



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:07 PM GMT

PDB ID : 1S6P
Title : CRYSTAL STRUCTURE OF HUMAN IMMUNODEFICIENCY VIRUS
TYPE 1 REVERSE TRANSCRIPTASE (RT) IN COMPLEX WITH
JANSSEN-R100943
Authors : Das, K.; Arnold, E.
Deposited on : 2004-01-26
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

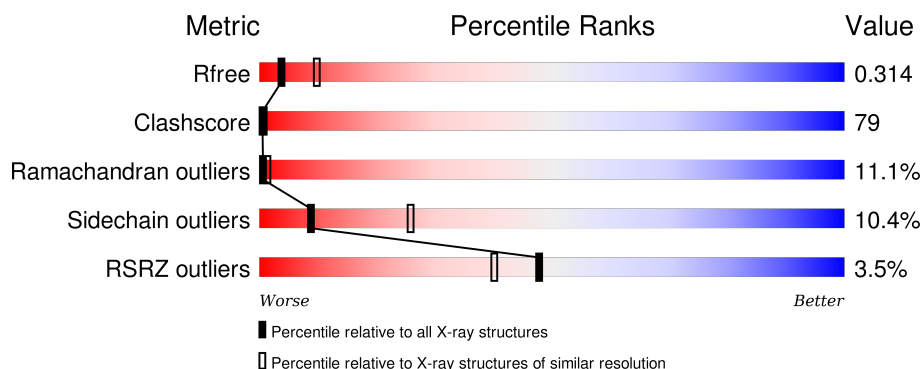
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 ≥ 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	<div> <div>4%</div> <div>21%</div> <div>62%</div> <div>15%</div> <div>..</div> </div>
2	B	430	<div> <div>3%</div> <div>19%</div> <div>59%</div> <div>20%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8202 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 POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	18	0	0
			4498	2913	748	830	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	17	0	0
			3529	2300	584	638	7			

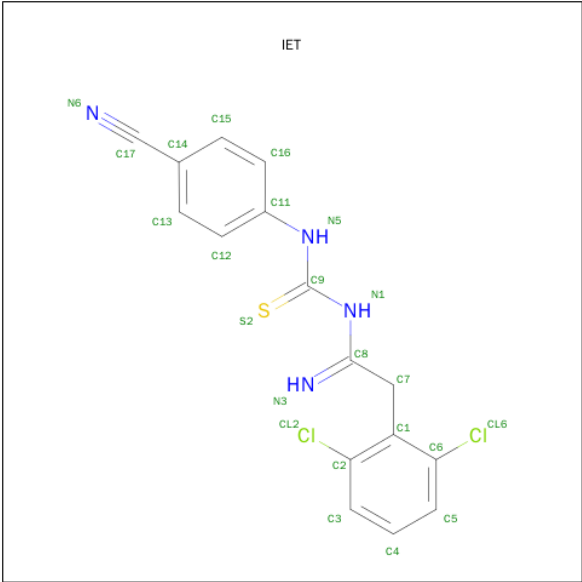
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 1-(4-CYANO-PHENYL)-3-[2-(2,6-DICHLORO-PHENYL)-1-IMINO-ETHYL]-THIOUREA (three-letter code: IET) (formula: C₁₆H₁₂Cl₂N₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	S	0	0
			23	16	2	4	1		

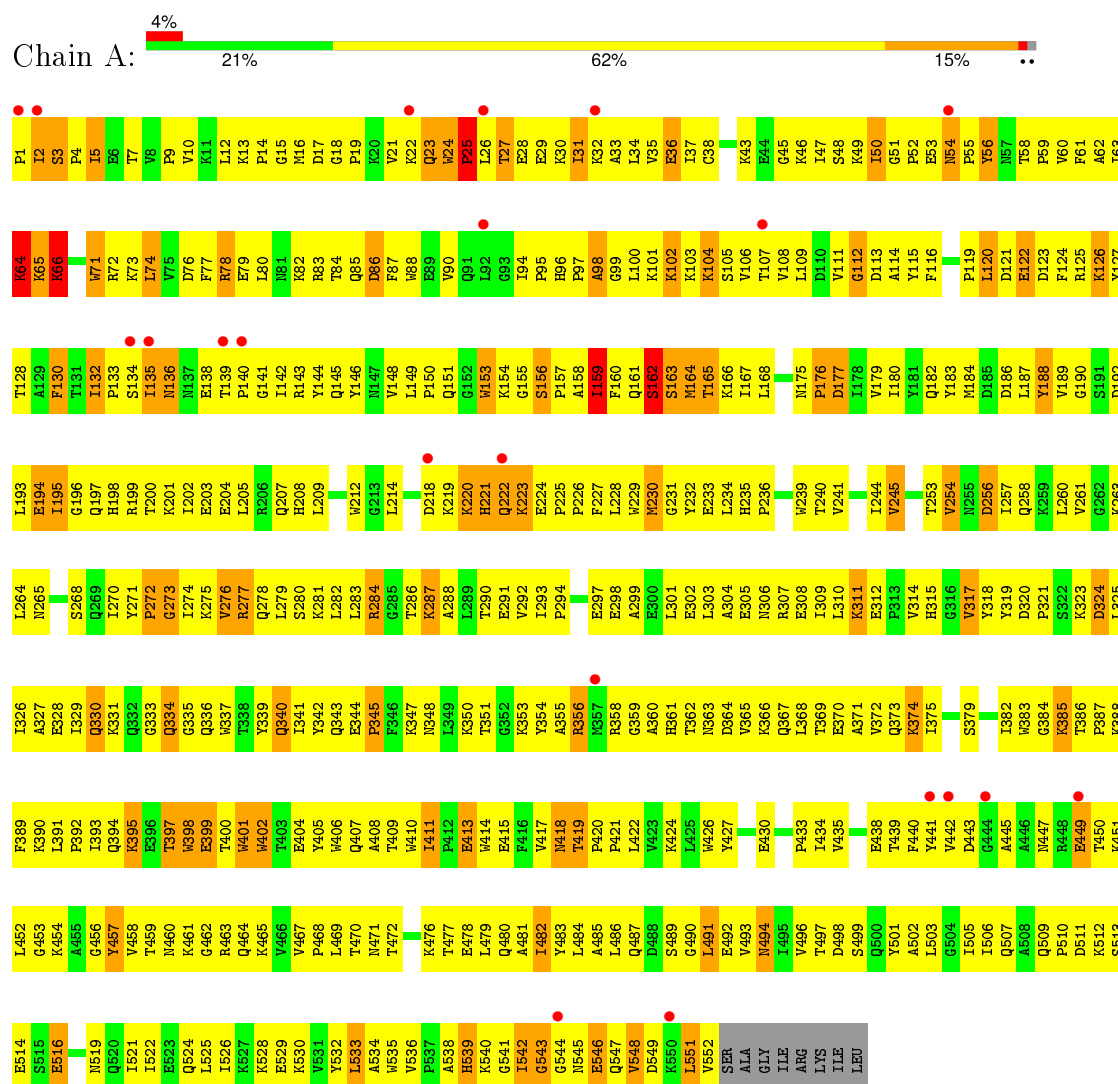
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	70	Total	O	0	0
			70	70		

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: POL polyprotein [Contains: Reverse transcriptase]





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.70Å 67.40Å 104.30Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.82	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-2.90) 87.2 (19.95-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.83Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.245 , 0.312 0.252 , 0.314	Depositor DCC
R_{free} test set	1584 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31794 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.67	1/4616 (0.0%)	0.90	8/6271 (0.1%)
2	B	0.66	2/3634 (0.1%)	0.95	9/4940 (0.2%)
All	All	0.67	3/8250 (0.0%)	0.92	17/11211 (0.2%)

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	1	0
2	B	0	1
All	All	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ILE	CG1-CD1	23.29	3.11	1.50
2	B	224	GLU	C-N	-5.33	1.24	1.34
2	B	225	PRO	N-CD	-5.15	1.40	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ILE	CB-CG1-CD1	-20.89	55.42	113.90
1	A	72	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	B	242	GLN	N-CA-C	7.12	130.24	111.00
1	A	287	LYS	O-C-N	6.82	133.61	122.70
2	B	83	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	284	ARG	NE-CZ-NH2	6.49	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	VAL	N-CA-C	6.30	128.01	111.00
1	A	221	HIS	N-CA-CB	-6.23	99.38	110.60
2	B	225	PRO	O-C-N	-6.10	109.51	121.10
2	B	225	PRO	CB-CA-C	-6.10	96.76	112.00
2	B	78	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	B	225	PRO	CA-N-CD	5.91	119.98	111.70
1	A	273	GLY	N-CA-C	5.87	127.78	113.10
1	A	162	SER	N-CA-C	-5.36	96.54	111.00
1	A	220	LYS	O-C-N	5.23	131.07	122.70
2	B	130	PHE	N-CA-C	-5.17	97.05	111.00
2	B	411	ILE	C-N-CD	5.10	139.11	128.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	31	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	PHE	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	4498	0	4560	697	0
2	B	3529	0	3568	615	0
3	A	1	0	0	0	0
4	A	23	0	12	5	0
5	A	81	0	0	8	0
5	B	70	0	0	5	0
All	All	8202	0	8140	1277	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 79.

All (1277) 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:64:LYS:O	1:A:66:LYS:HG2	1.34	1.25
2:B:139:THR:CG2	2:B:140:PRO:HD2	1.66	1.24
1:A:222:GLN:O	1:A:224:GLU:HG3	1.41	1.16
1:A:497:THR:HG22	1:A:499:SER:H	1.09	1.16
2:B:358:ARG:HG2	2:B:359:GLY:H	1.09	1.16
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.23	1.15
2:B:206:ARG:HE	2:B:218:ASP:HB2	1.09	1.14
2:B:296:THR:HG22	2:B:297:GLU:H	1.10	1.14
1:A:90:VAL:HG11	1:A:161:GLN:HE22	1.13	1.13
1:A:362:THR:HG22	1:A:363:ASN:H	0.97	1.13
2:B:135:ILE:H	2:B:135:ILE:CD1	1.61	1.12
2:B:195:ILE:HG23	2:B:196:GLY:H	1.10	1.11
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.28	1.10
2:B:135:ILE:N	2:B:135:ILE:HD12	1.66	1.09
1:A:454:LYS:HB2	1:A:552:VAL:HG13	1.16	1.07
2:B:220:LYS:HE3	2:B:231:GLY:HA2	1.35	1.07
1:A:288:ALA:HB1	1:A:291:GLU:HB2	1.38	1.06
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.33	1.06
1:A:442:VAL:HG22	1:A:481:ALA:HB1	1.38	1.05
1:A:397:THR:HG21	1:A:424:LYS:HA	1.36	1.03
1:A:84:THR:HG23	1:A:154:LYS:HE2	1.35	1.03
1:A:411:ILE:HD13	1:A:411:ILE:H	1.23	1.02
1:A:64:LYS:C	1:A:66:LYS:HG2	1.78	1.02
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.42	1.02
2:B:297:GLU:HG3	2:B:298:GLU:H	1.22	1.00
2:B:326:ILE:HB	2:B:342:TYR:CE1	1.96	1.00
2:B:295:LEU:HD12	2:B:300:GLU:HG2	1.43	1.00
1:A:492:GLU:HG3	1:A:530:LYS:HB2	1.44	0.99
2:B:216:THR:HB	2:B:218:ASP:OD2	1.62	0.98
2:B:74:LEU:HD21	2:B:411:ILE:HD11	1.47	0.97
1:A:108:VAL:HG12	1:A:188:TYR:CG	1.99	0.97
2:B:221:HIS:ND1	2:B:229:TRP:HB2	1.80	0.97
2:B:358:ARG:HA	2:B:362:THR:HB	1.47	0.96
2:B:135:ILE:H	2:B:135:ILE:HD12	0.81	0.95
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.44	0.95
2:B:326:ILE:HB	2:B:342:TYR:HE1	1.30	0.94
1:A:362:THR:HG22	1:A:363:ASN:N	1.80	0.94
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.30	0.94
1:A:19:PRO:O	1:A:56:TYR:HB3	1.67	0.93
2:B:253:THR:O	2:B:257:ILE:HG22	1.68	0.93
1:A:362:THR:CG2	1:A:363:ASN:H	1.80	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:O	2:B:367:GLN:HG3	1.68	0.92
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.49	0.92
2:B:296:THR:CG2	2:B:297:GLU:H	1.82	0.92
1:A:411:ILE:H	1:A:411:ILE:CD1	1.82	0.91
2:B:174:GLN:O	2:B:176:PRO:HD3	1.70	0.91
1:A:90:VAL:HG11	1:A:161:GLN:NE2	1.85	0.91
1:A:422:LEU:HD23	1:A:424:LYS:HD3	1.51	0.91
2:B:171:PHE:HB2	2:B:208:HIS:HD2	1.35	0.90
1:A:449:GLU:HG3	1:A:450:THR:N	1.83	0.90
2:B:31:ILE:O	2:B:35:VAL:HG23	1.72	0.90
2:B:275:LYS:HG2	2:B:277:ARG:HH21	1.35	0.90
2:B:358:ARG:HG2	2:B:359:GLY:N	1.87	0.89
2:B:139:THR:CG2	2:B:140:PRO:CD	2.50	0.88
1:A:53:GLU:HG3	1:A:54:ASN:H	1.38	0.88
1:A:442:VAL:CG2	1:A:481:ALA:HB1	2.02	0.88
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.04	0.88
2:B:12:LEU:HD12	2:B:83:ARG:O	1.73	0.88
1:A:64:LYS:O	1:A:66:LYS:N	2.06	0.88
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.37	0.88
1:A:115:TYR:OH	1:A:151:GLN:HG3	1.74	0.88
2:B:260:LEU:HG	2:B:264:LEU:HD11	1.56	0.87
1:A:38:CYS:HB3	1:A:144:TYR:CE1	2.10	0.87
1:A:240:THR:HG22	1:A:241:VAL:N	1.90	0.87
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.05	0.86
1:A:134:SER:OG	1:A:139:THR:HB	1.75	0.86
1:A:441:TYR:HB3	1:A:548:VAL:HG11	1.56	0.86
1:A:258:GLN:HG2	1:A:283:LEU:HD22	1.56	0.86
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.56	0.86
1:A:254:VAL:HG23	1:A:293:ILE:HD11	1.58	0.86
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.39	0.85
2:B:373:GLN:NE2	2:B:406:TRP:HA	1.90	0.85
2:B:183:TYR:HD1	2:B:380:ILE:HG23	1.40	0.85
2:B:296:THR:HG22	2:B:297:GLU:N	1.89	0.85
2:B:221:HIS:CE1	2:B:229:TRP:HB2	2.11	0.85
1:A:291:GLU:O	1:A:293:ILE:HD12	1.77	0.85
1:A:497:THR:HG22	1:A:499:SER:N	1.92	0.84
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.07	0.84
1:A:195:ILE:O	1:A:199:ARG:HG2	1.74	0.84
2:B:195:ILE:HG23	2:B:196:GLY:N	1.91	0.84
2:B:380:ILE:O	2:B:384:GLY:HA2	1.78	0.84
2:B:298:GLU:O	2:B:302:GLU:N	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:241:VAL:H	1.39	0.84
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.57	0.84
2:B:1:PRO:HD3	2:B:117:SER:HA	1.59	0.84
2:B:104:LYS:CB	2:B:192:ASP:HA	2.07	0.83
1:A:218:ASP:O	1:A:221:HIS:HB2	1.77	0.83
1:A:27:THR:HB	1:A:29:GLU:HG2	1.61	0.83
1:A:545:ASN:O	1:A:548:VAL:HG22	1.79	0.82
1:A:479:LEU:O	1:A:521:ILE:HD11	1.79	0.82
2:B:174:GLN:HE21	2:B:174:GLN:HA	1.44	0.82
2:B:101:LYS:O	2:B:236:PRO:HB2	1.80	0.82
2:B:206:ARG:NE	2:B:218:ASP:HB2	1.93	0.82
1:A:60:VAL:HG22	1:A:130:PHE:HB2	1.62	0.81
1:A:447:ASN:HB3	1:A:450:THR:HB	1.60	0.81
1:A:31:ILE:O	1:A:35:VAL:HG23	1.79	0.81
2:B:332:GLN:HG2	2:B:338:THR:HG23	1.60	0.81
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.16	0.81
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.95	0.81
2:B:178:ILE:HD13	2:B:191:SER:HB3	1.61	0.81
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.45	0.81
1:A:356:ARG:CZ	1:A:358:ARG:HG3	2.11	0.81
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.09	0.81
1:A:368:LEU:O	1:A:372:VAL:HG23	1.80	0.81
1:A:96:HIS:HB3	1:A:382:ILE:HD12	1.63	0.81
1:A:288:ALA:HB1	1:A:291:GLU:CB	2.11	0.81
1:A:108:VAL:CG1	1:A:188:TYR:CD2	2.64	0.81
1:A:320:ASP:H	1:A:343:GLN:HE22	1.27	0.81
1:A:441:TYR:HB3	1:A:548:VAL:CG1	2.10	0.80
2:B:27:THR:HG22	2:B:29:GLU:H	1.47	0.80
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.47	0.80
2:B:171:PHE:HB2	2:B:208:HIS:CD2	2.16	0.80
2:B:326:ILE:CB	2:B:342:TYR:HE1	1.94	0.79
1:A:29:GLU:HG3	1:A:30:LYS:N	1.97	0.79
1:A:434:ILE:HG21	1:A:492:GLU:HG2	1.61	0.79
2:B:103:LYS:HG3	2:B:190:GLY:O	1.83	0.79
1:A:64:LYS:O	1:A:66:LYS:CG	2.26	0.79
1:A:23:GLN:O	1:A:25:PRO:HD3	1.81	0.79
2:B:201:LYS:HA	2:B:201:LYS:HE2	1.64	0.79
1:A:540:LYS:HD3	2:B:265:ASN:HD21	1.48	0.78
1:A:476:LYS:HE3	1:A:516:GLU:OE2	1.83	0.78
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.12	0.78
1:A:28:GLU:HG2	1:A:135:ILE:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:O	2:B:295:LEU:HG	1.83	0.78
2:B:339:TYR:CG	2:B:375:ILE:HD11	2.19	0.78
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.64	0.77
2:B:376:THR:HG22	2:B:380:ILE:CD1	2.14	0.77
1:A:2:ILE:HG22	1:A:3:SER:H	1.47	0.77
1:A:132:ILE:CG2	1:A:142:ILE:HB	2.15	0.77
2:B:195:ILE:CG2	2:B:196:GLY:H	1.96	0.77
2:B:335:GLY:O	2:B:355:ALA:HA	1.85	0.77
1:A:12:LEU:HG	1:A:124:PHE:HE1	1.47	0.77
2:B:175:ASN:H	2:B:175:ASN:HD22	1.31	0.77
1:A:439:THR:O	1:A:459:THR:HG22	1.85	0.77
1:A:28:GLU:HA	1:A:31:ILE:CG2	2.14	0.77
1:A:189:VAL:HG21	1:A:205:LEU:CD2	2.15	0.77
2:B:139:THR:HG23	2:B:140:PRO:CD	2.12	0.76
2:B:69:THR:O	2:B:70:LYS:HG3	1.84	0.76
2:B:23:GLN:CG	2:B:133:PRO:HG3	2.14	0.76
2:B:261:VAL:HG13	2:B:276:VAL:CG1	2.14	0.76
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.68	0.76
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.01	0.76
2:B:66:LYS:HD3	2:B:69:THR:HB	1.67	0.76
1:A:104:LYS:HD3	1:A:192:ASP:O	1.84	0.76
2:B:221:HIS:N	2:B:221:HIS:CD2	2.53	0.76
2:B:23:GLN:HG2	2:B:133:PRO:HG3	1.68	0.76
1:A:156:SER:H	1:A:157:PRO:HD2	1.51	0.76
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.65	0.76
2:B:131:THR:OG1	2:B:143:ARG:HG2	1.86	0.75
2:B:267:ALA:HB2	2:B:426:TRP:CZ2	2.21	0.75
1:A:286:THR:HG22	1:A:287:LYS:N	2.00	0.75
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.17	0.75
1:A:29:GLU:HG3	1:A:30:LYS:H	1.51	0.75
2:B:282:LEU:O	2:B:293:ILE:HD11	1.85	0.75
1:A:101:LYS:O	1:A:103:LYS:HG2	1.86	0.75
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.20	0.75
1:A:132:ILE:HG22	1:A:142:ILE:HB	1.68	0.75
1:A:286:THR:CG2	1:A:287:LYS:N	2.49	0.75
1:A:195:ILE:HD12	1:A:199:ARG:HH21	1.51	0.75
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.69	0.75
1:A:53:GLU:HG3	1:A:54:ASN:N	2.00	0.75
1:A:34:LEU:HD21	1:A:62:ALA:CB	2.16	0.74
2:B:271:TYR:HB3	2:B:274:ILE:HD13	1.67	0.74
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD22	1:A:214:LEU:HD12	1.69	0.74
2:B:139:THR:HG22	2:B:140:PRO:CD	2.14	0.74
1:A:331:LYS:HE3	1:A:364:ASP:OD1	1.87	0.74
2:B:351:THR:HG22	2:B:351:THR:O	1.87	0.74
2:B:31:ILE:HG22	2:B:35:VAL:CG2	2.18	0.74
1:A:84:THR:CG2	1:A:154:LYS:HE2	2.17	0.74
2:B:33:ALA:O	2:B:37:ILE:HG13	1.88	0.74
1:A:108:VAL:CG1	1:A:188:TYR:CG	2.70	0.73
2:B:358:ARG:CG	2:B:359:GLY:H	1.96	0.73
2:B:69:THR:HG23	2:B:70:LYS:N	2.03	0.73
1:A:339:TYR:O	1:A:340:GLN:HG3	1.88	0.73
1:A:108:VAL:HG12	1:A:188:TYR:CB	2.18	0.73
1:A:132:ILE:HD13	1:A:133:PRO:HD2	1.70	0.73
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.17	0.73
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.22	0.73
1:A:240:THR:CG2	1:A:241:VAL:H	2.00	0.73
2:B:244:ILE:HD13	2:B:244:ILE:H	1.53	0.73
2:B:393:ILE:HG12	2:B:398:TRP:HB2	1.70	0.73
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.54	0.73
2:B:369:THR:O	2:B:373:GLN:HG3	1.89	0.73
1:A:64:LYS:HA	1:A:66:LYS:HD3	1.70	0.73
2:B:277:ARG:H	2:B:277:ARG:HD3	1.53	0.73
2:B:302:GLU:O	2:B:306:ASN:HB2	1.89	0.73
2:B:380:ILE:HD12	2:B:380:ILE:H	1.54	0.73
2:B:80:LEU:HD11	2:B:124:PHE:HZ	1.54	0.73
1:A:442:VAL:HG12	1:A:496:VAL:O	1.87	0.72
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.23	0.72
2:B:103:LYS:HG3	2:B:190:GLY:C	2.09	0.72
1:A:64:LYS:HG3	1:A:66:LYS:HG3	1.71	0.72
1:A:17:ASP:O	1:A:83:ARG:HD3	1.89	0.72
2:B:358:ARG:CA	2:B:362:THR:HB	2.19	0.72
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.71	0.72
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.70	0.72
1:A:427:TYR:CE1	1:A:525:LEU:HD13	2.25	0.72
1:A:164:MET:HE3	1:A:168:LEU:HD11	1.72	0.72
1:A:64:LYS:CG	1:A:64:LYS:O	2.37	0.72
2:B:278:GLN:NE2	2:B:297:GLU:HG3	2.04	0.72
1:A:356:ARG:NE	1:A:358:ARG:HG3	2.05	0.72
1:A:84:THR:HG21	1:A:154:LYS:HB3	1.71	0.72
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.69	0.72
2:B:311:LYS:O	2:B:313:PRO:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.71	0.72
2:B:297:GLU:CG	2:B:298:GLU:H	2.01	0.71
2:B:96:HIS:HD1	2:B:181:TYR:HE2	1.38	0.71
1:A:3:SER:OG	1:A:5:ILE:HG13	1.90	0.71
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.54	0.71
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.25	0.71
1:A:30:LYS:O	1:A:33:ALA:HB3	1.91	0.71
1:A:23:GLN:H	1:A:23:GLN:CD	1.93	0.71
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.56	0.71
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.71	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
2:B:109:LEU:HB2	2:B:218:ASP:OD2	1.91	0.71
1:A:50:ILE:HA	5:A:1095:HOH:O	1.91	0.71
2:B:278:GLN:HE21	2:B:298:GLU:HB2	1.55	0.71
2:B:109:LEU:HD13	2:B:206:ARG:HG2	1.73	0.71
1:A:399:GLU:CD	1:A:402:TRP:HE1	1.92	0.71
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.26	0.71
2:B:365:VAL:HG12	2:B:365:VAL:O	1.90	0.70
2:B:174:GLN:NE2	2:B:174:GLN:HA	2.06	0.70
1:A:96:HIS:HB3	1:A:382:ILE:CD1	2.21	0.70
2:B:1:PRO:HD3	2:B:117:SER:CA	2.20	0.70
2:B:91:GLN:C	2:B:91:GLN:HE21	1.95	0.70
2:B:278:GLN:NE2	2:B:297:GLU:CG	2.54	0.70
2:B:297:GLU:HG3	2:B:298:GLU:N	2.02	0.70
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.27	0.70
2:B:332:GLN:O	2:B:424:LYS:HE2	1.90	0.70
1:A:64:LYS:HG2	1:A:64:LYS:O	1.92	0.70
2:B:339:TYR:CD1	2:B:375:ILE:HD11	2.26	0.70
2:B:1:PRO:O	2:B:2:ILE:HD13	1.91	0.70
1:A:55:PRO:HG2	1:A:143:ARG:HH22	1.57	0.70
1:A:290:THR:HG22	1:A:290:THR:O	1.91	0.69
1:A:124:PHE:CE2	1:A:153:TRP:CZ2	2.79	0.69
2:B:168:LEU:HD11	2:B:180:ILE:HG21	1.74	0.69
2:B:340:GLN:HE21	2:B:340:GLN:N	1.90	0.69
1:A:34:LEU:HD12	1:A:132:ILE:HG12	1.75	0.69
1:A:326:ILE:N	1:A:326:ILE:HD12	2.07	0.69
2:B:69:THR:HG23	2:B:70:LYS:H	1.57	0.69
1:A:491:LEU:O	1:A:529:GLU:HB3	1.93	0.69
2:B:271:TYR:HB3	2:B:274:ILE:CD1	2.22	0.69
1:A:363:ASN:ND2	1:A:365:VAL:H	1.90	0.69
1:A:84:THR:HG23	1:A:154:LYS:CE	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.28	0.69
2:B:295:LEU:O	2:B:295:LEU:CG	2.41	0.69
2:B:241:VAL:O	2:B:243:PRO:HD3	1.91	0.69
1:A:222:GLN:O	1:A:223:LYS:C	2.31	0.69
1:A:108:VAL:HG23	1:A:222:GLN:HB3	1.75	0.69
1:A:128:THR:HB	1:A:146:TYR:HB2	1.75	0.69
2:B:260:LEU:HG	2:B:264:LEU:CD1	2.23	0.69
1:A:197:GLN:O	1:A:200:THR:HG22	1.92	0.69
1:A:483:TYR:HB2	1:A:521:ILE:HG13	1.74	0.69
2:B:376:THR:HG22	2:B:380:ILE:HD11	1.74	0.69
1:A:388:LYS:HE2	5:A:1092:HOH:O	1.93	0.69
1:A:395:LYS:HA	1:A:414:TRP:HZ2	1.56	0.69
1:A:74:LEU:O	1:A:74:LEU:HD23	1.92	0.69
2:B:393:ILE:HG23	2:B:416:PHE:HD1	1.57	0.68
1:A:433:PRO:HB3	2:B:255:ASN:ND2	2.08	0.68
2:B:76:ASP:CG	2:B:78:ARG:HH21	1.96	0.68
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.27	0.68
1:A:87:PHE:CE2	1:A:159:ILE:HD11	2.29	0.68
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.24	0.68
2:B:181:TYR:HD1	2:B:182:GLN:N	1.92	0.68
1:A:208:HIS:CE1	1:A:212:TRP:HE1	2.11	0.68
2:B:111:VAL:O	2:B:113:ASP:N	2.27	0.68
2:B:125:ARG:O	2:B:127:TYR:N	2.27	0.68
2:B:248:GLU:HB2	5:B:1086:HOH:O	1.95	0.67
1:A:96:HIS:HD1	1:A:97:PRO:N	1.92	0.67
2:B:206:ARG:CB	2:B:206:ARG:HH11	2.07	0.67
1:A:34:LEU:HD22	1:A:73:LYS:HB2	1.76	0.67
1:A:193:LEU:HD22	1:A:197:GLN:NE2	2.09	0.67
1:A:64:LYS:HB3	1:A:71:TRP:CD1	2.29	0.67
1:A:422:LEU:CD2	1:A:424:LYS:HD3	2.24	0.67
1:A:17:ASP:OD2	1:A:56:TYR:HE2	1.77	0.67
1:A:406:TRP:CZ2	2:B:418:ASN:O	2.47	0.67
2:B:254:VAL:O	2:B:258:GLN:HG3	1.95	0.67
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.28	0.67
2:B:377:THR:O	2:B:378:GLU:C	2.30	0.67
1:A:95:PRO:HG2	1:A:229:TRP:HH2	1.59	0.67
1:A:497:THR:CG2	1:A:499:SER:HB3	2.25	0.67
2:B:175:ASN:ND2	2:B:175:ASN:H	1.92	0.67
1:A:87:PHE:HE2	1:A:159:ILE:HD11	1.59	0.67
1:A:453:GLY:O	1:A:454:LYS:HD3	1.95	0.66
1:A:96:HIS:HD1	1:A:98:ALA:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.76	0.66
2:B:260:LEU:CG	2:B:264:LEU:HD11	2.25	0.66
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.34	0.66
2:B:277:ARG:O	2:B:281:LYS:HG3	1.96	0.66
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.25	0.66
2:B:206:ARG:HE	2:B:218:ASP:CB	1.99	0.66
1:A:38:CYS:HB3	1:A:144:TYR:HE1	1.58	0.66
2:B:326:ILE:CG2	2:B:342:TYR:HE1	2.08	0.66
2:B:69:THR:CG2	2:B:70:LYS:H	2.08	0.66
1:A:108:VAL:HG11	1:A:188:TYR:CD2	2.30	0.66
2:B:206:ARG:CB	2:B:206:ARG:NH1	2.58	0.66
1:A:363:ASN:HB3	1:A:366:LYS:HG3	1.78	0.66
2:B:176:PRO:O	2:B:178:ILE:N	2.28	0.66
1:A:219:LYS:O	1:A:220:LYS:C	2.34	0.66
2:B:340:GLN:HG2	2:B:427:TYR:CE1	2.31	0.65
2:B:341:ILE:O	2:B:349:LEU:HB2	1.96	0.65
1:A:435:VAL:HA	2:B:290:THR:OG1	1.96	0.65
1:A:29:GLU:CG	1:A:30:LYS:H	2.08	0.65
2:B:252:TRP:O	2:B:292:VAL:HG13	1.95	0.65
2:B:109:LEU:HB2	2:B:218:ASP:CG	2.17	0.65
2:B:358:ARG:H	2:B:358:ARG:HE	1.43	0.65
2:B:202:ILE:O	2:B:205:LEU:N	2.30	0.65
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.26	0.65
1:A:254:VAL:O	1:A:258:GLN:HG3	1.96	0.65
2:B:376:THR:CG2	2:B:380:ILE:HD11	2.26	0.65
2:B:100:LEU:HD13	2:B:179:VAL:HG21	1.79	0.65
1:A:340:GLN:HA	1:A:351:THR:HA	1.78	0.65
2:B:308:GLU:HG3	2:B:309:ILE:N	2.12	0.65
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.27	0.65
1:A:539:HIS:O	1:A:542:ILE:HG12	1.97	0.65
2:B:220:LYS:HE3	2:B:231:GLY:CA	2.21	0.65
2:B:115:TYR:HE2	2:B:157:PRO:CA	2.09	0.65
1:A:434:ILE:HG12	1:A:530:LYS:HB3	1.79	0.65
1:A:28:GLU:HA	1:A:31:ILE:HG23	1.78	0.65
1:A:27:THR:CB	1:A:29:GLU:HG2	2.27	0.65
2:B:324:ASP:O	2:B:343:GLN:HG2	1.96	0.65
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.31	0.65
2:B:232:TYR:HE2	2:B:234:LEU:HD21	1.60	0.65
1:A:356:ARG:HD2	1:A:362:THR:OG1	1.97	0.65
1:A:254:VAL:HG13	1:A:283:LEU:HD13	1.79	0.65
1:A:398:TRP:CZ2	1:A:411:ILE:HD12	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:SER:OG	2:B:198:HIS:ND1	2.30	0.64
1:A:397:THR:CG2	1:A:424:LYS:HA	2.23	0.64
2:B:66:LYS:HD3	2:B:69:THR:CB	2.27	0.64
2:B:299:ALA:HA	2:B:302:GLU:HB2	1.78	0.64
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.32	0.64
1:A:542:ILE:O	1:A:546:GLU:HB2	1.98	0.64
2:B:78:ARG:HD3	2:B:412:PRO:O	1.96	0.64
1:A:406:TRP:CE3	2:B:420:PRO:HD2	2.33	0.64
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.18	0.64
2:B:100:LEU:HD12	2:B:100:LEU:O	1.98	0.64
1:A:108:VAL:CG2	1:A:222:GLN:HB3	2.27	0.64
2:B:342:TYR:HD1	2:B:342:TYR:O	1.81	0.64
1:A:420:PRO:HA	1:A:421:PRO:C	2.19	0.64
1:A:95:PRO:HG2	1:A:229:TRP:CH2	2.33	0.63
2:B:358:ARG:O	2:B:362:THR:CB	2.45	0.63
2:B:364:ASP:O	2:B:366:LYS:N	2.31	0.63
1:A:64:LYS:HG3	1:A:66:LYS:CG	2.29	0.63
2:B:85:GLN:O	2:B:89:GLU:HB2	1.98	0.63
1:A:224:GLU:O	1:A:226:PRO:O	2.17	0.63
2:B:197:GLN:O	2:B:200:THR:HB	1.97	0.63
2:B:85:GLN:CG	2:B:154:LYS:HB3	2.22	0.63
1:A:130:PHE:H	1:A:130:PHE:HD1	1.46	0.63
2:B:31:ILE:C	2:B:35:VAL:HG23	2.18	0.63
1:A:301:LEU:O	1:A:304:ALA:HB3	1.97	0.63
2:B:110:ASP:C	2:B:110:ASP:OD1	2.36	0.63
1:A:405:TYR:CE2	1:A:407:GLN:HB3	2.34	0.63
1:A:175:ASN:N	1:A:176:PRO:CD	2.60	0.63
1:A:443:ASP:HB2	1:A:548:VAL:HG23	1.81	0.63
1:A:539:HIS:O	1:A:542:ILE:HG23	1.98	0.63
2:B:220:LYS:HG3	2:B:231:GLY:HA3	1.79	0.63
1:A:282:LEU:C	1:A:284:ARG:H	2.02	0.63
1:A:163:SER:O	1:A:167:ILE:HG12	1.99	0.63
1:A:99:GLY:HA3	1:A:382:ILE:CG2	2.29	0.63
2:B:5:ILE:HB	2:B:119:PRO:HD2	1.80	0.63
2:B:221:HIS:HD1	2:B:229:TRP:HB2	1.61	0.62
1:A:276:VAL:O	1:A:276:VAL:HG12	1.99	0.62
1:A:51:GLY:O	1:A:53:GLU:N	2.31	0.62
1:A:319:TYR:OH	1:A:385:LYS:HD3	1.98	0.62
1:A:55:PRO:HG2	1:A:143:ARG:NH2	2.14	0.62
2:B:275:LYS:HA	2:B:277:ARG:NH2	2.14	0.62
1:A:198:HIS:CD2	1:A:202:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:LYS:O	2:B:224:GLU:OE1	2.17	0.62
1:A:254:VAL:H	1:A:293:ILE:HD13	1.64	0.62
1:A:142:ILE:HD12	1:A:142:ILE:H	1.63	0.62
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.80	0.62
1:A:319:TYR:CD1	1:A:325:LEU:HD21	2.35	0.62
2:B:220:LYS:CE	2:B:231:GLY:HA2	2.22	0.61
2:B:175:ASN:ND2	2:B:175:ASN:N	2.48	0.61
1:A:479:LEU:HD21	1:A:502:ALA:HA	1.83	0.61
2:B:115:TYR:O	2:B:117:SER:N	2.29	0.61
1:A:434:ILE:HD13	1:A:494:ASN:ND2	2.14	0.61
1:A:32:LYS:HA	1:A:35:VAL:CG2	2.31	0.61
2:B:24:TRP:HE1	2:B:399:GLU:HG3	1.63	0.61
1:A:244:ILE:HG23	1:A:263:LYS:HE2	1.82	0.61
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.63	0.61
1:A:189:VAL:HG21	1:A:205:LEU:HD23	1.81	0.61
1:A:33:ALA:O	1:A:37:ILE:HG12	2.01	0.61
1:A:298:GLU:CD	1:A:298:GLU:N	2.53	0.61
2:B:195:ILE:HG13	2:B:199:ARG:CD	2.30	0.61
1:A:97:PRO:HA	1:A:100:LEU:HG	1.83	0.61
2:B:195:ILE:O	2:B:197:GLN:N	2.33	0.61
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.36	0.61
1:A:142:ILE:HD12	1:A:142:ILE:N	2.16	0.61
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.83	0.61
2:B:281:LYS:O	2:B:284:ARG:HB2	1.99	0.61
2:B:194:GLU:O	2:B:195:ILE:C	2.37	0.61
2:B:402:TRP:CH2	2:B:411:ILE:HD12	2.36	0.60
1:A:226:PRO:HB2	1:A:233:GLU:HG2	1.84	0.60
1:A:98:ALA:CB	1:A:350:LYS:HB2	2.31	0.60
2:B:252:TRP:CE3	2:B:252:TRP:HA	2.37	0.60
2:B:160:PHE:O	2:B:161:GLN:O	2.19	0.60
1:A:122:GLU:HA	1:A:125:ARG:CD	2.31	0.60
1:A:2:ILE:HG22	1:A:3:SER:N	2.14	0.60
2:B:221:HIS:HD2	2:B:221:HIS:N	1.98	0.60
2:B:76:ASP:O	2:B:76:ASP:CG	2.39	0.60
2:B:364:ASP:C	2:B:366:LYS:H	2.05	0.60
2:B:282:LEU:HD11	2:B:293:ILE:HG12	1.83	0.60
1:A:417:VAL:HG12	1:A:419:THR:H	1.66	0.60
1:A:253:THR:OG1	1:A:290:THR:HA	2.01	0.60
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.60
2:B:242:GLN:CG	2:B:242:GLN:O	2.49	0.60
1:A:23:GLN:H	1:A:23:GLN:NE2	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG21	1:A:347:LYS:HD3	1.83	0.60
2:B:391:LEU:HB3	2:B:393:ILE:HG22	1.84	0.60
2:B:149:LEU:CD1	2:B:159:ILE:HB	2.32	0.60
2:B:349:LEU:HD12	2:B:383:TRP:CZ2	2.37	0.60
2:B:30:LYS:HG3	2:B:62:ALA:HB3	1.82	0.60
1:A:286:THR:CG2	1:A:287:LYS:H	2.14	0.60
2:B:252:TRP:HE3	2:B:252:TRP:HA	1.66	0.59
2:B:336:GLN:HA	2:B:354:TYR:O	2.02	0.59
2:B:194:GLU:O	2:B:195:ILE:O	2.20	0.59
1:A:126:LYS:HG3	1:A:127:TYR:CE2	2.38	0.59
2:B:198:HIS:O	2:B:201:LYS:N	2.35	0.59
2:B:244:ILE:O	2:B:244:ILE:HG12	2.01	0.59
1:A:433:PRO:HB3	2:B:255:ASN:HD22	1.65	0.59
2:B:282:LEU:HD11	2:B:294:PRO:HD2	1.83	0.59
2:B:161:GLN:O	2:B:162:SER:C	2.40	0.59
2:B:332:GLN:OE1	2:B:332:GLN:HA	2.01	0.59
1:A:64:LYS:C	1:A:66:LYS:N	2.50	0.59
2:B:80:LEU:HD11	2:B:124:PHE:CZ	2.36	0.59
1:A:109:LEU:HD21	1:A:202:ILE:CG2	2.33	0.59
2:B:66:LYS:HB3	2:B:69:THR:HG22	1.84	0.59
2:B:326:ILE:HB	2:B:342:TYR:CD1	2.38	0.59
1:A:116:PHE:O	1:A:148:VAL:HG21	2.03	0.59
2:B:277:ARG:CD	2:B:277:ARG:H	2.11	0.59
1:A:128:THR:CB	1:A:146:TYR:HB2	2.33	0.59
2:B:69:THR:CG2	2:B:70:LYS:N	2.63	0.59
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.38	0.59
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.38	0.59
1:A:254:VAL:H	1:A:293:ILE:CD1	2.16	0.59
2:B:282:LEU:HG	2:B:293:ILE:HD13	1.84	0.59
2:B:385:LYS:NZ	2:B:385:LYS:HB3	2.17	0.59
2:B:13:LYS:HG3	2:B:14:PRO:HD2	1.85	0.59
1:A:108:VAL:HA	1:A:188:TYR:HA	1.84	0.59
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.38	0.59
2:B:242:GLN:HG2	2:B:242:GLN:O	2.02	0.59
1:A:356:ARG:HG3	1:A:367:GLN:HG2	1.85	0.58
1:A:64:LYS:C	1:A:66:LYS:H	2.05	0.58
2:B:266:TRP:HD1	2:B:422:LEU:HD23	1.65	0.58
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.34	0.58
1:A:58:THR:HG22	1:A:76:ASP:O	2.03	0.58
1:A:134:SER:HB3	1:A:138:GLU:HB3	1.84	0.58
1:A:513:SER:N	1:A:519:ASN:HD21	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PHE:CZ	2:B:205:LEU:HB2	2.38	0.58
1:A:261:VAL:HG22	1:A:279:LEU:HD22	1.86	0.58
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.38	0.58
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.37	0.58
1:A:430:GLU:HA	1:A:430:GLU:OE1	2.03	0.58
1:A:410:TRP:HB3	2:B:365:VAL:HG21	1.85	0.58
1:A:200:THR:HG23	1:A:201:LYS:N	2.18	0.58
2:B:46:LYS:NZ	2:B:116:PHE:HD2	2.01	0.58
1:A:354:TYR:HB2	1:A:374:LYS:HZ1	1.69	0.58
2:B:340:GLN:NE2	2:B:340:GLN:N	2.51	0.58
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.04	0.58
1:A:61:PHE:HB2	1:A:74:LEU:O	2.04	0.58
2:B:273:GLY:C	2:B:274:ILE:HD12	2.23	0.58
1:A:132:ILE:HG22	1:A:142:ILE:O	2.04	0.58
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.39	0.58
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.33	0.58
1:A:130:PHE:N	1:A:130:PHE:HD1	2.02	0.58
1:A:245:VAL:H	1:A:263:LYS:NZ	2.01	0.58
2:B:366:LYS:O	2:B:370:GLU:HG3	2.04	0.57
2:B:217:PRO:O	2:B:219:LYS:N	2.36	0.57
2:B:206:ARG:NH2	2:B:216:THR:O	2.37	0.57
1:A:363:ASN:HD22	1:A:365:VAL:H	1.52	0.57
2:B:149:LEU:H	2:B:149:LEU:HD23	1.69	0.57
1:A:402:TRP:O	1:A:402:TRP:HE3	1.88	0.57
2:B:192:ASP:O	2:B:193:LEU:HD23	2.03	0.57
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.68	0.57
2:B:168:LEU:O	2:B:172:LYS:HG3	2.04	0.57
2:B:379:SER:O	2:B:380:ILE:C	2.43	0.57
2:B:395:LYS:O	2:B:399:GLU:HB2	2.04	0.57
1:A:297:GLU:CD	1:A:297:GLU:H	2.07	0.57
2:B:169:GLU:C	2:B:171:PHE:H	2.06	0.57
2:B:161:GLN:O	2:B:164:MET:N	2.35	0.57
2:B:80:LEU:HD12	2:B:80:LEU:O	2.03	0.57
1:A:179:VAL:HG21	4:A:701:IET:N3	2.20	0.57
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.19	0.57
1:A:447:ASN:CB	1:A:450:THR:HB	2.32	0.57
1:A:88:TRP:CD1	2:B:143:ARG:HD2	2.39	0.57
1:A:353:LYS:O	1:A:374:LYS:NZ	2.38	0.57
1:A:203:GLU:OE2	1:A:207:GLN:NE2	2.37	0.57
2:B:206:ARG:HB2	2:B:206:ARG:HH11	1.70	0.57
1:A:411:ILE:HD13	1:A:411:ILE:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HG13	1:A:196:GLY:N	2.19	0.57
2:B:90:VAL:O	2:B:91:GLN:C	2.43	0.57
1:A:497:THR:HG21	1:A:499:SER:HB3	1.87	0.57
1:A:493:VAL:C	1:A:494:ASN:HD22	2.09	0.57
2:B:238:LYS:O	2:B:240:THR:N	2.38	0.57
1:A:254:VAL:N	1:A:293:ILE:HD13	2.20	0.56
2:B:183:TYR:CE2	2:B:184:MET:HE2	2.40	0.56
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.40	0.56
1:A:360:ALA:HA	1:A:514:GLU:CD	2.26	0.56
2:B:253:THR:HA	2:B:292:VAL:HA	1.86	0.56
2:B:376:THR:O	2:B:379:SER:HB2	2.05	0.56
2:B:59:PRO:HB2	2:B:76:ASP:HB3	1.87	0.56
2:B:116:PHE:CE1	2:B:151:GLN:HG3	2.41	0.56
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.87	0.56
2:B:198:HIS:O	2:B:200:THR:N	2.39	0.56
2:B:201:LYS:HE2	2:B:201:LYS:CA	2.34	0.56
2:B:149:LEU:N	2:B:149:LEU:HD23	2.20	0.56
1:A:492:GLU:OE2	1:A:530:LYS:HD2	2.05	0.56
1:A:438:GLU:OE2	1:A:461:LYS:HB2	2.05	0.56
1:A:524:GLN:O	1:A:528:LYS:HG2	2.06	0.56
1:A:7:THR:HG22	1:A:119:PRO:CB	2.36	0.56
1:A:182:GLN:HB3	5:A:1044:HOH:O	2.05	0.56
2:B:111:VAL:C	2:B:113:ASP:N	2.58	0.56
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.87	0.56
1:A:28:GLU:HA	1:A:31:ILE:HG21	1.87	0.56
1:A:454:LYS:HB2	1:A:552:VAL:CG1	2.11	0.56
2:B:402:TRP:CZ3	2:B:411:ILE:HD12	2.40	0.56
1:A:32:LYS:HA	1:A:35:VAL:HG23	1.86	0.56
1:A:218:ASP:O	1:A:221:HIS:CB	2.50	0.56
1:A:511:ASP:OD1	1:A:512:LYS:HG2	2.05	0.56
1:A:180:ILE:HD12	1:A:180:ILE:N	2.21	0.56
1:A:545:ASN:O	1:A:549:ASP:OD2	2.24	0.56
2:B:279:LEU:HD13	2:B:299:ALA:HB1	1.87	0.56
2:B:41:MET:HE3	2:B:46:LYS:HD3	1.88	0.56
2:B:111:VAL:O	2:B:112:GLY:C	2.44	0.56
1:A:130:PHE:N	1:A:130:PHE:CD1	2.73	0.56
1:A:121:ASP:C	1:A:123:ASP:H	2.09	0.56
1:A:198:HIS:CE1	1:A:202:ILE:HD11	2.40	0.56
2:B:13:LYS:HG2	2:B:14:PRO:O	2.06	0.56
2:B:328:GLU:HG2	2:B:390:LYS:HD3	1.86	0.56
1:A:426:TRP:O	1:A:427:TYR:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:GLY:HA2	2:B:284:ARG:HA	1.88	0.56
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.41	0.56
1:A:244:ILE:HA	1:A:263:LYS:HE2	1.87	0.56
2:B:377:THR:HA	2:B:380:ILE:HD13	1.88	0.55
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.55
2:B:205:LEU:O	2:B:208:HIS:HB3	2.05	0.55
2:B:315:HIS:HB3	5:B:1076:HOH:O	2.06	0.55
2:B:393:ILE:HG23	2:B:416:PHE:CD1	2.41	0.55
1:A:324:ASP:OD2	1:A:324:ASP:N	2.38	0.55
1:A:362:THR:CG2	1:A:363:ASN:N	2.51	0.55
2:B:332:GLN:OE1	2:B:424:LYS:HG2	2.06	0.55
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.41	0.55
1:A:543:GLY:O	2:B:284:ARG:HA	2.07	0.55
1:A:3:SER:OG	1:A:4:PRO:HD2	2.05	0.55
1:A:183:TYR:N	1:A:186:ASP:O	2.40	0.55
1:A:282:LEU:C	1:A:284:ARG:N	2.59	0.55
1:A:226:PRO:CB	1:A:233:GLU:HG2	2.36	0.55
1:A:86:ASP:OD2	1:A:86:ASP:N	2.40	0.55
1:A:434:ILE:HD12	1:A:434:ILE:H	1.71	0.55
1:A:112:GLY:O	1:A:115:TYR:CE2	2.60	0.55
1:A:320:ASP:N	1:A:343:GLN:HE22	2.02	0.55
1:A:401:TRP:HA	1:A:401:TRP:CE3	2.42	0.55
2:B:296:THR:CG2	2:B:297:GLU:N	2.57	0.55
2:B:183:TYR:C	2:B:183:TYR:CD2	2.78	0.55
2:B:342:TYR:C	2:B:342:TYR:CD1	2.77	0.55
1:A:244:ILE:CG2	1:A:310:LEU:HD21	2.37	0.55
1:A:1:PRO:HA	1:A:46:LYS:NZ	2.22	0.55
2:B:283:LEU:O	2:B:285:GLY:N	2.40	0.54
1:A:532:TYR:HE1	2:B:255:ASN:HD21	1.52	0.54
1:A:258:GLN:HE21	1:A:283:LEU:HD11	1.73	0.54
2:B:149:LEU:HB2	2:B:156:SER:HB3	1.89	0.54
2:B:38:CYS:O	2:B:39:THR:C	2.45	0.54
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.72	0.54
2:B:168:LEU:CD2	2:B:209:LEU:HD21	2.38	0.54
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.90	0.54
1:A:490:GLY:C	1:A:492:GLU:H	2.11	0.54
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.89	0.54
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.95	0.54
2:B:169:GLU:O	2:B:171:PHE:N	2.34	0.54
2:B:100:LEU:HD13	2:B:179:VAL:CG2	2.38	0.54
1:A:509:GLN:N	1:A:510:PRO:HD3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.70	0.54
2:B:156:SER:N	2:B:157:PRO:HD2	2.22	0.54
2:B:183:TYR:O	2:B:184:MET:HB2	2.07	0.54
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.90	0.54
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.36	0.54
1:A:325:LEU:HD13	1:A:383:TRP:CE3	2.42	0.54
2:B:214:LEU:HD23	2:B:214:LEU:N	2.23	0.54
1:A:194:GLU:O	1:A:197:GLN:N	2.41	0.54
1:A:401:TRP:CZ3	1:A:509:GLN:NE2	2.76	0.54
2:B:47:ILE:CG2	2:B:146:TYR:CD1	2.91	0.54
2:B:371:ALA:O	2:B:375:ILE:HD12	2.08	0.54
1:A:55:PRO:HG2	1:A:143:ARG:HH12	1.73	0.54
2:B:180:ILE:CG2	2:B:187:LEU:HD22	2.37	0.54
2:B:198:HIS:O	2:B:199:ARG:C	2.44	0.54
1:A:363:ASN:HB3	1:A:366:LYS:CG	2.38	0.54
1:A:434:ILE:HD13	1:A:494:ASN:HD21	1.73	0.54
1:A:450:THR:HG22	1:A:452:LEU:CG	2.38	0.54
2:B:12:LEU:CD1	2:B:83:ARG:O	2.53	0.54
1:A:24:TRP:O	1:A:25:PRO:C	2.45	0.54
2:B:183:TYR:CE1	2:B:380:ILE:HG13	2.43	0.53
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.23	0.53
2:B:314:VAL:O	2:B:314:VAL:HG23	2.08	0.53
2:B:257:ILE:CD1	2:B:279:LEU:HG	2.38	0.53
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.42	0.53
2:B:220:LYS:HG3	2:B:231:GLY:CA	2.39	0.53
1:A:288:ALA:CB	1:A:291:GLU:CB	2.78	0.53
2:B:326:ILE:HG22	2:B:327:ALA:N	2.23	0.53
2:B:331:LYS:HE3	2:B:364:ASP:OD1	2.08	0.53
1:A:503:LEU:HD12	1:A:507:GLN:HG2	1.90	0.53
2:B:110:ASP:HA	2:B:186:ASP:HA	1.90	0.53
1:A:164:MET:HE3	1:A:187:LEU:HD13	1.89	0.53
1:A:298:GLU:CD	1:A:298:GLU:H	2.11	0.53
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.89	0.53
1:A:272:PRO:O	1:A:274:ILE:N	2.41	0.53
1:A:401:TRP:HA	1:A:401:TRP:HE3	1.72	0.53
1:A:82:LYS:O	1:A:82:LYS:HD3	2.08	0.53
1:A:108:VAL:HG12	1:A:188:TYR:HA	1.90	0.53
2:B:261:VAL:O	2:B:265:ASN:HB2	2.08	0.53
2:B:205:LEU:O	2:B:208:HIS:N	2.35	0.53
1:A:253:THR:HG22	1:A:256:ASP:OD2	2.08	0.53
2:B:32:LYS:O	2:B:36:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:O	1:A:372:VAL:N	2.42	0.53
2:B:116:PHE:HE1	2:B:151:GLN:HG3	1.72	0.53
2:B:73:LYS:HE2	2:B:75:VAL:CG2	2.39	0.53
2:B:168:LEU:HD13	2:B:180:ILE:HD12	1.91	0.53
2:B:183:TYR:CE2	2:B:184:MET:CE	2.92	0.53
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.91	0.53
2:B:111:VAL:O	2:B:114:ALA:N	2.36	0.53
1:A:201:LYS:HD3	1:A:204:GLU:OE1	2.09	0.53
1:A:458:VAL:HG23	1:A:551:LEU:HD11	1.90	0.53
1:A:279:LEU:N	1:A:302:GLU:OE2	2.32	0.53
1:A:12:LEU:HD21	1:A:127:TYR:CD1	2.44	0.53
2:B:150:PRO:O	2:B:156:SER:OG	2.19	0.53
1:A:94:ILE:HD12	1:A:94:ILE:N	2.24	0.53
1:A:162:SER:O	1:A:163:SER:C	2.46	0.53
2:B:174:GLN:HE21	2:B:174:GLN:CA	2.11	0.53
2:B:164:MET:O	2:B:166:LYS:N	2.42	0.53
2:B:366:LYS:HG3	2:B:405:TYR:CE2	2.44	0.53
1:A:543:GLY:C	2:B:284:ARG:HA	2.28	0.52
1:A:398:TRP:O	1:A:400:THR:N	2.42	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
1:A:244:ILE:HG23	1:A:263:LYS:HG2	1.89	0.52
1:A:179:VAL:HG11	4:A:701:IET:N3	2.25	0.52
1:A:96:HIS:HD1	1:A:96:HIS:C	2.13	0.52
1:A:331:LYS:HG2	1:A:333:GLY:H	1.75	0.52
1:A:545:ASN:ND2	1:A:549:ASP:OD2	2.42	0.52
2:B:421:PRO:HG2	2:B:422:LEU:H	1.74	0.52
1:A:363:ASN:HD22	1:A:365:VAL:N	2.08	0.52
2:B:277:ARG:HA	2:B:280:SER:OG	2.10	0.52
2:B:263:LYS:HB3	2:B:426:TRP:CE3	2.45	0.52
1:A:275:LYS:O	1:A:276:VAL:HG23	2.09	0.52
1:A:434:ILE:HD12	1:A:434:ILE:N	2.24	0.52
1:A:19:PRO:O	1:A:56:TYR:CB	2.49	0.52
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.40	0.52
1:A:331:LYS:HE2	1:A:333:GLY:CA	2.36	0.52
1:A:254:VAL:HA	1:A:257:ILE:CG2	2.32	0.52
2:B:282:LEU:O	2:B:293:ILE:CD1	2.55	0.52
1:A:540:LYS:HD3	2:B:265:ASN:ND2	2.21	0.52
2:B:278:GLN:HG2	2:B:299:ALA:N	2.25	0.52
2:B:149:LEU:HD13	2:B:159:ILE:HB	1.91	0.52
2:B:241:VAL:C	2:B:243:PRO:HD3	2.29	0.52
2:B:56:TYR:O	2:B:57:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG12	1:A:188:TYR:CA	2.40	0.52
1:A:225:PRO:HG3	1:A:227:PHE:CE2	2.45	0.52
2:B:268:SER:HA	2:B:271:TYR:O	2.09	0.52
1:A:121:ASP:O	1:A:123:ASP:N	2.41	0.52
2:B:23:GLN:HE21	2:B:24:TRP:N	2.07	0.52
2:B:46:LYS:CE	2:B:116:PHE:HD2	2.23	0.52
2:B:391:LEU:HB3	2:B:393:ILE:CG2	2.39	0.52
2:B:376:THR:HG21	2:B:410:TRP:CH2	2.45	0.52
1:A:371:ALA:O	1:A:375:ILE:HD13	2.10	0.52
1:A:208:HIS:O	1:A:212:TRP:HD1	1.91	0.52
1:A:96:HIS:CE1	1:A:98:ALA:H	2.28	0.52
1:A:456:GLY:HA2	1:A:484:LEU:HD23	1.91	0.52
1:A:276:VAL:CG1	1:A:276:VAL:O	2.58	0.52
2:B:17:ASP:O	2:B:18:GLY:O	2.27	0.52
1:A:271:TYR:CE2	1:A:314:VAL:HG23	2.45	0.52
1:A:164:MET:CE	1:A:187:LEU:HD13	2.39	0.51
1:A:354:TYR:HB2	1:A:374:LYS:NZ	2.25	0.51
2:B:295:LEU:O	2:B:295:LEU:CD2	2.59	0.51
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.93	0.51
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.92	0.51
1:A:151:GLN:HG2	1:A:151:GLN:O	2.09	0.51
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.31	0.51
2:B:247:PRO:HB2	2:B:252:TRP:CZ2	2.45	0.51
2:B:253:THR:H	2:B:256:ASP:HB2	1.74	0.51
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.91	0.51
2:B:183:TYR:HE2	2:B:184:MET:HE2	1.76	0.51
2:B:379:SER:HA	2:B:383:TRP:CE3	2.45	0.51
1:A:329:ILE:HG12	1:A:391:LEU:CD2	2.40	0.51
1:A:490:GLY:O	1:A:492:GLU:N	2.44	0.51
2:B:361:HIS:O	2:B:363:ASN:N	2.43	0.51
2:B:395:LYS:NZ	2:B:399:GLU:OE1	2.34	0.51
1:A:406:TRP:HZ2	2:B:418:ASN:O	1.93	0.51
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.45	0.51
1:A:460:ASN:C	1:A:462:GLY:H	2.14	0.51
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.92	0.51
1:A:369:THR:O	1:A:370:GLU:C	2.49	0.51
1:A:101:LYS:O	1:A:102:LYS:C	2.49	0.51
1:A:411:ILE:N	1:A:411:ILE:CD1	2.59	0.51
1:A:125:ARG:O	1:A:145:GLN:HG3	2.10	0.51
1:A:244:ILE:HG22	1:A:310:LEU:HD21	1.92	0.51
1:A:513:SER:CA	1:A:519:ASN:HD21	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LYS:HB3	2:B:426:TRP:HE3	1.75	0.51
1:A:195:ILE:O	1:A:198:HIS:HB3	2.10	0.51
1:A:481:ALA:O	1:A:482:ILE:C	2.48	0.51
1:A:32:LYS:O	1:A:36:GLU:HG2	2.11	0.51
1:A:408:ALA:CB	2:B:337:TRP:HH2	2.24	0.51
2:B:63:ILE:O	2:B:71:TRP:HE3	1.93	0.51
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.46	0.51
2:B:275:LYS:O	2:B:276:VAL:HG23	2.11	0.51
2:B:263:LYS:HE2	2:B:425:LEU:HD13	1.92	0.51
2:B:104:LYS:HB2	2:B:192:ASP:CA	2.21	0.51
2:B:317:VAL:O	2:B:317:VAL:HG23	2.11	0.51
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.41	0.51
2:B:221:HIS:CD2	2:B:221:HIS:H	2.26	0.51
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.51
1:A:55:PRO:HG2	1:A:143:ARG:NH1	2.26	0.51
2:B:66:LYS:CB	2:B:69:THR:CG2	2.89	0.51
1:A:162:SER:O	1:A:164:MET:N	2.44	0.50
1:A:318:TYR:CE1	4:A:701:IET:H16	2.45	0.50
2:B:380:ILE:HD11	2:B:386:THR:HG22	1.93	0.50
1:A:38:CYS:CB	1:A:144:TYR:HE1	2.23	0.50
2:B:295:LEU:O	2:B:295:LEU:HD23	2.11	0.50
1:A:501:TYR:O	1:A:505:ILE:HG12	2.11	0.50
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.40	0.50
2:B:284:ARG:HG3	2:B:284:ARG:HH11	1.77	0.50
2:B:8:VAL:O	2:B:10:VAL:HG23	2.11	0.50
1:A:86:ASP:HA	1:A:154:LYS:HZ2	1.75	0.50
1:A:34:LEU:CG	1:A:62:ALA:HB2	2.40	0.50
2:B:278:GLN:HG3	2:B:299:ALA:HB2	1.92	0.50
2:B:79:GLU:C	2:B:81:ASN:N	2.64	0.50
1:A:450:THR:HG22	1:A:452:LEU:HG	1.93	0.50
2:B:49:LYS:HE2	2:B:142:ILE:HG22	1.93	0.50
1:A:318:TYR:OH	4:A:701:IET:H15	2.11	0.50
2:B:257:ILE:HD11	2:B:279:LEU:HG	1.93	0.50
2:B:342:TYR:C	2:B:342:TYR:HD1	2.14	0.50
2:B:365:VAL:CG1	2:B:365:VAL:O	2.59	0.50
1:A:28:GLU:CG	1:A:135:ILE:O	2.57	0.50
1:A:29:GLU:CG	1:A:30:LYS:N	2.64	0.50
1:A:360:ALA:O	1:A:514:GLU:HG2	2.11	0.50
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.46	0.50
1:A:139:THR:C	1:A:141:GLY:N	2.65	0.50
1:A:84:THR:O	1:A:154:LYS:NZ	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:TRP:CE3	1:A:155:GLY:O	2.65	0.50
1:A:51:GLY:C	1:A:53:GLU:H	2.13	0.50
2:B:325:LEU:HD23	2:B:343:GLN:HG3	1.94	0.50
2:B:156:SER:H	2:B:157:PRO:HD2	1.77	0.50
2:B:329:ILE:HD11	2:B:389:PHE:CD2	2.47	0.50
1:A:77:PHE:CZ	1:A:150:PRO:CB	2.94	0.50
1:A:55:PRO:CG	1:A:143:ARG:NH1	2.75	0.50
1:A:391:LEU:O	1:A:393:ILE:N	2.41	0.50
1:A:97:PRO:HA	1:A:100:LEU:CG	2.41	0.50
1:A:497:THR:HG22	1:A:498:ASP:N	2.26	0.50
2:B:183:TYR:HE2	2:B:184:MET:HG3	1.74	0.50
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.94	0.50
1:A:150:PRO:HG2	1:A:153:TRP:HB2	1.94	0.50
1:A:457:TYR:C	1:A:457:TYR:CD2	2.86	0.50
1:A:90:VAL:O	1:A:90:VAL:HG22	2.12	0.50
2:B:169:GLU:CB	2:B:170:PRO:HD3	2.42	0.50
2:B:149:LEU:HB3	2:B:156:SER:HA	1.94	0.50
2:B:181:TYR:CD1	2:B:182:GLN:N	2.77	0.50
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.12	0.50
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.93	0.49
1:A:261:VAL:HG21	1:A:280:SER:HB3	1.93	0.49
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.76	0.49
1:A:55:PRO:CG	1:A:143:ARG:HH12	2.24	0.49
1:A:481:ALA:O	1:A:484:LEU:HB3	2.12	0.49
1:A:356:ARG:NH1	1:A:358:ARG:HB2	2.26	0.49
1:A:135:ILE:O	1:A:136:ASN:ND2	2.44	0.49
1:A:513:SER:HB3	1:A:519:ASN:ND2	2.27	0.49
1:A:229:TRP:O	1:A:231:GLY:N	2.44	0.49
1:A:319:TYR:CE2	1:A:321:PRO:HA	2.47	0.49
1:A:50:ILE:HD12	1:A:50:ILE:N	2.26	0.49
2:B:385:LYS:HZ3	2:B:385:LYS:HB3	1.77	0.49
2:B:245:VAL:O	2:B:245:VAL:HG13	2.12	0.49
1:A:543:GLY:CA	2:B:284:ARG:HA	2.42	0.49
2:B:372:VAL:HG12	2:B:373:GLN:N	2.27	0.49
1:A:139:THR:HG22	1:A:141:GLY:H	1.77	0.49
1:A:200:THR:HG23	1:A:201:LYS:H	1.76	0.49
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.78	0.49
2:B:66:LYS:CB	2:B:69:THR:HG22	2.42	0.49
1:A:339:TYR:C	1:A:340:GLN:HG3	2.33	0.49
2:B:160:PHE:O	2:B:161:GLN:C	2.49	0.49
2:B:46:LYS:HZ3	2:B:116:PHE:HD2	1.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:O	1:A:225:PRO:C	2.50	0.49
1:A:384:GLY:HA3	2:B:135:ILE:CG2	2.43	0.49
2:B:125:ARG:HD3	2:B:146:TYR:O	2.12	0.49
2:B:47:ILE:O	2:B:47:ILE:HG13	2.12	0.49
1:A:38:CYS:CB	1:A:144:TYR:CE1	2.92	0.49
2:B:255:ASN:HB2	2:B:289:LEU:O	2.12	0.49
1:A:179:VAL:C	1:A:180:ILE:HD12	2.32	0.49
2:B:358:ARG:O	2:B:359:GLY:C	2.51	0.49
1:A:12:LEU:HB3	1:A:83:ARG:O	2.13	0.49
2:B:282:LEU:CD1	2:B:293:ILE:HG12	2.41	0.49
1:A:413:GLU:HG2	1:A:413:GLU:H	1.33	0.49
2:B:191:SER:HG	2:B:198:HIS:HD1	1.53	0.49
1:A:290:THR:CG2	1:A:290:THR:O	2.61	0.49
1:A:402:TRP:O	1:A:402:TRP:CE3	2.65	0.49
1:A:104:LYS:HG3	1:A:192:ASP:HA	1.95	0.49
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.47	0.49
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.95	0.49
2:B:274:ILE:HA	2:B:306:ASN:HD21	1.78	0.49
2:B:172:LYS:NZ	5:B:1070:HOH:O	2.46	0.48
1:A:49:LYS:HG2	1:A:144:TYR:CE2	2.48	0.48
1:A:149:LEU:HA	1:A:150:PRO:HD2	1.72	0.48
1:A:58:THR:CG2	1:A:76:ASP:O	2.61	0.48
2:B:305:GLU:HA	2:B:308:GLU:HG2	1.95	0.48
1:A:478:GLU:HB3	1:A:499:SER:HB2	1.95	0.48
2:B:84:THR:HG22	2:B:85:GLN:N	2.28	0.48
1:A:502:ALA:O	1:A:506:ILE:HG12	2.12	0.48
2:B:76:ASP:O	2:B:78:ARG:N	2.42	0.48
2:B:248:GLU:O	2:B:249:LYS:C	2.52	0.48
1:A:200:THR:O	1:A:204:GLU:HG3	2.13	0.48
2:B:319:TYR:OH	2:B:385:LYS:HD2	2.13	0.48
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.14	0.48
2:B:354:TYR:CG	2:B:355:ALA:N	2.81	0.48
2:B:37:ILE:O	2:B:40:GLU:HB3	2.12	0.48
1:A:1:PRO:HA	1:A:46:LYS:HZ1	1.78	0.48
1:A:64:LYS:HA	1:A:66:LYS:CD	2.41	0.48
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.44	0.48
1:A:260:LEU:HD23	1:A:279:LEU:HD21	1.95	0.48
1:A:218:ASP:N	5:A:1036:HOH:O	2.36	0.48
1:A:320:ASP:H	1:A:343:GLN:NE2	2.02	0.48
1:A:43:LYS:C	1:A:45:GLY:H	2.16	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:HG2	1:A:161:GLN:O	2.13	0.48
2:B:425:LEU:HD23	2:B:425:LEU:O	2.14	0.48
1:A:283:LEU:HD12	1:A:283:LEU:O	2.14	0.48
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.96	0.48
1:A:19:PRO:CG	1:A:80:LEU:HA	2.44	0.48
2:B:57:ASN:C	2:B:57:ASN:ND2	2.66	0.48
1:A:64:LYS:CA	1:A:66:LYS:HG2	2.44	0.48
1:A:239:TRP:O	1:A:240:THR:OG1	2.30	0.48
2:B:216:THR:C	2:B:218:ASP:H	2.17	0.48
1:A:261:VAL:HG13	1:A:276:VAL:CG1	2.43	0.48
2:B:332:GLN:HG2	2:B:338:THR:CG2	2.39	0.48
2:B:426:TRP:HD1	2:B:427:TYR:CD2	2.32	0.48
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.14	0.48
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.95	0.48
1:A:34:LEU:HD12	1:A:132:ILE:CG1	2.44	0.48
1:A:331:LYS:CE	1:A:333:GLY:HA2	2.42	0.48
1:A:111:VAL:O	1:A:114:ALA:N	2.47	0.48
1:A:441:TYR:CE1	1:A:544:GLY:HA3	2.49	0.48
1:A:402:TRP:CE3	1:A:402:TRP:C	2.86	0.48
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.48	0.48
2:B:115:TYR:CE2	2:B:157:PRO:HA	2.30	0.47
2:B:183:TYR:HD2	2:B:183:TYR:C	2.17	0.47
1:A:107:THR:HG1	1:A:198:HIS:CD2	2.32	0.47
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.94	0.47
2:B:54:ASN:ND2	2:B:126:LYS:HA	2.29	0.47
1:A:494:ASN:HD22	1:A:494:ASN:N	2.12	0.47
1:A:410:TRP:HB3	2:B:365:VAL:CG2	2.44	0.47
2:B:354:TYR:CD1	2:B:355:ALA:N	2.83	0.47
1:A:270:ILE:HD12	1:A:351:THR:HG23	1.95	0.47
1:A:485:ALA:O	1:A:486:LEU:C	2.50	0.47
2:B:267:ALA:O	2:B:271:TYR:HB2	2.15	0.47
1:A:120:LEU:O	1:A:121:ASP:C	2.52	0.47
1:A:122:GLU:CG	1:A:122:GLU:O	2.62	0.47
1:A:375:ILE:HG21	1:A:389:PHE:CE1	2.48	0.47
1:A:458:VAL:HG11	1:A:547:GLN:HG2	1.96	0.47
1:A:107:THR:CB	1:A:202:ILE:HD13	2.45	0.47
1:A:160:PHE:CE1	1:A:182:GLN:OE1	2.68	0.47
1:A:188:TYR:CD2	4:A:701:IET:H5	2.50	0.47
1:A:445:ALA:H	1:A:552:VAL:HG11	1.80	0.47
1:A:435:VAL:HG22	2:B:290:THR:CG2	2.31	0.47
1:A:513:SER:H	1:A:519:ASN:HD21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:PRO:C	2:B:219:LYS:H	2.18	0.47
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.96	0.47
1:A:439:THR:HG21	1:A:441:TYR:CE2	2.49	0.47
2:B:401:TRP:O	2:B:402:TRP:C	2.50	0.47
2:B:369:THR:O	2:B:369:THR:HG22	2.14	0.47
1:A:274:ILE:HG23	1:A:306:ASN:OD1	2.14	0.47
1:A:244:ILE:HA	1:A:263:LYS:CE	2.44	0.47
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.97	0.47
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.49	0.47
2:B:418:ASN:O	2:B:419:THR:HB	2.15	0.47
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.13	0.47
1:A:281:LYS:O	1:A:284:ARG:HB3	2.15	0.47
1:A:102:LYS:N	1:A:318:TYR:HD1	2.13	0.47
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.35	0.47
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.49	0.47
1:A:363:ASN:ND2	1:A:365:VAL:HB	2.29	0.47
1:A:139:THR:HG22	1:A:140:PRO:CD	2.45	0.47
2:B:130:PHE:CZ	2:B:144:TYR:CB	2.97	0.47
2:B:195:ILE:CG1	2:B:199:ARG:NE	2.77	0.47
2:B:380:ILE:N	2:B:380:ILE:HD12	2.28	0.47
2:B:380:ILE:O	2:B:384:GLY:CA	2.58	0.47
2:B:307:ARG:HG2	2:B:307:ARG:O	2.14	0.47
2:B:179:VAL:HG23	2:B:179:VAL:O	2.15	0.47
2:B:157:PRO:HG3	2:B:184:MET:HA	1.96	0.47
1:A:34:LEU:CD1	1:A:132:ILE:HG12	2.44	0.47
1:A:124:PHE:O	1:A:124:PHE:CD2	2.68	0.47
1:A:7:THR:HG22	1:A:119:PRO:CG	2.45	0.47
1:A:229:TRP:O	1:A:232:TYR:N	2.48	0.46
2:B:168:LEU:HD23	2:B:209:LEU:HD21	1.97	0.46
2:B:195:ILE:HG13	2:B:199:ARG:HD2	1.96	0.46
1:A:458:VAL:HG21	1:A:547:GLN:HG3	1.97	0.46
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.15	0.46
1:A:85:GLN:HE22	2:B:53:GLU:HA	1.80	0.46
1:A:309:ILE:HG22	1:A:310:LEU:N	2.30	0.46
1:A:326:ILE:HB	1:A:342:TYR:CD1	2.50	0.46
1:A:208:HIS:CE1	1:A:212:TRP:NE1	2.82	0.46
1:A:164:MET:CE	1:A:168:LEU:HD11	2.42	0.46
2:B:274:ILE:HA	2:B:306:ASN:ND2	2.30	0.46
2:B:76:ASP:C	2:B:78:ARG:H	2.19	0.46
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.46
2:B:13:LYS:CG	2:B:14:PRO:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ILE:HG23	2:B:189:VAL:HG12	1.98	0.46
1:A:298:GLU:O	1:A:299:ALA:C	2.53	0.46
2:B:366:LYS:HB2	2:B:405:TYR:CZ	2.50	0.46
1:A:418:ASN:O	1:A:420:PRO:HD3	2.16	0.46
2:B:223:LYS:HA	2:B:223:LYS:HD3	1.70	0.46
1:A:334:GLN:C	1:A:336:GLN:N	2.69	0.46
2:B:221:HIS:HD2	2:B:221:HIS:H	1.61	0.46
2:B:124:PHE:O	2:B:125:ARG:C	2.54	0.46
2:B:47:ILE:HG22	2:B:146:TYR:CD1	2.50	0.46
1:A:450:THR:O	1:A:451:LYS:C	2.53	0.46
1:A:373:GLN:HG2	2:B:394:GLN:HE21	1.80	0.46
1:A:64:LYS:O	1:A:65:LYS:C	2.52	0.46
1:A:180:ILE:CG2	1:A:187:LEU:HD11	2.46	0.46
1:A:228:LEU:HD23	1:A:232:TYR:O	2.15	0.46
2:B:168:LEU:HD13	2:B:180:ILE:CD1	2.45	0.46
1:A:433:PRO:CB	2:B:255:ASN:ND2	2.78	0.46
1:A:470:THR:O	1:A:471:ASN:HB3	2.14	0.46
2:B:245:VAL:O	2:B:245:VAL:HG22	2.15	0.46
1:A:9:PRO:O	1:A:9:PRO:HG2	2.16	0.46
1:A:440:PHE:CD2	1:A:459:THR:HG23	2.51	0.46
2:B:109:LEU:HD12	2:B:218:ASP:OD2	2.14	0.46
2:B:161:GLN:O	2:B:163:SER:N	2.48	0.46
2:B:31:ILE:HG22	2:B:35:VAL:HG22	1.97	0.46
1:A:24:TRP:O	1:A:26:LEU:N	2.49	0.46
1:A:175:ASN:O	1:A:177:ASP:N	2.48	0.46
1:A:98:ALA:HB2	1:A:350:LYS:HB2	1.98	0.46
1:A:480:GLN:O	1:A:481:ALA:C	2.54	0.46
2:B:263:LYS:O	2:B:426:TRP:CZ3	2.68	0.46
1:A:335:GLY:O	1:A:355:ALA:HA	2.15	0.46
2:B:331:LYS:O	2:B:424:LYS:HG3	2.16	0.46
1:A:401:TRP:HE3	1:A:404:GLU:HG3	1.81	0.46
2:B:54:ASN:OD1	2:B:56:TYR:HB2	2.16	0.46
2:B:358:ARG:NE	2:B:358:ARG:H	2.13	0.46
2:B:201:LYS:O	2:B:205:LEU:N	2.49	0.46
2:B:378:GLU:O	2:B:382:ILE:HG13	2.16	0.46
2:B:330:GLN:N	2:B:330:GLN:OE1	2.49	0.46
1:A:339:TYR:CE2	1:A:375:ILE:HG13	2.51	0.46
2:B:254:VAL:O	2:B:257:ILE:HG23	2.16	0.46
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.46
1:A:490:GLY:C	1:A:492:GLU:N	2.70	0.46
2:B:329:ILE:CD1	2:B:389:PHE:HD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:HB2	2:B:69:THR:CG2	2.46	0.46
1:A:348:ASN:ND2	1:A:351:THR:HG22	2.31	0.46
1:A:219:LYS:HB3	5:A:1088:HOH:O	2.16	0.46
1:A:361:HIS:CD2	1:A:505:ILE:HD12	2.51	0.46
1:A:111:VAL:O	1:A:113:ASP:N	2.49	0.46
1:A:311:LYS:NZ	5:A:1040:HOH:O	2.49	0.46
1:A:64:LYS:CA	1:A:66:LYS:HD3	2.43	0.45
2:B:205:LEU:O	2:B:206:ARG:C	2.53	0.45
1:A:394:GLN:O	1:A:397:THR:N	2.44	0.45
2:B:61:PHE:CE1	2:B:76:ASP:HB2	2.42	0.45
1:A:503:LEU:HD23	1:A:535:TRP:HB2	1.98	0.45
2:B:72:ARG:NH2	2:B:409:THR:HG22	2.31	0.45
1:A:319:TYR:CE1	1:A:325:LEU:HD21	2.52	0.45
1:A:379:SER:OG	1:A:387:PRO:HD3	2.16	0.45
2:B:22:LYS:HA	2:B:22:LYS:HD3	1.68	0.45
1:A:434:ILE:CG1	1:A:530:LYS:HD3	2.46	0.45
1:A:12:LEU:HG	1:A:124:PHE:CE1	2.38	0.45
2:B:23:GLN:HG2	2:B:133:PRO:CG	2.43	0.45
2:B:115:TYR:C	2:B:117:SER:H	2.19	0.45
2:B:181:TYR:CD1	2:B:181:TYR:C	2.88	0.45
1:A:12:LEU:H	1:A:12:LEU:HD12	1.80	0.45
1:A:124:PHE:CE2	1:A:153:TRP:CE2	3.04	0.45
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.97	0.45
1:A:408:ALA:HB2	2:B:337:TRP:CH2	2.52	0.45
1:A:306:ASN:O	1:A:310:LEU:HB2	2.15	0.45
1:A:491:LEU:HD12	1:A:491:LEU:H	1.80	0.45
1:A:513:SER:N	1:A:519:ASN:ND2	2.64	0.45
1:A:94:ILE:HG21	1:A:230:MET:HE2	1.98	0.45
2:B:227:PHE:O	2:B:228:LEU:HG	2.16	0.45
2:B:266:TRP:O	2:B:268:SER:N	2.49	0.45
2:B:146:TYR:CE1	2:B:150:PRO:HB3	2.52	0.45
2:B:164:MET:C	2:B:166:LYS:N	2.70	0.45
2:B:376:THR:CG2	2:B:380:ILE:CD1	2.87	0.45
1:A:34:LEU:CD2	1:A:62:ALA:CB	2.85	0.45
1:A:27:THR:C	1:A:29:GLU:H	2.18	0.45
2:B:41:MET:HE2	2:B:41:MET:HB3	1.86	0.45
1:A:491:LEU:O	1:A:529:GLU:CB	2.63	0.45
1:A:203:GLU:O	1:A:207:GLN:HG2	2.16	0.45
1:A:13:LYS:HD2	1:A:16:MET:HE1	1.98	0.45
2:B:279:LEU:HA	2:B:279:LEU:HD12	1.82	0.45
2:B:358:ARG:O	2:B:362:THR:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:OG1	1:A:410:TRP:N	2.48	0.45
1:A:134:SER:HB3	1:A:138:GLU:OE1	2.16	0.45
1:A:457:TYR:C	1:A:457:TYR:HD2	2.18	0.45
2:B:139:THR:HG22	2:B:140:PRO:N	2.29	0.45
2:B:220:LYS:CB	2:B:221:HIS:HD2	2.29	0.45
1:A:12:LEU:N	1:A:12:LEU:HD12	2.31	0.45
2:B:31:ILE:O	2:B:32:LYS:C	2.55	0.45
2:B:47:ILE:HG21	2:B:146:TYR:CD1	2.52	0.45
1:A:450:THR:O	1:A:450:THR:HG22	2.17	0.45
2:B:66:LYS:HB2	2:B:69:THR:HG21	1.98	0.45
1:A:286:THR:HG23	1:A:287:LYS:H	1.81	0.45
1:A:265:ASN:O	1:A:268:SER:N	2.47	0.45
1:A:229:TRP:HE3	1:A:234:LEU:HD11	1.82	0.45
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.98	0.45
2:B:208:HIS:CE1	2:B:212:TRP:HD1	2.34	0.45
1:A:398:TRP:CD1	1:A:399:GLU:N	2.85	0.45
1:A:307:ARG:O	1:A:308:GLU:C	2.55	0.45
2:B:60:VAL:HG23	2:B:60:VAL:O	2.16	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
2:B:54:ASN:HD21	2:B:126:LYS:CA	2.30	0.45
2:B:402:TRP:O	2:B:403:THR:C	2.54	0.45
1:A:105:SER:OG	1:A:198:HIS:CG	2.70	0.45
1:A:195:ILE:HA	1:A:198:HIS:HB3	1.97	0.45
1:A:270:ILE:O	1:A:272:PRO:HD3	2.17	0.45
1:A:426:TRP:HB3	1:A:526:ILE:HD12	1.99	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HE2	2.17	0.45
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.52	0.45
2:B:266:TRP:C	2:B:268:SER:H	2.20	0.45
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.45
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.99	0.44
2:B:200:THR:O	2:B:204:GLU:N	2.34	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CE1	2.52	0.44
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.81	0.44
2:B:376:THR:HG22	2:B:380:ILE:HD13	1.97	0.44
2:B:374:LYS:O	2:B:375:ILE:C	2.54	0.44
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.48	0.44
2:B:66:LYS:HA	5:B:1037:HOH:O	2.17	0.44
2:B:38:CYS:O	2:B:40:GLU:N	2.50	0.44
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.79	0.44
2:B:109:LEU:HD12	2:B:216:THR:HG21	1.99	0.44
2:B:220:LYS:HB2	2:B:221:HIS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.88	0.44
2:B:58:THR:HG22	2:B:59:PRO:HD2	1.98	0.44
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.53	0.44
2:B:27:THR:HG22	2:B:28:GLU:N	2.32	0.44
2:B:346:PHE:N	2:B:346:PHE:CD1	2.85	0.44
1:A:161:GLN:O	1:A:162:SER:O	2.36	0.44
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.99	0.44
1:A:43:LYS:C	1:A:45:GLY:N	2.71	0.44
2:B:54:ASN:HD21	2:B:126:LYS:HA	1.82	0.44
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.53	0.44
1:A:62:ALA:O	1:A:63:ILE:CG2	2.66	0.44
1:A:121:ASP:C	1:A:123:ASP:N	2.71	0.44
1:A:96:HIS:ND1	1:A:96:HIS:C	2.71	0.44
1:A:536:VAL:HG12	1:A:541:GLY:HA3	1.99	0.44
1:A:132:ILE:HD13	1:A:133:PRO:CD	2.44	0.44
1:A:127:TYR:N	1:A:127:TYR:CD2	2.84	0.44
1:A:148:VAL:O	1:A:150:PRO:CD	2.66	0.44
1:A:194:GLU:O	1:A:195:ILE:C	2.56	0.44
2:B:72:ARG:NH2	2:B:409:THR:CG2	2.81	0.44
1:A:328:GLU:HG2	1:A:390:LYS:CB	2.44	0.44
1:A:482:ILE:CD1	1:A:502:ALA:HB1	2.47	0.44
2:B:169:GLU:O	2:B:172:LYS:N	2.50	0.44
2:B:195:ILE:O	2:B:196:GLY:C	2.54	0.44
2:B:53:GLU:OE1	2:B:53:GLU:N	2.37	0.44
1:A:452:LEU:HD23	1:A:470:THR:HA	1.99	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.65	0.44
1:A:254:VAL:CA	1:A:257:ILE:HG22	2.38	0.44
2:B:79:GLU:O	2:B:81:ASN:N	2.51	0.44
2:B:86:ASP:O	2:B:89:GLU:HB3	2.17	0.44
1:A:17:ASP:CG	1:A:18:GLY:H	2.21	0.44
1:A:450:THR:O	1:A:452:LEU:HG	2.17	0.44
1:A:2:ILE:HD11	1:A:45:GLY:O	2.18	0.44
2:B:107:THR:HA	2:B:232:TYR:O	2.18	0.44
1:A:282:LEU:O	1:A:284:ARG:N	2.51	0.44
2:B:228:LEU:HA	2:B:228:LEU:HD23	1.85	0.44
1:A:469:LEU:CD1	1:A:477:THR:HG22	2.46	0.44
2:B:13:LYS:HG2	2:B:14:PRO:N	2.30	0.44
2:B:73:LYS:HE2	2:B:75:VAL:HG23	1.99	0.44
1:A:122:GLU:HG2	1:A:122:GLU:O	2.17	0.44
1:A:19:PRO:HG3	1:A:80:LEU:HA	2.00	0.44
1:A:55:PRO:HG2	1:A:143:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:HB3	1:A:323:LYS:HZ2	1.83	0.44
1:A:244:ILE:CA	1:A:263:LYS:HE2	2.48	0.44
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.76	0.44
2:B:278:GLN:HE22	2:B:297:GLU:CG	2.30	0.43
2:B:58:THR:HA	2:B:59:PRO:HD3	1.75	0.43
2:B:364:ASP:C	2:B:366:LYS:N	2.65	0.43
1:A:513:SER:H	1:A:519:ASN:ND2	2.16	0.43
1:A:292:VAL:O	1:A:294:PRO:HD3	2.18	0.43
1:A:27:THR:C	1:A:29:GLU:N	2.71	0.43
2:B:72:ARG:HH21	2:B:151:GLN:HE22	1.65	0.43
2:B:308:GLU:C	2:B:310:LEU:N	2.71	0.43
1:A:102:LYS:O	1:A:103:LYS:HD3	2.18	0.43
2:B:300:GLU:OE1	2:B:300:GLU:O	2.36	0.43
1:A:433:PRO:CB	2:B:255:ASN:HD22	2.31	0.43
1:A:139:THR:C	1:A:141:GLY:H	2.21	0.43
2:B:103:LYS:HE3	2:B:179:VAL:HG13	1.98	0.43
1:A:326:ILE:N	1:A:326:ILE:CD1	2.76	0.43
2:B:311:LYS:NZ	5:B:1079:HOH:O	2.50	0.43
1:A:175:ASN:C	1:A:177:ASP:H	2.22	0.43
2:B:198:HIS:CD2	2:B:198:HIS:C	2.90	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB2	2.00	0.43
1:A:130:PHE:HE1	1:A:144:TYR:HB2	1.77	0.43
2:B:142:ILE:HG12	2:B:142:ILE:H	1.58	0.43
2:B:269:GLN:HB3	2:B:346:PHE:CD2	2.53	0.43
1:A:315:HIS:CD2	5:A:1029:HOH:O	2.71	0.43
2:B:92:LEU:HB2	2:B:158:ALA:HB1	1.99	0.43
1:A:363:ASN:HD22	1:A:366:LYS:H	1.67	0.43
2:B:329:ILE:HD11	2:B:389:PHE:HD2	1.83	0.43
1:A:54:ASN:N	1:A:55:PRO:CD	2.81	0.43
1:A:156:SER:O	1:A:157:PRO:C	2.56	0.43
1:A:50:ILE:HD12	1:A:50:ILE:H	1.83	0.43
1:A:482:ILE:HD11	1:A:502:ALA:HB1	2.01	0.43
2:B:425:LEU:CD2	2:B:425:LEU:O	2.66	0.43
2:B:115:TYR:OH	2:B:184:MET:O	2.16	0.43
1:A:23:GLN:NE2	1:A:23:GLN:O	2.44	0.43
1:A:97:PRO:C	1:A:99:GLY:H	2.22	0.43
2:B:426:TRP:CD1	2:B:427:TYR:N	2.86	0.43
2:B:164:MET:O	2:B:167:ILE:N	2.51	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
1:A:312:GLU:H	1:A:312:GLU:HG2	1.59	0.43
1:A:406:TRP:C	1:A:406:TRP:CE3	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	1:A:166:LYS:N	2.32	0.43
1:A:477:THR:C	1:A:479:LEU:N	2.72	0.43
2:B:274:ILE:HD12	2:B:274:ILE:N	2.33	0.43
1:A:325:LEU:CD1	1:A:383:TRP:CE3	3.02	0.43
1:A:395:LYS:HA	1:A:414:TRP:CZ2	2.45	0.43
2:B:316:GLY:HA2	2:B:318:TYR:HE1	1.84	0.43
1:A:497:THR:HG22	1:A:499:SER:HB3	2.01	0.43
2:B:277:ARG:HD3	2:B:277:ARG:N	2.27	0.43
2:B:231:GLY:O	2:B:233:GLU:HG3	2.19	0.43
2:B:203:GLU:OE2	2:B:207:GLN:HG2	2.19	0.42
2:B:220:LYS:CB	2:B:221:HIS:CD2	3.02	0.42
1:A:264:LEU:CD1	1:A:279:LEU:HD13	2.49	0.42
1:A:261:VAL:CG2	1:A:279:LEU:HD22	2.48	0.42
2:B:79:GLU:O	2:B:80:LEU:C	2.57	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.51	0.42
1:A:334:GLN:C	1:A:336:GLN:H	2.21	0.42
2:B:358:ARG:C	2:B:362:THR:HB	2.39	0.42
1:A:279:LEU:HB2	1:A:302:GLU:OE2	2.18	0.42
2:B:349:LEU:HD12	2:B:383:TRP:CE2	2.53	0.42
1:A:398:TRP:NE1	1:A:402:TRP:HD1	2.18	0.42
1:A:142:ILE:CD1	1:A:142:ILE:H	2.29	0.42
1:A:134:SER:O	1:A:135:ILE:C	2.58	0.42
1:A:200:THR:CG2	1:A:201:LYS:N	2.82	0.42
1:A:477:THR:O	1:A:480:GLN:N	2.53	0.42
2:B:218:ASP:O	2:B:220:LYS:N	2.51	0.42
1:A:193:LEU:O	1:A:198:HIS:HB2	2.19	0.42
1:A:460:ASN:C	1:A:462:GLY:N	2.73	0.42
2:B:202:ILE:O	2:B:203:GLU:C	2.57	0.42
2:B:183:TYR:HE1	2:B:380:ILE:HG13	1.83	0.42
1:A:434:ILE:HG13	1:A:530:LYS:HD3	2.01	0.42
1:A:433:PRO:HG3	2:B:255:ASN:ND2	2.34	0.42
1:A:319:TYR:HD1	1:A:325:LEU:HD21	1.84	0.42
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.51	0.42
1:A:541:GLY:O	1:A:545:ASN:HB3	2.19	0.42
2:B:111:VAL:C	2:B:113:ASP:H	2.23	0.42
1:A:85:GLN:O	1:A:154:LYS:CE	2.67	0.42
2:B:53:GLU:O	2:B:55:PRO:HD3	2.20	0.42
1:A:433:PRO:CG	2:B:255:ASN:ND2	2.82	0.42
2:B:34:LEU:HD21	2:B:61:PHE:O	2.20	0.42
1:A:126:LYS:HG3	1:A:127:TYR:CD2	2.55	0.42
2:B:208:HIS:C	2:B:208:HIS:ND1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.42
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.42
2:B:96:HIS:CE1	2:B:384:GLY:N	2.88	0.42
1:A:139:THR:CG2	1:A:140:PRO:CD	2.92	0.42
1:A:369:THR:O	1:A:373:GLN:N	2.45	0.42
2:B:68:SER:O	2:B:69:THR:C	2.57	0.42
2:B:23:GLN:HG3	2:B:133:PRO:HG3	1.95	0.42
2:B:64:LYS:HG3	2:B:71:TRP:CE3	2.55	0.42
1:A:541:GLY:C	1:A:543:GLY:H	2.23	0.42
2:B:257:ILE:HG23	2:B:258:GLN:N	2.35	0.42
2:B:198:HIS:C	2:B:200:THR:N	2.71	0.42
2:B:85:GLN:HG3	2:B:154:LYS:HD2	2.01	0.42
2:B:366:LYS:CG	2:B:405:TYR:CD2	3.01	0.42
2:B:49:LYS:HE3	2:B:144:TYR:CZ	2.55	0.42
1:A:390:LYS:HA	1:A:415:GLU:O	2.20	0.42
2:B:257:ILE:CD1	2:B:261:VAL:HG23	2.50	0.42
2:B:278:GLN:HG3	2:B:278:GLN:O	2.19	0.42
2:B:171:PHE:CE2	2:B:205:LEU:CA	3.03	0.42
1:A:47:ILE:HB	1:A:145:GLN:O	2.19	0.42
1:A:341:ILE:HG12	1:A:383:TRP:CH2	2.55	0.42
2:B:345:PRO:C	2:B:346:PHE:HD1	2.22	0.42
1:A:98:ALA:HB1	1:A:350:LYS:HB2	2.02	0.42
2:B:358:ARG:CG	2:B:359:GLY:N	2.63	0.42
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.40	0.42
2:B:386:THR:HA	2:B:387:PRO:HD3	1.78	0.42
1:A:73:LYS:HE3	1:A:130:PHE:CE2	2.55	0.42
1:A:120:LEU:HD13	1:A:150:PRO:HD2	2.01	0.42
1:A:331:LYS:HG3	1:A:337:TRP:CZ2	2.55	0.42
2:B:60:VAL:O	2:B:60:VAL:CG2	2.67	0.42
2:B:7:THR:HG22	2:B:119:PRO:HB2	2.01	0.42
1:A:233:GLU:N	1:A:240:THR:O	2.44	0.42
1:A:442:VAL:HG22	1:A:443:ASP:N	2.35	0.42
1:A:456:GLY:HA2	1:A:484:LEU:CD2	2.50	0.42
2:B:34:LEU:HD21	2:B:62:ALA:HB2	2.01	0.42
1:A:122:GLU:HA	1:A:125:ARG:NE	2.34	0.42
2:B:320:ASP:O	2:B:343:GLN:NE2	2.51	0.42
1:A:543:GLY:O	2:B:284:ARG:O	2.37	0.41
2:B:253:THR:HB	2:B:291:GLU:O	2.20	0.41
1:A:96:HIS:HD1	1:A:98:ALA:N	2.13	0.41
1:A:441:TYR:HB2	1:A:458:VAL:O	2.21	0.41
1:A:126:LYS:H	1:A:126:LYS:HG2	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:O	1:A:373:GLN:HB3	2.20	0.41
1:A:344:GLU:HA	1:A:345:PRO:HD2	1.58	0.41
1:A:164:MET:CE	1:A:187:LEU:HD22	2.50	0.41
2:B:195:ILE:CG2	2:B:196:GLY:N	2.64	0.41
1:A:434:ILE:CD1	1:A:494:ASN:HD21	2.33	0.41
2:B:375:ILE:CG2	2:B:389:PHE:HE2	2.33	0.41
2:B:151:GLN:O	2:B:152:GLY:C	2.57	0.41
2:B:92:LEU:CB	2:B:158:ALA:HB1	2.50	0.41
1:A:499:SER:OG	1:A:499:SER:O	2.36	0.41
2:B:385:LYS:NZ	2:B:385:LYS:CB	2.83	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CG	2.56	0.41
1:A:183:TYR:CD2	1:A:229:TRP:CD1	3.08	0.41
2:B:372:VAL:O	2:B:374:LYS:N	2.53	0.41
2:B:244:ILE:HD13	2:B:244:ILE:N	2.30	0.41
1:A:315:HIS:H	1:A:315:HIS:CD2	2.38	0.41
1:A:168:LEU:HD13	1:A:180:ILE:HG21	2.02	0.41
1:A:183:TYR:CD2	1:A:229:TRP:HD1	2.39	0.41
1:A:482:ILE:O	1:A:483:TYR:C	2.57	0.41
2:B:275:LYS:HA	2:B:277:ARG:CZ	2.50	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.03	0.41
1:A:48:SER:O	1:A:144:TYR:HA	2.21	0.41
2:B:328:GLU:OE1	2:B:342:TYR:OH	2.30	0.41
1:A:435:VAL:HG13	2:B:290:THR:OG1	2.20	0.41
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.56	0.41
1:A:224:GLU:N	1:A:225:PRO:HD3	2.34	0.41
1:A:229:TRP:C	1:A:231:GLY:N	2.73	0.41
1:A:483:TYR:CB	1:A:521:ILE:HG12	2.43	0.41
1:A:32:LYS:O	1:A:36:GLU:CG	2.69	0.41
1:A:503:LEU:HD21	1:A:535:TRP:HB2	1.98	0.41
2:B:283:LEU:O	2:B:285:GLY:O	2.39	0.41
2:B:149:LEU:HD12	2:B:156:SER:O	2.20	0.41
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.51	0.41
2:B:50:ILE:HG13	2:B:143:ARG:HB3	2.03	0.41
2:B:72:ARG:HH22	2:B:409:THR:CG2	2.34	0.41
1:A:309:ILE:O	1:A:312:GLU:CG	2.68	0.41
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.56	0.41
1:A:325:LEU:C	1:A:326:ILE:HD12	2.41	0.41
2:B:91:GLN:NE2	2:B:91:GLN:O	2.48	0.41
2:B:269:GLN:HG2	2:B:346:PHE:CD2	2.56	0.41
1:A:229:TRP:C	1:A:231:GLY:H	2.24	0.41
1:A:162:SER:CB	2:B:52:PRO:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:HG21	2:B:283:LEU:CD1	2.50	0.41
2:B:276:VAL:HG12	2:B:276:VAL:O	2.21	0.41
1:A:253:THR:OG1	1:A:290:THR:CA	2.68	0.41
1:A:275:LYS:O	1:A:276:VAL:CG2	2.68	0.41
2:B:295:LEU:N	2:B:295:LEU:HD23	2.36	0.41
2:B:375:ILE:HG21	2:B:389:PHE:HE2	1.84	0.41
2:B:260:LEU:CD1	2:B:264:LEU:HD11	2.50	0.41
1:A:107:THR:O	1:A:189:VAL:N	2.33	0.41
1:A:196:GLY:C	1:A:198:HIS:N	2.74	0.41
1:A:472:THR:OG1	1:A:476:LYS:HB3	2.21	0.41
2:B:38:CYS:HA	2:B:41:MET:HG3	2.02	0.41
1:A:219:LYS:HA	5:A:1088:HOH:O	2.21	0.41
1:A:277:ARG:HA	1:A:277:ARG:HD2	1.92	0.41
1:A:443:ASP:HB2	1:A:548:VAL:CG2	2.50	0.41
2:B:306:ASN:HA	2:B:306:ASN:HD22	1.64	0.41
1:A:356:ARG:NE	1:A:358:ARG:CG	2.79	0.41
1:A:261:VAL:HG13	1:A:276:VAL:HG11	2.01	0.41
2:B:85:GLN:O	2:B:88:TRP:C	2.59	0.41
2:B:371:ALA:O	2:B:375:ILE:HB	2.21	0.41
1:A:21:VAL:HG12	1:A:22:LYS:N	2.36	0.41
2:B:23:GLN:HG3	2:B:24:TRP:O	2.20	0.41
1:A:307:ARG:C	1:A:309:ILE:N	2.74	0.41
1:A:485:ALA:O	1:A:487:GLN:N	2.54	0.40
1:A:257:ILE:O	1:A:261:VAL:HG23	2.21	0.40
2:B:183:TYR:HD1	2:B:380:ILE:CG2	2.23	0.40
1:A:142:ILE:CD1	1:A:142:ILE:N	2.84	0.40
2:B:66:LYS:HB3	2:B:67:ASP:H	1.62	0.40
1:A:326:ILE:HG22	1:A:327:ALA:N	2.36	0.40
2:B:198:HIS:CD2	2:B:199:ARG:N	2.89	0.40
1:A:450:THR:HG22	1:A:452:LEU:CB	2.52	0.40
1:A:438:GLU:CD	1:A:463:ARG:HH21	2.23	0.40
2:B:253:THR:HG22	2:B:292:VAL:HG22	2.03	0.40
2:B:156:SER:HB2	2:B:157:PRO:CD	2.51	0.40
1:A:2:ILE:CG2	1:A:3:SER:H	2.25	0.40
1:A:15:GLY:O	1:A:16:MET:C	2.60	0.40
1:A:481:ALA:O	1:A:484:LEU:N	2.54	0.40
2:B:171:PHE:O	2:B:171:PHE:CD1	2.74	0.40
1:A:193:LEU:CB	1:A:197:GLN:HB3	2.46	0.40
1:A:303:LEU:O	1:A:307:ARG:HG2	2.21	0.40
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.48	0.40
2:B:187:LEU:HA	2:B:187:LEU:HD23	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ARG:HD3	2:B:147:ASN:OD1	2.21	0.40
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.03	0.40
2:B:149:LEU:C	2:B:150:PRO:O	2.60	0.40
2:B:181:TYR:O	2:B:188:TYR:N	2.51	0.40
1:A:135:ILE:HG22	1:A:136:ASN:N	2.37	0.40
1:A:104:LYS:CG	1:A:192:ASP:HA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/560 (98%)	404 (74%)	92 (17%)	54 (10%)	1	2
2	B	425/430 (99%)	277 (65%)	94 (22%)	54 (13%)	0	1
All	All	975/990 (98%)	681 (70%)	186 (19%)	108 (11%)	0	1

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	25	PRO
1	A	52	PRO
1	A	65	LYS
1	A	112	GLY
1	A	153	TRP
1	A	162	SER
1	A	163	SER
1	A	273	GLY
1	A	359	GLY
1	A	538	ALA
2	B	66	LYS

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Mol	Chain	Res	Type
2	B	68	SER
2	B	71	TRP
2	B	77	PHE
2	B	116	PHE
2	B	126	LYS
2	B	161	GLN
2	B	176	PRO
2	B	177	ASP
2	B	195	ILE
2	B	218	ASP
2	B	242	GLN
2	B	267	ALA
2	B	284	ARG
2	B	297	GLU
2	B	362	THR
2	B	365	VAL
2	B	404	GLU
2	B	421	PRO
1	A	98	ALA
1	A	122	GLU
1	A	164	MET
1	A	195	ILE
1	A	223	LYS
1	A	230	MET
1	A	276	VAL
1	A	277	ARG
1	A	399	GLU
1	A	491	LEU
1	A	546	GLU
2	B	18	GLY
2	B	85	GLN
2	B	112	GLY
2	B	154	LYS
2	B	162	SER
2	B	165	THR
2	B	174	GLN
2	B	196	GLY
2	B	202	ILE
2	B	228	LEU
2	B	232	TYR
2	B	239	TRP
2	B	250	ASP

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Mol	Chain	Res	Type
2	B	345	PRO
1	A	2	ILE
1	A	64	LYS
1	A	66	LYS
1	A	78	ARG
1	A	102	LYS
1	A	156	SER
1	A	158	ALA
1	A	222	GLN
1	A	272	PRO
1	A	311	LYS
1	A	324	ASP
1	A	398	TRP
1	A	539	HIS
2	B	125	ARG
2	B	173	LYS
2	B	199	ARG
2	B	249	LYS
2	B	294	PRO
1	A	14	PRO
1	A	27	THR
1	A	104	LYS
1	A	176	PRO
1	A	254	VAL
1	A	465	LYS
1	A	482	ILE
2	B	122	GLU
2	B	170	PRO
2	B	251	SER
2	B	276	VAL
1	A	184	MET
1	A	194	GLU
1	A	345	PRO
1	A	392	PRO
1	A	542	ILE
2	B	184	MET
2	B	222	GLN
2	B	236	PRO
2	B	33	ALA
2	B	141	GLY
1	A	159	ILE
1	A	543	GLY

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Mol	Chain	Res	Type
1	A	24	TRP
1	A	54	ASN
1	A	135	ILE
1	A	236	PRO
2	B	111	VAL
2	B	155	GLY
1	A	419	THR
2	B	241	VAL
2	B	245	VAL
2	B	225	PRO
2	B	412	PRO
2	B	423	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	494/500 (99%)	449 (91%)	45 (9%)	12	34
2	B	389/392 (99%)	342 (88%)	47 (12%)	6	18
All	All	883/892 (99%)	791 (90%)	92 (10%)	9	26

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	23	GLN
1	A	25	PRO
1	A	36	GLU
1	A	50	ILE
1	A	56	TYR
1	A	64	LYS
1	A	66	LYS
1	A	71	TRP
1	A	74	LEU
1	A	86	ASP

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Mol	Chain	Res	Type
1	A	120	LEU
1	A	126	LYS
1	A	130	PHE
1	A	132	ILE
1	A	136	ASN
1	A	159	ILE
1	A	165	THR
1	A	177	ASP
1	A	188	TYR
1	A	245	VAL
1	A	256	ASP
1	A	317	VAL
1	A	330	GLN
1	A	334	GLN
1	A	340	GLN
1	A	356	ARG
1	A	374	LYS
1	A	385	LYS
1	A	386	THR
1	A	395	LYS
1	A	397	THR
1	A	401	TRP
1	A	402	TRP
1	A	411	ILE
1	A	413	GLU
1	A	418	ASN
1	A	449	GLU
1	A	457	TYR
1	A	494	ASN
1	A	516	GLU
1	A	522	ILE
1	A	533	LEU
1	A	548	VAL
1	A	551	LEU
2	B	9	PRO
2	B	24	TRP
2	B	50	ILE
2	B	57	ASN
2	B	58	THR
2	B	63	ILE
2	B	67	ASP
2	B	73	LYS

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Mol	Chain	Res	Type
2	B	74	LEU
2	B	86	ASP
2	B	91	GLN
2	B	110	ASP
2	B	131	THR
2	B	135	ILE
2	B	142	ILE
2	B	149	LEU
2	B	169	GLU
2	B	175	ASN
2	B	181	TYR
2	B	183	TYR
2	B	186	ASP
2	B	189	VAL
2	B	198	HIS
2	B	208	HIS
2	B	215	THR
2	B	221	HIS
2	B	224	GLU
2	B	232	TYR
2	B	239	TRP
2	B	244	ILE
2	B	252	TRP
2	B	257	ILE
2	B	277	ARG
2	B	308	GLU
2	B	322	SER
2	B	332	GLN
2	B	340	GLN
2	B	342	TYR
2	B	349	LEU
2	B	358	ARG
2	B	362	THR
2	B	366	LYS
2	B	383	TRP
2	B	385	LYS
2	B	409	THR
2	B	425	LEU
2	B	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	235	HIS
1	A	258	GLN
1	A	315	HIS
1	A	330	GLN
1	A	343	GLN
1	A	363	ASN
1	A	471	ASN
1	A	487	GLN
1	A	494	ASN
1	A	500	GLN
1	A	507	GLN
1	A	519	ASN
2	B	23	GLN
2	B	91	GLN
2	B	136	ASN
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	208	HIS
2	B	221	HIS
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	330	GLN
2	B	336	GLN
2	B	340	GLN
2	B	348	ASN
2	B	394	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	IET	A	701	-	22,24,24	4.00	11 (50%)	29,32,32	2.19	6 (20%)

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	IET	A	701	-	-	0/12/14/14	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	IET	C6-CL6	-9.16	1.51	1.73
4	A	701	IET	C2-CL2	-9.12	1.51	1.73
4	A	701	IET	C7-C8	-9.11	1.39	1.50
4	A	701	IET	C9-N1	-2.92	1.34	1.39
4	A	701	IET	C4-C3	2.03	1.43	1.38
4	A	701	IET	C3-C2	2.30	1.44	1.39
4	A	701	IET	C6-C1	2.45	1.44	1.39
4	A	701	IET	C7-C1	3.21	1.58	1.52
4	A	701	IET	C16-C15	3.56	1.45	1.38
4	A	701	IET	C2-C1	3.76	1.46	1.39
4	A	701	IET	C16-C11	4.13	1.46	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	701	IET	C9-N1-C8	-5.83	121.42	128.84
4	A	701	IET	C7-C1-C6	-3.19	116.63	121.62
4	A	701	IET	S2-C9-N5	-2.54	116.50	124.22
4	A	701	IET	C7-C1-C2	3.04	126.39	121.62
4	A	701	IET	N5-C9-N1	5.03	123.15	115.28
4	A	701	IET	C1-C7-C8	6.10	124.82	113.72

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	701	IET	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	552/560 (98%)	-0.09	21 (3%)	44 37	37, 83, 109, 111	5 (0%)
2	B	427/430 (99%)	-0.16	13 (3%)	54 47	19, 69, 110, 111	4 (0%)
All	All	979/990 (98%)	-0.12	34 (3%)	48 40	19, 78, 110, 111	9 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	6.8
1	A	444	GLY	5.8
2	B	3	SER	4.1
1	A	107	THR	3.7
2	B	4	PRO	3.6
2	B	419	THR	3.5
1	A	442	VAL	3.5
2	B	2	ILE	3.5
1	A	550	LYS	3.5
2	B	305	GLU	3.3
1	A	26	LEU	3.3
1	A	134	SER	3.0
1	A	357	MET	2.9
2	B	427	TYR	2.9
1	A	139	THR	2.9
1	A	140	PRO	2.7
1	A	92	LEU	2.5
1	A	54	ASN	2.5
2	B	266	TRP	2.5
2	B	210	LEU	2.4
2	B	242	GLN	2.4
1	A	449	GLU	2.3
1	A	135	ILE	2.2
1	A	22	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLY	2.2
2	B	359	GLY	2.1
1	A	441	TYR	2.1
1	A	32	LYS	2.1
1	A	1	PRO	2.1
2	B	189	VAL	2.1
1	A	218	ASP	2.0
1	A	2	ILE	2.0
1	A	222	GLN	2.0
2	B	219	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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(Å ²)	Q<0.9
4	IET	A	701	23/23	0.86	0.24	0.34	63,78,84,92	0
3	MG	A	601	1/1	0.90	0.14	-	79,79,79,79	0

6.5 Other polymers ⓘ

There are no such residues in this entry.