:LEU:HB3	2:B:156:SER:CB	2.40	0.51
2:B:350:LYS:HE2	2:B:378:GLU:OE2	2.10	0.51
1:A:163:SER:O	1:A:167:ILE:HD13	2.10	0.51
2:B:139:THR:HG23	2:B:140:PRO:CD	2.38	0.51
1:A:245:VAL:HG23	1:A:263:LYS:NZ	2.25	0.51
1:A:125:ARG:O	1:A:127:TYR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HG2	1:A:522:ILE:CD1	2.36	0.51
1:A:41:MET:O	1:A:43:LYS:N	2.44	0.51
1:A:465:LYS:CG	1:A:466:VAL:N	2.73	0.51
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.76	0.51
1:A:195:ILE:HG13	1:A:199:ARG:NE	2.25	0.51
1:A:361:HIS:CE1	1:A:513:SER:OG	2.62	0.51
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.58	0.51
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.75	0.51
1:A:301:LEU:O	1:A:304:ALA:HB3	2.10	0.51
2:B:248:GLU:O	2:B:249:LYS:HG3	2.11	0.51
2:B:64:LYS:O	2:B:65:LYS:C	2.49	0.51
1:A:203:GLU:O	1:A:206:ARG:HG2	2.11	0.51
2:B:277:ARG:HH11	2:B:277:ARG:CG	2.24	0.51
2:B:195:ILE:O	2:B:196:GLY:C	2.49	0.51
2:B:395:LYS:HB3	2:B:416:PHE:CD2	2.46	0.50
1:A:22:LYS:HG3	1:A:23:GLN:OE1	2.11	0.50
2:B:194:GLU:O	2:B:195:ILE:C	2.50	0.50
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.92	0.50
1:A:267:ALA:HB3	1:A:274:ILE:CD1	2.40	0.50
2:B:277:ARG:HA	2:B:280:SER:OG	2.11	0.50
2:B:257:ILE:HG13	2:B:293:ILE:HD11	1.93	0.50
2:B:88:TRP:N	2:B:88:TRP:CD2	2.79	0.50
1:A:45:GLY:O	1:A:46:LYS:C	2.49	0.50
2:B:378:GLU:O	2:B:381:VAL:N	2.43	0.50
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.46	0.50
1:A:477:THR:O	1:A:480:GLN:HB2	2.11	0.50
1:A:264:LEU:C	1:A:266:TRP:H	2.15	0.50
1:A:158:ALA:O	1:A:160:PHE:N	2.44	0.50
2:B:326:ILE:HB	2:B:342:TYR:HE1	1.77	0.50
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.45	0.50
1:A:111:VAL:CG2	1:A:187:LEU:HD13	2.30	0.50
1:A:508:ALA:O	1:A:509:GLN:C	2.49	0.50
1:A:58:THR:CG2	1:A:76:ASP:O	2.54	0.50
1:A:148:VAL:O	1:A:150:PRO:CD	2.56	0.50
1:A:10:VAL:O	1:A:11:LYS:HG3	2.12	0.50
2:B:353:LYS:HZ2	2:B:426:TRP:HH2	1.60	0.50
1:A:22:LYS:HG3	1:A:23:GLN:N	2.27	0.50
2:B:269:GLN:CD	2:B:346:PHE:HE2	2.15	0.50
1:A:88:TRP:CE3	1:A:88:TRP:HA	2.47	0.49
2:B:330:GLN:NE2	2:B:340:GLN:OE1	2.45	0.49
2:B:234:LEU:O	2:B:236:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:CG	1:A:139:THR:H	2.24	0.49
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.40	0.49
1:A:25:PRO:O	1:A:26:LEU:HD23	2.11	0.49
1:A:50:ILE:HG21	1:A:54:ASN:OD1	2.11	0.49
2:B:10:VAL:HG12	2:B:11:LYS:H	1.76	0.49
1:A:535:TRP:CG	1:A:536:VAL:N	2.81	0.49
1:A:113:ASP:O	1:A:114:ALA:C	2.50	0.49
1:A:64:LYS:O	1:A:67:ASP:O	2.31	0.49
1:A:107:THR:OG1	1:A:202:ILE:HD13	2.12	0.49
2:B:50:ILE:CD1	2:B:143:ARG:HB3	2.43	0.49
1:A:253:THR:O	1:A:256:ASP:N	2.46	0.49
2:B:113:ASP:O	2:B:114:ALA:C	2.51	0.49
2:B:344:GLU:OE1	2:B:345:PRO:HD3	2.13	0.49
1:A:203:GLU:O	1:A:206:ARG:CG	2.61	0.49
1:A:334:GLN:HB3	1:A:512:LYS:HZ3	1.76	0.49
2:B:139:THR:CG2	2:B:140:PRO:HD2	2.41	0.49
2:B:136:ASN:O	2:B:136:ASN:CG	2.51	0.49
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.48	0.49
1:A:277:ARG:NH2	1:A:514:GLU:OE1	2.45	0.49
2:B:233:GLU:CD	2:B:235:HIS:NE2	2.66	0.49
1:A:50:ILE:HB	1:A:143:ARG:HB3	1.94	0.49
2:B:296:THR:CG2	2:B:297:GLU:N	2.76	0.49
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.47	0.49
1:A:306:ASN:HD22	1:A:307:ARG:N	2.09	0.49
1:A:325:LEU:C	1:A:326:ILE:HG13	2.33	0.49
1:A:171:PHE:O	1:A:175:ASN:ND2	2.46	0.49
2:B:195:ILE:HG22	2:B:199:ARG:HE	1.76	0.49
1:A:452:LEU:CD2	1:A:471:ASN:H	2.25	0.49
1:A:190:GLY:CA	4:A:562:HBY:H143	2.42	0.49
2:B:160:PHE:O	2:B:162:SER:N	2.46	0.49
1:A:319:TYR:CD1	1:A:343:GLN:NE2	2.81	0.49
2:B:398:TRP:CZ2	2:B:402:TRP:HB2	2.48	0.49
1:A:120:LEU:HG	1:A:148:VAL:C	2.32	0.48
1:A:244:ILE:HD13	1:A:310:LEU:HD22	1.95	0.48
1:A:370:GLU:O	1:A:373:GLN:HB3	2.14	0.48
1:A:482:ILE:CD1	1:A:497:THR:HG21	2.36	0.48
1:A:518:VAL:O	1:A:522:ILE:HG13	2.13	0.48
1:A:522:ILE:O	1:A:522:ILE:HG22	2.12	0.48
2:B:27:THR:OG1	2:B:29:GLU:HG3	2.12	0.48
1:A:454:LYS:HE2	1:A:553:SER:HB3	1.94	0.48
2:B:50:ILE:CD1	2:B:143:ARG:NH2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG12	1:A:318:TYR:N	2.20	0.48
1:A:475:GLN:O	1:A:478:GLU:N	2.46	0.48
2:B:255:ASN:O	2:B:258:GLN:HB2	2.14	0.48
2:B:48:SER:O	2:B:144:TYR:HA	2.14	0.48
1:A:221:HIS:C	1:A:222:GLN:CG	2.82	0.48
2:B:350:LYS:CE	2:B:378:GLU:OE2	2.61	0.48
1:A:90:VAL:CG1	1:A:184:MET:CE	2.90	0.48
2:B:303:LEU:HG	2:B:307:ARG:HH21	1.78	0.48
1:A:101:LYS:HD2	1:A:101:LYS:H	1.79	0.48
2:B:178:ILE:HG12	2:B:191:SER:HB3	1.94	0.48
1:A:120:LEU:O	1:A:121:ASP:C	2.52	0.48
1:A:23:GLN:HB3	1:A:131:THR:CG2	2.44	0.48
1:A:517:LEU:HA	1:A:520:GLN:HG3	1.96	0.48
2:B:393:ILE:CG2	2:B:398:TRP:HB2	2.44	0.48
1:A:454:LYS:HB3	1:A:468:PRO:HA	1.96	0.48
1:A:197:GLN:O	1:A:200:THR:CB	2.53	0.47
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.40	0.47
2:B:277:ARG:HG3	2:B:277:ARG:NH1	2.27	0.47
1:A:126:LYS:HB2	1:A:127:TYR:CE1	2.49	0.47
1:A:126:LYS:HB2	1:A:127:TYR:CD1	2.49	0.47
2:B:97:PRO:HG2	2:B:181:CYS:CB	2.44	0.47
1:A:527:LYS:HB2	1:A:527:LYS:HE3	1.60	0.47
1:A:220:LYS:C	1:A:221:HIS:O	2.51	0.47
2:B:57:ASN:HA	2:B:129:ALA:O	2.14	0.47
1:A:188:TYR:N	1:A:188:TYR:CD1	2.82	0.47
2:B:18:GLY:HA2	2:B:127:TYR:HD1	1.75	0.47
1:A:406:TRP:C	1:A:406:TRP:CE3	2.87	0.47
1:A:329:ILE:HD11	1:A:375:ILE:CD1	2.44	0.47
1:A:330:GLN:HG2	1:A:338:THR:HG23	1.97	0.47
1:A:237:ASP:C	1:A:238:LYS:HG2	2.35	0.47
1:A:521:ILE:C	1:A:523:GLU:H	2.16	0.47
2:B:50:ILE:HD11	2:B:143:ARG:NE	2.29	0.47
1:A:108:VAL:C	1:A:109:LEU:HD23	2.34	0.47
1:A:107:THR:HG22	1:A:108:VAL:H	1.77	0.47
1:A:175:ASN:N	1:A:176:PRO:HD3	2.28	0.47
2:B:302:GLU:O	2:B:303:LEU:C	2.52	0.47
2:B:302:GLU:O	2:B:305:GLU:OE2	2.32	0.47
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.14	0.47
1:A:194:GLU:O	1:A:196:GLY:N	2.48	0.47
2:B:198:HIS:O	2:B:199:ARG:C	2.52	0.47
2:B:342:TYR:C	2:B:342:TYR:CD1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:O	1:A:115:TYR:C	2.52	0.47
1:A:499:SER:HG	1:A:502:ALA:H	1.58	0.47
2:B:423:VAL:HG13	2:B:427:TYR:HD2	1.79	0.47
1:A:126:LYS:C	1:A:127:TYR:HD1	2.17	0.47
2:B:118:VAL:CB	2:B:149:LEU:HD12	2.39	0.47
2:B:370:GLU:O	2:B:374:LYS:HB2	2.15	0.47
1:A:183:TYR:CE1	1:A:184:MET:HG3	2.49	0.47
1:A:29:GLU:HG3	1:A:30:LYS:N	2.26	0.47
2:B:205:LEU:O	2:B:208:HIS:N	2.48	0.47
1:A:455:ALA:O	1:A:467:VAL:HG22	2.15	0.47
2:B:287:LYS:HD2	2:B:291:GLU:OE2	2.14	0.47
1:A:460:ASN:C	1:A:462:GLY:H	2.18	0.47
2:B:5:ILE:HG22	2:B:5:ILE:O	2.15	0.47
2:B:158:ALA:O	2:B:159:ILE:C	2.50	0.47
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.96	0.47
1:A:320:ASP:O	1:A:322:SER:N	2.47	0.47
2:B:237:ASP:OD1	2:B:238:LYS:N	2.47	0.47
1:A:275:LYS:C	1:A:276:VAL:HG23	2.35	0.47
1:A:4:PRO:HG2	1:A:5:ILE:HG13	1.96	0.47
1:A:298:GLU:O	1:A:301:LEU:HB3	2.15	0.47
1:A:499:SER:O	1:A:500:GLN:C	2.53	0.46
1:A:304:ALA:O	1:A:307:ARG:HB3	2.15	0.46
1:A:47:ILE:HB	1:A:145:GLN:O	2.15	0.46
1:A:252:TRP:HZ3	1:A:295:LEU:CD2	2.25	0.46
1:A:252:TRP:CD1	1:A:256:ASP:OD1	2.68	0.46
2:B:114:ALA:HB2	2:B:214:LEU:HG	1.96	0.46
1:A:387:PRO:HG2	1:A:389:PHE:CE2	2.49	0.46
1:A:275:LYS:O	1:A:276:VAL:CG2	2.63	0.46
2:B:234:LEU:HD12	2:B:381:VAL:HG21	1.96	0.46
2:B:64:LYS:C	2:B:66:LYS:N	2.65	0.46
1:A:492:GLU:HA	1:A:530:LYS:O	2.15	0.46
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.49	0.46
1:A:195:ILE:HD13	1:A:223:LYS:HZ1	1.78	0.46
1:A:306:ASN:O	1:A:310:LEU:HG	2.15	0.46
1:A:50:ILE:CG2	1:A:54:ASN:HB2	2.44	0.46
2:B:270:ILE:HA	2:B:347:LYS:HZ1	1.81	0.46
1:A:460:ASN:ND2	1:A:460:ASN:H	2.13	0.46
2:B:311:LYS:O	2:B:312:GLU:CG	2.63	0.46
2:B:27:THR:O	2:B:31:ILE:HG12	2.15	0.46
1:A:170:PRO:HA	1:A:173:LYS:HB2	1.96	0.46
1:A:195:ILE:O	1:A:199:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ILE:CD1	1:A:310:LEU:HD22	2.46	0.46
1:A:50:ILE:HG21	1:A:54:ASN:CG	2.34	0.46
1:A:507:GLN:O	1:A:509:GLN:HG3	2.15	0.46
1:A:521:ILE:C	1:A:523:GLU:N	2.69	0.46
1:A:417:VAL:HG12	1:A:417:VAL:O	2.15	0.46
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.97	0.46
1:A:480:GLN:NE2	1:A:517:LEU:HD13	2.30	0.46
1:A:521:ILE:O	1:A:523:GLU:N	2.49	0.46
2:B:270:ILE:HA	2:B:347:LYS:NZ	2.31	0.46
1:A:264:LEU:C	1:A:266:TRP:N	2.69	0.46
2:B:118:VAL:CG1	2:B:149:LEU:HD11	2.46	0.46
1:A:291:GLU:CG	1:A:292:VAL:N	2.77	0.46
2:B:380:ILE:O	2:B:384:GLY:HA2	2.16	0.46
1:A:58:THR:HA	1:A:59:PRO:HD2	1.73	0.46
1:A:542:ILE:O	1:A:544:GLY:N	2.49	0.46
1:A:118:VAL:O	1:A:148:VAL:HA	2.16	0.46
2:B:248:GLU:C	2:B:249:LYS:HG3	2.36	0.46
2:B:87:PHE:O	2:B:90:VAL:N	2.49	0.46
2:B:118:VAL:CB	2:B:149:LEU:CD1	2.90	0.45
2:B:346:PHE:CD1	2:B:346:PHE:N	2.83	0.45
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.31	0.45
2:B:182:GLN:HB2	2:B:187:LEU:CD2	2.35	0.45
1:A:95:PRO:HD2	1:A:229:TRP:CH2	2.48	0.45
1:A:522:ILE:O	1:A:526:ILE:HD13	2.16	0.45
1:A:88:TRP:CD1	2:B:143:ARG:HD3	2.50	0.45
2:B:170:PRO:O	2:B:173:LYS:HB3	2.17	0.45
1:A:93:GLY:O	1:A:94:ILE:C	2.53	0.45
1:A:127:TYR:N	1:A:127:TYR:CD1	2.84	0.45
2:B:100:LEU:HD23	2:B:100:LEU:C	2.36	0.45
2:B:30:LYS:HD3	2:B:62:ALA:HB3	1.98	0.45
1:A:194:GLU:O	1:A:195:ILE:C	2.54	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.45	0.45
2:B:314:VAL:CG1	2:B:315:HIS:N	2.61	0.45
2:B:115:TYR:C	2:B:117:SER:H	2.19	0.45
1:A:237:ASP:O	1:A:237:ASP:OD1	2.34	0.45
1:A:270:ILE:HG13	1:A:314:VAL:CG2	2.47	0.45
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.51	0.45
1:A:195:ILE:O	1:A:199:ARG:CD	2.65	0.45
1:A:218:ASP:C	1:A:220:LYS:N	2.62	0.45
1:A:238:LYS:HE2	1:A:315:HIS:HD1	1.82	0.45
1:A:229:TRP:O	1:A:230:MET:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLY:O	1:A:385:LYS:HB3	2.17	0.45
1:A:431:LYS:HA	1:A:431:LYS:HD2	1.59	0.45
1:A:108:VAL:CG2	1:A:227:PHE:CZ	3.00	0.45
2:B:257:ILE:HG22	2:B:283:LEU:HD11	1.99	0.45
1:A:205:LEU:HG	1:A:209:LEU:HD11	1.98	0.45
1:A:132:ILE:HG21	1:A:142:ILE:HD12	1.99	0.45
1:A:54:ASN:HA	1:A:55:PRO:HD3	1.83	0.45
1:A:482:ILE:O	1:A:485:ALA:HB3	2.17	0.45
1:A:171:PHE:CG	1:A:205:LEU:HD13	2.52	0.45
1:A:552:VAL:O	1:A:554:ALA:N	2.50	0.45
2:B:342:TYR:C	2:B:342:TYR:HD1	2.21	0.45
1:A:210:LEU:O	1:A:210:LEU:HD12	2.17	0.45
1:A:190:GLY:N	4:A:562:HBV:H143	2.32	0.44
2:B:101:LYS:HE3	2:B:101:LYS:HB2	1.66	0.44
1:A:42:GLU:O	1:A:43:LYS:C	2.56	0.44
1:A:195:ILE:CD1	1:A:223:LYS:HE2	2.47	0.44
1:A:261:VAL:O	1:A:263:LYS:N	2.50	0.44
2:B:50:ILE:HD11	2:B:143:ARG:HE	1.82	0.44
2:B:257:ILE:CG1	2:B:293:ILE:HD11	2.47	0.44
1:A:171:PHE:CZ	1:A:175:ASN:OD1	2.70	0.44
2:B:83:ARG:HG3	2:B:83:ARG:HH11	1.82	0.44
2:B:419:THR:HA	2:B:420:PRO:HD3	1.62	0.44
1:A:116:PHE:HD2	1:A:148:VAL:HG21	1.82	0.44
2:B:277:ARG:NH1	2:B:277:ARG:CG	2.79	0.44
2:B:233:GLU:CD	2:B:235:HIS:CE1	2.91	0.44
1:A:395:LYS:HB2	1:A:414:TRP:CH2	2.52	0.44
2:B:18:GLY:HA2	2:B:127:TYR:CD1	2.52	0.44
2:B:164:MET:CE	2:B:182:GLN:OE1	2.66	0.44
2:B:126:LYS:HG2	2:B:127:TYR:CD2	2.52	0.44
1:A:365:VAL:O	1:A:366:LYS:C	2.55	0.44
1:A:191:SER:HG	1:A:198:HIS:CE1	2.33	0.44
1:A:113:ASP:O	1:A:116:PHE:N	2.49	0.44
1:A:472:THR:HG23	1:A:473:THR:H	1.81	0.44
1:A:37:ILE:HD11	1:A:71:TRP:O	2.17	0.44
2:B:179:VAL:HG23	2:B:179:VAL:O	2.17	0.44
1:A:107:THR:OG1	1:A:202:ILE:CD1	2.66	0.44
1:A:113:ASP:O	1:A:115:TYR:N	2.51	0.44
2:B:365:VAL:HG11	2:B:401:TRP:CB	2.47	0.44
1:A:253:THR:HG21	1:A:290:THR:HG23	2.00	0.44
2:B:214:LEU:C	2:B:214:LEU:HD23	2.38	0.44
1:A:215:THR:CG2	1:A:216:THR:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:ASN:OD1	2:B:309:ILE:HD12	2.18	0.44
2:B:344:GLU:HA	2:B:345:PRO:HD3	1.85	0.44
1:A:480:GLN:O	1:A:484:LEU:N	2.50	0.44
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.99	0.44
2:B:64:LYS:HB3	2:B:66:LYS:O	2.18	0.44
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.98	0.44
2:B:369:THR:O	2:B:373:GLN:HG3	2.17	0.44
1:A:224:GLU:N	1:A:225:PRO:HD3	2.33	0.44
1:A:295:LEU:HD23	1:A:300:GLU:OE2	2.17	0.44
2:B:41:MET:HB3	2:B:47:ILE:CG1	2.46	0.44
1:A:296:THR:HG23	1:A:299:ALA:HB2	1.99	0.44
1:A:211:ARG:C	1:A:213:GLY:H	2.21	0.44
2:B:378:GLU:O	2:B:379:SER:C	2.57	0.44
1:A:40:GLU:O	1:A:43:LYS:HG3	2.18	0.44
1:A:23:GLN:HB3	1:A:131:THR:HG21	2.00	0.44
1:A:397:THR:HG21	1:A:424:LYS:HA	2.00	0.43
1:A:150:PRO:O	1:A:151:GLN:C	2.54	0.43
2:B:248:GLU:O	2:B:249:LYS:HG2	2.18	0.43
2:B:253:THR:O	2:B:257:ILE:HG12	2.18	0.43
2:B:101:LYS:O	2:B:236:PRO:HB3	2.19	0.43
1:A:517:LEU:C	1:A:519:ASN:N	2.71	0.43
1:A:229:TRP:O	1:A:232:TYR:N	2.43	0.43
1:A:282:LEU:O	1:A:284:ARG:N	2.51	0.43
2:B:284:ARG:HG3	2:B:284:ARG:HH11	1.83	0.43
1:A:49:LYS:HG3	1:A:49:LYS:O	2.19	0.43
1:A:249:LYS:HA	1:A:249:LYS:HE3	2.01	0.43
1:A:208:HIS:CD2	1:A:212:TRP:CD1	3.05	0.43
2:B:65:LYS:HG3	2:B:72:ARG:HB2	2.00	0.43
2:B:303:LEU:HG	2:B:307:ARG:NH2	2.33	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:HB2	2.53	0.43
2:B:345:PRO:C	2:B:346:PHE:HD1	2.21	0.43
2:B:269:GLN:NE2	2:B:346:PHE:HE2	2.16	0.43
1:A:168:LEU:O	1:A:169:GLU:C	2.57	0.43
1:A:120:LEU:HG	1:A:148:VAL:O	2.19	0.43
1:A:270:ILE:HG23	1:A:314:VAL:CG2	2.48	0.43
1:A:548:VAL:O	1:A:552:VAL:HG23	2.19	0.43
2:B:110:ASP:HA	2:B:186:ASP:HB3	2.01	0.43
1:A:434:ILE:HG21	1:A:437:ALA:HB2	2.00	0.43
1:A:444:GLY:HA2	1:A:454:LYS:O	2.18	0.43
1:A:108:VAL:HG23	1:A:227:PHE:CZ	2.54	0.43
1:A:195:ILE:HD13	1:A:223:LYS:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:O	1:A:257:ILE:HG22	2.19	0.43
1:A:411:ILE:CG2	1:A:411:ILE:O	2.67	0.43
1:A:116:PHE:O	1:A:148:VAL:CG1	2.63	0.43
1:A:390:LYS:HE2	1:A:417:VAL:CG2	2.48	0.43
2:B:150:PRO:HG2	2:B:153:TRP:HB3	1.99	0.43
2:B:58:THR:HA	2:B:59:PRO:HD3	1.85	0.43
1:A:115:TYR:HB3	1:A:149:LEU:O	2.19	0.43
1:A:88:TRP:HA	1:A:88:TRP:HE3	1.83	0.43
2:B:131:THR:HA	2:B:142:ILE:O	2.18	0.43
1:A:306:ASN:C	1:A:308:GLU:N	2.72	0.43
2:B:253:THR:N	2:B:256:ASP:HB2	2.34	0.43
1:A:64:LYS:HA	1:A:72:ARG:H	1.84	0.43
1:A:31:ILE:CD1	1:A:133:PRO:HD2	2.47	0.43
2:B:109:LEU:HD12	2:B:205:LEU:HD23	2.01	0.43
1:A:370:GLU:HG3	2:B:394:GLN:NE2	2.33	0.43
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.43
2:B:225:PRO:HA	2:B:226:PRO:HD3	1.81	0.43
1:A:19:PRO:HD3	1:A:83:ARG:HG3	2.00	0.42
1:A:224:GLU:N	1:A:225:PRO:CD	2.81	0.42
1:A:236:PRO:C	1:A:238:LYS:N	2.71	0.42
2:B:169:GLU:O	2:B:173:LYS:N	2.43	0.42
1:A:270:ILE:HG23	1:A:314:VAL:HG21	2.01	0.42
2:B:255:ASN:O	2:B:258:GLN:N	2.52	0.42
2:B:276:VAL:O	2:B:279:LEU:N	2.42	0.42
2:B:100:LEU:HD22	2:B:381:VAL:HG13	2.01	0.42
1:A:63:ILE:O	1:A:63:ILE:CG1	2.62	0.42
2:B:269:GLN:NE2	2:B:346:PHE:CE2	2.87	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD12	1.78	0.42
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.99	0.42
2:B:131:THR:OG1	2:B:143:ARG:CD	2.65	0.42
2:B:240:THR:HG22	2:B:241:VAL:H	1.84	0.42
1:A:200:THR:O	1:A:203:GLU:CB	2.67	0.42
2:B:163:SER:O	2:B:167:ILE:HG13	2.19	0.42
2:B:248:GLU:C	2:B:249:LYS:CG	2.87	0.42
1:A:320:ASP:C	1:A:322:SER:N	2.72	0.42
2:B:107:THR:CG2	2:B:232:TYR:HE1	2.28	0.42
2:B:87:PHE:HB2	2:B:88:TRP:CE3	2.53	0.42
1:A:411:ILE:HG23	1:A:411:ILE:O	2.19	0.42
1:A:68:SER:C	1:A:70:LYS:H	2.22	0.42
2:B:244:ILE:O	2:B:244:ILE:CG1	2.66	0.42
1:A:506:ILE:O	1:A:509:GLN:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:VAL:O	2:B:263:LYS:NZ	2.46	0.42
2:B:165:THR:O	2:B:166:LYS:C	2.58	0.42
1:A:408:ALA:O	2:B:393:ILE:HD13	2.19	0.42
1:A:438:GLU:CG	1:A:459:THR:OG1	2.64	0.42
1:A:174:GLN:C	1:A:175:ASN:ND2	2.72	0.42
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.20	0.42
1:A:90:VAL:CG1	1:A:184:MET:HE3	2.50	0.42
1:A:34:LEU:CD1	1:A:132:ILE:HD11	2.49	0.42
1:A:271:TYR:CD2	1:A:310:LEU:HD23	2.55	0.42
2:B:301:LEU:O	2:B:302:GLU:C	2.56	0.42
1:A:357:MET:SD	1:A:357:MET:O	2.77	0.42
1:A:218:ASP:O	1:A:220:LYS:N	2.52	0.42
1:A:264:LEU:O	1:A:267:ALA:N	2.52	0.42
2:B:330:GLN:CG	2:B:338:THR:OG1	2.67	0.42
1:A:362:THR:CG2	1:A:367:GLN:HG3	2.49	0.42
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.50	0.42
1:A:337:TRP:O	1:A:353:LYS:HA	2.19	0.42
1:A:296:THR:O	1:A:299:ALA:HB3	2.20	0.42
1:A:257:ILE:O	1:A:261:VAL:HG22	2.19	0.42
2:B:255:ASN:O	2:B:256:ASP:C	2.58	0.42
2:B:88:TRP:N	2:B:88:TRP:HE3	2.14	0.42
2:B:205:LEU:O	2:B:206:ARG:C	2.58	0.42
1:A:13:LYS:HA	1:A:14:PRO:HD3	1.84	0.42
1:A:306:ASN:ND2	1:A:306:ASN:H	2.18	0.42
1:A:45:GLY:O	1:A:147:ASN:HB2	2.20	0.42
1:A:5:ILE:CG2	1:A:6:GLU:H	2.33	0.42
1:A:17:ASP:OD1	1:A:18:GLY:N	2.52	0.42
2:B:197:GLN:O	2:B:198:HIS:C	2.58	0.42
1:A:437:ALA:CB	1:A:494:ASN:HD22	2.32	0.42
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.39	0.42
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.33	0.42
1:A:4:PRO:O	1:A:5:ILE:O	2.38	0.42
1:A:337:TRP:N	1:A:354:TYR:O	2.53	0.42
2:B:217:PRO:CD	2:B:218:ASP:H	2.33	0.42
2:B:270:ILE:O	2:B:347:LYS:NZ	2.53	0.42
1:A:83:ARG:H	1:A:83:ARG:HG2	1.58	0.41
1:A:200:THR:O	1:A:203:GLU:HB3	2.20	0.41
1:A:135:ILE:O	1:A:135:ILE:HG22	2.20	0.41
1:A:87:PHE:CE1	1:A:155:GLY:HA3	2.55	0.41
2:B:154:LYS:HE2	2:B:184:MET:CE	2.50	0.41
2:B:76:ASP:OD1	2:B:76:ASP:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:O	1:A:449:GLU:N	2.53	0.41
1:A:227:PHE:O	1:A:233:GLU:HA	2.20	0.41
1:A:311:LYS:O	1:A:313:PRO:HD3	2.20	0.41
1:A:458:VAL:HG23	1:A:458:VAL:O	2.20	0.41
1:A:33:ALA:O	1:A:37:ILE:HG13	2.21	0.41
1:A:67:ASP:HB3	1:A:70:LYS:O	2.20	0.41
1:A:475:GLN:O	1:A:476:LYS:C	2.58	0.41
1:A:483:TYR:CE2	1:A:487:GLN:NE2	2.89	0.41
1:A:242:GLN:N	1:A:243:PRO:HD3	2.29	0.41
1:A:174:GLN:C	1:A:175:ASN:HD22	2.22	0.41
1:A:213:GLY:O	1:A:214:LEU:HD23	2.20	0.41
1:A:442:VAL:CG2	1:A:497:THR:HG22	2.51	0.41
2:B:156:SER:N	2:B:157:PRO:HD2	2.36	0.41
1:A:54:ASN:ND2	1:A:129:ALA:CB	2.79	0.41
1:A:406:TRP:O	1:A:406:TRP:HE3	2.02	0.41
2:B:306:ASN:O	2:B:310:LEU:HD13	2.21	0.41
1:A:507:GLN:C	1:A:509:GLN:N	2.72	0.41
1:A:365:VAL:HG23	1:A:365:VAL:H	1.58	0.41
2:B:33:ALA:O	2:B:37:ILE:HG12	2.20	0.41
1:A:178:ILE:HG13	1:A:190:GLY:O	2.20	0.41
2:B:65:LYS:CD	2:B:72:ARG:HG3	2.43	0.41
1:A:52:PRO:HG2	1:A:53:GLU:H	1.84	0.41
1:A:557:ARG:HH11	1:A:557:ARG:CG	2.33	0.41
2:B:347:LYS:HD3	2:B:347:LYS:HA	1.83	0.41
1:A:203:GLU:OE1	1:A:206:ARG:HD3	2.21	0.41
2:B:23:GLN:NE2	2:B:131:THR:O	2.53	0.41
1:A:390:LYS:HB3	1:A:390:LYS:HE2	1.84	0.41
1:A:68:SER:C	1:A:70:LYS:N	2.73	0.41
2:B:122:GLU:HG3	2:B:125:ARG:NH2	2.35	0.41
1:A:139:THR:CB	1:A:140:PRO:CD	2.97	0.41
2:B:17:ASP:O	2:B:83:ARG:CD	2.64	0.41
2:B:329:ILE:HD11	2:B:375:ILE:HD12	2.02	0.41
1:A:116:PHE:HA	1:A:148:VAL:HG21	2.01	0.41
1:A:499:SER:C	1:A:501:TYR:N	2.69	0.41
1:A:480:GLN:HE22	1:A:517:LEU:HD13	1.84	0.41
2:B:97:PRO:HB2	2:B:100:LEU:HB2	2.03	0.41
2:B:353:LYS:NZ	2:B:426:TRP:HH2	2.18	0.41
1:A:556:ILE:O	1:A:558:LYS:N	2.54	0.41
1:A:84:THR:C	1:A:85:GLN:O	2.58	0.41
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.03	0.41
1:A:478:GLU:O	1:A:482:ILE:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HG11	1:A:485:ALA:HB2	2.02	0.41
1:A:460:ASN:N	1:A:460:ASN:ND2	2.68	0.41
1:A:282:LEU:C	1:A:284:ARG:N	2.74	0.41
2:B:164:MET:HE2	2:B:182:GLN:OE1	2.20	0.41
1:A:266:TRP:C	1:A:266:TRP:CD1	2.94	0.41
1:A:264:LEU:O	1:A:266:TRP:N	2.54	0.41
2:B:253:THR:H	2:B:256:ASP:CG	2.24	0.41
2:B:261:VAL:HG12	2:B:276:VAL:HG21	2.03	0.41
1:A:320:ASP:O	1:A:321:PRO:C	2.58	0.41
1:A:325:LEU:O	1:A:326:ILE:HG13	2.21	0.41
2:B:398:TRP:CE2	2:B:402:TRP:HB2	2.56	0.41
2:B:317:VAL:CG1	2:B:317:VAL:O	2.69	0.41
1:A:268:SER:HB3	1:A:353:LYS:HZ2	1.86	0.41
1:A:105:SER:OG	1:A:198:HIS:CE1	2.74	0.41
1:A:175:ASN:O	1:A:178:ILE:HG22	2.20	0.41
1:A:57:ASN:HA	1:A:129:ALA:O	2.21	0.41
1:A:310:LEU:O	1:A:311:LYS:C	2.59	0.40
1:A:8:VAL:O	1:A:9:PRO:C	2.59	0.40
1:A:362:THR:HG21	1:A:367:GLN:CG	2.51	0.40
2:B:13:LYS:CB	2:B:14:PRO:HD2	2.16	0.40
1:A:341:ILE:O	1:A:349:LEU:CD1	2.64	0.40
2:B:52:PRO:C	2:B:54:ASN:N	2.74	0.40
1:A:543:GLY:HA3	2:B:283:LEU:O	2.21	0.40
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.86	0.40
1:A:447:ASN:C	1:A:449:GLU:H	2.25	0.40
1:A:518:VAL:HG12	1:A:518:VAL:O	2.21	0.40
2:B:401:TRP:O	2:B:404:GLU:N	2.55	0.40
1:A:406:TRP:CZ3	1:A:407:GLN:CB	3.04	0.40
1:A:555:GLY:C	1:A:556:ILE:HG13	2.41	0.40

All (3) 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:227:PHE:N	2:B:251:SER:N[2_656]	1.59	0.61
2:B:227:PHE:C	2:B:250:ASP:N[2_656]	2.05	0.15
2:B:226:PRO:O	2:B:249:LYS:C[2_656]	2.14	0.06



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/560 (99%)	383 (69%)	118 (21%)	55 (10%)	1	3
2	B	425/447 (95%)	304 (72%)	82 (19%)	39 (9%)	1	4
All	All	981/1007 (97%)	687 (70%)	200 (20%)	94 (10%)	1	3

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	27	THR
1	A	29	GLU
1	A	43	LYS
1	A	46	LYS
1	A	68	SER
1	A	85	GLN
1	A	126	LYS
1	A	138	GLU
1	A	158	ALA
1	A	159	ILE
1	A	236	PRO
1	A	237	ASP
1	A	476	LYS
1	A	543	GLY
1	A	553	SER
2	B	14	PRO
2	B	114	ALA
2	B	161	GLN
2	B	195	ILE
2	B	218	ASP
2	B	221	HIS
2	B	223	LYS
2	B	226	PRO
2	B	402	TRP

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Mol	Chain	Res	Type
2	B	420	PRO
1	A	4	PRO
1	A	42	GLU
1	A	123	ASP
1	A	149	LEU
1	A	254	VAL
1	A	262	GLY
1	A	276	VAL
1	A	348	ASN
1	A	518	VAL
2	B	78	ARG
2	B	116	PHE
2	B	196	GLY
2	B	302	GLU
2	B	333	GLY
1	A	53	GLU
1	A	91	GLN
1	A	153	TRP
1	A	235	HIS
1	A	265	ASN
1	A	431	LYS
1	A	448	ARG
1	A	475	GLN
2	B	9	PRO
2	B	77	PHE
2	B	85	GLN
2	B	97	PRO
2	B	103	ASN
2	B	164	MET
2	B	300	GLU
1	A	51	GLY
1	A	78	ARG
1	A	114	ALA
1	A	176	PRO
1	A	219	LYS
1	A	242	GLN
1	A	243	PRO
1	A	557	ARG
2	B	83	ARG
2	B	88	TRP
2	B	155	GLY
2	B	173	LYS

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Mol	Chain	Res	Type
2	B	214	LEU
2	B	358	ARG
2	B	378	GLU
2	B	379	SER
1	A	8	VAL
1	A	221	HIS
1	A	294	PRO
2	B	175	ASN
2	B	193	LEU
2	B	225	PRO
1	A	9	PRO
1	A	49	LYS
1	A	195	ILE
1	A	554	ALA
2	B	5	ILE
2	B	89	GLU
2	B	312	GLU
1	A	150	PRO
1	A	169	GLU
1	A	345	PRO
2	B	170	PRO
1	A	111	VAL
2	B	276	VAL
1	A	444	GLY
2	B	133	PRO
1	A	213	GLY
1	A	522	ILE

### 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	490/500 (98%)	438 (89%)	52 (11%)	8	31
2	B	379/404 (94%)	323 (85%)	56 (15%)	4	17
All	All	869/904 (96%)	761 (88%)	108 (12%)	6	24

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	66	LYS
1	A	67	ASP
1	A	78	ARG
1	A	82	LYS
1	A	83	ARG
1	A	103	ASN
1	A	116	PHE
1	A	127	TYR
1	A	131	THR
1	A	132	ILE
1	A	145	GLN
1	A	156	SER
1	A	162	SER
1	A	167	ILE
1	A	173	LYS
1	A	175	ASN
1	A	181	CYS
1	A	182	GLN
1	A	187	LEU
1	A	199	ARG
1	A	203	GLU
1	A	206	ARG
1	A	210	LEU
1	A	238	LYS
1	A	245	VAL
1	A	247	PRO
1	A	249	LYS
1	A	256	ASP
1	A	306	ASN
1	A	315	HIS
1	A	321	PRO
1	A	330	GLN
1	A	340	GLN
1	A	362	THR
1	A	391	LEU
1	A	396	GLU
1	A	398	TRP
1	A	409	THR
1	A	414	TRP
1	A	457	TYR
1	A	460	ASN

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Mol	Chain	Res	Type
1	A	464	GLN
1	A	471	ASN
1	A	474	ASN
1	A	477	THR
1	A	488	ASP
1	A	514	GLU
1	A	516	GLU
1	A	529	GLU
1	A	548	VAL
1	A	557	ARG
2	B	2	ILE
2	B	22	LYS
2	B	29	GLU
2	B	40	GLU
2	B	41	MET
2	B	57	ASN
2	B	58	THR
2	B	63	ILE
2	B	67	ASP
2	B	85	GLN
2	B	88	TRP
2	B	101	LYS
2	B	110	ASP
2	B	113	ASP
2	B	123	ASP
2	B	138	GLU
2	B	161	GLN
2	B	162	SER
2	B	181	CYS
2	B	186	ASP
2	B	194	GLU
2	B	200	THR
2	B	206	ARG
2	B	210	LEU
2	B	215	THR
2	B	216	THR
2	B	217	PRO
2	B	219	LYS
2	B	221	HIS
2	B	224	GLU
2	B	240	THR
2	B	250	ASP

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Mol	Chain	Res	Type
2	B	253	THR
2	B	255	ASN
2	B	261	VAL
2	B	265	ASN
2	B	271	TYR
2	B	277	ARG
2	B	284	ARG
2	B	290	THR
2	B	293	ILE
2	B	295	LEU
2	B	297	GLU
2	B	305	GLU
2	B	307	ARG
2	B	330	GLN
2	B	332	GLN
2	B	342	TYR
2	B	346	PHE
2	B	348	ASN
2	B	394	GLN
2	B	395	LYS
2	B	403	THR
2	B	405	TYR
2	B	410	TRP
2	B	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	96	HIS
1	A	145	GLN
1	A	221	HIS
1	A	235	HIS
1	A	269	GLN
1	A	306	ASN
1	A	332	GLN
1	A	373	GLN
1	A	407	GLN
1	A	418	ASN
1	A	460	ASN
1	A	464	GLN
1	A	471	ASN

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Mol	Chain	Res	Type
1	A	474	ASN
1	A	487	GLN
2	B	85	GLN
2	B	96	HIS
2	B	137	ASN
2	B	161	GLN
2	B	269	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
4	HBY	A	562	-	21,23,23	3.64	13 (61%)	24,32,32	3.29	6 (25%)

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
4	HBY	A	562	-	-	0/13/29/29	0/1/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	562	HBY	O2-C9	-6.01	1.22	1.34
4	A	562	HBY	C13-S2	-3.71	1.76	1.80
4	A	562	HBY	C8-C3	2.36	1.43	1.39
4	A	562	HBY	C8-C7	2.38	1.43	1.38
4	A	562	HBY	C7-C6	2.93	1.44	1.38
4	A	562	HBY	C4-N1	2.97	1.47	1.42
4	A	562	HBY	C5-C6	3.05	1.44	1.38
4	A	562	HBY	C5-C4	3.09	1.44	1.39
4	A	562	HBY	C3-N2	3.20	1.45	1.39
4	A	562	HBY	C9-N1	3.22	1.42	1.37
4	A	562	HBY	C3-C4	3.93	1.44	1.40
4	A	562	HBY	O1-C9	8.29	1.34	1.21
4	A	562	HBY	C2-S1	8.50	1.78	1.66

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	562	HBY	C3-N2-C2	-9.49	115.72	124.70
4	A	562	HBY	C14-S2-C13	-5.61	92.09	101.21
4	A	562	HBY	O2-C9-O1	-4.75	114.93	124.69
4	A	562	HBY	C3-C4-N1	-2.35	114.58	118.10
4	A	562	HBY	C15-O3-C6	2.55	123.49	117.51
4	A	562	HBY	O2-C9-N1	9.13	121.88	110.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	562	HBY	5	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	558/560 (99%)	-0.06	17 (3%)	54	25	36, 93, 124, 124	1 (0%)
2	B	427/447 (95%)	-0.15	11 (2%)	59	29	30, 77, 123, 124	3 (0%)
All	All	985/1007 (97%)	-0.10	28 (2%)	56	27	30, 86, 124, 124	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	PRO	5.2
2	B	225	PRO	4.9
2	B	91	GLN	4.2
1	A	18	GLY	3.7
1	A	133	PRO	3.4
1	A	140	PRO	3.4
1	A	129	ALA	3.3
1	A	291	GLU	3.2
2	B	218	ASP	3.1
1	A	130	PHE	3.1
2	B	358	ARG	2.9
1	A	68	SER	2.8
2	B	230	MET	2.8
2	B	409	THR	2.7
1	A	139	THR	2.7
1	A	132	ILE	2.6
2	B	309	ILE	2.5
1	A	54	ASN	2.4
1	A	193	LEU	2.3
2	B	231	GLY	2.3
1	A	66	LYS	2.3
1	A	142	ILE	2.2
2	B	2	ILE	2.2
1	A	67	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	357	MET	2.1
1	A	285	GLY	2.0
1	A	63	ILE	2.0
1	A	553	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HBV	A	562	22/22	0.93	0.32	0.87	88,91,96,98	0
3	MN	A	561	1/1	0.87	0.20	-	89,89,89,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.