



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:27 am BST

PDB ID : 2UZY  
Title : Structure of the human receptor tyrosine kinase Met in complex with the  
Listeria monocytogenes invasion protein inlb: low resolution, Crystal form II  
Authors : Niemann, H.H.; Jager, V.; Butler, P.J.G.; van den Heuvel, J.; Schmidt, S.;  
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Deposited on : 2007-05-02  
Resolution : 4.00 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

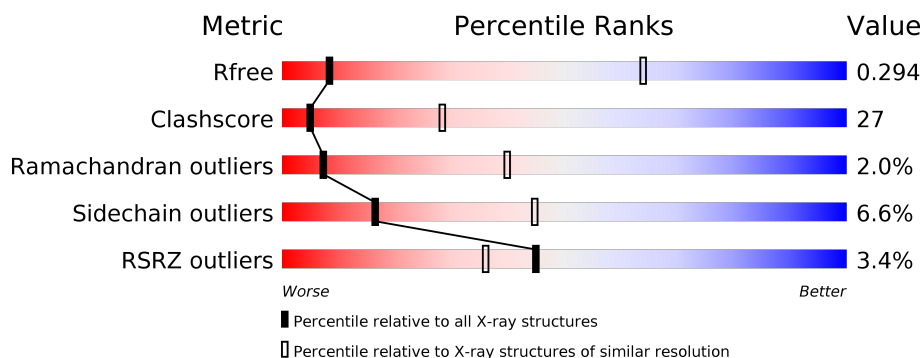
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	289	<div> <div>4%</div> <div> <div>55%</div> <div>41%</div> <div>••</div> </div> </div>
1	C	289	<div> <div>%</div> <div> <div>57%</div> <div>39%</div> <div>••</div> </div> </div>
2	B	727	<div> <div>3%</div> <div> <div>43%</div> <div>38%</div> <div>5%</div> <div>13%</div> </div> </div>
2	D	727	<div> <div>4%</div> <div> <div>43%</div> <div>37%</div> <div>5%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14329 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 INTERNALIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			
1	C	286	Total	C	N	O	S	0	0	0
			2252	1435	378	437	2			

- Molecule 2 is a protein called HEPATOCYTE GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	630	Total	C	N	O	S	0	0	0
			4959	3151	835	938	35			
2	D	618	Total	C	N	O	S	0	0	0
			4866	3097	818	918	33			

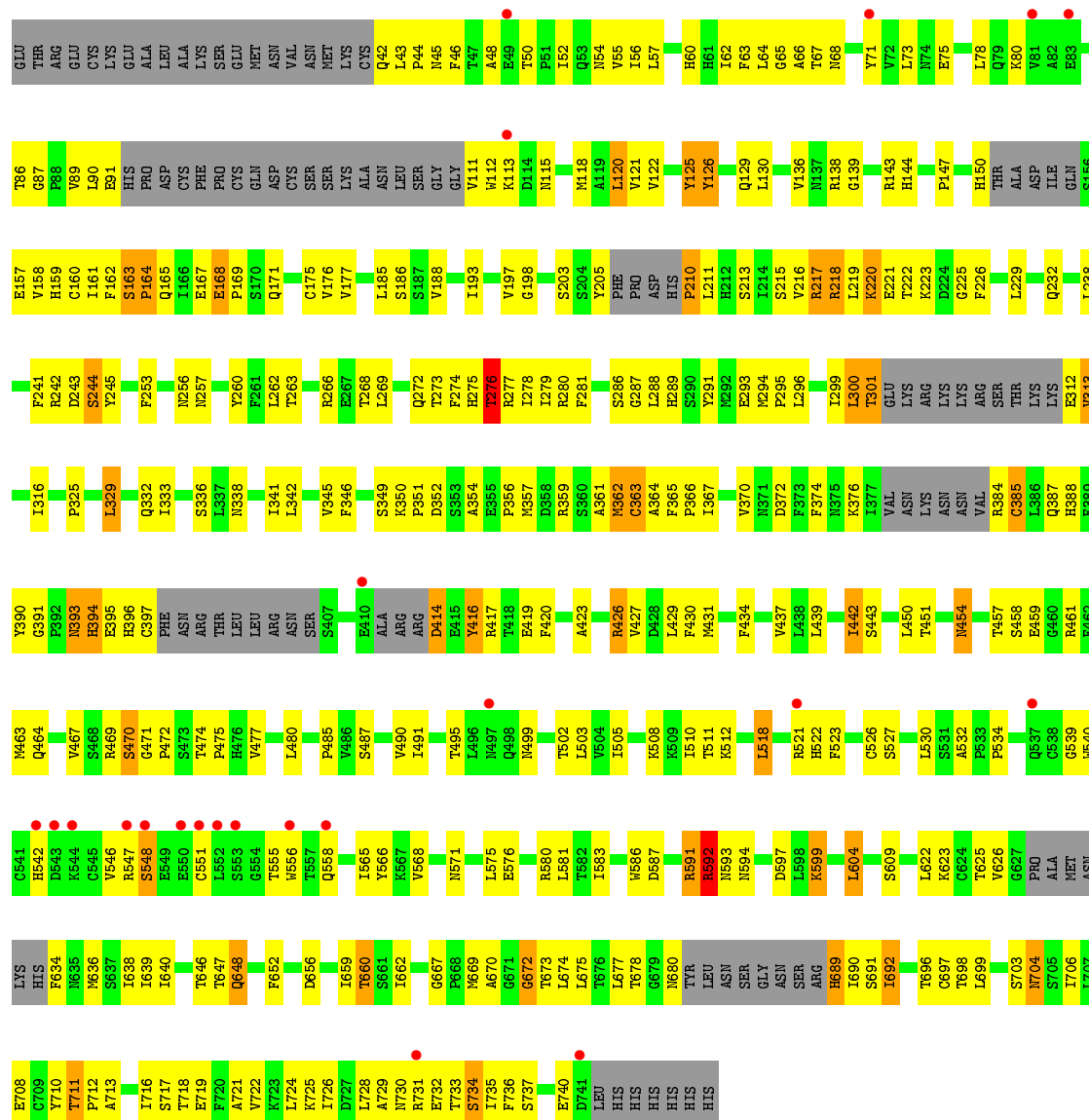
There are 4 discrepancies between the modelled and reference sequences:

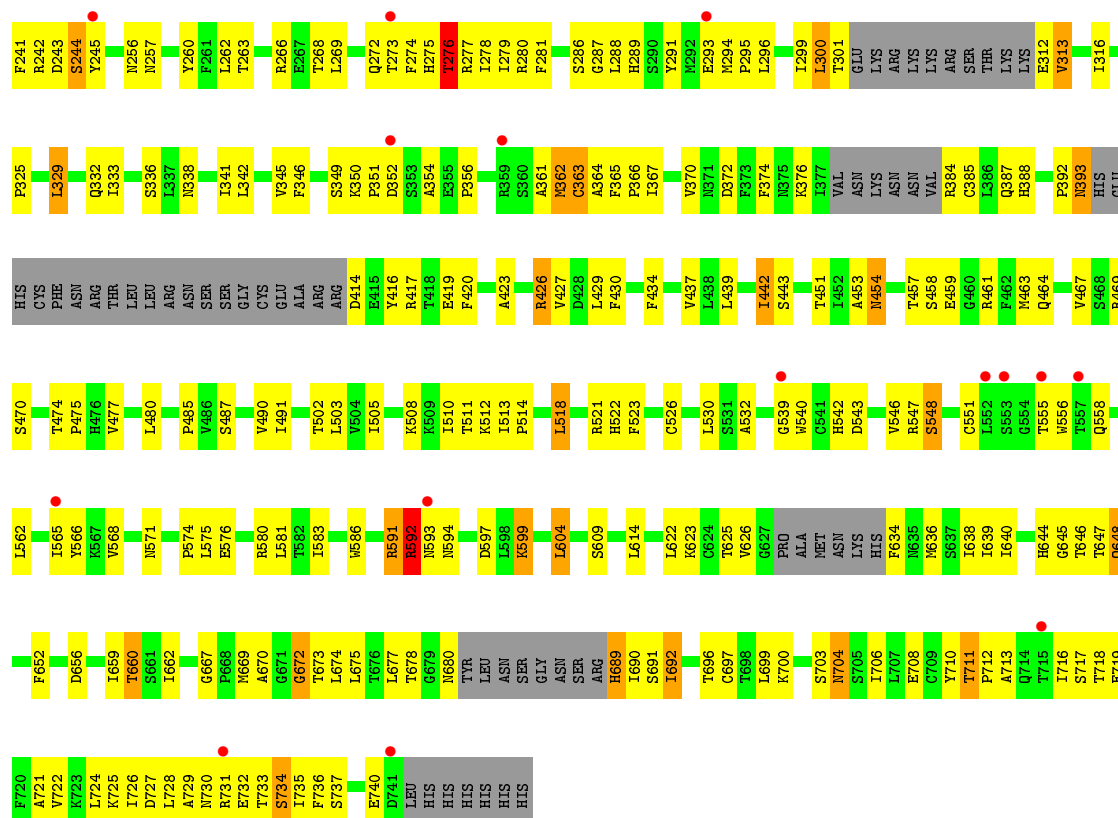
Chain	Residue	Modelled	Actual	Comment	Reference
B	41	CYS	TYR	conflict	UNP P08581
B	344	ALA	GLY	conflict	UNP P08581
D	41	CYS	TYR	conflict	UNP P08581
D	344	ALA	GLY	conflict	UNP P08581



- Molecule 1: INTERNALIN B







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.00Å 144.98Å 150.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 4.00 48.16 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-4.00) 99.6 (48.16-4.00)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.251 , 0.301 0.257 , 0.294	Depositor DCC
$R_{free}$ test set	1302 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.6	Xtriage
Anisotropy	0.833	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 92.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.088 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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	0.23	0/2288	0.42	0/3105
1	C	0.24	0/2288	0.42	0/3105
2	B	0.33	1/5068 (0.0%)	0.47	1/6868 (0.0%)
2	D	0.33	2/4972 (0.0%)	0.48	0/6738
All	All	0.30	3/14616 (0.0%)	0.46	1/19816 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	LYS	C-N	12.95	1.63	1.34
2	D	113	LYS	C-N	9.64	1.56	1.34
2	D	111	VAL	CB-CG2	-5.24	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	414	ASP	N-CA-C	-6.07	94.61	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	B	300	LEU	Peptide
2	D	300	LEU	Peptide

## 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	2252	0	2323	125	0
1	C	2252	0	2323	111	0
2	B	4959	0	4832	301	0
2	D	4866	0	4760	270	0
All	All	14329	0	14238	781	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 27.

All (781) 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:310:ARG:HG3	1:A:310:ARG:HH11	1.32	0.94
1:C:310:ARG:HH11	1:C:310:ARG:HG3	1.33	0.92
1:A:193:LEU:HD22	1:A:198:ILE:HD11	1.53	0.90
1:C:193:LEU:HD22	1:C:198:ILE:HD11	1.52	0.90
2:B:521:ARG:HE	2:B:546:VAL:HG23	1.37	0.90
1:A:299:TYR:HE1	2:B:469:ARG:HD2	1.38	0.87
2:D:521:ARG:HE	2:D:546:VAL:HG23	1.37	0.87
2:B:390:TYR:HB3	2:B:394:HIS:HE2	1.40	0.85
2:D:275:HIS:HE1	2:D:295:PRO:HB3	1.43	0.84
2:B:275:HIS:CE1	2:B:295:PRO:HB3	2.13	0.84
2:B:275:HIS:HE1	2:B:295:PRO:HB3	1.43	0.84
2:B:390:TYR:HB3	2:B:394:HIS:NE2	1.93	0.83
2:D:345:VAL:HG11	2:D:439:LEU:HB2	1.61	0.83
2:D:275:HIS:CE1	2:D:295:PRO:HB3	2.13	0.83
2:B:65:GLY:HA3	2:B:120:LEU:HD21	1.62	0.82
2:D:65:GLY:HA3	2:D:120:LEU:HD21	1.62	0.82
1:A:310:ARG:CG	1:A:310:ARG:HH11	1.93	0.82
1:C:157:ILE:HG12	1:C:181:VAL:HG11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:VAL:HG11	2:B:439:LEU:HB2	1.61	0.81
2:B:291:TYR:HB3	2:B:417:ARG:HG3	1.63	0.80
2:D:291:TYR:HB3	2:D:417:ARG:HG3	1.63	0.80
1:A:157:ILE:HG12	1:A:181:VAL:HG11	1.63	0.80
2:D:689:HIS:O	2:D:689:HIS:CG	2.34	0.80
1:C:310:ARG:HH11	1:C:310:ARG:CG	1.93	0.80
2:D:724:LEU:HD12	2:D:726:ILE:HD11	1.64	0.80
2:B:689:HIS:O	2:B:689:HIS:CG	2.34	0.80
2:B:52:ILE:HD13	2:B:66:ALA:HB2	1.64	0.79
1:A:238:PHE:HZ	2:B:469:ARG:HB3	1.47	0.79
2:B:724:LEU:HD12	2:B:726:ILE:HD11	1.64	0.79
1:C:226:LEU:H	1:C:226:LEU:HD12	1.48	0.78
1:C:247:ILE:HB	1:C:317:GLN:HE21	1.49	0.78
1:A:226:LEU:HD12	1:A:226:LEU:H	1.48	0.78
1:A:285:TRP:HB3	1:A:287:LEU:HD13	1.66	0.77
1:C:285:TRP:HB3	1:C:287:LEU:HD13	1.66	0.77
1:A:247:ILE:HB	1:A:317:GLN:HE21	1.49	0.77
2:D:52:ILE:HD13	2:D:66:ALA:HB2	1.65	0.77
1:C:113:ILE:HG13	1:C:137:SER:HB2	1.68	0.75
2:D:660:THR:HG23	2:D:678:THR:HB	1.69	0.75
2:B:176:VAL:HA	2:B:217:ARG:HH12	1.51	0.75
2:B:551:CYS:SG	2:B:556:TRP:HB2	2.27	0.74
2:D:176:VAL:HA	2:D:217:ARG:HH12	1.51	0.74
2:B:443:SER:HB2	2:B:454:ASN:ND2	2.02	0.74
2:D:551:CYS:SG	2:D:556:TRP:HB2	2.27	0.74
1:A:113:ILE:HG13	1:A:137:SER:HB2	1.69	0.74
2:B:660:THR:HG23	2:B:678:THR:HB	1.69	0.74
2:D:443:SER:HB2	2:D:454:ASN:ND2	2.02	0.74
2:B:458:SER:HA	2:B:485:PRO:HB3	1.71	0.73
2:D:604:LEU:HD22	2:D:609:SER:HA	1.70	0.73
2:D:458:SER:HA	2:D:485:PRO:HB3	1.71	0.73
1:A:247:ILE:HB	1:A:317:GLN:NE2	2.05	0.72
2:B:604:LEU:HD22	2:B:609:SER:HA	1.70	0.72
1:C:247:ILE:HB	1:C:317:GLN:NE2	2.05	0.71
2:B:591:ARG:O	2:B:592:ARG:HB2	1.90	0.71
2:D:316:ILE:HD13	2:D:349:SER:HB3	1.71	0.71
2:B:542:HIS:HB2	2:B:555:THR:HG21	1.72	0.71
2:B:539:GLY:HA3	2:B:556:TRP:NE1	2.06	0.71
2:D:539:GLY:HA3	2:D:556:TRP:NE1	2.06	0.71
2:B:316:ILE:HG21	2:B:356:PRO:HG3	1.73	0.70
2:B:316:ILE:HD13	2:B:349:SER:HB3	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:542:HIS:HB2	2:D:555:THR:HG21	1.72	0.70
2:D:591:ARG:O	2:D:592:ARG:HB2	1.90	0.70
2:B:521:ARG:NE	2:B:546:VAL:HG23	2.07	0.70
2:D:316:ILE:HG21	2:D:356:PRO:HG3	1.73	0.70
2:D:503:LEU:HB3	2:D:510:ILE:HD11	1.75	0.69
1:A:310:ARG:NE	2:B:431:MET:HG2	2.07	0.69
2:B:118:MET:CB	2:B:177:VAL:HG11	2.23	0.69
2:B:397:CYS:HA	2:B:416:TYR:CZ	2.27	0.69
1:C:80:GLN:HE21	1:C:82:ILE:HD11	1.58	0.69
2:D:118:MET:CB	2:D:177:VAL:HG11	2.23	0.69
2:D:521:ARG:NE	2:D:546:VAL:HG23	2.07	0.68
1:A:299:TYR:CE1	2:B:469:ARG:HD2	2.27	0.68
2:B:503:LEU:HB3	2:B:510:ILE:HD11	1.74	0.68
2:D:260:TYR:HA	2:D:279:ILE:O	1.94	0.68
1:A:301:PRO:HA	1:A:310:ARG:HA	1.76	0.68
2:B:260:TYR:HA	2:B:279:ILE:O	1.94	0.68
1:C:124:TRP:HZ2	2:D:604:LEU:HD23	1.59	0.67
2:B:674:LEU:HD11	2:B:708:GLU:HB3	1.74	0.67
2:B:396:HIS:CG	2:B:397:CYS:N	2.62	0.67
2:D:57:LEU:HD13	2:D:62:ILE:HD13	1.77	0.67
2:D:674:LEU:HD11	2:D:708:GLU:HB3	1.74	0.67
1:C:301:PRO:HA	1:C:310:ARG:HA	1.76	0.67
2:B:57:LEU:HD13	2:B:62:ILE:HD13	1.77	0.67
2:B:299:ILE:HG22	2:B:313:VAL:HA	1.77	0.67
2:D:393:ASN:HD22	2:D:393:ASN:H	1.42	0.67
1:A:80:GLN:HE21	1:A:82:ILE:HD11	1.58	0.66
2:D:299:ILE:HG22	2:D:313:VAL:HA	1.77	0.66
2:D:477:VAL:HG13	2:D:518:LEU:HD21	1.77	0.66
2:B:390:TYR:CB	2:B:394:HIS:HE2	2.08	0.66
2:B:477:VAL:HG13	2:B:518:LEU:HD21	1.77	0.66
2:B:52:ILE:HD12	2:B:64:LEU:HB3	1.77	0.66
2:D:52:ILE:HD12	2:D:64:LEU:HB3	1.76	0.66
1:C:192:SER:O	1:C:193:LEU:HG	1.96	0.66
2:B:575:LEU:HD21	2:B:656:ASP:HB2	1.77	0.65
2:B:534:PRO:HD3	2:B:594:ASN:HD21	1.60	0.65
1:C:254:VAL:HG22	1:C:284:LYS:HG2	1.77	0.65
1:A:204:LEU:HA	1:A:207:LEU:HD22	1.77	0.65
1:C:204:LEU:HA	1:C:207:LEU:HD22	1.77	0.65
2:D:56:ILE:HD13	2:D:120:LEU:HB3	1.78	0.65
2:D:575:LEU:HD21	2:D:656:ASP:HB2	1.77	0.65
1:A:192:SER:O	1:A:193:LEU:HG	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:VAL:HG22	1:A:284:LYS:HG2	1.78	0.64
2:D:118:MET:HB3	2:D:177:VAL:HG11	1.78	0.64
2:D:546:VAL:HG22	2:D:547:ARG:H	1.63	0.64
2:B:697:CYS:CB	2:B:712:PRO:HD3	2.28	0.64
1:C:235:LEU:HD12	1:C:236:GLU:H	1.63	0.64
2:B:463:MET:HB2	2:B:475:PRO:HB3	1.78	0.64
2:B:56:ILE:HD13	2:B:120:LEU:HB3	1.78	0.64
2:D:697:CYS:CB	2:D:712:PRO:HD3	2.28	0.64
2:B:118:MET:HB3	2:B:177:VAL:HG11	1.78	0.64
2:B:287:GLY:HA2	2:B:289:HIS:NE2	2.13	0.64
2:B:393:ASN:H	2:B:393:ASN:HD22	1.43	0.64
2:B:721:ALA:HB1	2:B:732:GLU:HB2	1.79	0.64
2:D:721:ALA:HB1	2:D:732:GLU:HB2	1.79	0.63
2:D:463:MET:HB2	2:D:475:PRO:HB3	1.78	0.63
2:B:143:ARG:HB2	2:B:159:HIS:HB2	1.80	0.63
2:D:291:TYR:HB3	2:D:417:ARG:CG	2.29	0.63
2:D:662:ILE:HD11	2:D:675:LEU:HD21	1.80	0.63
1:C:36:GLU:HG3	1:C:95:GLN:HB3	1.80	0.63
1:A:36:GLU:HG3	1:A:95:GLN:HB3	1.80	0.63
2:B:341:ILE:HD13	2:B:366:PRO:HA	1.79	0.63
2:B:291:TYR:HB3	2:B:417:ARG:CG	2.29	0.63
2:D:287:GLY:HA2	2:D:289:HIS:NE2	2.13	0.63
2:D:341:ILE:HD13	2:D:366:PRO:HA	1.79	0.63
1:A:310:ARG:NH1	1:A:310:ARG:CG	2.60	0.63
2:D:138:ARG:HG3	2:D:175:CYS:HB3	1.80	0.63
2:B:138:ARG:HG3	2:B:175:CYS:HB3	1.80	0.62
2:B:662:ILE:HD11	2:B:675:LEU:HD21	1.80	0.62
2:B:638:ILE:O	2:B:648:GLN:HA	1.99	0.62
2:D:143:ARG:HB2	2:D:159:HIS:HB2	1.80	0.62
1:A:235:LEU:HD12	1:A:236:GLU:H	1.63	0.62
2:B:546:VAL:HG22	2:B:547:ARG:H	1.63	0.62
1:A:246:PRO:HA	1:A:318:PRO:HB2	1.82	0.62
1:C:246:PRO:HA	1:C:318:PRO:HB2	1.82	0.62
1:C:86:SER:HB2	1:C:88:ILE:HG13	1.81	0.62
2:D:593:ASN:O	2:D:594:ASN:HB2	2.00	0.62
2:D:638:ILE:O	2:D:648:GLN:HA	1.99	0.62
1:C:94:ILE:HD12	1:C:97:LEU:HD13	1.82	0.61
2:D:176:VAL:HG22	2:D:217:ARG:NH1	2.16	0.61
1:A:86:SER:HB2	1:A:88:ILE:HG13	1.81	0.61
2:B:176:VAL:HG22	2:B:217:ARG:NH1	2.16	0.61
2:B:593:ASN:O	2:B:594:ASN:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:HIS:HE1	2:D:295:PRO:CB	2.14	0.61
2:D:680:ASN:HA	2:D:704:ASN:O	2.01	0.61
1:A:56:THR:HG21	1:A:83:ALA:HB2	1.83	0.60
2:B:719:GLU:HG2	2:B:737:SER:CB	2.31	0.60
2:D:568:VAL:HG13	2:D:583:ILE:HG12	1.83	0.60
2:D:719:GLU:HG2	2:D:737:SER:CB	2.31	0.60
1:A:157:ILE:H	1:A:157:ILE:HD13	1.66	0.60
2:B:568:VAL:HG13	2:B:583:ILE:HG12	1.83	0.60
2:B:680:ASN:HA	2:B:704:ASN:O	2.01	0.60
2:D:417:ARG:HD2	2:D:417:ARG:N	2.17	0.60
2:B:417:ARG:N	2:B:417:ARG:HD2	2.17	0.60
1:C:285:TRP:HB3	1:C:287:LEU:CD1	2.32	0.60
2:B:699:LEU:O	2:D:239:PRO:HD2	2.02	0.60
1:C:279:GLU:HB3	1:C:284:LYS:HE3	1.83	0.60
1:A:94:ILE:HD12	1:A:97:LEU:HD13	1.82	0.60
1:A:53:PHE:O	1:A:57:ILE:HG12	2.01	0.60
1:C:157:ILE:H	1:C:157:ILE:HD13	1.66	0.59
2:B:329:LEU:O	2:B:333:ILE:HG12	2.03	0.59
2:D:329:LEU:O	2:D:333:ILE:HG12	2.02	0.59
2:D:238:LEU:HG	2:D:388:HIS:O	2.03	0.59
2:B:43:LEU:HD23	2:B:43:LEU:H	1.67	0.59
1:C:56:THR:HG21	1:C:83:ALA:HB2	1.83	0.59
2:D:43:LEU:HD23	2:D:43:LEU:H	1.67	0.59
1:A:238:PHE:CZ	2:B:469:ARG:HB3	2.32	0.59
2:B:716:ILE:HG22	2:B:717:SER:H	1.67	0.59
1:C:213:LEU:HD11	1:C:215:LEU:HD21	1.84	0.59
1:C:53:PHE:O	1:C:57:ILE:HG12	2.01	0.59
2:D:673:THR:O	2:D:711:THR:HG22	2.02	0.59
1:A:279:GLU:HB3	1:A:284:LYS:HE3	1.84	0.59
2:D:518:LEU:HD23	2:D:522:HIS:NE2	2.17	0.59
2:B:238:LEU:HG	2:B:388:HIS:O	2.03	0.59
2:D:716:ILE:HG22	2:D:717:SER:H	1.68	0.59
2:B:275:HIS:HE1	2:B:295:PRO:CB	2.13	0.59
2:B:673:THR:O	2:B:711:THR:HG22	2.02	0.59
1:A:213:LEU:HD11	1:A:215:LEU:HD21	1.84	0.58
1:A:285:TRP:HB3	1:A:287:LEU:CD1	2.32	0.58
2:B:397:CYS:HA	2:B:416:TYR:CE2	2.37	0.58
2:B:394:HIS:ND1	2:D:672:GLY:HA2	2.19	0.58
2:D:281:PHE:HB3	2:D:291:TYR:HA	1.86	0.58
2:D:345:VAL:CG1	2:D:439:LEU:HB2	2.31	0.58
2:B:697:CYS:HA	2:B:712:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:TYR:HD2	1:C:301:PRO:HD3	1.69	0.58
2:D:161:ILE:HG23	2:D:225:GLY:HA2	1.85	0.58
2:D:55:VAL:HG22	2:D:64:LEU:HD22	1.86	0.58
2:B:281:PHE:HB3	2:B:291:TYR:HA	1.86	0.58
1:A:299:TYR:HD2	1:A:301:PRO:HD3	1.69	0.58
2:B:518:LEU:H	2:B:518:LEU:HD22	1.69	0.58
2:B:161:ILE:HG23	2:B:225:GLY:HA2	1.85	0.57
2:D:111:VAL:HG22	2:D:112:TRP:N	2.19	0.57
2:B:55:VAL:HG22	2:B:64:LEU:HD22	1.86	0.57
2:B:62:ILE:HB	2:B:73:LEU:HB2	1.87	0.57
2:D:176:VAL:HA	2:D:217:ARG:NH1	2.19	0.57
2:D:697:CYS:HA	2:D:712:PRO:HG3	1.85	0.57
2:B:450:LEU:HD11	2:B:534:PRO:HD2	1.86	0.57
1:C:136:SER:O	1:C:139:LYS:HG3	2.04	0.57
1:A:136:SER:O	1:A:139:LYS:HG3	2.04	0.57
1:C:157:ILE:CG1	1:C:181:VAL:HG11	2.33	0.57
2:B:345:VAL:CG1	2:B:439:LEU:HB2	2.31	0.57
1:C:271:ILE:HD11	2:D:426:ARG:NH2	2.20	0.57
2:D:443:SER:HB2	2:D:454:ASN:HD21	1.68	0.57
2:D:580:ARG:HG3	2:D:625:THR:HG22	1.86	0.57
2:D:726:ILE:H	2:D:726:ILE:HD12	1.69	0.57
2:D:547:ARG:HG2	2:D:548:SER:H	1.70	0.56
2:D:62:ILE:HB	2:D:73:LEU:HB2	1.87	0.56
2:D:518:LEU:H	2:D:518:LEU:HD22	1.69	0.56
2:B:580:ARG:HG3	2:B:625:THR:HG22	1.86	0.56
2:B:726:ILE:H	2:B:726:ILE:HD12	1.69	0.56
2:B:167:GLU:O	2:B:168:GLU:HB2	2.05	0.56
2:B:547:ARG:HG3	2:B:547:ARG:HH11	1.71	0.56
2:B:575:LEU:HD21	2:B:656:ASP:CB	2.36	0.56
2:D:168:GLU:OE1	2:D:168:GLU:HA	2.06	0.56
2:D:575:LEU:HD21	2:D:656:ASP:CB	2.36	0.56
2:B:176:VAL:HA	2:B:217:ARG:NH1	2.18	0.56
1:C:148:SER:HA	1:C:170:TYR:HB2	1.88	0.56
2:D:332:GLN:OE1	2:D:469:ARG:HB2	2.05	0.56
2:D:692:ILE:HD12	2:D:712:PRO:HD2	1.88	0.56
2:B:443:SER:HB2	2:B:454:ASN:HD21	1.69	0.55
2:B:724:LEU:HB3	2:B:726:ILE:CD1	2.36	0.55
2:D:547:ARG:HG2	2:D:548:SER:N	2.21	0.55
1:A:310:ARG:HE	2:B:431:MET:HG2	1.69	0.55
2:B:332:GLN:OE1	2:B:469:ARG:HB2	2.05	0.55
2:B:547:ARG:HG2	2:B:548:SER:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:LEU:HD21	2:D:467:VAL:HG12	1.88	0.55
1:A:271:ILE:HG12	2:B:426:ARG:HH22	1.71	0.55
2:B:168:GLU:OE1	2:B:168:GLU:HA	2.06	0.55
1:A:310:ARG:NH2	2:B:431:MET:SD	2.80	0.55
2:B:547:ARG:HG2	2:B:548:SER:H	1.70	0.55
2:B:692:ILE:HD12	2:B:712:PRO:HD2	1.88	0.55
1:A:148:SER:HA	1:A:170:TYR:HB2	1.88	0.55
2:D:547:ARG:HH11	2:D:547:ARG:HG3	1.71	0.55
2:B:429:LEU:CD2	2:B:469:ARG:HE	2.20	0.55
1:C:38:ILE:O	1:C:38:ILE:HG13	2.07	0.55
1:A:157:ILE:CG1	1:A:181:VAL:HG11	2.33	0.55
2:B:670:ALA:O	2:B:713:ALA:HA	2.06	0.55
2:B:669:MET:SD	2:B:740:GLU:HB2	2.47	0.55
2:B:203:SER:HA	2:B:242:ARG:HG2	1.90	0.54
2:D:670:ALA:O	2:D:713:ALA:HA	2.07	0.54
2:B:396:HIS:CE1	2:B:416:TYR:CD1	2.95	0.54
2:B:329:LEU:HD21	2:B:467:VAL:HG12	1.87	0.54
2:B:667:GLY:HA3	2:B:736:PHE:HZ	1.72	0.54
2:D:56:ILE:CD1	2:D:120:LEU:HB3	2.37	0.54
2:D:647:THR:HG22	2:D:648:GLN:H	1.72	0.54
2:B:138:ARG:HH22	2:B:205:TYR:C	2.10	0.54
2:B:692:ILE:HG22	2:B:722:VAL:HG13	1.88	0.54
2:B:454:ASN:HB3	2:B:464:GLN:HG2	1.90	0.54
2:D:692:ILE:HG22	2:D:722:VAL:HG13	1.88	0.54
2:D:724:LEU:HB3	2:D:726:ILE:CD1	2.36	0.54
2:D:662:ILE:HG22	2:D:734:SER:HB2	1.90	0.54
2:D:669:MET:SD	2:D:740:GLU:HB2	2.47	0.54
2:B:56:ILE:CD1	2:B:120:LEU:HB3	2.37	0.54
2:D:203:SER:HA	2:D:242:ARG:HG2	1.90	0.54
2:D:454:ASN:HB3	2:D:464:GLN:HG2	1.90	0.54
2:D:667:GLY:HA3	2:D:736:PHE:HZ	1.72	0.54
1:A:38:ILE:O	1:A:38:ILE:HG13	2.07	0.54
2:B:120:LEU:HD12	2:B:130:LEU:HD11	1.90	0.54
2:B:176:VAL:HG22	2:B:217:ARG:HH12	1.73	0.54
2:D:120:LEU:HD12	2:D:130:LEU:HD11	1.90	0.54
2:D:138:ARG:HH22	2:D:205:TYR:C	2.10	0.54
2:D:219:LEU:HG	2:D:220:LYS:N	2.22	0.54
2:D:241:PHE:HA	2:D:244:SER:OG	2.07	0.54
2:B:721:ALA:HA	2:B:735:ILE:HG13	1.90	0.54
1:C:310:ARG:NH1	1:C:310:ARG:CG	2.61	0.54
1:C:48:PHE:HA	1:C:92:GLN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:634:PHE:HB3	2:D:636:MET:HG3	1.90	0.54
2:B:241:PHE:HA	2:B:244:SER:OG	2.07	0.54
2:B:634:PHE:HB3	2:B:636:MET:HG3	1.90	0.54
2:B:662:ILE:HG22	2:B:734:SER:HB2	1.90	0.54
1:C:299:TYR:CD2	1:C:301:PRO:HD3	2.43	0.54
2:D:345:VAL:HG11	2:D:439:LEU:CB	2.36	0.54
2:D:721:ALA:HA	2:D:735:ILE:HG13	1.90	0.54
2:D:256:ASN:O	2:D:257:ASN:HB2	2.08	0.53
2:D:429:LEU:CD2	2:D:469:ARG:HE	2.20	0.53
1:A:94:ILE:HA	1:A:97:LEU:HD13	1.90	0.53
1:C:94:ILE:HA	1:C:97:LEU:HD13	1.90	0.53
2:D:430:PHE:CG	2:D:434:PHE:HE1	2.26	0.53
2:B:256:ASN:O	2:B:257:ASN:HB2	2.08	0.53
1:C:147:LEU:HD11	1:C:149:LEU:HG	1.91	0.53
2:D:638:ILE:HD11	2:D:652:PHE:HB2	1.90	0.53
1:A:147:LEU:HD11	1:A:149:LEU:HG	1.91	0.53
2:B:647:THR:HG22	2:B:648:GLN:H	1.72	0.53
2:B:697:CYS:HB2	2:B:712:PRO:HD3	1.91	0.53
1:C:169:LEU:HD11	1:C:171:LEU:HD21	1.91	0.53
2:D:269:LEU:HD11	2:D:387:GLN:HB3	1.91	0.53
2:D:697:CYS:HB2	2:D:712:PRO:HD3	1.91	0.53
2:B:86:THR:HB	2:B:115:ASN:HD22	1.73	0.53
1:C:213:LEU:HD12	1:C:214:TYR:H	1.74	0.53
1:A:150:GLU:HG2	1:A:172:GLY:H	1.74	0.53
2:B:219:LEU:HG	2:B:220:LYS:N	2.23	0.53
1:C:150:GLU:HG2	1:C:172:GLY:H	1.74	0.53
1:C:299:TYR:HE2	1:C:301:PRO:HG3	1.74	0.53
2:D:363:CYS:HB3	2:D:427:VAL:O	2.09	0.53
1:A:150:GLU:HG2	1:A:172:GLY:N	2.23	0.52
2:B:278:ILE:C	2:B:279:ILE:HD12	2.30	0.52
2:B:419:GLU:HG2	2:B:420:PHE:H	1.74	0.52
2:B:430:PHE:CG	2:B:434:PHE:HE1	2.26	0.52
2:B:638:ILE:HD11	2:B:652:PHE:HB2	1.90	0.52
1:C:150:GLU:HG2	1:C:172:GLY:N	2.23	0.52
2:D:86:THR:HB	2:D:115:ASN:HD22	1.73	0.52
2:D:692:ILE:CD1	2:D:712:PRO:HD2	2.39	0.52
1:A:169:LEU:HD11	1:A:171:LEU:HD21	1.91	0.52
1:A:299:TYR:CD2	1:A:301:PRO:HD3	2.43	0.52
2:D:597:ASP:OD2	2:D:599:LYS:HB2	2.09	0.52
2:B:269:LEU:HD11	2:B:387:GLN:HB3	1.91	0.52
2:D:176:VAL:HG22	2:D:217:ARG:HH12	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:HA	1:A:92:GLN:O	2.08	0.52
2:B:719:GLU:HG2	2:B:737:SER:HB3	1.92	0.52
2:D:229:LEU:HB2	2:D:286:SER:CB	2.40	0.52
2:D:719:GLU:HG2	2:D:737:SER:HB3	1.92	0.52
2:B:55:VAL:HG21	2:B:510:ILE:HD12	1.92	0.52
2:B:673:THR:HG22	2:B:711:THR:HG21	1.92	0.52
1:C:113:ILE:HG13	1:C:137:SER:CB	2.39	0.52
2:D:419:GLU:HG2	2:D:420:PHE:H	1.74	0.52
2:D:363:CYS:HA	2:D:429:LEU:HG	1.92	0.52
2:B:229:LEU:HB2	2:B:286:SER:CB	2.40	0.52
2:B:692:ILE:CD1	2:B:712:PRO:HD2	2.40	0.52
2:D:659:ILE:HD11	2:D:724:LEU:HD23	1.92	0.52
2:B:518:LEU:HD23	2:B:522:HIS:NE2	2.24	0.52
2:B:597:ASP:OD2	2:B:599:LYS:HB2	2.09	0.52
1:A:124:TRP:HZ2	2:B:604:LEU:HD23	1.75	0.52
2:B:691:SER:CB	2:B:696:THR:HA	2.40	0.52
2:D:89:VAL:CG1	2:D:90:LEU:N	2.72	0.52
2:B:391:GLY:O	2:B:394:HIS:HD2	1.93	0.51
2:B:89:VAL:CG1	2:B:90:LEU:N	2.73	0.51
1:A:169:LEU:HG	1:A:171:LEU:HG	1.91	0.51
1:A:213:LEU:HD12	1:A:214:TYR:H	1.74	0.51
2:D:673:THR:HG22	2:D:711:THR:HG21	1.92	0.51
1:A:223:LEU:HD11	1:A:311:PHE:CG	2.46	0.51
2:B:325:PRO:HG2	2:B:336:SER:O	2.10	0.51
2:B:363:CYS:HB3	2:B:427:VAL:O	2.09	0.51
2:B:396:HIS:CG	2:B:397:CYS:H	2.27	0.51
2:B:363:CYS:HA	2:B:429:LEU:HG	1.92	0.51
2:D:55:VAL:HG21	2:D:510:ILE:HD12	1.92	0.51
2:B:697:CYS:HB3	2:B:712:PRO:HD3	1.93	0.51
1:C:169:LEU:HG	1:C:171:LEU:HG	1.91	0.51
2:D:229:LEU:HB2	2:D:286:SER:HB3	1.92	0.51
1:A:299:TYR:HE2	1:A:301:PRO:HG3	1.74	0.51
2:D:691:SER:CB	2:D:696:THR:HA	2.40	0.51
2:D:279:ILE:HG13	2:D:293:GLU:HG2	1.92	0.51
2:B:232:GLN:HB3	2:B:417:ARG:HH22	1.76	0.51
2:B:229:LEU:HB2	2:B:286:SER:HB3	1.92	0.51
2:B:279:ILE:HG13	2:B:293:GLU:HG2	1.92	0.51
2:D:176:VAL:HG13	2:D:217:ARG:NH1	2.26	0.51
2:D:278:ILE:C	2:D:279:ILE:HD12	2.30	0.51
1:A:299:TYR:HD1	2:B:469:ARG:NH1	2.08	0.51
2:D:216:VAL:HG23	2:D:288:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:697:CYS:HB3	2:D:712:PRO:HD3	1.93	0.51
2:D:295:PRO:HB2	2:D:423:ALA:CB	2.40	0.51
2:D:732:GLU:CD	2:D:732:GLU:H	2.14	0.51
2:B:176:VAL:HG13	2:B:217:ARG:NH1	2.26	0.51
2:B:295:PRO:HB2	2:B:423:ALA:CB	2.41	0.51
2:B:568:VAL:HG22	2:B:583:ILE:HG23	1.93	0.51
2:B:659:ILE:HD11	2:B:724:LEU:HD23	1.92	0.51
2:D:568:VAL:HG22	2:D:583:ILE:HG23	1.93	0.50
2:D:697:CYS:HB2	2:D:710:TYR:O	2.11	0.50
1:A:53:PHE:HB2	1:A:88:ILE:HG23	1.94	0.50
2:B:216:VAL:HG23	2:B:288:LEU:HD11	1.92	0.50
1:A:127:LEU:HD13	1:A:132:VAL:HG21	1.94	0.50
2:B:329:LEU:HD12	2:B:333:ILE:HD13	1.93	0.50
1:C:127:LEU:HD13	1:C:132:VAL:HG21	1.94	0.50
2:D:232:GLN:HB3	2:D:417:ARG:HH22	1.76	0.50
1:A:299:TYR:CD1	2:B:469:ARG:NH1	2.80	0.50
1:C:53:PHE:HB2	1:C:88:ILE:HG23	1.94	0.50
1:C:218:ASN:O	1:C:240:GLN:HA	2.12	0.50
2:D:539:GLY:HA3	2:D:556:TRP:CE2	2.46	0.50
2:B:732:GLU:CD	2:B:732:GLU:H	2.14	0.50
1:C:251:SER:HA	1:C:287:LEU:O	2.10	0.50
2:D:325:PRO:HG2	2:D:336:SER:O	2.10	0.50
1:A:251:SER:HA	1:A:287:LEU:O	2.11	0.50
2:B:697:CYS:HB2	2:B:710:TYR:O	2.11	0.50
2:D:329:LEU:HD12	2:D:333:ILE:HD13	1.94	0.50
1:A:123:GLY:O	1:A:144:LEU:HD12	2.12	0.50
2:B:539:GLY:HA3	2:B:556:TRP:CE2	2.46	0.50
1:C:223:LEU:HD11	1:C:311:PHE:CG	2.46	0.50
1:A:218:ASN:O	1:A:240:GLN:HA	2.12	0.49
2:B:163:SER:HB3	2:B:164:PRO:CD	2.42	0.49
1:C:272:ILE:HG22	1:C:273:SER:N	2.27	0.49
1:A:125:LEU:HD12	1:A:126:PHE:N	2.27	0.49
1:A:266:LEU:HD13	1:A:281:PRO:HB3	1.93	0.49
2:B:457:THR:HG22	2:B:458:SER:N	2.28	0.49
2:B:689:HIS:ND1	2:B:725:LYS:HB3	2.27	0.49
2:D:689:HIS:ND1	2:D:725:LYS:HB3	2.27	0.49
2:B:345:VAL:HG11	2:B:439:LEU:CB	2.36	0.49
1:A:238:PHE:CE2	2:B:470:SER:HA	2.48	0.49
1:C:266:LEU:HD13	1:C:281:PRO:HB3	1.93	0.49
2:D:463:MET:HA	2:D:477:VAL:O	2.13	0.49
1:A:190:THR:HG22	1:A:191:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HG22	1:A:273:SER:N	2.27	0.49
2:B:547:ARG:CG	2:B:548:SER:H	2.26	0.49
1:C:125:LEU:HD12	1:C:126:PHE:N	2.28	0.49
1:C:123:GLY:O	1:C:144:LEU:HD12	2.12	0.49
2:D:262:LEU:HD11	2:D:342:LEU:HD21	1.95	0.49
2:D:457:THR:HG22	2:D:458:SER:N	2.28	0.49
1:A:235:LEU:HD12	1:A:236:GLU:N	2.28	0.49
2:B:203:SER:OG	2:B:243:ASP:HB2	2.13	0.49
2:B:262:LEU:HD11	2:B:342:LEU:HD21	1.95	0.49
2:B:419:GLU:HG2	2:B:420:PHE:N	2.28	0.49
1:C:114:LYS:N	1:C:115:PRO:CD	2.76	0.49
1:A:244:ASN:HB2	1:A:317:GLN:OE1	2.13	0.49
2:B:171:GLN:HA	2:B:210:PRO:HG3	1.95	0.49
2:B:518:LEU:HD23	2:B:522:HIS:CD2	2.47	0.49
1:A:310:ARG:NH1	1:A:310:ARG:CB	2.76	0.48
1:A:114:LYS:N	1:A:115:PRO:CD	2.76	0.48
2:B:457:THR:C	2:B:459:GLU:H	2.17	0.48
1:C:310:ARG:NH1	1:C:310:ARG:CB	2.76	0.48
2:D:171:GLN:HA	2:D:210:PRO:HG3	1.95	0.48
2:D:547:ARG:CG	2:D:548:SER:H	2.26	0.48
1:A:113:ILE:HG13	1:A:137:SER:CB	2.39	0.48
2:B:118:MET:HB2	2:B:177:VAL:HG11	1.96	0.48
2:B:565:ILE:HG12	2:B:640:ILE:HD12	1.94	0.48
1:C:244:ASN:HB2	1:C:317:GLN:OE1	2.13	0.48
2:D:203:SER:OG	2:D:243:ASP:HB2	2.13	0.48
2:D:565:ILE:HG12	2:D:640:ILE:HD12	1.94	0.48
1:A:85:ASN:HA	1:A:107:GLY:O	2.14	0.48
2:B:44:PRO:HB2	2:B:512:LYS:HB3	1.95	0.48
2:D:457:THR:C	2:D:459:GLU:H	2.17	0.48
1:C:58:LYS:HD2	1:C:58:LYS:C	2.34	0.48
2:B:647:THR:HG22	2:B:648:GLN:N	2.29	0.48
2:D:419:GLU:HG2	2:D:420:PHE:N	2.28	0.48
2:D:44:PRO:HB2	2:D:512:LYS:HB3	1.95	0.48
2:B:534:PRO:HD3	2:B:594:ASN:ND2	2.27	0.48
2:D:699:LEU:HD22	2:D:708:GLU:O	2.14	0.48
2:B:176:VAL:CA	2:B:217:ARG:HH12	2.24	0.48
2:B:361:ALA:O	2:B:362:MET:HB2	2.14	0.48
2:B:341:ILE:CG2	2:B:364:ALA:HB1	2.44	0.48
2:B:126:TYR:CE1	2:B:221:GLU:HA	2.49	0.47
1:C:271:ILE:CD1	2:D:426:ARG:NH2	2.76	0.47
2:B:395:GLU:OE1	2:B:395:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:MET:HA	2:B:477:VAL:O	2.13	0.47
2:B:726:ILE:C	2:B:728:LEU:H	2.18	0.47
2:D:126:TYR:CE1	2:D:221:GLU:HA	2.49	0.47
2:D:161:ILE:HG23	2:D:225:GLY:CA	2.44	0.47
2:D:276:THR:HG21	2:D:346:PHE:HE2	1.80	0.47
2:D:518:LEU:HD23	2:D:522:HIS:CD2	2.49	0.47
1:A:158:ASN:O	1:A:161:VAL:HG12	2.15	0.47
2:B:699:LEU:HD22	2:B:708:GLU:O	2.14	0.47
1:C:85:ASN:HA	1:C:107:GLY:O	2.14	0.47
1:A:58:LYS:HD2	1:A:58:LYS:C	2.34	0.47
2:B:161:ILE:HG23	2:B:225:GLY:CA	2.44	0.47
1:C:113:ILE:CG1	1:C:137:SER:HB2	2.43	0.47
2:D:86:THR:HB	2:D:115:ASN:ND2	2.30	0.47
2:D:342:LEU:HB3	2:D:365:PHE:HB2	1.96	0.47
2:D:341:ILE:CG2	2:D:364:ALA:HB1	2.44	0.47
2:D:592:ARG:HD2	2:D:592:ARG:HA	1.50	0.47
2:B:639:ILE:HD12	2:B:639:ILE:N	2.30	0.47
2:D:52:ILE:HB	2:D:505:ILE:HG21	1.97	0.47
2:B:262:LEU:HD11	2:B:342:LEU:HD11	1.97	0.47
2:B:429:LEU:HD22	2:B:469:ARG:HE	1.80	0.47
1:C:158:ASN:O	1:C:161:VAL:HG12	2.14	0.47
2:D:262:LEU:HD11	2:D:342:LEU:HD11	1.97	0.47
2:D:716:ILE:HG21	2:D:718:THR:HG22	1.97	0.47
2:B:161:ILE:HG21	2:B:226:PHE:CE1	2.50	0.47
2:B:581:LEU:O	2:B:623:LYS:HA	2.15	0.47
2:B:384:ARG:NH2	2:B:387:GLN:HE22	2.13	0.47
2:B:52:ILE:HB	2:B:505:ILE:HG21	1.97	0.47
1:C:190:THR:HG22	1:C:191:LEU:N	2.29	0.47
2:D:361:ALA:O	2:D:362:MET:HB2	2.15	0.47
2:D:639:ILE:N	2:D:639:ILE:HD12	2.30	0.47
1:A:36:GLU:HG3	1:A:95:GLN:CB	2.45	0.46
2:B:725:LYS:NZ	2:B:729:ALA:HB2	2.31	0.46
1:A:266:LEU:CD1	1:A:281:PRO:HB3	2.45	0.46
2:B:216:VAL:HG12	2:B:216:VAL:O	2.16	0.46
2:D:581:LEU:HD21	2:D:652:PHE:CE1	2.50	0.46
2:B:165:GLN:HG2	2:B:171:GLN:O	2.16	0.46
1:C:266:LEU:CD1	1:C:281:PRO:HB3	2.45	0.46
2:D:129:GLN:HE22	2:D:143:ARG:HE	1.64	0.46
2:D:217:ARG:O	2:D:217:ARG:HG2	2.16	0.46
2:D:429:LEU:HD22	2:D:469:ARG:HE	1.80	0.46
2:D:647:THR:HG22	2:D:648:GLN:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:O	2:B:217:ARG:HG2	2.16	0.46
2:B:294:MET:HA	2:B:295:PRO:HD3	1.81	0.46
2:B:385:CYS:SG	2:B:396:HIS:HD2	2.37	0.46
2:B:716:ILE:HG21	2:B:718:THR:HG22	1.97	0.46
1:C:235:LEU:HD12	1:C:236:GLU:N	2.28	0.46
1:C:310:ARG:HB2	1:C:310:ARG:NH1	2.31	0.46
2:D:161:ILE:HG21	2:D:226:PHE:CE1	2.50	0.46
2:B:698:THR:HG21	2:D:392:PRO:HD2	1.97	0.46
1:A:310:ARG:HB2	1:A:310:ARG:NH1	2.31	0.46
2:B:126:TYR:HE2	2:B:193:ILE:HG13	1.81	0.46
2:B:125:TYR:CD1	2:B:188:VAL:HG11	2.50	0.46
2:B:461:ARG:HG2	2:B:480:LEU:HD23	1.97	0.46
2:B:48:ALA:HB1	2:B:71:TYR:CZ	2.51	0.46
2:D:48:ALA:HB1	2:D:71:TYR:CZ	2.51	0.46
2:D:526:CYS:HA	2:D:540:TRP:CE3	2.50	0.46
2:D:591:ARG:C	2:D:591:ARG:HD3	2.36	0.46
2:D:725:LYS:NZ	2:D:729:ALA:HB2	2.31	0.46
2:B:342:LEU:HB3	2:B:365:PHE:HB2	1.95	0.46
2:B:571:ASN:O	2:B:652:PHE:HA	2.16	0.46
2:D:384:ARG:NH2	2:D:387:GLN:HE22	2.13	0.46
2:D:562:LEU:HD22	2:D:645:GLY:HA3	1.98	0.46
2:B:86:THR:HB	2:B:115:ASN:ND2	2.30	0.46
2:B:260:TYR:CE2	2:B:280:ARG:HG3	2.50	0.46
2:B:269:LEU:CD1	2:B:387:GLN:HB3	2.46	0.46
2:B:526:CYS:HA	2:B:540:TRP:CE3	2.50	0.46
2:B:581:LEU:HD21	2:B:652:PHE:CE1	2.50	0.46
2:D:126:TYR:HE2	2:D:193:ILE:HG13	1.81	0.46
2:D:216:VAL:O	2:D:216:VAL:HG12	2.15	0.46
2:D:260:TYR:CE2	2:D:280:ARG:HG3	2.51	0.46
2:D:726:ILE:C	2:D:728:LEU:H	2.18	0.46
1:A:201:ILE:HB	1:A:204:LEU:HD12	1.98	0.46
1:A:267:VAL:HG22	1:A:300:GLN:HG2	1.98	0.46
2:D:461:ARG:HG2	2:D:480:LEU:HD23	1.97	0.46
2:D:581:LEU:O	2:D:623:LYS:HA	2.15	0.46
2:B:689:HIS:CD2	2:B:689:HIS:O	2.69	0.46
2:D:269:LEU:CD1	2:D:387:GLN:HB3	2.46	0.46
2:B:276:THR:HG21	2:B:346:PHE:HE2	1.80	0.46
2:B:458:SER:O	2:B:485:PRO:HG3	2.16	0.46
1:C:43:PRO:HA	1:C:68:ASP:O	2.15	0.46
1:C:36:GLU:HG3	1:C:95:GLN:CB	2.45	0.46
2:D:546:VAL:HG22	2:D:547:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ILE:HB	1:C:204:LEU:HD12	1.98	0.45
2:B:278:ILE:HB	2:B:296:LEU:HD11	1.98	0.45
2:D:125:TYR:CD1	2:D:188:VAL:HG11	2.51	0.45
2:D:365:PHE:CE2	2:D:426:ARG:HG2	2.51	0.45
2:D:571:ASN:O	2:D:652:PHE:HA	2.16	0.45
1:A:43:PRO:HA	1:A:68:ASP:O	2.16	0.45
1:A:215:LEU:HB2	1:A:237:LEU:HD23	1.98	0.45
2:B:591:ARG:C	2:B:591:ARG:HD3	2.36	0.45
1:C:267:VAL:HG13	1:C:300:GLN:HB2	1.98	0.45
2:D:144:HIS:ND1	2:D:158:VAL:HG22	2.31	0.45
2:D:580:ARG:HG3	2:D:625:THR:CG2	2.46	0.45
1:A:238:PHE:CD2	2:B:470:SER:HA	2.52	0.45
1:A:286:HIS:O	1:A:288:PRO:HD3	2.17	0.45
1:A:38:ILE:HG12	1:A:72:GLN:OE1	2.17	0.45
1:C:267:VAL:HG22	1:C:300:GLN:HG2	1.98	0.45
2:D:245:TYR:CD2	2:D:266:ARG:HB3	2.52	0.45
2:D:574:PRO:HG2	2:D:727:ASP:HB2	1.99	0.45
1:A:169:LEU:HD21	1:A:171:LEU:HD11	1.98	0.45
1:A:239:SER:HA	1:A:312:HIS:ND1	2.32	0.45
2:B:129:GLN:HE22	2:B:143:ARG:HE	1.63	0.45
1:C:310:ARG:HH11	1:C:310:ARG:CB	2.29	0.45
1:C:38:ILE:HG12	1:C:72:GLN:OE1	2.17	0.45
2:D:458:SER:O	2:D:485:PRO:HG3	2.16	0.45
1:C:286:HIS:O	1:C:288:PRO:HD3	2.17	0.45
1:C:48:PHE:CE2	1:C:57:ILE:HG13	2.52	0.45
2:D:139:GLY:HA3	2:D:177:VAL:O	2.16	0.45
1:A:157:ILE:N	1:A:157:ILE:HD13	2.31	0.45
1:A:271:ILE:HG12	2:B:426:ARG:NH2	2.31	0.45
1:A:310:ARG:HH11	1:A:310:ARG:CB	2.30	0.45
2:B:144:HIS:ND1	2:B:158:VAL:HG22	2.31	0.45
2:B:365:PHE:CE2	2:B:426:ARG:HG2	2.51	0.45
2:B:546:VAL:HG22	2:B:547:ARG:N	2.31	0.45
2:B:581:LEU:HD21	2:B:652:PHE:HE1	1.82	0.45
2:D:659:ILE:CD1	2:D:724:LEU:HD23	2.47	0.45
1:A:202:VAL:N	1:A:203:PRO:CD	2.80	0.45
1:A:268:THR:HA	1:A:269:PRO:HD3	1.85	0.45
1:A:61:LEU:HD21	1:A:78:ILE:HD11	1.99	0.45
2:B:659:ILE:CD1	2:B:724:LEU:HD23	2.47	0.45
1:C:149:LEU:HB3	1:C:154:ILE:HD11	1.99	0.45
1:C:215:LEU:HB2	1:C:237:LEU:HD23	1.98	0.45
2:D:672:GLY:N	2:D:711:THR:HG23	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:GLY:HA3	2:B:177:VAL:O	2.16	0.44
2:B:300:LEU:H	2:B:312:GLU:N	2.15	0.44
2:B:527:SER:OG	2:B:587:ASP:HA	2.17	0.44
1:C:169:LEU:HD21	1:C:171:LEU:HD11	1.98	0.44
1:C:61:LEU:HD21	1:C:78:ILE:HD11	1.99	0.44
2:D:211:LEU:HA	2:D:211:LEU:HD23	1.86	0.44
1:A:149:LEU:HB3	1:A:154:ILE:HD11	1.99	0.44
1:A:267:VAL:HG13	1:A:300:GLN:HB2	1.98	0.44
2:B:121:VAL:HG11	2:B:186:SER:HB2	2.00	0.44
1:C:239:SER:HA	1:C:312:HIS:ND1	2.32	0.44
1:C:35:MET:HA	1:C:35:MET:HE3	2.00	0.44
2:B:165:GLN:HB3	2:B:169:PRO:HA	1.98	0.44
2:B:272:GLN:OE1	2:B:272:GLN:HA	2.18	0.44
2:B:672:GLY:N	2:B:711:THR:HG23	2.32	0.44
1:C:231:ASN:HD22	1:C:231:ASN:HA	1.61	0.44
2:D:121:VAL:HG11	2:D:186:SER:HB2	1.99	0.44
2:D:300:LEU:H	2:D:312:GLU:N	2.15	0.44
1:A:125:LEU:HD12	1:A:126:PHE:H	1.82	0.44
2:B:580:ARG:HG3	2:B:625:THR:CG2	2.47	0.44
2:D:547:ARG:CG	2:D:548:SER:N	2.80	0.44
2:D:689:HIS:O	2:D:689:HIS:CD2	2.69	0.44
1:A:299:TYR:OH	1:A:310:ARG:HD2	2.17	0.44
2:B:393:ASN:HD22	2:B:393:ASN:N	2.14	0.44
2:B:732:GLU:O	2:B:732:GLU:HG2	2.18	0.44
2:D:732:GLU:HG2	2:D:732:GLU:O	2.17	0.44
1:A:48:PHE:CE2	1:A:57:ILE:HG13	2.52	0.44
2:B:159:HIS:HB3	2:B:160:CYS:H	1.65	0.44
2:B:547:ARG:CG	2:B:548:SER:N	2.80	0.44
2:B:726:ILE:N	2:B:726:ILE:HD12	2.32	0.44
2:D:691:SER:HB2	2:D:696:THR:HA	1.99	0.44
2:D:730:ASN:ND2	2:D:731:ARG:H	2.16	0.44
2:B:245:TYR:CD2	2:B:266:ARG:HB3	2.52	0.44
2:B:46:PHE:CE1	2:B:80:LYS:HB2	2.53	0.44
2:D:197:VAL:HB	2:D:215:SER:OG	2.18	0.44
1:A:113:ILE:CG1	1:A:137:SER:HB2	2.43	0.44
1:A:301:PRO:HG2	2:B:301:THR:HG23	1.98	0.44
2:B:350:LYS:HB3	2:B:351:PRO:HD2	2.00	0.44
1:C:157:ILE:N	1:C:157:ILE:HD13	2.31	0.44
1:C:202:VAL:N	1:C:203:PRO:CD	2.80	0.44
1:C:201:ILE:HD12	1:C:226:LEU:HD11	2.00	0.44
1:C:96:TYR:C	1:C:98:PRO:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:HIS:HB3	2:D:160:CYS:H	1.65	0.44
2:D:168:GLU:HA	2:D:169:PRO:HD3	1.89	0.44
2:D:325:PRO:HG3	2:D:341:ILE:HG13	2.00	0.44
1:A:97:LEU:O	1:A:100:VAL:HG12	2.18	0.44
2:B:197:VAL:HB	2:B:215:SER:OG	2.18	0.44
2:B:232:GLN:HB3	2:B:417:ARG:NH2	2.33	0.44
1:C:125:LEU:HD12	1:C:126:PHE:H	1.82	0.43
2:D:176:VAL:CA	2:D:217:ARG:HH12	2.24	0.43
2:D:232:GLN:HB3	2:D:417:ARG:NH2	2.33	0.43
2:D:294:MET:HB2	2:D:374:PHE:CE2	2.53	0.43
2:B:471:GLY:HA2	2:B:472:PRO:HD3	1.90	0.43
2:B:730:ASN:ND2	2:B:731:ARG:H	2.16	0.43
2:D:272:GLN:OE1	2:D:272:GLN:HA	2.18	0.43
2:D:43:LEU:HD23	2:D:43:LEU:N	2.33	0.43
2:D:50:THR:HA	2:D:508:LYS:HE3	2.00	0.43
1:A:310:ARG:CZ	1:A:310:ARG:HB2	2.48	0.43
2:B:461:ARG:HG2	2:B:480:LEU:CD2	2.49	0.43
2:B:691:SER:HB2	2:B:696:THR:HA	1.99	0.43
1:C:299:TYR:OH	1:C:310:ARG:HD2	2.17	0.43
2:D:350:LYS:HB3	2:D:351:PRO:HD2	2.00	0.43
2:D:46:PHE:CE1	2:D:80:LYS:HB2	2.53	0.43
2:D:581:LEU:HD21	2:D:652:PHE:HE1	1.82	0.43
1:A:204:LEU:CA	1:A:207:LEU:HD22	2.45	0.43
1:A:297:ILE:HD11	1:A:314:ARG:HD3	1.99	0.43
2:B:677:LEU:HD13	2:B:724:LEU:HD21	2.00	0.43
2:B:163:SER:CB	2:B:164:PRO:CD	2.97	0.43
2:B:198:GLY:HA2	2:B:213:SER:O	2.18	0.43
2:B:263:THR:O	2:B:276:THR:HA	2.19	0.43
2:B:325:PRO:HG3	2:B:341:ILE:HG13	2.00	0.43
1:C:297:ILE:HD11	1:C:314:ARG:HD3	2.00	0.43
2:D:274:PHE:CG	2:D:354:ALA:HB2	2.54	0.43
1:A:231:ASN:HA	1:A:231:ASN:HD22	1.61	0.43
2:B:294:MET:HB2	2:B:374:PHE:CE2	2.53	0.43
2:B:50:THR:HA	2:B:508:LYS:HE3	2.00	0.43
2:B:703:SER:HB3	2:B:706:ILE:O	2.19	0.43
1:C:97:LEU:O	1:C:100:VAL:HG12	2.18	0.43
2:D:198:GLY:HA2	2:D:213:SER:O	2.18	0.43
2:D:263:THR:O	2:D:276:THR:HA	2.19	0.43
1:A:201:ILE:HD12	1:A:226:LEU:HD11	2.00	0.43
2:B:454:ASN:H	2:B:454:ASN:ND2	2.15	0.43
2:B:722:VAL:O	2:B:732:GLU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ILE:HG21	1:C:276:GLY:HA3	2.01	0.43
1:C:84:ASN:ND2	2:D:644:HIS:HA	2.34	0.43
1:A:96:TYR:C	1:A:98:PRO:HD3	2.39	0.43
2:B:274:PHE:CG	2:B:354:ALA:HB2	2.54	0.43
2:D:278:ILE:HB	2:D:296:LEU:HD11	1.99	0.43
2:B:716:ILE:HG22	2:B:717:SER:N	2.33	0.43
1:C:97:LEU:HD12	1:C:97:LEU:N	2.34	0.43
2:D:454:ASN:H	2:D:454:ASN:ND2	2.15	0.43
1:C:234:VAL:HG21	2:D:614:LEU:HB2	2.00	0.43
2:D:726:ILE:HD12	2:D:726:ILE:N	2.32	0.43
1:A:272:ILE:HG21	1:A:276:GLY:HA3	2.01	0.43
1:A:310:ARG:CZ	2:B:431:MET:SD	3.07	0.43
2:D:118:MET:HB2	2:D:177:VAL:HG11	1.96	0.43
2:D:530:LEU:HD22	2:D:558:GLN:HA	2.00	0.43
1:A:254:VAL:HG13	1:A:282:ASN:HB3	2.01	0.42
1:C:101:THR:HG22	1:C:121:ASN:O	2.19	0.42
1:C:257:ASN:HB3	1:C:266:LEU:HD22	2.01	0.42
2:D:677:LEU:HD13	2:D:724:LEU:HD21	2.01	0.42
1:A:101:THR:HG22	1:A:121:ASN:O	2.19	0.42
2:B:111:VAL:HG22	2:B:112:TRP:N	2.34	0.42
2:B:733:THR:O	2:B:734:SER:C	2.57	0.42
2:D:111:VAL:HG22	2:D:112:TRP:H	1.84	0.42
2:B:238:LEU:HD22	2:D:700:LYS:HA	2.00	0.42
2:D:703:SER:HB3	2:D:706:ILE:O	2.18	0.42
1:A:195:ASP:H	1:A:217:LYS:HB2	1.84	0.42
1:A:237:LEU:O	1:A:311:PHE:HA	2.20	0.42
2:B:43:LEU:N	2:B:43:LEU:HD23	2.33	0.42
1:C:237:LEU:O	1:C:311:PHE:HA	2.19	0.42
2:D:46:PHE:CZ	2:D:73:LEU:HD21	2.55	0.42
2:D:722:VAL:O	2:D:732:GLU:HA	2.19	0.42
1:C:310:ARG:CZ	1:C:310:ARG:HB2	2.49	0.42
1:A:97:LEU:HD12	1:A:97:LEU:N	2.34	0.42
2:B:692:ILE:HD13	2:B:692:ILE:O	2.19	0.42
1:C:195:ASP:H	1:C:217:LYS:HB2	1.84	0.42
2:D:434:PHE:HB3	2:D:437:VAL:CG1	2.50	0.42
2:D:56:ILE:HD12	2:D:122:VAL:HG23	2.02	0.42
2:D:68:ASN:HB3	2:D:87:GLY:HA2	2.00	0.42
1:A:35:MET:HA	1:A:35:MET:HE3	2.01	0.42
2:B:443:SER:HB2	2:B:454:ASN:HD22	1.83	0.42
2:D:56:ILE:HG13	2:D:63:PHE:HB2	2.02	0.42
2:D:692:ILE:O	2:D:692:ILE:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:733:THR:O	2:D:734:SER:C	2.57	0.42
2:B:724:LEU:HB3	2:B:726:ILE:HD12	2.02	0.42
2:D:273:THR:HG22	2:D:352:ASP:HA	2.01	0.42
2:D:461:ARG:HG2	2:D:480:LEU:CD2	2.49	0.42
1:A:270:GLU:OE2	2:B:469:ARG:NH2	2.53	0.42
2:B:530:LEU:HD22	2:B:558:GLN:HA	2.01	0.42
1:C:254:VAL:HG13	1:C:282:ASN:HB3	2.01	0.42
1:A:190:THR:HG22	1:A:191:LEU:H	1.85	0.42
2:B:143:ARG:HD2	2:B:223:LYS:O	2.20	0.42
2:D:662:ILE:HD11	2:D:675:LEU:CD2	2.48	0.42
2:B:56:ILE:HD12	2:B:122:VAL:HG23	2.02	0.41
2:B:566:TYR:HB2	2:B:586:TRP:CZ3	2.55	0.41
2:B:592:ARG:HA	2:B:592:ARG:HD2	1.50	0.41
2:B:68:ASN:HB3	2:B:87:GLY:HA2	2.01	0.41
2:D:221:GLU:H	2:D:221:GLU:CD	2.24	0.41
2:D:266:ARG:HG3	2:D:268:THR:O	2.20	0.41
2:D:716:ILE:HG22	2:D:717:SER:N	2.33	0.41
1:A:125:LEU:HD11	1:A:127:LEU:HG	2.01	0.41
1:A:200:ASP:OD1	1:A:202:VAL:HG23	2.20	0.41
1:A:257:ASN:HB3	1:A:266:LEU:HD22	2.01	0.41
2:B:165:GLN:HE21	2:B:167:GLU:HB2	1.85	0.41
2:B:78:LEU:HD23	2:B:78:LEU:HA	1.92	0.41
2:B:275:HIS:CG	2:B:276:THR:H	2.38	0.41
2:B:56:ILE:HG13	2:B:63:PHE:HB2	2.02	0.41
2:B:662:ILE:HD11	2:B:675:LEU:CD2	2.48	0.41
1:C:190:THR:HG22	1:C:191:LEU:H	1.85	0.41
1:C:301:PRO:HB3	1:C:310:ARG:HG2	2.02	0.41
2:B:434:PHE:HB3	2:B:437:VAL:CG1	2.50	0.41
2:B:474:THR:HG23	2:B:475:PRO:HD2	2.02	0.41
2:B:548:SER:HA	2:B:556:TRP:CZ2	2.55	0.41
1:C:125:LEU:HD11	1:C:127:LEU:HG	2.01	0.41
2:D:287:GLY:HA2	2:D:289:HIS:HE2	1.84	0.41
2:D:513:ILE:HA	2:D:514:PRO:HD3	1.87	0.41
2:D:566:TYR:HB2	2:D:586:TRP:CZ3	2.55	0.41
1:A:147:LEU:HD12	1:A:148:SER:N	2.36	0.41
1:A:35:MET:HG3	1:A:35:MET:O	2.21	0.41
2:B:266:ARG:HG3	2:B:268:THR:O	2.21	0.41
2:B:278:ILE:HD13	2:B:370:VAL:HG11	2.03	0.41
2:B:46:PHE:CZ	2:B:73:LEU:HD21	2.55	0.41
2:D:474:THR:HG23	2:D:475:PRO:HD2	2.02	0.41
2:B:442:ILE:HD13	2:B:443:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:THR:H	2:D:711:THR:CG2	2.33	0.41
1:A:301:PRO:HB3	1:A:310:ARG:HG2	2.03	0.41
2:B:218:ARG:NH2	2:B:229:LEU:HD21	2.36	0.41
1:C:204:LEU:CA	1:C:207:LEU:HD22	2.45	0.41
1:C:226:LEU:H	1:C:226:LEU:CD1	2.25	0.41
1:C:240:GLN:HG2	1:C:312:HIS:O	2.21	0.41
2:D:91:GLU:HB2	2:D:111:VAL:HG12	2.03	0.41
2:D:278:ILE:HD13	2:D:370:VAL:HG11	2.03	0.41
2:D:548:SER:HA	2:D:556:TRP:CZ2	2.55	0.41
2:B:91:GLU:CD	2:B:136:VAL:HG13	2.41	0.41
2:B:273:THR:HG22	2:B:352:ASP:HA	2.01	0.41
2:B:491:ILE:O	2:B:502:THR:HA	2.20	0.41
2:B:487:SER:OG	2:B:505:ILE:HB	2.20	0.41
2:B:54:ASN:HB2	2:B:120:LEU:HD23	2.02	0.41
2:B:60:HIS:HA	2:B:75:GLU:OE2	2.21	0.41
1:C:147:LEU:HD12	1:C:148:SER:N	2.35	0.41
2:D:217:ARG:H	2:D:217:ARG:HD2	1.85	0.41
2:D:277:ARG:HG2	2:D:295:PRO:HA	2.03	0.41
1:A:318:PRO:O	1:A:319:LEU:HD23	2.21	0.41
2:B:161:ILE:O	2:B:162:PHE:HB2	2.21	0.41
2:B:217:ARG:HD2	2:B:217:ARG:H	1.85	0.41
2:B:372:ASP:O	2:B:376:LYS:HG3	2.21	0.41
2:B:673:THR:H	2:B:711:THR:CG2	2.33	0.41
2:D:275:HIS:CG	2:D:276:THR:H	2.38	0.41
2:D:491:ILE:O	2:D:502:THR:HA	2.20	0.41
2:D:523:PHE:CZ	2:D:532:ALA:HB2	2.56	0.41
2:D:704:ASN:HD22	2:D:704:ASN:H	1.68	0.41
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.87	0.41
2:B:260:TYR:CZ	2:B:280:ARG:HG3	2.55	0.41
2:B:342:LEU:HB2	2:B:367:ILE:HD11	2.03	0.41
2:B:523:PHE:CZ	2:B:532:ALA:HB2	2.56	0.41
1:C:147:LEU:HD11	1:C:149:LEU:CG	2.50	0.41
2:D:372:ASP:O	2:D:376:LYS:HG3	2.21	0.41
2:D:442:ILE:HD13	2:D:443:SER:N	2.36	0.41
2:D:487:SER:OG	2:D:505:ILE:HB	2.21	0.41
1:A:240:GLN:HG2	1:A:312:HIS:O	2.21	0.41
2:B:357:MET:HE3	2:B:359:ARG:HD3	2.03	0.41
2:B:640:ILE:O	2:B:646:THR:HA	2.21	0.41
1:C:200:ASP:OD1	1:C:202:VAL:HG23	2.20	0.41
2:D:143:ARG:HD2	2:D:223:LYS:O	2.20	0.41
2:D:60:HIS:HA	2:D:75:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD11	1:A:149:LEU:CG	2.50	0.40
1:A:166:LEU:O	1:A:187:LYS:HB3	2.21	0.40
1:C:318:PRO:O	1:C:319:LEU:HD23	2.21	0.40
2:D:54:ASN:HB2	2:D:120:LEU:HD23	2.02	0.40
2:D:50:THR:HB	2:D:67:THR:HB	2.04	0.40
2:B:495:THR:OG1	2:B:499:ASN:HB2	2.21	0.40
2:B:50:THR:HB	2:B:67:THR:HB	2.03	0.40
2:B:704:ASN:HD22	2:B:704:ASN:H	1.68	0.40
1:C:201:ILE:HG21	1:C:220:ILE:HD12	2.03	0.40
2:D:91:GLU:CD	2:D:136:VAL:HG13	2.41	0.40
2:D:218:ARG:NH2	2:D:229:LEU:HD21	2.36	0.40
2:D:443:SER:HB2	2:D:454:ASN:HD22	1.83	0.40
2:D:64:LEU:HD11	2:D:73:LEU:HD11	2.02	0.40
1:A:229:LEU:HB3	1:A:232:LEU:HG	2.03	0.40
2:B:185:LEU:HD11	2:B:253:PHE:N	2.36	0.40
2:B:277:ARG:HG2	2:B:295:PRO:HA	2.02	0.40
2:B:64:LEU:HD11	2:B:73:LEU:HD11	2.02	0.40
1:C:35:MET:O	1:C:35:MET:HG3	2.21	0.40
2:D:342:LEU:HB2	2:D:367:ILE:HD11	2.03	0.40
2:D:543:ASP:OD2	2:D:543:ASP:N	2.54	0.40
2:D:640:ILE:O	2:D:646:THR:HA	2.21	0.40
2:B:43:LEU:HB2	2:B:44:PRO:HD2	2.03	0.40
2:D:393:ASN:HD22	2:D:393:ASN:N	2.14	0.40
2:D:443:SER:O	2:D:453:ALA:HA	2.22	0.40
2:D:711:THR:HA	2:D:712:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

## 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	284/289 (98%)	226 (80%)	54 (19%)	4 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	284/289 (98%)	227 (80%)	53 (19%)	4 (1%)	11	46
2	B	610/727 (84%)	494 (81%)	101 (17%)	15 (2%)	5	35
2	D	598/727 (82%)	489 (82%)	96 (16%)	13 (2%)	6	37
All	All	1776/2032 (87%)	1436 (81%)	304 (17%)	36 (2%)	7	40

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	LEU
2	B	163	SER
2	B	164	PRO
2	B	211	LEU
2	B	276	THR
1	C	193	LEU
2	D	211	LEU
2	D	276	THR
1	A	211	GLN
2	B	126	TYR
2	B	147	PRO
2	B	470	SER
2	B	734	SER
1	C	211	GLN
2	D	126	TYR
2	D	147	PRO
2	D	470	SER
2	D	734	SER
2	B	672	GLY
2	D	672	GLY
2	B	125	TYR
2	B	244	SER
2	B	548	SER
2	B	592	ARG
2	B	690	ILE
2	D	125	TYR
2	D	244	SER
2	D	548	SER
2	D	592	ARG
1	A	191	LEU
2	B	626	VAL
1	C	191	LEU
2	D	626	VAL

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Mol	Chain	Res	Type
2	D	690	ILE
1	A	305	GLY
1	C	305	GLY

### 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	264/265 (100%)	251 (95%)	13 (5%)	25	52
1	C	264/265 (100%)	251 (95%)	13 (5%)	25	52
2	B	566/654 (86%)	524 (93%)	42 (7%)	13	41
2	D	555/654 (85%)	514 (93%)	41 (7%)	13	41
All	All	1649/1838 (90%)	1540 (93%)	109 (7%)	16	45

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	109	LYS
1	A	135	LEU
1	A	157	ILE
1	A	180	THR
1	A	181	VAL
1	A	207	LEU
1	A	226	LEU
1	A	247	ILE
1	A	249	HIS
1	A	302	VAL
1	A	310	ARG
1	A	312	HIS
2	B	42	GLN
2	B	45	ASN
2	B	120	LEU
2	B	150	HIS
2	B	157	GLU

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Mol	Chain	Res	Type
2	B	168	GLU
2	B	210	PRO
2	B	217	ARG
2	B	218	ARG
2	B	220	LYS
2	B	222	THR
2	B	276	THR
2	B	301	THR
2	B	313	VAL
2	B	329	LEU
2	B	338	ASN
2	B	362	MET
2	B	363	CYS
2	B	385	CYS
2	B	393	ASN
2	B	394	HIS
2	B	414	ASP
2	B	416	TYR
2	B	426	ARG
2	B	442	ILE
2	B	451	THR
2	B	454	ASN
2	B	490	VAL
2	B	511	THR
2	B	518	LEU
2	B	576	GLU
2	B	591	ARG
2	B	592	ARG
2	B	599	LYS
2	B	604	LEU
2	B	622	LEU
2	B	648	GLN
2	B	660	THR
2	B	689	HIS
2	B	692	ILE
2	B	704	ASN
2	B	711	THR
1	C	37	THR
1	C	109	LYS
1	C	135	LEU
1	C	157	ILE
1	C	180	THR

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Mol	Chain	Res	Type
1	C	181	VAL
1	C	207	LEU
1	C	226	LEU
1	C	247	ILE
1	C	249	HIS
1	C	302	VAL
1	C	310	ARG
1	C	312	HIS
2	D	42	GLN
2	D	45	ASN
2	D	120	LEU
2	D	150	HIS
2	D	157	GLU
2	D	168	GLU
2	D	210	PRO
2	D	217	ARG
2	D	218	ARG
2	D	220	LYS
2	D	222	THR
2	D	276	THR
2	D	301	THR
2	D	313	VAL
2	D	329	LEU
2	D	338	ASN
2	D	362	MET
2	D	363	CYS
2	D	385	CYS
2	D	393	ASN
2	D	414	ASP
2	D	416	TYR
2	D	426	ARG
2	D	442	ILE
2	D	451	THR
2	D	454	ASN
2	D	490	VAL
2	D	511	THR
2	D	518	LEU
2	D	576	GLU
2	D	591	ARG
2	D	592	ARG
2	D	599	LYS
2	D	604	LEU

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Mol	Chain	Res	Type
2	D	622	LEU
2	D	648	GLN
2	D	660	THR
2	D	689	HIS
2	D	692	ILE
2	D	704	ASN
2	D	711	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	80	GLN
1	A	121	ASN
1	A	158	ASN
1	A	211	GLN
1	A	231	ASN
1	A	257	ASN
2	B	42	GLN
2	B	45	ASN
2	B	58	HIS
2	B	61	HIS
2	B	129	GLN
2	B	165	GLN
2	B	171	GLN
2	B	265	GLN
2	B	338	ASN
2	B	387	GLN
2	B	393	ASN
2	B	396	HIS
2	B	433	GLN
2	B	454	ASN
2	B	464	GLN
2	B	559	GLN
2	B	571	ASN
2	B	594	ASN
2	B	644	HIS
2	B	704	ASN
2	B	730	ASN
1	C	76	ASN
1	C	80	GLN
1	C	121	ASN

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Mol	Chain	Res	Type
1	C	158	ASN
1	C	211	GLN
1	C	231	ASN
1	C	257	ASN
2	D	42	GLN
2	D	45	ASN
2	D	58	HIS
2	D	61	HIS
2	D	129	GLN
2	D	171	GLN
2	D	265	GLN
2	D	338	ASN
2	D	387	GLN
2	D	393	ASN
2	D	433	GLN
2	D	454	ASN
2	D	464	GLN
2	D	559	GLN
2	D	571	ASN
2	D	644	HIS
2	D	704	ASN
2	D	730	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	113:LYS	C	114:ASP	N	1.63

## 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	286/289 (98%)	0.11	11 (3%) 40 32	89, 125, 174, 201	0
1	C	286/289 (98%)	0.02	2 (0%) 87 82	76, 112, 158, 191	0
2	B	630/727 (86%)	0.27	22 (3%) 44 35	87, 139, 208, 245	0
2	D	618/727 (85%)	0.34	27 (4%) 34 28	87, 137, 191, 236	0
All	All	1820/2032 (89%)	0.23	62 (3%) 45 36	76, 132, 192, 245	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	VAL	5.9
2	B	552	LEU	5.1
2	D	555	THR	4.9
2	D	135	SER	4.3
2	B	544	LYS	4.0
2	D	741	ASP	3.9
2	B	113	LYS	3.8
2	B	537	GLN	3.8
2	B	558	GLN	3.5
2	B	551	CYS	3.5
2	D	170	SER	3.3
2	D	83	GLU	3.3
1	C	64	LYS	3.1
2	D	593	ASN	3.0
2	D	359	ARG	3.0
2	D	49	GLU	2.9
1	A	175	LYS	2.9
2	D	88	PRO	2.8
2	B	550	GLU	2.8
2	B	71	TYR	2.8
2	B	410	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	289	GLU	2.7
2	D	273	THR	2.7
2	B	548	SER	2.6
1	A	320	LYS	2.6
2	D	161	ILE	2.6
2	D	114	ASP	2.6
2	B	556	TRP	2.6
1	C	320	LYS	2.6
2	B	553	SER	2.5
2	D	565	ILE	2.5
2	D	352	ASP	2.5
2	B	547	ARG	2.4
1	A	36	GLU	2.4
2	B	542	HIS	2.4
2	D	539	GLY	2.4
1	A	87	ASP	2.3
2	D	137	ASN	2.3
1	A	66	VAL	2.3
2	D	553	SER	2.3
2	D	731	ARG	2.3
2	B	81	VAL	2.3
1	A	250	GLN	2.3
2	D	293	GLU	2.3
2	B	83	GLU	2.2
2	D	552	LEU	2.2
2	D	557	THR	2.2
2	B	521	ARG	2.1
2	D	715	THR	2.1
2	B	741	ASP	2.1
1	A	288	PRO	2.1
1	A	89	LYS	2.1
1	A	278	TYR	2.1
2	D	171	GLN	2.1
1	A	251	SER	2.1
2	B	731	ARG	2.1
2	D	245	TYR	2.1
2	B	543	ASP	2.0
2	D	84	TYR	2.0
2	B	497	ASN	2.0
2	D	115	ASN	2.0
2	B	49	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.