Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:26 AM EDT

PDB ID	:	1E9S
Title	:	Bacterial conjugative coupling protein TrwBdeltaN70. Unbound monoclinic form.
Authors	:	Gomis-Rueth, F.X.; Moncalian, G.; Cabezon, E.; de la Cruz, F.; Coll, M.
Deposited on	:	2000-10-26
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

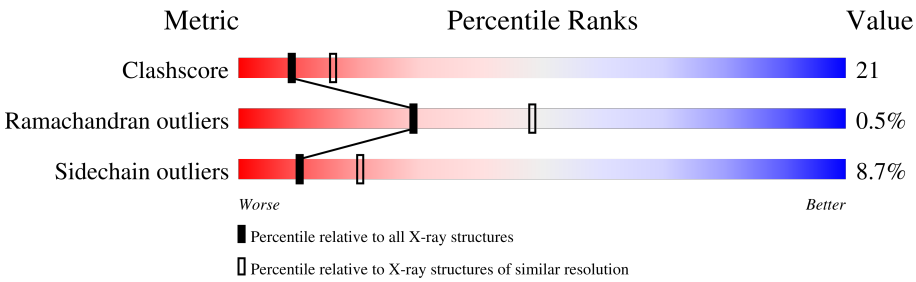
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	437	66% 28% • •
1	B	437	64% 27% 5% •
1	D	437	61% 30% 5% 5%
1	E	437	63% 28% 7% •
1	F	437	64% 29% 5% •
1	G	437	57% 36% 5% •
1	H	437	57% 36% • •
1	I	437	60% 33% • •

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Mol	Chain	Length	Quality of chain
1	J	437	60% 33%
1	K	437	56% 36%
1	L	437	55% 38% 5%
1	M	437	59% 33% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 41513 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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3353	2118	602	623	10	0	0	0
1	B	422	3318	2097	596	615	10	0	0	0
1	D	417	3279	2075	586	608	10	0	0	0
1	E	425	3340	2110	600	620	10	0	0	0
1	F	427	3348	2114	602	622	10	0	0	0
1	G	427	3352	2116	603	623	10	0	0	0
1	H	424	3329	2103	598	618	10	0	0	0
1	I	424	3328	2102	598	618	10	0	0	0
1	J	424	3328	2102	598	618	10	0	0	0
1	K	422	3316	2096	595	615	10	0	0	0
1	L	426	3344	2112	601	621	10	0	0	0
1	M	425	3332	2104	599	619	10	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	157	157	157	0	0
2	B	135	135	135	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	D	139	139	139	0	0
			Total	O		
2	E	133	133	133	0	0
			Total	O		
2	F	193	193	193	0	0
			Total	O		
2	G	167	167	167	0	0
			Total	O		
2	H	124	124	124	0	0
			Total	O		
2	I	113	113	113	0	0
			Total	O		
2	J	102	102	102	0	0
			Total	O		
2	K	84	84	84	0	0
			Total	O		
2	L	86	86	86	0	0
			Total	O		
2	M	113	113	113	0	0

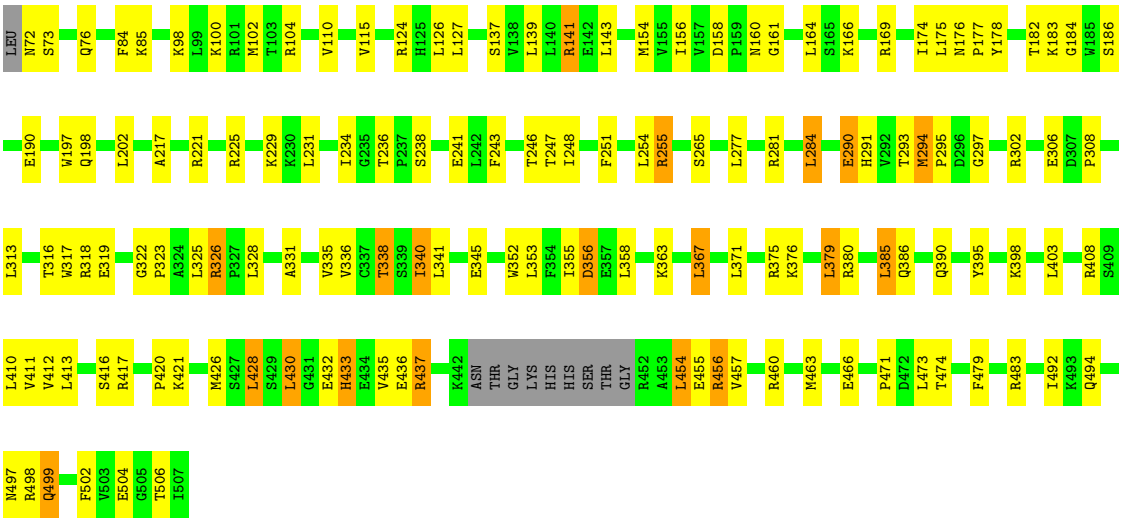
3 Residue-property plots (i)

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

Note EDS was not executed.

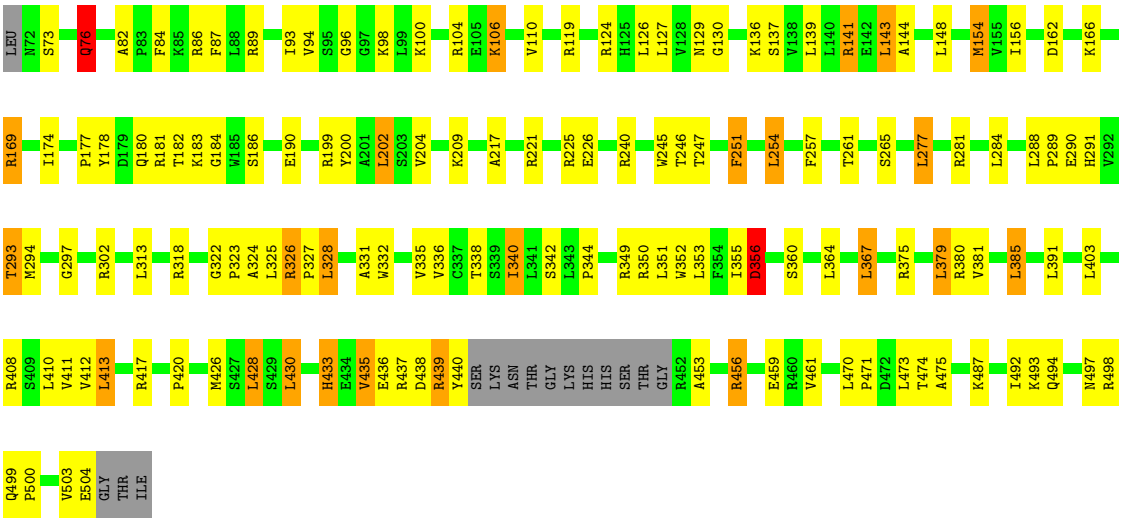
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain A: 66% 28%



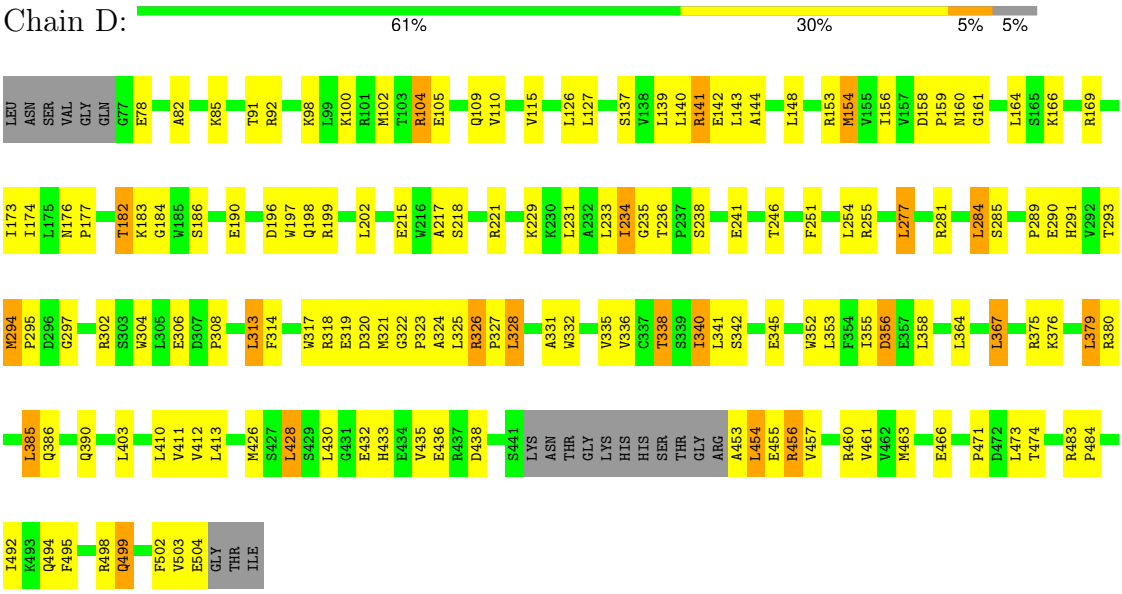
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain B: 64% 27% 5%



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain D:

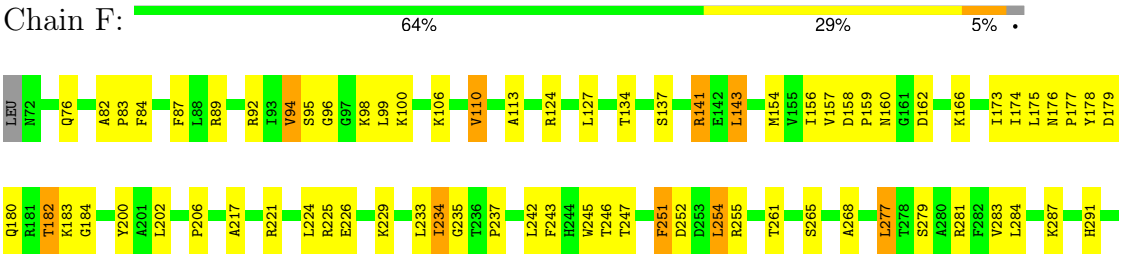


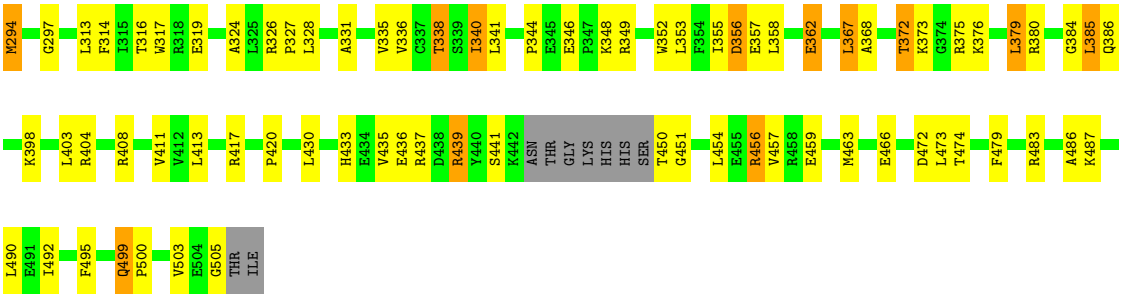
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain E:

• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

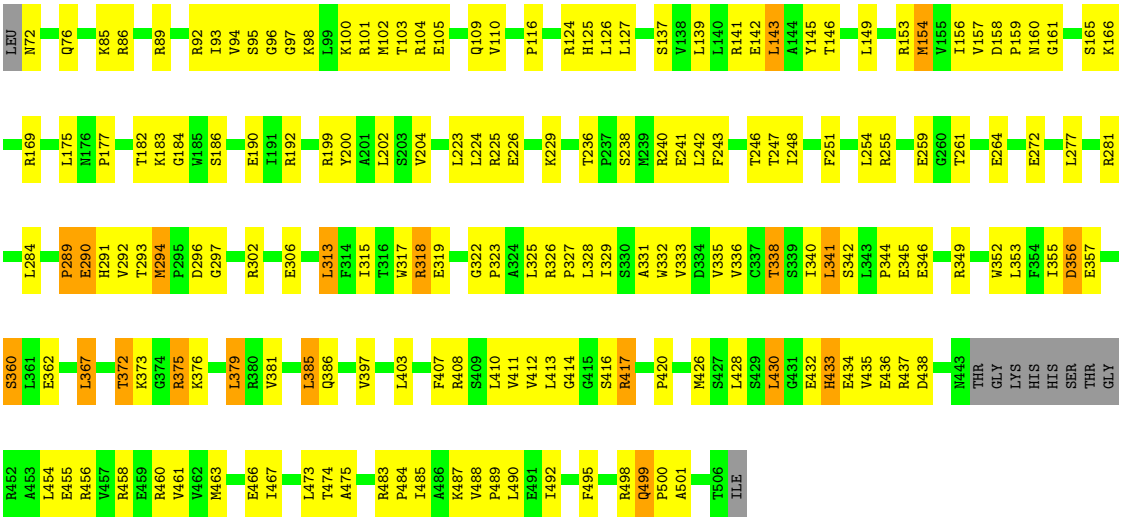
Chain F:





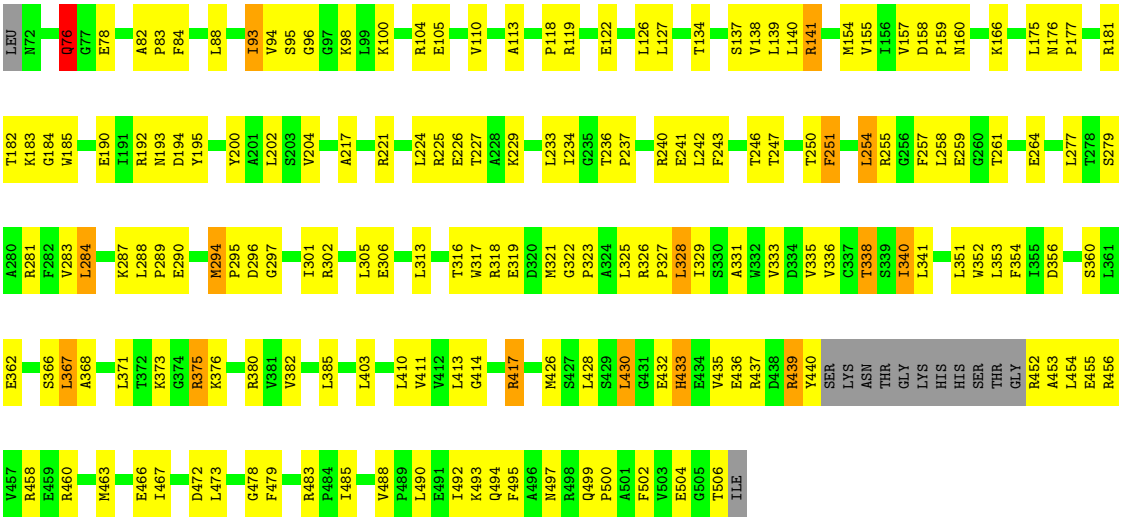
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain G:



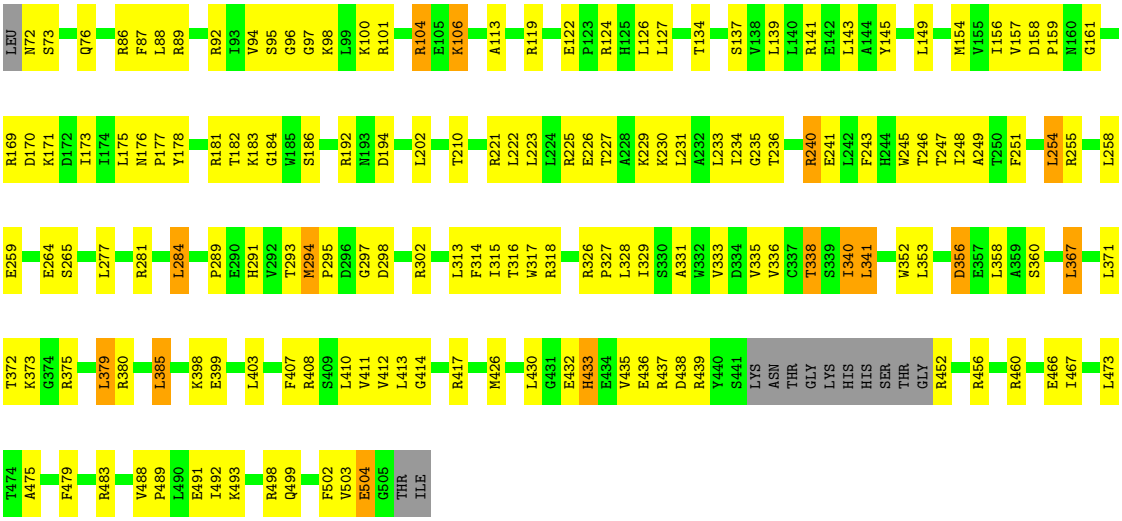
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain H:



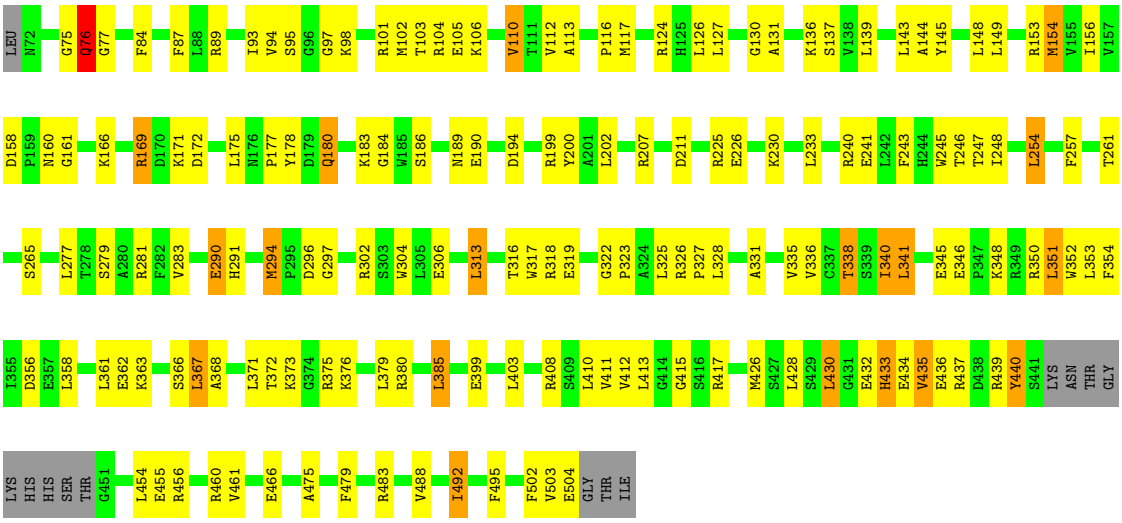
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain I:



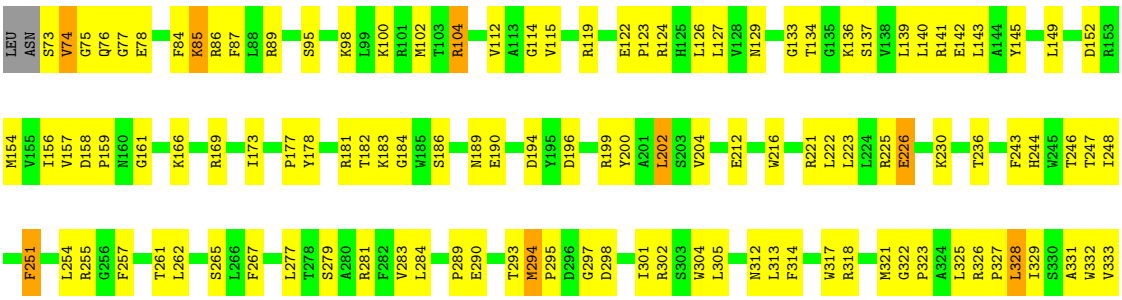
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

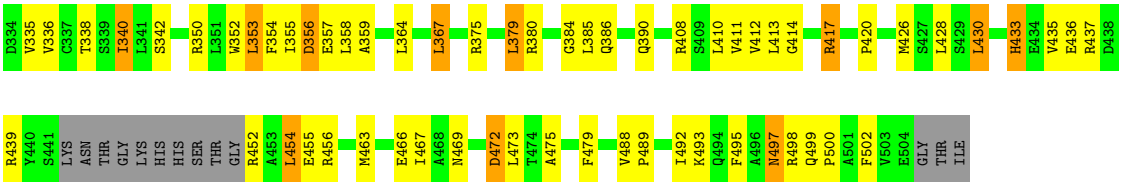
Chain J:



• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

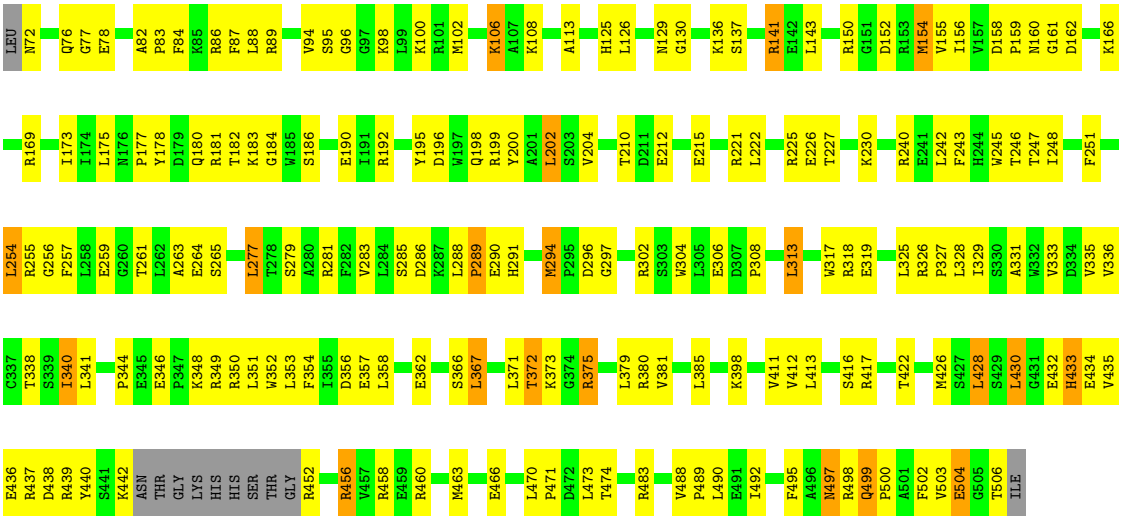
Chain K:





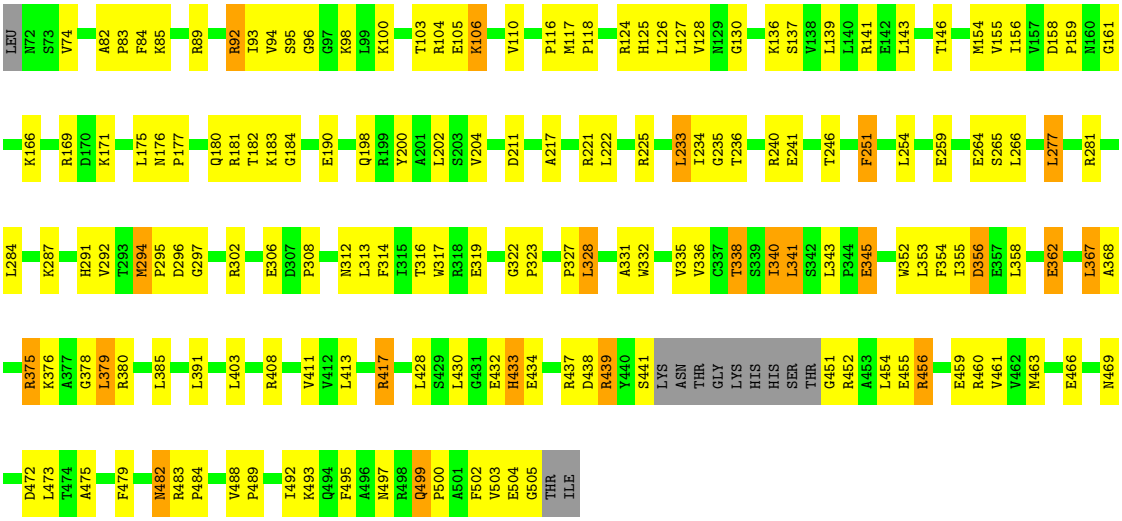
- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain L:



- Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain M:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.40Å 153.40Å 162.50Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.2 (50.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41513	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.42	0/3418	0.67	1/4617 (0.0%)
1	B	0.42	0/3383	0.66	0/4572
1	D	0.41	0/3344	0.69	1/4520 (0.0%)
1	E	0.41	0/3405	0.66	1/4601 (0.0%)
1	F	0.42	0/3413	0.69	1/4611 (0.0%)
1	G	0.41	0/3417	0.66	0/4617
1	H	0.40	0/3394	0.65	1/4587 (0.0%)
1	I	0.39	0/3393	0.66	0/4585
1	J	0.40	0/3393	0.64	0/4585
1	K	0.40	0/3381	0.63	0/4569
1	L	0.40	0/3409	0.65	0/4606
1	M	0.41	0/3397	0.64	0/4590
All	All	0.41	0/40747	0.66	5/55060 (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
1	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	F	157	VAL	N-CA-C	-5.22	96.91	111.00
1	D	104	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	157	VAL	N-CA-C	-5.10	97.22	111.00
1	H	157	VAL	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	200	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3353	0	3385	109	0
1	B	3318	0	3346	140	0
1	D	3279	0	3307	111	0
1	E	3340	0	3371	141	0
1	F	3348	0	3377	123	0
1	G	3352	0	3380	150	0
1	H	3329	0	3356	145	0
1	I	3328	0	3354	137	0
1	J	3328	0	3354	142	0
1	K	3316	0	3345	191	0
1	L	3344	0	3374	173	0
1	M	3332	0	3357	161	0
2	A	157	0	0	9	0
2	B	135	0	0	7	0
2	D	139	0	0	10	0
2	E	133	0	0	8	0
2	F	193	0	0	9	0
2	G	167	0	0	10	0
2	H	124	0	0	8	0
2	I	113	0	0	8	0
2	J	102	0	0	6	0
2	K	84	0	0	5	0
2	L	86	0	0	4	0
2	M	113	0	0	4	0
All	All	41513	0	40306	1647	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 21.

All (1647) 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:J:76:GLN:HG2	1:J:77:GLY:H	1.07	1.16
1:I:106:LYS:H	1:I:106:LYS:HD3	1.04	1.15
1:E:127:LEU:HD11	1:E:385:LEU:HD22	1.27	1.09
1:J:492:ILE:HD13	1:J:492:ILE:H	1.14	1.08
1:F:372:THR:HG22	1:F:373:LYS:HG3	1.40	1.03
1:G:127:LEU:HD11	1:G:385:LEU:HD22	1.36	1.03
1:M:106:LYS:HD3	1:M:106:LYS:H	1.17	1.01
1:J:127:LEU:HD11	1:J:385:LEU:HD22	1.39	1.01
1:K:436:GLU:HG2	1:K:454:LEU:HD22	1.41	1.00
1:E:106:LYS:H	1:E:106:LYS:HD3	1.23	0.99
1:L:412:VAL:HG22	1:L:426:MET:HE3	1.44	0.99
1:J:226:GLU:HG3	1:J:261:THR:HB	1.45	0.99
1:H:367:LEU:HD13	1:H:403:LEU:HD11	1.49	0.94
1:F:173:ILE:HD12	1:F:183:LYS:HE3	1.49	0.94
1:B:226:GLU:HG3	1:B:261:THR:HB	1.51	0.93
1:F:235:GLY:HA2	2:I:2009:HOH:O	1.67	0.93
1:K:173:ILE:HD12	1:K:183:LYS:HE3	1.51	0.92
1:B:124:ARG:HH21	1:B:408:ARG:HH12	1.17	0.91
1:M:169:ARG:HH21	1:M:171:LYS:HD3	1.33	0.91
1:K:154:MET:HE3	1:K:156:ILE:HD11	1.53	0.91
1:I:134:THR:HG21	1:I:413:LEU:O	1.72	0.90
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.36	0.90
1:F:176:ASN:H	1:F:182:THR:HG23	1.35	0.90
1:K:412:VAL:HG22	1:K:426:MET:HE3	1.53	0.89
1:A:290:GLU:HG2	1:A:325:LEU:HD23	1.54	0.89
1:L:442:LYS:HD2	1:M:452:ARG:HH21	1.37	0.89
1:L:497:ASN:N	1:L:497:ASN:HD22	1.69	0.89
1:B:290:GLU:HG2	1:B:325:LEU:HD23	1.52	0.88
1:I:246:THR:O	1:I:281:ARG:HD2	1.73	0.88
1:E:180:GLN:HB2	1:E:504:GLU:HB2	1.54	0.88
1:E:226:GLU:HG3	1:E:261:THR:HB	1.56	0.88
1:I:154:MET:CE	1:I:156:ILE:HD11	2.04	0.88
1:E:412:VAL:HG22	1:E:426:MET:CE	2.01	0.88
1:I:106:LYS:HD3	1:I:106:LYS:N	1.89	0.88
1:J:76:GLN:HG2	1:J:77:GLY:N	1.87	0.87
1:K:226:GLU:HG3	1:K:261:THR:HB	1.54	0.87
1:H:294:MET:HE2	1:H:295:PRO:HD2	1.57	0.87
1:E:246:THR:O	1:E:281:ARG:HD2	1.73	0.86
1:G:357:GLU:HG3	2:G:2122:HOH:O	1.75	0.86
1:K:357:GLU:HG3	2:K:2066:HOH:O	1.75	0.86
1:G:72:ASN:HD21	1:G:438:ASP:HB2	1.39	0.86
1:K:169:ARG:HD3	1:K:498:ARG:HH22	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:O	1:A:281:ARG:HD2	1.75	0.85
1:L:226:GLU:HG3	1:L:261:THR:HB	1.56	0.85
1:E:154:MET:HE3	1:E:156:ILE:HD11	1.59	0.85
1:K:182:THR:HG22	1:K:183:LYS:O	1.77	0.85
1:G:372:THR:HG22	1:G:373:LYS:HG3	1.58	0.85
1:M:259:GLU:HA	1:M:264:GLU:HG3	1.59	0.85
1:J:290:GLU:HG2	1:J:325:LEU:HD23	1.59	0.85
1:B:124:ARG:NH2	1:B:408:ARG:HH12	1.74	0.84
1:B:412:VAL:HG22	1:B:426:MET:HE3	1.59	0.84
1:L:106:LYS:H	1:L:106:LYS:HD3	1.43	0.84
1:B:96:GLY:O	1:B:100:LYS:HG3	1.78	0.84
1:M:432:GLU:HG2	1:M:460:ARG:HD3	1.61	0.83
1:G:340:ILE:HD13	1:G:379:LEU:HG	1.61	0.83
1:K:169:ARG:HG3	1:K:169:ARG:HH11	1.42	0.83
1:L:290:GLU:HG2	1:L:325:LEU:HD23	1.59	0.83
1:L:240:ARG:NH1	1:L:240:ARG:HB2	1.93	0.83
1:D:290:GLU:HG2	1:D:325:LEU:HD23	1.61	0.82
1:J:246:THR:O	1:J:281:ARG:HD2	1.78	0.82
1:D:367:LEU:HD13	1:D:403:LEU:HD11	1.60	0.82
1:M:106:LYS:H	1:M:106:LYS:CD	1.88	0.82
1:E:177:PRO:HB3	1:E:294:MET:HG2	1.61	0.81
1:F:499:GLN:HG3	1:F:500:PRO:HD2	1.62	0.81
1:H:246:THR:O	1:H:281:ARG:HD2	1.79	0.81
1:I:94:VAL:HG13	1:I:98:LYS:HB3	1.61	0.81
1:B:240:ARG:HB2	1:B:240:ARG:HH11	1.46	0.81
1:J:336:VAL:O	1:J:340:ILE:HG23	1.80	0.80
1:L:108:LYS:HE3	1:L:150:ARG:HG3	1.63	0.80
1:D:127:LEU:HD11	1:D:385:LEU:HD22	1.63	0.80
1:G:94:VAL:CG1	1:G:98:LYS:HB3	2.12	0.80
1:E:240:ARG:NH1	1:E:240:ARG:HB2	1.97	0.80
1:G:327:PRO:HG2	2:G:2115:HOH:O	1.82	0.80
1:K:169:ARG:HD3	1:K:498:ARG:NH2	1.96	0.80
1:K:246:THR:O	1:K:281:ARG:HD2	1.82	0.80
1:F:237:PRO:HG3	1:I:104:ARG:NH2	1.97	0.80
1:J:160:ASN:HD21	1:J:319:GLU:CD	1.85	0.80
1:D:498:ARG:O	1:D:499:GLN:HG2	1.82	0.79
1:H:463:MET:HB2	1:H:466:GLU:HG3	1.64	0.79
1:L:259:GLU:HA	1:L:264:GLU:HG3	1.64	0.79
1:B:154:MET:HB3	1:B:352:TRP:HB2	1.65	0.79
1:A:154:MET:CE	1:A:156:ILE:HD11	2.13	0.79
1:F:237:PRO:HG3	1:I:104:ARG:HH21	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:255:ARG:HH11	1:L:277:LEU:HD12	1.48	0.79
1:G:259:GLU:HA	1:G:264:GLU:HG3	1.65	0.78
1:A:127:LEU:HD11	1:A:385:LEU:HD22	1.64	0.78
1:F:176:ASN:H	1:F:182:THR:CG2	1.96	0.78
1:E:154:MET:CE	1:E:156:ILE:HD11	2.14	0.78
1:F:225:ARG:O	1:F:229:LYS:HG3	1.82	0.78
1:B:336:VAL:O	1:B:340:ILE:HG23	1.83	0.78
1:B:412:VAL:HG22	1:B:426:MET:CE	2.14	0.78
1:H:177:PRO:HB3	1:H:294:MET:HG2	1.65	0.78
1:H:375:ARG:HB2	1:H:375:ARG:HH11	1.48	0.78
1:L:182:THR:HG22	1:L:183:LYS:O	1.84	0.78
1:L:240:ARG:HB2	1:L:240:ARG:HH11	1.50	0.77
1:M:175:LEU:HD12	1:M:313:LEU:HD21	1.65	0.77
1:K:127:LEU:HD11	1:K:385:LEU:HD13	1.65	0.77
1:I:124:ARG:NH2	1:I:408:ARG:HH12	1.82	0.77
1:M:110:VAL:HG11	1:M:143:LEU:HD23	1.65	0.77
1:B:437:ARG:HD2	1:D:456:ARG:NH1	1.99	0.77
1:F:234:ILE:O	1:F:234:ILE:HG22	1.83	0.77
1:J:84:PHE:HB3	1:J:437:ARG:NH1	2.00	0.77
1:A:198:GLN:HG2	2:G:2012:HOH:O	1.85	0.77
1:A:291:HIS:HD2	2:A:2040:HOH:O	1.68	0.77
1:F:127:LEU:HD11	1:F:385:LEU:HD22	1.67	0.77
1:G:290:GLU:HG2	1:G:325:LEU:HD23	1.67	0.76
1:K:497:ASN:N	1:K:497:ASN:HD22	1.83	0.76
1:I:127:LEU:HD11	1:I:385:LEU:CD2	2.15	0.76
1:M:502:PHE:CE2	1:M:504:GLU:HB2	2.21	0.76
1:I:502:PHE:CE2	1:I:504:GLU:HB3	2.20	0.76
1:G:499:GLN:HG3	1:G:500:PRO:HD2	1.67	0.76
1:K:473:LEU:HD11	1:K:492:ILE:HD11	1.67	0.76
1:G:154:MET:CE	1:G:156:ILE:HD11	2.16	0.75
1:K:73:SER:HB3	1:K:85:LYS:HA	1.68	0.75
1:D:246:THR:O	1:D:281:ARG:HD2	1.86	0.75
1:E:412:VAL:HG22	1:E:426:MET:HE2	1.68	0.75
1:G:182:THR:HG22	1:G:183:LYS:O	1.87	0.75
1:D:154:MET:CE	1:D:156:ILE:HD11	2.17	0.75
1:H:127:LEU:HD11	1:H:385:LEU:HD22	1.67	0.75
1:K:230:LYS:HD3	1:K:257:PHE:CE2	2.22	0.75
1:G:154:MET:HE2	1:G:156:ILE:HD11	1.69	0.75
1:L:336:VAL:O	1:L:340:ILE:HG23	1.85	0.75
1:B:327:PRO:HG2	2:B:2088:HOH:O	1.86	0.75
1:G:226:GLU:HG3	1:G:261:THR:HB	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:THR:HG22	1:I:183:LYS:O	1.86	0.75
1:I:473:LEU:HD11	1:I:492:ILE:HD11	1.67	0.75
1:K:166:LYS:HE2	1:K:497:ASN:ND2	2.02	0.75
1:M:126:LEU:HD11	1:M:411:VAL:HG23	1.69	0.74
1:M:154:MET:HB3	1:M:352:TRP:HB2	1.68	0.74
1:A:367:LEU:HD13	1:A:403:LEU:HD11	1.69	0.74
1:L:412:VAL:HG22	1:L:426:MET:CE	2.16	0.74
1:M:92:ARG:HB2	1:M:484:PRO:HB3	1.70	0.74
1:M:156:ILE:HG22	1:M:158:ASP:HB2	1.69	0.74
1:I:318:ARG:HD3	1:I:502:PHE:CE2	2.22	0.74
1:I:372:THR:HG23	1:I:373:LYS:HG3	1.70	0.74
1:K:412:VAL:HG22	1:K:426:MET:CE	2.16	0.74
1:K:84:PHE:CG	1:K:435:VAL:HG21	2.23	0.74
1:M:177:PRO:HA	1:M:294:MET:HE2	1.69	0.74
1:D:473:LEU:HD11	1:D:492:ILE:HD11	1.68	0.73
1:K:452:ARG:NH1	1:K:452:ARG:HB3	2.03	0.73
1:A:169:ARG:HG3	1:A:498:ARG:HH22	1.52	0.73
1:A:410:LEU:HD11	1:A:426:MET:HE1	1.71	0.73
1:M:327:PRO:HG2	2:M:2073:HOH:O	1.87	0.73
1:I:154:MET:HE3	1:I:156:ILE:HD11	1.70	0.73
1:K:134:THR:HG21	1:K:413:LEU:HB3	1.70	0.73
1:M:336:VAL:O	1:M:340:ILE:HG23	1.88	0.73
1:G:246:THR:O	1:G:281:ARG:HD2	1.89	0.73
1:H:440:TYR:HA	1:H:452:ARG:HB2	1.71	0.73
1:I:225:ARG:O	1:I:229:LYS:HG3	1.89	0.73
1:H:177:PRO:HA	1:H:294:MET:HE2	1.71	0.73
1:A:154:MET:HE3	1:A:156:ILE:HD11	1.71	0.72
1:J:190:GLU:OE1	1:J:302:ARG:HG3	1.87	0.72
1:J:200:TYR:HE1	1:J:335:VAL:HG13	1.54	0.72
1:A:225:ARG:HD2	2:A:2067:HOH:O	1.88	0.72
1:I:124:ARG:HG3	1:I:124:ARG:HH11	1.54	0.72
1:K:74:VAL:HG12	1:K:75:GLY:H	1.54	0.72
1:K:134:THR:HG21	1:K:413:LEU:O	1.89	0.72
1:D:190:GLU:OE1	1:D:302:ARG:HG3	1.90	0.72
1:F:234:ILE:O	1:F:234:ILE:CG2	2.38	0.72
1:L:246:THR:O	1:L:281:ARG:HD2	1.90	0.72
1:M:124:ARG:HH21	1:M:375:ARG:HG3	1.54	0.72
1:M:413:LEU:HD23	1:M:475:ALA:HB2	1.72	0.72
1:H:294:MET:CE	1:H:295:PRO:HD2	2.19	0.72
1:K:78:GLU:HA	1:K:78:GLU:OE1	1.89	0.72
1:I:255:ARG:HH11	1:I:255:ARG:HG3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:LEU:HD11	1:J:411:VAL:HG23	1.71	0.72
1:M:352:TRP:CE2	1:M:380:ARG:HD3	2.25	0.72
1:G:126:LEU:HD11	1:G:411:VAL:HG23	1.71	0.71
1:B:246:THR:O	1:B:281:ARG:HD2	1.90	0.71
1:B:106:LYS:HE3	1:B:106:LYS:H	1.54	0.71
1:G:94:VAL:HG12	1:G:95:SER:N	2.05	0.71
1:I:158:ASP:OD2	1:I:161:GLY:HA2	1.91	0.71
1:K:78:GLU:HG3	1:K:95:SER:CA	2.20	0.71
1:I:154:MET:HE2	1:I:156:ILE:HD11	1.71	0.71
1:K:129:ASN:HB3	1:K:426:MET:HE1	1.73	0.71
1:D:154:MET:HE3	1:D:156:ILE:HD11	1.72	0.71
1:A:473:LEU:HD11	1:A:492:ILE:HD11	1.73	0.70
1:F:160:ASN:HD21	1:F:319:GLU:HG3	1.56	0.70
1:D:432:GLU:HG2	1:D:460:ARG:HD3	1.72	0.70
1:E:412:VAL:HG22	1:E:426:MET:HE3	1.73	0.70
1:G:410:LEU:HD11	1:G:426:MET:HE1	1.73	0.70
1:J:154:MET:HE3	1:J:156:ILE:HD11	1.71	0.70
1:I:259:GLU:HA	1:I:264:GLU:HG3	1.73	0.70
1:A:412:VAL:HG22	1:A:426:MET:CE	2.21	0.70
1:K:75:GLY:HA3	1:K:84:PHE:H	1.55	0.70
1:B:240:ARG:HB2	1:B:240:ARG:NH1	2.05	0.70
1:G:72:ASN:ND2	1:G:438:ASP:HB2	2.04	0.70
1:A:432:GLU:HG2	1:A:460:ARG:HD3	1.72	0.70
1:F:420:PRO:HB2	1:G:428:LEU:HD22	1.74	0.70
1:J:76:GLN:CG	1:J:77:GLY:H	1.92	0.69
1:A:498:ARG:O	1:A:499:GLN:HG2	1.92	0.69
1:F:226:GLU:HG3	1:F:261:THR:HB	1.72	0.69
1:M:379:LEU:HD22	1:M:380:ARG:N	2.07	0.69
1:E:230:LYS:HD3	1:E:257:PHE:CZ	2.27	0.69
1:E:240:ARG:HB2	1:E:240:ARG:HH11	1.55	0.69
1:A:318:ARG:HD2	1:A:502:PHE:CE2	2.28	0.69
1:F:336:VAL:O	1:F:340:ILE:HG23	1.91	0.69
1:M:294:MET:CE	1:M:295:PRO:HD2	2.22	0.69
1:A:190:GLU:OE1	1:A:302:ARG:HG3	1.92	0.69
1:B:190:GLU:OE1	1:B:302:ARG:HG3	1.93	0.69
1:J:154:MET:HB3	1:J:352:TRP:HB2	1.73	0.69
1:M:190:GLU:OE1	1:M:302:ARG:HG3	1.92	0.69
1:I:173:ILE:HD12	1:I:183:LYS:HE3	1.73	0.69
1:J:436:GLU:HB3	1:J:454:LEU:HD21	1.73	0.69
1:K:85:LYS:HD2	1:K:454:LEU:HD21	1.75	0.69
1:I:106:LYS:H	1:I:106:LYS:CD	1.84	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:ARG:HD3	2:G:2116:HOH:O	1.93	0.69
1:B:225:ARG:HD2	2:B:2058:HOH:O	1.92	0.69
1:I:367:LEU:HD13	1:I:403:LEU:HD11	1.75	0.69
1:G:372:THR:HG22	1:G:373:LYS:CG	2.23	0.68
1:H:279:SER:O	1:H:283:VAL:HG23	1.93	0.68
1:H:336:VAL:O	1:H:340:ILE:HG23	1.94	0.68
1:J:331:ALA:O	1:J:335:VAL:HG23	1.93	0.68
1:L:255:ARG:NH1	1:L:277:LEU:HD12	2.07	0.68
1:H:155:VAL:HG13	1:H:313:LEU:HD12	1.75	0.68
1:M:502:PHE:HE2	1:M:504:GLU:HB2	1.59	0.68
1:K:78:GLU:HG3	1:K:95:SER:HA	1.75	0.68
1:L:190:GLU:OE1	1:L:302:ARG:HG3	1.94	0.68
1:B:126:LEU:HD11	1:B:411:VAL:HG23	1.76	0.68
1:E:443:ASN:OD1	1:F:451:GLY:HA3	1.92	0.68
1:J:492:ILE:H	1:J:492:ILE:CD1	1.92	0.68
1:K:313:LEU:HD23	1:K:314:PHE:N	2.08	0.68
1:I:124:ARG:HG3	1:I:124:ARG:NH1	2.09	0.68
1:J:412:VAL:HG22	1:J:426:MET:CE	2.24	0.68
1:F:246:THR:O	1:F:281:ARG:HD2	1.92	0.68
1:D:412:VAL:HG22	1:D:426:MET:CE	2.23	0.68
1:E:432:GLU:HG2	1:E:460:ARG:HD3	1.76	0.68
1:J:94:VAL:HG13	1:J:98:LYS:HB3	1.76	0.68
1:M:504:GLU:HG3	1:M:505:GLY:N	2.09	0.67
1:A:412:VAL:HG22	1:A:426:MET:HE3	1.77	0.67
1:E:110:VAL:HG11	1:E:143:LEU:HD23	1.76	0.67
1:K:413:LEU:HD12	1:K:475:ALA:HB2	1.77	0.67
1:L:473:LEU:HD11	1:L:492:ILE:HD11	1.74	0.67
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.59	0.67
1:D:169:ARG:HG3	1:D:498:ARG:NH2	2.10	0.67
1:J:230:LYS:HD3	1:J:257:PHE:CE1	2.30	0.67
1:J:327:PRO:HG2	2:J:2070:HOH:O	1.94	0.67
1:K:173:ILE:HG23	1:K:183:LYS:HG3	1.75	0.67
1:B:124:ARG:NH2	1:B:408:ARG:NH1	2.43	0.67
1:A:293:THR:HG21	2:A:2091:HOH:O	1.94	0.67
1:B:180:GLN:HE21	1:B:504:GLU:HG3	1.59	0.67
1:I:145:TYR:CZ	1:I:149:LEU:HD21	2.30	0.67
1:J:184:GLY:HA3	1:J:297:GLY:HA3	1.76	0.67
1:L:432:GLU:HG2	1:L:460:ARG:HD3	1.76	0.67
1:I:94:VAL:CG1	1:I:98:LYS:HB3	2.25	0.66
1:L:497:ASN:N	1:L:497:ASN:ND2	2.42	0.66
1:E:106:LYS:H	1:E:106:LYS:CD	2.01	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ARG:HH11	1:F:141:ARG:HG2	1.60	0.66
1:A:169:ARG:HG3	1:A:498:ARG:NH2	2.09	0.66
1:H:290:GLU:HG2	1:H:325:LEU:HD23	1.76	0.66
1:B:87:PHE:HA	1:B:435:VAL:HG23	1.77	0.66
1:H:439:ARG:HD3	1:H:453:ALA:O	1.96	0.66
1:F:173:ILE:HG23	1:F:183:LYS:HG3	1.75	0.66
1:A:410:LEU:HD11	1:A:426:MET:CE	2.26	0.66
1:A:502:PHE:CE2	1:A:504:GLU:HB2	2.31	0.66
1:F:82:ALA:HB2	1:G:456:ARG:HD2	1.77	0.66
1:L:160:ASN:HD21	1:L:319:GLU:CD	1.99	0.66
1:B:94:VAL:CG2	1:B:98:LYS:HD3	2.25	0.66
1:D:176:ASN:H	1:D:182:THR:HG23	1.60	0.66
1:F:134:THR:HA	1:F:472:ASP:OD1	1.96	0.66
1:H:158:ASP:HB3	1:H:316:THR:HG22	1.76	0.66
1:J:372:THR:HG22	1:J:373:LYS:HG3	1.78	0.66
1:K:74:VAL:HG12	1:K:75:GLY:N	2.10	0.66
1:F:346:GLU:OE2	1:F:348:LYS:HB2	1.96	0.65
1:H:294:MET:HG3	1:H:328:LEU:HD11	1.78	0.65
1:L:503:VAL:O	1:L:504:GLU:HB2	1.96	0.65
1:E:255:ARG:HG3	1:E:255:ARG:HH11	1.61	0.65
1:G:367:LEU:HD13	1:G:403:LEU:HD11	1.78	0.65
1:L:180:GLN:HB2	1:L:504:GLU:HB2	1.76	0.65
1:M:251:PHE:CE1	1:M:277:LEU:HD13	2.30	0.65
1:B:184:GLY:HA3	1:B:297:GLY:HA3	1.79	0.65
1:J:200:TYR:CE1	1:J:335:VAL:HG13	2.32	0.65
1:J:432:GLU:HG2	1:J:460:ARG:HD3	1.79	0.65
1:B:182:THR:HG22	1:B:183:LYS:O	1.97	0.65
1:M:106:LYS:HD3	1:M:106:LYS:N	2.02	0.65
1:H:94:VAL:HG13	1:H:98:LYS:HB3	1.79	0.64
1:K:452:ARG:HB3	1:K:452:ARG:HH11	1.60	0.64
1:A:398:LYS:HG3	2:G:2134:HOH:O	1.97	0.64
1:A:436:GLU:HB3	1:A:454:LEU:HD21	1.79	0.64
1:H:138:VAL:HG21	1:H:492:ILE:HG12	1.79	0.64
1:L:184:GLY:HA3	1:L:297:GLY:HA3	1.79	0.64
1:L:463:MET:HB2	1:L:466:GLU:HG3	1.79	0.64
1:I:101:ARG:O	1:I:104:ARG:HG2	1.97	0.64
1:I:139:LEU:HD11	1:I:411:VAL:HG11	1.80	0.64
1:G:473:LEU:HD11	1:G:492:ILE:HD11	1.79	0.64
1:K:251:PHE:CE2	1:K:277:LEU:HD12	2.33	0.64
1:L:96:GLY:O	1:L:100:LYS:HG3	1.97	0.64
1:M:222:LEU:HA	1:M:225:ARG:NH1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:TYR:O	1:H:204:VAL:HG23	1.98	0.64
1:K:433:HIS:HD2	1:K:433:HIS:O	1.80	0.64
1:E:379:LEU:HD22	1:E:380:ARG:N	2.12	0.63
1:H:302:ARG:O	1:H:306:GLU:HG3	1.98	0.63
1:E:357:GLU:OE2	1:E:386:GLN:HG3	1.98	0.63
1:I:255:ARG:HG3	1:I:255:ARG:NH1	2.12	0.63
1:A:98:LYS:O	1:A:102:MET:HG3	1.98	0.63
1:B:413:LEU:HD12	1:B:475:ALA:HB2	1.78	0.63
1:D:318:ARG:HD2	1:D:502:PHE:CE2	2.34	0.63
1:E:106:LYS:HD3	1:E:106:LYS:N	2.06	0.63
1:F:154:MET:HE3	1:F:156:ILE:HD11	1.80	0.63
1:L:338:THR:HG23	1:L:366:SER:OG	1.97	0.63
1:G:166:LYS:HD3	1:G:495:PHE:HB2	1.80	0.63
1:G:413:LEU:HD12	1:G:475:ALA:HB2	1.79	0.63
1:J:154:MET:CE	1:J:156:ILE:HD11	2.28	0.63
1:L:442:LYS:HD2	1:M:452:ARG:NH2	2.11	0.63
1:H:281:ARG:NH2	1:I:265:SER:HB3	2.14	0.63
1:D:336:VAL:O	1:D:340:ILE:HG23	1.99	0.63
1:G:110:VAL:CG1	1:G:143:LEU:HD23	2.29	0.63
1:J:199:ARG:HE	1:J:338:THR:CG2	2.12	0.63
1:G:412:VAL:HG22	1:G:426:MET:CE	2.29	0.63
1:L:88:LEU:HD21	1:L:436:GLU:HG3	1.81	0.63
1:B:124:ARG:HH21	1:B:408:ARG:NH1	1.92	0.62
1:E:113:ALA:HA	1:E:490:LEU:HD23	1.81	0.62
1:G:329:ILE:O	1:G:333:VAL:HG23	1.99	0.62
1:M:294:MET:HE2	1:M:295:PRO:HD2	1.79	0.62
1:E:94:VAL:HG13	1:E:98:LYS:HB3	1.82	0.62
1:L:195:TYR:HE1	1:L:199:ARG:HH11	1.47	0.62
1:M:124:ARG:HH22	1:M:375:ARG:NH1	1.95	0.62
1:I:412:VAL:HG22	1:I:426:MET:HE3	1.80	0.62
1:D:436:GLU:HG2	1:D:454:LEU:HD22	1.81	0.62
1:E:350:ARG:HG2	1:E:380:ARG:NH2	2.15	0.62
1:H:176:ASN:H	1:H:182:THR:CG2	2.12	0.62
1:L:247:THR:HG22	1:L:248:ILE:HD13	1.80	0.62
1:M:94:VAL:CG2	1:M:98:LYS:HD3	2.29	0.62
1:H:432:GLU:OE1	1:H:458:ARG:HD2	1.99	0.62
1:K:177:PRO:HG3	1:K:325:LEU:HD21	1.81	0.62
1:M:118:PRO:HG2	1:M:483:ARG:NH1	2.14	0.62
1:B:106:LYS:H	1:B:106:LYS:CE	2.11	0.62
1:B:180:GLN:HE21	1:B:504:GLU:HB2	1.63	0.62
1:B:326:ARG:HD3	2:B:2086:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:HB3	1:E:352:TRP:HB2	1.81	0.62
1:I:124:ARG:NH2	1:I:408:ARG:NH1	2.46	0.62
1:F:137:SER:O	1:F:141:ARG:HB2	2.00	0.62
1:I:126:LEU:HD11	1:I:411:VAL:HG23	1.82	0.62
1:F:245:TRP:O	1:F:254:LEU:HG	2.00	0.62
1:H:181:ARG:NH1	1:H:500:PRO:HG2	2.15	0.62
1:H:327:PRO:HG2	2:H:2085:HOH:O	1.99	0.62
1:I:221:ARG:O	1:I:225:ARG:HG2	1.99	0.62
1:L:372:THR:HG22	1:L:373:LYS:CG	2.30	0.62
1:B:180:GLN:HE21	1:B:504:GLU:CG	2.13	0.62
1:B:433:HIS:NE2	1:B:459:GLU:HG3	2.15	0.62
1:D:326:ARG:HD3	2:D:2083:HOH:O	2.00	0.62
1:G:432:GLU:HG2	1:G:460:ARG:HD3	1.80	0.62
1:H:84:PHE:CG	1:H:435:VAL:HG11	2.35	0.62
1:K:289:PRO:O	1:K:293:THR:HG23	2.00	0.62
1:M:438:ASP:OD1	1:M:454:LEU:HD23	1.99	0.62
1:F:176:ASN:N	1:F:182:THR:HG23	2.11	0.61
1:G:154:MET:HB3	1:G:352:TRP:HB2	1.82	0.61
1:J:177:PRO:HG2	1:J:178:TYR:CD1	2.35	0.61
1:D:182:THR:HG21	1:D:294:MET:HE1	1.80	0.61
1:I:173:ILE:CD1	1:I:183:LYS:HE3	2.30	0.61
1:D:255:ARG:HH11	1:D:255:ARG:HG3	1.65	0.61
1:L:372:THR:HG22	1:L:373:LYS:HG3	1.83	0.61
1:H:177:PRO:HA	1:H:294:MET:CE	2.29	0.61
1:H:436:GLU:OE2	1:H:456:ARG:NH1	2.32	0.61
1:K:139:LEU:HD11	1:K:411:VAL:HG11	1.81	0.61
1:L:154:MET:HB3	1:L:352:TRP:HB2	1.83	0.61
1:A:154:MET:HE2	1:A:156:ILE:HD11	1.81	0.61
1:A:158:ASP:OD2	1:A:161:GLY:HA2	2.01	0.61
1:D:169:ARG:HG3	1:D:498:ARG:HH22	1.65	0.61
1:F:436:GLU:HG2	1:F:456:ARG:HD3	1.81	0.61
1:M:104:ARG:NH1	1:M:105:GLU:O	2.34	0.61
1:E:254:LEU:HD22	1:E:258:LEU:HG	1.83	0.61
1:J:437:ARG:HG3	1:J:437:ARG:HH11	1.64	0.61
1:D:290:GLU:HG2	1:D:325:LEU:CD2	2.29	0.61
1:G:243:PHE:O	1:G:247:THR:HB	2.01	0.61
1:D:141:ARG:HG2	1:D:141:ARG:HH11	1.66	0.61
1:D:184:GLY:HA3	1:D:297:GLY:HA3	1.83	0.61
1:I:154:MET:HB3	1:I:352:TRP:HB2	1.82	0.61
1:L:126:LEU:HD11	1:L:411:VAL:HG23	1.83	0.61
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:HD12	1:B:221:ARG:CD	2.31	0.60
1:G:97:GLY:O	1:G:101:ARG:HG3	1.99	0.60
1:J:169:ARG:NH2	1:J:171:LYS:NZ	2.49	0.60
1:B:137:SER:O	1:B:141:ARG:HB2	2.00	0.60
1:K:182:THR:HG21	1:K:294:MET:CE	2.31	0.60
1:K:357:GLU:OE2	1:K:386:GLN:HG3	2.00	0.60
1:H:254:LEU:HD12	1:H:281:ARG:HD3	1.82	0.60
1:L:497:ASN:HD22	1:L:497:ASN:H	1.50	0.60
1:B:344:PRO:O	1:B:349:ARG:NH2	2.33	0.60
1:F:357:GLU:HG3	2:F:2143:HOH:O	2.01	0.60
1:I:336:VAL:O	1:I:340:ILE:HG23	2.00	0.60
1:A:85:LYS:HE2	1:A:454:LEU:HG	1.83	0.60
1:E:124:ARG:HG3	1:E:124:ARG:HH11	1.66	0.60
1:F:463:MET:HB2	1:F:466:GLU:HG3	1.84	0.60
1:I:456:ARG:HD2	1:I:456:ARG:N	2.17	0.60
1:F:175:LEU:HD12	1:F:313:LEU:HD21	1.84	0.60
1:L:154:MET:CE	1:L:156:ILE:HD11	2.32	0.60
2:A:2130:HOH:O	1:G:417:ARG:HG2	2.00	0.60
1:E:380:ARG:HG3	1:E:380:ARG:HH11	1.66	0.60
1:E:438:ASP:OD1	1:E:454:LEU:HD12	2.02	0.60
1:F:124:ARG:HB3	1:F:408:ARG:HG3	1.83	0.60
1:G:110:VAL:HG11	1:G:143:LEU:HD23	1.82	0.60
1:G:190:GLU:OE1	1:G:302:ARG:HG3	2.01	0.60
1:E:426:MET:O	1:E:430:LEU:HD22	2.02	0.60
1:I:412:VAL:HG22	1:I:426:MET:CE	2.31	0.60
1:M:251:PHE:CZ	1:M:277:LEU:HD13	2.37	0.60
1:M:338:THR:O	1:M:341:LEU:HB2	2.02	0.60
1:B:324:ALA:HB2	2:D:2045:HOH:O	2.02	0.60
1:D:411:VAL:HG12	1:D:413:LEU:CD1	2.32	0.60
1:J:410:LEU:HD11	1:J:426:MET:HE1	1.84	0.60
1:H:154:MET:HB3	1:H:352:TRP:HB2	1.82	0.59
1:J:291:HIS:HE1	2:J:2074:HOH:O	1.85	0.59
1:A:421:LYS:HB3	2:A:2136:HOH:O	2.01	0.59
1:K:169:ARG:HG3	1:K:169:ARG:NH1	2.12	0.59
1:M:83:PRO:O	1:M:437:ARG:HD3	2.02	0.59
1:G:225:ARG:O	1:G:229:LYS:HB2	2.02	0.59
1:I:169:ARG:HH12	1:I:171:LYS:CG	2.15	0.59
1:J:139:LEU:HD11	1:J:411:VAL:HG11	1.84	0.59
1:M:417:ARG:NH2	1:M:469:ASN:OD1	2.36	0.59
1:H:94:VAL:CG1	1:H:95:SER:N	2.66	0.59
1:K:85:LYS:CD	1:K:454:LEU:HD21	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:86:ARG:HG2	1:K:86:ARG:HH11	1.67	0.59
1:K:134:THR:HG22	1:K:134:THR:O	2.03	0.59
1:K:154:MET:CE	1:K:156:ILE:HD11	2.29	0.59
1:K:230:LYS:HE2	1:K:257:PHE:O	2.02	0.59
1:B:202:LEU:HD12	1:B:221:ARG:HD3	1.84	0.59
1:D:498:ARG:C	1:D:499:GLN:HG2	2.23	0.59
1:H:243:PHE:O	1:H:247:THR:HB	2.03	0.59
1:B:351:LEU:HD12	1:B:379:LEU:HD23	1.84	0.59
1:B:440:TYR:O	1:D:453:ALA:HB1	2.03	0.59
1:D:410:LEU:HD11	1:D:426:MET:HE1	1.84	0.59
1:E:106:LYS:HG2	1:E:107:ALA:H	1.67	0.59
1:F:82:ALA:O	1:F:437:ARG:NH1	2.36	0.59
1:G:375:ARG:NH2	1:G:376:LYS:NZ	2.51	0.59
1:I:432:GLU:HG2	1:I:460:ARG:HD3	1.83	0.59
1:M:246:THR:O	1:M:281:ARG:HD2	2.02	0.59
1:D:98:LYS:O	1:D:102:MET:HG3	2.03	0.59
1:D:197:TRP:CE2	1:D:229:LYS:HG2	2.37	0.59
1:H:94:VAL:HG12	1:H:95:SER:O	2.03	0.59
1:A:160:ASN:HD21	1:A:319:GLU:CD	2.05	0.59
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.66	0.59
1:G:137:SER:O	1:G:141:ARG:HB2	2.02	0.59
1:H:426:MET:O	1:H:430:LEU:HD22	2.03	0.59
1:M:110:VAL:CG1	1:M:143:LEU:HD23	2.33	0.59
1:E:180:GLN:HB2	1:E:504:GLU:CB	2.30	0.58
1:I:177:PRO:HG2	1:I:178:TYR:CD1	2.38	0.58
1:K:182:THR:HG21	1:K:294:MET:HE2	1.84	0.58
1:F:162:ASP:HB3	2:F:2041:HOH:O	2.02	0.58
1:F:439:ARG:NH1	1:F:439:ARG:HB2	2.18	0.58
1:B:104:ARG:HD2	2:B:2009:HOH:O	2.01	0.58
1:G:413:LEU:HD12	1:G:475:ALA:CB	2.33	0.58
1:H:76:GLN:C	1:H:78:GLU:H	2.07	0.58
1:K:200:TYR:O	1:K:204:VAL:HG23	2.03	0.58
1:L:173:ILE:HD12	1:L:183:LYS:NZ	2.18	0.58
1:A:463:MET:HB2	1:A:466:GLU:HG3	1.85	0.58
1:D:255:ARG:HG3	1:D:255:ARG:NH1	2.17	0.58
1:H:251:PHE:HE2	1:H:255:ARG:HH12	1.51	0.58
1:H:331:ALA:O	1:H:335:VAL:HG23	2.02	0.58
1:M:182:THR:HG21	1:M:294:MET:CE	2.33	0.58
1:G:104:ARG:HG2	1:G:104:ARG:HH11	1.68	0.58
1:A:126:LEU:HD11	1:A:411:VAL:HG23	1.85	0.58
1:E:124:ARG:HB3	1:E:408:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:PRO:CB	1:G:428:LEU:HD22	2.33	0.58
1:K:329:ILE:O	1:K:333:VAL:HG23	2.02	0.58
1:F:357:GLU:OE2	1:F:386:GLN:HG3	2.04	0.58
1:G:223:LEU:HD23	1:G:284:LEU:HD22	1.85	0.58
1:L:357:GLU:HG3	2:L:2059:HOH:O	2.03	0.58
1:M:504:GLU:HG3	1:M:505:GLY:H	1.69	0.58
1:K:134:THR:CG2	1:K:413:LEU:HB3	2.34	0.58
1:M:493:LYS:HD3	1:M:495:PHE:CZ	2.39	0.58
1:F:338:THR:O	1:F:341:LEU:HB2	2.03	0.58
1:J:186:SER:H	1:J:189:ASN:ND2	2.02	0.58
1:F:96:GLY:O	1:F:100:LYS:HG3	2.04	0.58
1:H:479:PHE:O	1:M:417:ARG:NH1	2.36	0.58
1:I:410:LEU:HD11	1:I:426:MET:HE1	1.85	0.58
1:L:84:PHE:CG	1:L:435:VAL:HG11	2.38	0.58
1:H:436:GLU:HG2	1:H:456:ARG:HD3	1.85	0.57
1:K:169:ARG:CD	1:K:498:ARG:HH22	2.15	0.57
1:K:499:GLN:HG3	1:K:500:PRO:HD2	1.86	0.57
1:L:226:GLU:CG	1:L:261:THR:HB	2.33	0.57
1:A:455:GLU:HG2	1:A:457:VAL:HG23	1.86	0.57
1:A:494:GLN:HA	1:A:494:GLN:OE1	2.02	0.57
1:B:318:ARG:HG2	1:B:318:ARG:HH11	1.70	0.57
1:E:367:LEU:HD22	1:E:371:LEU:HG	1.86	0.57
1:G:159:PRO:HG3	1:G:317:TRP:CH2	2.39	0.57
1:B:410:LEU:HD11	1:B:426:MET:HE1	1.86	0.57
1:J:169:ARG:NH2	1:J:171:LYS:HZ3	2.02	0.57
1:B:106:LYS:HE3	1:B:106:LYS:N	2.19	0.57
1:K:104:ARG:HG2	1:K:104:ARG:HH11	1.69	0.57
1:L:466:GLU:OE2	1:M:89:ARG:HD2	2.05	0.57
1:M:182:THR:HG22	1:M:183:LYS:O	2.05	0.57
1:A:408:ARG:HD2	1:G:416:SER:HB2	1.86	0.57
1:F:473:LEU:HD11	1:F:492:ILE:HD11	1.86	0.57
1:I:281:ARG:NH2	1:J:265:SER:HB3	2.20	0.57
1:M:322:GLY:N	1:M:323:PRO:HD2	2.19	0.57
1:J:169:ARG:NH1	1:J:172:ASP:OD2	2.38	0.57
1:L:94:VAL:HG22	1:L:95:SER:H	1.69	0.57
1:M:156:ILE:HG13	1:M:354:PHE:HB2	1.87	0.57
1:A:306:GLU:O	1:A:308:PRO:HD3	2.05	0.57
1:I:338:THR:O	1:I:341:LEU:HB2	2.04	0.57
1:B:154:MET:HE2	1:B:156:ILE:HD11	1.87	0.57
1:E:313:LEU:HD23	1:E:314:PHE:N	2.20	0.57
1:M:331:ALA:O	1:M:335:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:SER:HB2	1:F:408:ARG:HD2	1.87	0.56
1:E:255:ARG:HG3	1:E:255:ARG:NH1	2.20	0.56
1:G:94:VAL:CG1	1:G:95:SER:N	2.68	0.56
1:A:176:ASN:H	1:A:182:THR:HG23	1.69	0.56
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.69	0.56
2:B:2087:HOH:O	1:D:198:GLN:HG2	2.04	0.56
1:D:345:GLU:OE2	1:D:376:LYS:HD2	2.04	0.56
1:E:184:GLY:HA3	1:E:297:GLY:HA3	1.87	0.56
1:E:399:GLU:HG3	2:E:2105:HOH:O	2.04	0.56
1:I:184:GLY:HA3	1:I:297:GLY:HA3	1.87	0.56
1:L:466:GLU:CD	1:M:89:ARG:HD2	2.25	0.56
1:L:488:VAL:HG13	1:L:489:PRO:HD2	1.86	0.56
1:M:287:LYS:HE3	1:M:362:GLU:OE2	2.05	0.56
1:D:463:MET:HB2	1:D:466:GLU:HG3	1.87	0.56
1:G:200:TYR:O	1:G:204:VAL:HG23	2.05	0.56
1:J:375:ARG:NH2	1:J:376:LYS:HE2	2.19	0.56
1:K:414:GLY:HA2	1:K:467:ILE:CG2	2.36	0.56
1:G:85:LYS:HE3	1:G:86:ARG:NH2	2.20	0.56
1:L:499:GLN:HG3	1:L:500:PRO:HD2	1.86	0.56
1:A:336:VAL:O	1:A:340:ILE:HG23	2.04	0.56
1:J:413:LEU:HD12	1:J:475:ALA:HB2	1.87	0.56
1:L:329:ILE:O	1:L:333:VAL:HG23	2.05	0.56
1:A:326:ARG:HD3	2:A:2101:HOH:O	2.06	0.56
1:I:96:GLY:O	1:I:100:LYS:HG3	2.05	0.56
1:L:255:ARG:HH11	1:L:277:LEU:CD1	2.17	0.56
1:M:141:ARG:HH11	1:M:141:ARG:HG2	1.70	0.56
1:A:85:LYS:CE	1:A:454:LEU:HG	2.36	0.56
1:B:470:LEU:HD21	1:B:487:LYS:HE3	1.87	0.56
1:D:182:THR:HG22	1:D:183:LYS:N	2.21	0.56
1:F:372:THR:CG2	1:F:373:LYS:HG3	2.25	0.56
1:B:94:VAL:HG22	1:B:98:LYS:HB3	1.88	0.56
1:B:290:GLU:HG2	1:B:325:LEU:CD2	2.30	0.56
1:D:126:LEU:HD11	1:D:411:VAL:HG23	1.86	0.56
1:H:432:GLU:HG2	1:H:460:ARG:HD3	1.87	0.56
1:K:326:ARG:N	1:K:327:PRO:HD2	2.20	0.56
1:L:221:ARG:O	1:L:225:ARG:HG2	2.06	0.56
1:F:94:VAL:HG22	1:F:98:LYS:HD3	1.88	0.56
1:G:177:PRO:HB3	1:G:294:MET:HG2	1.88	0.56
1:H:254:LEU:CD1	1:H:281:ARG:HD3	2.36	0.56
1:J:97:GLY:O	1:J:101:ARG:HG3	2.06	0.56
1:M:124:ARG:NH2	1:M:375:ARG:NH1	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLU:OE2	1:E:89:ARG:HD2	2.06	0.55
1:E:233:LEU:C	1:E:235:GLY:H	2.08	0.55
1:J:413:LEU:HD12	1:J:475:ALA:CB	2.35	0.55
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.21	0.55
1:G:94:VAL:HG12	1:G:98:LYS:HB3	1.88	0.55
1:G:410:LEU:HD21	1:G:426:MET:HE3	1.89	0.55
1:J:243:PHE:O	1:J:247:THR:HB	2.07	0.55
1:K:77:GLY:O	1:K:78:GLU:HB2	2.06	0.55
1:K:318:ARG:HB2	1:K:321:MET:HE2	1.87	0.55
1:F:217:ALA:O	1:F:221:ARG:HG3	2.06	0.55
1:F:346:GLU:OE1	1:F:346:GLU:HA	2.06	0.55
1:G:436:GLU:OE2	1:G:456:ARG:NH1	2.39	0.55
1:J:177:PRO:CA	1:J:294:MET:HE2	2.36	0.55
1:J:254:LEU:HD12	1:J:281:ARG:HH11	1.72	0.55
1:K:177:PRO:HG2	1:K:178:TYR:CD1	2.42	0.55
1:L:82:ALA:O	1:L:437:ARG:NH1	2.39	0.55
1:H:190:GLU:OE1	1:H:302:ARG:HG3	2.07	0.55
1:K:304:TRP:CZ2	1:K:313:LEU:HB2	2.41	0.55
1:M:463:MET:HB2	1:M:466:GLU:HG3	1.87	0.55
1:A:176:ASN:H	1:A:182:THR:CG2	2.19	0.55
1:H:160:ASN:HD21	1:H:319:GLU:CD	2.09	0.55
1:H:224:LEU:HD12	1:H:242:LEU:HD21	1.89	0.55
1:I:177:PRO:HB3	1:I:294:MET:HG2	1.89	0.55
1:B:331:ALA:O	1:B:335:VAL:HG23	2.07	0.55
1:I:240:ARG:HH11	1:I:240:ARG:HG3	1.72	0.55
1:K:463:MET:HB2	1:K:466:GLU:HG3	1.89	0.55
1:L:173:ILE:HG23	1:L:183:LYS:CG	2.36	0.55
1:M:177:PRO:HB3	1:M:294:MET:HG2	1.88	0.55
1:A:236:THR:CG2	1:A:241:GLU:HG3	2.36	0.55
1:F:324:ALA:HB2	2:G:2049:HOH:O	2.06	0.55
1:L:83:PRO:O	1:L:437:ARG:HD3	2.07	0.55
1:A:217:ALA:O	1:A:221:ARG:HG3	2.07	0.55
1:F:83:PRO:O	1:F:437:ARG:HD3	2.07	0.55
1:H:176:ASN:H	1:H:182:THR:HG23	1.72	0.55
1:I:182:THR:HG22	1:I:183:LYS:N	2.22	0.55
1:K:413:LEU:HD12	1:K:475:ALA:CB	2.36	0.55
1:L:177:PRO:HB3	1:L:294:MET:HG2	1.88	0.55
1:L:198:GLN:HE21	1:L:202:LEU:HD22	1.72	0.55
1:M:124:ARG:NH2	1:M:375:ARG:HG3	2.20	0.55
1:F:154:MET:CE	1:F:156:ILE:HD11	2.36	0.55
1:G:105:GLU:HB2	1:G:109:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:LYS:HE2	1:H:497:ASN:HD21	1.72	0.55
1:K:222:LEU:HA	1:K:225:ARG:NH1	2.22	0.55
1:K:226:GLU:CG	1:K:261:THR:HB	2.33	0.55
1:K:384:GLY:O	1:K:385:LEU:HD12	2.07	0.55
1:B:84:PHE:CD2	1:B:435:VAL:HG21	2.42	0.55
1:B:217:ALA:O	1:B:221:ARG:HG3	2.07	0.55
1:H:83:PRO:O	1:H:437:ARG:HD3	2.07	0.55
1:I:157:VAL:HG12	1:I:317:TRP:CH2	2.41	0.55
1:I:291:HIS:HE1	2:I:2041:HOH:O	1.89	0.55
1:B:180:GLN:NE2	1:B:504:GLU:HB2	2.22	0.54
1:B:291:HIS:HE1	2:B:2046:HOH:O	1.90	0.54
1:J:254:LEU:HD12	1:J:281:ARG:NH1	2.23	0.54
1:F:156:ILE:HG22	1:F:158:ASP:HB2	1.90	0.54
1:B:254:LEU:HD12	1:B:281:ARG:NH1	2.22	0.54
1:D:412:VAL:HG22	1:D:426:MET:HE2	1.88	0.54
1:J:254:LEU:CD1	1:J:281:ARG:HD3	2.37	0.54
1:K:78:GLU:HG3	1:K:95:SER:N	2.22	0.54
1:L:154:MET:HE3	1:L:156:ILE:HD11	1.88	0.54
1:L:177:PRO:HG2	1:L:178:TYR:HD1	1.73	0.54
1:B:154:MET:CE	1:B:156:ILE:HD11	2.37	0.54
1:F:233:LEU:C	1:F:235:GLY:H	2.10	0.54
1:G:412:VAL:HG22	1:G:426:MET:HE3	1.89	0.54
1:H:84:PHE:CB	1:H:435:VAL:HG11	2.37	0.54
1:J:247:THR:HG22	1:J:248:ILE:HD13	1.88	0.54
1:J:454:LEU:HD23	1:J:455:GLU:N	2.23	0.54
1:J:492:ILE:HD13	1:J:492:ILE:N	2.00	0.54
1:A:139:LEU:C	1:A:139:LEU:HD23	2.28	0.54
1:G:72:ASN:N	2:G:2001:HOH:O	2.41	0.54
1:B:73:SER:O	1:B:76:GLN:NE2	2.40	0.54
1:D:355:ILE:O	1:D:356:ASP:C	2.46	0.54
1:E:350:ARG:HG2	1:E:380:ARG:CZ	2.38	0.54
1:H:281:ARG:HH22	1:I:265:SER:HB3	1.72	0.54
1:H:411:VAL:HG12	1:H:413:LEU:CD1	2.37	0.54
1:L:180:GLN:HB2	1:L:504:GLU:CG	2.36	0.54
1:L:470:LEU:HD23	1:L:471:PRO:HD2	1.88	0.54
1:B:200:TYR:O	1:B:204:VAL:HG23	2.07	0.54
1:D:231:LEU:HD23	1:D:234:ILE:HD11	1.90	0.54
1:D:236:THR:CG2	1:D:241:GLU:HG3	2.38	0.54
1:F:252:ASP:HB2	2:F:2106:HOH:O	2.08	0.54
1:H:368:ALA:HB3	2:H:2091:HOH:O	2.08	0.54
1:H:454:LEU:O	1:M:439:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:H	1:B:106:LYS:CD	2.20	0.54
1:B:180:GLN:HE21	1:B:504:GLU:CB	2.19	0.54
1:G:96:GLY:O	1:G:100:LYS:HG3	2.08	0.54
1:G:126:LEU:HD11	1:G:411:VAL:CG2	2.37	0.54
1:K:184:GLY:HA3	1:K:297:GLY:HA3	1.90	0.54
1:L:290:GLU:HG2	1:L:325:LEU:CD2	2.37	0.54
1:L:338:THR:O	1:L:341:LEU:HB2	2.08	0.54
1:A:291:HIS:HE1	2:A:2105:HOH:O	1.90	0.54
1:F:327:PRO:HG2	2:F:2136:HOH:O	2.08	0.54
1:H:94:VAL:CG1	1:H:98:LYS:HB3	2.37	0.54
1:A:331:ALA:O	1:A:335:VAL:HG23	2.07	0.54
1:E:410:LEU:HD11	1:E:426:MET:HE1	1.90	0.54
1:E:417:ARG:NH1	1:F:479:PHE:O	2.41	0.54
1:G:291:HIS:HE1	2:G:2117:HOH:O	1.91	0.54
1:J:440:TYR:HE2	1:K:454:LEU:HD12	1.72	0.54
1:E:281:ARG:NH2	1:F:265:SER:HB3	2.23	0.53
1:J:145:TYR:CE2	1:J:149:LEU:HD11	2.44	0.53
1:E:86:ARG:O	1:E:435:VAL:HG22	2.08	0.53
1:E:177:PRO:CA	1:E:294:MET:HE2	2.39	0.53
1:G:226:GLU:HG3	1:G:261:THR:CB	2.38	0.53
1:G:463:MET:HB2	1:G:466:GLU:HG3	1.89	0.53
1:J:177:PRO:HA	1:J:294:MET:HE2	1.90	0.53
1:M:177:PRO:HA	1:M:294:MET:CE	2.39	0.53
1:I:230:LYS:O	1:I:234:ILE:HG23	2.08	0.53
1:J:166:LYS:HD3	1:J:495:PHE:HB2	1.90	0.53
1:L:173:ILE:HD12	1:L:183:LYS:HZ2	1.73	0.53
1:B:127:LEU:HD11	1:B:385:LEU:HD22	1.91	0.53
1:B:328:LEU:HD13	1:B:332:TRP:CH2	2.44	0.53
1:D:177:PRO:HB3	1:D:294:MET:HG2	1.90	0.53
1:D:503:VAL:O	1:D:504:GLU:HB3	2.09	0.53
1:E:94:VAL:HG22	1:E:98:LYS:HD3	1.90	0.53
1:G:331:ALA:O	1:G:335:VAL:HG23	2.09	0.53
1:F:154:MET:HB3	1:F:352:TRP:HB2	1.91	0.53
1:F:384:GLY:O	1:F:385:LEU:HD13	2.08	0.53
1:G:142:GLU:O	1:G:146:THR:HG23	2.08	0.53
1:K:173:ILE:HG12	1:K:304:TRP:HE1	1.74	0.53
1:L:198:GLN:HE21	1:L:202:LEU:CD2	2.21	0.53
1:D:291:HIS:HD2	2:D:2037:HOH:O	1.91	0.53
1:E:170:ASP:HB3	2:E:2029:HOH:O	2.07	0.53
1:G:338:THR:O	1:G:341:LEU:HB2	2.09	0.53
1:J:145:TYR:CZ	1:J:149:LEU:HD11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:PRO:HG2	1:J:178:TYR:HD1	1.71	0.53
1:M:181:ARG:NH1	1:M:500:PRO:HG2	2.24	0.53
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.74	0.53
1:D:196:ASP:HA	1:D:199:ARG:HB3	1.91	0.53
1:D:233:LEU:C	1:D:235:GLY:H	2.12	0.53
1:F:113:ALA:HA	1:F:490:LEU:HD23	1.91	0.53
1:H:96:GLY:O	1:H:100:LYS:HG3	2.08	0.53
1:H:466:GLU:OE2	1:I:89:ARG:HD2	2.09	0.53
1:I:466:GLU:CD	1:J:89:ARG:HD2	2.30	0.53
1:K:158:ASP:OD2	1:K:161:GLY:HA2	2.09	0.53
1:K:173:ILE:CG2	1:K:183:LYS:HG3	2.39	0.53
1:K:336:VAL:O	1:K:340:ILE:HG23	2.08	0.53
1:D:154:MET:HE2	1:D:156:ILE:HD11	1.89	0.53
1:F:224:LEU:HD12	1:F:242:LEU:HD21	1.91	0.53
1:I:259:GLU:HA	1:I:264:GLU:CG	2.39	0.53
1:K:358:LEU:HD11	1:K:367:LEU:HD11	1.90	0.53
1:E:281:ARG:HH21	1:F:265:SER:HB3	1.73	0.52
1:K:379:LEU:HD23	1:K:380:ARG:H	1.74	0.52
1:L:129:ASN:HB3	1:L:426:MET:CE	2.40	0.52
1:D:173:ILE:HD12	1:D:183:LYS:HE2	1.90	0.52
1:I:88:LEU:HD21	1:I:436:GLU:HG3	1.91	0.52
1:K:152:ASP:OD1	1:K:350:ARG:NE	2.40	0.52
1:K:173:ILE:HG13	1:K:304:TRP:NE1	2.24	0.52
1:K:202:LEU:HD12	1:K:221:ARG:HD3	1.90	0.52
1:L:243:PHE:O	1:L:247:THR:HB	2.08	0.52
1:M:236:THR:HG21	1:M:241:GLU:HG3	1.91	0.52
1:B:110:VAL:CG1	1:B:143:LEU:HD23	2.39	0.52
1:F:291:HIS:HD2	2:F:2061:HOH:O	1.91	0.52
1:G:367:LEU:CD1	1:G:403:LEU:HD11	2.39	0.52
1:I:437:ARG:HD3	1:J:456:ARG:CZ	2.40	0.52
1:M:155:VAL:C	1:M:156:ILE:HD12	2.30	0.52
1:M:200:TYR:O	1:M:204:VAL:HG23	2.10	0.52
1:G:159:PRO:HG3	1:G:317:TRP:CZ2	2.45	0.52
1:I:498:ARG:O	1:I:499:GLN:HG3	2.09	0.52
1:K:85:LYS:HG3	1:K:436:GLU:O	2.10	0.52
1:K:414:GLY:HA2	1:K:467:ILE:HG22	1.91	0.52
1:L:452:ARG:HH11	1:L:452:ARG:HG2	1.73	0.52
1:A:345:GLU:OE2	1:A:376:LYS:HD2	2.09	0.52
1:G:247:THR:HG22	1:G:248:ILE:HD13	1.92	0.52
1:J:281:ARG:NH2	1:K:265:SER:HB3	2.24	0.52
1:K:145:TYR:CE1	1:K:149:LEU:HD21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:ILE:HB	1:M:461:VAL:HG11	1.90	0.52
1:M:176:ASN:H	1:M:182:THR:HG23	1.74	0.52
1:D:78:GLU:HA	2:D:2001:HOH:O	2.08	0.52
1:G:145:TYR:CZ	1:G:149:LEU:HD11	2.44	0.52
1:G:160:ASN:HD21	1:G:319:GLU:HG3	1.75	0.52
1:H:410:LEU:HD21	1:H:426:MET:HE3	1.90	0.52
1:J:466:GLU:OE2	1:K:89:ARG:HD2	2.09	0.52
1:D:358:LEU:HB3	1:D:385:LEU:CD1	2.40	0.52
1:F:413:LEU:N	1:F:413:LEU:HD12	2.25	0.52
1:G:92:ARG:HB2	1:G:484:PRO:HB3	1.91	0.52
1:G:94:VAL:HG12	1:G:95:SER:H	1.75	0.52
1:H:318:ARG:HE	1:H:321:MET:HE3	1.74	0.52
1:K:190:GLU:OE1	1:K:302:ARG:HG3	2.09	0.52
1:K:353:LEU:HD22	1:K:355:ILE:HG13	1.91	0.52
1:A:85:LYS:NZ	1:A:454:LEU:HG	2.24	0.52
1:A:236:THR:HG22	1:A:241:GLU:HG3	1.92	0.52
1:A:386:GLN:HB2	1:A:390:GLN:OE1	2.10	0.52
1:F:94:VAL:CG2	1:F:98:LYS:HD3	2.40	0.52
1:F:463:MET:HE3	1:G:458:ARG:HD3	1.92	0.52
1:K:226:GLU:OE2	1:K:262:LEU:HB2	2.10	0.52
1:K:466:GLU:OE2	1:L:89:ARG:HD2	2.10	0.52
1:I:352:TRP:CE2	1:I:380:ARG:HD3	2.45	0.52
1:K:247:THR:HG22	1:K:248:ILE:HD13	1.91	0.52
1:L:471:PRO:HG2	1:L:474:THR:OG1	2.10	0.52
1:A:281:ARG:NH2	1:B:265:SER:HB3	2.25	0.52
1:B:433:HIS:HD2	1:B:433:HIS:O	1.93	0.52
1:G:94:VAL:HG13	1:G:98:LYS:HD3	1.92	0.52
1:K:196:ASP:O	1:K:200:TYR:HD2	1.93	0.52
1:K:331:ALA:O	1:K:335:VAL:HG23	2.10	0.52
1:A:175:LEU:HA	1:A:182:THR:HG23	1.91	0.51
1:A:177:PRO:HB3	1:A:294:MET:HG2	1.91	0.51
1:D:412:VAL:HG22	1:D:426:MET:HE3	1.90	0.51
1:K:173:ILE:CG1	1:K:304:TRP:HE1	2.23	0.51
1:M:126:LEU:HD11	1:M:411:VAL:CG2	2.39	0.51
1:A:243:PHE:O	1:A:247:THR:HB	2.10	0.51
1:F:344:PRO:O	1:F:349:ARG:NH2	2.43	0.51
1:F:439:ARG:HB2	1:F:439:ARG:CZ	2.39	0.51
1:G:340:ILE:HD13	1:G:379:LEU:CG	2.38	0.51
1:H:283:VAL:O	1:H:287:LYS:HG2	2.10	0.51
1:H:440:TYR:HA	1:H:452:ARG:CB	2.39	0.51
1:K:133:GLY:O	1:K:472:ASP:OD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:212:GLU:O	1:L:215:GLU:HB3	2.10	0.51
1:M:177:PRO:CA	1:M:294:MET:HE2	2.40	0.51
1:M:182:THR:HG21	1:M:294:MET:HE1	1.91	0.51
1:M:246:THR:HB	1:M:284:LEU:HD23	1.92	0.51
1:M:367:LEU:HD13	1:M:403:LEU:HD11	1.92	0.51
1:A:411:VAL:HG12	1:A:413:LEU:CD1	2.41	0.51
1:F:411:VAL:HG12	1:F:413:LEU:CD1	2.40	0.51
1:H:82:ALA:O	1:H:437:ARG:NH1	2.44	0.51
1:J:156:ILE:HG22	1:J:158:ASP:HB2	1.92	0.51
1:J:254:LEU:HD12	1:J:281:ARG:HD3	1.93	0.51
1:K:184:GLY:HA2	1:K:295:PRO:O	2.10	0.51
1:L:96:GLY:HA3	1:L:488:VAL:HG22	1.92	0.51
1:M:385:LEU:HD21	1:M:391:LEU:HD22	1.91	0.51
1:E:87:PHE:HA	1:E:435:VAL:CG2	2.41	0.51
1:J:126:LEU:HD11	1:J:411:VAL:CG2	2.38	0.51
1:L:380:ARG:HH11	1:L:380:ARG:HG3	1.74	0.51
1:M:358:LEU:HD11	1:M:367:LEU:HD11	1.91	0.51
1:H:439:ARG:HG2	1:H:453:ALA:HB3	1.93	0.51
1:I:222:LEU:HA	1:I:225:ARG:NH1	2.26	0.51
1:I:491:GLU:OE2	1:I:493:LYS:HD3	2.11	0.51
1:J:84:PHE:HB3	1:J:437:ARG:HH12	1.76	0.51
1:K:159:PRO:HG3	1:K:317:TRP:CH2	2.46	0.51
1:L:437:ARG:HD2	1:M:456:ARG:NH2	2.26	0.51
1:H:126:LEU:HD11	1:H:411:VAL:HG23	1.92	0.51
1:J:158:ASP:OD2	1:J:161:GLY:HA2	2.10	0.51
1:J:412:VAL:HG22	1:J:426:MET:HE3	1.90	0.51
1:J:440:TYR:CE2	1:K:454:LEU:HD12	2.45	0.51
1:A:412:VAL:HG22	1:A:426:MET:HE2	1.91	0.51
1:E:503:VAL:O	1:E:504:GLU:CB	2.58	0.51
1:K:433:HIS:C	1:K:433:HIS:CD2	2.84	0.51
1:D:494:GLN:HA	1:D:494:GLN:OE1	2.11	0.51
1:I:294:MET:SD	1:I:295:PRO:HD2	2.51	0.51
1:K:433:HIS:O	1:K:433:HIS:CD2	2.62	0.51
1:K:455:GLU:HG3	1:K:455:GLU:O	2.10	0.51
1:L:129:ASN:HB3	1:L:426:MET:HE1	1.92	0.51
1:L:159:PRO:HG3	1:L:317:TRP:CH2	2.45	0.51
1:B:433:HIS:C	1:B:433:HIS:CD2	2.84	0.51
1:D:100:LYS:HG2	1:D:115:VAL:HA	1.93	0.51
1:D:277:LEU:HD22	1:D:277:LEU:O	2.10	0.51
1:D:291:HIS:HE1	2:D:2049:HOH:O	1.94	0.51
1:D:302:ARG:O	1:D:306:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:SER:HB3	2:E:2075:HOH:O	2.10	0.51
1:I:86:ARG:HB2	1:I:86:ARG:CZ	2.40	0.51
1:K:84:PHE:HA	1:K:437:ARG:HG3	1.93	0.51
1:K:497:ASN:N	1:K:497:ASN:ND2	2.55	0.51
1:L:256:GLY:O	1:L:259:GLU:HB2	2.11	0.51
1:H:139:LEU:HD23	1:H:139:LEU:C	2.30	0.51
1:J:241:GLU:HA	1:J:241:GLU:OE1	2.10	0.51
1:M:313:LEU:HD23	1:M:314:PHE:N	2.26	0.51
1:M:482:ASN:C	1:M:482:ASN:HD22	2.14	0.51
1:F:466:GLU:OE2	1:G:89:ARG:HD2	2.11	0.50
1:G:432:GLU:OE1	1:G:458:ARG:HD2	2.11	0.50
1:M:158:ASP:OD2	1:M:161:GLY:HA2	2.11	0.50
1:A:84:PHE:HA	1:A:437:ARG:HG3	1.93	0.50
1:B:247:THR:HG21	2:D:2064:HOH:O	2.11	0.50
1:D:154:MET:HB3	1:D:352:TRP:HB2	1.93	0.50
1:E:124:ARG:HB3	1:E:408:ARG:CG	2.41	0.50
1:F:184:GLY:HA3	1:F:297:GLY:HA3	1.92	0.50
1:J:87:PHE:HA	1:J:435:VAL:HG22	1.93	0.50
1:J:175:LEU:HD12	1:J:313:LEU:HD21	1.93	0.50
1:J:345:GLU:OE2	1:J:376:LYS:HD2	2.12	0.50
1:L:177:PRO:HG2	1:L:178:TYR:CD1	2.46	0.50
1:D:328:LEU:HD13	1:D:332:TRP:CH2	2.46	0.50
1:I:134:THR:CG2	1:I:413:LEU:O	2.55	0.50
1:I:483:ARG:NH1	2:I:2111:HOH:O	2.44	0.50
1:L:226:GLU:HG3	1:L:261:THR:CB	2.35	0.50
1:B:413:LEU:CD1	1:B:475:ALA:HB2	2.40	0.50
1:F:473:LEU:HA	1:F:490:LEU:HD12	1.93	0.50
1:H:118:PRO:HB3	1:H:483:ARG:NH1	2.26	0.50
1:L:318:ARG:HD2	1:L:502:PHE:CE2	2.46	0.50
1:L:439:ARG:NH2	1:M:456:ARG:H	2.09	0.50
1:M:110:VAL:HG11	1:M:143:LEU:CD2	2.39	0.50
1:A:504:GLU:HG3	1:A:506:THR:H	1.76	0.50
1:F:182:THR:HG22	1:F:183:LYS:H	1.77	0.50
1:H:221:ARG:HD2	2:H:2057:HOH:O	2.11	0.50
1:I:313:LEU:HD23	1:I:314:PHE:N	2.27	0.50
1:I:414:GLY:HA2	1:I:467:ILE:HG22	1.93	0.50
1:J:291:HIS:HD2	2:J:2027:HOH:O	1.93	0.50
1:K:255:ARG:NH1	1:K:267:PHE:O	2.34	0.50
1:M:127:LEU:HD11	1:M:385:LEU:HD22	1.93	0.50
1:A:184:GLY:HA3	1:A:297:GLY:HA3	1.92	0.50
1:B:322:GLY:N	1:B:323:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ASN:ND2	1:G:319:GLU:HG3	2.27	0.50
1:I:145:TYR:CE2	1:I:149:LEU:HD11	2.47	0.50
1:I:488:VAL:HG13	1:I:489:PRO:HD2	1.94	0.50
1:L:173:ILE:HG23	1:L:183:LYS:HG2	1.93	0.50
1:L:503:VAL:O	1:L:504:GLU:CB	2.60	0.50
1:M:217:ALA:O	1:M:221:ARG:HG3	2.12	0.50
1:D:164:LEU:HD11	1:D:174:ILE:HD11	1.93	0.50
1:D:352:TRP:CE2	1:D:380:ARG:HD3	2.46	0.50
1:F:441:SER:O	1:F:450:THR:HG23	2.12	0.50
1:J:112:VAL:HA	2:J:2009:HOH:O	2.12	0.50
1:K:318:ARG:HD2	1:K:502:PHE:CE2	2.46	0.50
1:L:84:PHE:CB	1:L:435:VAL:HG11	2.41	0.50
1:M:488:VAL:HG13	1:M:489:PRO:HD2	1.93	0.50
1:D:144:ALA:O	1:D:148:LEU:HG	2.12	0.50
1:E:411:VAL:HG12	1:E:413:LEU:HD13	1.92	0.50
1:G:182:THR:HG22	1:G:183:LYS:N	2.26	0.50
1:I:291:HIS:HD2	2:I:2031:HOH:O	1.93	0.50
1:K:436:GLU:HG2	1:K:454:LEU:CD2	2.28	0.50
1:K:456:ARG:HD2	1:K:456:ARG:N	2.26	0.50
1:L:196:ASP:O	1:L:200:TYR:HD2	1.95	0.50
1:L:362:GLU:OE2	2:L:2061:HOH:O	2.19	0.50
1:D:182:THR:HG22	1:D:183:LYS:H	1.75	0.50
1:E:498:ARG:O	1:E:499:GLN:HG2	2.11	0.50
1:F:224:LEU:CD1	1:F:242:LEU:HD21	2.42	0.50
1:H:254:LEU:O	1:H:258:LEU:HG	2.12	0.50
1:H:367:LEU:HD22	1:H:371:LEU:HG	1.94	0.50
1:I:134:THR:HG22	1:I:134:THR:O	2.11	0.50
1:J:113:ALA:O	1:J:488:VAL:HG11	2.12	0.50
1:J:350:ARG:HG2	1:J:380:ARG:CZ	2.41	0.50
1:J:399:GLU:HG3	2:J:2085:HOH:O	2.11	0.50
1:A:247:THR:HG22	1:A:248:ILE:HD13	1.93	0.49
1:B:326:ARG:HD2	1:B:360:SER:O	2.11	0.49
1:F:177:PRO:HB3	1:F:294:MET:HG2	1.94	0.49
1:L:137:SER:O	1:L:141:ARG:HB2	2.12	0.49
1:F:160:ASN:ND2	1:F:319:GLU:HG3	2.24	0.49
1:I:119:ARG:HD3	1:I:122:GLU:OE2	2.13	0.49
1:I:329:ILE:O	1:I:333:VAL:HG23	2.12	0.49
1:I:452:ARG:HG3	1:I:452:ARG:O	2.13	0.49
1:J:483:ARG:HH11	1:J:483:ARG:HG2	1.76	0.49
1:K:488:VAL:HG13	1:K:489:PRO:HD2	1.94	0.49
1:L:87:PHE:HA	1:L:435:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PRO:HG3	1:D:317:TRP:CH2	2.47	0.49
1:E:357:GLU:HG3	2:E:2093:HOH:O	2.12	0.49
1:H:414:GLY:HA2	1:H:467:ILE:HG23	1.94	0.49
1:K:230:LYS:HD3	1:K:257:PHE:CZ	2.47	0.49
1:B:141:ARG:HH11	1:B:141:ARG:CG	2.15	0.49
1:H:175:LEU:HG	1:H:313:LEU:HD21	1.93	0.49
1:L:198:GLN:NE2	1:L:202:LEU:HD22	2.28	0.49
1:L:279:SER:O	1:L:283:VAL:HG23	2.12	0.49
1:D:436:GLU:HG2	1:D:454:LEU:CD2	2.42	0.49
1:G:94:VAL:CG1	1:G:95:SER:H	2.26	0.49
1:J:98:LYS:O	1:J:102:MET:HG3	2.12	0.49
1:L:306:GLU:O	1:L:308:PRO:HD3	2.12	0.49
1:M:504:GLU:CG	1:M:505:GLY:N	2.73	0.49
1:D:85:LYS:HE2	1:D:454:LEU:HD21	1.95	0.49
1:D:379:LEU:HD22	1:D:380:ARG:N	2.28	0.49
1:K:294:MET:HG3	1:K:328:LEU:HD11	1.95	0.49
1:M:93:ILE:HB	1:M:461:VAL:CG1	2.42	0.49
1:A:290:GLU:HG2	1:A:325:LEU:CD2	2.34	0.49
1:E:325:LEU:HA	2:E:2086:HOH:O	2.13	0.49
1:G:85:LYS:HD3	1:G:454:LEU:HD21	1.95	0.49
1:H:182:THR:HG22	1:H:183:LYS:N	2.26	0.49
1:H:493:LYS:HD3	1:H:495:PHE:CZ	2.47	0.49
1:I:433:HIS:HD2	1:I:433:HIS:O	1.95	0.49
1:J:322:GLY:N	1:J:323:PRO:HD2	2.27	0.49
1:M:184:GLY:HA2	1:M:295:PRO:O	2.13	0.49
1:D:246:THR:HB	1:D:284:LEU:HD23	1.95	0.49
1:E:287:LYS:HE3	1:E:362:GLU:OE2	2.13	0.49
1:E:413:LEU:HD12	1:E:475:ALA:HB2	1.94	0.49
1:G:224:LEU:CD1	1:G:242:LEU:HD21	2.43	0.49
1:K:304:TRP:CH2	1:K:313:LEU:HB2	2.46	0.49
1:K:379:LEU:HD23	1:K:380:ARG:N	2.26	0.49
1:M:176:ASN:O	1:M:182:THR:OG1	2.23	0.49
1:A:436:GLU:CB	1:A:454:LEU:HD21	2.43	0.49
1:B:226:GLU:CG	1:B:261:THR:HB	2.34	0.49
1:D:324:ALA:HB2	2:E:2039:HOH:O	2.13	0.49
1:E:470:LEU:HD23	1:E:471:PRO:HD2	1.95	0.49
1:I:233:LEU:C	1:I:235:GLY:H	2.16	0.49
1:I:249:ALA:O	1:I:281:ARG:NH2	2.35	0.49
1:K:129:ASN:HB3	1:K:426:MET:CE	2.42	0.49
1:K:129:ASN:CB	1:K:426:MET:HE1	2.40	0.49
1:B:438:ASP:HB3	1:B:440:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:357:GLU:HG2	1:G:386:GLN:NE2	2.28	0.49
1:H:224:LEU:CD1	1:H:242:LEU:HD21	2.43	0.49
1:H:453:ALA:HA	1:M:441:SER:HA	1.95	0.49
1:J:177:PRO:N	1:J:294:MET:HE2	2.28	0.49
1:K:417:ARG:NH2	1:K:469:ASN:HD21	2.10	0.49
1:M:236:THR:O	1:M:236:THR:HG22	2.13	0.49
1:M:294:MET:HE1	1:M:295:PRO:HD2	1.93	0.49
1:E:353:LEU:HB2	1:E:379:LEU:HD21	1.95	0.48
1:K:169:ARG:NH1	1:K:169:ARG:CG	2.76	0.48
1:L:200:TYR:O	1:L:204:VAL:HG23	2.13	0.48
1:K:246:THR:HB	1:K:284:LEU:HD23	1.94	0.48
1:L:227:THR:CG2	1:L:242:LEU:HD12	2.43	0.48
1:E:433:HIS:HD2	1:E:433:HIS:O	1.96	0.48
1:J:94:VAL:HG13	1:J:95:SER:N	2.28	0.48
1:K:364:LEU:HB2	1:K:367:LEU:HB2	1.95	0.48
1:L:113:ALA:HA	1:L:490:LEU:HD23	1.93	0.48
1:L:180:GLN:HB2	1:L:504:GLU:CB	2.41	0.48
1:A:420:PRO:HB2	1:B:428:LEU:HD13	1.95	0.48
1:D:331:ALA:O	1:D:335:VAL:HG23	2.12	0.48
1:F:124:ARG:HB3	1:F:408:ARG:CG	2.43	0.48
1:I:104:ARG:HB2	1:I:104:ARG:CZ	2.43	0.48
1:K:84:PHE:CG	1:K:435:VAL:CG2	2.94	0.48
1:K:173:ILE:HD12	1:K:183:LYS:CE	2.35	0.48
1:L:452:ARG:HG2	1:L:452:ARG:NH1	2.28	0.48
1:A:322:GLY:N	1:A:323:PRO:HD2	2.28	0.48
1:D:338:THR:O	1:D:341:LEU:HB2	2.13	0.48
1:H:246:THR:HB	1:H:284:LEU:HD23	1.95	0.48
1:H:439:ARG:NE	1:H:455:GLU:HB3	2.29	0.48
1:J:492:ILE:CD1	1:J:492:ILE:N	2.70	0.48
1:K:177:PRO:HB3	1:K:294:MET:HG2	1.96	0.48
1:L:222:LEU:HD11	1:L:263:ALA:HB2	1.95	0.48
1:L:470:LEU:HD22	1:L:474:THR:HB	1.96	0.48
1:M:328:LEU:O	1:M:331:ALA:HB3	2.14	0.48
1:D:306:GLU:O	1:D:308:PRO:HD3	2.13	0.48
1:E:110:VAL:CG1	1:E:143:LEU:HD23	2.41	0.48
1:E:443:ASN:HA	1:F:451:GLY:HA2	1.95	0.48
1:F:166:LYS:HD2	1:F:495:PHE:HB2	1.96	0.48
1:G:192:ARG:NH2	1:G:306:GLU:OE1	2.47	0.48
1:L:433:HIS:HD2	1:L:433:HIS:O	1.97	0.48
1:A:73:SER:C	1:A:76:GLN:HE22	2.16	0.48
1:A:479:PHE:O	1:G:417:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:GLN:HG3	1:E:77:GLY:H	1.78	0.48
1:E:110:VAL:HG11	1:E:143:LEU:CD2	2.44	0.48
1:E:212:GLU:O	1:E:215:GLU:HB3	2.14	0.48
1:G:397:VAL:HG23	2:G:2138:HOH:O	2.12	0.48
1:K:85:LYS:CE	1:K:454:LEU:HD21	2.44	0.48
1:K:358:LEU:HD11	1:K:367:LEU:CD1	2.43	0.48
1:L:439:ARG:NH2	1:M:455:GLU:HA	2.29	0.48
1:A:471:PRO:HG2	1:A:474:THR:OG1	2.13	0.48
1:E:367:LEU:HD13	1:E:403:LEU:HD11	1.96	0.48
1:G:461:VAL:HG11	1:G:485:ILE:HD11	1.96	0.48
1:H:175:LEU:HA	1:H:182:THR:HG23	1.96	0.48
1:H:225:ARG:HD2	2:H:2059:HOH:O	2.12	0.48
1:K:202:LEU:HD12	1:K:221:ARG:CD	2.44	0.48
1:L:158:ASP:OD2	1:L:161:GLY:HA2	2.14	0.48
1:L:344:PRO:O	1:L:349:ARG:NH2	2.46	0.48
1:A:137:SER:O	1:A:141:ARG:HB2	2.14	0.48
1:B:247:THR:CG2	2:D:2064:HOH:O	2.61	0.48
1:D:326:ARG:HB3	1:D:327:PRO:HD3	1.96	0.48
1:E:437:ARG:HD2	1:F:456:ARG:NH2	2.29	0.48
1:I:182:THR:CG2	1:I:183:LYS:N	2.77	0.48
1:J:169:ARG:HH21	1:J:171:LYS:NZ	2.10	0.48
1:A:182:THR:HG22	1:A:183:LYS:N	2.29	0.48
1:E:76:GLN:HG3	1:E:78:GLU:HG2	1.95	0.48
1:E:177:PRO:N	1:E:294:MET:HE2	2.29	0.48
1:G:488:VAL:HG13	1:G:489:PRO:HD2	1.96	0.48
1:K:246:THR:CB	1:K:284:LEU:HD23	2.44	0.48
1:K:301:ILE:O	1:K:305:LEU:HG	2.14	0.48
1:K:318:ARG:HD3	1:K:321:MET:HE2	1.96	0.48
1:D:236:THR:HG21	1:D:241:GLU:HG3	1.95	0.47
1:I:73:SER:O	1:I:76:GLN:HG2	2.14	0.47
1:K:420:PRO:HB2	1:L:428:LEU:HD13	1.96	0.47
1:E:105:GLU:HG2	1:E:106:LYS:HD3	1.96	0.47
1:F:182:THR:HG21	1:F:294:MET:HE1	1.95	0.47
1:G:175:LEU:HD12	1:G:313:LEU:HD21	1.94	0.47
1:J:233:LEU:HD23	1:J:233:LEU:HA	1.70	0.47
1:K:212:GLU:HG2	1:K:216:TRP:CZ2	2.48	0.47
1:L:175:LEU:HD12	1:L:313:LEU:HD21	1.95	0.47
1:B:503:VAL:O	1:B:504:GLU:HB3	2.14	0.47
1:G:236:THR:CG2	1:G:241:GLU:HG3	2.44	0.47
1:M:438:ASP:OD2	1:M:452:ARG:HD2	2.14	0.47
1:B:169:ARG:HG3	1:B:169:ARG:NH1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:O	1:B:356:ASP:C	2.53	0.47
1:E:327:PRO:HG2	2:E:2086:HOH:O	2.15	0.47
1:F:173:ILE:HG23	1:F:183:LYS:CG	2.44	0.47
1:F:375:ARG:HD2	1:F:375:ARG:O	2.13	0.47
1:H:251:PHE:CD2	1:H:255:ARG:NH1	2.82	0.47
1:H:301:ILE:O	1:H:305:LEU:HG	2.14	0.47
1:I:243:PHE:O	1:I:247:THR:HB	2.14	0.47
1:J:352:TRP:HB3	1:J:354:PHE:CE1	2.49	0.47
1:H:502:PHE:HE2	1:H:504:GLU:HB2	1.79	0.47
1:A:231:LEU:HD23	1:A:234:ILE:HD11	1.96	0.47
1:B:119:ARG:HH12	1:B:350:ARG:HH11	1.61	0.47
1:B:141:ARG:CG	1:B:141:ARG:NH1	2.77	0.47
1:B:251:PHE:CZ	1:B:277:LEU:HD12	2.50	0.47
1:B:470:LEU:CD2	1:B:487:LYS:HE3	2.45	0.47
1:E:355:ILE:O	1:E:356:ASP:C	2.52	0.47
1:F:251:PHE:CZ	1:F:277:LEU:HD13	2.49	0.47
1:H:439:ARG:CZ	1:H:455:GLU:HB3	2.44	0.47
1:J:199:ARG:HE	1:J:338:THR:HG22	1.78	0.47
1:L:94:VAL:CG2	1:L:98:LYS:HD3	2.45	0.47
1:L:285:SER:HB2	1:M:266:LEU:HD11	1.96	0.47
1:L:411:VAL:HG12	1:L:413:LEU:CD1	2.45	0.47
1:A:72:ASN:N	2:A:2001:HOH:O	2.47	0.47
1:B:139:LEU:HD11	1:B:411:VAL:HG11	1.95	0.47
1:B:141:ARG:HG2	1:B:141:ARG:NH1	2.13	0.47
1:B:291:HIS:CE1	2:B:2046:HOH:O	2.68	0.47
1:E:101:ARG:HD2	2:E:2006:HOH:O	2.14	0.47
1:E:124:ARG:HG3	1:E:124:ARG:NH1	2.29	0.47
1:E:166:LYS:HD2	1:E:495:PHE:HB2	1.97	0.47
1:F:110:VAL:HG13	1:F:143:LEU:HD23	1.97	0.47
1:G:165:SER:OG	1:G:501:ALA:HB2	2.15	0.47
1:G:346:GLU:OE1	1:G:346:GLU:HA	2.14	0.47
1:H:326:ARG:HD2	1:H:360:SER:O	2.14	0.47
1:I:327:PRO:HG2	2:I:2078:HOH:O	2.14	0.47
1:L:182:THR:CG2	1:L:183:LYS:N	2.78	0.47
1:M:92:ARG:HG3	1:M:92:ARG:HH11	1.80	0.47
1:M:117:MET:HG3	1:M:479:PHE:CE1	2.49	0.47
1:B:144:ALA:O	1:B:148:LEU:HG	2.15	0.47
1:B:166:LYS:HE2	1:B:497:ASN:HD21	1.80	0.47
1:F:283:VAL:O	1:F:287:LYS:HG2	2.15	0.47
1:G:169:ARG:HG2	1:G:498:ARG:NH2	2.30	0.47
1:G:490:LEU:HD12	1:G:490:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:351:LEU:HD13	1:H:352:TRP:N	2.28	0.47
1:M:103:THR:OG1	1:M:116:PRO:HG2	2.15	0.47
1:D:499:GLN:HE21	1:D:499:GLN:HB3	1.52	0.47
1:H:110:VAL:HG12	2:H:2008:HOH:O	2.13	0.47
1:H:127:LEU:O	1:H:410:LEU:HD12	2.15	0.47
1:H:217:ALA:O	1:H:221:ARG:HG3	2.15	0.47
1:J:410:LEU:HD21	1:J:426:MET:HE3	1.96	0.47
1:L:173:ILE:HG23	1:L:183:LYS:HG3	1.97	0.47
1:M:358:LEU:HD11	1:M:367:LEU:CD1	2.44	0.47
1:D:176:ASN:H	1:D:182:THR:CG2	2.26	0.47
1:G:98:LYS:O	1:G:102:MET:HG3	2.15	0.47
1:H:478:GLY:C	1:M:417:ARG:HH11	2.19	0.47
1:I:439:ARG:NH1	1:J:439:ARG:HH22	2.13	0.47
1:B:289:PRO:O	1:B:293:THR:HG23	2.15	0.46
1:F:313:LEU:HD23	1:F:314:PHE:N	2.30	0.46
1:F:355:ILE:O	1:F:356:ASP:C	2.52	0.46
1:G:236:THR:HG22	1:G:236:THR:O	2.14	0.46
1:G:430:LEU:HD12	1:G:430:LEU:HA	1.84	0.46
1:I:94:VAL:CG1	1:I:95:SER:N	2.77	0.46
1:I:227:THR:O	1:I:231:LEU:HG	2.15	0.46
1:L:72:ASN:ND2	1:L:440:TYR:HE1	2.13	0.46
1:L:196:ASP:HA	1:L:199:ARG:HB3	1.97	0.46
1:A:338:THR:O	1:A:341:LEU:HB2	2.14	0.46
1:B:129:ASN:HB3	1:B:426:MET:CE	2.45	0.46
1:D:82:ALA:N	1:E:88:LEU:HD13	2.29	0.46
1:E:94:VAL:HG13	1:E:95:SER:N	2.29	0.46
1:G:315:ILE:HG23	1:G:332:TRP:CE3	2.50	0.46
1:K:304:TRP:HZ2	1:K:312:ASN:C	2.19	0.46
1:L:175:LEU:HA	1:L:182:THR:HG23	1.97	0.46
1:M:137:SER:O	1:M:141:ARG:HB2	2.15	0.46
1:A:85:LYS:HZ3	1:A:454:LEU:HG	1.80	0.46
1:B:177:PRO:HG2	1:B:178:TYR:CD1	2.50	0.46
1:D:386:GLN:HB2	1:D:390:GLN:OE1	2.16	0.46
1:E:179:ASP:O	1:E:182:THR:HG22	2.16	0.46
1:G:182:THR:HG21	1:G:294:MET:HE1	1.96	0.46
1:G:199:ARG:HE	1:G:338:THR:HB	1.81	0.46
1:G:344:PRO:O	1:G:349:ARG:NH2	2.42	0.46
1:I:331:ALA:O	1:I:335:VAL:HG23	2.15	0.46
1:I:358:LEU:HD11	1:I:367:LEU:HD11	1.97	0.46
1:I:414:GLY:HA2	1:I:467:ILE:CG2	2.45	0.46
1:J:437:ARG:NH1	1:J:437:ARG:HG3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:ARG:HG2	1:L:498:ARG:HH22	1.80	0.46
1:G:414:GLY:HA2	1:G:467:ILE:HG23	1.98	0.46
1:H:118:PRO:HB3	1:H:483:ARG:HH12	1.79	0.46
1:H:192:ARG:HG2	1:H:302:ARG:NH1	2.30	0.46
1:H:226:GLU:OE1	1:H:261:THR:HB	2.14	0.46
1:I:94:VAL:HG22	1:I:98:LYS:HD3	1.96	0.46
1:K:78:GLU:OE1	1:K:78:GLU:CA	2.57	0.46
1:M:385:LEU:HD12	2:M:2080:HOH:O	2.15	0.46
1:D:85:LYS:HD3	1:D:438:ASP:OD1	2.16	0.46
1:D:166:LYS:HD2	1:D:495:PHE:HB2	1.97	0.46
1:E:355:ILE:O	1:E:356:ASP:O	2.34	0.46
1:F:94:VAL:HG13	1:F:95:SER:N	2.30	0.46
1:G:94:VAL:HG11	1:G:98:LYS:HB3	1.91	0.46
1:G:124:ARG:HB3	1:G:408:ARG:HG3	1.98	0.46
1:G:159:PRO:HG2	1:G:356:ASP:OD2	2.16	0.46
1:I:289:PRO:O	1:I:293:THR:HG23	2.16	0.46
1:J:503:VAL:O	1:J:504:GLU:CB	2.62	0.46
1:K:104:ARG:HG2	1:K:104:ARG:NH1	2.31	0.46
1:K:182:THR:CG2	1:K:183:LYS:N	2.78	0.46
1:L:372:THR:HG22	1:L:373:LYS:HG2	1.97	0.46
1:L:439:ARG:HH22	1:M:456:ARG:H	1.62	0.46
1:M:182:THR:HG21	1:M:294:MET:HE3	1.98	0.46
1:B:379:LEU:HD13	1:B:381:VAL:HG23	1.97	0.46
1:D:92:ARG:HB2	1:D:484:PRO:HB3	1.97	0.46
1:K:136:LYS:O	1:K:140:LEU:HD13	2.15	0.46
1:K:380:ARG:HG3	1:K:380:ARG:HH11	1.81	0.46
1:K:413:LEU:CD1	1:K:475:ALA:HB2	2.44	0.46
1:L:291:HIS:HD2	2:L:2024:HOH:O	1.97	0.46
1:M:345:GLU:CD	1:M:376:LYS:HD2	2.35	0.46
1:B:110:VAL:HG12	1:B:143:LEU:HD23	1.96	0.46
1:B:420:PRO:HB2	1:D:428:LEU:HD13	1.97	0.46
1:E:117:MET:HG3	1:E:479:PHE:CE1	2.50	0.46
1:E:503:VAL:O	1:E:504:GLU:HB2	2.15	0.46
1:F:279:SER:O	1:F:283:VAL:HG23	2.15	0.46
1:G:322:GLY:N	1:G:323:PRO:HD2	2.30	0.46
1:H:322:GLY:N	1:H:323:PRO:HD2	2.30	0.46
1:I:127:LEU:HD11	1:I:385:LEU:HD23	1.93	0.46
1:J:75:GLY:O	1:J:76:GLN:C	2.54	0.46
1:L:304:TRP:CZ2	1:L:313:LEU:HB2	2.51	0.46
1:L:338:THR:HG23	1:L:366:SER:CB	2.45	0.46
1:D:139:LEU:HD22	1:D:140:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:THR:HG22	1:D:236:THR:O	2.16	0.46
1:E:157:VAL:HG12	1:E:317:TRP:HH2	1.80	0.46
1:H:113:ALA:O	1:H:488:VAL:HG11	2.16	0.46
1:H:439:ARG:O	1:H:452:ARG:HB3	2.15	0.46
1:K:126:LEU:HD11	1:K:411:VAL:HG23	1.98	0.46
1:L:227:THR:HG22	1:L:242:LEU:HD12	1.98	0.46
1:B:318:ARG:HG2	1:B:318:ARG:NH1	2.31	0.46
1:E:326:ARG:HD2	1:E:360:SER:O	2.16	0.46
1:E:493:LYS:HD3	1:E:495:PHE:CZ	2.51	0.46
1:G:86:ARG:NE	1:G:436:GLU:OE1	2.46	0.46
1:G:157:VAL:HG12	1:G:317:TRP:CH2	2.51	0.46
1:K:86:ARG:HH11	1:K:86:ARG:CG	2.27	0.46
1:K:221:ARG:HD2	2:K:2037:HOH:O	2.16	0.46
1:E:301:ILE:HD12	1:E:335:VAL:HG11	1.98	0.46
1:G:110:VAL:HG11	1:G:143:LEU:CD2	2.46	0.46
1:G:357:GLU:CG	1:G:386:GLN:HE21	2.29	0.46
1:J:177:PRO:HB3	1:J:294:MET:HG2	1.98	0.46
1:K:182:THR:HG22	1:K:183:LYS:N	2.31	0.46
1:M:233:LEU:C	1:M:235:GLY:H	2.20	0.46
1:M:437:ARG:O	1:M:455:GLU:HG2	2.16	0.46
1:A:416:SER:HB2	1:B:408:ARG:HD2	1.98	0.45
1:D:160:ASN:HD21	1:D:319:GLU:CD	2.18	0.45
1:E:452:ARG:HH11	1:E:452:ARG:HB3	1.81	0.45
1:F:99:LEU:HD22	1:F:486:ALA:HB3	1.97	0.45
1:H:433:HIS:HD2	1:H:433:HIS:O	1.99	0.45
1:H:473:LEU:C	1:H:490:LEU:HD13	2.36	0.45
1:I:181:ARG:CZ	1:I:503:VAL:HG23	2.45	0.45
1:K:98:LYS:O	1:K:102:MET:HG3	2.17	0.45
1:L:154:MET:HE2	1:L:156:ILE:HD11	1.98	0.45
1:L:497:ASN:ND2	1:L:497:ASN:H	2.10	0.45
1:D:91:THR:HB	1:D:461:VAL:HG21	1.98	0.45
1:D:158:ASP:OD2	1:D:161:GLY:HA2	2.17	0.45
1:D:455:GLU:HG2	1:D:457:VAL:HG23	1.99	0.45
1:E:177:PRO:HA	1:E:294:MET:HE2	1.99	0.45
1:E:199:ARG:HE	1:E:338:THR:HB	1.81	0.45
1:F:234:ILE:HG13	2:I:2011:HOH:O	2.16	0.45
1:F:457:VAL:HG12	1:F:459:GLU:CG	2.45	0.45
1:G:94:VAL:CG1	1:G:98:LYS:HD3	2.46	0.45
1:H:184:GLY:HA3	1:H:297:GLY:HA3	1.98	0.45
1:H:439:ARG:NH2	1:M:439:ARG:CZ	2.79	0.45
1:I:372:THR:CG2	1:I:373:LYS:HG3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:VAL:HG22	1:J:98:LYS:HD3	1.97	0.45
1:K:243:PHE:O	1:K:247:THR:HB	2.17	0.45
1:K:247:THR:HG22	1:K:248:ILE:CD1	2.46	0.45
1:L:259:GLU:HA	1:L:264:GLU:CG	2.41	0.45
1:M:455:GLU:HG3	1:M:455:GLU:O	2.15	0.45
1:F:179:ASP:O	1:F:182:THR:OG1	2.35	0.45
1:F:180:GLN:NE2	1:F:505:GLY:HA3	2.31	0.45
1:G:240:ARG:HG2	1:G:292:VAL:HG13	1.97	0.45
1:G:289:PRO:O	1:G:293:THR:HG23	2.16	0.45
1:I:466:GLU:OE2	1:J:89:ARG:HD2	2.17	0.45
1:K:124:ARG:HB3	1:K:408:ARG:HG3	1.98	0.45
1:E:148:LEU:HD11	1:E:154:MET:HE1	1.97	0.45
1:E:498:ARG:C	1:E:499:GLN:HG2	2.37	0.45
1:G:412:VAL:HG22	1:G:426:MET:HE2	1.98	0.45
1:H:354:PHE:CE1	1:H:382:VAL:HG21	2.52	0.45
1:I:159:PRO:HG3	1:I:317:TRP:CZ2	2.51	0.45
1:K:74:VAL:CG1	1:K:75:GLY:H	2.21	0.45
1:A:246:THR:HB	1:A:284:LEU:HD23	1.98	0.45
1:B:433:HIS:CD2	1:B:459:GLU:HG3	2.52	0.45
1:D:471:PRO:HG2	1:D:474:THR:OG1	2.17	0.45
1:I:379:LEU:HD22	1:I:380:ARG:N	2.32	0.45
1:L:152:ASP:OD1	1:L:350:ARG:CZ	2.64	0.45
1:L:195:TYR:CD1	1:L:195:TYR:C	2.89	0.45
1:M:200:TYR:OH	1:M:302:ARG:HD2	2.16	0.45
1:B:352:TRP:CE2	1:B:380:ARG:HD3	2.52	0.45
1:F:411:VAL:HG12	1:F:413:LEU:HD12	1.97	0.45
1:I:176:ASN:O	1:I:182:THR:OG1	2.19	0.45
1:J:440:TYR:CD1	1:J:440:TYR:C	2.89	0.45
1:L:155:VAL:HG23	1:L:351:LEU:HD11	1.99	0.45
1:L:182:THR:HG22	1:L:183:LYS:N	2.31	0.45
1:M:198:GLN:CD	1:M:225:ARG:HH21	2.20	0.45
1:M:240:ARG:HG2	1:M:292:VAL:HG13	1.98	0.45
1:A:358:LEU:HB3	1:A:385:LEU:CD1	2.47	0.45
1:D:176:ASN:O	1:D:182:THR:OG1	2.28	0.45
1:E:329:ILE:O	1:E:333:VAL:HG23	2.17	0.45
1:H:318:ARG:HE	1:H:321:MET:CE	2.28	0.45
1:J:358:LEU:HD21	1:J:403:LEU:HD21	1.98	0.45
1:M:180:GLN:NE2	1:M:504:GLU:O	2.50	0.45
1:M:236:THR:CG2	1:M:241:GLU:HG3	2.46	0.45
1:D:217:ALA:O	1:D:221:ARG:HG3	2.16	0.45
1:F:379:LEU:HD22	1:F:380:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:ASN:H	1:H:182:THR:HG21	1.79	0.45
1:I:247:THR:HG22	1:I:248:ILE:HD13	1.97	0.45
1:I:316:THR:O	1:I:317:TRP:HB3	2.17	0.45
1:J:240:ARG:HG3	1:J:240:ARG:HH11	1.82	0.45
1:B:84:PHE:HA	1:B:437:ARG:HG3	1.98	0.45
1:E:99:LEU:HD22	1:E:486:ALA:HB3	1.98	0.45
1:E:433:HIS:NE2	1:E:459:GLU:HG3	2.32	0.45
1:E:438:ASP:OD1	1:E:454:LEU:CD1	2.65	0.45
1:H:338:THR:HG23	1:H:366:SER:OG	2.17	0.45
1:K:322:GLY:N	1:K:323:PRO:HD2	2.32	0.45
1:A:236:THR:HG22	1:A:236:THR:O	2.17	0.45
1:B:76:GLN:HE21	1:B:76:GLN:HB2	1.58	0.45
1:D:137:SER:O	1:D:141:ARG:HB2	2.16	0.45
1:D:182:THR:HG21	1:D:294:MET:CE	2.47	0.45
1:G:93:ILE:HG13	1:G:485:ILE:HG13	1.98	0.45
1:K:352:TRP:HB3	1:K:354:PHE:CE1	2.52	0.45
1:M:124:ARG:HD3	1:M:124:ARG:HA	1.74	0.45
1:M:316:THR:O	1:M:317:TRP:HB3	2.16	0.45
1:A:433:HIS:HD2	1:A:433:HIS:O	2.00	0.44
1:F:180:GLN:NE2	1:F:505:GLY:O	2.49	0.44
1:G:104:ARG:HG2	1:G:104:ARG:NH1	2.32	0.44
1:G:379:LEU:HD13	1:G:381:VAL:HG23	1.98	0.44
1:G:474:THR:HG21	1:G:487:LYS:NZ	2.32	0.44
1:K:112:VAL:HA	2:K:2012:HOH:O	2.16	0.44
1:K:290:GLU:HG3	1:K:325:LEU:HD23	1.99	0.44
1:A:141:ARG:NH1	2:A:2025:HOH:O	2.49	0.44
1:L:240:ARG:HH11	1:L:240:ARG:CB	2.27	0.44
1:A:379:LEU:HD22	1:A:380:ARG:N	2.33	0.44
1:B:93:ILE:HB	1:B:461:VAL:HG11	1.98	0.44
1:D:215:GLU:O	1:D:218:SER:HB2	2.16	0.44
1:E:73:SER:O	1:E:74:VAL:HG23	2.17	0.44
1:E:243:PHE:O	1:E:247:THR:HB	2.18	0.44
1:E:379:LEU:CD2	1:E:380:ARG:N	2.78	0.44
1:F:82:ALA:HB3	1:F:437:ARG:NH1	2.32	0.44
1:H:229:LYS:O	1:H:233:LEU:HG	2.17	0.44
1:H:436:GLU:CD	1:H:456:ARG:HH11	2.20	0.44
1:H:458:ARG:HD3	1:M:463:MET:HE3	2.00	0.44
1:H:502:PHE:CE2	1:H:504:GLU:HB2	2.53	0.44
1:I:226:GLU:OE1	1:I:226:GLU:HA	2.17	0.44
1:L:460:ARG:HG3	1:L:460:ARG:HH11	1.82	0.44
1:A:430:LEU:HD12	1:A:430:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:ILE:HG13	1:I:234:ILE:O	2.17	0.44
1:J:302:ARG:O	1:J:306:GLU:HG3	2.16	0.44
1:K:186:SER:HB3	2:K:2053:HOH:O	2.16	0.44
1:L:150:ARG:NE	1:L:350:ARG:NH1	2.66	0.44
1:M:92:ARG:HG3	1:M:92:ARG:NH1	2.32	0.44
1:A:182:THR:HG21	1:A:294:MET:HE1	1.98	0.44
1:A:302:ARG:O	1:A:306:GLU:HG3	2.17	0.44
1:B:130:GLY:HA3	1:B:413:LEU:HB2	1.98	0.44
1:B:430:LEU:HD12	1:B:430:LEU:HA	1.87	0.44
1:B:473:LEU:HD11	1:B:492:ILE:HD11	1.98	0.44
1:E:154:MET:HE2	1:E:156:ILE:HD11	1.95	0.44
1:F:499:GLN:HG3	1:F:500:PRO:CD	2.41	0.44
1:G:139:LEU:C	1:G:139:LEU:HD23	2.38	0.44
1:G:184:GLY:HA3	1:G:297:GLY:HA3	1.99	0.44
1:G:433:HIS:HD2	1:G:433:HIS:O	2.01	0.44
1:J:368:ALA:HB3	2:J:2077:HOH:O	2.16	0.44
1:K:137:SER:O	1:K:141:ARG:HB2	2.17	0.44
1:K:181:ARG:NH2	1:K:500:PRO:O	2.42	0.44
1:M:82:ALA:O	1:M:437:ARG:NH1	2.50	0.44
1:M:302:ARG:O	1:M:306:GLU:HG3	2.18	0.44
1:E:76:GLN:CG	1:E:77:GLY:H	2.31	0.44
1:E:226:GLU:HG3	1:E:261:THR:CB	2.38	0.44
1:F:106:LYS:HE3	2:F:2013:HOH:O	2.17	0.44
1:I:113:ALA:O	1:I:488:VAL:HG11	2.18	0.44
1:I:137:SER:O	1:I:141:ARG:HB2	2.18	0.44
1:K:139:LEU:CD1	1:K:411:VAL:HG11	2.46	0.44
1:L:210:THR:HG21	1:M:211:ASP:OD2	2.17	0.44
1:M:169:ARG:NH1	1:M:312:ASN:HD21	2.16	0.44
1:F:141:ARG:HG2	1:F:141:ARG:NH1	2.31	0.44
1:F:159:PRO:HG2	1:F:356:ASP:OD2	2.18	0.44
1:H:155:VAL:HG13	1:H:313:LEU:CD1	2.44	0.44
1:J:338:THR:O	1:J:341:LEU:HB2	2.18	0.44
1:L:371:LEU:HD23	1:L:381:VAL:HG21	2.00	0.44
1:M:74:VAL:HB	1:M:84:PHE:O	2.18	0.44
1:B:503:VAL:O	1:B:504:GLU:CB	2.65	0.44
1:E:106:LYS:HG2	1:E:107:ALA:N	2.30	0.44
1:E:190:GLU:OE1	1:E:302:ARG:HG3	2.18	0.44
1:E:441:SER:OG	1:E:442:LYS:N	2.44	0.44
1:F:87:PHE:CE2	1:F:92:ARG:HG2	2.53	0.44
1:G:158:ASP:OD2	1:G:161:GLY:HA2	2.17	0.44
1:H:122:GLU:HB3	1:H:380:ARG:HE	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:THR:HG23	1:H:257:PHE:CE2	2.53	0.44
1:M:159:PRO:HG3	1:M:317:TRP:CH2	2.53	0.44
1:M:499:GLN:HG3	1:M:500:PRO:HD2	2.00	0.44
1:B:471:PRO:HG2	1:B:474:THR:OG1	2.18	0.44
1:E:78:GLU:OE1	1:E:95:SER:HB3	2.18	0.44
1:E:198:GLN:NE2	1:E:202:LEU:HD22	2.32	0.44
1:F:255:ARG:NH2	1:F:268:ALA:HB1	2.33	0.44
1:F:368:ALA:HB3	2:F:2149:HOH:O	2.16	0.44
1:G:236:THR:HG22	1:G:241:GLU:HG3	2.00	0.44
1:H:439:ARG:NH2	1:M:439:ARG:NH2	2.66	0.44
1:I:159:PRO:HG3	1:I:317:TRP:CH2	2.53	0.44
1:I:313:LEU:HD22	1:I:315:ILE:HG13	2.00	0.44
1:A:380:ARG:HG3	1:A:380:ARG:HH11	1.82	0.43
1:E:304:TRP:CZ2	1:E:313:LEU:HB2	2.52	0.43
1:H:417:ARG:NH1	1:I:479:PHE:O	2.51	0.43
1:K:173:ILE:CG1	1:K:304:TRP:NE1	2.79	0.43
1:L:94:VAL:HG22	1:L:98:LYS:HB3	2.00	0.43
1:M:156:ILE:CG2	1:M:158:ASP:HB2	2.43	0.43
1:M:368:ALA:HB3	2:M:2088:HOH:O	2.17	0.43
1:H:159:PRO:O	1:H:160:ASN:HB2	2.18	0.43
1:H:338:THR:O	1:H:341:LEU:HB2	2.19	0.43
1:K:173:ILE:HG23	1:K:183:LYS:CG	2.44	0.43
1:L:483:ARG:NH1	2:L:2082:HOH:O	2.50	0.43
1:B:254:LEU:CD1	1:B:281:ARG:HD3	2.48	0.43
1:B:288:LEU:N	1:B:289:PRO:CD	2.81	0.43
1:D:289:PRO:O	1:D:293:THR:HG23	2.17	0.43
1:E:217:ALA:O	1:E:221:ARG:HG3	2.18	0.43
1:F:177:PRO:HG2	1:F:178:TYR:CD2	2.53	0.43
1:H:137:SER:O	1:H:141:ARG:HB2	2.18	0.43
1:H:250:THR:HG23	2:H:2066:HOH:O	2.18	0.43
1:H:410:LEU:HD11	1:H:426:MET:HE1	1.99	0.43
1:I:94:VAL:CG2	1:I:98:LYS:HD3	2.48	0.43
1:K:236:THR:O	1:K:236:THR:HG22	2.19	0.43
1:M:176:ASN:H	1:M:182:THR:CG2	2.31	0.43
1:M:482:ASN:C	1:M:482:ASN:ND2	2.71	0.43
1:B:86:ARG:O	1:B:435:VAL:HG22	2.18	0.43
1:B:326:ARG:N	1:B:327:PRO:HD2	2.33	0.43
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.83	0.43
1:F:331:ALA:O	1:F:335:VAL:HG23	2.18	0.43
1:G:461:VAL:CG1	1:G:485:ILE:HD11	2.49	0.43
1:H:93:ILE:HG12	1:H:485:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:VAL:HG12	1:H:95:SER:N	2.33	0.43
1:H:105:GLU:OE2	1:H:119:ARG:HG3	2.18	0.43
1:L:141:ARG:HG2	1:L:141:ARG:HH11	1.83	0.43
1:A:265:SER:HB3	1:G:281:ARG:NH2	2.34	0.43
1:G:355:ILE:O	1:G:356:ASP:C	2.56	0.43
1:H:139:LEU:HD11	1:H:411:VAL:HG11	2.00	0.43
1:I:159:PRO:HG2	1:I:356:ASP:OD2	2.19	0.43
1:I:175:LEU:HD12	1:I:313:LEU:HD21	1.99	0.43
1:I:245:TRP:O	1:I:254:LEU:HG	2.18	0.43
1:J:76:GLN:CG	1:J:77:GLY:N	2.63	0.43
1:L:84:PHE:CB	1:L:435:VAL:CG1	2.97	0.43
1:L:412:VAL:CG2	1:L:426:MET:HE3	2.32	0.43
1:M:379:LEU:HD22	1:M:380:ARG:H	1.81	0.43
1:M:473:LEU:HD11	1:M:492:ILE:HD11	2.00	0.43
1:D:322:GLY:N	1:D:323:PRO:HD2	2.33	0.43
1:D:358:LEU:HB3	1:D:385:LEU:HD11	2.00	0.43
1:F:316:THR:O	1:F:317:TRP:HB3	2.19	0.43
1:M:433:HIS:CD2	1:M:459:GLU:HG3	2.53	0.43
1:D:436:GLU:HG3	1:D:456:ARG:HG3	2.00	0.43
1:F:99:LEU:CD2	1:F:486:ALA:HB3	2.49	0.43
1:F:398:LYS:HA	1:F:398:LYS:HD3	1.77	0.43
1:G:247:THR:HG22	1:G:248:ILE:CD1	2.48	0.43
1:H:185:TRP:NE1	1:H:190:GLU:OE2	2.43	0.43
1:I:326:ARG:HB3	1:I:327:PRO:CD	2.49	0.43
1:J:93:ILE:HB	1:J:461:VAL:HG11	2.01	0.43
1:J:226:GLU:CG	1:J:261:THR:HB	2.32	0.43
1:L:88:LEU:HD11	1:L:436:GLU:HG3	2.01	0.43
1:L:367:LEU:HD22	1:L:371:LEU:HD11	2.01	0.43
1:M:328:LEU:HD22	1:M:332:TRP:CE2	2.54	0.43
1:H:182:THR:HG21	1:H:294:MET:HE3	2.01	0.43
1:I:210:THR:HG21	1:J:211:ASP:OD2	2.19	0.43
1:J:110:VAL:HG12	1:J:117:MET:HB3	2.00	0.43
1:J:158:ASP:O	1:J:316:THR:HA	2.18	0.43
1:K:281:ARG:NH2	1:L:265:SER:HB3	2.33	0.43
1:L:143:LEU:HD22	1:L:354:PHE:HZ	1.83	0.43
1:B:380:ARG:HH11	1:B:380:ARG:CG	2.32	0.43
1:B:439:ARG:HG3	1:B:453:ALA:O	2.19	0.43
1:D:173:ILE:HG22	1:D:174:ILE:N	2.33	0.43
1:E:159:PRO:HG2	1:E:356:ASP:OD2	2.19	0.43
1:E:315:ILE:HG23	1:E:332:TRP:CE3	2.53	0.43
1:E:473:LEU:CD1	1:E:492:ILE:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:LEU:HD13	1:F:403:LEU:HD11	2.01	0.43
1:I:169:ARG:NH1	1:I:171:LYS:CG	2.81	0.43
1:I:417:ARG:NH1	1:J:479:PHE:O	2.51	0.43
2:I:2107:HOH:O	1:J:124:ARG:HG3	2.19	0.43
1:J:440:TYR:CE2	1:K:454:LEU:HB2	2.54	0.43
1:K:254:LEU:CD1	1:K:281:ARG:HD3	2.49	0.43
1:L:166:LYS:HD2	1:L:495:PHE:HB2	2.00	0.43
1:L:175:LEU:CD1	1:L:313:LEU:HD21	2.48	0.43
1:L:358:LEU:HB3	1:L:385:LEU:CD1	2.48	0.43
1:L:367:LEU:HD22	1:L:371:LEU:HG	2.00	0.43
1:L:430:LEU:HD12	1:L:430:LEU:HA	1.85	0.43
1:M:124:ARG:HB3	1:M:408:ARG:HG3	2.01	0.43
1:M:413:LEU:CD2	1:M:475:ALA:HB2	2.46	0.43
1:B:245:TRP:CZ3	1:B:257:PHE:HB2	2.54	0.43
1:B:385:LEU:HD21	1:B:391:LEU:HD22	2.01	0.43
1:E:466:GLU:OE2	1:F:89:ARG:HD2	2.19	0.43
1:H:193:ASN:HB2	1:H:195:TYR:CE1	2.54	0.43
1:I:87:PHE:CZ	1:I:92:ARG:HG3	2.53	0.43
1:J:153:ARG:NH2	1:J:304:TRP:CE2	2.87	0.43
1:J:367:LEU:HD22	1:J:371:LEU:HG	2.00	0.43
1:L:130:GLY:O	1:L:136:LYS:HE2	2.19	0.43
1:M:85:LYS:NZ	1:M:454:LEU:HD21	2.34	0.43
1:A:499:GLN:HE21	1:A:499:GLN:HB3	1.55	0.42
1:B:139:LEU:O	1:B:139:LEU:HD23	2.18	0.42
1:D:139:LEU:HD11	1:D:411:VAL:HG11	2.01	0.42
1:E:233:LEU:C	1:E:235:GLY:N	2.72	0.42
1:H:84:PHE:CB	1:H:435:VAL:CG1	2.97	0.42
1:H:134:THR:HA	1:H:472:ASP:OD1	2.19	0.42
1:H:329:ILE:O	1:H:333:VAL:HG23	2.19	0.42
1:I:439:ARG:CZ	1:J:439:ARG:HH22	2.31	0.42
1:K:359:ALA:HB1	1:K:390:GLN:HG2	2.00	0.42
1:L:159:PRO:HG3	1:L:317:TRP:CZ2	2.54	0.42
1:L:492:ILE:O	1:L:492:ILE:HG22	2.18	0.42
1:M:130:GLY:HA3	1:M:413:LEU:HB2	2.01	0.42
1:M:139:LEU:C	1:M:139:LEU:HD23	2.40	0.42
1:B:174:ILE:O	1:B:182:THR:HA	2.19	0.42
1:B:351:LEU:C	1:B:351:LEU:HD13	2.40	0.42
1:E:290:GLU:HB3	1:E:328:LEU:HD12	2.00	0.42
1:F:243:PHE:O	1:F:247:THR:HB	2.18	0.42
1:G:272:GLU:OE1	1:G:272:GLU:HA	2.19	0.42
1:H:494:GLN:HA	1:H:494:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:VAL:HG12	1:I:317:TRP:HH2	1.80	0.42
1:J:479:PHE:HB2	1:J:483:ARG:HD2	2.01	0.42
1:L:98:LYS:O	1:L:102:MET:HG3	2.19	0.42
1:M:181:ARG:CZ	1:M:503:VAL:HG23	2.49	0.42
1:B:119:ARG:HH12	1:B:350:ARG:NH1	2.17	0.42
1:D:142:GLU:HB2	2:D:2136:HOH:O	2.19	0.42
1:D:199:ARG:NH2	1:D:342:SER:OG	2.51	0.42
1:G:76:GLN:HE21	1:G:76:GLN:HB2	1.60	0.42
1:H:251:PHE:CE2	1:H:255:ARG:NH1	2.83	0.42
1:J:103:THR:OG1	1:J:116:PRO:HG2	2.18	0.42
1:K:114:GLY:N	1:K:142:GLU:OE2	2.46	0.42
1:B:162:ASP:O	1:B:166:LYS:HG2	2.19	0.42
1:B:181:ARG:NH1	1:B:500:PRO:HG2	2.35	0.42
1:B:182:THR:CG2	1:B:183:LYS:N	2.82	0.42
1:B:199:ARG:NH2	1:B:342:SER:OG	2.37	0.42
1:B:498:ARG:HG2	1:B:499:GLN:HG3	2.02	0.42
1:D:320:ASP:OD1	1:D:321:MET:HG3	2.19	0.42
1:F:180:GLN:HB2	1:F:503:VAL:HG12	2.01	0.42
1:G:238:SER:OG	1:G:241:GLU:HG2	2.20	0.42
1:I:367:LEU:HD22	1:I:371:LEU:CD1	2.49	0.42
1:J:130:GLY:O	1:J:136:LYS:HE3	2.20	0.42
1:K:223:LEU:HD23	1:K:284:LEU:HD22	2.02	0.42
1:D:313:LEU:HD23	1:D:314:PHE:N	2.34	0.42
1:E:413:LEU:HD12	1:E:475:ALA:CB	2.50	0.42
1:F:473:LEU:CD1	1:F:492:ILE:HD11	2.50	0.42
1:G:355:ILE:O	1:G:356:ASP:O	2.38	0.42
1:H:373:LYS:HD3	1:M:319:GLU:CD	2.40	0.42
1:J:94:VAL:CG1	1:J:95:SER:N	2.81	0.42
1:J:131:ALA:HB2	1:J:415:GLY:HA2	2.00	0.42
1:J:245:TRP:CZ3	1:J:257:PHE:HB2	2.54	0.42
1:L:198:GLN:O	1:L:202:LEU:HD22	2.19	0.42
1:L:326:ARG:N	1:L:327:PRO:HD2	2.35	0.42
1:M:340:ILE:HA	1:M:343:LEU:HG	2.01	0.42
1:A:456:ARG:NH1	1:G:437:ARG:HD2	2.35	0.42
1:B:364:LEU:HD12	1:B:367:LEU:HG	2.01	0.42
1:E:294:MET:HG3	1:E:328:LEU:HD11	2.02	0.42
1:E:375:ARG:NH2	1:E:376:LYS:NZ	2.67	0.42
1:H:288:LEU:N	1:H:289:PRO:CD	2.83	0.42
1:H:435:VAL:CG1	1:H:436:GLU:N	2.82	0.42
1:J:417:ARG:NH1	1:K:479:PHE:O	2.52	0.42
1:K:100:LYS:HG2	1:K:115:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:143:LEU:O	1:K:143:LEU:HD23	2.20	0.42
1:K:439:ARG:HA	1:L:456:ARG:HH22	1.83	0.42
1:L:77:GLY:C	1:L:78:GLU:HG3	2.39	0.42
1:L:113:ALA:HA	1:L:490:LEU:CD2	2.49	0.42
1:M:352:TRP:CZ2	1:M:380:ARG:HD3	2.54	0.42
1:M:355:ILE:O	1:M:356:ASP:C	2.57	0.42
1:A:197:TRP:CE2	1:A:229:LYS:HG2	2.54	0.42
1:B:350:ARG:HG2	1:B:380:ARG:CZ	2.49	0.42
1:D:364:LEU:HB2	1:D:367:LEU:HB2	2.02	0.42
1:F:375:ARG:NH2	1:F:376:LYS:HE2	2.34	0.42
1:G:103:THR:OG1	1:G:116:PRO:HG2	2.20	0.42
1:G:157:VAL:HG12	1:G:317:TRP:HH2	1.85	0.42
1:I:456:ARG:HD2	1:I:456:ARG:H	1.85	0.42
1:K:74:VAL:CG1	1:K:75:GLY:N	2.77	0.42
1:K:463:MET:HE3	1:L:458:ARG:HD3	2.01	0.42
1:M:96:GLY:O	1:M:100:LYS:HG3	2.19	0.42
1:M:184:GLY:HA3	1:M:297:GLY:HA3	2.02	0.42
1:M:306:GLU:O	1:M:308:PRO:HD3	2.20	0.42
1:B:87:PHE:CD1	1:B:87:PHE:C	2.93	0.42
1:E:87:PHE:HA	1:E:435:VAL:HG23	2.02	0.42
1:E:175:LEU:HD12	1:E:313:LEU:HD21	2.02	0.42
1:E:336:VAL:O	1:E:340:ILE:HG23	2.19	0.42
1:E:344:PRO:O	1:E:349:ARG:NH2	2.52	0.42
1:F:206:PRO:HG2	1:F:362:GLU:OE2	2.19	0.42
1:G:182:THR:CG2	1:G:183:LYS:N	2.83	0.42
1:I:399:GLU:HG3	2:I:2096:HOH:O	2.18	0.42
1:K:279:SER:O	1:K:283:VAL:HG23	2.19	0.42
1:M:460:ARG:HH11	1:M:460:ARG:HG3	1.85	0.42
1:A:363:LYS:HG3	1:A:395:TYR:CD2	2.55	0.42
1:E:130:GLY:HA3	1:E:413:LEU:HB2	2.02	0.42
1:E:433:HIS:CD2	1:E:433:HIS:C	2.92	0.42
1:H:159:PRO:HG3	1:H:317:TRP:CZ2	2.54	0.42
1:H:499:GLN:HG2	1:H:500:PRO:HD2	2.01	0.42
2:H:2097:HOH:O	1:I:398:LYS:HD2	2.20	0.42
1:I:223:LEU:HD23	1:I:284:LEU:CD2	2.50	0.42
1:K:86:ARG:CG	1:K:86:ARG:NH1	2.83	0.42
1:L:435:VAL:CG1	1:L:436:GLU:N	2.83	0.42
1:B:367:LEU:HD13	1:B:403:LEU:HD11	2.02	0.42
1:D:105:GLU:HB2	1:D:109:GLN:NE2	2.35	0.42
1:E:113:ALA:HA	1:E:490:LEU:CD2	2.49	0.42
1:F:358:LEU:HD11	1:F:367:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:THR:HG21	1:F:487:LYS:CE	2.50	0.42
1:H:159:PRO:HG3	1:H:317:TRP:CH2	2.55	0.42
1:I:192:ARG:HG2	1:I:302:ARG:NH1	2.34	0.42
1:I:254:LEU:HD22	1:I:258:LEU:HG	2.01	0.42
1:J:316:THR:O	1:J:317:TRP:HB3	2.20	0.42
1:J:326:ARG:NH1	1:J:361:LEU:O	2.53	0.42
1:J:346:GLU:OE2	1:J:348:LYS:HB2	2.20	0.42
1:J:408:ARG:HG3	1:J:408:ARG:HH11	1.84	0.42
1:K:75:GLY:C	1:K:77:GLY:H	2.23	0.42
1:K:412:VAL:HG13	1:K:426:MET:HE2	2.02	0.42
1:L:178:TYR:CD1	1:L:178:TYR:N	2.88	0.42
1:A:164:LEU:HD11	1:A:174:ILE:HD11	2.01	0.41
1:F:173:ILE:CG2	1:F:183:LYS:HG3	2.47	0.41
1:G:318:ARG:HG2	1:G:318:ARG:HH11	1.85	0.41
1:H:184:GLY:HA2	1:H:295:PRO:O	2.20	0.41
1:I:124:ARG:HH11	1:I:124:ARG:CG	2.27	0.41
1:I:358:LEU:HD11	1:I:367:LEU:CD1	2.50	0.41
1:K:157:VAL:HB	1:K:356:ASP:H	1.85	0.41
1:L:181:ARG:CZ	1:L:503:VAL:HG23	2.49	0.41
1:L:344:PRO:O	1:L:346:GLU:HG2	2.20	0.41
1:L:432:GLU:OE1	1:L:458:ARG:HD2	2.20	0.41
1:A:294:MET:SD	1:A:295:PRO:HD2	2.60	0.41
1:D:503:VAL:O	1:D:504:GLU:CB	2.67	0.41
1:E:410:LEU:HD11	1:E:426:MET:CE	2.50	0.41
1:E:433:HIS:CD2	1:E:459:GLU:HG3	2.56	0.41
1:J:160:ASN:ND2	1:J:319:GLU:CD	2.65	0.41
1:K:430:LEU:HD12	1:K:430:LEU:HA	1.83	0.41
1:A:182:THR:HG22	1:A:183:LYS:O	2.21	0.41
1:A:316:THR:O	1:A:317:TRP:HB3	2.20	0.41
1:A:355:ILE:O	1:A:356:ASP:C	2.58	0.41
1:B:245:TRP:O	1:B:254:LEU:HG	2.20	0.41
1:D:326:ARG:CD	2:D:2083:HOH:O	2.65	0.41
1:E:180:GLN:HB2	1:E:504:GLU:CG	2.50	0.41
1:F:173:ILE:HG22	1:F:174:ILE:N	2.36	0.41
1:G:455:GLU:O	1:G:455:GLU:HG3	2.19	0.41
1:H:259:GLU:HA	1:H:264:GLU:CD	2.40	0.41
1:H:376:LYS:HD3	1:H:376:LYS:HA	1.90	0.41
1:J:105:GLU:HG2	1:J:106:LYS:N	2.35	0.41
1:J:169:ARG:NH1	1:J:169:ARG:HB2	2.35	0.41
1:J:433:HIS:HD2	1:J:433:HIS:O	2.03	0.41
1:K:410:LEU:HD21	1:K:426:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:VAL:O	1:G:340:ILE:HG23	2.19	0.41
1:I:127:LEU:HD13	1:I:407:PHE:CG	2.56	0.41
1:J:207:ARG:HB2	1:J:363:LYS:HG2	2.02	0.41
1:K:254:LEU:C	1:K:254:LEU:HD23	2.41	0.41
1:L:473:LEU:CD1	1:L:492:ILE:HD11	2.47	0.41
1:M:128:VAL:O	1:M:136:LYS:HE2	2.21	0.41
1:B:180:GLN:HG3	1:B:504:GLU:OE1	2.21	0.41
1:G:156:ILE:HG22	1:G:158:ASP:HB2	2.02	0.41
1:G:433:HIS:CD2	1:G:433:HIS:C	2.94	0.41
1:K:87:PHE:CD1	1:K:87:PHE:C	2.94	0.41
1:K:182:THR:HG21	1:K:294:MET:HE1	2.02	0.41
1:K:352:TRP:CE2	1:K:380:ARG:HD3	2.55	0.41
1:K:414:GLY:HA2	1:K:467:ILE:HG23	2.02	0.41
1:L:84:PHE:HB3	1:L:437:ARG:HG3	2.02	0.41
1:L:422:THR:O	1:L:426:MET:HG2	2.20	0.41
1:B:413:LEU:HD12	1:B:475:ALA:CB	2.48	0.41
1:B:436:GLU:OE2	1:B:456:ARG:HD2	2.21	0.41
1:E:250:THR:HA	2:F:2110:HOH:O	2.20	0.41
1:E:251:PHE:CZ	1:E:277:LEU:HD13	2.56	0.41
1:E:473:LEU:HD11	1:E:492:ILE:HD11	2.02	0.41
1:J:430:LEU:HD12	1:J:430:LEU:HA	1.86	0.41
1:K:230:LYS:CE	1:K:257:PHE:O	2.68	0.41
1:L:230:LYS:HD3	1:L:257:PHE:CE2	2.55	0.41
1:A:367:LEU:HD22	1:A:371:LEU:CD1	2.51	0.41
1:A:433:HIS:CD2	1:A:433:HIS:C	2.94	0.41
1:B:84:PHE:CG	1:B:435:VAL:HG21	2.55	0.41
1:B:136:LYS:HG2	1:B:413:LEU:CD2	2.51	0.41
1:E:452:ARG:HH11	1:E:452:ARG:CB	2.34	0.41
1:G:175:LEU:CD1	1:G:313:LEU:HD21	2.51	0.41
1:H:259:GLU:HG2	1:H:264:GLU:OE2	2.21	0.41
1:K:318:ARG:HG2	1:K:318:ARG:HH11	1.85	0.41
1:L:375:ARG:NH1	1:L:375:ARG:HG3	2.35	0.41
1:M:291:HIS:CE1	2:M:2041:HOH:O	2.73	0.41
1:A:178:TYR:OH	1:A:290:GLU:OE2	2.31	0.41
1:B:180:GLN:HG3	1:B:504:GLU:CB	2.50	0.41
1:D:184:GLY:HA2	1:D:295:PRO:O	2.20	0.41
1:H:234:ILE:HD11	1:H:236:THR:OG1	2.21	0.41
1:H:375:ARG:HB2	1:H:375:ARG:NH1	2.25	0.41
1:I:72:ASN:OD1	1:I:438:ASP:HB2	2.20	0.41
1:K:199:ARG:NH2	1:K:342:SER:OG	2.52	0.41
1:K:379:LEU:CD2	1:K:380:ARG:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:493:LYS:HB3	1:K:495:PHE:CE1	2.56	0.41
1:M:94:VAL:HG13	1:M:95:SER:O	2.20	0.41
1:A:124:ARG:HB3	1:A:408:ARG:HG3	2.02	0.41
1:A:139:LEU:HD23	1:A:139:LEU:O	2.21	0.41
1:A:154:MET:HB3	1:A:352:TRP:HB2	2.03	0.41
1:A:352:TRP:CE2	1:A:380:ARG:HD3	2.56	0.41
1:A:428:LEU:HD13	1:G:420:PRO:HB2	2.03	0.41
1:B:84:PHE:CD2	1:B:435:VAL:CG2	3.04	0.41
1:E:75:GLY:O	1:E:76:GLN:C	2.59	0.41
1:E:76:GLN:HG3	1:E:77:GLY:N	2.35	0.41
1:F:84:PHE:CD1	1:F:84:PHE:N	2.89	0.41
1:G:125:HIS:HB2	1:G:407:PHE:HA	2.03	0.41
1:G:175:LEU:HA	1:G:182:THR:HG23	2.03	0.41
1:J:84:PHE:CG	1:J:435:VAL:HG11	2.56	0.41
1:J:279:SER:O	1:J:283:VAL:HG23	2.21	0.41
1:K:122:GLU:N	1:K:123:PRO:HD2	2.35	0.41
1:L:106:LYS:H	1:L:106:LYS:CD	2.23	0.41
1:L:245:TRP:O	1:L:254:LEU:HG	2.21	0.41
1:L:281:ARG:NH2	1:M:265:SER:HB3	2.36	0.41
1:L:416:SER:HB2	1:M:408:ARG:HD2	2.03	0.41
1:L:452:ARG:HG2	1:L:452:ARG:O	2.21	0.41
1:M:166:LYS:HG3	1:M:495:PHE:HB3	2.02	0.41
1:M:380:ARG:HG3	1:M:380:ARG:HH11	1.85	0.41
1:B:180:GLN:HG3	1:B:504:GLU:HB2	2.03	0.41
1:E:144:ALA:O	1:E:148:LEU:HG	2.21	0.41
1:G:110:VAL:HG13	1:G:146:THR:OG1	2.21	0.41
1:G:483:ARG:NH1	2:G:2163:HOH:O	2.53	0.41
1:H:88:LEU:HD13	1:M:82:ALA:HB2	2.02	0.41
1:I:145:TYR:CE1	1:I:149:LEU:HD21	2.54	0.41
1:I:236:THR:HB	1:I:241:GLU:OE2	2.21	0.41
1:J:180:GLN:NE2	1:J:504:GLU:OE1	2.54	0.41
1:J:183:LYS:HD3	1:J:183:LYS:HA	1.98	0.41
1:K:328:LEU:HD13	1:K:332:TRP:CH2	2.56	0.41
1:K:340:ILE:HG13	1:K:379:LEU:HD12	2.02	0.41
1:K:454:LEU:HA	1:K:454:LEU:HD23	1.89	0.41
1:M:259:GLU:HA	1:M:264:GLU:CG	2.41	0.41
1:M:378:GLY:O	1:M:380:ARG:NH1	2.54	0.41
1:B:82:ALA:O	1:B:437:ARG:NH1	2.54	0.40
1:E:86:ARG:HG3	1:E:86:ARG:HH11	1.86	0.40
1:F:404:ARG:NH1	2:F:2165:HOH:O	2.48	0.40
1:G:326:ARG:HD2	1:G:360:SER:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:LEU:CD1	1:M:82:ALA:HB2	2.51	0.40
1:H:104:ARG:NH1	2:H:2006:HOH:O	2.54	0.40
1:H:352:TRP:HB3	1:H:354:PHE:CE2	2.55	0.40
1:I:433:HIS:CD2	1:I:433:HIS:C	2.94	0.40
1:J:199:ARG:HE	1:J:338:THR:HG21	1.83	0.40
1:J:437:ARG:O	1:J:455:GLU:HG2	2.20	0.40
1:M:277:LEU:O	1:M:277:LEU:HD22	2.21	0.40
1:A:184:GLY:HA2	1:A:295:PRO:O	2.21	0.40
1:D:78:GLU:HG2	2:D:2001:HOH:O	2.20	0.40
1:E:183:LYS:HD3	1:E:183:LYS:HA	1.90	0.40
1:G:153:ARG:C	1:G:154:MET:HG2	2.41	0.40
1:J:144:ALA:O	1:J:148:LEU:HG	2.21	0.40
1:J:226:GLU:HG3	1:J:261:THR:CB	2.33	0.40
1:K:134:THR:O	1:K:134:THR:CG2	2.66	0.40
1:K:186:SER:H	1:K:189:ASN:ND2	2.19	0.40
1:K:244:HIS:HD2	2:K:2043:HOH:O	2.03	0.40
1:L:166:LYS:HD2	1:L:495:PHE:CB	2.52	0.40
1:L:398:LYS:HD3	1:L:398:LYS:HA	1.83	0.40
1:M:94:VAL:HG22	1:M:98:LYS:HB3	2.04	0.40
1:A:166:LYS:HD3	1:A:497:ASN:HD22	1.85	0.40
1:E:129:ASN:HB3	1:E:426:MET:HE1	2.03	0.40
1:G:199:ARG:NH2	1:G:342:SER:OG	2.47	0.40
1:I:413:LEU:HD12	1:I:475:ALA:CB	2.51	0.40
1:L:331:ALA:O	1:L:335:VAL:HG23	2.22	0.40
1:M:106:LYS:CD	1:M:106:LYS:N	2.67	0.40
1:M:110:VAL:HG13	1:M:146:THR:OG1	2.21	0.40
1:A:100:LYS:HG2	1:A:115:VAL:HA	2.04	0.40
1:A:466:GLU:OE2	1:B:89:ARG:HD2	2.21	0.40
1:D:153:ARG:NH2	1:D:304:TRP:CE2	2.89	0.40
1:D:238:SER:HB3	1:D:241:GLU:HB2	2.03	0.40
1:E:471:PRO:HG2	1:E:474:THR:OG1	2.22	0.40
1:H:439:ARG:HH22	1:M:439:ARG:NH2	2.19	0.40
1:J:318:ARG:HD2	1:J:502:PHE:CZ	2.57	0.40
1:J:350:ARG:HG2	1:J:380:ARG:NH2	2.37	0.40
1:J:483:ARG:HH11	1:J:483:ARG:CG	2.34	0.40
1:K:119:ARG:HD3	1:K:122:GLU:OE2	2.21	0.40
1:K:463:MET:SD	1:L:434:GLU:HG3	2.62	0.40
1:L:288:LEU:N	1:L:289:PRO:CD	2.85	0.40
1:M:441:SER:HB2	1:M:451:GLY:HA3	2.02	0.40
1:B:385:LEU:HD12	1:B:385:LEU:HA	1.90	0.40
1:F:474:THR:HG21	1:F:487:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:MET:HE3	1:G:156:ILE:HD11	1.99	0.40
1:G:357:GLU:CG	1:G:386:GLN:NE2	2.85	0.40
1:I:97:GLY:O	1:I:101:ARG:HG3	2.22	0.40
1:J:154:MET:HA	1:J:351:LEU:HD22	2.03	0.40
1:K:352:TRP:CZ2	1:K:380:ARG:HD3	2.57	0.40
1:L:192:ARG:HG2	1:L:302:ARG:NH1	2.35	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	423/437 (97%)	407 (96%)	15 (4%)	1 (0%)	47	68
1	B	418/437 (96%)	397 (95%)	19 (4%)	2 (0%)	29	48
1	D	413/437 (94%)	395 (96%)	15 (4%)	3 (1%)	22	39
1	E	421/437 (96%)	401 (95%)	16 (4%)	4 (1%)	15	28
1	F	423/437 (97%)	401 (95%)	20 (5%)	2 (0%)	29	48
1	G	423/437 (97%)	410 (97%)	12 (3%)	1 (0%)	47	68
1	H	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	29	48
1	I	420/437 (96%)	398 (95%)	20 (5%)	2 (0%)	29	48
1	J	420/437 (96%)	402 (96%)	16 (4%)	2 (0%)	29	48
1	K	418/437 (96%)	401 (96%)	15 (4%)	2 (0%)	29	48
1	L	422/437 (97%)	405 (96%)	14 (3%)	3 (1%)	22	39
1	M	421/437 (96%)	403 (96%)	15 (4%)	3 (1%)	22	39
All	All	5042/5244 (96%)	4818 (96%)	197 (4%)	27 (0%)	29	48

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	356	ASP
1	E	76	GLN
1	E	356	ASP
1	G	356	ASP
1	H	76	GLN
1	J	76	GLN
1	K	74	VAL
1	A	356	ASP
1	B	356	ASP
1	E	442	LYS
1	F	234	ILE
1	F	356	ASP
1	H	356	ASP
1	I	356	ASP
1	J	356	ASP
1	K	356	ASP
1	L	356	ASP
1	L	504	GLU
1	M	125	HIS
1	M	356	ASP
1	D	182	THR
1	D	234	ILE
1	I	504	GLU
1	L	125	HIS
1	B	76	GLN
1	E	234	ILE
1	M	234	ILE

5.3.2 Protein sidechains (i)

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	356/364 (98%)	323 (91%)	33 (9%)	9 17
1	B	352/364 (97%)	316 (90%)	36 (10%)	7 14
1	D	348/364 (96%)	317 (91%)	31 (9%)	9 19
1	E	355/364 (98%)	327 (92%)	28 (8%)	12 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	355/364 (98%)	324 (91%)	31 (9%)	10 20
1	G	356/364 (98%)	324 (91%)	32 (9%)	9 19
1	H	353/364 (97%)	325 (92%)	28 (8%)	12 24
1	I	353/364 (97%)	326 (92%)	27 (8%)	13 25
1	J	353/364 (97%)	318 (90%)	35 (10%)	8 15
1	K	352/364 (97%)	329 (94%)	23 (6%)	17 33
1	L	355/364 (98%)	322 (91%)	33 (9%)	9 17
1	M	353/364 (97%)	323 (92%)	30 (8%)	10 21
All	All	4241/4368 (97%)	3874 (91%)	367 (9%)	10 20

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	110	VAL
1	A	141	ARG
1	A	143	LEU
1	A	186	SER
1	A	202	LEU
1	A	238	SER
1	A	251	PHE
1	A	254	LEU
1	A	255	ARG
1	A	277	LEU
1	A	284	LEU
1	A	290	GLU
1	A	294	MET
1	A	313	LEU
1	A	326	ARG
1	A	328	LEU
1	A	338	THR
1	A	340	ILE
1	A	353	LEU
1	A	367	LEU
1	A	375	ARG
1	A	379	LEU
1	A	385	LEU
1	A	417	ARG
1	A	428	LEU

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	433	HIS
1	A	435	VAL
1	A	454	LEU
1	A	456	ARG
1	A	483	ARG
1	A	499	GLN
1	B	76	GLN
1	B	106	LYS
1	B	141	ARG
1	B	143	LEU
1	B	154	MET
1	B	169	ARG
1	B	186	SER
1	B	202	LEU
1	B	209	LYS
1	B	251	PHE
1	B	254	LEU
1	B	277	LEU
1	B	284	LEU
1	B	293	THR
1	B	294	MET
1	B	313	LEU
1	B	326	ARG
1	B	328	LEU
1	B	338	THR
1	B	340	ILE
1	B	353	LEU
1	B	356	ASP
1	B	367	LEU
1	B	375	ARG
1	B	379	LEU
1	B	385	LEU
1	B	413	LEU
1	B	417	ARG
1	B	428	LEU
1	B	430	LEU
1	B	433	HIS
1	B	435	VAL
1	B	439	ARG
1	B	456	ARG
1	B	493	LYS

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Mol	Chain	Res	Type
1	B	494	GLN
1	D	104	ARG
1	D	110	VAL
1	D	141	ARG
1	D	143	LEU
1	D	154	MET
1	D	186	SER
1	D	202	LEU
1	D	251	PHE
1	D	254	LEU
1	D	277	LEU
1	D	284	LEU
1	D	285	SER
1	D	294	MET
1	D	313	LEU
1	D	326	ARG
1	D	328	LEU
1	D	338	THR
1	D	340	ILE
1	D	353	LEU
1	D	367	LEU
1	D	375	ARG
1	D	379	LEU
1	D	385	LEU
1	D	428	LEU
1	D	430	LEU
1	D	433	HIS
1	D	435	VAL
1	D	454	LEU
1	D	456	ARG
1	D	483	ARG
1	D	499	GLN
1	E	78	GLU
1	E	94	VAL
1	E	106	LYS
1	E	129	ASN
1	E	143	LEU
1	E	154	MET
1	E	186	SER
1	E	202	LEU
1	E	233	LEU
1	E	251	PHE

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Mol	Chain	Res	Type
1	E	254	LEU
1	E	277	LEU
1	E	284	LEU
1	E	294	MET
1	E	328	LEU
1	E	338	THR
1	E	353	LEU
1	E	367	LEU
1	E	379	LEU
1	E	385	LEU
1	E	413	LEU
1	E	417	ARG
1	E	430	LEU
1	E	433	HIS
1	E	435	VAL
1	E	454	LEU
1	E	456	ARG
1	E	483	ARG
1	F	76	GLN
1	F	94	VAL
1	F	110	VAL
1	F	141	ARG
1	F	143	LEU
1	F	182	THR
1	F	202	LEU
1	F	251	PHE
1	F	254	LEU
1	F	277	LEU
1	F	284	LEU
1	F	294	MET
1	F	326	ARG
1	F	328	LEU
1	F	338	THR
1	F	340	ILE
1	F	353	LEU
1	F	362	GLU
1	F	367	LEU
1	F	372	THR
1	F	379	LEU
1	F	385	LEU
1	F	417	ARG
1	F	430	LEU

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Mol	Chain	Res	Type
1	F	433	HIS
1	F	435	VAL
1	F	439	ARG
1	F	454	LEU
1	F	456	ARG
1	F	483	ARG
1	F	499	GLN
1	G	143	LEU
1	G	154	MET
1	G	186	SER
1	G	202	LEU
1	G	251	PHE
1	G	254	LEU
1	G	255	ARG
1	G	277	LEU
1	G	289	PRO
1	G	290	GLU
1	G	294	MET
1	G	296	ASP
1	G	313	LEU
1	G	318	ARG
1	G	328	LEU
1	G	338	THR
1	G	341	LEU
1	G	345	GLU
1	G	353	LEU
1	G	360	SER
1	G	362	GLU
1	G	367	LEU
1	G	372	THR
1	G	375	ARG
1	G	379	LEU
1	G	385	LEU
1	G	417	ARG
1	G	430	LEU
1	G	433	HIS
1	G	434	GLU
1	G	435	VAL
1	G	499	GLN
1	H	76	GLN
1	H	93	ILE
1	H	140	LEU

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Mol	Chain	Res	Type
1	H	141	ARG
1	H	194	ASP
1	H	202	LEU
1	H	237	PRO
1	H	240	ARG
1	H	241	GLU
1	H	251	PHE
1	H	254	LEU
1	H	277	LEU
1	H	284	LEU
1	H	294	MET
1	H	296	ASP
1	H	328	LEU
1	H	338	THR
1	H	340	ILE
1	H	353	LEU
1	H	362	GLU
1	H	367	LEU
1	H	375	ARG
1	H	417	ARG
1	H	428	LEU
1	H	430	LEU
1	H	433	HIS
1	H	439	ARG
1	H	506	THR
1	I	104	ARG
1	I	106	LYS
1	I	143	LEU
1	I	170	ASP
1	I	186	SER
1	I	194	ASP
1	I	202	LEU
1	I	240	ARG
1	I	251	PHE
1	I	254	LEU
1	I	277	LEU
1	I	284	LEU
1	I	294	MET
1	I	298	ASP
1	I	328	LEU
1	I	338	THR
1	I	340	ILE

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Mol	Chain	Res	Type
1	I	341	LEU
1	I	353	LEU
1	I	360	SER
1	I	367	LEU
1	I	375	ARG
1	I	379	LEU
1	I	385	LEU
1	I	430	LEU
1	I	433	HIS
1	I	435	VAL
1	J	76	GLN
1	J	104	ARG
1	J	110	VAL
1	J	137	SER
1	J	143	LEU
1	J	154	MET
1	J	169	ARG
1	J	180	GLN
1	J	194	ASP
1	J	202	LEU
1	J	225	ARG
1	J	254	LEU
1	J	277	LEU
1	J	290	GLU
1	J	294	MET
1	J	296	ASP
1	J	313	LEU
1	J	328	LEU
1	J	338	THR
1	J	340	ILE
1	J	341	LEU
1	J	351	LEU
1	J	353	LEU
1	J	362	GLU
1	J	366	SER
1	J	367	LEU
1	J	379	LEU
1	J	385	LEU
1	J	428	LEU
1	J	430	LEU
1	J	433	HIS
1	J	434	GLU

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Mol	Chain	Res	Type
1	J	435	VAL
1	J	440	TYR
1	J	492	ILE
1	K	76	GLN
1	K	85	LYS
1	K	104	ARG
1	K	194	ASP
1	K	202	LEU
1	K	226	GLU
1	K	251	PHE
1	K	294	MET
1	K	298	ASP
1	K	328	LEU
1	K	338	THR
1	K	340	ILE
1	K	353	LEU
1	K	367	LEU
1	K	375	ARG
1	K	379	LEU
1	K	417	ARG
1	K	428	LEU
1	K	430	LEU
1	K	433	HIS
1	K	454	LEU
1	K	472	ASP
1	K	497	ASN
1	L	76	GLN
1	L	86	ARG
1	L	106	LYS
1	L	141	ARG
1	L	154	MET
1	L	162	ASP
1	L	186	SER
1	L	202	LEU
1	L	251	PHE
1	L	254	LEU
1	L	277	LEU
1	L	286	ASP
1	L	289	PRO
1	L	294	MET
1	L	296	ASP
1	L	313	LEU

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Mol	Chain	Res	Type
1	L	328	LEU
1	L	340	ILE
1	L	348	LYS
1	L	353	LEU
1	L	367	LEU
1	L	372	THR
1	L	375	ARG
1	L	379	LEU
1	L	417	ARG
1	L	428	LEU
1	L	430	LEU
1	L	433	HIS
1	L	438	ASP
1	L	456	ARG
1	L	497	ASN
1	L	499	GLN
1	L	506	THR
1	M	92	ARG
1	M	106	LYS
1	M	202	LEU
1	M	233	LEU
1	M	251	PHE
1	M	254	LEU
1	M	277	LEU
1	M	294	MET
1	M	296	ASP
1	M	328	LEU
1	M	338	THR
1	M	340	ILE
1	M	341	LEU
1	M	345	GLU
1	M	353	LEU
1	M	362	GLU
1	M	367	LEU
1	M	375	ARG
1	M	379	LEU
1	M	417	ARG
1	M	428	LEU
1	M	430	LEU
1	M	433	HIS
1	M	434	GLU
1	M	439	ARG

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Mol	Chain	Res	Type
1	M	456	ARG
1	M	472	ASP
1	M	482	ASN
1	M	497	ASN
1	M	499	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	160	ASN
1	A	291	HIS
1	A	497	ASN
1	A	499	GLN
1	B	76	GLN
1	B	180	GLN
1	B	291	HIS
1	B	497	ASN
1	D	160	ASN
1	D	291	HIS
1	D	497	ASN
1	D	499	GLN
1	E	160	ASN
1	E	244	HIS
1	E	291	HIS
1	E	497	ASN
1	F	76	GLN
1	F	160	ASN
1	F	180	GLN
1	F	291	HIS
1	F	433	HIS
1	F	499	GLN
1	G	76	GLN
1	G	244	HIS
1	G	291	HIS
1	G	309	ASN
1	G	386	GLN
1	G	497	ASN
1	G	499	GLN
1	H	160	ASN
1	H	180	GLN
1	H	291	HIS

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Mol	Chain	Res	Type
1	H	433	HIS
1	H	494	GLN
1	H	497	ASN
1	H	499	GLN
1	I	76	GLN
1	I	189	ASN
1	I	291	HIS
1	I	433	HIS
1	I	497	ASN
1	I	499	GLN
1	J	76	GLN
1	J	129	ASN
1	J	160	ASN
1	J	180	GLN
1	J	189	ASN
1	J	291	HIS
1	K	76	GLN
1	K	129	ASN
1	K	189	ASN
1	K	291	HIS
1	K	433	HIS
1	K	469	ASN
1	K	497	ASN
1	L	76	GLN
1	L	160	ASN
1	L	291	HIS
1	L	386	GLN
1	L	433	HIS
1	L	494	GLN
1	L	497	ASN
1	L	499	GLN
1	M	180	GLN
1	M	291	HIS
1	M	312	ASN
1	M	482	ASN
1	M	494	GLN
1	M	499	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.