



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BML  
Title : COMPLEX OF THE CATALYTIC DOMAIN OF HUMAN PLASMIN AND  
STREPTOKINASE  
Authors : Wang, X.; Zhang, X.C.  
Deposited on : 1999-05-25  
Resolution : 2.90 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

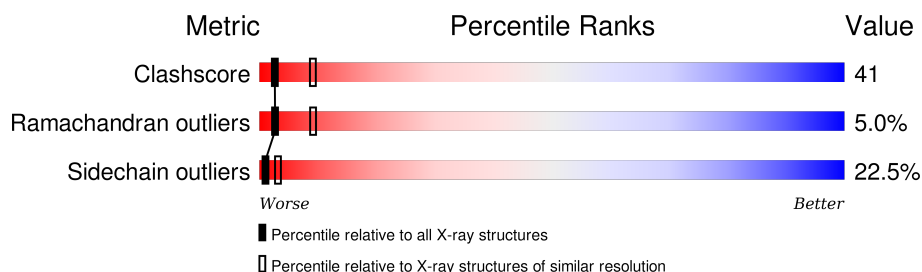
# 1 Overall quality at a glance

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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	 45% 42% 12%
1	B	250	 42% 49% 9% •
2	C	362	 26% 43% 17% • 12%
2	D	362	 31% 41% 14% • 12%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8940 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 PLASMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1917	1217	339	347	14			
1	B	250	Total	C	N	O	S	0	0	0
			1917	1217	339	347	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	ALA	SER	MUTATION	UNP P00747
B	741	ALA	SER	MUTATION	UNP P00747

- Molecule 2 is a protein called STREPTOKINASE.

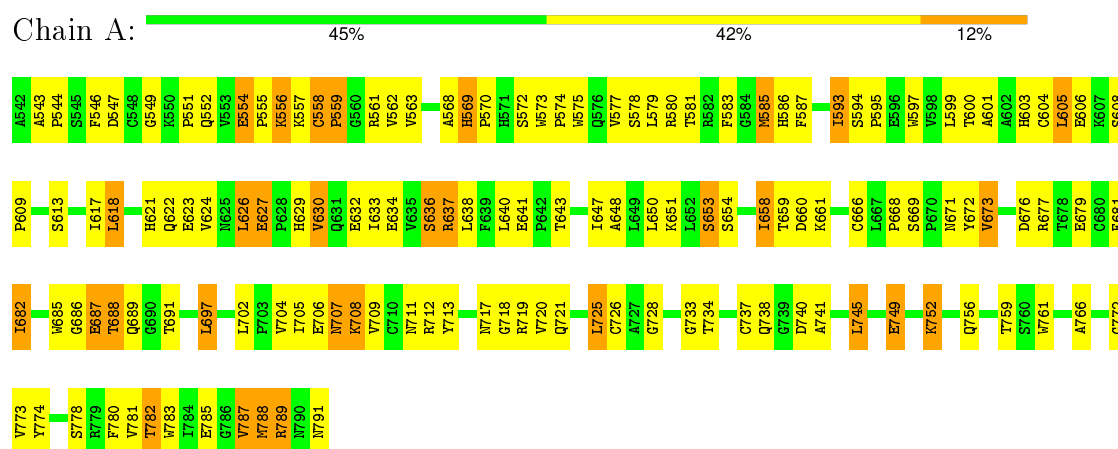
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	318	Total	C	N	O	S	0	0	0
			2553	1610	426	514	3			
2	D	318	Total	C	N	O	S	0	0	0
			2553	1610	426	514	3			

### 3 Residue-property plots

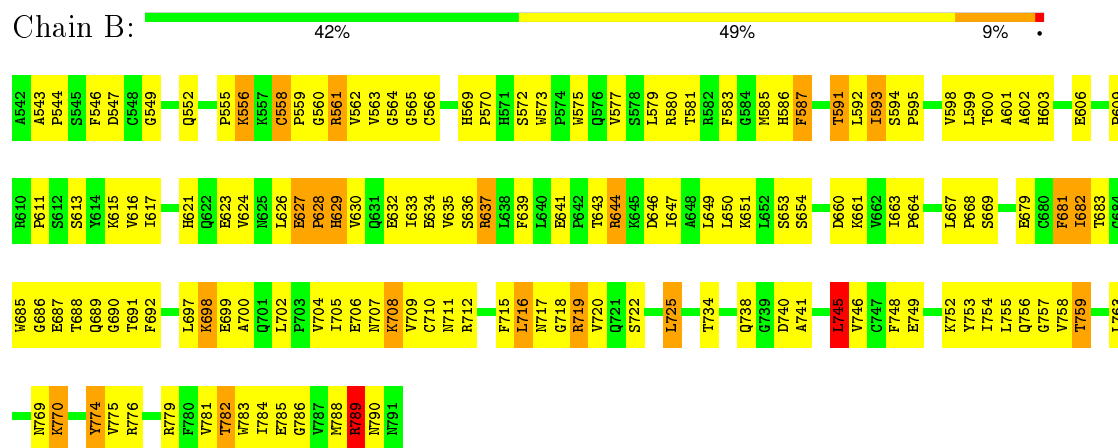
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

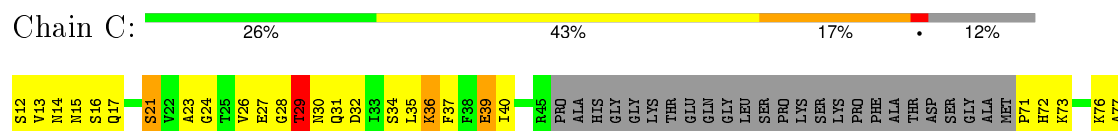
#### • Molecule 1: PLASMIN

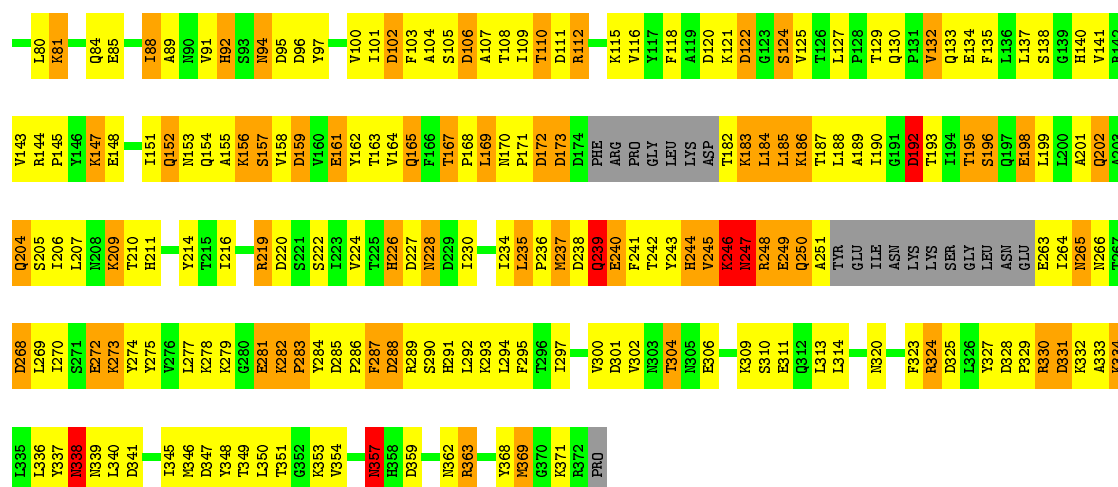


#### • Molecule 1: PLASMIN



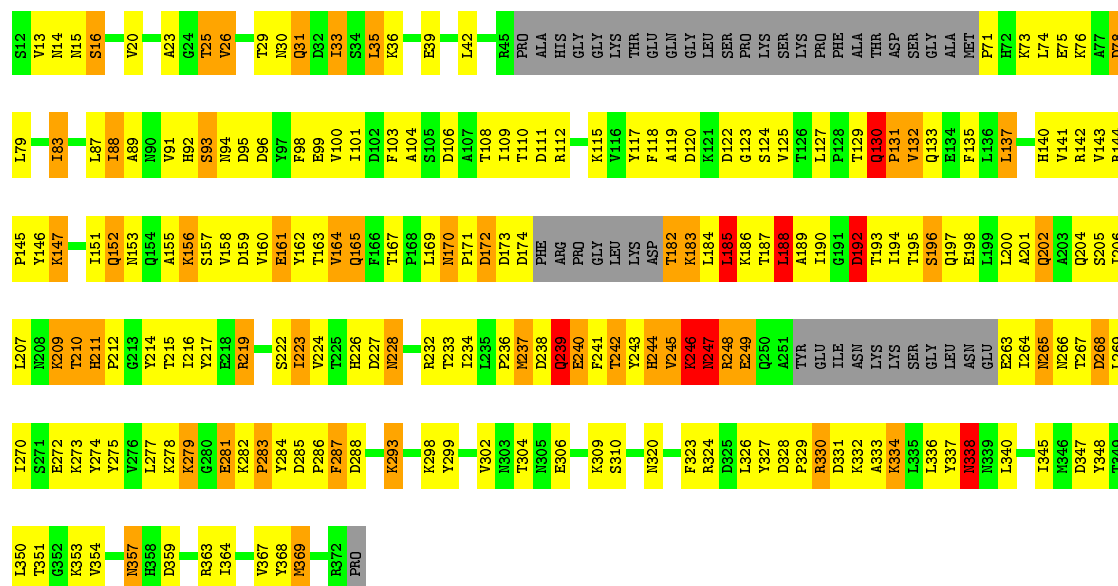
#### • Molecule 2: STREPTOKINASE





## • Molecule 2: STREPTOKINASE

Chain D: 31% 41% 14% 12%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.03 Å   125.05 Å   86.79 Å 90.00°   105.41°   90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	91.3 (20.00-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.201 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 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	0.50	0/1967	0.76	2/2673 (0.1%)
1	B	0.50	0/1967	0.74	2/2673 (0.1%)
2	C	0.44	0/2597	0.67	0/3522
2	D	0.43	0/2597	0.70	2/3522 (0.1%)
All	All	0.47	0/9128	0.72	6/12390 (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	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	745	LEU	N-CA-C	-6.63	93.09	111.00
1	A	569	HIS	N-CA-C	-5.71	95.60	111.00
1	B	745	LEU	N-CA-C	-5.56	95.99	111.00
2	D	130	GLN	N-CA-C	5.40	125.59	111.00
1	B	716	LEU	CA-CB-CG	-5.25	103.23	115.30
2	D	25	THR	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	327	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1917	0	1892	122	0
1	B	1917	0	1892	141	0
2	C	2553	0	2485	241	0
2	D	2553	0	2485	233	0
All	All	8940	0	8754	726	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 41.

All (726) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:170:ASN:HB2	2:C:171:PRO:HD2	1.24	1.13
2:D:170:ASN:HB2	2:D:171:PRO:HD2	1.14	1.10
1:B:749:GLU:HG2	1:B:754:ILE:HD13	1.33	1.05
2:D:186:LYS:HB3	2:D:188:LEU:HD21	1.40	1.03
2:C:302:VAL:HG22	2:C:368:TYR:HB3	1.45	0.96
2:D:170:ASN:HB2	2:D:171:PRO:CD	1.95	0.96
1:B:598:VAL:HB	1:B:650:LEU:HB2	1.48	0.95
2:C:304:THR:HB	2:C:306:GLU:HG2	1.50	0.93
2:D:282:LYS:HB3	2:D:283:PRO:HD2	1.48	0.92
1:B:611:PRO:HB3	1:B:635:VAL:HG12	1.50	0.91
2:C:224:VAL:HG22	2:C:270:ILE:HD12	1.55	0.87
2:C:101:ILE:HD11	2:C:144:ARG:HG2	1.56	0.87
2:C:348:TYR:HB3	2:C:369:MET:HG2	1.56	0.86
2:C:357:ASN:HD21	2:C:359:ASP:HB3	1.39	0.86
2:D:224:VAL:HG22	2:D:270:ILE:HD12	1.58	0.85
2:D:71:PRO:N	2:D:129:THR:HG22	1.91	0.85
1:B:711:ASN:HD21	1:B:720:VAL:H	1.25	0.84
2:C:282:LYS:HB3	2:C:283:PRO:HD2	1.57	0.84
1:A:682:ILE:HD11	1:A:702:LEU:HG	1.61	0.82
2:D:323:PHE:CD1	2:D:350:LEU:HD11	2.15	0.81
2:C:170:ASN:HB2	2:C:171:PRO:CD	2.06	0.81
2:D:247:ASN:O	2:D:248:ARG:HB3	1.80	0.80
2:C:283:PRO:HG2	2:C:286:PRO:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:LYS:HB3	2:D:188:LEU:CD2	2.12	0.79
2:D:357:ASN:HD22	2:D:359:ASP:H	1.27	0.79
2:C:302:VAL:CG2	2:C:368:TYR:HB3	2.11	0.79
2:D:170:ASN:CB	2:D:171:PRO:HD2	2.06	0.79
2:C:226:HIS:HB3	2:C:248:ARG:NH1	1.99	0.78
2:C:36:LYS:NZ	2:C:89:ALA:HB3	1.99	0.77
2:D:196:SER:HB2	2:D:240:GLU:OE2	1.83	0.77
1:A:637:ARG:HB2	1:A:651:LYS:HB3	1.68	0.75
1:A:577:VAL:HG22	1:A:618:LEU:HD23	1.67	0.75
1:B:746:VAL:CG1	1:B:753:TYR:HB3	2.17	0.75
1:B:586:HIS:CD2	1:B:587:PHE:N	2.54	0.75
2:D:91:VAL:HG13	2:D:96:ASP:HB2	1.68	0.75
2:C:91:VAL:HG13	2:C:96:ASP:HB2	1.67	0.74
1:A:622:GLN:HG3	2:C:313:LEU:HD21	1.69	0.74
2:C:238:ASP:O	2:C:239:GLN:HB3	1.87	0.74
2:D:351:THR:HG22	2:D:353:LYS:HD3	1.69	0.73
1:B:549:GLY:HA2	1:B:575:TRP:CZ3	2.24	0.73
1:B:746:VAL:HG11	1:B:753:TYR:HB3	1.71	0.73
1:A:666:CYS:SG	1:A:752:LYS:HD3	2.29	0.72
2:D:75:GLU:HB2	2:D:78:ASP:OD2	1.89	0.72
1:A:711:ASN:HD21	1:A:720:VAL:H	1.35	0.72
2:C:340:LEU:HG	2:C:345:ILE:HD12	1.72	0.71
2:D:106:ASP:HB3	2:D:140:HIS:H	1.55	0.71
2:D:130:GLN:O	2:D:132:VAL:HG23	1.90	0.71
2:C:247:ASN:O	2:C:248:ARG:HB3	1.88	0.71
1:B:634:GLU:HG2	1:B:635:VAL:H	1.54	0.71
2:C:245:VAL:HG12	2:C:246:LYS:H	1.56	0.71
2:D:348:TYR:HB3	2:D:369:MET:HG2	1.72	0.71
2:C:170:ASN:CB	2:C:171:PRO:HD2	2.13	0.71
2:C:350:LEU:HA	2:C:369:MET:HE2	1.73	0.71
1:A:637:ARG:NH2	1:A:638:LEU:H	1.89	0.70
1:A:595:PRO:HG3	1:A:658:ILE:HD11	1.74	0.70
2:C:132:VAL:O	2:C:132:VAL:HG12	1.89	0.70
2:D:264:ILE:HG22	2:D:265:ASN:H	1.54	0.70
1:B:681:PHE:C	1:B:682:ILE:HD13	2.12	0.70
1:A:741:ALA:HA	1:A:759:THR:HG22	1.72	0.70
2:D:281:GLU:O	2:D:282:LYS:HG3	1.92	0.70
1:B:679:GLU:HA	1:B:679:GLU:OE1	1.91	0.70
1:B:769:ASN:O	1:B:770:LYS:HG2	1.90	0.70
1:A:733:GLY:H	1:A:766:ALA:HB1	1.57	0.70
2:D:196:SER:O	2:D:200:LEU:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ASN:HD21	2:C:234:ILE:H	1.40	0.69
2:C:291:HIS:ND1	2:C:292:LEU:HD23	2.07	0.69
2:D:263:GLU:HG3	2:D:264:ILE:N	2.07	0.69
2:C:16:SER:OG	2:C:132:VAL:HA	1.92	0.69
2:C:184:LEU:HD12	2:C:185:LEU:N	2.07	0.69
1:B:634:GLU:HG2	1:B:635:VAL:N	2.06	0.69
2:C:104:ALA:C	2:C:106:ASP:H	1.97	0.68
1:B:682:ILE:N	1:B:682:ILE:HD13	2.07	0.68
2:D:302:VAL:HG22	2:D:368:TYR:HB3	1.76	0.68
2:D:338:ASN:HB3	2:D:350:LEU:HG	1.76	0.68
2:C:297:ILE:O	2:C:310:SER:HA	1.93	0.68
2:D:101:ILE:HD11	2:D:144:ARG:HG2	1.76	0.68
2:D:190:ILE:O	2:D:245:VAL:HB	1.93	0.67
2:C:23:ALA:HB3	2:C:140:HIS:CD2	2.30	0.67
2:D:331:ASP:HA	2:D:334:LYS:HD3	1.76	0.67
1:A:543:ALA:HB3	1:A:544:PRO:HD3	1.75	0.67
1:B:745:LEU:HD23	1:B:774:TYR:CE2	2.30	0.67
2:D:153:ASN:O	2:D:249:GLU:HG3	1.95	0.67
2:C:36:LYS:HZ1	2:C:89:ALA:HB3	1.57	0.67
2:C:339:ASN:ND2	2:C:341:ASP:HB2	2.10	0.66
2:D:223:ILE:HG23	2:D:234:ILE:HA	1.75	0.66
2:D:152:GLN:HA	2:D:152:GLN:NE2	2.10	0.66
2:D:35:LEU:HD22	2:D:87:LEU:HD13	1.76	0.66
2:D:198:GLU:O	2:D:201:ALA:HB3	1.95	0.66
1:B:580:ARG:HD2	1:B:617:ILE:HD13	1.76	0.66
1:A:725:LEU:CD2	1:A:774:TYR:HB2	2.24	0.66
2:D:151:ILE:HG23	2:D:249:GLU:OE1	1.95	0.66
2:C:282:LYS:HB3	2:C:283:PRO:CD	2.25	0.66
2:D:162:TYR:CE1	2:D:164:VAL:HB	2.31	0.65
1:A:676:ASP:HB2	1:A:706:GLU:HB2	1.78	0.65
1:B:707:ASN:H	1:B:707:ASN:HD22	1.44	0.65
2:C:226:HIS:CD2	2:C:246:LYS:HD3	2.32	0.65
2:C:357:ASN:ND2	2:C:359:ASP:HB3	2.10	0.65
1:B:774:TYR:N	1:B:774:TYR:CD1	2.65	0.65
2:C:196:SER:HB2	2:C:240:GLU:OE2	1.96	0.65
2:D:162:TYR:HE1	2:D:164:VAL:HB	1.62	0.64
1:A:605:LEU:HD13	1:A:638:LEU:HD22	1.78	0.64
1:A:682:ILE:HD11	1:A:702:LEU:CG	2.27	0.64
1:A:637:ARG:HH21	1:A:638:LEU:H	1.45	0.64
2:C:111:ASP:OD2	2:C:115:LYS:HB3	1.98	0.64
1:B:626:LEU:HD11	1:B:630:VAL:HG11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:92:HIS:O	2:D:234:ILE:HD13	1.97	0.64
2:C:153:ASN:O	2:C:249:GLU:HA	1.97	0.64
2:C:77:ALA:O	2:C:81:LYS:HB2	1.98	0.64
2:D:163:THR:HB	2:D:182:THR:HB	1.80	0.64
1:A:586:HIS:CE1	1:A:685:TRP:HB2	2.31	0.64
1:A:562:VAL:O	1:A:688:THR:HA	1.98	0.64
2:D:144:ARG:HH11	2:D:144:ARG:HG3	1.62	0.64
2:D:104:ALA:C	2:D:106:ASP:H	2.02	0.63
1:B:626:LEU:CD1	1:B:630:VAL:HG11	2.28	0.63
2:C:347:ASP:O	2:C:371:LYS:HA	1.98	0.63
1:B:603:HIS:HA	1:B:606:GLU:HG3	1.78	0.63
2:D:163:THR:CB	2:D:182:THR:HB	2.29	0.63
1:A:761:TRP:CZ2	1:A:773:VAL:HG21	2.34	0.63
2:D:245:VAL:HG12	2:D:246:LYS:H	1.64	0.63
1:B:711:ASN:HD21	1:B:720:VAL:N	1.96	0.63
1:B:682:ILE:HG23	1:B:745:LEU:HD22	1.80	0.63
2:C:284:TYR:O	2:C:286:PRO:HD2	1.98	0.63
2:C:112:ARG:O	2:C:112:ARG:HG2	1.98	0.63
1:B:668:PRO:HB3	1:B:754:ILE:HG21	1.80	0.62
2:D:192:ASP:O	2:D:245:VAL:HG23	1.99	0.62
1:A:725:LEU:HD21	1:A:774:TYR:HB2	1.80	0.62
2:D:145:PRO:O	2:D:147:LYS:HG2	1.99	0.62
2:C:207:LEU:HD11	2:C:214:TYR:O	1.99	0.62
1:B:628:PRO:O	1:B:630:VAL:N	2.32	0.62
2:C:172:ASP:CG	2:C:173:ASP:N	2.53	0.62
2:D:15:ASN:HD22	2:D:16:SER:H	1.45	0.62
2:C:190:ILE:O	2:C:245:VAL:HB	1.99	0.62
1:A:759:THR:HA	1:A:774:TYR:CD2	2.35	0.62
1:A:756:GLN:HA	1:A:756:GLN:HE21	1.65	0.62
2:C:338:ASN:HD22	2:C:338:ASN:C	2.02	0.62
1:B:633:ILE:HG22	1:B:634:GLU:H	1.62	0.62
2:D:163:THR:HG22	2:D:269:LEU:HD11	1.80	0.62
2:C:302:VAL:HG23	2:C:369:MET:O	1.99	0.62
2:C:158:VAL:HG11	2:C:268:ASP:OD1	2.00	0.62
2:C:188:LEU:HB3	2:C:192:ASP:OD2	2.00	0.62
2:D:282:LYS:HB3	2:D:283:PRO:CD	2.28	0.61
1:B:748:PHE:HB2	1:B:753:TYR:CE1	2.35	0.61
2:C:172:ASP:CG	2:C:173:ASP:H	2.02	0.61
2:C:269:LEU:C	2:C:270:ILE:HD13	2.21	0.61
1:B:709:VAL:O	1:B:712:ARG:HG3	2.00	0.61
2:D:357:ASN:OD1	2:D:364:ILE:HB	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:GLN:HA	1:A:756:GLN:NE2	2.16	0.61
1:B:637:ARG:NE	1:B:637:ARG:HA	2.16	0.61
2:D:187:THR:O	2:D:187:THR:HG22	2.01	0.61
2:D:269:LEU:HD12	2:D:270:ILE:N	2.16	0.61
1:B:633:ILE:HG22	1:B:634:GLU:N	2.15	0.61
2:D:238:ASP:O	2:D:239:GLN:HB3	1.99	0.61
2:D:184:LEU:O	2:D:185:LEU:HD23	2.01	0.61
2:D:20:VAL:HA	2:D:137:LEU:HB3	1.83	0.61
1:A:572:SER:C	1:A:574:PRO:HD3	2.21	0.61
2:C:148:GLU:H	2:C:148:GLU:CD	2.04	0.61
2:C:309:LYS:HG2	2:C:310:SER:H	1.65	0.60
1:B:639:PHE:HB2	1:B:649:LEU:HB2	1.84	0.60
2:C:286:PRO:HB2	2:C:287:PHE:CE1	2.37	0.60
2:D:264:ILE:HG22	2:D:265:ASN:N	2.16	0.60
1:A:554:GLU:OE2	1:A:555:PRO:HD2	2.00	0.60
1:B:581:THR:HG23	1:B:585:MET:O	2.02	0.60
1:B:626:LEU:HD11	1:B:630:VAL:CG1	2.32	0.60
2:C:162:TYR:CE1	2:C:164:VAL:HB	2.36	0.60
1:A:637:ARG:HH21	1:A:638:LEU:HB2	1.65	0.60
1:A:593:ILE:HG22	1:A:594:SER:N	2.17	0.60
1:B:556:LYS:O	1:B:699:GLU:OE2	2.20	0.60
1:A:549:GLY:HA2	1:A:575:TRP:CZ3	2.37	0.60
1:B:749:GLU:CG	1:B:754:ILE:HD13	2.23	0.59
2:D:75:GLU:OE1	2:D:75:GLU:HA	2.02	0.59
2:C:101:ILE:HD11	2:C:144:ARG:CG	2.31	0.59
2:D:137:LEU:HD12	2:D:137:LEU:C	2.22	0.59
2:D:155:ALA:O	2:D:190:ILE:HD11	2.02	0.59
2:C:284:TYR:C	2:C:286:PRO:HD2	2.22	0.59
2:D:323:PHE:CE1	2:D:350:LEU:HD21	2.37	0.59
1:A:603:HIS:HA	1:A:606:GLU:HG3	1.84	0.59
2:D:283:PRO:CG	2:D:286:PRO:HG3	2.33	0.59
2:D:159:ASP:OD1	2:D:187:THR:HG23	2.02	0.59
1:B:754:ILE:N	1:B:754:ILE:HD12	2.18	0.59
2:C:192:ASP:OD1	2:C:192:ASP:N	2.34	0.59
2:D:357:ASN:ND2	2:D:359:ASP:H	1.99	0.59
2:C:284:TYR:CD2	2:C:285:ASP:HB2	2.37	0.59
2:D:31:GLN:HA	2:D:31:GLN:OE1	2.01	0.59
1:A:577:VAL:CG2	1:A:618:LEU:HD23	2.33	0.59
1:B:615:LYS:HG2	1:B:617:ILE:HD11	1.85	0.59
2:D:172:ASP:CG	2:D:173:ASP:H	2.06	0.59
2:D:173:ASP:O	2:D:174:ASP:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:331:ASP:HA	2:C:334:LYS:HD3	1.83	0.59
2:C:248:ARG:NH1	2:C:268:ASP:OD1	2.36	0.59
2:D:357:ASN:ND2	2:D:359:ASP:HB3	2.18	0.59
2:C:153:ASN:O	2:C:249:GLU:HG3	2.03	0.59
2:D:204:GLN:NE2	2:D:207:LEU:HD12	2.18	0.59
2:C:302:VAL:HG12	2:C:302:VAL:O	2.03	0.58
2:D:263:GLU:O	2:D:264:ILE:HD13	2.04	0.58
2:C:159:ASP:HA	2:C:187:THR:HG23	1.83	0.58
1:B:616:VAL:C	1:B:617:ILE:HD12	2.23	0.58
2:D:236:PRO:HB3	2:D:239:GLN:NE2	2.17	0.58
1:A:709:VAL:O	1:A:712:ARG:HG3	2.02	0.58
2:C:151:ILE:HG21	2:C:248:ARG:O	2.03	0.58
2:D:193:THR:HG22	2:D:244:HIS:HB3	1.86	0.58
2:C:198:GLU:O	2:C:201:ALA:HB3	2.04	0.58
2:C:294:LEU:HD12	2:C:295:PHE:N	2.19	0.58
1:A:641:GLU:HB2	1:A:647:ILE:CG2	2.34	0.58
2:D:91:VAL:HG13	2:D:96:ASP:CB	2.34	0.58
2:D:214:TYR:CD1	2:D:278:LYS:HA	2.38	0.58
2:D:340:LEU:HB3	2:D:345:ILE:HB	1.84	0.58
1:B:710:CYS:SG	1:B:716:LEU:HD12	2.44	0.58
2:C:76:LYS:HE3	2:C:103:PHE:HD2	1.69	0.57
2:C:323:PHE:HA	2:C:336:LEU:O	2.04	0.57
2:D:265:ASN:HD22	2:D:265:ASN:H	1.52	0.57
2:C:162:TYR:HE2	2:C:199:LEU:HD22	1.69	0.57
2:C:324:ARG:N	2:C:336:LEU:O	2.35	0.57
2:C:152:GLN:NE2	2:C:152:GLN:HA	2.19	0.57
1:B:543:ALA:HB3	1:B:544:PRO:HD3	1.86	0.57
2:C:121:LYS:HE2	2:C:121:LYS:HA	1.86	0.57
1:B:725:LEU:HD21	1:B:774:TYR:HB2	1.86	0.57
1:A:586:HIS:C	1:A:586:HIS:CD2	2.77	0.57
2:C:154:GLN:OE1	2:C:154:GLN:HA	2.05	0.57
2:C:164:VAL:HG23	2:C:272:GLU:HB3	1.87	0.57
2:C:284:TYR:CE2	2:C:285:ASP:HB2	2.40	0.56
1:B:759:THR:HA	1:B:774:TYR:CD2	2.40	0.56
2:C:328:ASP:OD1	2:C:330:ARG:HD3	2.05	0.56
2:D:15:ASN:ND2	2:D:16:SER:H	2.03	0.56
1:A:563:VAL:O	1:A:734:THR:HA	2.06	0.56
1:B:577:VAL:CG1	1:B:616:VAL:HG13	2.35	0.56
1:A:586:HIS:CD2	1:A:587:PHE:N	2.73	0.56
1:A:668:PRO:HD2	1:A:781:VAL:HG22	1.86	0.56
2:D:304:THR:HB	2:D:306:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:VAL:HG13	2:D:141:VAL:HG11	1.87	0.56
2:D:165:GLN:CB	2:D:273:LYS:HG3	2.36	0.56
1:A:685:TRP:CE2	1:A:697:LEU:HB2	2.40	0.56
2:C:246:LYS:HB3	2:C:248:ARG:NH2	2.21	0.56
1:B:784:ILE:HG22	1:B:785:GLU:N	2.19	0.56
1:B:649:LEU:O	1:B:650:LEU:HD23	2.05	0.56
1:A:687:GLU:HB3	1:A:737:CYS:HB3	1.87	0.56
2:C:363:ARG:CG	2:C:363:ARG:HH11	2.18	0.56
2:D:15:ASN:ND2	2:D:16:SER:N	2.53	0.56
1:A:733:GLY:N	1:A:766:ALA:HB1	2.21	0.56
1:B:562:VAL:HG23	1:B:740:ASP:OD2	2.06	0.56
1:A:637:ARG:CZ	1:A:638:LEU:H	2.19	0.55
2:C:35:LEU:HD12	2:C:36:LYS:H	1.72	0.55
2:D:88:ILE:O	2:D:91:VAL:HG23	2.05	0.55
1:B:682:ILE:HD11	1:B:702:LEU:HG	1.88	0.55
2:C:88:ILE:O	2:C:88:ILE:HG23	2.06	0.55
2:C:72:HIS:HD2	2:C:73:LYS:N	2.04	0.55
2:C:71:PRO:N	2:C:129:THR:HG22	2.21	0.55
1:A:756:GLN:CA	1:A:756:GLN:HE21	2.19	0.55
2:D:171:PRO:O	2:D:172:ASP:HB2	2.07	0.55
2:C:183:LYS:H	2:C:183:LYS:HD3	1.70	0.55
2:C:226:HIS:HB3	2:C:248:ARG:HH12	1.70	0.55
2:D:130:GLN:O	2:D:132:VAL:N	2.40	0.55
2:D:188:LEU:HB3	2:D:192:ASP:CG	2.26	0.55
2:C:183:LYS:HG2	2:C:184:LEU:N	2.22	0.55
1:B:591:THR:HG21	1:B:755:LEU:HD13	1.89	0.55
2:D:23:ALA:HB3	2:D:140:HIS:CD2	2.41	0.55
2:D:130:GLN:OE1	2:D:130:GLN:HA	2.07	0.54
2:C:302:VAL:HG21	2:C:351:THR:OG1	2.07	0.54
2:D:219:ARG:NH2	2:D:274:TYR:OH	2.40	0.54
2:D:265:ASN:H	2:D:265:ASN:ND2	2.05	0.54
2:C:226:HIS:NE2	2:C:246:LYS:HD3	2.23	0.54
1:B:609:PRO:HB2	2:D:237:MET:HE1	1.88	0.54
2:C:192:ASP:O	2:C:244:HIS:HA	2.06	0.54
2:C:108:THR:HG23	2:C:116:VAL:HG13	1.89	0.54
2:C:28:GLY:O	2:C:30:ASN:N	2.41	0.54
1:B:599:LEU:HD11	1:B:647:ILE:HG12	1.89	0.54
2:C:294:LEU:HD12	2:C:295:PHE:H	1.73	0.54
2:C:37:PHE:C	2:C:37:PHE:CD1	2.81	0.54
1:A:761:TRP:NE1	1:A:773:VAL:HG11	2.23	0.54
2:C:204:GLN:HE22	2:C:207:LEU:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:325:ASP:HB3	2:C:331:ASP:OD2	2.08	0.54
2:D:165:GLN:HB2	2:D:273:LYS:HG3	1.89	0.54
1:B:668:PRO:HD2	1:B:781:VAL:CG2	2.38	0.53
2:C:323:PHE:HA	2:C:336:LEU:HB2	1.90	0.53
2:D:284:TYR:O	2:D:286:PRO:HD2	2.07	0.53
2:C:188:LEU:HD13	2:C:192:ASP:HB2	1.90	0.53
1:B:711:ASN:ND2	1:B:718:GLY:CA	2.71	0.53
2:C:236:PRO:HB3	2:C:239:GLN:NE2	2.22	0.53
1:A:711:ASN:ND2	1:A:718:GLY:HA2	2.23	0.53
1:B:691:THR:HG22	1:B:692:PHE:N	2.23	0.53
2:D:161:GLU:HB3	2:D:269:LEU:HD13	1.90	0.53
2:D:245:VAL:HG12	2:D:246:LYS:N	2.23	0.53
2:C:183:LYS:HE2	2:C:206:ILE:HD11	1.90	0.53
2:C:106:ASP:HB3	2:C:140:HIS:H	1.74	0.53
1:B:686:GLY:HA3	1:B:740:ASP:OD1	2.09	0.53
1:B:782:THR:HG22	1:B:783:TRP:N	2.23	0.53
2:D:73:LYS:HA	2:D:125:VAL:O	2.09	0.53
2:D:172:ASP:CG	2:D:173:ASP:N	2.62	0.53
1:B:681:PHE:N	1:B:681:PHE:CD1	2.76	0.53
2:C:94:ASN:ND2	2:C:234:ILE:H	2.06	0.53
2:D:151:ILE:HD12	2:D:249:GLU:N	2.22	0.53
2:C:151:ILE:HG13	2:C:248:ARG:N	2.24	0.53
2:C:357:ASN:ND2	2:C:359:ASP:CB	2.71	0.53
2:D:351:THR:CG2	2:D:353:LYS:HD3	2.35	0.53
2:D:101:ILE:HB	2:D:142:ARG:HB3	1.90	0.53
1:A:627:GLU:O	1:A:630:VAL:HB	2.08	0.53
2:D:338:ASN:CB	2:D:350:LEU:HG	2.39	0.53
2:C:127:LEU:HD22	2:C:135:PHE:CD2	2.44	0.53
2:D:189:ALA:H	2:D:192:ASP:CG	2.12	0.53
1:B:711:ASN:ND2	1:B:718:GLY:HA2	2.24	0.52
2:D:155:ALA:HB1	2:D:266:ASN:OD1	2.08	0.52
1:A:605:LEU:HD12	1:A:640:LEU:HD21	1.91	0.52
1:B:707:ASN:HD21	1:B:776:ARG:HH22	1.56	0.52
2:D:188:LEU:HB3	2:D:192:ASP:OD2	2.09	0.52
1:B:581:THR:CG2	1:B:585:MET:HB2	2.40	0.52
2:D:100:VAL:HG13	2:D:141:VAL:CG1	2.40	0.52
2:D:285:ASP:O	2:D:286:PRO:C	2.48	0.52
2:C:186:LYS:HB3	2:C:188:LEU:HD21	1.91	0.52
2:C:237:MET:HG3	2:C:238:ASP:H	1.75	0.52
2:C:204:GLN:HA	2:C:204:GLN:HE21	1.74	0.52
2:D:186:LYS:HD2	2:D:188:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ASN:HD22	1:B:718:GLY:CA	2.23	0.52
1:A:586:HIS:HD2	1:A:587:PHE:N	2.08	0.52
2:D:284:TYR:C	2:D:286:PRO:HD2	2.31	0.52
2:C:159:ASP:CA	2:C:187:THR:HG23	2.39	0.52
2:D:309:LYS:HG2	2:D:310:SER:H	1.75	0.52
2:D:246:LYS:O	2:D:247:ASN:HB2	2.09	0.52
1:A:640:LEU:O	1:A:641:GLU:C	2.48	0.52
1:A:641:GLU:HB2	1:A:647:ILE:HG23	1.90	0.52
2:C:288:ASP:HB3	2:C:291:HIS:NE2	2.25	0.52
2:C:72:HIS:HD2	2:C:73:LYS:H	1.58	0.52
1:B:594:SER:HB2	1:B:595:PRO:HD2	1.91	0.52
2:C:161:GLU:HG3	2:C:183:LYS:O	2.09	0.52
2:C:346:MET:O	2:C:347:ASP:HB2	2.10	0.52
2:C:137:LEU:HD12	2:C:138:SER:N	2.25	0.52
2:D:163:THR:OG1	2:D:182:THR:HB	2.10	0.51
2:C:184:LEU:HD12	2:C:185:LEU:H	1.71	0.51
1:B:641:GLU:HA	1:B:783:TRP:CZ2	2.45	0.51
2:D:79:LEU:O	2:D:83:ILE:HG13	2.11	0.51
2:C:161:GLU:HB3	2:C:269:LEU:CD1	2.40	0.51
1:A:637:ARG:NE	1:A:638:LEU:H	2.08	0.51
2:D:269:LEU:HD12	2:D:270:ILE:H	1.74	0.51
2:D:99:GLU:HG3	2:D:146:TYR:HA	1.93	0.51
1:B:602:ALA:HB3	1:B:646:ASP:HA	1.93	0.51
2:D:302:VAL:CG2	2:D:368:TYR:HB3	2.40	0.51
1:B:668:PRO:O	1:B:781:VAL:HG21	2.10	0.51
1:A:706:GLU:OE1	1:A:708:LYS:HB2	2.10	0.51
2:C:162:TYR:HE1	2:C:164:VAL:HB	1.74	0.51
1:A:682:ILE:HD11	1:A:702:LEU:CD1	2.40	0.51
1:A:774:TYR:CD1	1:A:774:TYR:N	2.78	0.51
2:D:15:ASN:HD22	2:D:16:SER:N	2.08	0.51
2:C:214:TYR:CD1	2:C:278:LYS:HA	2.45	0.51
2:C:13:VAL:O	2:C:15:ASN:N	2.43	0.51
2:D:283:PRO:HG2	2:D:286:PRO:HG3	1.93	0.51
2:C:163:THR:O	2:C:163:THR:HG23	2.10	0.51
1:A:640:LEU:HD23	1:A:648:ALA:HB2	1.93	0.51
2:D:76:LYS:HB2	2:D:123:GLY:O	2.10	0.51
1:A:556:LYS:O	1:A:556:LYS:HG3	2.10	0.51
2:D:324:ARG:HG3	2:D:331:ASP:O	2.11	0.50
1:B:637:ARG:HB2	1:B:651:LYS:CB	2.41	0.50
2:D:159:ASP:HA	2:D:187:THR:HG23	1.93	0.50
2:D:211:HIS:HB2	2:D:214:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:PRO:O	2:C:147:LYS:HG2	2.11	0.50
1:A:641:GLU:OE1	1:A:643:THR:N	2.43	0.50
2:C:36:LYS:HZ3	2:C:89:ALA:HB3	1.73	0.50
2:D:293:LYS:N	2:D:293:LYS:HD2	2.26	0.50
1:A:579:LEU:HD23	1:A:587:PHE:CZ	2.46	0.50
1:A:685:TRP:CZ2	1:A:697:LEU:HB2	2.47	0.50
1:B:641:GLU:HB2	1:B:647:ILE:HG22	1.93	0.50
2:D:163:THR:O	2:D:163:THR:HG23	2.11	0.50
1:B:598:VAL:CB	1:B:650:LEU:HB2	2.32	0.50
2:D:323:PHE:CG	2:D:350:LEU:HD11	2.46	0.50
2:C:153:ASN:HB3	2:C:249:GLU:CG	2.42	0.50
2:D:26:VAL:HG11	2:D:98:PHE:HE2	1.76	0.50
2:D:216:ILE:HG23	2:D:274:TYR:HB3	1.93	0.50
2:D:194:ILE:HG22	2:D:195:THR:N	2.27	0.50
2:D:153:ASN:O	2:D:249:GLU:HA	2.12	0.50
2:C:245:VAL:HG12	2:C:246:LYS:N	2.25	0.50
2:D:144:ARG:HG3	2:D:144:ARG:NH1	2.26	0.50
2:C:338:ASN:HD22	2:C:339:ASN:N	2.09	0.50
1:A:686:GLY:HA3	1:A:740:ASP:OD1	2.12	0.50
2:D:99:GLU:O	2:D:143:VAL:HA	2.12	0.50
2:C:155:ALA:HA	2:C:250:GLN:HA	1.93	0.50
2:D:357:ASN:ND2	2:D:359:ASP:CB	2.75	0.50
2:D:158:VAL:HA	2:D:266:ASN:O	2.11	0.49
2:D:71:PRO:HA	2:D:127:LEU:O	2.12	0.49
2:C:311:GLU:OE2	2:C:313:LEU:HD11	2.12	0.49
2:C:219:ARG:NH2	2:C:274:TYR:OH	2.45	0.49
2:D:111:ASP:HB3	2:D:135:PHE:HE1	1.77	0.49
2:D:357:ASN:HD21	2:D:359:ASP:HB3	1.75	0.49
2:D:309:LYS:HG2	2:D:310:SER:N	2.27	0.49
2:D:226:HIS:CD2	2:D:246:LYS:HD3	2.47	0.49
1:A:676:ASP:O	1:A:677:ARG:HB2	2.12	0.49
2:C:162:TYR:CE2	2:C:199:LEU:HD22	2.46	0.49
2:C:195:THR:H	2:C:198:GLU:HG3	1.78	0.49
2:C:88:ILE:O	2:C:88:ILE:CG2	2.59	0.49
2:D:269:LEU:C	2:D:270:ILE:HD13	2.33	0.49
2:D:284:TYR:CD2	2:D:285:ASP:N	2.80	0.49
2:D:26:VAL:O	2:D:29:THR:O	2.30	0.49
1:A:660:ASP:N	1:A:660:ASP:OD1	2.46	0.49
2:C:300:VAL:HG12	2:C:301:ASP:O	2.12	0.49
2:C:244:HIS:CD2	2:C:244:HIS:N	2.79	0.49
2:C:247:ASN:O	2:C:248:ARG:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:338:ASN:HB3	2:C:350:LEU:HD11	1.94	0.49
2:D:117:TYR:N	2:D:117:TYR:CD1	2.80	0.49
1:A:597:TRP:CZ3	1:A:651:LYS:HB2	2.47	0.49
1:B:564:GLY:H	1:B:691:THR:HG21	1.77	0.49
2:D:163:THR:HA	2:D:182:THR:HA	1.95	0.49
2:D:36:LYS:NZ	2:D:89:ALA:HB3	2.27	0.49
2:D:244:HIS:O	2:D:245:VAL:C	2.51	0.49
2:D:91:VAL:CG1	2:D:96:ASP:HB2	2.39	0.49
2:C:204:GLN:NE2	2:C:207:LEU:HD12	2.28	0.49
2:D:265:ASN:ND2	2:D:265:ASN:N	2.58	0.49
2:C:157:SER:OG	2:C:187:THR:HG22	2.12	0.49
1:B:757:GLY:HA2	1:B:775:VAL:O	2.13	0.49
1:B:682:ILE:CD1	1:B:682:ILE:N	2.72	0.48
1:B:641:GLU:OE1	1:B:643:THR:N	2.46	0.48
2:C:338:ASN:HB3	2:C:350:LEU:CD1	2.43	0.48
2:C:244:HIS:O	2:C:245:VAL:C	2.51	0.48
2:C:286:PRO:HB2	2:C:287:PHE:CD1	2.47	0.48
2:D:93:SER:OG	2:D:94:ASN:N	2.46	0.48
2:D:73:LYS:HG3	2:D:125:VAL:O	2.14	0.48
1:A:600:THR:OG1	1:A:601:ALA:N	2.46	0.48
1:B:629:HIS:CD2	1:B:661:LYS:HD2	2.48	0.48
2:C:359:ASP:HB3	2:C:362:ASN:O	2.13	0.48
2:C:363:ARG:NH1	2:C:363:ARG:CG	2.77	0.48
1:A:557:LYS:O	1:A:559:PRO:HD3	2.14	0.48
1:B:663:ILE:CG2	1:B:664:PRO:HD2	2.44	0.48
2:C:154:GLN:O	2:C:250:GLN:HB2	2.12	0.48
1:A:781:VAL:O	1:A:785:GLU:HG3	2.14	0.48
2:D:327:TYR:O	2:D:329:PRO:HD3	2.13	0.48
2:D:210:THR:O	2:D:212:PRO:HD3	2.13	0.48
2:D:161:GLU:HB2	2:D:268:ASP:O	2.13	0.48
2:C:76:LYS:HE2	2:C:102:ASP:OD1	2.13	0.48
1:B:577:VAL:HG13	1:B:616:VAL:HG13	1.95	0.48
1:B:543:ALA:N	1:B:544:PRO:HD2	2.29	0.48
2:C:17:GLN:HB2	2:C:40:ILE:O	2.13	0.48
2:C:151:ILE:HG13	2:C:248:ARG:CA	2.44	0.48
2:C:101:ILE:O	2:C:102:ASP:HB2	2.14	0.48
2:D:298:LYS:HE3	2:D:364:ILE:CG2	2.43	0.48
2:C:94:ASN:OD1	2:C:234:ILE:O	2.32	0.48
2:C:153:ASN:HB3	2:C:249:GLU:HG3	1.94	0.48
2:D:202:GLN:HB2	2:D:202:GLN:HE21	1.51	0.48
2:D:202:GLN:O	2:D:206:ILE:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:PRO:O	1:A:638:LEU:HD12	2.14	0.48
2:C:132:VAL:HG12	2:D:330:ARG:HB3	1.96	0.48
2:D:99:GLU:OE1	2:D:144:ARG:NH2	2.46	0.48
1:A:677:ARG:HD3	1:A:677:ARG:N	2.29	0.48
1:B:707:ASN:HD22	1:B:707:ASN:N	2.11	0.48
2:D:226:HIS:HB3	2:D:248:ARG:NH1	2.29	0.47
1:B:711:ASN:ND2	1:B:720:VAL:H	2.03	0.47
1:B:575:TRP:O	1:B:577:VAL:HG23	2.14	0.47
2:C:109:ILE:O	2:C:110:THR:HG23	2.14	0.47
2:D:320:ASN:HB3	2:D:333:ALA:O	2.13	0.47
1:A:629:HIS:CD2	1:A:661:LYS:HD2	2.49	0.47
2:D:336:LEU:HD22	2:D:367:VAL:CG2	2.44	0.47
1:A:636:SER:OG	1:A:653:SER:HA	2.14	0.47
2:C:357:ASN:HD21	2:C:359:ASP:CB	2.19	0.47
2:D:122:ASP:C	2:D:124:SER:H	2.16	0.47
1:B:563:VAL:HG22	1:B:689:GLN:HB2	1.96	0.47
1:A:577:VAL:CG1	1:A:578:SER:N	2.78	0.47
1:A:623:GLU:OE1	2:C:332:LYS:HE2	2.13	0.47
1:A:668:PRO:HD2	1:A:781:VAL:CG2	2.44	0.47
2:C:110:THR:HG22	2:C:116:VAL:HA	1.96	0.47
1:B:563:VAL:O	1:B:734:THR:HA	2.14	0.47
2:C:122:ASP:HB2	2:C:124:SER:OG	2.14	0.47
2:C:244:HIS:CD2	2:C:244:HIS:H	2.33	0.47
2:C:104:ALA:C	2:C:106:ASP:N	2.66	0.47
1:B:543:ALA:HB3	1:B:544:PRO:CD	2.44	0.47
2:C:169:LEU:HD12	2:C:277:LEU:HD13	1.96	0.47
2:C:158:VAL:HA	2:C:266:ASN:O	2.14	0.47
2:D:16:SER:O	2:D:42:LEU:HB2	2.15	0.47
2:C:165:GLN:CB	2:C:273:LYS:HG3	2.44	0.47
2:C:118:PHE:CD1	2:C:118:PHE:N	2.82	0.47
2:C:224:VAL:HG23	2:C:235:LEU:HD11	1.97	0.47
1:A:711:ASN:ND2	1:A:719:ARG:H	2.12	0.47
1:A:551:PRO:HA	1:A:574:PRO:HG2	1.96	0.47
2:D:207:LEU:HD11	2:D:214:TYR:C	2.35	0.47
2:D:195:THR:HG22	2:D:242:THR:HB	1.97	0.47
2:C:193:THR:HG22	2:C:244:HIS:HB3	1.97	0.47
2:C:329:PRO:O	2:C:332:LYS:HD2	2.15	0.47
2:C:251:ALA:C	2:C:263:GLU:HB3	2.34	0.46
1:B:711:ASN:O	1:B:717:ASN:HA	2.14	0.46
2:C:363:ARG:NH1	2:C:363:ARG:HG3	2.30	0.46
1:A:679:GLU:OE1	1:A:679:GLU:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:ARG:HB2	2:C:334:LYS:HB2	1.96	0.46
2:C:184:LEU:C	2:C:185:LEU:HG	2.30	0.46
2:D:94:ASN:HD21	2:D:234:ILE:H	1.62	0.46
1:B:637:ARG:NE	1:B:637:ARG:CA	2.78	0.46
2:D:222:SER:HB3	2:D:272:GLU:HG2	1.97	0.46
2:C:151:ILE:HG21	2:C:248:ARG:C	2.35	0.46
2:D:111:ASP:HB3	2:D:135:PHE:CE1	2.50	0.46
1:B:789:ARG:HG3	1:B:789:ARG:O	2.15	0.46
1:B:708:LYS:HA	1:B:708:LYS:HD2	1.61	0.46
2:D:226:HIS:NE2	2:D:246:LYS:HD3	2.31	0.46
2:D:26:VAL:HG23	2:D:31:GLN:O	2.16	0.46
2:C:72:HIS:CD2	2:C:73:LYS:N	2.82	0.46
2:D:111:ASP:CB	2:D:135:PHE:HE1	2.28	0.46
2:C:80:LEU:HA	2:C:80:LEU:HD23	1.75	0.46
2:D:197:GLN:O	2:D:200:LEU:HB3	2.15	0.46
1:A:761:TRP:CE2	1:A:773:VAL:HG11	2.51	0.46
1:A:686:GLY:O	1:A:687:GLU:C	2.54	0.46
2:D:354:VAL:HG12	2:D:367:VAL:HA	1.97	0.46
2:D:151:ILE:CD1	2:D:248:ARG:HA	2.46	0.46
1:A:556:LYS:HB3	1:A:569:HIS:CE1	2.51	0.46
1:B:560:GLY:O	1:B:561:ARG:C	2.54	0.46
1:A:580:ARG:HD2	1:A:617:ILE:HD13	1.98	0.46
2:C:158:VAL:HG23	2:C:189:ALA:O	2.15	0.46
1:B:741:ALA:HA	1:B:759:THR:HG22	1.97	0.46
1:B:627:GLU:HB3	1:B:628:PRO:HD2	1.98	0.46
1:A:568:ALA:HB3	1:A:697:LEU:HD23	1.98	0.46
1:B:592:LEU:HD23	1:B:664:PRO:HB3	1.96	0.46
2:D:244:HIS:H	2:D:244:HIS:CD2	2.34	0.46
1:A:597:TRP:CZ2	1:A:788:MET:HA	2.50	0.46
2:D:284:TYR:CD2	2:D:285:ASP:HB2	2.51	0.46
2:C:284:TYR:C	2:C:286:PRO:CD	2.84	0.46
2:D:132:VAL:HG12	2:D:132:VAL:O	2.15	0.46
2:D:99:GLU:CD	2:D:144:ARG:NH2	2.70	0.46
2:D:207:LEU:HD11	2:D:214:TYR:O	2.16	0.46
2:C:264:ILE:O	2:C:264:ILE:HD12	2.16	0.46
1:A:702:LEU:HD13	1:A:728:GLY:HA2	1.97	0.45
1:B:746:VAL:HG13	1:B:753:TYR:HB3	1.93	0.45
2:C:161:GLU:HB3	2:C:269:LEU:HD12	1.98	0.45
2:D:104:ALA:C	2:D:106:ASP:N	2.69	0.45
2:C:196:SER:HG	2:C:241:PHE:H	1.64	0.45
1:A:587:PHE:HE1	1:A:604:CYS:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:VAL:HG21	2:D:332:LYS:HB3	1.97	0.45
2:C:165:GLN:HB3	2:C:273:LYS:HG3	1.99	0.45
2:D:193:THR:HG22	2:D:244:HIS:CB	2.46	0.45
1:A:726:CYS:HA	1:A:772:GLY:O	2.17	0.45
1:A:713:TYR:HA	1:A:717:ASN:OD1	2.16	0.45
1:B:745:LEU:HD23	1:B:774:TYR:CD2	2.52	0.45
2:C:207:LEU:HD11	2:C:214:TYR:C	2.36	0.45
2:D:247:ASN:HD22	2:D:247:ASN:HA	1.59	0.45
2:C:331:ASP:OD1	2:C:334:LYS:HE2	2.17	0.45
1:B:746:VAL:HG22	1:B:755:LEU:HA	1.98	0.45
2:D:130:GLN:C	2:D:132:VAL:N	2.68	0.45
1:A:687:GLU:OE2	1:A:689:GLN:N	2.42	0.45
2:C:73:LYS:HA	2:C:125:VAL:O	2.16	0.45
2:D:75:GLU:HB2	2:D:78:ASP:CG	2.36	0.45
1:B:644:ARG:HD3	2:D:33:ILE:HG23	1.98	0.45
2:D:118:PHE:CD1	2:D:118:PHE:N	2.84	0.45
2:D:226:HIS:CE1	2:D:233:THR:OG1	2.70	0.44
1:B:711:ASN:HD22	1:B:718:GLY:N	2.15	0.44
1:A:583:PHE:N	1:A:583:PHE:CD1	2.85	0.44
2:C:246:LYS:HB3	2:C:247:ASN:H	1.66	0.44
2:C:100:VAL:HA	2:C:143:VAL:HG12	1.99	0.44
2:C:284:TYR:CD2	2:C:285:ASP:N	2.85	0.44
1:B:580:ARG:CD	1:B:617:ILE:HD13	2.46	0.44
1:B:628:PRO:C	1:B:630:VAL:H	2.20	0.44
2:D:277:LEU:C	2:D:279:LYS:H	2.21	0.44
2:C:338:ASN:C	2:C:338:ASN:ND2	2.71	0.44
2:C:101:ILE:O	2:C:102:ASP:CB	2.66	0.44
1:A:682:ILE:HG23	1:A:745:LEU:CD2	2.47	0.44
2:C:71:PRO:HA	2:C:127:LEU:O	2.17	0.44
2:D:109:ILE:HG21	2:D:127:LEU:HD21	1.99	0.44
1:B:586:HIS:CD2	1:B:586:HIS:C	2.90	0.44
2:C:104:ALA:O	2:C:106:ASP:N	2.46	0.44
1:B:592:LEU:CD2	1:B:664:PRO:HB3	2.47	0.44
2:C:270:ILE:N	2:C:270:ILE:HD13	2.32	0.44
2:D:117:TYR:CD2	2:D:127:LEU:HD23	2.52	0.44
1:A:638:LEU:HD23	1:A:650:LEU:CD2	2.47	0.44
1:A:745:LEU:HA	1:A:745:LEU:HD22	1.73	0.44
2:D:263:GLU:HG3	2:D:264:ILE:H	1.80	0.44
2:D:207:LEU:HD22	2:D:207:LEU:O	2.17	0.44
2:D:194:ILE:O	2:D:242:THR:HA	2.18	0.44
2:D:320:ASN:HD22	2:D:320:ASN:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:GLU:OE2	1:B:689:GLN:N	2.49	0.44
1:A:581:THR:OG1	1:A:585:MET:SD	2.58	0.44
2:C:202:GLN:HB2	2:C:202:GLN:HE21	1.57	0.44
1:A:783:TRP:O	1:A:787:VAL:HG23	2.18	0.44
1:B:566:CYS:O	1:B:698:LYS:HG3	2.18	0.44
1:B:586:HIS:HD2	1:B:587:PHE:N	2.09	0.44
2:C:39:GLU:H	2:C:39:GLU:HG2	1.52	0.44
2:D:188:LEU:HD13	2:D:192:ASP:HB3	1.98	0.44
2:C:250:GLN:HE21	2:C:263:GLU:N	2.16	0.44
2:D:265:ASN:HD22	2:D:265:ASN:N	2.12	0.44
2:D:130:GLN:O	2:D:131:PRO:C	2.55	0.43
1:B:660:ASP:HA	1:B:663:ILE:HD11	2.00	0.43
2:C:151:ILE:HG22	2:C:151:ILE:O	2.17	0.43
1:B:691:THR:HG22	1:B:692:PHE:H	1.82	0.43
2:D:76:LYS:HE3	2:D:103:PHE:HD2	1.83	0.43
1:B:592:LEU:HD23	1:B:664:PRO:CA	2.48	0.43
2:D:244:HIS:N	2:D:244:HIS:CD2	2.85	0.43
1:A:676:ASP:OD1	1:A:677:ARG:NH1	2.51	0.43
1:A:595:PRO:HG3	1:A:658:ILE:CD1	2.44	0.43
2:C:196:SER:OG	2:C:240:GLU:HG3	2.18	0.43
2:C:204:GLN:O	2:C:207:LEU:HB3	2.17	0.43
2:C:159:ASP:HA	2:C:187:THR:HA	1.99	0.43
1:B:623:GLU:O	1:B:623:GLU:HG2	2.18	0.43
2:C:155:ALA:HB1	2:C:266:ASN:OD1	2.17	0.43
2:C:101:ILE:HG12	2:C:143:VAL:HA	2.00	0.43
1:A:707:ASN:HD22	1:A:707:ASN:N	2.16	0.43
2:C:323:PHE:CE2	2:C:350:LEU:HD22	2.53	0.43
2:D:75:GLU:OE1	2:D:124:SER:HB3	2.18	0.43
1:B:785:GLU:O	1:B:786:GLY:C	2.57	0.43
2:C:339:ASN:HD21	2:C:341:ASP:HB2	1.81	0.43
1:A:658:ILE:N	1:A:658:ILE:CD1	2.80	0.43
1:B:725:LEU:HD23	1:B:725:LEU:H	1.84	0.43
2:C:121:LYS:HE2	2:C:121:LYS:CA	2.49	0.43
2:C:169:LEU:HD23	2:C:275:TYR:CD1	2.54	0.43
1:A:570:PRO:HG3	1:A:621:HIS:NE2	2.34	0.43
1:A:681:PHE:N	1:A:681:PHE:CD1	2.87	0.43
2:C:320:ASN:N	2:C:320:ASN:HD22	2.17	0.43
1:B:758:VAL:O	1:B:759:THR:C	2.56	0.43
2:C:156:LYS:HB2	2:C:265:ASN:ND2	2.33	0.43
2:D:224:VAL:HG11	2:D:243:TYR:CZ	2.54	0.43
2:D:115:LYS:HG2	2:D:117:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:PRO:CG	2:C:286:PRO:HG3	2.39	0.43
2:C:287:PHE:CD1	2:C:287:PHE:N	2.86	0.43
1:A:741:ALA:HA	1:A:759:THR:CG2	2.45	0.43
2:C:330:ARG:C	2:C:332:LYS:H	2.22	0.43
1:B:555:PRO:HA	1:B:572:SER:HB2	2.00	0.43
2:C:167:THR:HA	2:C:168:PRO:HD3	1.81	0.43
1:B:682:ILE:HD12	1:B:745:LEU:HD22	2.00	0.43
2:C:289:ARG:HA	2:C:292:LEU:HG	2.01	0.43
1:A:672:TYR:H	1:A:778:SER:HB2	1.83	0.43
1:A:673:VAL:HG12	1:A:673:VAL:O	2.19	0.43
2:D:122:ASP:C	2:D:124:SER:N	2.72	0.42
2:C:107:ALA:HA	2:C:138:SER:O	2.19	0.42
1:B:558:CYS:HA	1:B:559:PRO:HD2	1.74	0.42
2:D:193:THR:HA	2:D:243:TYR:O	2.19	0.42
2:C:351:THR:HG22	2:C:353:LYS:HD3	2.01	0.42
2:D:165:GLN:HB3	2:D:273:LYS:HG3	2.01	0.42
2:C:161:GLU:HB2	2:C:268:ASP:O	2.18	0.42
2:D:196:SER:HG	2:D:241:PHE:H	1.66	0.42
1:A:599:LEU:HD12	1:A:648:ALA:O	2.19	0.42
2:D:206:ILE:HA	2:D:209:LYS:HB2	2.01	0.42
1:B:788:MET:C	1:B:790:ASN:H	2.23	0.42
1:B:711:ASN:ND2	1:B:719:ARG:N	2.67	0.42
1:B:725:LEU:CD2	1:B:774:TYR:HB2	2.50	0.42
2:C:292:LEU:HD12	2:C:314:LEU:CD1	2.49	0.42
1:B:628:PRO:C	1:B:630:VAL:N	2.73	0.42
1:A:761:TRP:NE1	1:A:773:VAL:CG1	2.82	0.42
2:D:29:THR:O	2:D:29:THR:HG23	2.20	0.42
2:C:127:LEU:HD22	2:C:135:PHE:CE2	2.54	0.42
1:B:685:TRP:CZ2	1:B:697:LEU:HD13	2.55	0.42
1:B:583:PHE:HE1	2:D:170:ASN:HA	1.85	0.42
2:C:163:THR:HG22	2:C:269:LEU:HD11	2.00	0.42
2:C:92:HIS:O	2:C:234:ILE:HD13	2.20	0.42
2:C:81:LYS:O	2:C:85:GLU:HG3	2.20	0.42
1:B:709:VAL:HG12	1:B:715:PHE:CE2	2.54	0.42
1:A:713:TYR:CE1	2:C:134:GLU:HG2	2.54	0.42
2:D:326:LEU:HD23	2:D:326:LEU:HA	1.85	0.42
2:D:284:TYR:C	2:D:286:PRO:CD	2.88	0.42
2:D:88:ILE:HD12	2:D:88:ILE:HA	1.76	0.42
1:A:573:TRP:N	1:A:574:PRO:HD3	2.33	0.42
2:C:84:GLN:O	2:C:85:GLU:C	2.58	0.42
1:A:624:VAL:HG21	2:C:332:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:243:TYR:CE2	2:C:245:VAL:HA	2.55	0.42
1:B:570:PRO:HG3	1:B:621:HIS:CD2	2.55	0.42
1:B:573:TRP:CG	1:B:683:THR:HG21	2.54	0.42
2:D:217:TYR:N	2:D:275:TYR:O	2.51	0.42
1:B:668:PRO:HD2	1:B:781:VAL:HG22	2.02	0.41
1:B:754:ILE:CD1	1:B:754:ILE:N	2.83	0.41
1:B:580:ARG:HG2	1:B:586:HIS:HA	2.02	0.41
2:D:87:LEU:HA	2:D:87:LEU:HD12	1.91	0.41
1:A:706:GLU:CD	1:A:708:LYS:H	2.23	0.41
2:C:169:LEU:HA	2:C:169:LEU:HD23	1.91	0.41
2:D:286:PRO:HB2	2:D:287:PHE:CE1	2.56	0.41
2:D:196:SER:O	2:D:200:LEU:CB	2.63	0.41
1:B:745:LEU:C	1:B:745:LEU:CD1	2.89	0.41
1:A:782:THR:HG22	1:A:783:TRP:N	2.35	0.41
2:C:24:GLY:O	2:C:32:ASP:HA	2.20	0.41
2:D:226:HIS:HE1	2:D:233:THR:OG1	2.04	0.41
2:D:200:LEU:HD12	2:D:200:LEU:O	2.21	0.41
2:D:353:LYS:O	2:D:368:TYR:HD2	2.04	0.41
2:D:328:ASP:OD1	2:D:330:ARG:HD3	2.21	0.41
1:B:682:ILE:HG12	1:B:700:ALA:O	2.19	0.41
2:C:30:ASN:HD22	2:C:30:ASN:HA	1.65	0.41
1:B:564:GLY:O	1:B:565:GLY:C	2.58	0.41
2:D:76:LYS:O	2:D:79:LEU:HB2	2.20	0.41
2:D:247:ASN:O	2:D:248:ARG:CB	2.57	0.41
2:D:153:ASN:HB3	2:D:249:GLU:HG3	2.02	0.41
2:D:281:GLU:C	2:D:282:LYS:HG3	2.41	0.41
2:D:119:ALA:HA	2:D:124:SER:O	2.21	0.41
1:A:711:ASN:ND2	1:A:718:GLY:CA	2.83	0.41
2:D:293:LYS:CD	2:D:293:LYS:N	2.83	0.41
2:D:299:TYR:HA	2:D:367:VAL:O	2.19	0.41
1:B:788:MET:O	1:B:790:ASN:N	2.54	0.41
1:A:704:VAL:CG1	1:A:705:ILE:N	2.84	0.41
2:C:243:TYR:CE1	2:C:245:VAL:O	2.73	0.41
1:A:637:ARG:HE	1:A:638:LEU:H	1.66	0.41
2:D:183:LYS:HB2	2:D:184:LEU:H	1.64	0.41
2:C:216:ILE:HG23	2:C:274:TYR:HB3	2.02	0.41
2:C:206:ILE:HA	2:C:209:LYS:HB2	2.03	0.41
2:C:148:GLU:N	2:C:148:GLU:OE1	2.50	0.41
2:C:320:ASN:HB3	2:C:333:ALA:O	2.20	0.41
1:B:579:LEU:HA	1:B:579:LEU:HD12	1.82	0.41
1:B:632:GLU:O	1:B:632:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:SER:OG	2:C:21:SER:O	2.37	0.41
2:C:250:GLN:NE2	2:C:251:ALA:C	2.74	0.41
2:C:281:GLU:O	2:C:282:LYS:HG3	2.20	0.41
2:D:159:ASP:OD1	2:D:187:THR:CG2	2.69	0.41
2:C:156:LYS:HB2	2:C:157:SER:H	1.68	0.41
2:D:245:VAL:CG1	2:D:246:LYS:H	2.28	0.41
2:C:323:PHE:CD2	2:C:350:LEU:CD1	3.04	0.41
2:D:357:ASN:HD22	2:D:359:ASP:N	2.06	0.41
1:A:711:ASN:HD21	1:A:720:VAL:N	2.12	0.41
1:A:606:GLU:O	2:C:92:HIS:HE1	2.04	0.41
2:C:71:PRO:CA	2:C:129:THR:HG22	2.50	0.41
1:A:626:LEU:HD11	1:A:630:VAL:HG11	2.03	0.41
1:B:660:ASP:N	1:B:660:ASP:OD1	2.53	0.41
2:C:26:VAL:CG1	2:C:29:THR:HG23	2.51	0.41
2:C:161:GLU:HB3	2:C:269:LEU:HD13	2.03	0.41
1:B:711:ASN:OD1	1:B:720:VAL:HB	2.21	0.41
1:B:587:PHE:C	1:B:587:PHE:CD1	2.93	0.41
1:B:581:THR:HG21	1:B:585:MET:HB2	2.03	0.41
2:D:33:ILE:CD1	2:D:33:ILE:N	2.84	0.41
2:C:323:PHE:CD1	2:C:323:PHE:N	2.88	0.40
2:C:183:LYS:N	2:C:183:LYS:HD3	2.34	0.40
2:D:357:ASN:ND2	2:D:359:ASP:N	2.68	0.40
1:A:641:GLU:HG3	1:A:780:PHE:CE2	2.56	0.40
1:A:733:GLY:CA	1:A:766:ALA:HB1	2.50	0.40
2:D:157:SER:OG	2:D:187:THR:HG22	2.21	0.40
1:B:593:ILE:HG12	1:B:599:LEU:HB2	2.03	0.40
2:D:336:LEU:HD22	2:D:367:VAL:HG21	2.02	0.40
2:C:220:ASP:HB3	2:C:273:LYS:O	2.21	0.40
1:B:600:THR:OG1	1:B:601:ALA:N	2.54	0.40
2:C:188:LEU:HD13	2:C:192:ASP:CB	2.50	0.40
2:D:196:SER:OG	2:D:240:GLU:HG3	2.20	0.40
1:A:637:ARG:HH21	1:A:638:LEU:CB	2.32	0.40
1:A:640:LEU:HD23	1:A:648:ALA:CB	2.51	0.40
1:B:705:ILE:HG22	1:B:710:CYS:HB2	2.04	0.40
2:D:160:VAL:HG23	2:D:186:LYS:O	2.21	0.40
2:C:285:ASP:N	2:C:286:PRO:CD	2.85	0.40
1:A:543:ALA:N	1:A:544:PRO:CD	2.84	0.40
1:B:609:PRO:HB3	2:D:92:HIS:CD2	2.56	0.40
1:B:569:HIS:O	1:B:572:SER:HB3	2.21	0.40
2:D:151:ILE:HG13	2:D:248:ARG:N	2.36	0.40
2:C:339:ASN:C	2:C:341:ASP:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:VAL:HG22	1:A:618:LEU:CD2	2.47	0.40
1:B:593:ILE:HD12	1:B:667:LEU:HD21	2.03	0.40
1:A:637:ARG:HH21	1:A:638:LEU:N	2.15	0.40
1:A:651:LYS:HE3	1:A:791:ASN:OXT	2.21	0.40
1:B:637:ARG:HB2	1:B:651:LYS:HB3	2.02	0.40
1:A:558:CYS:HA	1:A:559:PRO:HD2	1.90	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	246/250 (98%)	212 (86%)	28 (11%)	6 (2%)	7	29
1	B	246/250 (98%)	203 (82%)	36 (15%)	7 (3%)	6	24
2	C	310/362 (86%)	235 (76%)	53 (17%)	22 (7%)	1	3
2	D	310/362 (86%)	244 (79%)	45 (14%)	21 (7%)	1	4
All	All	1112/1224 (91%)	894 (80%)	162 (15%)	56 (5%)	3	9

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	629	HIS
1	B	789	ARG
2	C	156	LYS
2	C	338	ASN
2	D	188	LEU
2	D	248	ARG
1	B	628	PRO
1	B	644	ARG
2	C	29	THR

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Mol	Chain	Res	Type
2	C	102	ASP
2	C	228	ASN
2	C	239	GLN
2	C	245	VAL
2	C	248	ARG
2	D	185	LEU
2	D	239	GLN
2	D	247	ASN
2	D	338	ASN
1	A	547	ASP
1	A	789	ARG
1	B	587	PHE
1	B	759	THR
2	C	14	ASN
2	C	105	SER
2	C	186	LYS
2	C	192	ASP
2	C	237	MET
2	C	279	LYS
2	C	337	TYR
2	D	156	LYS
2	D	228	ASN
2	D	237	MET
2	D	245	VAL
2	D	246	LYS
2	D	283	PRO
2	D	337	TYR
1	A	559	PRO
1	A	749	GLU
2	C	247	ASN
2	C	283	PRO
2	D	192	ASP
1	A	687	GLU
2	C	172	ASP
2	C	246	LYS
2	C	331	ASP
2	D	14	ASN
2	D	132	VAL
2	D	172	ASP
2	D	279	LYS
1	A	787	VAL
2	C	132	VAL

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Mol	Chain	Res	Type
2	C	357	ASN
2	D	13	VAL
2	D	170	ASN
1	B	690	GLY
2	D	131	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	168 (80%)	41 (20%)	1	5
1	B	209/209 (100%)	174 (83%)	35 (17%)	3	8
2	C	288/327 (88%)	207 (72%)	81 (28%)	0	1
2	D	288/327 (88%)	221 (77%)	67 (23%)	1	3
All	All	994/1072 (93%)	770 (78%)	224 (22%)	1	3

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	546	PHE
1	A	552	GLN
1	A	554	GLU
1	A	556	LYS
1	A	558	CYS
1	A	561	ARG
1	A	585	MET
1	A	593	ILE
1	A	605	LEU
1	A	608	SER
1	A	613	SER
1	A	618	LEU
1	A	626	LEU
1	A	627	GLU
1	A	630	VAL
1	A	632	GLU

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Mol	Chain	Res	Type
1	A	633	ILE
1	A	634	GLU
1	A	636	SER
1	A	637	ARG
1	A	653	SER
1	A	654	SER
1	A	658	ILE
1	A	659	THR
1	A	669	SER
1	A	671	ASN
1	A	673	VAL
1	A	682	ILE
1	A	688	THR
1	A	691	THR
1	A	697	LEU
1	A	707	ASN
1	A	708	LYS
1	A	721	GLN
1	A	725	LEU
1	A	738	GLN
1	A	749	GLU
1	A	752	LYS
1	A	782	THR
1	A	788	MET
1	A	789	ARG
1	B	546	PHE
1	B	547	ASP
1	B	552	GLN
1	B	556	LYS
1	B	558	CYS
1	B	561	ARG
1	B	591	THR
1	B	593	ILE
1	B	613	SER
1	B	627	GLU
1	B	636	SER
1	B	637	ARG
1	B	653	SER
1	B	654	SER
1	B	669	SER
1	B	681	PHE
1	B	682	ILE

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Mol	Chain	Res	Type
1	B	688	THR
1	B	698	LYS
1	B	704	VAL
1	B	706	GLU
1	B	708	LYS
1	B	719	ARG
1	B	722	SER
1	B	725	LEU
1	B	738	GLN
1	B	745	LEU
1	B	752	LYS
1	B	756	GLN
1	B	763	LEU
1	B	770	LYS
1	B	774	TYR
1	B	779	ARG
1	B	782	THR
1	B	789	ARG
2	C	12	SER
2	C	21	SER
2	C	27	GLU
2	C	29	THR
2	C	31	GLN
2	C	34	SER
2	C	36	LYS
2	C	39	GLU
2	C	81	LYS
2	C	88	ILE
2	C	92	HIS
2	C	94	ASN
2	C	95	ASP
2	C	97	TYR
2	C	106	ASP
2	C	110	THR
2	C	112	ARG
2	C	120	ASP
2	C	122	ASP
2	C	124	SER
2	C	130	GLN
2	C	133	GLN
2	C	141	VAL
2	C	147	LYS

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Mol	Chain	Res	Type
2	C	152	GLN
2	C	157	SER
2	C	159	ASP
2	C	161	GLU
2	C	165	GLN
2	C	167	THR
2	C	169	LEU
2	C	173	ASP
2	C	182	THR
2	C	183	LYS
2	C	184	LEU
2	C	185	LEU
2	C	192	ASP
2	C	195	THR
2	C	196	SER
2	C	198	GLU
2	C	202	GLN
2	C	204	GLN
2	C	205	SER
2	C	209	LYS
2	C	210	THR
2	C	211	HIS
2	C	219	ARG
2	C	222	SER
2	C	226	HIS
2	C	227	ASP
2	C	228	ASN
2	C	230	ILE
2	C	235	LEU
2	C	239	GLN
2	C	240	GLU
2	C	242	THR
2	C	244	HIS
2	C	246	LYS
2	C	247	ASN
2	C	249	GLU
2	C	250	GLN
2	C	265	ASN
2	C	268	ASP
2	C	272	GLU
2	C	273	LYS
2	C	281	GLU

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Mol	Chain	Res	Type
2	C	282	LYS
2	C	287	PHE
2	C	288	ASP
2	C	290	SER
2	C	293	LYS
2	C	304	THR
2	C	324	ARG
2	C	330	ARG
2	C	334	LYS
2	C	338	ASN
2	C	349	THR
2	C	354	VAL
2	C	357	ASN
2	C	363	ARG
2	C	369	MET
2	D	16	SER
2	D	25	THR
2	D	26	VAL
2	D	30	ASN
2	D	31	GLN
2	D	33	ILE
2	D	35	LEU
2	D	39	GLU
2	D	74	LEU
2	D	78	ASP
2	D	83	ILE
2	D	88	ILE
2	D	93	SER
2	D	95	ASP
2	D	108	THR
2	D	110	THR
2	D	112	ARG
2	D	120	ASP
2	D	130	GLN
2	D	133	GLN
2	D	137	LEU
2	D	147	LYS
2	D	152	GLN
2	D	156	LYS
2	D	161	GLU
2	D	164	VAL
2	D	165	GLN

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Mol	Chain	Res	Type
2	D	167	THR
2	D	169	LEU
2	D	182	THR
2	D	183	LYS
2	D	185	LEU
2	D	188	LEU
2	D	192	ASP
2	D	196	SER
2	D	202	GLN
2	D	205	SER
2	D	209	LYS
2	D	210	THR
2	D	211	HIS
2	D	215	THR
2	D	219	ARG
2	D	223	ILE
2	D	227	ASP
2	D	228	ASN
2	D	232	ARG
2	D	239	GLN
2	D	240	GLU
2	D	242	THR
2	D	244	HIS
2	D	246	LYS
2	D	247	ASN
2	D	249	GLU
2	D	265	ASN
2	D	267	THR
2	D	268	ASP
2	D	281	GLU
2	D	287	PHE
2	D	288	ASP
2	D	293	LYS
2	D	330	ARG
2	D	334	LYS
2	D	338	ASN
2	D	347	ASP
2	D	357	ASN
2	D	363	ARG
2	D	369	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	586	HIS
1	A	625	ASN
1	A	701	GLN
1	A	707	ASN
1	A	711	ASN
1	A	756	GLN
1	A	769	ASN
1	B	586	HIS
1	B	621	HIS
1	B	625	ASN
1	B	671	ASN
1	B	707	ASN
1	B	711	ASN
1	B	729	HIS
1	B	756	GLN
1	B	769	ASN
2	C	17	GLN
2	C	30	ASN
2	C	72	HIS
2	C	86	GLN
2	C	94	ASN
2	C	133	GLN
2	C	204	GLN
2	C	208	ASN
2	C	226	HIS
2	C	239	GLN
2	C	247	ASN
2	C	250	GLN
2	C	265	ASN
2	C	303	ASN
2	C	320	ASN
2	C	338	ASN
2	C	357	ASN
2	D	15	ASN
2	D	30	ASN
2	D	92	HIS
2	D	94	ASN
2	D	133	GLN
2	D	152	GLN
2	D	165	GLN
2	D	204	GLN
2	D	226	HIS
2	D	239	GLN

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Mol	Chain	Res	Type
2	D	244	HIS
2	D	247	ASN
2	D	250	GLN
2	D	265	ASN
2	D	305	ASN
2	D	320	ASN
2	D	338	ASN
2	D	357	ASN
2	D	358	HIS

### 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](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.