



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LNN
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of apo form of GS
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 3.10 Å(reported)

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

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

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

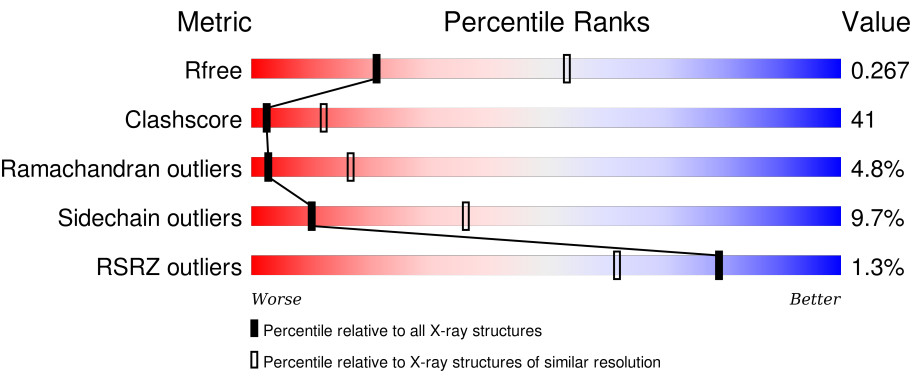
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	443	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>36%55%7% ..</div></div>
1	B	443	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>41%51%7% .</div></div>
1	C	443	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>39%50%10% .</div></div>
1	D	443	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>36%55%8% .</div></div>
1	E	443	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>37%51%10% ..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	443	
1	G	443	
1	H	443	
1	I	443	
1	J	443	
1	K	443	
1	L	443	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	C	501	-	-	-	X
3	SO4	D	501	-	-	-	X
3	SO4	F	503	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 42284 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	B	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	C	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	D	439	Total	C	N	O	S	0	0	0
			3505	2240	586	663	16			
1	E	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	F	437	Total	C	N	O	S	0	0	0
			3491	2230	584	661	16			
1	G	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	H	437	Total	C	N	O	S	0	0	0
			3491	2230	584	661	16			
1	I	436	Total	C	N	O	S	0	0	0
			3485	2227	583	660	15			
1	J	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	K	438	Total	C	N	O	S	0	0	0
			3498	2235	585	662	16			
1	L	440	Total	C	N	O	S	0	0	0
			3509	2242	587	664	16			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	B	3	Total	Mg	0	0
			3	3		
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	27	Total	O	0	0
			27	27		
4	C	28	Total	O	0	0
			28	28		
4	D	20	Total	O	0	0
			20	20		
4	E	17	Total	O	0	0
			17	17		
4	F	24	Total	O	0	0
			24	24		
4	G	21	Total	O	0	0
			21	21		
4	H	20	Total	O	0	0
			20	20		
4	I	23	Total	O	0	0
			23	23		
4	J	12	Total	O	0	0
			12	12		
4	K	22	Total	O	0	0
			22	22		
4	L	22	Total	O	0	0
			22	22		

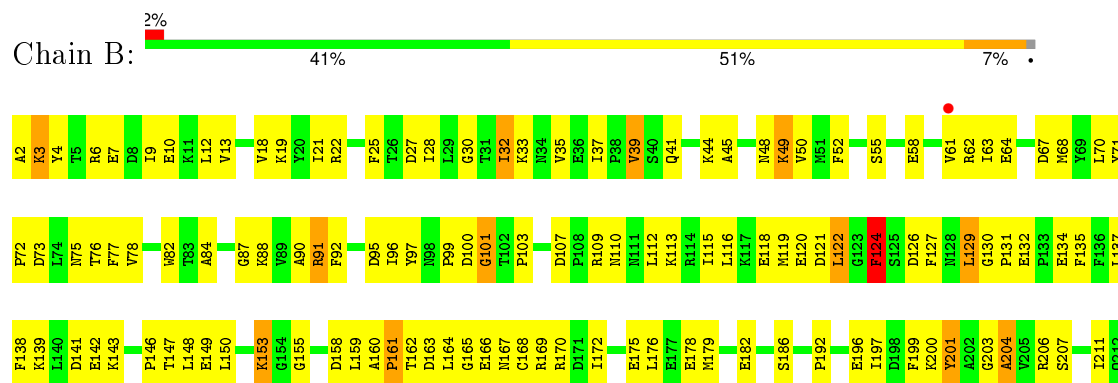
3 Residue-property plots

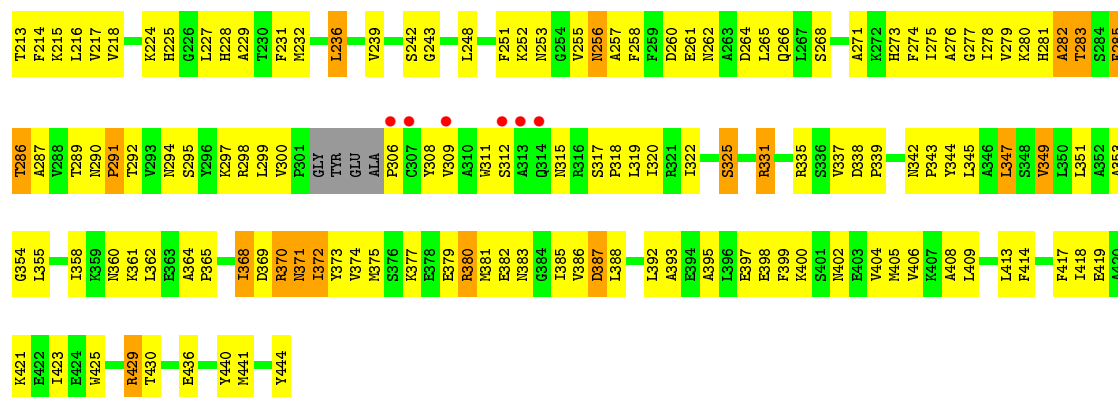
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Glutamine synthetase

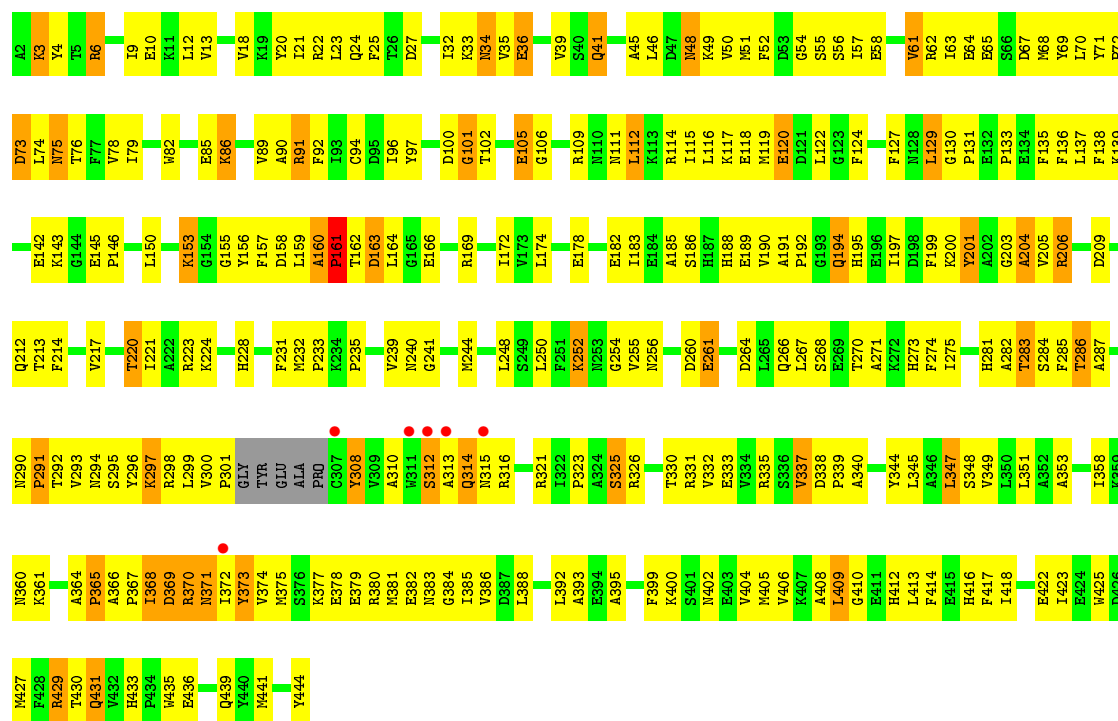


• Molecule 1: Glutamine synthetase

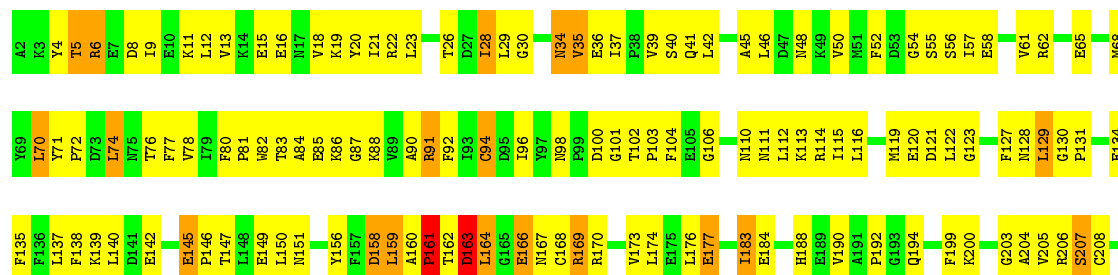


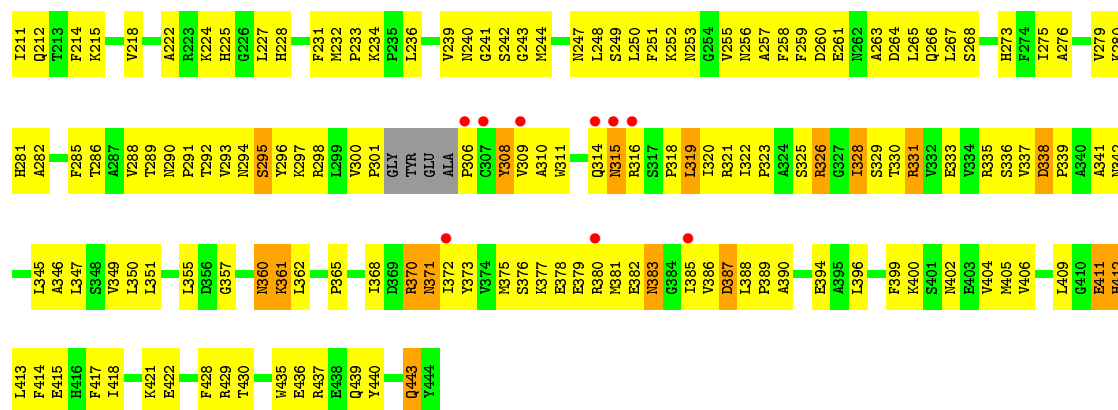


• Molecule 1: Glutamine synthetase

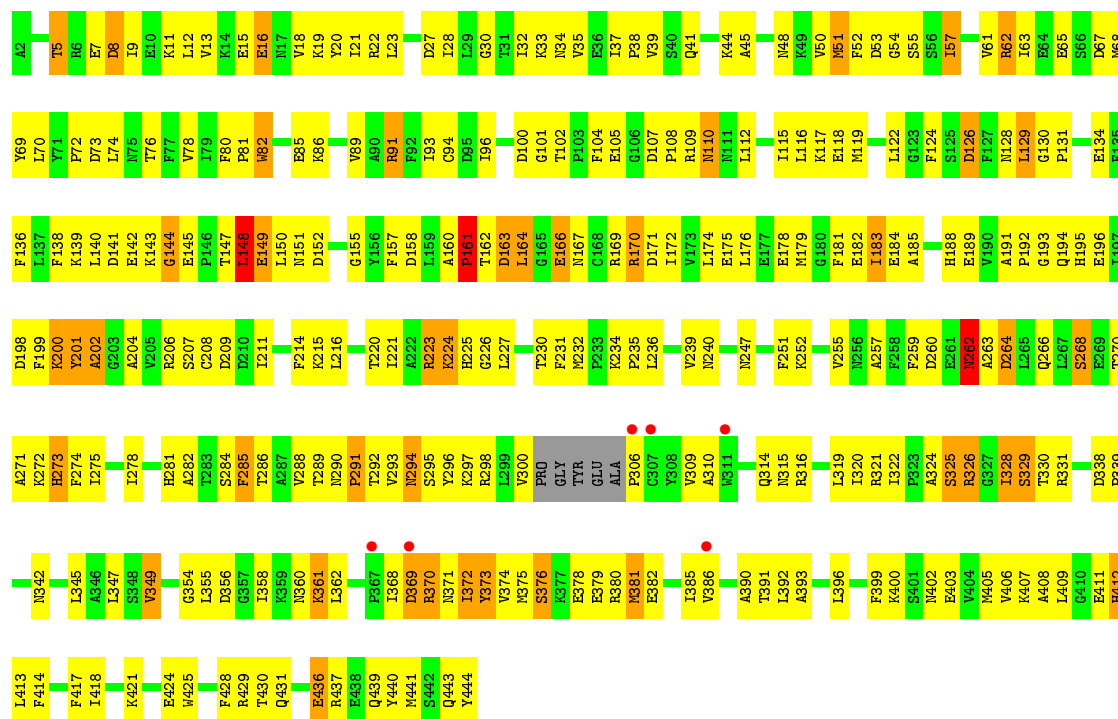


• Molecule 1: Glutamine synthetase

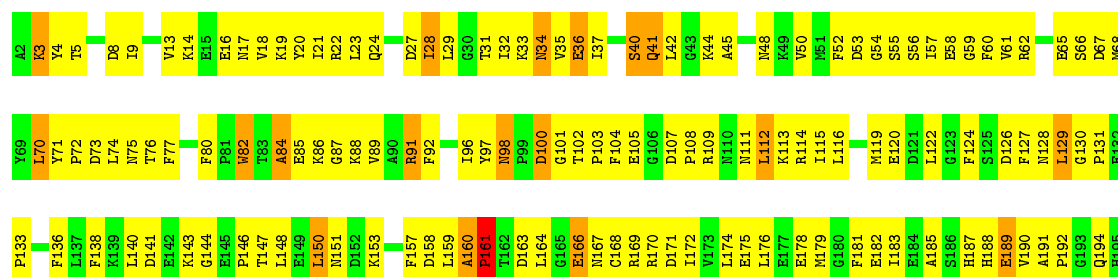


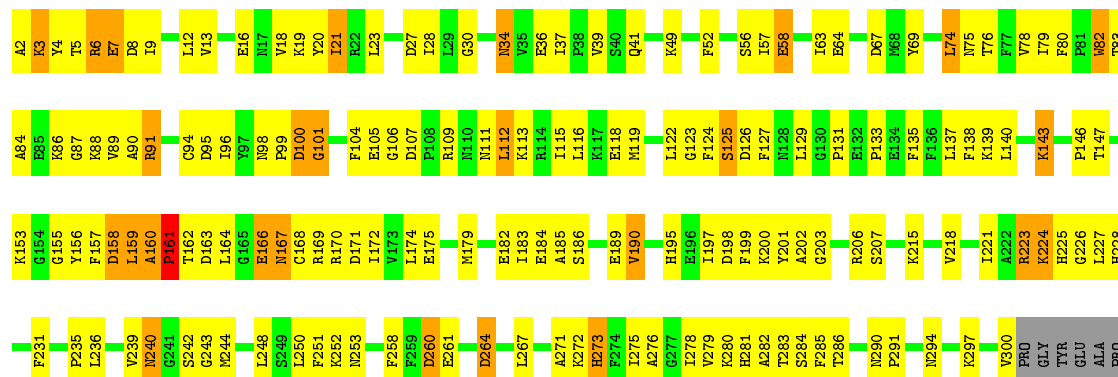


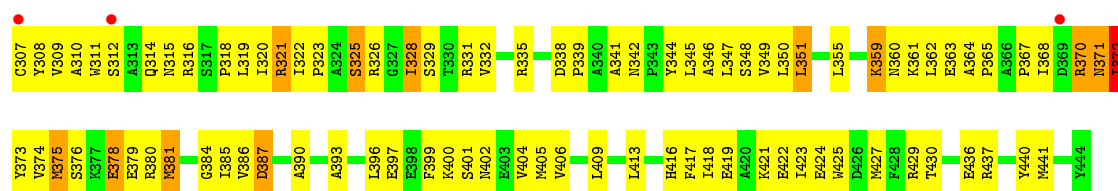
• Molecule 1: Glutamine synthetase



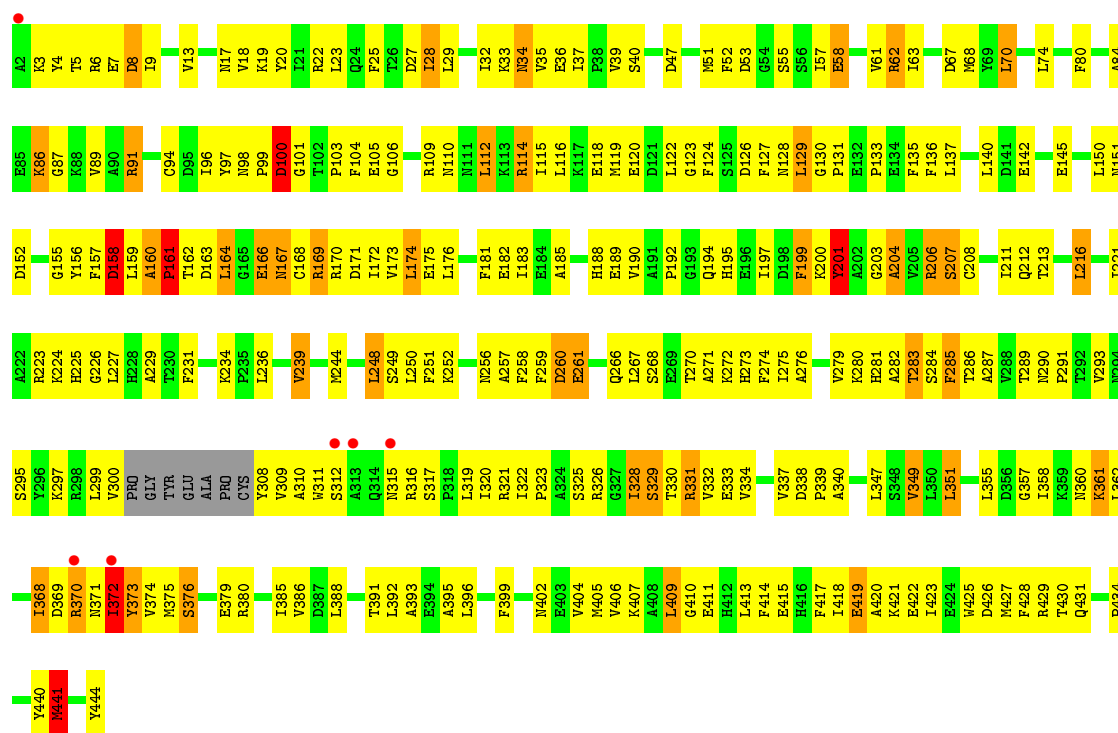
• Molecule 1: Glutamine synthetase



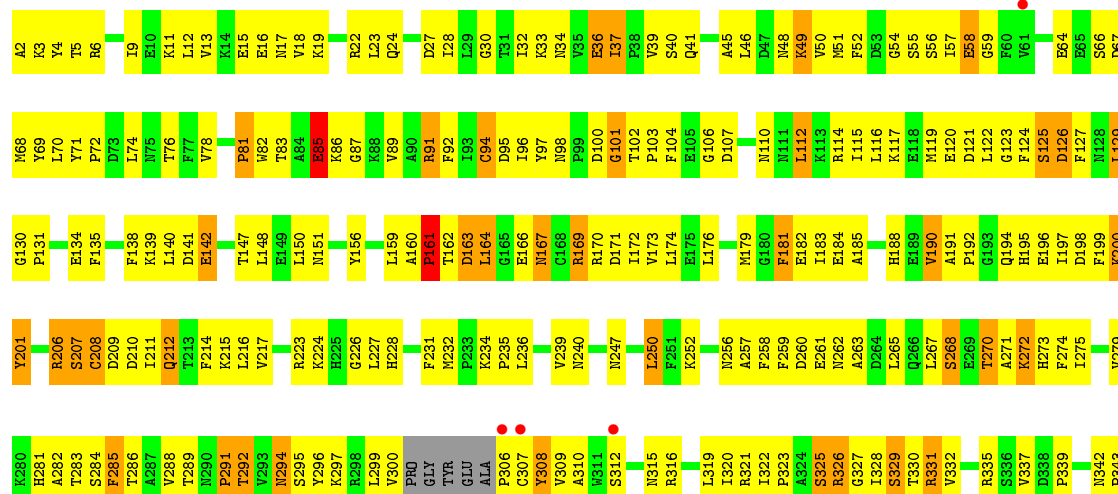


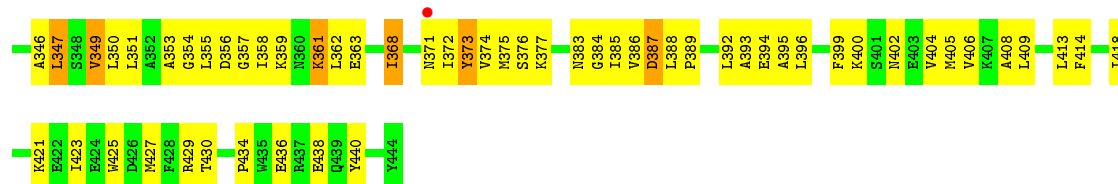


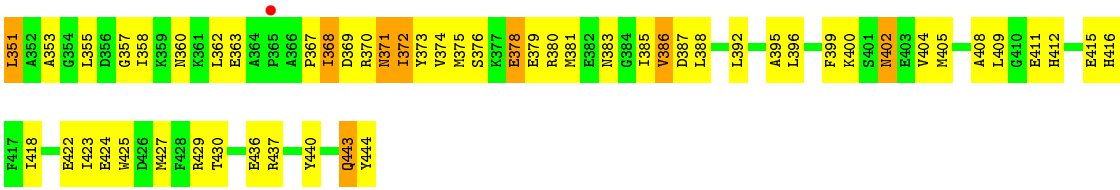
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.99Å 138.38Å 138.74Å 119.80° 90.19° 93.85°	Depositor
Resolution (Å)	84.25 – 3.10 84.25 – 3.10	Depositor EDS
% Data completeness (in resolution range)	85.7 (84.25-3.10) 71.7 (84.25-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.13Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.267 0.217 , 0.267	Depositor DCC
R_{free} test set	8288 reflections (7.53%)	DCC
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.6	EDS
Estimated twinning fraction	0.327 for -h,-k-l,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 110085 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42284	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4

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	0.39	0/3586	0.61	0/4849
1	B	0.40	0/3586	0.62	0/4849
1	C	0.42	0/3578	0.62	0/4838
1	D	0.41	0/3586	0.61	0/4849
1	E	0.41	0/3578	0.60	0/4837
1	F	0.43	0/3570	0.62	0/4826
1	G	0.41	0/3578	0.61	0/4837
1	H	0.41	0/3570	0.62	0/4826
1	I	0.42	0/3564	0.63	0/4818
1	J	0.43	0/3578	0.63	1/4837 (0.0%)
1	K	0.39	0/3578	0.61	0/4837
1	L	0.42	0/3590	0.63	0/4854
All	All	0.41	0/42942	0.62	1/58057 (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	L	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	2	ALA	CA-C-N	-6.09	103.80	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	296	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3443	310	0
1	B	3505	0	3443	285	0
1	C	3498	0	3435	295	0
1	D	3505	0	3443	308	0
1	E	3498	0	3436	329	0
1	F	3491	0	3428	342	0
1	G	3498	0	3436	303	0
1	H	3491	0	3428	294	0
1	I	3485	0	3423	298	0
1	J	3498	0	3436	318	0
1	K	3498	0	3436	314	0
1	L	3509	0	3446	301	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	A	17	0	0	4	0
4	B	27	0	0	1	0
4	C	28	0	0	1	0
4	D	20	0	0	3	0
4	E	17	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	24	0	0	1	0
4	G	21	0	0	4	0
4	H	20	0	0	2	0
4	I	23	0	0	2	0
4	J	12	0	0	1	0
4	K	22	0	0	1	0
4	L	22	0	0	2	0
All	All	42284	0	41233	3435	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (3435) 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:K:83:THR:HG21	1:K:89:VAL:H	1.13	1.09
1:F:286:THR:HG23	1:F:290:ASN:HD22	1.19	1.07
1:I:173:VAL:HG13	1:I:183:ILE:HD12	1.31	1.07
1:I:372:ILE:HG22	1:I:385:ILE:HD13	1.37	1.05
1:G:371:ASN:HD22	1:G:375:MET:HB3	1.18	1.04
1:E:9:ILE:HG13	1:E:74:LEU:HD12	1.39	1.04
1:C:372:ILE:HG22	1:C:385:ILE:HD13	1.40	1.02
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.37	1.02
1:E:319:LEU:HG	1:E:320:ILE:HD12	1.40	1.02
1:G:27:ASP:HA	1:G:57:ILE:HG23	1.41	1.02
1:J:98:ASN:HD22	1:J:102:THR:HG23	1.24	1.02
1:B:126:ASP:HB2	1:B:251:PHE:HB2	1.37	1.02
1:G:258:PHE:HB2	1:G:271:ALA:HB2	1.40	1.01
1:J:272:LYS:HA	1:J:275:ILE:HD12	1.42	1.01
1:F:13:VAL:HG13	1:F:18:VAL:HB	1.43	1.00
1:B:153:LYS:H	1:B:153:LYS:HE2	1.23	0.99
1:J:182:GLU:HB3	1:J:200:LYS:HE2	1.44	0.99
1:H:182:GLU:HB3	1:H:200:LYS:HD2	1.42	0.98
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.28	0.97
1:A:160:ALA:HB1	1:A:161:PRO:HD2	1.45	0.97
1:H:321:ARG:HG2	1:H:335:ARG:HD2	1.45	0.97
1:K:315:ASN:HD21	1:K:370:ARG:H	1.10	0.95
1:H:140:LEU:HD21	1:H:223:ARG:NH2	1.81	0.95
1:H:129:LEU:HD13	1:H:131:PRO:HD3	1.46	0.94
1:I:328:ILE:H	1:I:328:ILE:HD13	1.32	0.94
1:L:52:PHE:HE2	1:L:56:SER:HG	1.13	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:LEU:HD22	1:I:131:PRO:HG3	1.49	0.94
1:K:370:ARG:HH21	1:K:374:VAL:HG22	1.32	0.93
1:K:160:ALA:HB1	1:K:161:PRO:HD2	1.50	0.93
1:D:129:LEU:HD13	1:D:131:PRO:HD3	1.51	0.92
1:H:5:THR:H	1:H:8:ASP:HB2	1.34	0.92
1:J:386:VAL:HG12	1:J:387:ASP:H	1.31	0.92
1:F:371:ASN:HD21	1:F:373:TYR:HB2	1.32	0.92
1:B:325:SER:HB2	1:B:331:ARG:NH2	1.85	0.92
1:J:281:HIS:CD2	1:J:402:ASN:HD21	1.88	0.92
1:F:146:PRO:HG3	1:F:228:HIS:CD2	2.04	0.92
1:G:182:GLU:HB3	1:G:200:LYS:HD2	1.52	0.91
1:K:33:LYS:HA	1:L:158:ASP:HA	1.53	0.91
1:L:315:ASN:HD21	1:L:370:ARG:HA	1.36	0.91
1:F:429:ARG:HH21	1:L:300:VAL:HG22	1.33	0.91
1:I:57:ILE:HD11	1:I:96:ILE:HG12	1.53	0.91
1:H:74:LEU:H	1:H:74:LEU:HD22	1.35	0.91
1:E:325:SER:HB2	1:E:331:ARG:HH22	1.34	0.90
1:K:316:ARG:HH11	1:K:316:ARG:H	1.16	0.90
1:J:281:HIS:HD2	1:J:402:ASN:HD21	1.20	0.90
1:J:371:ASN:HD22	1:J:374:VAL:HG22	1.34	0.90
1:H:13:VAL:HG13	1:H:18:VAL:HB	1.51	0.90
1:B:370:ARG:HH22	1:B:375:MET:HG3	1.36	0.90
1:I:63:ILE:HG22	1:J:316:ARG:HD3	1.55	0.89
1:G:370:ARG:H	1:G:370:ARG:HD3	1.35	0.89
1:F:300:VAL:HG22	1:L:429:ARG:NH2	1.88	0.89
1:J:377:LYS:H	1:J:377:LYS:HD2	1.37	0.88
1:I:86:LYS:HB3	1:J:174:LEU:HD13	1.55	0.88
1:J:160:ALA:HB3	1:J:169:ARG:HH12	1.38	0.88
1:I:248:LEU:HD11	1:I:334:VAL:HG23	1.54	0.88
1:J:13:VAL:HG13	1:J:18:VAL:HB	1.52	0.88
1:L:55:SER:HB2	1:L:62:ARG:HG3	1.56	0.88
1:G:281:HIS:NE2	1:G:404:VAL:HG11	1.88	0.87
1:B:201:TYR:HB2	4:B:602:HOH:O	1.73	0.87
1:F:300:VAL:HG22	1:L:429:ARG:HH22	1.39	0.87
1:A:306:PRO:HB3	1:A:319:LEU:HA	1.53	0.87
1:B:429:ARG:HH21	1:H:390:ALA:HB1	1.37	0.87
1:D:150:LEU:HD13	1:D:192:PRO:HB2	1.56	0.87
1:F:286:THR:HG23	1:F:290:ASN:ND2	1.89	0.86
1:E:57:ILE:HD11	1:E:96:ILE:HG12	1.55	0.86
1:G:310:ALA:HB1	1:G:368:ILE:HG12	1.55	0.86
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:HIS:HD2	1:E:402:ASN:HD21	1.20	0.86
1:K:313:ALA:HA	1:K:321:ARG:HG3	1.56	0.86
1:E:319:LEU:HG	1:E:320:ILE:CD1	2.05	0.85
1:G:32:ILE:HD13	1:G:216:LEU:HD12	1.56	0.85
1:D:319:LEU:HD23	1:D:320:ILE:HG12	1.59	0.85
1:B:3:LYS:HB3	1:B:75:ASN:OD1	1.77	0.84
1:E:129:LEU:HD23	1:E:347:LEU:HD21	1.59	0.84
1:G:160:ALA:HB1	1:G:161:PRO:HD2	1.57	0.84
1:B:182:GLU:HB3	1:B:200:LYS:HD2	1.59	0.84
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.59	0.84
1:B:153:LYS:N	1:B:153:LYS:HE2	1.92	0.84
1:E:316:ARG:HB3	1:E:372:ILE:HD11	1.60	0.84
1:J:236:LEU:HB2	1:J:239:VAL:HG21	1.60	0.84
1:F:368:ILE:HG23	1:F:372:ILE:HD11	1.57	0.84
1:J:54:GLY:O	1:J:57:ILE:HG12	1.77	0.83
1:J:9:ILE:HG13	1:J:74:LEU:HD12	1.58	0.83
1:F:3:LYS:HB3	1:F:75:ASN:OD1	1.77	0.83
1:J:236:LEU:HB2	1:J:239:VAL:CG2	2.06	0.83
1:L:57:ILE:HD11	1:L:96:ILE:HG12	1.60	0.83
1:G:371:ASN:HB3	1:G:375:MET:HG2	1.60	0.83
1:I:280:LYS:HE3	1:I:281:HIS:HE2	1.43	0.83
1:F:45:ALA:HA	1:F:50:VAL:HG23	1.59	0.83
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.61	0.83
1:B:236:LEU:HD12	1:B:239:VAL:HG21	1.61	0.83
1:H:129:LEU:CD1	1:H:131:PRO:HD3	2.09	0.83
1:B:27:ASP:OD1	1:B:33:LYS:HE3	1.79	0.83
1:L:27:ASP:HA	1:L:57:ILE:HG23	1.60	0.82
1:G:236:LEU:HB2	1:G:239:VAL:CG2	2.09	0.82
1:F:182:GLU:HB3	1:F:200:LYS:HD2	1.60	0.82
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.59	0.82
1:L:386:VAL:HG12	1:L:387:ASP:H	1.43	0.82
1:J:275:ILE:O	1:J:279:VAL:HG23	1.80	0.82
1:F:300:VAL:HG21	1:L:430:THR:HG22	1.60	0.82
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.61	0.82
1:L:375:MET:HG3	1:L:379:GLU:HG3	1.60	0.82
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.14	0.81
1:K:83:THR:HG21	1:K:89:VAL:N	1.94	0.81
1:B:150:LEU:HD13	1:B:192:PRO:O	1.80	0.81
1:L:52:PHE:CZ	1:L:54:GLY:HA2	2.14	0.81
1:J:306:PRO:HG2	1:J:335:ARG:HB2	1.61	0.81
1:L:127:PHE:CE2	1:L:351:LEU:HG	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:SER:HB2	1:G:331:ARG:NH2	1.94	0.81
1:F:297:LYS:HD3	1:L:429:ARG:O	1.79	0.81
1:E:310:ALA:HB1	1:E:368:ILE:HG12	1.63	0.81
1:A:252:LYS:NZ	1:A:252:LYS:HB2	1.96	0.81
1:G:236:LEU:HB2	1:G:239:VAL:HG21	1.62	0.81
1:B:132:GLU:HB3	1:B:196:GLU:OE1	1.80	0.81
1:G:129:LEU:HD13	1:G:131:PRO:HD3	1.63	0.81
1:B:370:ARG:HH22	1:B:375:MET:CG	1.95	0.80
1:L:51:MET:HE1	1:L:67:ASP:HB3	1.61	0.80
1:C:402:ASN:O	1:C:406:VAL:HG23	1.82	0.80
1:B:325:SER:HB2	1:B:331:ARG:HH22	1.46	0.80
1:C:51:MET:HE3	1:C:67:ASP:HB3	1.64	0.80
1:B:281:HIS:NE2	1:B:404:VAL:HG21	1.97	0.80
1:H:41:GLN:HE22	1:I:200:LYS:NZ	1.78	0.80
1:L:166:GLU:O	1:L:168:CYS:N	2.14	0.80
1:E:286:THR:HG23	1:E:290:ASN:HD22	1.47	0.80
1:J:212:GLN:HA	1:J:212:GLN:OE1	1.81	0.80
1:E:314:GLN:HE22	1:E:321:ARG:HH21	1.30	0.80
1:H:160:ALA:HB1	1:H:161:PRO:HD2	1.63	0.80
1:C:310:ALA:HB2	1:C:385:ILE:HG23	1.64	0.79
1:I:5:THR:HG23	1:I:8:ASP:H	1.47	0.79
1:F:16:GLU:O	1:F:88:LYS:HE2	1.82	0.79
1:K:152:ASP:HB3	1:K:161:PRO:HG3	1.64	0.79
1:E:406:VAL:HG22	1:E:414:PHE:CE1	2.18	0.79
1:D:273:HIS:O	1:D:276:ALA:HB3	1.82	0.79
1:G:371:ASN:ND2	1:G:375:MET:HB3	1.97	0.79
1:E:314:GLN:NE2	1:E:321:ARG:HH21	1.81	0.79
1:J:389:PRO:HB2	1:J:394:GLU:HB3	1.64	0.79
1:E:140:LEU:HD12	1:E:226:GLY:C	2.03	0.79
1:I:27:ASP:HA	1:I:57:ILE:HG23	1.63	0.79
1:L:83:THR:HG21	1:L:89:VAL:HB	1.65	0.79
1:A:310:ALA:HB3	1:A:372:ILE:HD13	1.62	0.78
1:B:345:LEU:HD22	1:B:409:LEU:HD21	1.64	0.78
1:A:355:LEU:O	1:A:359:LYS:HG2	1.83	0.78
1:J:190:VAL:HG13	1:J:191:ALA:H	1.47	0.78
1:C:281:HIS:CE1	1:C:404:VAL:HG11	2.18	0.78
1:F:57:ILE:HD11	1:F:96:ILE:HG12	1.64	0.78
1:K:270:THR:HG22	1:K:358:ILE:HD12	1.63	0.78
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.14	0.78
1:J:98:ASN:ND2	1:J:102:THR:HG23	1.98	0.78
1:F:286:THR:CG2	1:F:290:ASN:HD22	1.95	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ILE:CG2	1:F:372:ILE:HD11	2.12	0.78
1:H:272:LYS:HE3	1:H:363:GLU:HA	1.64	0.78
1:H:98:ASN:HD21	1:H:104:PHE:HA	1.46	0.78
1:J:156:TYR:HB2	1:J:190:VAL:HA	1.65	0.78
1:L:67:ASP:O	1:L:68:MET:HG3	1.83	0.78
1:K:357:GLY:HA2	1:K:362:LEU:HD13	1.64	0.78
1:L:291:PRO:O	1:L:392:LEU:HD13	1.84	0.78
1:G:250:LEU:HB2	1:G:258:PHE:CZ	2.19	0.78
1:E:372:ILE:HD12	1:E:373:TYR:N	1.99	0.78
1:I:150:LEU:HD13	1:I:192:PRO:O	1.83	0.78
1:G:132:GLU:HA	1:G:198:ASP:HB3	1.64	0.77
1:H:380:ARG:NH1	1:H:380:ARG:HB2	1.98	0.77
1:G:160:ALA:HB2	1:G:188:HIS:HD2	1.50	0.77
1:C:436:GLU:OE2	1:I:297:LYS:HE3	1.85	0.77
1:F:232:MET:CE	1:L:440:TYR:HB2	2.13	0.77
1:A:135:PHE:HB3	1:A:231:PHE:CE1	2.19	0.77
1:E:257:ALA:O	1:E:270:THR:HB	1.84	0.77
1:G:13:VAL:HG13	1:G:18:VAL:HB	1.65	0.77
1:D:111:ASN:HD21	1:D:409:LEU:HA	1.50	0.77
1:F:309:VAL:HB	1:F:386:VAL:HG23	1.65	0.77
1:A:41:GLN:HE22	1:F:200:LYS:HE2	1.48	0.77
1:K:115:ILE:HG22	1:K:351:LEU:HD12	1.64	0.77
1:E:136:PHE:CD1	1:E:235:PRO:HG2	2.20	0.77
1:D:241:GLY:HA3	1:D:298:ARG:HG3	1.66	0.77
1:E:91:ARG:HD2	1:E:91:ARG:C	2.05	0.77
1:A:200:LYS:HZ1	1:B:41:GLN:HE22	1.32	0.77
1:L:78:VAL:HG13	1:L:91:ARG:HG3	1.66	0.77
1:K:316:ARG:HH12	1:K:372:ILE:HG13	1.49	0.77
1:E:160:ALA:HB1	1:E:161:PRO:HD2	1.67	0.77
1:G:86:LYS:HG3	1:H:174:LEU:HB3	1.66	0.77
1:K:127:PHE:CZ	1:K:248:LEU:HD22	2.19	0.77
1:B:271:ALA:O	1:B:275:ILE:HD12	1.85	0.77
1:I:406:VAL:HG22	1:I:414:PHE:CE1	2.20	0.77
1:C:164:LEU:HD11	1:D:224:LYS:HD3	1.65	0.77
1:D:91:ARG:HD2	1:D:91:ARG:C	2.05	0.77
1:F:160:ALA:HB1	1:F:161:PRO:HD2	1.65	0.76
1:E:273:HIS:CD2	1:E:361:LYS:HA	2.20	0.76
1:J:328:ILE:HD12	1:J:329:SER:N	2.00	0.76
1:H:273:HIS:CD2	1:H:361:LYS:HA	2.20	0.76
1:A:372:ILE:HG23	1:A:385:ILE:HD13	1.67	0.76
1:C:429:ARG:HH22	1:I:300:VAL:HA	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:ILE:O	1:I:13:VAL:HG23	1.85	0.76
1:B:159:LEU:CD1	1:C:22:ARG:HH11	1.99	0.76
1:G:399:PHE:HZ	1:G:409:LEU:HD22	1.49	0.76
1:G:21:ILE:HD13	1:G:42:LEU:HD13	1.66	0.76
1:J:30:GLY:HA2	1:J:342:ASN:ND2	2.01	0.76
1:L:109:ARG:HD2	1:L:344:TYR:CE2	2.21	0.75
1:H:309:VAL:HG23	1:H:386:VAL:O	1.86	0.75
1:B:429:ARG:HH12	1:H:300:VAL:HG23	1.51	0.75
1:C:136:PHE:HB3	1:C:138:PHE:HE1	1.52	0.75
1:A:273:HIS:CD2	1:A:361:LYS:HA	2.21	0.75
1:E:96:ILE:H	1:E:96:ILE:HD12	1.50	0.75
1:H:98:ASN:ND2	1:H:104:PHE:HA	2.00	0.75
1:J:176:LEU:HB2	1:J:183:ILE:HD11	1.68	0.75
1:A:129:LEU:HG	1:A:347:LEU:HD21	1.69	0.75
1:J:83:THR:HG21	1:J:89:VAL:HB	1.66	0.75
1:H:372:ILE:HD13	1:H:372:ILE:H	1.50	0.75
1:J:160:ALA:HB3	1:J:169:ARG:NH1	2.02	0.75
1:E:281:HIS:CD2	1:E:402:ASN:HD21	2.04	0.75
1:C:105:GLU:OE1	1:C:412:HIS:HB2	1.86	0.75
1:F:434:PRO:HA	1:F:437:ARG:HH12	1.51	0.75
1:G:4:TYR:HB3	1:G:9:ILE:HD11	1.69	0.75
1:H:242:SER:O	1:H:339:PRO:HD2	1.87	0.75
1:K:11:LYS:HG3	1:K:15:GLU:OE2	1.87	0.75
1:E:21:ILE:HD13	1:E:39:VAL:HA	1.68	0.74
1:F:98:ASN:N	1:F:98:ASN:HD22	1.83	0.74
1:F:232:MET:HE3	1:L:440:TYR:HB2	1.68	0.74
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.69	0.74
1:K:273:HIS:CD2	1:K:361:LYS:HA	2.21	0.74
1:D:129:LEU:HD22	1:D:130:GLY:N	2.03	0.74
1:F:312:SER:HB2	1:F:368:ILE:HB	1.69	0.74
1:I:225:HIS:O	1:I:227:LEU:HG	1.88	0.74
1:A:380:ARG:NH1	1:A:380:ARG:HB2	2.03	0.73
1:B:129:LEU:HG	1:B:347:LEU:HD21	1.70	0.73
1:H:106:GLY:O	1:H:413:LEU:HD21	1.86	0.73
1:E:136:PHE:HD1	1:E:235:PRO:HG2	1.52	0.73
1:E:100:ASP:O	1:E:102:THR:HG23	1.88	0.73
1:H:41:GLN:HE22	1:I:200:LYS:HZ2	1.34	0.73
1:D:309:VAL:HG13	1:D:319:LEU:HD22	1.70	0.73
1:A:206:ARG:HG2	1:A:206:ARG:HH11	1.52	0.73
1:I:260:ASP:O	1:I:266:GLN:HA	1.88	0.73
1:J:70:LEU:O	1:J:72:PRO:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ARG:HA	1:F:385:ILE:HB	1.71	0.73
1:E:76:THR:O	1:E:78:VAL:HG23	1.89	0.73
1:L:150:LEU:HD13	1:L:192:PRO:O	1.86	0.73
1:I:68:MET:HE3	1:I:98:ASN:HA	1.70	0.73
1:K:3:LYS:H	1:K:75:ASN:HB3	1.53	0.73
1:C:129:LEU:HD22	1:C:131:PRO:HD3	1.69	0.73
1:J:121:ASP:O	1:J:122:LEU:HD22	1.89	0.73
1:D:252:LYS:O	1:D:255:VAL:HG22	1.88	0.73
1:J:125:SER:H	1:J:252:LYS:HA	1.53	0.73
1:K:129:LEU:HD22	1:K:347:LEU:HD21	1.70	0.73
1:F:98:ASN:HD21	1:F:104:PHE:HA	1.54	0.73
1:D:328:ILE:HD12	1:D:329:SER:H	1.52	0.73
1:J:282:ALA:HA	1:J:285:PHE:CZ	2.23	0.72
1:B:148:LEU:HD21	1:H:437:ARG:HD3	1.71	0.72
1:E:158:ASP:OD1	1:F:33:LYS:HE2	1.89	0.72
1:K:247:ASN:HB3	1:K:331:ARG:HG3	1.70	0.72
1:D:243:GLY:HA3	1:D:298:ARG:HH12	1.55	0.72
1:D:310:ALA:HB1	1:D:368:ILE:HG21	1.71	0.72
1:E:371:ASN:HB3	1:E:375:MET:SD	2.28	0.72
1:B:377:LYS:O	1:B:381:MET:HG2	1.88	0.72
1:F:308:TYR:HA	1:F:387:ASP:HA	1.70	0.72
1:H:172:ILE:HD12	1:H:218:VAL:HA	1.72	0.72
1:J:310:ALA:HB1	1:J:368:ILE:HG21	1.71	0.72
1:D:259:PHE:CE2	1:D:326:ARG:HB3	2.24	0.72
1:L:287:ALA:HB2	1:L:395:ALA:HB1	1.70	0.72
1:L:116:LEU:O	1:L:119:MET:HG2	1.89	0.72
1:D:390:ALA:HB1	1:J:429:ARG:HE	1.55	0.72
1:B:349:VAL:HG22	1:B:405:MET:SD	2.30	0.72
1:E:191:ALA:HB2	1:E:240:ASN:HB3	1.70	0.72
1:H:57:ILE:HD11	1:H:96:ILE:HG12	1.70	0.72
1:G:128:ASN:HA	1:G:202:ALA:O	1.89	0.72
1:I:355:LEU:HD23	1:I:358:ILE:HD12	1.71	0.72
1:F:22:ARG:HD2	1:F:80:PHE:HE1	1.53	0.72
1:A:3:LYS:HB3	1:A:3:LYS:NZ	2.05	0.72
1:I:267:LEU:HD11	1:I:322:ILE:HD13	1.70	0.72
1:C:182:GLU:HG3	1:C:200:LYS:HD2	1.69	0.72
1:I:96:ILE:H	1:I:96:ILE:HD12	1.54	0.72
1:A:429:ARG:NH2	1:G:300:VAL:HG22	2.05	0.72
1:K:67:ASP:O	1:K:68:MET:HG3	1.90	0.72
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.71	0.72
1:C:55:SER:HB2	1:C:62:ARG:HG2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:LEU:O	1:H:116:LEU:HG	1.90	0.71
1:L:375:MET:HG2	1:L:380:ARG:HG2	1.71	0.71
1:L:51:MET:CE	1:L:67:ASP:HB3	2.20	0.71
1:D:140:LEU:HD21	1:D:228:HIS:HB2	1.72	0.71
1:C:366:ALA:HB1	1:C:367:PRO:HD2	1.70	0.71
1:K:310:ALA:HB2	1:K:372:ILE:HG21	1.71	0.71
1:A:429:ARG:HH22	1:G:300:VAL:HG22	1.56	0.71
1:G:183:ILE:HD12	1:G:183:ILE:H	1.55	0.71
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.73	0.71
1:D:236:LEU:HB2	1:D:239:VAL:CG2	2.20	0.71
1:L:82:TRP:HH2	1:L:217:VAL:HG22	1.55	0.71
1:J:72:PRO:HA	1:J:94:CYS:HB3	1.71	0.71
1:G:91:ARG:C	1:G:91:ARG:HD2	2.11	0.71
1:G:23:LEU:HB2	1:G:35:VAL:HG13	1.73	0.71
1:B:211:ILE:HG22	1:B:215:LYS:HE3	1.73	0.71
1:A:294:ASN:HB2	1:G:436:GLU:OE2	1.91	0.71
1:A:300:VAL:HG22	1:G:429:ARG:HH22	1.56	0.71
1:G:375:MET:HB2	1:G:379:GLU:HB2	1.73	0.71
1:B:160:ALA:HB1	1:B:161:PRO:HD2	1.72	0.71
1:K:316:ARG:NH1	1:K:316:ARG:H	1.88	0.71
1:L:189:GLU:HB2	1:L:194:GLN:HB3	1.72	0.71
1:I:248:LEU:O	1:I:331:ARG:HB2	1.91	0.71
1:J:52:PHE:CE2	1:J:54:GLY:HA2	2.26	0.71
1:D:345:LEU:HD22	1:D:409:LEU:HD22	1.73	0.70
1:F:437:ARG:HH11	1:F:437:ARG:HB2	1.56	0.70
1:C:150:LEU:CD1	1:C:192:PRO:HG2	2.21	0.70
1:G:402:ASN:O	1:G:406:VAL:HG23	1.91	0.70
1:G:34:ASN:HD22	1:G:34:ASN:C	1.93	0.70
1:L:91:ARG:C	1:L:91:ARG:HD2	2.11	0.70
1:E:236:LEU:O	1:E:239:VAL:HG22	1.91	0.70
1:A:45:ALA:HA	1:A:50:VAL:HG23	1.72	0.70
1:J:371:ASN:ND2	1:J:374:VAL:HG22	2.05	0.70
1:J:231:PHE:HB3	1:J:339:PRO:CB	2.20	0.70
1:A:252:LYS:HE3	1:A:253:ASN:HD22	1.56	0.70
1:C:267:LEU:HD21	1:C:326:ARG:NH1	2.07	0.70
1:L:402:ASN:ND2	1:L:404:VAL:HG12	2.07	0.70
1:A:34:ASN:HD22	1:A:34:ASN:C	1.94	0.70
1:C:380:ARG:HB2	1:C:380:ARG:HH11	1.55	0.70
1:G:375:MET:SD	1:G:380:ARG:HG2	2.31	0.70
1:F:129:LEU:HD22	1:F:131:PRO:HD3	1.73	0.70
1:A:224:LYS:HB2	1:F:164:LEU:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:TYR:H	1:B:201:TYR:HD1	1.39	0.70
1:C:182:GLU:CG	1:C:200:LYS:HD2	2.22	0.70
1:E:320:ILE:HG22	1:E:321:ARG:N	2.07	0.70
1:A:372:ILE:HG22	1:A:380:ARG:HH21	1.56	0.70
1:L:323:PRO:HD2	1:L:331:ARG:O	1.92	0.70
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.74	0.70
1:A:112:LEU:O	1:A:116:LEU:HG	1.92	0.70
1:J:414:PHE:O	1:J:418:ILE:HG12	1.91	0.70
1:B:368:ILE:HG21	1:B:385:ILE:HD11	1.73	0.70
1:F:59:GLY:O	1:F:62:ARG:HG3	1.91	0.70
1:J:310:ALA:HA	1:J:368:ILE:HG13	1.74	0.70
1:D:289:THR:O	1:D:341:ALA:HB2	1.92	0.70
1:C:58:GLU:O	1:C:61:VAL:HG23	1.91	0.70
1:D:142:GLU:CD	1:D:142:GLU:H	1.95	0.70
1:I:328:ILE:H	1:I:328:ILE:CD1	2.05	0.69
1:A:252:LYS:O	1:A:252:LYS:HG3	1.90	0.69
1:H:279:VAL:HG13	1:H:309:VAL:HG12	1.72	0.69
1:C:73:ASP:OD2	1:C:76:THR:HG23	1.90	0.69
1:K:404:VAL:HG23	1:K:405:MET:HE3	1.73	0.69
1:B:281:HIS:CD2	1:B:402:ASN:HD21	2.09	0.69
1:J:119:MET:SD	1:J:127:PHE:HB2	2.32	0.69
1:L:378:GLU:OE1	1:L:381:MET:HG3	1.92	0.69
1:K:85:GLU:HG2	1:L:170:ARG:HH12	1.58	0.69
1:K:325:SER:HB2	1:K:331:ARG:HH22	1.57	0.69
1:K:325:SER:HB2	1:K:331:ARG:NH2	2.06	0.69
1:K:404:VAL:HG23	1:K:405:MET:CE	2.22	0.69
1:A:127:PHE:CD2	1:A:351:LEU:HD13	2.28	0.69
1:G:368:ILE:HD13	1:G:372:ILE:HD11	1.72	0.69
1:H:310:ALA:HB1	1:H:368:ILE:HG12	1.72	0.69
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.73	0.69
1:I:375:MET:HB3	1:I:379:GLU:HB3	1.75	0.69
1:F:136:PHE:HB3	1:F:138:PHE:CE1	2.26	0.69
1:J:281:HIS:HD2	1:J:402:ASN:ND2	1.91	0.69
1:H:272:LYS:HD3	1:H:272:LYS:C	2.13	0.69
1:G:377:LYS:HA	1:G:380:ARG:NH1	2.08	0.69
1:A:231:PHE:HB3	1:A:339:PRO:HB2	1.73	0.69
1:J:129:LEU:HD23	1:J:130:GLY:N	2.07	0.69
1:C:293:VAL:HG23	1:I:440:TYR:OH	1.92	0.69
1:D:231:PHE:HB3	1:D:339:PRO:HB2	1.74	0.69
1:K:293:VAL:HG11	1:K:428:PHE:CD2	2.28	0.69
1:E:325:SER:HB3	1:E:329:SER:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ASN:O	1:G:115:ILE:HD13	1.93	0.69
1:B:236:LEU:HB2	1:B:239:VAL:CG2	2.23	0.69
1:D:119:MET:SD	1:D:127:PHE:HB2	2.33	0.69
1:E:440:TYR:HB2	1:K:232:MET:HE2	1.73	0.69
1:D:21:ILE:HD13	1:D:42:LEU:HD13	1.74	0.69
1:B:429:ARG:HH21	1:H:390:ALA:CB	2.06	0.68
1:E:96:ILE:N	1:E:96:ILE:HD12	2.08	0.68
1:L:353:ALA:HB2	1:L:405:MET:HE1	1.75	0.68
1:C:287:ALA:HB2	1:C:395:ALA:HB1	1.75	0.68
1:G:55:SER:O	1:G:62:ARG:HG2	1.91	0.68
1:D:247:ASN:HB3	1:D:331:ARG:HG3	1.75	0.68
1:H:437:ARG:NH1	4:H:602:HOH:O	2.26	0.68
1:D:236:LEU:O	1:D:239:VAL:HG22	1.92	0.68
1:E:440:TYR:HB2	1:K:232:MET:CE	2.22	0.68
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.28	0.68
1:D:13:VAL:HG13	1:D:18:VAL:HB	1.75	0.68
1:F:423:ILE:HD12	1:F:423:ILE:C	2.13	0.68
1:I:80:PHE:HE1	1:I:91:ARG:HG2	1.57	0.68
1:L:368:ILE:HD12	1:L:368:ILE:H	1.59	0.68
1:L:125:SER:HB3	1:L:251:PHE:O	1.93	0.68
1:L:129:LEU:HG	1:L:347:LEU:HD21	1.76	0.68
1:G:370:ARG:N	1:G:370:ARG:HD3	2.08	0.68
1:L:386:VAL:HG12	1:L:387:ASP:N	2.08	0.68
1:I:281:HIS:CE1	1:I:404:VAL:HG11	2.28	0.68
1:B:178:GLU:OE1	1:C:86:LYS:HD3	1.93	0.68
1:C:372:ILE:CG2	1:C:385:ILE:HD13	2.22	0.68
1:K:315:ASN:ND2	1:K:370:ARG:H	1.86	0.68
1:E:129:LEU:HD13	1:E:130:GLY:N	2.08	0.68
1:J:182:GLU:O	1:J:200:LYS:HB2	1.92	0.68
1:I:167:ASN:OD1	1:I:170:ARG:HB3	1.93	0.68
1:G:323:PRO:HG3	1:G:331:ARG:HG2	1.75	0.68
1:K:316:ARG:HH11	1:K:316:ARG:N	1.90	0.68
1:J:67:ASP:O	1:J:68:MET:HG3	1.93	0.68
1:B:441:MET:O	1:H:228:HIS:HE1	1.77	0.68
1:A:363:GLU:CD	1:A:363:GLU:H	1.96	0.68
1:E:314:GLN:HE22	1:E:321:ARG:NH2	1.91	0.68
1:C:402:ASN:OD1	1:C:404:VAL:HG12	1.94	0.68
1:K:233:PRO:C	1:K:235:PRO:HD3	2.14	0.68
1:G:34:ASN:ND2	1:G:34:ASN:C	2.47	0.67
1:C:169:ARG:HH22	1:C:188:HIS:HB2	1.59	0.67
1:C:129:LEU:O	1:C:201:TYR:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:THR:HG22	1:D:88:LYS:HD3	1.76	0.67
1:G:260:ASP:O	1:G:266:GLN:HA	1.94	0.67
1:D:300:VAL:HG13	1:D:301:PRO:HD2	1.73	0.67
1:G:160:ALA:HB1	1:G:161:PRO:CD	2.24	0.67
1:E:52:PHE:CE2	1:E:54:GLY:HA2	2.30	0.67
1:I:114:ARG:HH11	1:I:114:ARG:HB3	1.58	0.67
1:K:316:ARG:NH1	1:K:316:ARG:HB2	2.08	0.67
1:H:312:SER:HB2	1:H:368:ILE:HG22	1.74	0.67
1:E:178:GLU:OE2	1:F:86:LYS:HD2	1.95	0.67
1:J:295:SER:O	1:J:299:LEU:HD13	1.94	0.67
1:E:309:VAL:HG21	1:E:386:VAL:HG23	1.75	0.67
1:K:316:ARG:HH11	1:K:316:ARG:HB2	1.59	0.67
1:A:419:GLU:O	1:A:423:ILE:HD13	1.93	0.67
1:K:109:ARG:HD2	1:K:344:TYR:CE2	2.30	0.67
1:E:320:ILE:CG2	1:E:321:ARG:N	2.58	0.67
1:I:280:LYS:HE3	1:I:281:HIS:NE2	2.09	0.67
1:C:13:VAL:HG13	1:C:18:VAL:HB	1.76	0.67
1:D:116:LEU:O	1:D:120:GLU:HG3	1.95	0.67
1:K:259:PHE:HD1	1:K:326:ARG:HD2	1.58	0.67
1:K:58:GLU:O	1:K:61:VAL:HG22	1.95	0.67
1:G:160:ALA:HB2	1:G:188:HIS:CD2	2.29	0.67
1:F:423:ILE:HD12	1:F:424:GLU:N	2.09	0.67
1:I:23:LEU:HB2	1:I:35:VAL:HG13	1.77	0.67
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.30	0.67
1:F:40:SER:O	1:F:41:GLN:HG2	1.93	0.67
1:C:423:ILE:O	1:C:427:MET:HG3	1.93	0.67
1:I:127:PHE:CD2	1:I:351:LEU:HG	2.29	0.67
1:B:319:LEU:HG	1:B:320:ILE:HG13	1.77	0.67
1:A:30:GLY:HA2	1:A:342:ASN:ND2	2.10	0.67
1:L:21:ILE:HG12	1:L:42:LEU:HD13	1.76	0.67
1:C:232:MET:HE3	1:C:235:PRO:HB3	1.76	0.67
1:H:30:GLY:HA2	1:H:342:ASN:ND2	2.09	0.67
1:I:310:ALA:HB2	1:I:368:ILE:HD12	1.75	0.67
1:K:112:LEU:O	1:K:116:LEU:HG	1.95	0.67
1:E:155:GLY:HA3	4:E:616:HOH:O	1.94	0.66
1:G:267:LEU:HD21	1:G:326:ARG:HH12	1.61	0.66
1:K:309:VAL:HG13	1:K:319:LEU:HD23	1.76	0.66
1:I:97:TYR:CZ	1:I:103:PRO:HG3	2.30	0.66
1:J:142:GLU:H	1:J:142:GLU:CD	1.97	0.66
1:L:129:LEU:HD12	1:L:347:LEU:HD11	1.76	0.66
1:A:431:GLN:HE21	1:A:432:VAL:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:ASN:O	1:D:406:VAL:HG23	1.96	0.66
1:H:260:ASP:HB3	1:H:267:LEU:O	1.96	0.66
1:A:200:LYS:NZ	1:B:41:GLN:HE22	1.93	0.66
1:C:32:ILE:N	1:C:32:ILE:HD12	2.10	0.66
1:E:444:TYR:OXT	1:K:231:PHE:HB2	1.95	0.66
1:K:323:PRO:HD2	1:K:331:ARG:O	1.96	0.66
1:C:160:ALA:HB1	1:C:161:PRO:HD2	1.77	0.66
1:K:402:ASN:OD1	1:K:404:VAL:HG22	1.96	0.66
1:C:232:MET:HE2	1:I:441:MET:HA	1.77	0.66
1:F:319:LEU:HD12	1:F:336:SER:HB3	1.78	0.66
1:E:57:ILE:CD1	1:E:96:ILE:HG12	2.24	0.66
1:L:349:VAL:HG22	1:L:405:MET:SD	2.34	0.66
1:D:265:LEU:O	1:D:267:LEU:HD13	1.94	0.66
1:G:224:LYS:HD2	1:H:164:LEU:HD11	1.78	0.66
1:A:32:ILE:HD13	1:A:216:LEU:HD13	1.77	0.66
1:B:414:PHE:O	1:B:418:ILE:HD13	1.95	0.66
1:H:244:MET:H	1:H:338:ASP:HA	1.61	0.66
1:D:183:ILE:HD11	1:E:38:PRO:HG3	1.77	0.66
1:F:189:GLU:HA	1:F:189:GLU:OE1	1.96	0.66
1:I:105:GLU:HB3	4:I:608:HOH:O	1.96	0.66
1:K:295:SER:O	1:K:299:LEU:HD13	1.95	0.66
1:H:322:ILE:HD13	1:H:332:VAL:HA	1.77	0.66
1:H:5:THR:OG1	1:H:7:GLU:HG3	1.96	0.66
1:L:189:GLU:HA	1:L:189:GLU:OE1	1.93	0.66
1:E:331:ARG:HG2	1:E:331:ARG:HH21	1.60	0.66
1:B:372:ILE:HG21	1:B:385:ILE:HG21	1.77	0.66
1:B:345:LEU:HD22	1:B:409:LEU:CD2	2.25	0.66
1:A:131:PRO:CB	1:A:211:ILE:HD11	2.25	0.66
1:D:411:GLU:O	1:D:415:GLU:HG2	1.96	0.66
1:I:182:GLU:HB3	1:I:200:LYS:HE2	1.76	0.66
1:J:160:ALA:CB	1:J:169:ARG:HH12	2.08	0.66
1:E:234:LYS:HE3	1:E:239:VAL:O	1.96	0.66
1:E:378:GLU:HA	1:E:381:MET:HB3	1.77	0.66
1:B:129:LEU:HD22	1:B:130:GLY:N	2.10	0.65
1:L:82:TRP:HE1	1:L:221:ILE:CD1	2.09	0.65
1:G:314:GLN:HE22	1:L:66:SER:HA	1.59	0.65
1:I:368:ILE:HG21	1:I:372:ILE:HG23	1.78	0.65
1:A:310:ALA:HB2	1:A:385:ILE:HG23	1.77	0.65
1:J:236:LEU:O	1:J:239:VAL:HG22	1.95	0.65
1:E:300:VAL:HG22	1:K:429:ARG:NH2	2.11	0.65
1:B:84:ALA:HB3	1:B:87:GLY:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:LEU:HB2	1:D:239:VAL:HG22	1.77	0.65
1:D:18:VAL:HA	1:D:88:LYS:HB2	1.78	0.65
1:B:68:MET:HG2	1:B:99:PRO:HD3	1.79	0.65
1:K:78:VAL:HB	1:K:91:ARG:HG3	1.77	0.65
1:L:313:ALA:HA	1:L:322:ILE:H	1.60	0.65
1:F:4:TYR:HB3	1:F:9:ILE:HD11	1.78	0.65
1:E:264:ASP:N	1:E:264:ASP:OD2	2.29	0.65
1:C:119:MET:SD	1:C:127:PHE:HB2	2.37	0.65
1:L:135:PHE:HB3	1:L:231:PHE:CE1	2.31	0.65
1:B:200:LYS:HE2	1:C:41:GLN:OE1	1.96	0.65
1:F:168:CYS:O	1:F:172:ILE:HG12	1.97	0.65
1:B:129:LEU:HD12	1:B:207:SER:HB3	1.79	0.65
1:C:331:ARG:HG2	1:C:331:ARG:HH21	1.61	0.65
1:K:315:ASN:HB3	1:K:318:PRO:HG3	1.78	0.65
1:I:248:LEU:CD1	1:I:334:VAL:HG23	2.26	0.65
1:I:274:PHE:CE2	1:I:332:VAL:HG21	2.32	0.65
1:E:129:LEU:CD2	1:E:347:LEU:HD21	2.26	0.65
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.31	0.65
1:A:37:ILE:HG22	1:F:185:ALA:HA	1.77	0.65
1:A:191:ALA:HB2	1:A:240:ASN:HB3	1.79	0.65
1:G:383:ASN:HB2	1:G:385:ILE:HG12	1.78	0.65
1:E:429:ARG:HH22	1:K:300:VAL:HG12	1.61	0.65
1:A:357:GLY:HA2	1:A:362:LEU:HB2	1.78	0.65
1:K:261:GLU:HA	1:K:266:GLN:NE2	2.12	0.65
1:A:400:LYS:HE2	1:A:418:ILE:HD13	1.79	0.65
1:D:205:VAL:HG23	1:D:206:ARG:H	1.61	0.65
1:F:205:VAL:HG13	1:F:206:ARG:N	2.12	0.65
1:C:273:HIS:NE2	1:C:361:LYS:HE3	2.10	0.65
1:G:267:LEU:HD21	1:G:326:ARG:NH1	2.11	0.65
1:G:421:LYS:HD3	1:G:424:GLU:OE2	1.96	0.65
1:H:328:ILE:H	1:H:328:ILE:HD13	1.61	0.65
1:L:271:ALA:O	1:L:275:ILE:HG12	1.96	0.65
1:C:314:GLN:HE22	1:D:65:GLU:C	2.01	0.65
1:K:136:PHE:HB2	1:K:230:THR:HG23	1.78	0.65
1:K:33:LYS:HG2	1:L:158:ASP:HB3	1.78	0.65
1:F:282:ALA:CB	1:F:319:LEU:HD21	2.27	0.65
1:A:22:ARG:HH22	1:F:167:ASN:HD21	1.44	0.65
1:H:37:ILE:HG22	1:I:185:ALA:HB2	1.79	0.65
1:H:315:ASN:HD22	1:H:373:TYR:HE1	1.45	0.65
1:B:159:LEU:HD12	1:C:22:ARG:HH11	1.62	0.64
1:I:114:ARG:NH1	1:I:114:ARG:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:MET:H	1:A:338:ASP:HA	1.61	0.64
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.78	0.64
1:A:431:GLN:NE2	1:A:432:VAL:H	1.94	0.64
1:B:289:THR:HB	1:B:337:VAL:HG22	1.78	0.64
1:A:131:PRO:CG	1:A:211:ILE:HD11	2.28	0.64
1:G:91:ARG:HD2	1:G:92:PHE:N	2.12	0.64
1:B:261:GLU:C	1:B:262:ASN:HD22	2.00	0.64
1:H:250:LEU:HB2	1:H:258:PHE:CE2	2.32	0.64
1:I:176:LEU:O	1:I:181:PHE:HB2	1.95	0.64
1:B:370:ARG:NH2	1:B:375:MET:HG3	2.10	0.64
1:C:160:ALA:HB2	1:C:169:ARG:HH22	1.61	0.64
1:L:399:PHE:HD2	1:L:418:ILE:HD11	1.62	0.64
1:C:297:LYS:HG2	1:I:431:GLN:O	1.96	0.64
1:A:161:PRO:HD3	4:A:616:HOH:O	1.96	0.64
1:H:272:LYS:HZ1	1:H:364:ALA:H	1.45	0.64
1:C:160:ALA:HB2	1:C:169:ARG:NH2	2.12	0.64
1:F:19:LYS:HG3	1:F:86:LYS:O	1.97	0.64
1:C:116:LEU:O	1:C:119:MET:HB3	1.97	0.64
1:G:122:LEU:HD11	1:G:359:LYS:HG3	1.79	0.64
1:F:338:ASP:HB2	1:F:339:PRO:HD2	1.80	0.64
1:D:127:PHE:CE2	1:D:351:LEU:HD23	2.33	0.64
1:E:158:ASP:HA	1:F:33:LYS:HG2	1.78	0.64
1:C:24:GLN:NE2	1:C:91:ARG:HH11	1.95	0.64
1:K:293:VAL:HG11	1:K:428:PHE:CE2	2.32	0.64
1:J:91:ARG:HD2	1:J:91:ARG:C	2.18	0.64
1:G:129:LEU:CD1	1:G:131:PRO:HD3	2.27	0.64
1:A:150:LEU:HD13	1:A:192:PRO:O	1.98	0.64
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.33	0.64
1:A:23:LEU:HB2	1:A:35:VAL:HG13	1.78	0.64
1:K:251:PHE:HA	1:K:255:VAL:O	1.97	0.64
1:L:306:PRO:HG2	1:L:335:ARG:O	1.98	0.64
1:J:160:ALA:HB1	1:J:161:PRO:HD2	1.79	0.64
1:H:396:LEU:O	1:H:400:LYS:HG2	1.97	0.64
1:C:409:LEU:O	1:C:413:LEU:HB2	1.98	0.64
1:C:261:GLU:HA	1:C:266:GLN:HE21	1.62	0.64
1:L:9:ILE:HA	1:L:12:LEU:HD12	1.80	0.64
1:C:136:PHE:HB3	1:C:138:PHE:CE1	2.31	0.64
1:A:34:ASN:ND2	1:A:34:ASN:C	2.51	0.64
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.45	0.64
1:D:45:ALA:HA	1:D:50:VAL:HG23	1.80	0.64
1:D:396:LEU:HD11	1:D:421:LYS:HB3	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:HIS:HE1	1:F:196:GLU:OE1	1.81	0.64
1:E:322:ILE:HD12	1:E:322:ILE:N	2.13	0.64
1:B:236:LEU:HB2	1:B:239:VAL:HG22	1.78	0.64
1:E:300:VAL:HG22	1:K:429:ARG:HH22	1.63	0.64
1:K:46:LEU:O	1:K:47:ASP:HB2	1.98	0.64
1:H:236:LEU:HB2	1:H:239:VAL:CG2	2.27	0.64
1:F:73:ASP:OD1	1:F:76:THR:HG23	1.97	0.64
1:L:315:ASN:ND2	1:L:370:ARG:HA	2.11	0.63
1:A:311:TRP:HB3	1:A:320:ILE:HB	1.80	0.63
1:F:377:LYS:HA	1:F:380:ARG:HG3	1.80	0.63
1:B:147:THR:CG2	1:B:149:GLU:HG3	2.28	0.63
1:C:241:GLY:HA3	1:C:298:ARG:HG3	1.81	0.63
1:I:135:PHE:HB3	1:I:231:PHE:CE1	2.33	0.63
1:K:309:VAL:HB	1:K:386:VAL:O	1.99	0.63
1:L:48:ASN:HB3	1:L:71:TYR:CE1	2.33	0.63
1:K:307:CYS:H	1:K:317:SER:HB2	1.63	0.63
1:J:72:PRO:CA	1:J:94:CYS:HB3	2.27	0.63
1:I:98:ASN:HB3	1:I:100:ASP:OD1	1.98	0.63
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.78	0.63
1:F:402:ASN:O	1:F:406:VAL:HG23	1.97	0.63
1:A:37:ILE:HG22	1:F:185:ALA:CB	2.29	0.63
1:I:279:VAL:HG13	1:I:309:VAL:HG12	1.81	0.63
1:I:295:SER:O	1:I:299:LEU:HD23	1.99	0.63
1:J:386:VAL:HG12	1:J:387:ASP:N	2.07	0.63
1:G:160:ALA:HB3	1:G:169:ARG:NH1	2.14	0.63
1:C:150:LEU:HD13	1:C:192:PRO:HG2	1.80	0.63
1:F:440:TYR:HB2	1:L:232:MET:HE3	1.79	0.63
1:B:19:LYS:HA	1:B:39:VAL:HG11	1.80	0.63
1:K:35:VAL:HG11	1:K:70:LEU:HD11	1.79	0.63
1:E:9:ILE:O	1:E:13:VAL:HG23	1.99	0.63
1:E:368:ILE:HG21	1:E:372:ILE:HG23	1.81	0.63
1:A:78:VAL:HG12	1:A:91:ARG:HG3	1.80	0.63
1:C:178:GLU:OE1	1:D:86:LYS:HD3	1.99	0.63
1:B:58:GLU:HB3	1:B:61:VAL:HG23	1.81	0.63
1:F:34:ASN:C	1:F:34:ASN:HD22	2.00	0.63
1:K:310:ALA:HB3	1:K:372:ILE:HD13	1.80	0.63
1:K:316:ARG:HE	1:K:370:ARG:CZ	2.11	0.63
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.80	0.63
1:I:129:LEU:HD22	1:I:131:PRO:CG	2.27	0.63
1:E:402:ASN:O	1:E:406:VAL:HG23	1.99	0.63
1:E:264:ASP:C	1:E:266:GLN:H	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:LEU:HD13	1:F:192:PRO:HB2	1.80	0.63
1:H:21:ILE:HG22	1:H:90:ALA:HB3	1.80	0.63
1:J:399:PHE:CE1	1:J:405:MET:HB3	2.34	0.63
1:G:406:VAL:HG22	1:G:414:PHE:CE1	2.33	0.63
1:F:98:ASN:ND2	1:F:98:ASN:N	2.47	0.63
1:E:430:THR:HG22	1:K:300:VAL:HG11	1.80	0.63
1:A:418:ILE:O	1:A:422:GLU:HG3	1.99	0.63
1:A:22:ARG:NH2	1:F:167:ASN:HD21	1.97	0.63
1:I:55:SER:O	1:I:58:GLU:HB2	1.97	0.63
1:G:306:PRO:HG2	1:G:335:ARG:HH21	1.64	0.63
1:F:129:LEU:HD23	1:F:130:GLY:N	2.14	0.62
1:E:290:ASN:HB3	1:E:295:SER:HB3	1.81	0.62
1:A:207:SER:O	1:A:211:ILE:HG12	1.99	0.62
1:D:300:VAL:CG1	1:D:301:PRO:HD2	2.28	0.62
1:D:183:ILE:CD1	1:E:38:PRO:HG3	2.29	0.62
1:B:19:LYS:HA	1:B:39:VAL:CG1	2.29	0.62
1:J:234:LYS:HB3	1:J:294:ASN:HD21	1.63	0.62
1:K:98:ASN:ND2	1:K:104:PHE:HA	2.14	0.62
1:K:298:ARG:O	1:K:298:ARG:HG3	1.97	0.62
1:E:129:LEU:HD12	1:E:131:PRO:HD3	1.81	0.62
1:B:311:TRP:CE3	1:B:322:ILE:HD13	2.34	0.62
1:A:159:LEU:HD21	1:B:22:ARG:HE	1.64	0.62
1:I:189:GLU:HB3	1:I:194:GLN:NE2	2.14	0.62
1:G:37:ILE:O	1:G:37:ILE:HG13	1.99	0.62
1:A:184:GLU:HG2	4:A:604:HOH:O	1.97	0.62
1:G:48:ASN:OD1	1:G:71:TYR:HA	1.98	0.62
1:E:9:ILE:CG1	1:E:74:LEU:HD12	2.24	0.62
1:I:274:PHE:HE2	1:I:332:VAL:HG21	1.64	0.62
1:C:169:ARG:HD2	1:D:36:GLU:OE1	1.99	0.62
1:F:434:PRO:HA	1:F:437:ARG:NH1	2.14	0.62
1:H:316:ARG:HB3	1:H:373:TYR:CD1	2.33	0.62
1:H:20:TYR:HB3	1:H:89:VAL:HG22	1.80	0.62
1:F:282:ALA:HB1	1:F:319:LEU:HD21	1.81	0.62
1:C:112:LEU:HD12	1:C:344:TYR:HD2	1.64	0.62
1:L:114:ARG:NH2	1:L:115:ILE:HD11	2.14	0.62
1:D:162:THR:O	1:D:164:LEU:N	2.29	0.62
1:E:285:PHE:HB2	1:E:349:VAL:HG13	1.81	0.62
1:F:33:LYS:NZ	1:F:56:SER:O	2.33	0.62
1:F:24:GLN:NE2	1:F:91:ARG:HH11	1.98	0.62
1:J:402:ASN:O	1:J:406:VAL:HG23	1.99	0.62
1:A:283:THR:HG22	1:A:388:LEU:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:370:ARG:HH11	1:H:370:ARG:HG3	1.65	0.62
1:A:431:GLN:HE21	1:A:432:VAL:H	1.48	0.62
1:J:104:PHE:CZ	1:J:106:GLY:HA3	2.35	0.62
1:B:232:MET:HE3	1:H:440:TYR:HB2	1.81	0.62
1:B:232:MET:CE	1:H:440:TYR:HB2	2.30	0.62
1:J:95:ASP:HB3	1:J:110:ASN:HD21	1.63	0.62
1:J:115:ILE:HD11	1:J:408:ALA:O	2.00	0.62
1:J:325:SER:HB3	1:J:329:SER:HB3	1.80	0.62
1:K:253:ASN:O	1:K:255:VAL:HG23	1.99	0.62
1:E:169:ARG:HH11	1:E:195:HIS:HD2	1.46	0.62
1:D:104:PHE:CZ	1:D:106:GLY:HA3	2.34	0.62
1:F:21:ILE:HG13	1:F:42:LEU:HD13	1.81	0.62
1:F:371:ASN:ND2	1:F:373:TYR:HB2	2.10	0.62
1:E:282:ALA:HA	1:E:285:PHE:CZ	2.35	0.62
1:H:380:ARG:HH11	1:H:380:ARG:HB2	1.64	0.62
1:L:372:ILE:CG2	1:L:385:ILE:HG21	2.30	0.62
1:F:183:ILE:HD12	1:F:197:ILE:HG22	1.80	0.62
1:L:355:LEU:HD23	1:L:358:ILE:HD12	1.82	0.62
1:D:273:HIS:CE1	1:D:361:LYS:HA	2.35	0.62
1:A:312:SER:HB3	1:A:315:ASN:HD22	1.64	0.62
1:B:197:ILE:HD12	1:B:214:PHE:CZ	2.35	0.62
1:H:138:PHE:HB3	1:H:147:THR:O	2.00	0.62
1:D:243:GLY:HA3	1:D:298:ARG:NH1	2.14	0.62
1:L:74:LEU:H	1:L:74:LEU:HD22	1.64	0.62
1:C:380:ARG:HB2	1:C:380:ARG:NH1	2.15	0.61
1:C:267:LEU:HD21	1:C:326:ARG:HH12	1.64	0.61
1:F:321:ARG:C	1:F:322:ILE:HD12	2.20	0.61
1:H:86:LYS:HE2	1:H:86:LYS:HA	1.81	0.61
1:H:4:TYR:HB3	1:H:9:ILE:HG13	1.82	0.61
1:H:308:TYR:HB3	1:H:385:ILE:HG23	1.81	0.61
1:E:161:PRO:O	1:E:167:ASN:ND2	2.33	0.61
1:D:289:THR:C	1:D:290:ASN:HD22	2.03	0.61
1:C:282:ALA:C	1:C:284:SER:H	2.03	0.61
1:C:96:ILE:N	1:C:96:ILE:HD12	2.14	0.61
1:L:9:ILE:HG21	1:L:92:PHE:HZ	1.64	0.61
1:G:267:LEU:HD11	1:G:322:ILE:HG21	1.83	0.61
1:I:57:ILE:CD1	1:I:96:ILE:HG12	2.27	0.61
1:A:252:LYS:HE3	1:A:253:ASN:ND2	2.15	0.61
1:H:160:ALA:HB1	1:H:161:PRO:CD	2.31	0.61
1:B:381:MET:HE2	1:B:381:MET:N	2.16	0.61
1:D:396:LEU:O	1:D:400:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PHE:HB2	1:B:92:PHE:HE2	1.65	0.61
1:I:287:ALA:HB2	1:I:395:ALA:HB1	1.82	0.61
1:L:236:LEU:HD12	1:L:239:VAL:HG21	1.83	0.61
1:L:316:ARG:HD3	1:L:370:ARG:HH22	1.66	0.61
1:L:273:HIS:HB3	1:L:357:GLY:O	2.00	0.61
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.82	0.61
1:H:202:ALA:HB3	1:H:207:SER:HB2	1.81	0.61
1:J:156:TYR:HA	1:J:188:HIS:O	2.00	0.61
1:I:35:VAL:HG11	1:I:70:LEU:CD2	2.30	0.61
1:F:244:MET:H	1:F:338:ASP:HA	1.65	0.61
1:E:20:TYR:O	1:E:89:VAL:HG13	2.01	0.61
1:B:164:LEU:HD11	1:C:224:LYS:HG3	1.83	0.61
1:F:399:PHE:CE1	1:F:405:MET:HB3	2.35	0.61
1:D:264:ASP:C	1:D:266:GLN:H	2.03	0.61
1:I:129:LEU:O	1:I:201:TYR:HA	2.00	0.61
1:B:315:ASN:HB3	1:B:318:PRO:HD3	1.83	0.61
1:I:127:PHE:CE2	1:I:351:LEU:HG	2.35	0.61
1:G:236:LEU:HB2	1:G:239:VAL:HG22	1.83	0.61
1:B:281:HIS:HD2	1:B:402:ASN:HD21	1.46	0.61
1:F:16:GLU:O	1:F:17:ASN:HB3	2.01	0.61
1:E:136:PHE:CE2	1:E:194:GLN:HB2	2.35	0.61
1:A:211:ILE:HG21	1:A:343:PRO:HG3	1.82	0.61
1:F:436:GLU:OE2	1:L:297:LYS:HE3	2.01	0.61
1:K:45:ALA:HA	1:K:50:VAL:HG21	1.82	0.61
1:J:176:LEU:O	1:J:181:PHE:HB2	1.99	0.61
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.36	0.61
1:E:139:LYS:HA	1:E:227:LEU:HD23	1.83	0.61
1:K:281:HIS:CD2	1:K:402:ASN:HD21	2.19	0.61
1:L:372:ILE:HG21	1:L:385:ILE:HG21	1.82	0.61
1:I:320:ILE:N	1:I:320:ILE:HD12	2.16	0.61
1:I:289:THR:HB	1:I:337:VAL:HG22	1.83	0.61
1:F:119:MET:HA	1:F:355:LEU:HD11	1.82	0.61
1:K:236:LEU:HB2	1:K:239:VAL:CG2	2.30	0.61
1:I:310:ALA:CB	1:I:368:ILE:HD12	2.31	0.61
1:G:311:TRP:CB	1:G:320:ILE:HB	2.31	0.61
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.81	0.61
1:A:45:ALA:HA	1:A:50:VAL:CG2	2.30	0.61
1:H:311:TRP:CZ2	1:H:367:PRO:HB3	2.36	0.61
1:C:337:VAL:HG12	1:C:338:ASP:N	2.16	0.61
1:E:148:LEU:HD22	1:E:148:LEU:H	1.64	0.61
1:A:5:THR:H	1:A:8:ASP:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PRO:HB3	1:A:211:ILE:HD11	1.83	0.61
1:A:400:LYS:HB3	1:A:418:ILE:CD1	2.30	0.61
1:B:120:GLU:C	1:B:122:LEU:H	2.02	0.61
1:H:183:ILE:N	1:H:183:ILE:HD12	2.15	0.61
1:K:160:ALA:HB1	1:K:161:PRO:CD	2.26	0.60
1:D:248:LEU:O	1:D:331:ARG:HB2	2.00	0.60
1:G:312:SER:HB3	1:G:315:ASN:HB2	1.82	0.60
1:B:163:ASP:OD1	1:C:89:VAL:HG21	2.01	0.60
1:F:236:LEU:HD12	1:F:239:VAL:HG22	1.82	0.60
1:I:32:ILE:HG21	1:I:216:LEU:HD12	1.82	0.60
1:B:436:GLU:OE2	1:H:297:LYS:HE3	2.01	0.60
1:A:252:LYS:HB2	1:A:252:LYS:HZ2	1.64	0.60
1:D:249:SER:HB3	1:D:331:ARG:HB3	1.84	0.60
1:H:57:ILE:CD1	1:H:96:ILE:HG12	2.31	0.60
1:A:127:PHE:CE2	1:A:351:LEU:HD13	2.37	0.60
1:C:231:PHE:HB2	1:I:444:TYR:OXT	2.01	0.60
1:D:260:ASP:O	1:D:266:GLN:HA	2.01	0.60
1:K:380:ARG:HA	1:K:383:ASN:HD22	1.65	0.60
1:G:169:ARG:HG3	1:G:195:HIS:ND1	2.16	0.60
1:I:349:VAL:HG22	1:I:405:MET:SD	2.41	0.60
1:H:166:GLU:OE2	1:H:227:LEU:HD11	2.01	0.60
1:I:150:LEU:CD1	1:I:192:PRO:HB2	2.32	0.60
1:C:159:LEU:HD11	1:D:22:ARG:HD3	1.83	0.60
1:J:129:LEU:HD23	1:J:130:GLY:H	1.67	0.60
1:D:259:PHE:CD2	1:D:326:ARG:HB3	2.36	0.60
1:I:118:GLU:O	1:I:122:LEU:HD13	2.02	0.60
1:L:323:PRO:HG3	1:L:331:ARG:HG3	1.82	0.60
1:B:197:ILE:HD12	1:B:214:PHE:CE1	2.36	0.60
1:A:9:ILE:HG13	1:A:74:LEU:HD12	1.82	0.60
1:K:150:LEU:CD1	1:K:192:PRO:HG2	2.31	0.60
1:G:20:TYR:CZ	1:G:36:GLU:HB3	2.36	0.60
1:D:316:ARG:NH1	1:E:63:ILE:HA	2.16	0.60
1:F:27:ASP:HB2	1:F:57:ILE:O	2.01	0.60
1:D:111:ASN:O	1:D:115:ILE:HD13	2.00	0.60
1:K:248:LEU:O	1:K:331:ARG:HB2	2.02	0.60
1:D:377:LYS:HG3	1:D:380:ARG:NH2	2.15	0.60
1:H:84:ALA:HB3	1:H:87:GLY:O	2.02	0.60
1:D:129:LEU:HD12	1:D:207:SER:HB3	1.82	0.60
1:J:236:LEU:HB2	1:J:239:VAL:HG22	1.80	0.60
1:F:283:THR:O	1:F:398:GLU:HG2	2.01	0.60
1:E:297:LYS:HE3	1:K:436:GLU:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ILE:HD12	1:B:96:ILE:H	1.65	0.60
1:K:37:ILE:HD13	1:K:41:GLN:HB2	1.82	0.60
1:H:2:ALA:N	4:H:613:HOH:O	2.34	0.60
1:I:316:ARG:HB3	1:I:373:TYR:CE1	2.37	0.60
1:J:57:ILE:HG13	1:J:96:ILE:HD13	1.84	0.60
1:F:440:TYR:OH	1:L:293:VAL:HB	2.02	0.60
1:A:329:SER:O	1:A:331:ARG:HG2	2.02	0.60
1:L:145:GLU:OE2	1:L:146:PRO:HD2	2.01	0.60
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.83	0.60
1:K:83:THR:HB	1:K:88:LYS:HA	1.84	0.60
1:B:430:THR:HG22	1:H:300:VAL:HG21	1.83	0.60
1:A:206:ARG:CG	1:A:206:ARG:HH11	2.13	0.60
1:G:224:LYS:CD	1:H:164:LEU:HD11	2.32	0.60
1:I:136:PHE:CE2	1:I:194:GLN:HB2	2.36	0.60
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.35	0.60
1:D:6:ARG:HH11	1:D:6:ARG:HG3	1.67	0.60
1:K:55:SER:O	1:K:62:ARG:HG2	2.02	0.60
1:L:286:THR:HG23	1:L:290:ASN:ND2	2.17	0.60
1:F:32:ILE:HD13	1:F:216:LEU:HD13	1.83	0.60
1:E:19:LYS:HD3	1:E:39:VAL:HG11	1.83	0.60
1:E:326:ARG:HG2	1:E:326:ARG:NH1	2.17	0.60
1:L:48:ASN:HB3	1:L:71:TYR:CD1	2.36	0.60
1:F:100:ASP:O	1:F:102:THR:N	2.34	0.60
1:J:206:ARG:HG3	1:J:206:ARG:HH11	1.65	0.60
1:A:319:LEU:HD22	1:A:320:ILE:CD1	2.31	0.60
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.32	0.60
1:K:119:MET:HG2	1:K:124:PHE:HB2	1.84	0.60
1:B:159:LEU:HD11	1:C:22:ARG:HH11	1.65	0.60
1:E:271:ALA:O	1:E:275:ILE:HG12	2.02	0.60
1:D:325:SER:HB3	1:D:331:ARG:HH21	1.66	0.60
1:H:96:ILE:HD12	1:H:96:ILE:N	2.17	0.60
1:H:21:ILE:HD13	1:H:21:ILE:H	1.66	0.60
1:E:176:LEU:O	1:E:181:PHE:HB2	2.01	0.59
1:B:139:LYS:O	1:B:147:THR:HB	2.02	0.59
1:D:183:ILE:H	1:D:183:ILE:HD13	1.66	0.59
1:C:197:ILE:HD12	1:C:214:PHE:CE1	2.37	0.59
1:G:282:ALA:HA	1:G:285:PHE:CZ	2.37	0.59
1:C:402:ASN:HD21	1:C:404:VAL:CG1	2.15	0.59
1:D:91:ARG:HD2	1:D:92:PHE:N	2.17	0.59
1:D:325:SER:HB3	1:D:331:ARG:NH2	2.16	0.59
1:H:127:PHE:HE2	1:H:347:LEU:HD12	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:PRO:HG3	1:H:228:HIS:CD2	2.36	0.59
1:H:328:ILE:N	1:H:328:ILE:HD13	2.17	0.59
1:C:260:ASP:HB2	1:C:268:SER:HB3	1.84	0.59
1:I:372:ILE:HG13	1:I:373:TYR:CE1	2.38	0.59
1:K:306:PRO:HB3	1:K:319:LEU:HA	1.85	0.59
1:A:300:VAL:HG22	1:G:429:ARG:HH12	1.66	0.59
1:K:383:ASN:HB2	1:K:385:ILE:HG13	1.83	0.59
1:D:372:ILE:HG13	1:D:373:TYR:HD1	1.66	0.59
1:I:160:ALA:HB1	1:I:161:PRO:HD2	1.83	0.59
1:E:314:GLN:NE2	1:F:65:GLU:HB3	2.16	0.59
1:G:258:PHE:HB3	1:G:270:THR:HB	1.83	0.59
1:F:96:ILE:N	1:F:96:ILE:HD12	2.17	0.59
1:F:437:ARG:HD3	1:L:148:LEU:HD21	1.84	0.59
1:H:127:PHE:CE2	1:H:347:LEU:HD12	2.38	0.59
1:I:163:ASP:HA	1:I:167:ASN:HD22	1.67	0.59
1:J:11:LYS:HG3	1:J:15:GLU:CD	2.22	0.59
1:G:325:SER:HB2	1:G:331:ARG:HH22	1.67	0.59
1:K:315:ASN:HD21	1:K:370:ARG:N	1.91	0.59
1:A:122:LEU:HD21	1:A:359:LYS:HB3	1.84	0.59
1:E:161:PRO:HB3	1:F:223:ARG:HH12	1.67	0.59
1:C:200:LYS:HE2	1:D:41:GLN:OE1	2.01	0.59
1:D:316:ARG:HH11	1:E:63:ILE:HA	1.66	0.59
1:G:368:ILE:HD13	1:G:372:ILE:CD1	2.31	0.59
1:G:57:ILE:C	1:G:59:GLY:H	2.06	0.59
1:D:83:THR:CG2	1:D:88:LYS:HD3	2.32	0.59
1:K:316:ARG:HD3	1:K:316:ARG:N	2.18	0.59
1:F:380:ARG:HH11	1:F:385:ILE:CG2	2.15	0.59
1:L:168:CYS:O	1:L:172:ILE:HG13	2.02	0.59
1:G:4:TYR:HB3	1:G:9:ILE:CD1	2.32	0.59
1:E:273:HIS:NE2	1:E:361:LYS:HA	2.18	0.59
1:J:368:ILE:HD12	1:J:385:ILE:HG23	1.83	0.59
1:C:85:GLU:O	1:C:86:LYS:HB2	2.01	0.59
1:L:306:PRO:HG2	1:L:335:ARG:C	2.23	0.59
1:E:293:VAL:HG23	1:K:440:TYR:OH	2.02	0.59
1:K:17:ASN:HD22	1:K:87:GLY:HA2	1.67	0.59
1:A:41:GLN:HE22	1:F:200:LYS:CE	2.15	0.59
1:K:260:ASP:O	1:K:266:GLN:HA	2.02	0.59
1:K:5:THR:HG22	1:K:8:ASP:CG	2.23	0.59
1:H:63:ILE:N	1:H:63:ILE:HD12	2.18	0.59
1:J:357:GLY:HA2	1:J:362:LEU:HG	1.85	0.59
1:J:371:ASN:ND2	1:J:374:VAL:H	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:PRO:HG2	1:E:199:PHE:HD1	1.68	0.59
1:A:244:MET:N	1:A:338:ASP:HA	2.17	0.59
1:L:136:PHE:HB3	1:L:138:PHE:HE1	1.68	0.59
1:F:115:ILE:HG22	1:F:351:LEU:HD13	1.84	0.59
1:I:376:SER:O	1:I:380:ARG:HG3	2.03	0.59
1:B:370:ARG:NH2	1:B:375:MET:SD	2.76	0.59
1:L:55:SER:CB	1:L:62:ARG:HG3	2.30	0.59
1:E:207:SER:O	1:E:211:ILE:HG12	2.03	0.59
1:A:191:ALA:HB3	1:A:194:GLN:HE21	1.68	0.59
1:I:282:ALA:C	1:I:284:SER:H	2.05	0.59
1:H:280:LYS:HG2	1:H:281:HIS:CD2	2.38	0.59
1:H:402:ASN:O	1:H:406:VAL:HG23	2.03	0.59
1:A:319:LEU:HB3	1:A:320:ILE:HD12	1.84	0.58
1:A:306:PRO:HG2	1:A:335:ARG:C	2.23	0.58
1:E:140:LEU:HD12	1:E:226:GLY:CA	2.33	0.58
1:L:443:GLN:HG2	1:L:444:TYR:CE2	2.38	0.58
1:E:273:HIS:NE2	1:E:361:LYS:HG2	2.16	0.58
1:D:68:MET:CE	1:D:98:ASN:HA	2.33	0.58
1:D:68:MET:HE3	1:D:98:ASN:HA	1.84	0.58
1:A:172:ILE:HD13	1:A:218:VAL:HG22	1.85	0.58
1:J:184:GLU:OE1	1:J:200:LYS:HG3	2.03	0.58
1:L:425:TRP:CZ3	1:L:429:ARG:HD2	2.38	0.58
1:K:360:ASN:N	1:K:360:ASN:HD22	2.00	0.58
1:F:218:VAL:HG12	1:F:219:LYS:N	2.16	0.58
1:A:138:PHE:CZ	1:A:236:LEU:HD11	2.38	0.58
1:D:139:LYS:HE3	1:D:149:GLU:HB3	1.84	0.58
1:F:96:ILE:HD13	1:F:107:ASP:CG	2.23	0.58
1:B:129:LEU:HD13	1:B:131:PRO:HD3	1.86	0.58
1:J:299:LEU:HD12	1:J:299:LEU:N	2.17	0.58
1:K:380:ARG:HA	1:K:383:ASN:ND2	2.18	0.58
1:C:9:ILE:HA	1:C:12:LEU:HD12	1.84	0.58
1:C:6:ARG:O	1:C:10:GLU:HG3	2.03	0.58
1:C:189:GLU:HB2	1:C:194:GLN:HB3	1.83	0.58
1:K:169:ARG:HH21	1:K:169:ARG:HG3	1.68	0.58
1:E:247:ASN:HD22	1:E:331:ARG:HE	1.51	0.58
1:J:9:ILE:HG21	1:J:92:PHE:HZ	1.68	0.58
1:E:396:LEU:HD11	1:E:421:LYS:HB3	1.84	0.58
1:D:310:ALA:O	1:D:318:PRO:HB2	2.03	0.58
1:L:127:PHE:CD2	1:L:351:LEU:HG	2.38	0.58
1:I:9:ILE:HG13	1:I:74:LEU:HD12	1.84	0.58
1:H:267:LEU:CD2	1:H:326:ARG:HH12	2.14	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:620:HOH:O	1:L:177:GLU:HG2	2.03	0.58
1:J:140:LEU:HD21	1:J:228:HIS:HB2	1.84	0.58
1:F:141:ASP:O	1:F:144:GLY:N	2.28	0.58
1:E:152:ASP:OD1	1:E:193:GLY:HA2	2.03	0.58
1:J:100:ASP:OD1	1:J:102:THR:HG22	2.03	0.58
1:B:429:ARG:NH1	1:H:300:VAL:HG23	2.16	0.58
1:G:160:ALA:O	1:G:161:PRO:C	2.42	0.58
1:D:114:ARG:HH21	1:D:115:ILE:HD11	1.68	0.58
1:F:437:ARG:CD	1:L:148:LEU:HD21	2.34	0.58
1:J:123:GLY:O	1:J:252:LYS:HG3	2.03	0.58
1:D:146:PRO:HG3	1:D:228:HIS:CD2	2.38	0.58
1:F:109:ARG:HH21	1:F:109:ARG:HG2	1.68	0.58
1:B:134:GLU:O	1:B:242:SER:HB3	2.04	0.58
1:D:52:PHE:HZ	1:D:57:ILE:HD11	1.68	0.58
1:J:346:ALA:O	1:J:350:LEU:HB2	2.03	0.58
1:G:371:ASN:HB3	1:G:375:MET:CG	2.33	0.58
1:I:27:ASP:OD1	1:I:33:LYS:HE3	2.04	0.58
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.84	0.58
1:I:189:GLU:OE1	1:I:190:VAL:HG23	2.03	0.58
1:C:375:MET:HE3	1:C:379:GLU:HB3	1.86	0.58
1:G:77:PHE:CZ	1:G:79:ILE:HD11	2.38	0.58
1:E:282:ALA:HA	1:E:285:PHE:CE1	2.38	0.58
1:K:380:ARG:HB3	1:K:385:ILE:HD12	1.85	0.58
1:E:232:MET:HE3	1:K:437:ARG:HA	1.85	0.58
1:C:191:ALA:HB2	1:C:240:ASN:HB3	1.85	0.58
1:I:261:GLU:HA	1:I:266:GLN:CG	2.24	0.58
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.50	0.58
1:B:429:ARG:NH2	1:H:390:ALA:HB1	2.15	0.58
1:E:429:ARG:HH12	1:K:300:VAL:HG12	1.69	0.58
1:L:250:LEU:C	1:L:251:PHE:HD1	2.07	0.58
1:C:3:LYS:HG2	1:C:4:TYR:CD1	2.39	0.58
1:E:122:LEU:HD12	1:E:355:LEU:HD22	1.85	0.58
1:E:68:MET:HE1	1:E:104:PHE:CD1	2.39	0.58
1:G:308:TYR:HD2	1:G:380:ARG:HD3	1.68	0.58
1:E:325:SER:HB2	1:E:331:ARG:NH2	2.14	0.58
1:E:140:LEU:HD22	1:E:144:GLY:O	2.04	0.58
1:L:287:ALA:HB2	1:L:395:ALA:CB	2.33	0.58
1:G:177:GLU:HB2	1:G:183:ILE:HD11	1.85	0.58
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.39	0.58
1:H:122:LEU:HD21	1:H:359:LYS:HD3	1.86	0.58
1:E:12:LEU:O	1:E:16:GLU:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:THR:C	1:H:7:GLU:H	2.07	0.58
1:J:404:VAL:HG13	1:J:405:MET:HE2	1.86	0.58
1:L:291:PRO:HG2	1:L:292:THR:H	1.69	0.58
1:H:279:VAL:HG13	1:H:309:VAL:CG1	2.32	0.58
1:G:265:LEU:N	1:G:265:LEU:HD12	2.19	0.58
1:G:380:ARG:HD2	1:G:387:ASP:OD2	2.04	0.57
1:K:325:SER:CB	1:K:331:ARG:HH22	2.17	0.57
1:D:22:ARG:O	1:D:91:ARG:HB2	2.04	0.57
1:J:119:MET:O	1:J:124:PHE:HB2	2.03	0.57
1:C:150:LEU:HD13	1:C:192:PRO:O	2.04	0.57
1:L:402:ASN:HD21	1:L:404:VAL:HG12	1.67	0.57
1:C:118:GLU:O	1:C:122:LEU:HD23	2.04	0.57
1:B:48:ASN:OD1	1:B:72:PRO:HD2	2.04	0.57
1:H:140:LEU:HD21	1:H:223:ARG:HH22	1.67	0.57
1:I:399:PHE:CE1	1:I:405:MET:HB3	2.39	0.57
1:E:429:ARG:O	1:K:297:LYS:HD3	2.04	0.57
1:F:34:ASN:ND2	1:F:34:ASN:C	2.57	0.57
1:D:52:PHE:CZ	1:D:54:GLY:HA2	2.38	0.57
1:C:124:PHE:CD2	1:C:250:LEU:HD13	2.39	0.57
1:L:118:GLU:O	1:L:122:LEU:HD23	2.03	0.57
1:G:370:ARG:CD	1:G:370:ARG:H	2.11	0.57
1:E:13:VAL:CG1	1:E:18:VAL:HB	2.32	0.57
1:K:323:PRO:HG3	1:K:331:ARG:NE	2.18	0.57
1:C:201:TYR:C	1:C:201:TYR:CD1	2.77	0.57
1:F:298:ARG:NH2	1:F:338:ASP:HB3	2.20	0.57
1:A:52:PHE:CE1	1:A:70:LEU:HD13	2.38	0.57
1:K:150:LEU:HD13	1:K:192:PRO:HG2	1.87	0.57
1:H:215:LYS:HG2	1:H:231:PHE:CE2	2.39	0.57
1:J:81:PRO:HG2	1:J:82:TRP:H	1.69	0.57
1:A:63:ILE:O	1:F:316:ARG:HD2	2.03	0.57
1:A:142:GLU:H	1:A:142:GLU:CD	2.08	0.57
1:D:129:LEU:CD1	1:D:131:PRO:HD3	2.31	0.57
1:I:112:LEU:HD21	1:I:347:LEU:HD12	1.86	0.57
1:K:319:LEU:O	1:K:320:ILE:HD13	2.03	0.57
1:K:45:ALA:HA	1:K:50:VAL:CG2	2.35	0.57
1:H:155:GLY:O	1:H:158:ASP:HB2	2.05	0.57
1:E:32:ILE:HD12	1:E:216:LEU:HD13	1.84	0.57
1:I:323:PRO:HD2	1:I:331:ARG:O	2.05	0.57
1:H:166:GLU:O	1:H:168:CYS:N	2.37	0.57
1:F:98:ASN:HD21	1:F:104:PHE:CA	2.17	0.57
1:F:232:MET:HE2	1:L:440:TYR:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLU:O	1:C:65:GLU:HG3	2.04	0.57
1:B:116:LEU:O	1:B:119:MET:HB3	2.04	0.57
1:A:274:PHE:CE1	1:A:354:GLY:HA3	2.39	0.57
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.87	0.57
1:A:436:GLU:CD	1:G:297:LYS:HZ2	2.08	0.57
1:K:28:ILE:HD11	1:K:417:PHE:CA	2.34	0.57
1:J:273:HIS:CE1	1:J:361:LYS:HA	2.39	0.57
1:I:347:LEU:O	1:I:347:LEU:HD13	2.04	0.57
1:L:51:MET:HE1	1:L:67:ASP:CB	2.32	0.57
1:D:34:ASN:C	1:D:34:ASN:ND2	2.56	0.57
1:C:63:ILE:HG22	1:C:64:GLU:HG3	1.87	0.57
1:D:212:GLN:OE1	1:D:212:GLN:HA	2.05	0.57
1:H:123:GLY:O	1:H:252:LYS:HG3	2.05	0.57
1:A:233:PRO:HG2	1:A:295:SER:OG	2.04	0.57
1:A:55:SER:O	1:A:58:GLU:HG2	2.05	0.57
1:K:310:ALA:CB	1:K:372:ILE:HG21	2.34	0.57
1:D:160:ALA:O	1:D:161:PRO:O	2.23	0.57
1:D:243:GLY:CA	1:D:298:ARG:NH1	2.68	0.57
1:B:164:LEU:HB2	1:C:82:TRP:CD1	2.38	0.57
1:I:22:ARG:NH1	1:J:159:LEU:HD21	2.20	0.57
1:B:142:GLU:HG3	1:B:143:LYS:N	2.20	0.57
1:A:205:VAL:HG23	4:A:602:HOH:O	2.04	0.57
1:G:342:ASN:C	1:G:342:ASN:HD22	2.08	0.57
1:K:316:ARG:HH11	1:K:316:ARG:CB	2.18	0.57
1:F:429:ARG:NH2	1:L:300:VAL:HG22	2.13	0.57
1:G:169:ARG:NE	1:L:36:GLU:OE1	2.38	0.57
1:E:440:TYR:OH	1:K:293:VAL:HG23	2.05	0.57
1:F:91:ARG:HD2	1:F:92:PHE:N	2.20	0.57
1:F:114:ARG:HH21	1:F:115:ILE:HD11	1.68	0.57
1:D:214:PHE:O	1:D:218:VAL:HG23	2.04	0.57
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.69	0.57
1:G:375:MET:HB2	1:G:379:GLU:CB	2.33	0.57
1:K:370:ARG:NH2	1:K:374:VAL:HG22	2.13	0.57
1:B:147:THR:HG21	1:B:149:GLU:HG3	1.85	0.57
1:I:309:VAL:HG23	1:I:386:VAL:O	2.04	0.57
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.38	0.57
1:H:223:ARG:HE	1:H:223:ARG:HA	1.70	0.57
1:A:311:TRP:CB	1:A:320:ILE:HB	2.35	0.57
1:F:380:ARG:HH11	1:F:380:ARG:HG2	1.69	0.57
1:J:96:ILE:HD12	1:J:107:ASP:HB2	1.86	0.57
1:A:135:PHE:HB3	1:A:231:PHE:CD1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:ARG:HH12	1:I:115:ILE:HD11	1.69	0.57
1:F:324:ALA:O	1:F:326:ARG:NE	2.38	0.57
1:F:5:THR:HG23	1:F:8:ASP:OD1	2.04	0.57
1:K:83:THR:CB	1:K:88:LYS:HA	2.34	0.56
1:G:383:ASN:HB2	1:G:385:ILE:CG1	2.35	0.56
1:J:282:ALA:HA	1:J:285:PHE:CE2	2.39	0.56
1:D:111:ASN:ND2	1:D:409:LEU:HA	2.17	0.56
1:C:52:PHE:CE2	1:C:54:GLY:HA2	2.40	0.56
1:I:58:GLU:HB3	1:I:62:ARG:HB2	1.86	0.56
1:C:68:MET:HG2	1:C:97:TYR:O	2.05	0.56
1:E:74:LEU:H	1:E:74:LEU:HD22	1.70	0.56
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.86	0.56
1:H:272:LYS:HZ1	1:H:276:ALA:HB2	1.70	0.56
1:I:4:TYR:HB3	1:I:9:ILE:HD11	1.87	0.56
1:F:437:ARG:HB2	1:F:437:ARG:NH1	2.20	0.56
1:L:136:PHE:HB3	1:L:138:PHE:CE1	2.41	0.56
1:H:119:MET:SD	1:H:127:PHE:HB2	2.44	0.56
1:E:264:ASP:C	1:E:266:GLN:N	2.59	0.56
1:F:23:LEU:HB2	1:F:35:VAL:HG13	1.86	0.56
1:I:173:VAL:HG13	1:I:183:ILE:CD1	2.22	0.56
1:F:380:ARG:HH11	1:F:385:ILE:HG21	1.70	0.56
1:J:320:ILE:HG22	1:J:321:ARG:N	2.20	0.56
1:H:169:ARG:NH2	1:H:195:HIS:ND1	2.53	0.56
1:I:100:ASP:OD1	1:I:100:ASP:N	2.37	0.56
1:J:129:LEU:HD22	1:J:131:PRO:HG3	1.87	0.56
1:J:131:PRO:HG2	1:J:211:ILE:HD11	1.87	0.56
1:A:115:ILE:HD11	1:A:408:ALA:O	2.05	0.56
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.40	0.56
1:H:64:GLU:OE2	1:I:315:ASN:HA	2.06	0.56
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.41	0.56
1:L:60:PHE:CE1	1:L:423:ILE:HD11	2.40	0.56
1:G:6:ARG:HG3	1:G:10:GLU:OE2	2.04	0.56
1:E:117:LYS:HD3	1:E:117:LYS:O	2.05	0.56
1:L:156:TYR:HE1	1:L:189:GLU:OE1	1.88	0.56
1:D:319:LEU:HD12	1:D:336:SER:HB3	1.86	0.56
1:L:57:ILE:CD1	1:L:96:ILE:HG12	2.34	0.56
1:B:402:ASN:O	1:B:406:VAL:HG23	2.05	0.56
1:L:78:VAL:CG1	1:L:91:ARG:HG3	2.36	0.56
1:G:62:ARG:O	1:G:63:ILE:HG23	2.05	0.56
1:C:282:ALA:O	1:C:284:SER:N	2.39	0.56
1:I:169:ARG:NH2	1:I:195:HIS:ND1	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:VAL:HG11	1:E:428:PHE:CD2	2.40	0.56
1:B:100:ASP:OD1	1:B:101:GLY:N	2.39	0.56
1:K:345:LEU:O	1:K:348:SER:HB2	2.05	0.56
1:J:46:LEU:HD21	1:J:74:LEU:HD11	1.87	0.56
1:J:116:LEU:O	1:J:120:GLU:HG3	2.06	0.56
1:B:58:GLU:O	1:B:61:VAL:HG22	2.05	0.56
1:E:232:MET:CE	1:K:437:ARG:HA	2.36	0.56
1:A:64:GLU:HG2	1:F:316:ARG:HA	1.87	0.56
1:K:276:ALA:HB2	1:K:364:ALA:HB2	1.86	0.56
1:H:52:PHE:HE2	1:H:56:SER:HG	1.53	0.56
1:A:380:ARG:HA	1:A:383:ASN:HB2	1.86	0.56
1:H:74:LEU:H	1:H:74:LEU:CD2	2.14	0.56
1:D:309:VAL:HG23	1:D:386:VAL:O	2.06	0.56
1:J:319:LEU:HD23	1:J:320:ILE:CD1	2.35	0.56
1:H:167:ASN:HB3	1:H:170:ARG:NH2	2.20	0.56
1:E:140:LEU:HD12	1:E:226:GLY:HA2	1.88	0.56
1:E:52:PHE:CD1	1:E:70:LEU:HD13	2.40	0.56
1:A:37:ILE:HG22	1:F:185:ALA:CA	2.35	0.56
1:D:6:ARG:NH1	1:D:6:ARG:HG3	2.21	0.56
1:L:23:LEU:HB2	1:L:35:VAL:CG2	2.35	0.56
1:D:100:ASP:OD2	1:D:101:GLY:N	2.39	0.56
1:A:442:SER:HB3	1:H:153:LYS:HD2	1.87	0.56
1:D:418:ILE:O	1:D:422:GLU:HG3	2.06	0.56
1:A:186:SER:HB2	1:A:197:ILE:HD13	1.86	0.56
1:F:160:ALA:CB	1:F:169:ARG:HH21	2.19	0.56
1:F:319:LEU:HG	1:F:320:ILE:HD12	1.87	0.56
1:C:313:ALA:O	1:C:314:GLN:HB2	2.06	0.56
1:K:252:LYS:O	1:K:253:ASN:HB2	2.04	0.56
1:E:138:PHE:CD2	1:E:148:LEU:HA	2.41	0.56
1:K:38:PRO:HD2	1:K:41:GLN:HG3	1.88	0.56
1:I:234:LYS:HE3	1:I:239:VAL:O	2.05	0.56
1:E:204:ALA:HB1	1:E:347:LEU:HD13	1.86	0.56
1:E:372:ILE:HD12	1:E:373:TYR:H	1.71	0.56
1:F:379:GLU:HG3	1:F:385:ILE:HD12	1.88	0.56
1:H:28:ILE:HG22	1:H:57:ILE:O	2.05	0.56
1:G:183:ILE:HD13	1:L:38:PRO:HG2	1.87	0.56
1:K:135:PHE:HB3	1:K:231:PHE:CE1	2.41	0.56
1:H:328:ILE:H	1:H:328:ILE:CD1	2.18	0.56
1:K:163:ASP:C	1:K:164:LEU:HD23	2.26	0.56
1:K:32:ILE:HD13	1:K:216:LEU:HD13	1.88	0.56
1:G:308:TYR:HE2	1:G:380:ARG:HE	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:SER:CB	1:G:331:ARG:HH22	2.17	0.56
1:A:319:LEU:O	1:A:319:LEU:HD23	2.06	0.56
1:K:49:LYS:HD3	1:K:69:TYR:CE2	2.41	0.56
1:D:377:LYS:HG3	1:D:380:ARG:HH21	1.69	0.56
1:C:377:LYS:O	1:C:381:MET:HG3	2.06	0.56
1:K:167:ASN:OD1	1:K:170:ARG:HB3	2.05	0.56
1:K:137:LEU:HD23	1:K:229:ALA:HA	1.88	0.56
1:I:175:GLU:HG3	1:I:221:ILE:HD11	1.88	0.56
1:B:372:ILE:CG2	1:B:385:ILE:HG21	2.36	0.56
1:L:83:THR:CG2	1:L:89:VAL:HB	2.35	0.56
1:D:323:PRO:HG2	1:D:331:ARG:NH2	2.21	0.56
1:F:120:GLU:C	1:F:122:LEU:H	2.09	0.56
1:D:429:ARG:O	1:J:297:LYS:HD3	2.06	0.56
1:I:208:CYS:HA	1:I:211:ILE:HG12	1.88	0.56
1:E:393:ALA:HB2	1:E:425:TRP:CE2	2.41	0.56
1:K:21:ILE:HD13	1:K:39:VAL:HA	1.87	0.55
1:G:32:ILE:HD13	1:G:216:LEU:CD1	2.33	0.55
1:F:55:SER:O	1:F:62:ARG:HG2	2.06	0.55
1:E:35:VAL:CG1	1:E:70:LEU:HD21	2.36	0.55
1:K:50:VAL:O	1:K:69:TYR:HA	2.05	0.55
1:I:319:LEU:C	1:I:320:ILE:HD12	2.27	0.55
1:I:236:LEU:HB2	1:I:239:VAL:HG22	1.88	0.55
1:I:415:GLU:HG3	4:I:620:HOH:O	2.05	0.55
1:K:82:TRP:HZ3	1:K:221:ILE:HD11	1.71	0.55
1:I:23:LEU:HB2	1:I:35:VAL:CG1	2.36	0.55
1:D:102:THR:HB	1:D:103:PRO:HD2	1.87	0.55
1:J:182:GLU:O	1:J:200:LYS:HD3	2.07	0.55
1:D:129:LEU:HD22	1:D:130:GLY:H	1.71	0.55
1:E:402:ASN:OD1	1:E:403:GLU:N	2.39	0.55
1:B:138:PHE:HB3	1:B:147:THR:O	2.06	0.55
1:C:115:ILE:HG22	1:C:351:LEU:HD12	1.89	0.55
1:C:261:GLU:HA	1:C:266:GLN:HG2	1.88	0.55
1:F:260:ASP:O	1:F:266:GLN:HA	2.06	0.55
1:J:307:CYS:O	1:J:388:LEU:HG	2.06	0.55
1:C:33:LYS:O	1:C:34:ASN:HB3	2.06	0.55
1:E:266:GLN:HB2	1:E:326:ARG:HD2	1.88	0.55
1:G:306:PRO:HG2	1:G:335:ARG:HD3	1.88	0.55
1:G:72:PRO:HA	1:G:94:CYS:HA	1.88	0.55
1:G:370:ARG:HH22	1:G:383:ASN:HD22	1.52	0.55
1:K:316:ARG:C	1:K:318:PRO:HD3	2.27	0.55
1:C:404:VAL:HG13	1:C:405:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:127:PHE:CE2	1:K:351:LEU:HB2	2.42	0.55
1:F:160:ALA:HB3	1:F:169:ARG:NH2	2.22	0.55
1:E:288:VAL:O	1:E:291:PRO:HD3	2.06	0.55
1:A:67:ASP:O	1:A:68:MET:HG3	2.07	0.55
1:I:182:GLU:O	1:I:200:LYS:HB2	2.07	0.55
1:B:138:PHE:CE2	1:B:150:LEU:HD23	2.41	0.55
1:C:25:PHE:CE1	1:C:33:LYS:HB2	2.42	0.55
1:J:83:THR:HB	1:J:89:VAL:HG23	1.88	0.55
1:D:249:SER:HA	1:D:258:PHE:CE1	2.42	0.55
1:L:74:LEU:H	1:L:74:LEU:CD2	2.20	0.55
1:A:314:GLN:HG2	1:B:64:GLU:OE1	2.07	0.55
1:F:293:VAL:HG12	1:L:440:TYR:OH	2.07	0.55
1:D:123:GLY:O	1:D:252:LYS:HG3	2.07	0.55
1:G:58:GLU:HB2	1:G:62:ARG:HG2	1.89	0.55
1:F:40:SER:C	1:F:41:GLN:HG2	2.27	0.55
1:F:440:TYR:HB2	1:L:232:MET:CE	2.35	0.55
1:K:98:ASN:HB2	1:K:102:THR:O	2.07	0.55
1:D:26:THR:HG23	1:D:30:GLY:HA2	1.88	0.55
1:K:54:GLY:C	1:K:56:SER:H	2.10	0.55
1:H:421:LYS:HD3	1:H:424:GLU:OE2	2.07	0.55
1:K:166:GLU:HB2	1:K:227:LEU:HD11	1.87	0.55
1:G:368:ILE:HD13	1:G:372:ILE:CG1	2.37	0.55
1:G:380:ARG:HB3	1:G:385:ILE:O	2.06	0.55
1:J:321:ARG:O	1:J:323:PRO:HD3	2.07	0.55
1:K:402:ASN:O	1:K:406:VAL:HG23	2.07	0.55
1:A:168:CYS:O	1:A:169:ARG:C	2.45	0.55
1:D:162:THR:C	1:D:164:LEU:H	2.10	0.55
1:E:292:THR:HB	1:K:440:TYR:CE1	2.42	0.55
1:C:6:ARG:HG3	1:C:10:GLU:OE2	2.07	0.55
1:H:118:GLU:O	1:H:122:LEU:HD13	2.07	0.55
1:I:291:PRO:O	1:I:392:LEU:HD13	2.06	0.55
1:F:251:PHE:HD2	1:F:254:GLY:O	1.88	0.55
1:E:62:ARG:HD3	1:E:62:ARG:O	2.06	0.55
1:G:45:ALA:HA	1:G:50:VAL:HG23	1.88	0.55
1:J:114:ARG:HH12	1:J:115:ILE:HD11	1.71	0.55
1:J:281:HIS:CE1	1:J:404:VAL:HG11	2.41	0.55
1:K:33:LYS:CA	1:L:158:ASP:HA	2.29	0.55
1:I:248:LEU:HD11	1:I:334:VAL:CG2	2.30	0.55
1:C:105:GLU:CD	1:C:412:HIS:HB2	2.27	0.55
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.42	0.55
1:E:232:MET:CE	1:K:440:TYR:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PHE:HA	1:B:252:LYS:HA	1.89	0.55
1:J:173:VAL:HG13	1:J:183:ILE:HD12	1.87	0.55
1:A:310:ALA:HB3	1:A:372:ILE:CD1	2.33	0.55
1:J:399:PHE:HZ	1:J:409:LEU:HD22	1.71	0.55
1:J:190:VAL:HG13	1:J:191:ALA:N	2.17	0.55
1:C:33:LYS:NZ	1:C:56:SER:O	2.40	0.55
1:L:150:LEU:CD1	1:L:192:PRO:HG2	2.37	0.55
1:I:338:ASP:OD2	1:I:340:ALA:HB3	2.06	0.55
1:K:109:ARG:HG2	1:K:109:ARG:HH21	1.72	0.55
1:E:170:ARG:HG2	1:E:170:ARG:HH11	1.72	0.55
1:C:400:LYS:HG3	1:C:418:ILE:HD12	1.88	0.55
1:E:126:ASP:OD1	1:E:251:PHE:HB2	2.07	0.55
1:I:122:LEU:HD22	1:I:355:LEU:HD22	1.88	0.54
1:F:319:LEU:HG	1:F:320:ILE:CD1	2.37	0.54
1:D:139:LYS:HE3	1:D:149:GLU:CB	2.38	0.54
1:F:342:ASN:HB3	1:F:345:LEU:HD12	1.89	0.54
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.88	0.54
1:L:82:TRP:CH2	1:L:217:VAL:HG22	2.40	0.54
1:B:264:ASP:C	1:B:266:GLN:H	2.09	0.54
1:A:78:VAL:HB	1:A:91:ARG:NH1	2.22	0.54
1:G:306:PRO:CG	1:G:335:ARG:HH21	2.20	0.54
1:A:137:LEU:HA	1:A:228:HIS:O	2.08	0.54
1:G:119:MET:SD	1:G:127:PHE:HB2	2.47	0.54
1:I:37:ILE:HG22	1:J:185:ALA:HB2	1.89	0.54
1:J:49:LYS:HA	1:J:49:LYS:HE3	1.89	0.54
1:I:286:THR:O	1:I:290:ASN:N	2.40	0.54
1:A:41:GLN:NE2	1:F:200:LYS:HE2	2.18	0.54
1:D:351:LEU:O	1:D:351:LEU:HD13	2.07	0.54
1:B:131:PRO:HG2	1:B:199:PHE:HD1	1.71	0.54
1:J:211:ILE:O	1:J:215:LYS:HG3	2.07	0.54
1:A:224:LYS:HB2	1:F:164:LEU:CD1	2.38	0.54
1:H:67:ASP:O	1:H:99:PRO:HG3	2.07	0.54
1:A:104:PHE:CZ	1:A:106:GLY:HA3	2.43	0.54
1:G:267:LEU:CD2	1:G:326:ARG:NH1	2.70	0.54
1:F:372:ILE:HA	1:F:375:MET:HG3	1.88	0.54
1:B:207:SER:O	1:B:211:ILE:HG13	2.08	0.54
1:C:201:TYR:C	1:C:201:TYR:HD1	2.11	0.54
1:J:383:ASN:HB2	1:J:385:ILE:HG12	1.90	0.54
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.90	0.54
1:I:114:ARG:CB	1:I:114:ARG:HH11	2.20	0.54
1:K:236:LEU:HB2	1:K:239:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:HG2	1:F:316:ARG:CA	2.38	0.54
1:B:295:SER:O	1:B:299:LEU:HD13	2.07	0.54
1:A:252:LYS:HZ3	1:A:252:LYS:HB2	1.73	0.54
1:K:270:THR:CG2	1:K:358:ILE:HD12	2.37	0.54
1:D:127:PHE:CZ	1:D:351:LEU:HD23	2.42	0.54
1:F:319:LEU:HD13	1:F:388:LEU:HD11	1.90	0.54
1:C:260:ASP:O	1:C:266:GLN:HA	2.08	0.54
1:L:114:ARG:HH21	1:L:115:ILE:HG13	1.73	0.54
1:J:396:LEU:HD11	1:J:421:LYS:HB3	1.88	0.54
1:K:18:VAL:HA	1:K:88:LYS:HB2	1.90	0.54
1:K:83:THR:HG22	1:K:89:VAL:HG23	1.90	0.54
1:K:310:ALA:CB	1:K:372:ILE:HD13	2.37	0.54
1:A:170:ARG:NH1	1:B:84:ALA:HB1	2.23	0.54
1:G:77:PHE:HZ	1:G:79:ILE:HD11	1.72	0.54
1:H:49:LYS:HD3	1:H:69:TYR:HE2	1.72	0.54
1:J:33:LYS:HE2	1:K:158:ASP:OD1	2.07	0.54
1:I:328:ILE:HG12	1:I:329:SER:N	2.20	0.54
1:E:400:LYS:HA	1:E:414:PHE:HZ	1.72	0.54
1:G:160:ALA:CB	1:G:188:HIS:HD2	2.18	0.54
1:D:115:ILE:CG2	1:D:351:LEU:HD12	2.38	0.54
1:E:170:ARG:O	1:E:174:LEU:HG	2.08	0.54
1:C:244:MET:HB2	1:C:339:PRO:HD3	1.88	0.54
1:C:145:GLU:HA	1:C:145:GLU:OE1	2.08	0.54
1:G:325:SER:CB	1:G:331:ARG:NH2	2.70	0.54
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.90	0.54
1:A:272:LYS:NZ	1:A:311:TRP:CH2	2.76	0.54
1:B:2:ALA:O	1:B:3:LYS:HB2	2.08	0.54
1:G:169:ARG:NH2	1:G:195:HIS:ND1	2.56	0.54
1:E:368:ILE:HG21	1:E:372:ILE:CG2	2.38	0.54
1:F:376:SER:O	1:F:380:ARG:HG3	2.07	0.54
1:H:384:GLY:O	1:H:386:VAL:HG23	2.08	0.54
1:D:128:ASN:HD22	1:D:203:GLY:HA2	1.73	0.54
1:H:236:LEU:HB2	1:H:239:VAL:HG21	1.89	0.54
1:H:236:LEU:HB2	1:H:239:VAL:HG22	1.89	0.54
1:D:104:PHE:CE2	1:D:106:GLY:HA3	2.43	0.54
1:L:423:ILE:C	1:L:423:ILE:HD12	2.27	0.54
1:B:95:ASP:O	1:B:97:TYR:HD1	1.90	0.54
1:J:39:VAL:HG13	1:J:40:SER:N	2.23	0.54
1:G:204:ALA:HB1	1:G:347:LEU:HD23	1.90	0.54
1:J:169:ARG:HG3	1:J:195:HIS:HB3	1.90	0.54
1:E:96:ILE:HD13	1:E:107:ASP:CG	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ILE:H	1:F:96:ILE:HD12	1.73	0.54
1:B:129:LEU:HG	1:B:347:LEU:CD2	2.37	0.54
1:D:256:ASN:ND2	1:D:328:ILE:O	2.41	0.54
1:B:278:ILE:CG2	1:B:320:ILE:HD11	2.38	0.54
1:H:258:PHE:HA	1:H:271:ALA:HB2	1.89	0.54
1:E:393:ALA:HB2	1:E:425:TRP:CD2	2.43	0.54
1:F:409:LEU:O	1:F:413:LEU:HB2	2.07	0.54
1:I:156:TYR:C	1:I:158:ASP:H	2.11	0.54
1:J:172:ILE:O	1:J:176:LEU:HG	2.07	0.54
1:E:199:PHE:HZ	1:E:214:PHE:CG	2.26	0.54
1:C:404:VAL:HG13	1:C:405:MET:HE2	1.90	0.54
1:H:27:ASP:HB2	1:H:57:ILE:O	2.07	0.54
1:H:323:PRO:HD2	1:H:331:ARG:O	2.08	0.54
1:A:323:PRO:HD2	1:A:331:ARG:O	2.08	0.54
1:G:127:PHE:N	4:G:608:HOH:O	2.36	0.54
1:F:393:ALA:HB2	1:F:425:TRP:CE2	2.43	0.54
1:A:281:HIS:O	1:A:284:SER:HB2	2.09	0.54
1:C:252:LYS:NZ	1:C:252:LYS:HB2	2.23	0.54
1:A:316:ARG:HD3	1:B:63:ILE:O	2.08	0.54
1:B:126:ASP:CB	1:B:251:PHE:HB2	2.25	0.53
1:G:256:ASN:ND2	1:G:330:THR:HB	2.23	0.53
1:G:325:SER:HB2	1:G:331:ARG:HH21	1.71	0.53
1:C:51:MET:CE	1:C:67:ASP:HB3	2.37	0.53
1:B:211:ILE:CG2	1:B:215:LYS:HE3	2.37	0.53
1:L:404:VAL:HG13	1:L:405:MET:HE2	1.90	0.53
1:K:85:GLU:CD	1:K:85:GLU:H	2.10	0.53
1:I:328:ILE:N	1:I:328:ILE:HD13	2.12	0.53
1:E:160:ALA:O	1:E:161:PRO:C	2.46	0.53
1:L:310:ALA:HB1	1:L:368:ILE:HB	1.90	0.53
1:C:97:TYR:HD2	1:C:101:GLY:O	1.91	0.53
1:E:55:SER:HB2	1:E:62:ARG:HB2	1.89	0.53
1:H:49:LYS:HD3	1:H:69:TYR:CE2	2.43	0.53
1:E:201:TYR:O	1:E:202:ALA:HB2	2.08	0.53
1:I:206:ARG:O	1:I:206:ARG:HD3	2.09	0.53
1:L:201:TYR:C	1:L:201:TYR:CD1	2.81	0.53
1:L:316:ARG:HG3	1:L:316:ARG:HH11	1.74	0.53
1:L:96:ILE:N	1:L:96:ILE:HD12	2.22	0.53
1:H:28:ILE:HD11	1:H:417:PHE:CA	2.39	0.53
1:I:440:TYR:HD1	1:I:444:TYR:CE2	2.25	0.53
1:B:178:GLU:CD	1:C:86:LYS:HD3	2.29	0.53
1:F:281:HIS:CE1	1:F:404:VAL:HG11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:81:PRO:HG2	1:J:82:TRP:CE3	2.44	0.53
1:K:378:GLU:HA	1:K:381:MET:HG2	1.91	0.53
1:B:291:PRO:HB2	1:B:421:LYS:HE3	1.90	0.53
1:L:6:ARG:HD2	1:L:46:LEU:HD13	1.89	0.53
1:E:345:LEU:HD22	1:E:409:LEU:HD22	1.88	0.53
1:E:319:LEU:CG	1:E:320:ILE:HD12	2.27	0.53
1:B:201:TYR:CD1	1:B:201:TYR:N	2.77	0.53
1:I:116:LEU:O	1:I:119:MET:HB3	2.09	0.53
1:A:338:ASP:HB2	1:A:339:PRO:CD	2.38	0.53
1:G:21:ILE:CD1	1:G:42:LEU:HD13	2.37	0.53
1:F:160:ALA:O	1:F:161:PRO:C	2.47	0.53
1:J:112:LEU:O	1:J:116:LEU:HG	2.09	0.53
1:L:231:PHE:HB3	1:L:339:PRO:CB	2.38	0.53
1:E:51:MET:SD	1:E:67:ASP:HB3	2.48	0.53
1:A:223:ARG:HG3	1:A:223:ARG:NH1	2.23	0.53
1:G:146:PRO:HG3	1:G:228:HIS:CD2	2.44	0.53
1:J:423:ILE:O	1:J:427:MET:HG3	2.07	0.53
1:D:275:ILE:O	1:D:279:VAL:HG23	2.08	0.53
1:J:404:VAL:HG13	1:J:405:MET:CE	2.38	0.53
1:F:182:GLU:HB3	1:F:200:LYS:CD	2.34	0.53
1:E:160:ALA:HB2	1:E:188:HIS:HD2	1.73	0.53
1:G:231:PHE:O	1:G:339:PRO:HG2	2.08	0.53
1:C:24:GLN:HE21	1:C:91:ARG:HB2	1.74	0.53
1:L:368:ILE:HG12	1:L:385:ILE:HG23	1.90	0.53
1:B:278:ILE:HG22	1:B:320:ILE:HD11	1.88	0.53
1:E:263:ALA:O	1:E:266:GLN:HA	2.09	0.53
1:H:371:ASN:OD1	1:H:373:TYR:HD1	1.91	0.53
1:K:348:SER:O	1:K:352:ALA:HB2	2.09	0.53
1:L:201:TYR:C	1:L:201:TYR:HD1	2.12	0.53
1:I:418:ILE:HG22	1:I:422:GLU:HG3	1.89	0.53
1:J:247:ASN:ND2	1:J:331:ARG:HD2	2.22	0.53
1:A:291:PRO:HG3	1:A:341:ALA:HA	1.90	0.53
1:L:215:LYS:O	1:L:219:LYS:HG2	2.09	0.53
1:A:107:ASP:OD2	1:A:110:ASN:N	2.41	0.53
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.90	0.53
1:E:5:THR:HG23	1:E:8:ASP:CG	2.29	0.53
1:G:156:TYR:C	1:G:158:ASP:H	2.12	0.53
1:K:399:PHE:CE1	1:K:405:MET:HB3	2.44	0.53
1:I:28:ILE:HD13	1:I:28:ILE:O	2.08	0.53
1:I:96:ILE:N	1:I:96:ILE:HD12	2.23	0.53
1:B:265:LEU:O	1:B:266:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LYS:HD2	1:D:86:LYS:O	2.08	0.53
1:D:375:MET:SD	1:D:379:GLU:HB3	2.48	0.53
1:I:123:GLY:O	1:I:252:LYS:HG3	2.08	0.53
1:A:399:PHE:HZ	1:A:409:LEU:HD12	1.73	0.53
1:G:182:GLU:O	1:G:200:LYS:HG3	2.09	0.53
1:F:9:ILE:HG13	1:F:74:LEU:HD12	1.91	0.53
1:L:380:ARG:HH11	1:L:380:ARG:CB	2.22	0.53
1:F:175:GLU:HG3	1:F:221:ILE:HD11	1.91	0.53
1:J:125:SER:HB3	1:J:126:ASP:OD1	2.09	0.53
1:A:35:VAL:HG11	1:A:70:LEU:CD2	2.39	0.53
1:H:20:TYR:CZ	1:H:36:GLU:HB3	2.44	0.53
1:C:197:ILE:HD12	1:C:214:PHE:CZ	2.43	0.53
1:A:146:PRO:HB3	1:A:228:HIS:ND1	2.23	0.53
1:F:151:ASN:HD22	1:F:166:GLU:CD	2.12	0.53
1:F:234:LYS:HB3	1:F:294:ASN:HD21	1.73	0.53
1:I:423:ILE:O	1:I:427:MET:HG3	2.08	0.53
1:D:349:VAL:HB	1:D:405:MET:SD	2.49	0.53
1:F:128:ASN:OD1	1:F:201:TYR:CE1	2.62	0.53
1:F:169:ARG:O	1:F:172:ILE:HB	2.09	0.53
1:H:282:ALA:HA	1:H:285:PHE:CE2	2.44	0.53
1:D:249:SER:HB3	1:D:331:ARG:CB	2.39	0.53
1:F:419:GLU:O	1:F:423:ILE:HG23	2.09	0.53
1:E:326:ARG:HH11	1:E:326:ARG:HG2	1.74	0.53
1:C:332:VAL:HG13	1:C:332:VAL:O	2.08	0.53
1:H:316:ARG:HB2	1:H:371:ASN:HD21	1.73	0.53
1:C:368:ILE:HD13	1:C:384:GLY:O	2.09	0.53
1:J:288:VAL:O	1:J:291:PRO:HD3	2.09	0.53
1:L:261:GLU:HA	1:L:266:GLN:HE21	1.73	0.53
1:I:34:ASN:C	1:I:34:ASN:ND2	2.62	0.53
1:I:35:VAL:HG11	1:I:70:LEU:HD23	1.90	0.53
1:I:35:VAL:HG13	1:I:35:VAL:O	2.08	0.53
1:D:281:HIS:NE2	1:D:404:VAL:HG21	2.24	0.53
1:K:82:TRP:CZ3	1:K:221:ILE:HD11	2.43	0.53
1:L:278:ILE:O	1:L:282:ALA:HB2	2.08	0.53
1:G:175:GLU:O	1:G:178:GLU:HB3	2.09	0.53
1:B:360:ASN:O	1:B:361:LYS:C	2.47	0.53
1:I:371:ASN:ND2	1:I:375:MET:HG2	2.23	0.52
1:J:377:LYS:H	1:J:377:LYS:CD	2.13	0.52
1:J:160:ALA:HB2	1:J:188:HIS:CD2	2.43	0.52
1:B:159:LEU:CD1	1:C:22:ARG:NH1	2.72	0.52
1:H:244:MET:N	1:H:338:ASP:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:95:ASP:OD1	1:K:109:ARG:HG2	2.09	0.52
1:E:259:PHE:O	1:E:268:SER:HB3	2.09	0.52
1:F:24:GLN:NE2	1:F:91:ARG:NH1	2.57	0.52
1:D:371:ASN:OD1	1:D:375:MET:HB2	2.09	0.52
1:B:243:GLY:CA	1:B:298:ARG:NH1	2.72	0.52
1:C:3:LYS:HG2	1:C:4:TYR:HD1	1.73	0.52
1:A:281:HIS:HD2	1:A:402:ASN:ND2	2.07	0.52
1:I:168:CYS:O	1:I:172:ILE:HG13	2.09	0.52
1:K:152:ASP:CB	1:K:161:PRO:HG3	2.37	0.52
1:F:297:LYS:HE3	1:L:436:GLU:OE2	2.09	0.52
1:F:183:ILE:HD12	1:F:197:ILE:CG2	2.39	0.52
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.39	0.52
1:E:160:ALA:HB1	1:E:161:PRO:CD	2.38	0.52
1:E:361:LYS:O	1:E:362:LEU:HD23	2.09	0.52
1:I:114:ARG:NH2	1:I:407:LYS:O	2.42	0.52
1:K:326:ARG:HG3	1:K:327:GLY:N	2.23	0.52
1:A:35:VAL:HG13	1:A:35:VAL:O	2.08	0.52
1:D:399:PHE:CE1	1:D:405:MET:HB3	2.44	0.52
1:G:368:ILE:O	1:G:369:ASP:HB2	2.09	0.52
1:A:380:ARG:HA	1:A:383:ASN:HD22	1.73	0.52
1:F:133:PRO:HG2	1:F:199:PHE:HE1	1.75	0.52
1:K:232:MET:HB3	1:K:235:PRO:HG3	1.91	0.52
1:D:83:THR:HB	1:D:87:GLY:O	2.09	0.52
1:C:115:ILE:HD11	1:C:408:ALA:O	2.09	0.52
1:J:162:THR:O	1:J:164:LEU:N	2.43	0.52
1:G:33:LYS:HD3	1:H:158:ASP:OD1	2.10	0.52
1:K:170:ARG:HG2	1:K:174:LEU:CD2	2.40	0.52
1:I:261:GLU:CA	1:I:266:GLN:HG2	2.27	0.52
1:J:272:LYS:CA	1:J:275:ILE:HD12	2.29	0.52
1:A:337:VAL:HG12	1:A:338:ASP:H	1.73	0.52
1:H:276:ALA:HA	1:H:364:ALA:HB2	1.91	0.52
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.90	0.52
1:E:234:LYS:HB3	1:E:294:ASN:HD21	1.74	0.52
1:K:259:PHE:CD1	1:K:326:ARG:HD2	2.42	0.52
1:G:33:LYS:HE3	1:H:156:TYR:O	2.10	0.52
1:I:166:GLU:O	1:I:168:CYS:N	2.42	0.52
1:C:435:TRP:CZ2	1:C:439:GLN:HG3	2.44	0.52
1:H:286:THR:HG23	1:H:290:ASN:ND2	2.25	0.52
1:B:248:LEU:O	1:B:331:ARG:HB2	2.09	0.52
1:D:318:PRO:O	1:D:335:ARG:HD2	2.10	0.52
1:B:236:LEU:HB2	1:B:239:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:PHE:HB3	1:F:138:PHE:HE1	1.75	0.52
1:L:274:PHE:HD1	1:L:358:ILE:HD11	1.75	0.52
1:E:164:LEU:HG	1:F:82:TRP:HB3	1.92	0.52
1:K:135:PHE:HB3	1:K:231:PHE:CD1	2.45	0.52
1:B:68:MET:SD	1:B:96:ILE:CG2	2.98	0.52
1:G:315:ASN:HB3	1:G:318:PRO:HD3	1.92	0.52
1:A:53:ASP:OD2	1:A:55:SER:HB3	2.09	0.52
1:F:261:GLU:HA	1:F:266:GLN:HE21	1.74	0.52
1:F:323:PRO:HD2	1:F:331:ARG:O	2.09	0.52
1:L:5:THR:HG23	1:L:8:ASP:OD2	2.09	0.52
1:K:322:ILE:HG22	1:K:322:ILE:O	2.10	0.52
1:B:160:ALA:O	1:B:161:PRO:C	2.47	0.52
1:C:297:LYS:HE2	1:I:429:ARG:O	2.09	0.52
1:A:150:LEU:CD1	1:A:192:PRO:HB2	2.39	0.52
1:G:333:GLU:HG2	1:G:335:ARG:HG2	1.90	0.52
1:B:243:GLY:HA3	1:B:298:ARG:NH1	2.23	0.52
1:L:237:PHE:CD1	1:L:238:GLY:N	2.78	0.52
1:H:79:ILE:O	1:H:79:ILE:HG22	2.08	0.52
1:L:34:ASN:C	1:L:34:ASN:ND2	2.63	0.52
1:L:73:ASP:HB3	1:L:76:THR:OG1	2.09	0.52
1:B:375:MET:HB3	1:B:379:GLU:HB2	1.92	0.52
1:E:27:ASP:HA	1:E:57:ILE:HG23	1.91	0.52
1:H:309:VAL:HG13	1:H:319:LEU:HD23	1.92	0.52
1:L:404:VAL:HG13	1:L:405:MET:CE	2.40	0.52
1:F:206:ARG:HB2	4:F:621:HOH:O	2.10	0.52
1:G:33:LYS:HD3	1:H:158:ASP:HA	1.92	0.52
1:A:274:PHE:HE2	1:A:332:VAL:HG21	1.74	0.52
1:G:157:PHE:CE1	1:L:35:VAL:HG12	2.45	0.52
1:B:291:PRO:O	1:B:392:LEU:HD13	2.09	0.52
1:A:86:LYS:HD2	1:F:178:GLU:OE1	2.10	0.52
1:E:278:ILE:HG23	1:E:285:PHE:CZ	2.45	0.52
1:E:285:PHE:HB3	1:E:405:MET:SD	2.50	0.52
1:I:406:VAL:HG22	1:I:414:PHE:CZ	2.44	0.52
1:A:37:ILE:HD13	1:A:37:ILE:H	1.74	0.52
1:D:23:LEU:HD13	1:D:70:LEU:HD23	1.92	0.52
1:C:244:MET:HE2	1:C:337:VAL:HG12	1.92	0.52
1:I:224:LYS:HD3	1:J:164:LEU:HD11	1.90	0.52
1:B:397:GLU:HA	1:B:400:LYS:HE2	1.91	0.52
1:L:184:GLU:OE1	1:L:200:LYS:HG2	2.10	0.52
1:K:53:ASP:CG	1:K:65:GLU:HG2	2.30	0.52
1:G:286:THR:HA	1:G:289:THR:OG1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:150:LEU:HD13	1:J:192:PRO:HG2	1.91	0.52
1:G:259:PHE:HB2	1:G:330:THR:HG21	1.91	0.52
1:I:127:PHE:HZ	1:I:248:LEU:HD23	1.75	0.52
1:D:306:PRO:O	1:D:388:LEU:HD12	2.09	0.52
1:F:380:ARG:NH1	1:F:385:ILE:HG21	2.25	0.52
1:H:372:ILE:HG13	1:H:385:ILE:HD12	1.90	0.52
1:F:160:ALA:HB3	1:F:169:ARG:HH21	1.74	0.52
1:I:140:LEU:HD12	1:I:226:GLY:C	2.30	0.52
1:L:82:TRP:HE1	1:L:221:ILE:HD11	1.74	0.52
1:C:58:GLU:HG2	1:C:416:HIS:CD2	2.44	0.52
1:L:285:PHE:C	1:L:285:PHE:CD1	2.84	0.52
1:D:297:LYS:HE3	1:J:436:GLU:OE1	2.08	0.52
1:F:397:GLU:HA	1:F:400:LYS:HD3	1.91	0.52
1:C:143:LYS:HA	1:C:143:LYS:HE2	1.90	0.52
1:A:379:GLU:HG2	1:A:379:GLU:O	2.08	0.52
1:F:13:VAL:HG21	1:F:42:LEU:HD21	1.92	0.52
1:H:129:LEU:C	1:H:129:LEU:HD13	2.29	0.52
1:H:8:ASP:O	1:H:12:LEU:HG	2.10	0.52
1:E:281:HIS:HD2	1:E:402:ASN:ND2	2.00	0.52
1:F:375:MET:O	1:F:380:ARG:NH2	2.43	0.52
1:H:370:ARG:O	1:H:372:ILE:HG23	2.10	0.52
1:D:127:PHE:CD2	1:D:351:LEU:HD23	2.45	0.52
1:C:22:ARG:NH1	1:C:36:GLU:OE2	2.43	0.52
1:F:52:PHE:CZ	1:F:54:GLY:HA2	2.46	0.52
1:E:345:LEU:HD22	1:E:409:LEU:CD2	2.40	0.52
1:H:78:VAL:HB	1:H:91:ARG:HG3	1.92	0.52
1:G:167:ASN:HD22	1:G:170:ARG:CZ	2.23	0.52
1:H:378:GLU:O	1:H:381:MET:HG3	2.09	0.52
1:J:97:TYR:CE2	1:J:103:PRO:HG3	2.45	0.51
1:A:386:VAL:HG12	1:A:387:ASP:N	2.24	0.51
1:D:135:PHE:HB3	1:D:231:PHE:CE1	2.45	0.51
1:L:131:PRO:HG2	1:L:199:PHE:HD2	1.75	0.51
1:H:397:GLU:HA	1:H:400:LYS:HZ1	1.75	0.51
1:G:120:GLU:HA	1:G:124:PHE:O	2.10	0.51
1:E:128:ASN:HA	1:E:202:ALA:O	2.09	0.51
1:L:34:ASN:ND2	1:L:34:ASN:O	2.43	0.51
1:G:76:THR:HG21	1:G:93:ILE:HB	1.92	0.51
1:G:311:TRP:HB3	1:G:320:ILE:HB	1.92	0.51
1:I:131:PRO:HD2	1:I:199:PHE:HB2	1.93	0.51
1:I:402:ASN:OD1	1:I:404:VAL:HG12	2.10	0.51
1:L:85:GLU:C	1:L:87:GLY:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:364:ALA:HB1	1:H:365:PRO:HD2	1.92	0.51
1:G:63:ILE:HG13	1:G:64:GLU:H	1.75	0.51
1:F:244:MET:N	1:F:338:ASP:HA	2.25	0.51
1:J:11:LYS:O	1:J:15:GLU:HG3	2.10	0.51
1:K:54:GLY:C	1:K:56:SER:N	2.63	0.51
1:L:285:PHE:C	1:L:285:PHE:HD1	2.12	0.51
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.92	0.51
1:A:250:LEU:HD12	1:A:258:PHE:CE2	2.46	0.51
1:K:147:THR:C	1:K:149:GLU:H	2.13	0.51
1:J:356:ASP:HA	1:J:359:LYS:HE2	1.92	0.51
1:E:285:PHE:CB	1:E:349:VAL:HG13	2.41	0.51
1:L:344:TYR:O	1:L:348:SER:HB2	2.09	0.51
1:A:343:PRO:O	1:A:347:LEU:HB2	2.10	0.51
1:K:3:LYS:HE2	1:K:4:TYR:OH	2.10	0.51
1:L:372:ILE:HG22	1:L:385:ILE:HD13	1.92	0.51
1:A:35:VAL:HG11	1:A:70:LEU:HD23	1.93	0.51
1:I:319:LEU:HB3	1:I:320:ILE:HD12	1.93	0.51
1:H:349:VAL:CG2	1:H:405:MET:SD	2.99	0.51
1:F:325:SER:O	1:F:326:ARG:HD3	2.10	0.51
1:I:155:GLY:O	1:I:158:ASP:HB2	2.11	0.51
1:J:434:PRO:O	1:J:438:GLU:HG3	2.11	0.51
1:J:349:VAL:HG23	1:J:409:LEU:CD1	2.40	0.51
1:F:379:GLU:HG3	1:F:385:ILE:CD1	2.41	0.51
1:L:375:MET:HG3	1:L:379:GLU:CG	2.38	0.51
1:E:91:ARG:NH1	1:E:93:ILE:HD11	2.25	0.51
1:B:135:PHE:HB3	1:B:231:PHE:CD1	2.45	0.51
1:D:236:LEU:HB2	1:D:239:VAL:HG21	1.90	0.51
1:A:110:ASN:O	1:A:113:LYS:HB2	2.11	0.51
1:F:48:ASN:HB3	1:F:71:TYR:CE1	2.46	0.51
1:B:286:THR:HG21	1:B:388:LEU:HD22	1.92	0.51
1:K:21:ILE:HD12	1:K:21:ILE:N	2.24	0.51
1:J:191:ALA:HB2	1:J:240:ASN:HB2	1.93	0.51
1:E:417:PHE:HD2	1:E:418:ILE:HD12	1.75	0.51
1:F:271:ALA:O	1:F:275:ILE:HG12	2.11	0.51
1:J:207:SER:O	1:J:210:ASP:N	2.43	0.51
1:H:162:THR:C	1:H:164:LEU:H	2.14	0.51
1:C:323:PRO:HD2	1:C:331:ARG:O	2.10	0.51
1:D:68:MET:CE	1:D:104:PHE:HB2	2.40	0.51
1:K:377:LYS:HA	1:K:380:ARG:NH2	2.25	0.51
1:D:52:PHE:CE2	1:D:54:GLY:HA2	2.45	0.51
1:F:267:LEU:HD21	1:F:326:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:291:PRO:HD3	2.10	0.51
1:A:421:LYS:HD3	1:A:424:GLU:OE2	2.10	0.51
1:D:211:ILE:HG22	1:D:215:LYS:HE3	1.91	0.51
1:I:150:LEU:HD13	1:I:192:PRO:HB2	1.93	0.51
1:D:22:ARG:NH1	1:D:36:GLU:OE2	2.43	0.51
1:H:116:LEU:HD22	1:H:119:MET:CE	2.40	0.51
1:L:383:ASN:HB2	1:L:385:ILE:CG1	2.40	0.51
1:D:406:VAL:HG22	1:D:414:PHE:CZ	2.45	0.51
1:F:114:ARG:NH2	1:F:407:LYS:O	2.44	0.51
1:K:380:ARG:HB2	1:K:380:ARG:NH1	2.26	0.51
1:I:160:ALA:O	1:I:161:PRO:C	2.49	0.51
1:H:345:LEU:O	1:H:349:VAL:HG12	2.11	0.51
1:L:23:LEU:HB2	1:L:35:VAL:HG22	1.92	0.51
1:G:203:GLY:O	1:G:204:ALA:C	2.48	0.51
1:B:300:VAL:HA	1:H:429:ARG:HH22	1.75	0.51
1:K:83:THR:CG2	1:K:89:VAL:H	2.04	0.51
1:C:380:ARG:CB	1:C:380:ARG:HH11	2.23	0.51
1:G:281:HIS:CD2	1:G:402:ASN:HD21	2.28	0.51
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.93	0.51
1:D:20:TYR:CZ	1:D:36:GLU:HB3	2.45	0.51
1:L:311:TRP:NE1	1:L:367:PRO:HA	2.25	0.51
1:D:406:VAL:HG22	1:D:414:PHE:CE1	2.45	0.51
1:H:397:GLU:CD	1:H:400:LYS:HZ1	2.14	0.51
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.51
1:I:203:GLY:O	1:I:207:SER:N	2.38	0.51
1:I:37:ILE:HG22	1:J:185:ALA:CB	2.41	0.51
1:L:242:SER:O	1:L:298:ARG:NE	2.44	0.51
1:A:237:PHE:CD1	1:A:238:GLY:N	2.79	0.51
1:L:30:GLY:HA2	1:L:342:ASN:ND2	2.25	0.51
1:B:393:ALA:HB2	1:B:425:TRP:CE2	2.45	0.51
1:K:19:LYS:HA	1:K:39:VAL:HB	1.91	0.51
1:L:316:ARG:HB2	1:L:370:ARG:NH1	2.26	0.51
1:A:38:PRO:HD2	1:A:41:GLN:HG3	1.93	0.51
1:L:51:MET:HE3	1:L:69:TYR:CE1	2.46	0.51
1:L:9:ILE:O	1:L:13:VAL:HG23	2.11	0.51
1:J:429:ARG:HD3	4:J:610:HOH:O	2.10	0.51
1:A:300:VAL:HG22	1:G:429:ARG:NH2	2.26	0.51
1:A:191:ALA:HB3	1:A:194:GLN:NE2	2.25	0.51
1:G:37:ILE:HG22	1:H:185:ALA:CB	2.41	0.51
1:J:162:THR:HG22	1:J:163:ASP:N	2.26	0.51
1:D:57:ILE:HD11	1:D:96:ILE:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ASN:ND2	1:G:104:PHE:HA	2.25	0.51
1:G:370:ARG:NH2	1:G:383:ASN:HD22	2.08	0.51
1:A:158:ASP:OD2	1:B:33:LYS:HE2	2.11	0.51
1:A:200:LYS:NZ	1:B:41:GLN:NE2	2.59	0.51
1:L:109:ARG:HG2	1:L:109:ARG:HH21	1.76	0.51
1:F:281:HIS:O	1:F:284:SER:N	2.42	0.51
1:D:128:ASN:ND2	1:D:203:GLY:HA2	2.26	0.51
1:L:306:PRO:O	1:L:388:LEU:HD12	2.11	0.51
1:D:315:ASN:ND2	1:D:370:ARG:HA	2.26	0.51
1:H:34:ASN:ND2	1:H:34:ASN:C	2.64	0.51
1:H:223:ARG:O	1:H:226:GLY:N	2.41	0.51
1:F:146:PRO:O	1:F:147:THR:HG23	2.10	0.51
1:B:370:ARG:NH2	1:B:375:MET:CG	2.71	0.51
1:I:116:LEU:HD23	1:I:351:LEU:HD11	1.93	0.51
1:F:386:VAL:HG23	1:F:386:VAL:O	2.11	0.51
1:E:147:THR:C	1:E:149:GLU:H	2.15	0.51
1:F:223:ARG:C	1:F:225:HIS:H	2.14	0.51
1:K:129:LEU:HD23	1:K:207:SER:OG	2.10	0.51
1:G:260:ASP:HB3	1:G:263:ALA:HB3	1.93	0.51
1:F:205:VAL:CG1	1:F:206:ARG:N	2.74	0.51
1:C:124:PHE:CE2	1:C:250:LEU:HD13	2.46	0.51
1:D:159:LEU:CD1	1:E:22:ARG:HH11	2.23	0.51
1:K:107:ASP:OD2	1:K:110:ASN:OD1	2.29	0.51
1:E:206:ARG:O	1:E:209:ASP:HB2	2.11	0.51
1:E:145:GLU:OE1	1:E:145:GLU:HA	2.11	0.51
1:G:406:VAL:HA	1:G:414:PHE:CD1	2.46	0.50
1:D:311:TRP:CD1	1:D:365:PRO:HG2	2.46	0.50
1:L:13:VAL:HG13	1:L:18:VAL:HB	1.93	0.50
1:D:34:ASN:O	1:D:34:ASN:ND2	2.44	0.50
1:E:356:ASP:O	1:E:360:ASN:HB2	2.11	0.50
1:F:437:ARG:HD3	1:L:148:LEU:CD2	2.41	0.50
1:H:243:GLY:C	1:H:339:PRO:HD3	2.32	0.50
1:D:253:ASN:O	1:D:255:VAL:HG13	2.11	0.50
1:E:374:VAL:HG23	1:E:375:MET:N	2.26	0.50
1:L:82:TRP:HE1	1:L:221:ILE:HD13	1.76	0.50
1:K:35:VAL:HG13	1:K:35:VAL:O	2.12	0.50
1:E:232:MET:HE3	1:K:440:TYR:HB2	1.93	0.50
1:L:23:LEU:HB3	1:L:70:LEU:HD23	1.93	0.50
1:L:371:ASN:HD21	1:L:374:VAL:HB	1.75	0.50
1:B:91:ARG:C	1:B:91:ARG:HD2	2.32	0.50
1:H:5:THR:O	1:H:7:GLU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:LYS:HE2	1:F:4:TYR:CE2	2.46	0.50
1:D:167:ASN:HD22	1:D:170:ARG:HB3	1.76	0.50
1:A:36:GLU:OE2	1:F:169:ARG:NH1	2.41	0.50
1:F:172:ILE:HD12	1:F:218:VAL:HA	1.92	0.50
1:F:53:ASP:OD1	1:F:62:ARG:NH2	2.43	0.50
1:G:315:ASN:HB3	1:G:318:PRO:HG3	1.93	0.50
1:H:351:LEU:CD2	1:H:355:LEU:HG	2.42	0.50
1:G:223:ARG:C	1:G:225:HIS:H	2.15	0.50
1:I:293:VAL:HG11	1:I:428:PHE:CD1	2.46	0.50
1:A:389:PRO:HA	1:A:394:GLU:OE1	2.11	0.50
1:G:267:LEU:CD2	1:G:326:ARG:HH12	2.24	0.50
1:J:160:ALA:O	1:J:161:PRO:O	2.30	0.50
1:G:237:PHE:CD2	1:G:238:GLY:N	2.79	0.50
1:D:160:ALA:HB3	1:D:169:ARG:HH22	1.76	0.50
1:H:372:ILE:HA	1:H:375:MET:SD	2.51	0.50
1:I:35:VAL:HG11	1:I:70:LEU:HD21	1.92	0.50
1:E:378:GLU:O	1:E:382:GLU:HG3	2.11	0.50
1:A:170:ARG:NH1	1:A:171:ASP:OD2	2.44	0.50
1:L:135:PHE:HB3	1:L:231:PHE:CD1	2.46	0.50
1:A:437:ARG:O	1:A:441:MET:HB2	2.11	0.50
1:G:375:MET:SD	1:G:380:ARG:HA	2.51	0.50
1:K:20:TYR:OH	1:K:36:GLU:HG3	2.11	0.50
1:B:371:ASN:HD22	1:B:372:ILE:N	2.10	0.50
1:J:169:ARG:HG3	1:J:169:ARG:HH21	1.76	0.50
1:L:376:SER:H	1:L:379:GLU:CG	2.25	0.50
1:G:399:PHE:HZ	1:G:409:LEU:CD2	2.21	0.50
1:H:399:PHE:HZ	1:H:409:LEU:HD12	1.76	0.50
1:F:60:PHE:CZ	1:F:423:ILE:HD11	2.46	0.50
1:L:306:PRO:HB3	1:L:319:LEU:HA	1.93	0.50
1:J:224:LYS:HB2	1:K:164:LEU:HD12	1.93	0.50
1:H:52:PHE:HE2	1:H:56:SER:OG	1.95	0.50
1:K:81:PRO:HG2	1:K:82:TRP:CE3	2.47	0.50
1:E:437:ARG:O	1:E:441:MET:HB3	2.12	0.50
1:G:211:ILE:HD13	1:G:244:MET:HE3	1.93	0.50
1:G:164:LEU:CD1	1:L:224:LYS:HD3	2.41	0.50
1:H:203:GLY:O	1:H:206:ARG:N	2.42	0.50
1:B:35:VAL:O	1:B:35:VAL:HG13	2.11	0.50
1:I:199:PHE:N	1:I:199:PHE:CD1	2.79	0.50
1:J:52:PHE:CZ	1:J:54:GLY:HA2	2.47	0.50
1:F:133:PRO:HD2	1:F:197:ILE:O	2.11	0.50
1:A:253:ASN:O	1:A:255:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:351:LEU:CD2	1:J:355:LEU:HG	2.40	0.50
1:I:267:LEU:HG	1:I:326:ARG:HH12	1.75	0.50
1:G:429:ARG:NH1	1:G:430:THR:HG22	2.26	0.50
1:J:234:LYS:HB3	1:J:294:ASN:ND2	2.27	0.50
1:B:165:GLY:HA3	1:C:223:ARG:HH21	1.77	0.50
1:J:176:LEU:CB	1:J:183:ILE:HD11	2.40	0.50
1:I:199:PHE:N	1:I:199:PHE:HD1	2.10	0.50
1:J:46:LEU:CD2	1:J:74:LEU:HD11	2.41	0.50
1:F:16:GLU:HG3	1:F:88:LYS:HE3	1.94	0.50
1:L:81:PRO:HG2	1:L:82:TRP:H	1.76	0.50
1:C:127:PHE:CE2	1:C:351:LEU:HB2	2.47	0.50
1:A:91:ARG:NH2	1:A:213:THR:OG1	2.43	0.50
1:I:216:LEU:HD11	1:J:159:LEU:HD13	1.93	0.50
1:I:169:ARG:HG3	1:I:195:HIS:CG	2.47	0.50
1:A:133:PRO:O	1:A:196:GLU:HG3	2.12	0.50
1:A:267:LEU:HD21	1:A:326:ARG:HH12	1.77	0.50
1:D:121:ASP:O	1:D:122:LEU:HD23	2.12	0.50
1:J:64:GLU:HG2	1:K:315:ASN:O	2.12	0.50
1:J:399:PHE:HE1	1:J:405:MET:HB3	1.76	0.50
1:J:236:LEU:HD12	1:J:239:VAL:HG21	1.93	0.50
1:C:326:ARG:HA	1:C:330:THR:OG1	2.11	0.50
1:L:286:THR:HG23	1:L:290:ASN:HD22	1.77	0.50
1:I:396:LEU:HD11	1:I:421:LYS:HB3	1.94	0.50
1:B:97:TYR:CE2	1:B:103:PRO:HG3	2.47	0.50
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.59	0.50
1:A:321:ARG:HG2	1:A:322:ILE:N	2.25	0.50
1:J:196:GLU:O	1:J:197:ILE:HD13	2.11	0.50
1:G:434:PRO:O	1:G:438:GLU:HG3	2.12	0.50
1:I:84:ALA:HB3	1:I:87:GLY:O	2.12	0.50
1:G:100:ASP:OD2	1:G:101:GLY:N	2.41	0.50
1:J:257:ALA:O	1:J:270:THR:HG23	2.12	0.50
1:I:142:GLU:N	1:I:142:GLU:OE2	2.38	0.50
1:K:372:ILE:O	1:K:373:TYR:HD2	1.94	0.50
1:F:45:ALA:HA	1:F:50:VAL:CG2	2.35	0.50
1:H:160:ALA:HB3	1:H:169:ARG:HH12	1.77	0.50
1:G:132:GLU:OE2	4:G:615:HOH:O	2.19	0.50
1:E:375:MET:HB3	1:E:379:GLU:HG2	1.94	0.50
1:F:22:ARG:HH11	1:F:22:ARG:HG2	1.76	0.50
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.94	0.50
1:H:95:ASP:OD1	1:H:109:ARG:HD3	2.12	0.50
1:A:164:LEU:HD11	1:B:224:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:O	1:A:279:VAL:HG23	2.12	0.50
1:L:156:TYR:CE1	1:L:189:GLU:OE1	2.64	0.50
1:G:404:VAL:HG22	1:G:405:MET:HE2	1.93	0.50
1:C:405:MET:HE2	1:C:405:MET:N	2.27	0.50
1:I:355:LEU:C	1:I:357:GLY:H	2.15	0.50
1:D:140:LEU:CD2	1:D:228:HIS:HB2	2.42	0.50
1:L:281:HIS:CE1	1:L:404:VAL:HG11	2.47	0.50
1:F:402:ASN:OD1	1:F:404:VAL:HG12	2.12	0.50
1:G:245:HIS:CD2	1:G:335:ARG:HB3	2.47	0.50
1:E:148:LEU:HD13	1:E:148:LEU:N	2.26	0.50
1:K:5:THR:HG23	1:K:8:ASP:H	1.77	0.50
1:I:236:LEU:HD12	1:I:239:VAL:HG21	1.94	0.50
1:A:435:TRP:O	1:A:439:GLN:HG2	2.12	0.50
1:D:200:LYS:CE	1:E:41:GLN:HE22	2.25	0.50
1:K:115:ILE:HG22	1:K:351:LEU:CD1	2.38	0.49
1:C:182:GLU:HG2	1:C:200:LYS:HD2	1.94	0.49
1:I:80:PHE:CE1	1:I:91:ARG:HG2	2.42	0.49
1:H:20:TYR:O	1:H:89:VAL:HG13	2.11	0.49
1:H:311:TRP:HB3	1:H:320:ILE:HB	1.93	0.49
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.46	0.49
1:C:3:LYS:HB3	1:C:75:ASN:OD1	2.12	0.49
1:I:156:TYR:O	1:I:158:ASP:N	2.44	0.49
1:L:261:GLU:O	1:L:266:GLN:HG2	2.12	0.49
1:G:112:LEU:HD12	1:G:344:TYR:HD2	1.77	0.49
1:H:184:GLU:HB2	1:H:199:PHE:O	2.12	0.49
1:A:328:ILE:C	1:A:328:ILE:HD12	2.32	0.49
1:H:111:ASN:O	1:H:115:ILE:HG12	2.11	0.49
1:I:368:ILE:HG21	1:I:372:ILE:CG2	2.42	0.49
1:G:27:ASP:HB2	1:G:57:ILE:HA	1.93	0.49
1:J:309:VAL:CG2	1:J:386:VAL:HB	2.42	0.49
1:H:74:LEU:HD22	1:H:74:LEU:N	2.17	0.49
1:D:161:PRO:HB2	1:D:167:ASN:OD1	2.12	0.49
1:D:174:LEU:HD13	1:E:86:LYS:HB2	1.94	0.49
1:J:208:CYS:HA	1:J:343:PRO:HB2	1.94	0.49
1:H:82:TRP:HE1	1:H:221:ILE:HD11	1.75	0.49
1:K:48:ASN:HB3	1:K:71:TYR:CD1	2.47	0.49
1:J:162:THR:CG2	1:J:163:ASP:N	2.75	0.49
1:K:338:ASP:C	1:K:338:ASP:OD2	2.50	0.49
1:B:252:LYS:O	1:B:253:ASN:HB2	2.12	0.49
1:B:393:ALA:HB2	1:B:425:TRP:CD2	2.46	0.49
1:H:224:LYS:HB2	1:I:164:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:391:THR:OG1	1:K:394:GLU:HB2	2.12	0.49
1:H:189:GLU:OE2	1:H:190:VAL:HG23	2.12	0.49
1:G:384:GLY:C	1:G:385:ILE:HD13	2.31	0.49
1:L:58:GLU:O	1:L:61:VAL:HG22	2.12	0.49
1:F:309:VAL:O	1:F:310:ALA:HB2	2.12	0.49
1:B:399:PHE:HZ	1:B:409:LEU:HD12	1.77	0.49
1:K:115:ILE:HD11	1:K:408:ALA:O	2.12	0.49
1:E:429:ARG:NH2	1:K:300:VAL:HG12	2.26	0.49
1:C:203:GLY:O	1:C:205:VAL:N	2.45	0.49
1:F:24:GLN:HE21	1:F:91:ARG:HH11	1.59	0.49
1:C:282:ALA:C	1:C:284:SER:N	2.66	0.49
1:E:293:VAL:HG11	1:E:428:PHE:CE2	2.47	0.49
1:H:76:THR:O	1:H:78:VAL:HG23	2.12	0.49
1:C:156:TYR:CE2	1:D:62:ARG:NH1	2.80	0.49
1:K:183:ILE:HD12	1:K:183:ILE:N	2.27	0.49
1:E:74:LEU:H	1:E:74:LEU:CD2	2.26	0.49
1:I:256:ASN:ND2	1:I:328:ILE:O	2.46	0.49
1:D:311:TRP:HA	1:D:320:ILE:HB	1.94	0.49
1:I:399:PHE:HZ	1:I:409:LEU:HD11	1.76	0.49
1:G:239:VAL:O	1:G:239:VAL:HG23	2.11	0.49
1:F:129:LEU:HD22	1:F:131:PRO:CD	2.42	0.49
1:C:402:ASN:ND2	1:C:404:VAL:HG12	2.28	0.49
1:B:409:LEU:O	1:B:413:LEU:HB2	2.12	0.49
1:J:129:LEU:O	1:J:201:TYR:HA	2.12	0.49
1:G:23:LEU:HB3	1:G:70:LEU:HD23	1.94	0.49
1:E:48:ASN:OD1	1:E:72:PRO:HD2	2.13	0.49
1:H:328:ILE:HD13	1:H:329:SER:H	1.76	0.49
1:A:52:PHE:CE1	1:A:70:LEU:CD1	2.95	0.49
1:F:85:GLU:C	1:F:87:GLY:H	2.15	0.49
1:E:271:ALA:O	1:E:272:LYS:C	2.50	0.49
1:B:109:ARG:HG3	1:B:344:TYR:CE2	2.48	0.49
1:B:107:ASP:HB3	1:B:110:ASN:HB2	1.95	0.49
1:E:45:ALA:HA	1:E:50:VAL:HG23	1.95	0.49
1:I:273:HIS:O	1:I:276:ALA:HB3	2.12	0.49
1:H:6:ARG:O	1:H:6:ARG:HG3	2.13	0.49
1:G:402:ASN:OD1	1:G:402:ASN:C	2.51	0.49
1:H:161:PRO:O	1:H:167:ASN:ND2	2.45	0.49
1:B:380:ARG:HA	1:B:383:ASN:HD22	1.77	0.49
1:I:52:PHE:CD1	1:I:70:LEU:HD22	2.48	0.49
1:E:326:ARG:HH11	1:E:326:ARG:CG	2.25	0.49
1:C:297:LYS:N	1:C:297:LYS:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ASP:C	1:D:266:GLN:N	2.64	0.49
1:I:320:ILE:HG22	1:I:321:ARG:N	2.26	0.49
1:I:308:TYR:OH	1:I:380:ARG:HD2	2.12	0.49
1:C:212:GLN:OE1	1:C:212:GLN:HA	2.11	0.49
1:D:293:VAL:HG23	1:J:440:TYR:OH	2.12	0.49
1:I:133:PRO:CA	1:I:244:MET:HG3	2.43	0.49
1:K:27:ASP:C	1:K:27:ASP:OD2	2.51	0.49
1:I:312:SER:OG	1:I:369:ASP:HA	2.13	0.49
1:G:145:GLU:HA	1:G:145:GLU:OE1	2.13	0.49
1:G:310:ALA:HB3	1:G:372:ILE:HD11	1.93	0.49
1:H:5:THR:C	1:H:7:GLU:N	2.65	0.49
1:F:197:ILE:HD12	1:F:214:PHE:CE1	2.48	0.49
1:A:360:ASN:O	1:A:361:LYS:C	2.50	0.49
1:F:280:LYS:HG3	1:F:281:HIS:CD2	2.46	0.49
1:H:235:PRO:O	1:H:236:LEU:HD23	2.12	0.49
1:F:119:MET:O	1:F:124:PHE:HB2	2.12	0.49
1:J:85:GLU:C	1:J:87:GLY:H	2.16	0.49
1:H:286:THR:HG23	1:H:290:ASN:HD22	1.77	0.49
1:G:309:VAL:HA	1:G:319:LEU:HD22	1.95	0.49
1:K:271:ALA:O	1:K:275:ILE:HG13	2.13	0.49
1:J:22:ARG:HH11	1:J:22:ARG:HG2	1.77	0.49
1:E:223:ARG:C	1:E:225:HIS:H	2.16	0.49
1:D:13:VAL:HG21	1:D:42:LEU:CD2	2.42	0.49
1:F:127:PHE:CD2	1:F:351:LEU:HG	2.47	0.49
1:A:138:PHE:CE2	1:A:236:LEU:HD11	2.47	0.49
1:K:25:PHE:HB2	1:K:96:ILE:HD11	1.94	0.49
1:A:232:MET:CE	1:A:235:PRO:HA	2.42	0.49
1:D:11:LYS:HG3	1:D:15:GLU:OE2	2.13	0.49
1:D:443:GLN:CA	1:D:443:GLN:HE21	2.25	0.49
1:E:142:GLU:H	1:E:142:GLU:CD	2.15	0.49
1:G:371:ASN:O	1:G:372:ILE:HB	2.13	0.49
1:F:146:PRO:CG	1:F:228:HIS:CD2	2.87	0.49
1:L:355:LEU:C	1:L:357:GLY:H	2.15	0.49
1:B:419:GLU:O	1:B:423:ILE:HG12	2.12	0.49
1:D:243:GLY:N	1:D:298:ARG:NH1	2.61	0.49
1:D:78:VAL:HG21	1:D:91:ARG:HH21	1.76	0.49
1:C:18:VAL:CG2	1:C:79:ILE:HD12	2.42	0.49
1:C:79:ILE:HD13	1:C:90:ALA:HB2	1.95	0.49
1:C:54:GLY:O	1:C:57:ILE:HG12	2.12	0.49
1:A:52:PHE:HE1	1:A:70:LEU:HD13	1.77	0.49
1:F:187:HIS:CE1	1:F:196:GLU:OE1	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:GLU:O	1:I:61:VAL:HG22	2.13	0.49
1:F:322:ILE:HD12	1:F:322:ILE:N	2.28	0.49
1:F:433:HIS:O	1:F:436:GLU:HB2	2.13	0.49
1:I:67:ASP:O	1:I:99:PRO:HG3	2.12	0.49
1:D:80:PHE:CD2	1:D:80:PHE:N	2.81	0.49
1:I:63:ILE:H	1:I:63:ILE:HD12	1.77	0.49
1:H:166:GLU:O	1:H:166:GLU:OE1	2.31	0.49
1:B:129:LEU:CD1	1:B:207:SER:HB3	2.42	0.49
1:J:129:LEU:HD22	1:J:131:PRO:CD	2.43	0.49
1:A:3:LYS:HB3	1:A:3:LYS:HZ3	1.74	0.49
1:K:282:ALA:C	1:K:284:SER:H	2.16	0.49
1:H:91:ARG:HD2	1:H:91:ARG:C	2.33	0.49
1:D:200:LYS:HE2	1:E:41:GLN:HE22	1.78	0.49
1:J:24:GLN:NE2	1:J:32:ILE:HD11	2.27	0.49
1:J:258:PHE:HA	1:J:271:ALA:HB2	1.93	0.49
1:G:73:ASP:HA	4:G:612:HOH:O	2.11	0.49
1:K:317:SER:N	1:K:318:PRO:HD3	2.28	0.49
1:J:78:VAL:HB	1:J:91:ARG:HG3	1.94	0.49
1:F:283:THR:HG23	1:F:309:VAL:HG21	1.95	0.49
1:L:124:PHE:CZ	1:L:358:ILE:HG21	2.48	0.49
1:D:351:LEU:O	1:D:355:LEU:HG	2.13	0.49
1:D:286:THR:HA	1:D:289:THR:OG1	2.12	0.49
1:C:18:VAL:HG21	1:C:79:ILE:CD1	2.42	0.49
1:F:52:PHE:CD1	1:F:70:LEU:HD13	2.48	0.49
1:G:174:LEU:HD23	1:L:86:LYS:HB3	1.95	0.49
1:E:380:ARG:O	1:E:385:ILE:O	2.31	0.49
1:A:27:ASP:OD1	1:A:31:THR:HB	2.12	0.49
1:B:315:ASN:HD22	1:B:318:PRO:HD3	1.78	0.48
1:B:370:ARG:HH12	1:B:375:MET:HG3	1.78	0.48
1:J:160:ALA:O	1:J:161:PRO:C	2.51	0.48
1:F:308:TYR:CD1	1:F:372:ILE:HG21	2.48	0.48
1:A:3:LYS:HB3	1:A:3:LYS:HZ2	1.76	0.48
1:A:23:LEU:HB2	1:A:35:VAL:CG1	2.43	0.48
1:D:199:PHE:HZ	1:D:214:PHE:HB2	1.78	0.48
1:F:66:SER:O	1:F:68:MET:N	2.47	0.48
1:A:281:HIS:CD2	1:A:402:ASN:HD21	2.30	0.48
1:B:308:TYR:HE1	1:B:373:TYR:CE1	2.31	0.48
1:L:140:LEU:HD12	1:L:226:GLY:HA2	1.94	0.48
1:B:45:ALA:HA	1:B:50:VAL:HG23	1.95	0.48
1:D:177:GLU:OE2	1:D:177:GLU:HA	2.13	0.48
1:G:375:MET:HE1	1:G:379:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:258:PHE:HB3	1:G:271:ALA:N	2.29	0.48
1:J:160:ALA:HB2	1:J:188:HIS:HD2	1.79	0.48
1:J:76:THR:O	1:J:78:VAL:HG23	2.13	0.48
1:G:281:HIS:CD2	1:G:404:VAL:HG11	2.47	0.48
1:C:160:ALA:HB1	1:C:161:PRO:CD	2.43	0.48
1:A:206:ARG:NH1	1:A:206:ARG:CG	2.74	0.48
1:C:129:LEU:HD22	1:C:131:PRO:CD	2.41	0.48
1:A:300:VAL:HG13	1:A:301:PRO:HD2	1.94	0.48
1:C:91:ARG:C	1:C:91:ARG:HD2	2.34	0.48
1:H:371:ASN:OD1	1:H:374:VAL:HG22	2.12	0.48
1:I:208:CYS:HA	1:I:211:ILE:CG1	2.43	0.48
1:G:203:GLY:O	1:G:206:ARG:N	2.46	0.48
1:F:48:ASN:OD1	1:F:72:PRO:HD2	2.12	0.48
1:J:268:SER:OG	1:J:270:THR:HG23	2.13	0.48
1:A:324:ALA:O	1:A:325:SER:O	2.31	0.48
1:F:129:LEU:HD23	1:F:130:GLY:H	1.78	0.48
1:L:380:ARG:HB3	1:L:380:ARG:HH11	1.77	0.48
1:J:306:PRO:CG	1:J:335:ARG:HB2	2.37	0.48
1:D:273:HIS:CE1	1:D:361:LYS:CA	2.96	0.48
1:J:30:GLY:CA	1:J:342:ASN:ND2	2.74	0.48
1:K:234:LYS:HB3	1:K:294:ASN:HD21	1.78	0.48
1:E:260:ASP:HB2	1:E:268:SER:HA	1.95	0.48
1:K:104:PHE:CZ	1:K:106:GLY:HA3	2.48	0.48
1:K:37:ILE:HG22	1:L:185:ALA:HA	1.94	0.48
1:K:138:PHE:HB3	1:K:147:THR:O	2.13	0.48
1:C:286:THR:HG22	1:C:290:ASN:ND2	2.28	0.48
1:J:199:PHE:HZ	1:J:214:PHE:CG	2.31	0.48
1:F:375:MET:HE2	1:F:385:ILE:HD11	1.94	0.48
1:C:402:ASN:C	1:C:402:ASN:OD1	2.51	0.48
1:E:78:VAL:HB	1:E:91:ARG:HG3	1.95	0.48
1:L:310:ALA:HB1	1:L:368:ILE:CB	2.43	0.48
1:D:173:VAL:HG13	1:D:183:ILE:HG13	1.96	0.48
1:H:21:ILE:HG12	1:H:21:ILE:O	2.13	0.48
1:G:178:GLU:HG2	1:L:86:LYS:HE2	1.94	0.48
1:C:291:PRO:HG2	1:C:292:THR:H	1.78	0.48
4:G:604:HOH:O	1:H:157:PHE:HZ	1.96	0.48
1:J:259:PHE:CE1	1:J:326:ARG:HB3	2.48	0.48
1:I:328:ILE:C	1:I:330:THR:H	2.16	0.48
1:E:331:ARG:NH2	1:E:331:ARG:HG2	2.28	0.48
1:I:63:ILE:N	1:I:63:ILE:HD12	2.28	0.48
1:F:297:LYS:HE3	1:L:436:GLU:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:LEU:O	1:K:119:MET:HB3	2.13	0.48
1:L:440:TYR:HD1	1:L:444:TYR:CE2	2.32	0.48
1:F:160:ALA:HB1	1:F:161:PRO:CD	2.39	0.48
1:E:375:MET:HA	1:E:379:GLU:OE1	2.13	0.48
1:C:321:ARG:O	1:C:323:PRO:HD3	2.13	0.48
1:A:27:ASP:CG	1:A:31:THR:HB	2.34	0.48
1:L:176:LEU:O	1:L:181:PHE:HB2	2.13	0.48
1:H:272:LYS:NZ	1:H:364:ALA:H	2.09	0.48
1:H:282:ALA:C	1:H:284:SER:H	2.17	0.48
1:E:19:LYS:HA	1:E:39:VAL:HB	1.94	0.48
1:K:129:LEU:HD11	1:K:246:CYS:HB3	1.95	0.48
1:D:325:SER:OG	1:D:329:SER:HB2	2.14	0.48
1:K:426:ASP:HA	1:K:429:ARG:HG2	1.95	0.48
1:L:396:LEU:O	1:L:400:LYS:HG3	2.12	0.48
1:L:310:ALA:HB2	1:L:385:ILE:HG22	1.96	0.48
1:I:282:ALA:HB1	1:I:319:LEU:HD21	1.96	0.48
1:I:311:TRP:HB3	1:I:320:ILE:HB	1.96	0.48
1:H:291:PRO:HG3	1:H:341:ALA:HA	1.94	0.48
1:D:437:ARG:HA	1:J:232:MET:HE3	1.96	0.48
1:G:271:ALA:O	1:G:275:ILE:HD12	2.14	0.48
1:J:173:VAL:HG13	1:J:183:ILE:CD1	2.44	0.48
1:K:22:ARG:NH1	1:K:36:GLU:OE2	2.45	0.48
1:F:97:TYR:CD1	1:F:103:PRO:HA	2.48	0.48
1:L:24:GLN:HE22	1:L:91:ARG:HH11	1.60	0.48
1:C:164:LEU:CD1	1:D:224:LYS:HD3	2.38	0.48
1:B:380:ARG:HA	1:B:383:ASN:ND2	2.29	0.48
1:G:23:LEU:HB2	1:G:35:VAL:CG1	2.41	0.48
1:A:111:ASN:O	1:A:115:ILE:HG12	2.14	0.48
1:D:242:SER:O	1:D:339:PRO:HD2	2.13	0.48
1:D:280:LYS:HD3	1:D:281:HIS:CE1	2.49	0.48
1:F:189:GLU:HB3	1:F:194:GLN:NE2	2.29	0.48
1:K:236:LEU:O	1:K:239:VAL:HG23	2.13	0.48
1:K:236:LEU:HB2	1:K:239:VAL:HG23	1.96	0.48
1:F:35:VAL:HG13	1:F:35:VAL:O	2.13	0.48
1:G:119:MET:HG2	1:G:124:PHE:HB2	1.95	0.48
1:A:402:ASN:OD1	1:A:404:VAL:HG12	2.13	0.48
1:C:100:ASP:O	1:C:102:THR:HG22	2.14	0.48
1:A:243:GLY:HA3	1:A:298:ARG:NH1	2.29	0.48
1:A:11:LYS:HZ3	1:A:15:GLU:HB2	1.79	0.48
1:J:167:ASN:O	1:J:171:ASP:OD1	2.31	0.48
1:D:208:CYS:SG	1:D:347:LEU:HD12	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:O	1:A:158:ASP:N	2.46	0.48
1:I:150:LEU:HD12	1:I:192:PRO:HB2	1.96	0.48
1:G:13:VAL:CG1	1:G:18:VAL:HB	2.41	0.48
1:A:131:PRO:HG2	1:A:211:ILE:HD11	1.96	0.48
1:K:234:LYS:N	1:K:235:PRO:HD3	2.29	0.48
1:D:205:VAL:HG23	1:D:206:ARG:N	2.26	0.48
1:G:20:TYR:OH	1:G:36:GLU:HB3	2.13	0.48
1:I:6:ARG:NH2	1:I:47:ASP:OD1	2.46	0.48
1:L:147:THR:C	1:L:149:GLU:H	2.16	0.48
1:E:319:LEU:C	1:E:320:ILE:HD12	2.34	0.48
1:H:41:GLN:NE2	1:I:200:LYS:NZ	2.56	0.48
1:K:22:ARG:NH1	1:L:159:LEU:HD13	2.28	0.48
1:F:429:ARG:HH21	1:L:300:VAL:CG2	2.15	0.48
1:J:207:SER:O	1:J:208:CYS:C	2.51	0.48
1:I:355:LEU:C	1:I:357:GLY:N	2.66	0.48
1:E:297:LYS:HE3	1:K:436:GLU:CD	2.34	0.48
1:J:51:MET:SD	1:J:67:ASP:HB3	2.54	0.48
1:G:261:GLU:O	1:G:266:GLN:HG2	2.13	0.48
1:C:109:ARG:HD2	1:C:344:TYR:CE2	2.49	0.48
1:D:292:THR:OG1	1:D:295:SER:HB2	2.13	0.48
1:D:251:PHE:N	1:D:251:PHE:CD1	2.82	0.48
1:L:189:GLU:HB3	1:L:194:GLN:NE2	2.29	0.48
1:G:158:ASP:N	1:G:158:ASP:OD1	2.47	0.48
1:J:135:PHE:HB3	1:J:231:PHE:CE1	2.49	0.48
1:B:55:SER:OG	1:B:62:ARG:NE	2.46	0.48
1:J:212:GLN:CA	1:J:212:GLN:OE1	2.58	0.48
1:H:137:LEU:HD12	1:H:195:HIS:HE2	1.79	0.48
1:D:77:PHE:CE1	1:D:90:ALA:HB1	2.49	0.48
1:L:418:ILE:O	1:L:422:GLU:HG3	2.13	0.48
1:J:299:LEU:CD1	1:J:299:LEU:N	2.77	0.48
1:H:250:LEU:HB2	1:H:258:PHE:CZ	2.48	0.48
1:K:98:ASN:C	1:K:100:ASP:H	2.16	0.48
1:E:272:LYS:O	1:E:275:ILE:HB	2.14	0.48
1:E:32:ILE:CD1	1:E:216:LEU:HD13	2.44	0.48
1:D:218:VAL:O	1:D:222:ALA:HB2	2.14	0.48
1:C:393:ALA:HB2	1:C:425:TRP:CE2	2.48	0.48
1:H:423:ILE:O	1:H:427:MET:HG3	2.14	0.48
1:F:286:THR:O	1:F:290:ASN:N	2.45	0.47
1:J:402:ASN:CG	1:J:405:MET:HG2	2.34	0.47
1:L:156:TYR:HB2	1:L:190:VAL:HA	1.96	0.47
1:A:311:TRP:HA	1:A:320:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ILE:HG23	1:E:285:PHE:CE2	2.49	0.47
1:K:311:TRP:HA	1:K:320:ILE:HB	1.96	0.47
1:F:370:ARG:NH1	1:F:375:MET:HE3	2.29	0.47
1:K:270:THR:HG22	1:K:358:ILE:CD1	2.40	0.47
1:B:279:VAL:HG13	1:B:309:VAL:HG12	1.95	0.47
1:J:121:ASP:C	1:J:122:LEU:HD22	2.34	0.47
1:H:28:ILE:HD11	1:H:417:PHE:HA	1.96	0.47
1:E:294:ASN:HD22	1:E:297:LYS:HG3	1.79	0.47
1:K:326:ARG:HD3	1:K:330:THR:OG1	2.14	0.47
1:A:78:VAL:HG12	1:A:91:ARG:CG	2.44	0.47
1:A:315:ASN:OD1	1:A:371:ASN:HA	2.14	0.47
1:I:319:LEU:CB	1:I:320:ILE:HD12	2.44	0.47
1:B:120:GLU:C	1:B:122:LEU:N	2.68	0.47
1:C:20:TYR:HB3	1:C:89:VAL:HG22	1.96	0.47
1:F:264:ASP:O	1:F:265:LEU:HB2	2.14	0.47
1:G:360:ASN:O	1:G:361:LYS:C	2.53	0.47
1:D:413:LEU:HA	1:D:413:LEU:HD23	1.73	0.47
1:J:138:PHE:CD2	1:J:148:LEU:HA	2.48	0.47
1:G:370:ARG:HG3	1:G:370:ARG:HH11	1.79	0.47
1:H:140:LEU:HD12	1:H:226:GLY:HA2	1.96	0.47
1:I:116:LEU:HD23	1:I:351:LEU:CD1	2.44	0.47
1:E:402:ASN:CG	1:E:405:MET:HG2	2.35	0.47
1:G:160:ALA:HB3	1:G:169:ARG:HH12	1.79	0.47
1:L:291:PRO:HG2	1:L:292:THR:HG23	1.96	0.47
1:D:134:GLU:HG3	1:D:243:GLY:O	2.13	0.47
1:K:404:VAL:HG23	1:K:405:MET:HE2	1.96	0.47
1:H:349:VAL:HG23	1:H:405:MET:SD	2.53	0.47
1:G:79:ILE:HD13	1:G:90:ALA:HB2	1.96	0.47
1:F:342:ASN:HD21	1:F:344:TYR:HD1	1.62	0.47
1:G:309:VAL:HB	1:G:386:VAL:HG23	1.95	0.47
1:C:295:SER:O	1:C:299:LEU:HD13	2.15	0.47
1:F:347:LEU:HD22	1:F:347:LEU:N	2.29	0.47
1:C:316:ARG:HG2	1:C:373:TYR:CG	2.49	0.47
1:G:368:ILE:HD13	1:G:372:ILE:HG13	1.96	0.47
1:I:126:ASP:HB2	1:I:251:PHE:HB2	1.96	0.47
1:B:315:ASN:HD22	1:B:318:PRO:CD	2.27	0.47
1:D:167:ASN:ND2	1:D:170:ARG:HB2	2.29	0.47
1:H:168:CYS:O	1:H:169:ARG:C	2.53	0.47
1:E:80:PHE:CE1	1:E:91:ARG:HB3	2.49	0.47
1:B:231:PHE:O	1:B:339:PRO:HG2	2.14	0.47
1:K:129:LEU:HB3	1:K:207:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:HIS:HE1	1:I:441:MET:O	1.96	0.47
1:C:114:ARG:HH21	1:C:115:ILE:HD11	1.78	0.47
1:B:262:ASN:HD22	1:B:262:ASN:N	2.08	0.47
1:G:306:PRO:HA	1:G:317:SER:HB2	1.96	0.47
1:D:176:LEU:HD11	1:D:214:PHE:CD1	2.49	0.47
1:B:300:VAL:HG11	1:H:430:THR:CG2	2.44	0.47
1:D:55:SER:HB2	1:D:62:ARG:HB2	1.95	0.47
1:L:325:SER:HB2	1:L:329:SER:HB3	1.96	0.47
1:J:48:ASN:HB3	1:J:71:TYR:CD1	2.49	0.47
1:G:148:LEU:N	1:G:148:LEU:HD22	2.29	0.47
1:J:36:GLU:HG2	1:K:186:SER:O	2.14	0.47
1:H:131:PRO:C	1:H:133:PRO:HD3	2.34	0.47
1:D:168:CYS:O	1:D:169:ARG:C	2.52	0.47
1:D:160:ALA:HB2	1:D:188:HIS:CD2	2.49	0.47
1:B:147:THR:HG22	1:B:149:GLU:HG3	1.94	0.47
1:E:140:LEU:HD12	1:E:227:LEU:N	2.29	0.47
1:F:172:ILE:O	1:F:176:LEU:HG	2.14	0.47
1:G:52:PHE:CD1	1:G:70:LEU:HD13	2.48	0.47
1:I:114:ARG:HH12	1:I:115:ILE:CD1	2.26	0.47
1:C:127:PHE:CE2	1:C:347:LEU:HD22	2.49	0.47
1:B:261:GLU:HA	1:B:266:GLN:HE22	1.80	0.47
1:G:245:HIS:NE2	1:G:335:ARG:HB3	2.29	0.47
1:F:91:ARG:C	1:F:91:ARG:HD2	2.34	0.47
1:C:244:MET:O	1:C:337:VAL:HB	2.13	0.47
1:B:308:TYR:HE1	1:B:373:TYR:CD1	2.32	0.47
1:B:203:GLY:O	1:B:206:ARG:N	2.47	0.47
1:D:156:TYR:HB2	1:D:190:VAL:HA	1.96	0.47
1:L:203:GLY:O	1:L:204:ALA:C	2.52	0.47
1:E:74:LEU:N	1:E:74:LEU:HD22	2.29	0.47
1:I:63:ILE:O	1:J:316:ARG:NH1	2.47	0.47
1:L:58:GLU:HG3	1:L:416:HIS:ND1	2.29	0.47
1:E:399:PHE:CE2	1:E:418:ILE:HD11	2.49	0.47
1:F:309:VAL:HG23	1:F:386:VAL:O	2.14	0.47
1:B:25:PHE:CE1	1:B:33:LYS:HB2	2.49	0.47
1:D:345:LEU:HD22	1:D:409:LEU:CD2	2.44	0.47
1:D:34:ASN:C	1:D:34:ASN:HD22	2.17	0.47
1:J:129:LEU:CD2	1:J:130:GLY:N	2.74	0.47
1:H:347:LEU:O	1:H:348:SER:C	2.52	0.47
1:H:271:ALA:O	1:H:275:ILE:HG12	2.14	0.47
1:F:353:ALA:HB2	1:F:405:MET:HE3	1.96	0.47
1:K:5:THR:H	1:K:8:ASP:HB2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:MET:HA	1:C:379:GLU:OE1	2.14	0.47
1:A:11:LYS:HD2	1:A:15:GLU:OE1	2.14	0.47
1:A:48:ASN:OD1	1:A:71:TYR:HA	2.14	0.47
1:A:105:GLU:H	1:A:105:GLU:CD	2.18	0.47
1:I:5:THR:H	1:I:8:ASP:HB2	1.80	0.47
1:H:360:ASN:O	1:H:361:LYS:C	2.51	0.47
1:K:291:PRO:CG	1:K:341:ALA:HA	2.40	0.47
1:C:203:GLY:O	1:C:204:ALA:C	2.53	0.47
1:C:274:PHE:CE2	1:C:332:VAL:HG11	2.49	0.47
1:D:84:ALA:C	1:D:86:LYS:H	2.18	0.47
1:F:23:LEU:HB3	1:F:70:LEU:HD23	1.95	0.47
1:K:168:CYS:SG	1:K:227:LEU:HD12	2.54	0.47
1:C:435:TRP:CE2	1:C:439:GLN:HG3	2.49	0.47
1:G:208:CYS:O	1:G:212:GLN:HG2	2.15	0.47
1:G:151:ASN:HD22	1:G:166:GLU:CD	2.17	0.47
1:E:5:THR:O	1:E:8:ASP:HB2	2.15	0.47
1:J:176:LEU:HD12	1:J:183:ILE:HD11	1.95	0.47
1:H:5:THR:H	1:H:8:ASP:CB	2.17	0.47
1:E:247:ASN:HD22	1:E:331:ARG:NE	2.12	0.47
1:D:167:ASN:HD22	1:D:170:ARG:CB	2.28	0.47
1:L:309:VAL:HG21	1:L:386:VAL:HB	1.96	0.47
1:A:337:VAL:HG12	1:A:338:ASP:N	2.30	0.47
1:L:355:LEU:C	1:L:357:GLY:N	2.67	0.47
1:C:402:ASN:HD21	1:C:404:VAL:HG12	1.78	0.47
1:H:139:LYS:HA	1:H:227:LEU:HD23	1.96	0.47
1:K:351:LEU:O	1:K:351:LEU:HD13	2.14	0.47
1:F:215:LYS:O	1:F:219:LYS:HB2	2.14	0.47
1:B:380:ARG:NH1	1:B:387:ASP:OD1	2.47	0.47
1:L:396:LEU:HD22	1:L:418:ILE:HD13	1.97	0.47
1:K:405:MET:HE2	1:K:405:MET:HA	1.96	0.47
1:D:4:TYR:CE2	1:D:12:LEU:HD11	2.50	0.47
1:C:321:ARG:O	1:C:333:GLU:HB3	2.14	0.47
1:E:170:ARG:HG2	1:E:170:ARG:NH1	2.29	0.47
1:A:5:THR:O	1:A:9:ILE:HG12	2.15	0.47
1:H:183:ILE:HG23	1:H:198:ASP:O	2.14	0.47
1:D:375:MET:HG2	1:D:376:SER:N	2.29	0.47
1:B:243:GLY:HA3	1:B:298:ARG:HH12	1.79	0.47
1:C:124:PHE:CZ	1:C:358:ILE:HD13	2.50	0.47
1:H:135:PHE:HB3	1:H:231:PHE:CD1	2.50	0.47
1:H:125:SER:OG	1:H:253:ASN:N	2.48	0.47
1:F:326:ARG:HD2	1:F:330:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:17:ASN:ND2	1:J:87:GLY:HA2	2.30	0.47
1:G:211:ILE:HD13	1:G:244:MET:CE	2.45	0.47
1:J:289:THR:HB	1:J:337:VAL:HG22	1.96	0.47
1:B:440:TYR:O	1:B:444:TYR:HB2	2.14	0.47
1:C:185:ALA:CB	1:D:37:ILE:HG22	2.45	0.47
1:H:175:GLU:O	1:H:179:MET:HG3	2.15	0.47
1:J:151:ASN:HD22	1:J:166:GLU:CD	2.17	0.47
1:G:3:LYS:HB3	1:G:75:ASN:ND2	2.29	0.47
1:I:370:ARG:N	1:I:370:ARG:HD3	2.29	0.47
1:A:306:PRO:HB3	1:A:319:LEU:CA	2.37	0.47
1:E:421:LYS:HD3	1:E:424:GLU:OE1	2.15	0.47
1:F:221:ILE:O	1:F:225:HIS:HD2	1.98	0.47
1:B:159:LEU:HD13	1:C:34:ASN:CG	2.34	0.47
1:A:150:LEU:HD12	1:A:192:PRO:HB2	1.96	0.47
1:D:159:LEU:HD13	1:E:22:ARG:HH11	1.80	0.47
1:J:24:GLN:HE21	1:J:32:ILE:HD11	1.80	0.47
1:B:277:GLY:HA3	1:B:353:ALA:O	2.14	0.47
1:G:57:ILE:O	1:G:59:GLY:N	2.47	0.47
1:A:160:ALA:HB2	1:A:188:HIS:CD2	2.50	0.47
1:J:285:PHE:HB2	1:J:349:VAL:CG1	2.45	0.47
1:G:156:TYR:CE2	1:L:62:ARG:NH1	2.83	0.47
1:E:208:CYS:SG	1:E:347:LEU:HD12	2.55	0.47
1:C:159:LEU:HD12	1:D:34:ASN:CG	2.35	0.47
1:E:440:TYR:HB2	1:K:232:MET:HE3	1.97	0.47
1:L:383:ASN:HB2	1:L:385:ILE:HD11	1.96	0.47
1:F:109:ARG:NH2	1:F:109:ARG:HG2	2.29	0.47
1:E:322:ILE:CD1	1:E:322:ILE:N	2.77	0.47
1:I:216:LEU:HD21	1:J:162:THR:OG1	2.15	0.47
1:E:32:ILE:HD13	1:E:216:LEU:HB2	1.96	0.47
1:B:119:MET:SD	1:B:127:PHE:HB2	2.54	0.47
1:B:142:GLU:HG3	1:B:143:LYS:H	1.80	0.47
1:G:291:PRO:HG3	1:G:341:ALA:HA	1.96	0.47
1:B:167:ASN:HD22	1:B:170:ARG:CZ	2.28	0.47
1:B:283:THR:HB	1:B:398:GLU:OE1	2.15	0.47
1:G:17:ASN:ND2	1:G:87:GLY:HA2	2.30	0.47
1:A:160:ALA:CB	1:A:188:HIS:CD2	2.98	0.47
1:K:319:LEU:HG	1:K:320:ILE:CD1	2.45	0.47
1:E:131:PRO:HG2	1:E:199:PHE:CD1	2.49	0.47
1:J:325:SER:HB3	1:J:329:SER:CB	2.45	0.47
1:C:27:ASP:OD1	1:C:33:LYS:HE3	2.15	0.47
1:H:325:SER:HB2	1:H:331:ARG:HH22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LYS:NZ	1:D:145:GLU:OE1	2.45	0.47
1:D:21:ILE:CD1	1:D:39:VAL:HA	2.45	0.47
1:E:48:ASN:O	1:E:69:TYR:HD2	1.97	0.47
1:B:258:PHE:HZ	1:B:274:PHE:CG	2.33	0.47
1:D:23:LEU:HB3	1:D:94:CYS:SG	2.55	0.47
1:C:174:LEU:O	1:C:178:GLU:HG2	2.14	0.47
1:C:9:ILE:O	1:C:12:LEU:N	2.47	0.47
1:L:226:GLY:O	1:L:227:LEU:HD23	2.15	0.47
1:C:369:ASP:CG	1:C:370:ARG:H	2.18	0.47
1:H:58:GLU:HG2	1:H:416:HIS:CD2	2.50	0.47
1:F:4:TYR:HB3	1:F:9:ILE:CD1	2.45	0.46
1:C:429:ARG:HH11	1:C:429:ARG:HG3	1.80	0.46
1:K:351:LEU:HD22	1:K:351:LEU:O	2.14	0.46
1:B:41:GLN:NE2	1:B:44:LYS:HD2	2.29	0.46
1:H:409:LEU:O	1:H:413:LEU:HB2	2.15	0.46
1:J:127:PHE:CE2	1:J:351:LEU:HG	2.50	0.46
1:E:236:LEU:HB2	1:E:239:VAL:HG21	1.97	0.46
1:K:215:LYS:HG2	1:K:231:PHE:CE2	2.50	0.46
1:L:311:TRP:HA	1:L:320:ILE:HB	1.97	0.46
1:H:37:ILE:HG22	1:I:185:ALA:CB	2.45	0.46
1:H:281:HIS:CE1	1:H:404:VAL:HG11	2.51	0.46
1:E:200:LYS:HG2	1:E:201:TYR:H	1.80	0.46
1:C:45:ALA:O	1:C:72:PRO:HG3	2.15	0.46
1:F:203:GLY:O	1:F:204:ALA:C	2.52	0.46
1:J:322:ILE:CD1	1:J:332:VAL:HG13	2.45	0.46
1:C:23:LEU:HB3	1:C:94:CYS:SG	2.55	0.46
1:G:143:LYS:HD3	1:G:143:LYS:N	2.29	0.46
1:B:49:LYS:HE2	1:B:49:LYS:HA	1.98	0.46
1:J:100:ASP:OD1	1:J:101:GLY:N	2.48	0.46
1:A:310:ALA:CB	1:A:372:ILE:HD13	2.40	0.46
1:A:368:ILE:HD12	1:A:385:ILE:HD11	1.96	0.46
1:H:4:TYR:CB	1:H:9:ILE:HG13	2.45	0.46
1:E:315:ASN:OD1	1:E:372:ILE:HG12	2.16	0.46
1:F:368:ILE:HG21	1:F:372:ILE:HD11	1.94	0.46
1:J:310:ALA:CA	1:J:368:ILE:HG13	2.43	0.46
1:H:96:ILE:HD13	1:H:107:ASP:CG	2.36	0.46
1:D:4:TYR:HB3	1:D:9:ILE:HD11	1.97	0.46
1:C:270:THR:O	1:C:274:PHE:HB2	2.15	0.46
1:A:57:ILE:HD13	1:A:96:ILE:HG13	1.96	0.46
1:K:48:ASN:HB3	1:K:71:TYR:CE1	2.50	0.46
1:H:236:LEU:O	1:H:239:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ASN:OD1	1:G:72:PRO:HD2	2.14	0.46
1:K:49:LYS:HD3	1:K:69:TYR:HE2	1.78	0.46
1:J:163:ASP:HA	1:J:170:ARG:NH1	2.31	0.46
1:I:160:ALA:CB	1:I:169:ARG:HH12	2.26	0.46
1:I:207:SER:O	1:I:211:ILE:HG12	2.16	0.46
1:K:54:GLY:O	1:K:56:SER:N	2.48	0.46
1:C:371:ASN:OD1	1:C:374:VAL:HG22	2.15	0.46
1:B:146:PRO:HG3	1:B:228:HIS:CD2	2.50	0.46
1:F:170:ARG:NH1	1:F:171:ASP:OD2	2.48	0.46
1:L:183:ILE:H	1:L:183:ILE:HD12	1.81	0.46
1:K:296:TYR:CD1	1:K:296:TYR:N	2.84	0.46
1:F:310:ALA:HB1	1:F:368:ILE:HG12	1.98	0.46
1:B:402:ASN:OD1	1:B:405:MET:HG2	2.15	0.46
1:H:160:ALA:CB	1:H:169:ARG:HH12	2.28	0.46
1:E:139:LYS:HB2	1:E:149:GLU:HB3	1.97	0.46
1:K:360:ASN:HB2	1:K:362:LEU:CD1	2.45	0.46
1:A:36:GLU:CD	1:F:169:ARG:HH12	2.18	0.46
1:J:328:ILE:C	1:J:328:ILE:HD12	2.35	0.46
1:H:172:ILE:HD13	1:H:221:ILE:HB	1.97	0.46
1:C:85:GLU:OE2	1:C:86:LYS:N	2.48	0.46
1:F:319:LEU:C	1:F:320:ILE:HD12	2.34	0.46
1:C:114:ARG:NH2	1:C:115:ILE:HD11	2.30	0.46
1:C:114:ARG:HH21	1:C:115:ILE:CD1	2.28	0.46
1:H:318:PRO:HB2	1:H:320:ILE:O	2.15	0.46
1:J:140:LEU:HD12	1:J:226:GLY:C	2.36	0.46
1:D:176:LEU:HD11	1:D:214:PHE:HD1	1.78	0.46
1:I:392:LEU:HD21	1:I:421:LYS:HB3	1.97	0.46
1:J:17:ASN:HD21	1:J:87:GLY:HA2	1.81	0.46
1:A:271:ALA:O	1:A:275:ILE:HG13	2.15	0.46
1:A:166:GLU:CD	1:A:167:ASN:H	2.19	0.46
1:B:162:THR:HG21	1:C:220:THR:OG1	2.15	0.46
1:G:46:LEU:HD22	1:G:74:LEU:HD11	1.97	0.46
1:K:83:THR:OG1	1:K:88:LYS:HD3	2.15	0.46
1:J:282:ALA:C	1:J:284:SER:H	2.18	0.46
1:C:444:TYR:OH	1:I:29:LEU:HD22	2.16	0.46
1:K:311:TRP:O	1:K:312:SER:HB3	2.14	0.46
1:J:72:PRO:N	1:J:94:CYS:HB3	2.31	0.46
1:F:131:PRO:HG2	1:F:199:PHE:CD1	2.50	0.46
1:D:168:CYS:SG	1:D:227:LEU:HD12	2.55	0.46
1:L:386:VAL:CG1	1:L:387:ASP:H	2.12	0.46
1:L:124:PHE:HZ	1:L:358:ILE:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:115:ILE:CG2	1:K:351:LEU:HD12	2.39	0.46
1:J:208:CYS:N	1:J:211:ILE:HD12	2.30	0.46
1:H:116:LEU:O	1:H:119:MET:HB3	2.15	0.46
1:F:420:ALA:O	1:F:423:ILE:HG13	2.15	0.46
1:D:164:LEU:HD23	1:E:220:THR:CG2	2.46	0.46
1:J:82:TRP:HE1	1:K:163:ASP:HB2	1.81	0.46
1:D:294:ASN:HB2	1:J:436:GLU:HB3	1.97	0.46
1:D:5:THR:O	1:D:8:ASP:N	2.48	0.46
1:F:188:HIS:HE1	1:F:191:ALA:O	1.97	0.46
1:E:115:ILE:O	1:E:118:GLU:HB3	2.15	0.46
1:I:371:ASN:HB2	1:I:374:VAL:HG22	1.97	0.46
1:I:201:TYR:C	1:I:201:TYR:CD1	2.88	0.46
1:F:430:THR:HG22	1:L:300:VAL:HG21	1.97	0.46
1:D:310:ALA:CB	1:D:368:ILE:HG21	2.42	0.46
1:F:370:ARG:HH21	1:F:372:ILE:CD1	2.29	0.46
1:I:285:PHE:HB2	1:I:349:VAL:HG13	1.96	0.46
1:B:239:VAL:HG23	1:B:239:VAL:O	2.14	0.46
1:H:272:LYS:NZ	1:H:276:ALA:HB2	2.31	0.46
1:L:91:ARG:HD2	1:L:92:PHE:N	2.29	0.46
1:H:278:ILE:O	1:H:282:ALA:HB2	2.15	0.46
1:H:116:LEU:HD22	1:H:119:MET:HE2	1.96	0.46
1:C:116:LEU:HD11	1:C:204:ALA:HB3	1.97	0.46
1:H:315:ASN:ND2	1:H:371:ASN:HA	2.31	0.46
1:H:63:ILE:HG22	1:H:64:GLU:HG3	1.97	0.46
1:J:82:TRP:HE1	1:K:163:ASP:CB	2.29	0.46
1:E:119:MET:HG2	1:E:124:PHE:HB2	1.98	0.46
1:H:182:GLU:HB3	1:H:200:LYS:CD	2.31	0.46
1:I:27:ASP:C	1:I:27:ASP:OD2	2.53	0.46
1:J:91:ARG:CD	1:J:91:ARG:C	2.82	0.46
1:K:312:SER:HB2	1:K:369:ASP:OD1	2.16	0.46
1:E:234:LYS:HB3	1:E:294:ASN:ND2	2.30	0.46
1:C:267:LEU:CD2	1:C:326:ARG:NH1	2.78	0.46
1:I:160:ALA:HB3	1:I:169:ARG:HH12	1.79	0.46
1:A:259:PHE:HE2	1:A:261:GLU:OE2	1.99	0.46
1:D:443:GLN:HA	1:D:443:GLN:HE21	1.81	0.46
1:A:108:PRO:O	1:A:344:TYR:HB3	2.16	0.46
1:A:80:PHE:HA	1:A:81:PRO:HD3	1.78	0.46
1:F:129:LEU:CD2	1:F:130:GLY:N	2.78	0.46
1:H:370:ARG:HH22	1:H:375:MET:CE	2.28	0.46
1:C:431:GLN:O	1:I:297:LYS:HD2	2.16	0.46
1:D:342:ASN:HB3	1:D:345:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:267:LEU:HG	1:I:326:ARG:NH1	2.31	0.46
1:C:274:PHE:HE2	1:C:332:VAL:HG11	1.80	0.46
1:C:111:ASN:OD1	1:C:409:LEU:HA	2.15	0.46
1:L:232:MET:SD	1:L:235:PRO:HA	2.56	0.46
1:J:273:HIS:CE1	1:J:361:LYS:CA	2.99	0.46
1:F:345:LEU:CD2	1:F:409:LEU:HD22	2.45	0.46
1:E:376:SER:O	1:E:380:ARG:HG3	2.16	0.46
1:B:287:ALA:HB2	1:B:395:ALA:HB1	1.98	0.46
1:C:380:ARG:HA	1:C:385:ILE:HD12	1.97	0.46
1:I:27:ASP:OD2	1:I:29:LEU:N	2.48	0.46
1:E:211:ILE:HG22	1:E:215:LYS:HE2	1.98	0.46
1:C:21:ILE:HD13	1:C:39:VAL:HA	1.97	0.46
1:B:138:PHE:CE2	1:B:150:LEU:CD2	2.99	0.46
1:C:433:HIS:N	1:C:436:GLU:OE1	2.48	0.46
1:E:189:GLU:HB3	1:E:194:GLN:OE1	2.15	0.46
1:H:282:ALA:HB1	1:H:319:LEU:HD21	1.97	0.46
1:I:124:PHE:CE1	1:I:358:ILE:HD13	2.51	0.46
1:I:357:GLY:HA2	1:I:362:LEU:HD13	1.98	0.46
1:A:300:VAL:CG2	1:G:429:ARG:HH12	2.28	0.46
1:D:288:VAL:O	1:D:291:PRO:HD3	2.15	0.46
1:H:332:VAL:HG13	1:H:332:VAL:O	2.16	0.46
1:K:98:ASN:O	1:K:100:ASP:N	2.49	0.46
1:J:33:LYS:HB3	1:K:157:PHE:O	2.16	0.46
1:I:418:ILE:HG22	1:I:422:GLU:CG	2.45	0.46
1:A:372:ILE:O	1:A:380:ARG:NH2	2.48	0.46
1:I:25:PHE:CE1	1:I:33:LYS:HB2	2.50	0.46
1:G:402:ASN:CG	1:G:405:MET:HG2	2.36	0.46
1:F:309:VAL:HB	1:F:386:VAL:CG2	2.41	0.46
1:J:23:LEU:HB3	1:J:70:LEU:HD23	1.97	0.46
1:C:160:ALA:O	1:C:161:PRO:C	2.54	0.46
1:B:159:LEU:HB2	1:C:32:ILE:O	2.15	0.46
1:B:159:LEU:HD12	1:C:22:ARG:NH1	2.27	0.46
1:C:62:ARG:HH21	1:C:65:GLU:HB3	1.81	0.46
1:C:127:PHE:HE2	1:C:347:LEU:HD22	1.80	0.46
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.97	0.46
1:I:282:ALA:O	1:I:284:SER:N	2.49	0.46
1:F:355:LEU:HD23	1:F:355:LEU:HA	1.67	0.46
1:G:315:ASN:HB3	1:G:318:PRO:CG	2.46	0.46
1:J:206:ARG:HG3	1:J:206:ARG:NH1	2.31	0.46
1:A:58:GLU:O	1:A:61:VAL:HG22	2.16	0.46
1:L:33:LYS:O	1:L:34:ASN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:ASP:O	1:L:75:ASN:N	2.49	0.46
1:D:232:MET:HE2	1:D:234:LYS:O	2.16	0.46
1:A:309:VAL:HG23	1:A:386:VAL:O	2.16	0.46
1:I:127:PHE:CZ	1:I:248:LEU:HD23	2.50	0.46
1:G:406:VAL:HG22	1:G:414:PHE:CZ	2.50	0.46
1:A:306:PRO:O	1:A:388:LEU:HD12	2.16	0.46
1:J:320:ILE:HG22	1:J:321:ARG:H	1.81	0.46
1:A:252:LYS:CE	1:A:253:ASN:ND2	2.78	0.46
1:J:368:ILE:CD1	1:J:385:ILE:HG23	2.46	0.46
1:L:287:ALA:HB2	1:L:395:ALA:C	2.36	0.46
1:E:436:GLU:HG2	1:K:294:ASN:HB2	1.98	0.46
1:C:399:PHE:HZ	1:C:409:LEU:HD11	1.81	0.46
1:K:151:ASN:HB2	1:K:166:GLU:OE2	2.16	0.46
1:E:201:TYR:HD2	1:E:201:TYR:H	1.63	0.46
1:B:300:VAL:HG11	1:H:430:THR:HG22	1.98	0.46
1:C:296:TYR:CE1	1:C:392:LEU:HA	2.51	0.46
1:J:167:ASN:HA	1:J:167:ASN:HD22	1.51	0.46
1:I:272:LYS:HA	1:I:275:ILE:HD12	1.97	0.46
1:C:142:GLU:H	1:C:142:GLU:CD	2.20	0.46
1:J:371:ASN:HD21	1:J:373:TYR:HB2	1.79	0.45
1:A:306:PRO:CB	1:A:319:LEU:HA	2.37	0.45
1:K:309:VAL:HG13	1:K:319:LEU:CD2	2.43	0.45
1:H:166:GLU:O	1:H:166:GLU:CD	2.54	0.45
1:C:429:ARG:O	1:I:297:LYS:HD3	2.16	0.45
1:G:13:VAL:HG21	1:G:42:LEU:HD21	1.97	0.45
1:G:86:LYS:HG3	1:H:174:LEU:CB	2.43	0.45
1:H:242:SER:O	1:H:339:PRO:CD	2.61	0.45
1:E:100:ASP:OD2	1:E:102:THR:HG23	2.16	0.45
1:K:51:MET:HA	1:K:68:MET:O	2.16	0.45
1:D:9:ILE:O	1:D:13:VAL:HG23	2.16	0.45
1:G:423:ILE:O	1:G:424:GLU:C	2.54	0.45
1:L:275:ILE:O	1:L:279:VAL:HG23	2.16	0.45
1:B:261:GLU:HA	1:B:266:GLN:NE2	2.31	0.45
1:K:35:VAL:CG1	1:K:70:LEU:HD11	2.46	0.45
1:L:114:ARG:NH2	1:L:115:ILE:CD1	2.78	0.45
1:J:140:LEU:HD11	1:J:227:LEU:O	2.16	0.45
1:D:436:GLU:OE2	1:J:297:LYS:HG3	2.15	0.45
1:J:19:LYS:HG3	1:J:87:GLY:HA3	1.97	0.45
1:A:259:PHE:CE2	1:A:261:GLU:OE2	2.69	0.45
1:G:166:GLU:HG2	1:G:168:CYS:H	1.81	0.45
1:F:140:LEU:HD12	1:F:226:GLY:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:O	1:C:160:ALA:O	2.33	0.45
1:A:356:ASP:O	1:A:360:ASN:HB2	2.16	0.45
1:J:112:LEU:HD11	1:J:208:CYS:SG	2.56	0.45
1:B:381:MET:C	1:B:382:GLU:HG3	2.37	0.45
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.75	0.45
1:I:80:PHE:HB2	1:I:89:VAL:O	2.15	0.45
1:D:308:TYR:HA	1:D:387:ASP:HA	1.98	0.45
1:D:138:PHE:HA	1:D:149:GLU:O	2.16	0.45
1:D:26:THR:OG1	1:D:212:GLN:NE2	2.47	0.45
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.16	0.45
1:H:273:HIS:NE2	1:H:361:LYS:HA	2.32	0.45
1:K:234:LYS:HB3	1:K:294:ASN:ND2	2.32	0.45
1:D:4:TYR:HB3	1:D:9:ILE:CD1	2.47	0.45
1:H:20:TYR:OH	1:H:36:GLU:HB3	2.16	0.45
1:I:282:ALA:C	1:I:284:SER:N	2.70	0.45
1:A:9:ILE:HG21	1:A:92:PHE:HZ	1.81	0.45
1:I:236:LEU:HB2	1:I:239:VAL:CG2	2.46	0.45
1:F:345:LEU:HD22	1:F:409:LEU:HD22	1.98	0.45
1:A:326:ARG:HD3	1:A:326:ARG:HA	1.82	0.45
1:D:184:GLU:HG3	1:E:44:LYS:NZ	2.31	0.45
1:E:252:LYS:O	1:E:255:VAL:HG22	2.16	0.45
1:L:130:GLY:O	1:L:247:ASN:ND2	2.49	0.45
1:J:37:ILE:HG13	1:J:41:GLN:HB2	1.97	0.45
1:G:147:THR:C	1:G:149:GLU:H	2.20	0.45
1:K:85:GLU:HG2	1:L:170:ARG:NH1	2.27	0.45
1:A:376:SER:HB3	1:A:378:GLU:OE1	2.17	0.45
1:K:309:VAL:HG22	1:K:319:LEU:HD22	1.98	0.45
1:C:402:ASN:CG	1:C:404:VAL:HG12	2.36	0.45
1:F:175:GLU:HG3	1:F:221:ILE:CD1	2.46	0.45
1:A:211:ILE:O	1:A:214:PHE:HB3	2.16	0.45
1:F:56:SER:HA	1:F:62:ARG:HD2	1.98	0.45
1:C:18:VAL:HG21	1:C:79:ILE:HD12	1.98	0.45
1:K:290:ASN:HB3	1:K:295:SER:HB3	1.99	0.45
1:C:127:PHE:CZ	1:C:248:LEU:HD22	2.51	0.45
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.80	0.45
1:E:169:ARG:NH2	1:F:36:GLU:OE2	2.45	0.45
1:B:110:ASN:O	1:B:113:LYS:HB2	2.17	0.45
1:H:79:ILE:O	1:H:80:PHE:C	2.55	0.45
1:D:184:GLU:OE1	1:D:200:LYS:HG2	2.16	0.45
1:J:308:TYR:CD1	1:J:372:ILE:HG21	2.51	0.45
1:L:345:LEU:HD22	1:L:409:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:GLU:HG2	1:E:196:GLU:HG3	1.99	0.45
1:G:172:ILE:O	1:G:176:LEU:HG	2.16	0.45
1:L:132:GLU:HB3	1:L:196:GLU:OE1	2.16	0.45
1:E:247:ASN:ND2	1:E:331:ARG:HE	2.14	0.45
1:G:237:PHE:O	1:G:239:VAL:N	2.49	0.45
1:A:20:TYR:OH	1:A:36:GLU:HG3	2.17	0.45
1:I:68:MET:HE2	1:I:104:PHE:HB2	1.98	0.45
1:E:429:ARG:NH1	1:K:300:VAL:HG12	2.32	0.45
1:F:84:ALA:HB3	1:F:87:GLY:O	2.16	0.45
1:B:176:LEU:HD11	1:B:214:PHE:CE1	2.51	0.45
1:F:119:MET:HA	1:F:355:LEU:CD1	2.46	0.45
1:K:244:MET:H	1:K:338:ASP:HA	1.80	0.45
1:G:45:ALA:HA	1:G:50:VAL:CG2	2.46	0.45
1:J:322:ILE:HD11	1:J:332:VAL:HG13	1.98	0.45
1:I:106:GLY:HA2	1:I:413:LEU:HG	1.98	0.45
1:G:440:TYR:O	1:G:441:MET:C	2.55	0.45
1:D:166:GLU:HA	1:D:225:HIS:CD2	2.52	0.45
1:I:368:ILE:O	1:I:368:ILE:HG22	2.17	0.45
1:K:127:PHE:HZ	1:K:248:LEU:HD22	1.73	0.45
1:A:169:ARG:NH2	1:A:195:HIS:ND1	2.64	0.45
1:C:321:ARG:HD3	1:C:333:GLU:OE1	2.17	0.45
1:A:280:LYS:HD2	1:A:362:LEU:HD21	1.98	0.45
1:G:204:ALA:HB1	1:G:347:LEU:CD2	2.47	0.45
1:K:258:PHE:CA	1:K:271:ALA:HB2	2.47	0.45
1:C:315:ASN:HD21	1:C:369:ASP:CB	2.29	0.45
1:C:255:VAL:HG12	1:C:256:ASN:H	1.81	0.45
1:G:95:ASP:OD1	1:G:109:ARG:NH2	2.49	0.45
1:A:380:ARG:HD3	1:A:387:ASP:OD1	2.17	0.45
1:A:320:ILE:N	1:A:320:ILE:HD12	2.32	0.45
1:E:96:ILE:H	1:E:96:ILE:CD1	2.22	0.45
1:E:406:VAL:HG22	1:E:414:PHE:CZ	2.51	0.45
1:E:260:ASP:O	1:E:266:GLN:HA	2.17	0.45
1:I:426:ASP:HA	1:I:429:ARG:HG2	1.98	0.45
1:E:170:ARG:NH1	1:F:84:ALA:HB1	2.31	0.45
1:J:163:ASP:O	1:J:164:LEU:HB2	2.17	0.45
1:H:78:VAL:HG12	1:H:79:ILE:N	2.32	0.45
1:K:396:LEU:HD22	1:K:418:ILE:HD13	1.98	0.45
1:B:30:GLY:N	1:B:342:ASN:HD22	2.15	0.45
1:A:276:ALA:HB2	1:A:364:ALA:HB2	1.97	0.45
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.99	0.45
1:F:230:THR:HG23	1:F:230:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:THR:C	1:L:85:GLU:OE2	2.55	0.45
1:H:368:ILE:HG21	1:H:372:ILE:HD12	1.98	0.45
1:D:259:PHE:HZ	1:D:261:GLU:HG3	1.82	0.45
1:D:145:GLU:OE2	1:D:146:PRO:HD2	2.17	0.45
1:K:282:ALA:HA	1:K:285:PHE:CE1	2.51	0.45
1:F:298:ARG:HD2	1:F:298:ARG:O	2.17	0.45
1:H:86:LYS:HB2	1:I:174:LEU:HD23	1.99	0.45
1:F:399:PHE:HE1	1:F:405:MET:HB3	1.80	0.45
1:H:404:VAL:HG13	1:H:405:MET:CE	2.47	0.45
1:D:96:ILE:HD13	1:D:96:ILE:N	2.32	0.45
1:B:297:LYS:HD3	1:H:429:ARG:O	2.17	0.45
1:K:419:GLU:O	1:K:423:ILE:HG12	2.16	0.45
1:C:383:ASN:N	1:C:383:ASN:HD22	2.14	0.45
1:C:383:ASN:ND2	1:C:383:ASN:N	2.64	0.45
1:C:35:VAL:HG13	1:C:35:VAL:O	2.17	0.45
1:J:406:VAL:HG22	1:J:414:PHE:CE1	2.51	0.45
1:J:6:ARG:HG3	1:J:46:LEU:HD13	1.99	0.45
1:B:430:THR:CG2	1:H:300:VAL:HG21	2.47	0.45
1:I:402:ASN:CG	1:I:405:MET:HG2	2.37	0.45
1:J:296:TYR:HE2	1:J:389:PRO:HG2	1.82	0.45
1:A:129:LEU:HD13	1:A:131:PRO:HG3	1.99	0.45
1:K:129:LEU:CD1	1:K:246:CYS:HB3	2.46	0.45
1:B:148:LEU:CD2	1:H:437:ARG:HD3	2.44	0.45
1:H:248:LEU:O	1:H:331:ARG:HB2	2.16	0.45
1:G:35:VAL:O	1:G:35:VAL:HG13	2.17	0.45
1:D:183:ILE:HD13	1:D:183:ILE:N	2.31	0.45
1:E:169:ARG:HH21	1:F:36:GLU:CD	2.19	0.45
1:E:201:TYR:C	1:E:201:TYR:CD2	2.88	0.45
1:C:316:ARG:HG2	1:C:373:TYR:CD2	2.52	0.45
1:B:213:THR:O	1:B:217:VAL:HG23	2.17	0.45
1:D:158:ASP:OD2	1:E:33:LYS:HE2	2.17	0.45
1:B:260:ASP:HB2	1:B:268:SER:CA	2.47	0.45
1:K:316:ARG:HE	1:K:370:ARG:NH1	2.14	0.45
1:B:312:SER:HB3	1:B:315:ASN:HB2	1.99	0.45
1:I:280:LYS:HG2	1:I:281:HIS:CD2	2.51	0.45
1:L:18:VAL:HG21	1:L:79:ILE:HD12	1.98	0.45
1:H:309:VAL:HG13	1:H:319:LEU:CD2	2.47	0.45
1:L:129:LEU:CG	1:L:347:LEU:HD21	2.46	0.45
1:E:70:LEU:O	1:E:72:PRO:HD3	2.17	0.45
1:K:48:ASN:OD1	1:K:71:TYR:HA	2.17	0.45
1:D:6:ARG:NE	1:D:46:LEU:HD13	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ILE:CD1	1:C:74:LEU:HB3	2.46	0.45
1:B:48:ASN:HB3	1:B:71:TYR:CD1	2.51	0.45
1:D:346:ALA:O	1:D:347:LEU:C	2.56	0.45
1:L:325:SER:HB2	1:L:329:SER:CB	2.48	0.45
1:E:175:GLU:O	1:E:179:MET:HB2	2.17	0.45
1:D:58:GLU:O	1:D:61:VAL:HG22	2.17	0.45
1:H:100:ASP:CG	1:H:101:GLY:H	2.21	0.45
1:I:410:GLY:O	1:I:411:GLU:C	2.55	0.45
1:D:322:ILE:N	1:D:322:ILE:HD12	2.32	0.45
1:G:328:ILE:C	1:G:330:THR:H	2.20	0.44
1:D:150:LEU:CD1	1:D:192:PRO:HB2	2.37	0.44
1:F:375:MET:HE2	1:F:385:ILE:CD1	2.47	0.44
1:B:309:VAL:HB	1:B:386:VAL:HG13	1.99	0.44
1:D:390:ALA:HB1	1:J:429:ARG:NE	2.29	0.44
1:E:429:ARG:HH12	1:K:300:VAL:CG1	2.30	0.44
1:F:402:ASN:OD1	1:F:404:VAL:CG1	2.65	0.44
1:B:68:MET:HE3	1:B:96:ILE:HG21	1.99	0.44
1:C:114:ARG:O	1:C:117:LYS:HB2	2.17	0.44
1:F:321:ARG:HD3	1:F:335:ARG:HD2	1.98	0.44
1:C:74:LEU:HD23	1:C:74:LEU:N	2.32	0.44
1:I:286:THR:HG23	1:I:290:ASN:ND2	2.31	0.44
1:D:211:ILE:O	1:D:215:LYS:HG3	2.17	0.44
1:G:223:ARG:O	1:G:226:GLY:N	2.50	0.44
1:D:437:ARG:NH1	1:J:235:PRO:O	2.45	0.44
1:C:100:ASP:O	1:C:102:THR:N	2.50	0.44
1:A:166:GLU:CD	1:A:167:ASN:N	2.71	0.44
1:C:217:VAL:HG12	1:C:221:ILE:HD12	1.99	0.44
1:J:260:ASP:CG	1:J:263:ALA:HB2	2.38	0.44
1:K:83:THR:O	1:K:84:ALA:HB3	2.16	0.44
1:A:160:ALA:O	1:A:161:PRO:O	2.35	0.44
1:L:375:MET:HG2	1:L:380:ARG:CG	2.46	0.44
1:B:150:LEU:HD13	1:B:192:PRO:HB2	1.98	0.44
1:F:189:GLU:HB3	1:F:194:GLN:HE21	1.82	0.44
1:K:91:ARG:HD2	1:K:91:ARG:C	2.37	0.44
1:E:169:ARG:HH11	1:E:195:HIS:CD2	2.32	0.44
1:H:311:TRP:HA	1:H:320:ILE:O	2.17	0.44
1:B:134:GLU:HG3	1:B:243:GLY:O	2.16	0.44
1:C:97:TYR:CD2	1:C:101:GLY:O	2.70	0.44
1:F:35:VAL:HG11	1:F:70:LEU:HD22	1.99	0.44
1:D:440:TYR:CE1	1:J:292:THR:HB	2.53	0.44
1:L:73:ASP:O	1:L:76:THR:N	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ARG:CB	1:G:223:ARG:HH11	2.31	0.44
1:E:5:THR:O	1:E:9:ILE:HG12	2.17	0.44
1:A:319:LEU:HD22	1:A:320:ILE:HD11	1.99	0.44
1:E:400:LYS:HA	1:E:414:PHE:CZ	2.52	0.44
1:D:167:ASN:ND2	1:D:170:ARG:CB	2.79	0.44
1:L:166:GLU:OE2	1:L:166:GLU:O	2.35	0.44
1:H:308:TYR:HA	1:H:387:ASP:HA	1.99	0.44
1:J:120:GLU:C	1:J:122:LEU:H	2.21	0.44
1:J:383:ASN:HB2	1:J:385:ILE:CG1	2.48	0.44
1:K:281:HIS:CE1	1:K:404:VAL:HG21	2.52	0.44
1:A:55:SER:CB	1:A:62:ARG:HE	2.31	0.44
1:L:423:ILE:O	1:L:427:MET:HG3	2.17	0.44
1:C:418:ILE:O	1:C:422:GLU:HG3	2.17	0.44
1:D:293:VAL:HG11	1:D:428:PHE:CG	2.52	0.44
1:A:27:ASP:OD2	1:A:27:ASP:C	2.55	0.44
1:C:286:THR:O	1:C:290:ASN:N	2.50	0.44
1:L:253:ASN:O	1:L:255:VAL:HG23	2.18	0.44
1:A:163:ASP:O	1:A:165:GLY:N	2.50	0.44
1:D:435:TRP:CE2	1:D:439:GLN:HG3	2.52	0.44
1:G:311:TRP:O	1:G:368:ILE:HG13	2.17	0.44
1:I:86:LYS:CB	1:J:174:LEU:HD13	2.38	0.44
1:A:319:LEU:C	1:A:319:LEU:HD23	2.38	0.44
1:G:32:ILE:HG22	1:H:159:LEU:HD12	1.98	0.44
1:L:355:LEU:O	1:L:357:GLY:N	2.51	0.44
1:C:25:PHE:CE1	1:C:33:LYS:CB	3.00	0.44
1:A:2:ALA:O	1:A:3:LYS:HB2	2.17	0.44
1:C:248:LEU:HB2	1:C:332:VAL:HG13	1.99	0.44
1:C:96:ILE:CD1	1:C:96:ILE:N	2.81	0.44
1:E:138:PHE:HD2	1:E:148:LEU:HA	1.81	0.44
1:D:372:ILE:HG13	1:D:373:TYR:N	2.33	0.44
1:F:326:ARG:HA	1:F:326:ARG:HD3	1.79	0.44
1:F:151:ASN:ND2	1:F:166:GLU:OE2	2.50	0.44
1:J:48:ASN:O	1:J:69:TYR:HD2	1.99	0.44
1:L:256:ASN:OD1	1:L:258:PHE:N	2.50	0.44
1:K:34:ASN:C	1:K:34:ASN:ND2	2.69	0.44
1:J:349:VAL:HG22	1:J:405:MET:SD	2.58	0.44
1:H:370:ARG:HH11	1:H:370:ARG:CG	2.28	0.44
1:D:115:ILE:HG23	1:D:351:LEU:HD12	2.00	0.44
1:E:374:VAL:HG23	1:E:375:MET:H	1.82	0.44
1:H:294:ASN:HA	1:H:297:LYS:HD3	1.99	0.44
1:D:308:TYR:CD1	1:D:372:ILE:HB	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:HZ	1:A:236:LEU:HD11	1.82	0.44
1:H:252:LYS:O	1:H:253:ASN:HB2	2.17	0.44
1:B:360:ASN:HB2	1:B:362:LEU:HD13	1.99	0.44
1:C:315:ASN:HD21	1:C:369:ASP:HA	1.82	0.44
1:F:418:ILE:HG22	1:F:422:GLU:OE1	2.17	0.44
1:F:237:PHE:CD2	1:F:238:GLY:N	2.85	0.44
1:G:323:PRO:HD2	1:G:331:ARG:O	2.18	0.44
1:I:279:VAL:HG13	1:I:309:VAL:CG1	2.45	0.44
1:F:440:TYR:HD1	1:F:444:TYR:HE2	1.65	0.44
1:G:162:THR:HG21	1:L:220:THR:OG1	2.17	0.44
1:J:138:PHE:HB3	1:J:147:THR:O	2.18	0.44
1:C:45:ALA:HA	1:C:50:VAL:HG23	2.00	0.44
1:I:250:LEU:HB2	1:I:258:PHE:CE2	2.53	0.44
1:A:397:GLU:O	1:A:401:SER:HB3	2.17	0.44
1:D:28:ILE:HG22	1:D:29:LEU:HG	1.99	0.44
1:E:443:GLN:O	1:E:443:GLN:HG2	2.16	0.44
1:E:370:ARG:NH1	1:E:370:ARG:HG3	2.32	0.44
1:E:298:ARG:HG2	1:E:298:ARG:O	2.18	0.44
1:I:251:PHE:CD1	1:I:256:ASN:HA	2.53	0.44
1:L:316:ARG:NH1	1:L:316:ARG:HG3	2.33	0.44
1:B:371:ASN:HD22	1:B:372:ILE:H	1.64	0.44
1:D:137:LEU:HD13	1:D:227:LEU:HD13	2.00	0.44
1:B:406:VAL:HG22	1:B:414:PHE:CE1	2.52	0.44
1:I:5:THR:HG22	1:I:8:ASP:CG	2.38	0.44
1:K:360:ASN:HB2	1:K:362:LEU:HD11	2.00	0.44
1:G:9:ILE:O	1:G:13:VAL:HG23	2.17	0.44
1:A:300:VAL:CG1	1:A:301:PRO:HD2	2.48	0.44
1:D:300:VAL:HG21	1:J:430:THR:HG22	1.99	0.44
1:E:70:LEU:HG	1:E:94:CYS:HB2	1.99	0.44
1:F:280:LYS:HE2	1:F:281:HIS:NE2	2.33	0.44
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.52	0.44
1:F:440:TYR:HD1	1:F:444:TYR:CE2	2.35	0.44
1:B:297:LYS:HE3	1:H:436:GLU:OE1	2.17	0.44
1:B:224:LYS:HE2	1:B:225:HIS:CE1	2.53	0.44
1:F:286:THR:HA	1:F:289:THR:OG1	2.18	0.44
1:G:370:ARG:NH2	1:G:383:ASN:ND2	2.66	0.44
1:E:314:GLN:NE2	1:E:321:ARG:NH2	2.55	0.44
1:G:250:LEU:O	1:G:257:ALA:HB3	2.18	0.44
1:J:399:PHE:CD1	1:J:405:MET:HB3	2.52	0.44
1:E:418:ILE:HD12	1:E:418:ILE:N	2.33	0.44
1:J:54:GLY:O	1:J:56:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PHE:HB2	1:B:349:VAL:HG11	2.00	0.44
1:H:380:ARG:HH11	1:H:380:ARG:CB	2.28	0.44
1:J:129:LEU:HD22	1:J:131:PRO:CG	2.48	0.44
1:E:309:VAL:CG2	1:E:386:VAL:HG23	2.46	0.44
1:D:23:LEU:HB2	1:D:35:VAL:HG13	2.00	0.44
1:I:282:ALA:CB	1:I:319:LEU:HD21	2.47	0.44
1:I:22:ARG:NH1	1:J:159:LEU:CD2	2.81	0.44
1:C:6:ARG:CD	1:C:46:LEU:HD13	2.48	0.44
1:G:286:THR:HG23	1:G:290:ASN:OD1	2.18	0.44
1:G:140:LEU:HD12	1:G:226:GLY:C	2.37	0.44
1:H:16:GLU:O	1:H:88:LYS:HG3	2.18	0.44
1:E:392:LEU:O	1:E:392:LEU:HG	2.18	0.44
1:G:115:ILE:N	1:G:115:ILE:HD12	2.32	0.44
1:E:80:PHE:HE1	1:E:91:ARG:HB3	1.82	0.44
1:A:36:GLU:HG2	1:A:36:GLU:H	1.67	0.44
1:A:31:THR:HG22	1:A:33:LYS:HG3	1.98	0.44
1:E:185:ALA:HB2	1:F:37:ILE:HG22	1.99	0.44
1:A:39:VAL:HG22	1:A:39:VAL:O	2.17	0.44
1:I:200:LYS:O	1:I:201:TYR:C	2.56	0.43
1:J:386:VAL:CG1	1:J:387:ASP:H	2.14	0.43
1:F:372:ILE:HG23	1:F:375:MET:SD	2.58	0.43
1:B:55:SER:HB2	1:B:62:ARG:HB2	2.00	0.43
1:D:76:THR:O	1:D:78:VAL:HG23	2.17	0.43
1:B:158:ASP:HA	1:C:33:LYS:HA	1.98	0.43
1:C:32:ILE:N	1:C:32:ILE:CD1	2.79	0.43
1:J:211:ILE:HG22	1:J:215:LYS:HE3	2.00	0.43
1:C:117:LYS:O	1:C:120:GLU:N	2.51	0.43
1:A:37:ILE:HG22	1:F:185:ALA:HB2	1.97	0.43
1:A:69:TYR:O	1:A:70:LEU:HD13	2.18	0.43
1:B:18:VAL:HG11	1:B:90:ALA:HB2	1.99	0.43
1:G:312:SER:CB	1:G:315:ASN:HB2	2.47	0.43
1:D:376:SER:O	1:D:380:ARG:HG3	2.18	0.43
1:C:377:LYS:C	1:C:381:MET:HE2	2.38	0.43
1:B:124:PHE:CZ	1:B:358:ILE:HD13	2.53	0.43
1:J:396:LEU:HD11	1:J:421:LYS:CB	2.48	0.43
1:L:259:PHE:CE1	1:L:326:ARG:HB3	2.53	0.43
1:A:102:THR:HG22	1:A:103:PRO:HD2	2.00	0.43
1:J:285:PHE:HB2	1:J:349:VAL:HG13	2.00	0.43
1:L:316:ARG:HG2	1:L:373:TYR:HB2	2.00	0.43
1:B:368:ILE:CG2	1:B:370:ARG:HG3	2.48	0.43
1:F:380:ARG:NH1	1:F:385:ILE:CG2	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:406:VAL:HG13	1:K:414:PHE:CD2	2.54	0.43
1:L:383:ASN:HB2	1:L:385:ILE:HG12	1.99	0.43
1:D:45:ALA:CA	1:D:50:VAL:HG23	2.46	0.43
1:D:46:LEU:HD22	1:D:74:LEU:HD21	2.00	0.43
1:K:28:ILE:HD11	1:K:417:PHE:HA	1.99	0.43
1:I:34:ASN:HD22	1:I:34:ASN:C	2.20	0.43
1:I:51:MET:SD	1:I:67:ASP:HB3	2.57	0.43
1:I:271:ALA:O	1:I:275:ILE:HD12	2.17	0.43
1:B:273:HIS:O	1:B:276:ALA:HB3	2.18	0.43
1:C:213:THR:O	1:C:217:VAL:HG23	2.18	0.43
1:K:189:GLU:HB3	1:K:194:GLN:NE2	2.33	0.43
1:A:44:LYS:HE2	1:A:49:LYS:O	2.18	0.43
1:F:153:LYS:HG2	1:F:153:LYS:O	2.18	0.43
1:G:308:TYR:CD2	1:G:380:ARG:HD3	2.52	0.43
1:J:183:ILE:HG22	1:J:184:GLU:N	2.32	0.43
1:H:223:ARG:O	1:H:225:HIS:N	2.52	0.43
1:D:388:LEU:HB3	1:D:389:PRO:HD2	2.00	0.43
1:A:252:LYS:NZ	1:A:253:ASN:ND2	2.65	0.43
1:C:402:ASN:OD1	1:C:404:VAL:CG1	2.65	0.43
1:K:351:LEU:O	1:K:355:LEU:HG	2.19	0.43
1:D:78:VAL:O	1:D:90:ALA:HA	2.18	0.43
1:J:256:ASN:ND2	1:J:330:THR:HB	2.33	0.43
1:B:129:LEU:HD22	1:B:130:GLY:H	1.80	0.43
1:C:55:SER:CB	1:C:62:ARG:HG2	2.46	0.43
1:C:48:ASN:O	1:C:69:TYR:HD2	2.01	0.43
1:K:262:ASN:O	1:K:263:ALA:HB2	2.18	0.43
1:D:23:LEU:HB3	1:D:70:LEU:HD23	2.00	0.43
1:D:72:PRO:HA	1:D:94:CYS:HA	2.01	0.43
1:I:287:ALA:HB2	1:I:395:ALA:CB	2.46	0.43
1:D:6:ARG:HE	1:D:46:LEU:HD13	1.83	0.43
1:J:82:TRP:HH2	1:J:217:VAL:HG22	1.83	0.43
1:H:206:ARG:O	1:H:206:ARG:HD3	2.19	0.43
1:I:133:PRO:HA	1:I:244:MET:HG3	2.00	0.43
1:A:80:PHE:HB3	1:A:82:TRP:CE3	2.53	0.43
1:E:184:GLU:OE2	1:F:44:LYS:HE3	2.18	0.43
1:B:4:TYR:HB3	1:B:9:ILE:HD11	1.98	0.43
1:E:407:LYS:HA	1:E:407:LYS:HE2	2.01	0.43
1:J:285:PHE:C	1:J:285:PHE:CD1	2.92	0.43
1:J:406:VAL:HG22	1:J:414:PHE:CZ	2.54	0.43
1:A:245:HIS:CD2	1:A:335:ARG:HA	2.54	0.43
1:D:321:ARG:O	1:D:333:GLU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:HA	1:B:227:LEU:HD23	2.00	0.43
1:H:307:CYS:O	1:H:387:ASP:HA	2.18	0.43
1:C:162:THR:O	1:C:164:LEU:N	2.51	0.43
1:B:290:ASN:OD1	1:B:338:ASP:OD1	2.37	0.43
1:L:311:TRP:H	1:L:368:ILE:HD13	1.84	0.43
1:L:333:GLU:HG2	1:L:335:ARG:HG2	2.01	0.43
1:D:45:ALA:HB2	1:D:50:VAL:HG21	2.01	0.43
1:G:162:THR:HG22	1:G:163:ASP:N	2.34	0.43
1:G:112:LEU:HD11	1:G:208:CYS:SG	2.59	0.43
1:D:8:ASP:O	1:D:11:LYS:HB3	2.19	0.43
1:B:115:ILE:O	1:B:118:GLU:HB2	2.17	0.43
1:F:359:LYS:C	1:F:360:ASN:HD22	2.21	0.43
1:L:137:LEU:HD23	1:L:229:ALA:HA	2.01	0.43
1:H:240:ASN:HA	1:H:240:ASN:HD22	1.58	0.43
1:A:376:SER:O	1:A:380:ARG:HB2	2.19	0.43
1:B:201:TYR:OH	1:B:331:ARG:NE	2.49	0.43
1:J:353:ALA:HB2	1:J:405:MET:HE1	2.01	0.43
1:A:319:LEU:HD22	1:A:320:ILE:HD12	1.98	0.43
1:J:28:ILE:HG12	1:J:57:ILE:O	2.19	0.43
1:D:161:PRO:HD3	4:D:620:HOH:O	2.18	0.43
1:I:5:THR:HG22	1:I:8:ASP:OD1	2.18	0.43
1:D:360:ASN:O	1:D:361:LYS:C	2.56	0.43
1:J:389:PRO:CB	1:J:394:GLU:HB3	2.41	0.43
1:G:132:GLU:HB3	1:G:196:GLU:OE1	2.19	0.43
1:I:9:ILE:HG13	1:I:74:LEU:CD1	2.48	0.43
1:G:426:ASP:HA	1:G:429:ARG:HG2	2.00	0.43
1:G:429:ARG:HG3	1:G:430:THR:N	2.33	0.43
1:D:233:PRO:HG3	1:D:338:ASP:OD2	2.19	0.43
1:K:58:GLU:OE1	1:K:416:HIS:CD2	2.72	0.43
1:F:163:ASP:HA	1:F:167:ASN:HD22	1.83	0.43
1:L:115:ILE:HD11	1:L:408:ALA:O	2.19	0.43
1:I:321:ARG:O	1:I:333:GLU:HB3	2.18	0.43
1:C:74:LEU:HA	1:C:92:PHE:HE2	1.82	0.43
1:C:239:VAL:O	1:C:240:ASN:C	2.57	0.43
1:C:414:PHE:CE2	1:C:418:ILE:HG13	2.53	0.43
1:A:402:ASN:C	1:A:402:ASN:OD1	2.56	0.43
1:C:252:LYS:C	1:C:254:GLY:H	2.20	0.43
1:L:205:VAL:O	1:L:206:ARG:C	2.57	0.43
1:L:258:PHE:O	1:L:330:THR:HG21	2.18	0.43
1:G:152:ASP:OD1	1:G:193:GLY:HA2	2.18	0.43
1:B:28:ILE:O	1:B:28:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:ILE:C	1:E:330:THR:H	2.21	0.43
1:G:322:ILE:HA	1:G:323:PRO:HD2	1.84	0.43
1:L:316:ARG:HG2	1:L:373:TYR:CB	2.48	0.43
1:F:430:THR:HG22	1:L:300:VAL:HG11	2.00	0.43
1:E:329:SER:O	1:E:331:ARG:NH2	2.51	0.43
1:I:249:SER:HB3	1:I:331:ARG:HB3	2.01	0.43
1:E:278:ILE:O	1:E:282:ALA:N	2.52	0.43
1:H:370:ARG:HH22	1:H:375:MET:HE3	1.84	0.43
1:F:223:ARG:C	1:F:225:HIS:N	2.71	0.43
1:I:68:MET:HB3	1:I:97:TYR:O	2.19	0.43
1:A:297:LYS:HD3	1:G:429:ARG:O	2.18	0.43
1:A:116:LEU:O	1:A:120:GLU:HG3	2.19	0.43
1:C:325:SER:HB2	1:C:331:ARG:HH22	1.83	0.43
1:K:261:GLU:HG3	1:K:262:ASN:ND2	2.34	0.43
1:F:440:TYR:CD1	1:F:444:TYR:HE2	2.35	0.43
1:E:67:ASP:O	1:E:68:MET:HG2	2.19	0.43
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.54	0.43
1:I:175:GLU:HG3	1:I:221:ILE:CD1	2.48	0.43
1:G:178:GLU:OE1	1:L:86:LYS:HE3	2.19	0.43
1:B:300:VAL:HG22	1:H:429:ARG:NH2	2.33	0.43
1:A:259:PHE:CE1	1:A:266:GLN:HB3	2.54	0.43
1:A:313:ALA:HA	1:A:321:ARG:HG3	2.00	0.43
1:F:37:ILE:O	1:F:37:ILE:HG13	2.17	0.43
1:I:212:GLN:O	1:I:213:THR:C	2.57	0.43
1:G:346:ALA:O	1:G:350:LEU:HB2	2.19	0.43
1:K:74:LEU:CD2	1:K:74:LEU:H	2.32	0.43
1:C:300:VAL:O	1:C:300:VAL:HG13	2.19	0.43
1:D:250:LEU:O	1:D:257:ALA:HB3	2.19	0.43
1:C:271:ALA:O	1:C:275:ILE:HG13	2.18	0.43
1:E:37:ILE:O	1:E:37:ILE:HG13	2.18	0.43
1:I:317:SER:C	1:I:373:TYR:OH	2.57	0.43
1:I:259:PHE:HA	1:I:330:THR:HG21	2.00	0.43
1:D:306:PRO:HB3	1:D:319:LEU:HA	2.01	0.43
1:D:160:ALA:O	1:D:161:PRO:C	2.57	0.43
1:L:360:ASN:HB2	1:L:362:LEU:HD13	2.01	0.43
1:F:97:TYR:C	1:F:98:ASN:HD22	2.22	0.43
1:I:100:ASP:HB2	1:I:101:GLY:H	1.32	0.43
1:B:160:ALA:HB3	1:B:169:ARG:NH1	2.34	0.43
1:B:351:LEU:CD2	1:B:355:LEU:HG	2.49	0.43
1:A:402:ASN:OD1	1:A:405:MET:HG2	2.19	0.43
1:L:73:ASP:O	1:L:76:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLY:O	1:B:204:ALA:C	2.57	0.43
1:G:2:ALA:HB1	1:G:75:ASN:OD1	2.19	0.43
1:G:66:SER:HA	1:H:314:GLN:OE1	2.19	0.43
1:F:181:PHE:CE2	1:F:210:ASP:HB3	2.53	0.43
1:E:53:ASP:CG	1:E:65:GLU:HG3	2.39	0.43
1:D:430:THR:HG22	1:J:300:VAL:HG22	2.01	0.43
1:I:128:ASN:HB2	1:I:249:SER:OG	2.18	0.43
1:A:156:TYR:C	1:A:158:ASP:H	2.22	0.43
1:J:319:LEU:HD23	1:J:320:ILE:HD11	1.99	0.43
1:H:372:ILE:O	1:H:380:ARG:HD3	2.19	0.43
1:F:232:MET:CE	1:L:437:ARG:HA	2.48	0.43
1:H:282:ALA:HA	1:H:285:PHE:CZ	2.53	0.43
1:H:113:LYS:O	1:H:116:LEU:HB2	2.19	0.43
1:D:244:MET:H	1:D:338:ASP:HA	1.83	0.43
1:K:326:ARG:NH1	1:K:326:ARG:HB2	2.33	0.43
1:H:162:THR:O	1:H:164:LEU:N	2.51	0.43
1:K:78:VAL:HB	1:K:91:ARG:CG	2.45	0.43
1:H:23:LEU:HD11	1:H:37:ILE:HD13	2.01	0.43
1:F:20:TYR:CZ	1:F:36:GLU:HB2	2.54	0.43
1:A:436:GLU:OE1	1:G:297:LYS:NZ	2.52	0.43
1:K:28:ILE:HG12	1:K:28:ILE:O	2.18	0.43
1:I:418:ILE:O	1:I:420:ALA:N	2.52	0.43
1:I:28:ILE:HD11	1:I:417:PHE:HB2	2.01	0.43
1:F:432:VAL:HB	1:L:237:PHE:HB2	2.00	0.43
1:G:162:THR:O	1:G:164:LEU:O	2.36	0.43
1:J:196:GLU:HG2	1:J:198:ASP:OD2	2.19	0.43
1:A:232:MET:HE1	1:A:235:PRO:HA	1.99	0.43
1:K:375:MET:HB2	1:K:379:GLU:HB2	2.01	0.43
1:E:183:ILE:HG22	1:E:198:ASP:O	2.19	0.43
1:L:100:ASP:O	1:L:102:THR:N	2.51	0.43
1:K:224:LYS:HG3	1:L:164:LEU:HD11	2.00	0.43
1:H:376:SER:HB3	1:H:379:GLU:HB2	2.00	0.43
1:J:354:GLY:O	1:J:358:ILE:HG12	2.18	0.43
1:H:143:LYS:HA	1:H:143:LYS:HE2	2.00	0.43
1:K:83:THR:HA	1:K:85:GLU:OE2	2.18	0.43
1:I:200:LYS:O	1:I:201:TYR:O	2.37	0.43
1:J:371:ASN:O	1:J:375:MET:HG3	2.19	0.43
1:H:9:ILE:O	1:H:13:VAL:HG23	2.18	0.43
1:B:374:VAL:HG23	1:B:375:MET:N	2.34	0.43
1:J:91:ARG:HD2	1:J:92:PHE:N	2.34	0.43
1:F:376:SER:O	1:F:379:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ILE:HG22	1:B:419:GLU:N	2.33	0.43
1:E:360:ASN:O	1:E:361:LYS:O	2.37	0.43
1:H:96:ILE:HD12	1:H:96:ILE:H	1.82	0.43
1:B:160:ALA:HB1	1:B:161:PRO:CD	2.44	0.43
1:D:260:ASP:HB2	1:D:268:SER:HB3	2.00	0.43
1:H:183:ILE:HD12	1:H:183:ILE:H	1.83	0.43
1:D:26:THR:HG1	1:D:212:GLN:HE21	1.66	0.43
1:A:58:GLU:HB3	1:A:61:VAL:HG23	2.00	0.43
1:A:145:GLU:OE1	1:A:146:PRO:HD2	2.19	0.43
1:D:297:LYS:HE3	1:J:436:GLU:CD	2.39	0.43
1:K:172:ILE:HG22	1:K:173:VAL:N	2.33	0.43
1:G:393:ALA:HB2	1:G:425:TRP:CE2	2.54	0.43
1:F:369:ASP:OD1	1:F:369:ASP:N	2.52	0.43
1:J:141:ASP:OD2	1:J:141:ASP:C	2.57	0.43
1:J:409:LEU:O	1:J:413:LEU:HB2	2.19	0.43
1:L:156:TYR:O	1:L:158:ASP:N	2.52	0.43
1:G:32:ILE:O	1:H:159:LEU:HB2	2.19	0.43
1:G:160:ALA:CB	1:G:169:ARG:HH12	2.32	0.43
1:J:52:PHE:CD1	1:J:70:LEU:HD13	2.53	0.43
1:F:201:TYR:CD1	1:F:201:TYR:C	2.93	0.43
1:G:131:PRO:HG2	1:G:199:PHE:HE1	1.84	0.43
1:B:285:PHE:HB2	1:B:349:VAL:HG13	2.00	0.43
1:E:136:PHE:CE1	1:E:235:PRO:HG2	2.53	0.43
1:E:273:HIS:NE2	1:E:361:LYS:CA	2.82	0.43
1:B:306:PRO:HB3	1:B:319:LEU:HA	2.01	0.43
1:A:37:ILE:N	1:A:37:ILE:HD13	2.33	0.43
1:H:21:ILE:HD12	1:H:39:VAL:HA	2.01	0.43
1:C:337:VAL:CG1	1:C:338:ASP:N	2.82	0.43
1:L:34:ASN:C	1:L:34:ASN:HD22	2.18	0.43
1:L:225:HIS:O	1:L:227:LEU:HG	2.19	0.43
1:G:151:ASN:ND2	1:G:166:GLU:OE1	2.52	0.43
1:A:102:THR:HG21	4:A:610:HOH:O	2.18	0.43
1:K:63:ILE:HG22	1:K:64:GLU:HG3	2.01	0.43
1:I:371:ASN:O	1:I:372:ILE:HG23	2.18	0.42
1:I:20:TYR:HB2	1:J:174:LEU:HD21	2.01	0.42
1:E:274:PHE:CE1	1:E:354:GLY:HA3	2.54	0.42
1:E:28:ILE:HD11	1:E:417:PHE:HB2	2.01	0.42
1:F:104:PHE:HD2	1:F:107:ASP:HB2	1.84	0.42
1:F:172:ILE:CD1	1:F:221:ILE:HB	2.49	0.42
1:I:140:LEU:HA	1:I:145:GLU:O	2.18	0.42
1:H:437:ARG:O	1:H:441:MET:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:ASP:CB	1:G:339:PRO:HD2	2.47	0.42
1:G:314:GLN:HE22	1:L:66:SER:CA	2.31	0.42
1:B:18:VAL:HG12	1:B:21:ILE:HD12	2.00	0.42
1:J:16:GLU:O	1:J:17:ASN:HB3	2.18	0.42
1:J:17:ASN:O	1:J:17:ASN:CG	2.57	0.42
1:C:315:ASN:HD21	1:C:369:ASP:CA	2.32	0.42
1:K:224:LYS:HG3	1:L:164:LEU:CD1	2.48	0.42
1:F:274:PHE:HD2	1:F:332:VAL:HG21	1.84	0.42
1:J:45:ALA:HA	1:J:50:VAL:HG23	2.00	0.42
1:F:28:ILE:HD11	1:F:417:PHE:HB2	2.00	0.42
1:E:112:LEU:O	1:E:116:LEU:HG	2.19	0.42
1:I:19:LYS:HA	1:I:39:VAL:HB	1.99	0.42
1:C:388:LEU:HA	1:C:388:LEU:HD23	1.85	0.42
1:G:325:SER:HB3	1:G:329:SER:HB2	2.00	0.42
1:I:129:LEU:CD2	1:I:131:PRO:HG3	2.35	0.42
1:J:349:VAL:HG23	1:J:409:LEU:HD13	2.00	0.42
1:J:402:ASN:C	1:J:402:ASN:OD1	2.58	0.42
1:I:116:LEU:O	1:I:120:GLU:HG2	2.19	0.42
1:E:354:GLY:O	1:E:358:ILE:HG13	2.19	0.42
1:H:370:ARG:O	1:H:372:ILE:N	2.52	0.42
1:C:169:ARG:HD3	1:C:186:SER:OG	2.19	0.42
1:G:35:VAL:HG11	1:G:70:LEU:CD2	2.49	0.42
1:E:236:LEU:HB2	1:E:239:VAL:CG2	2.49	0.42
1:D:12:LEU:O	1:D:16:GLU:HB2	2.19	0.42
1:A:191:ALA:H	1:A:194:GLN:NE2	2.17	0.42
1:H:328:ILE:HG12	1:H:329:SER:N	2.35	0.42
1:L:423:ILE:HD12	1:L:424:GLU:N	2.34	0.42
1:A:186:SER:HB2	1:A:196:GLU:O	2.19	0.42
1:A:402:ASN:CG	1:A:405:MET:HG2	2.40	0.42
1:L:282:ALA:HA	1:L:285:PHE:CZ	2.54	0.42
1:L:411:GLU:O	1:L:415:GLU:HB2	2.19	0.42
1:D:194:GLN:HE22	1:D:240:ASN:HB3	1.84	0.42
1:C:133:PRO:HG3	1:C:199:PHE:HE1	1.83	0.42
1:G:287:ALA:HB2	1:G:395:ALA:HB1	2.00	0.42
1:B:6:ARG:HG2	1:B:10:GLU:OE1	2.18	0.42
1:K:84:ALA:O	1:K:85:GLU:C	2.58	0.42
1:F:289:THR:O	1:F:341:ALA:HB2	2.19	0.42
1:L:55:SER:HA	1:L:58:GLU:OE2	2.19	0.42
1:E:107:ASP:OD1	1:E:108:PRO:HD2	2.20	0.42
1:I:399:PHE:CZ	1:I:409:LEU:HD11	2.54	0.42
1:B:147:THR:C	1:B:149:GLU:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:HIS:NE2	1:C:404:VAL:HG11	2.33	0.42
1:J:328:ILE:C	1:J:330:THR:H	2.22	0.42
1:G:409:LEU:O	1:G:413:LEU:HB2	2.19	0.42
1:J:351:LEU:HD23	1:J:355:LEU:HG	2.01	0.42
1:L:272:LYS:HZ3	1:L:311:TRP:HH2	1.58	0.42
1:H:316:ARG:HD2	1:H:316:ARG:HA	1.90	0.42
1:K:216:LEU:HA	1:K:216:LEU:HD12	1.88	0.42
1:A:265:LEU:HD12	1:A:265:LEU:N	2.34	0.42
1:A:259:PHE:CE1	1:A:326:ARG:HB3	2.54	0.42
1:B:276:ALA:HB2	1:B:364:ALA:HB2	2.01	0.42
1:B:73:ASP:O	1:B:76:THR:OG1	2.30	0.42
1:A:126:ASP:HB2	1:A:251:PHE:HB2	1.99	0.42
1:G:256:ASN:O	1:G:258:PHE:N	2.52	0.42
1:J:115:ILE:O	1:J:115:ILE:HG22	2.19	0.42
1:F:430:THR:CG2	1:L:300:VAL:HG11	2.48	0.42
1:B:374:VAL:HG23	1:B:375:MET:HG3	2.02	0.42
1:L:58:GLU:HB3	1:L:61:VAL:HG23	2.01	0.42
1:G:402:ASN:OD1	1:G:405:MET:HG2	2.19	0.42
1:D:320:ILE:HG22	1:D:321:ARG:N	2.34	0.42
1:E:131:PRO:HG3	1:E:211:ILE:HD11	2.01	0.42
1:F:9:ILE:HG13	1:F:74:LEU:CD1	2.50	0.42
1:E:80:PHE:CD1	1:E:80:PHE:N	2.88	0.42
1:E:80:PHE:HA	1:E:81:PRO:HD3	1.85	0.42
1:E:297:LYS:HD2	1:K:431:GLN:O	2.19	0.42
1:H:267:LEU:HD21	1:H:326:ARG:HH12	1.82	0.42
1:C:114:ARG:HH12	1:C:410:GLY:CA	2.32	0.42
1:F:436:GLU:CD	1:L:297:LYS:HE3	2.40	0.42
1:F:54:GLY:HA3	1:F:68:MET:HE2	2.02	0.42
1:I:208:CYS:CA	1:I:211:ILE:HG12	2.49	0.42
1:I:156:TYR:C	1:I:158:ASP:N	2.72	0.42
1:B:37:ILE:CD1	1:B:45:ALA:HB2	2.50	0.42
1:E:124:PHE:HD2	1:E:252:LYS:HB2	1.84	0.42
1:A:317:SER:N	1:A:318:PRO:CD	2.83	0.42
1:G:191:ALA:HB3	1:G:194:GLN:NE2	2.33	0.42
1:G:54:GLY:HA3	1:G:68:MET:CE	2.49	0.42
1:E:163:ASP:OD1	1:F:89:VAL:HG21	2.19	0.42
1:G:57:ILE:C	1:G:59:GLY:N	2.72	0.42
1:G:267:LEU:O	1:G:268:SER:O	2.38	0.42
1:H:41:GLN:HE22	1:I:200:LYS:HZ3	1.66	0.42
1:E:396:LEU:O	1:E:400:LYS:HG3	2.19	0.42
1:D:319:LEU:HD12	1:D:336:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:HIS:ND1	1:C:353:ALA:HA	2.35	0.42
1:L:85:GLU:N	1:L:85:GLU:CD	2.73	0.42
1:B:275:ILE:O	1:B:279:VAL:HG23	2.20	0.42
1:F:281:HIS:O	1:F:282:ALA:C	2.58	0.42
1:F:285:PHE:C	1:F:285:PHE:CD1	2.93	0.42
1:A:168:CYS:O	1:A:170:ARG:N	2.53	0.42
1:C:70:LEU:HA	1:C:70:LEU:HD12	1.88	0.42
1:B:264:ASP:C	1:B:266:GLN:N	2.73	0.42
1:B:18:VAL:HG11	1:B:90:ALA:CB	2.49	0.42
1:E:20:TYR:HB3	1:E:89:VAL:HG22	2.01	0.42
1:D:110:ASN:O	1:D:113:LYS:HB2	2.19	0.42
1:A:256:ASN:OD1	1:A:258:PHE:HB2	2.19	0.42
1:D:412:HIS:O	1:D:413:LEU:C	2.58	0.42
1:G:148:LEU:HD22	1:G:148:LEU:H	1.84	0.42
1:J:37:ILE:HG13	1:J:41:GLN:CB	2.49	0.42
1:G:138:PHE:HB3	1:G:147:THR:O	2.18	0.42
1:B:76:THR:O	1:B:78:VAL:HG23	2.20	0.42
1:A:140:LEU:HD12	1:A:226:GLY:HA2	2.01	0.42
1:L:173:VAL:HG22	1:L:197:ILE:HD13	2.02	0.42
1:F:410:GLY:O	1:F:411:GLU:C	2.57	0.42
1:A:381:MET:CE	1:A:381:MET:HA	2.49	0.42
1:F:426:ASP:O	1:F:430:THR:HG23	2.19	0.42
1:H:3:LYS:HG2	1:H:4:TYR:CE1	2.54	0.42
1:J:9:ILE:HG13	1:J:74:LEU:CD1	2.41	0.42
1:E:172:ILE:O	1:E:176:LEU:HG	2.19	0.42
1:F:434:PRO:HD2	4:L:607:HOH:O	2.19	0.42
1:J:310:ALA:HB2	1:J:385:ILE:HG22	2.01	0.42
1:L:399:PHE:CD2	1:L:418:ILE:HD11	2.50	0.42
1:C:76:THR:O	1:C:78:VAL:HG23	2.19	0.42
1:L:126:ASP:HB2	1:L:251:PHE:HB2	2.00	0.42
1:F:280:LYS:HE2	1:F:281:HIS:HE2	1.84	0.42
1:D:260:ASP:OD1	1:D:263:ALA:HB2	2.20	0.42
1:K:258:PHE:HA	1:K:271:ALA:HB2	2.01	0.42
1:J:326:ARG:HB3	1:J:327:GLY:H	1.67	0.42
1:E:162:THR:HG22	1:E:163:ASP:N	2.35	0.42
1:G:410:GLY:O	1:G:412:HIS:N	2.53	0.42
1:E:296:TYR:HB3	1:E:390:ALA:O	2.19	0.42
1:E:306:PRO:HB3	1:E:319:LEU:CA	2.48	0.42
1:J:282:ALA:HA	1:J:285:PHE:CE1	2.54	0.42
1:B:18:VAL:HG12	1:B:21:ILE:CD1	2.49	0.42
1:L:146:PRO:HB3	1:L:228:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:ASP:O	1:K:164:LEU:HD23	2.20	0.42
1:J:291:PRO:HG2	1:J:292:THR:H	1.84	0.42
1:B:400:LYS:HB2	1:B:400:LYS:HE3	1.80	0.42
1:A:264:ASP:C	1:A:266:GLN:N	2.73	0.42
1:E:142:GLU:N	1:E:142:GLU:CD	2.73	0.42
1:B:168:CYS:O	1:B:172:ILE:HG13	2.19	0.42
1:I:257:ALA:O	1:I:270:THR:HB	2.20	0.42
1:H:264:ASP:OD2	1:H:264:ASP:N	2.52	0.42
1:J:400:LYS:HA	1:J:414:PHE:CZ	2.55	0.42
1:G:32:ILE:HG21	1:G:216:LEU:HD13	2.01	0.42
1:D:318:PRO:HG2	1:D:320:ILE:O	2.19	0.42
1:L:355:LEU:HD23	1:L:355:LEU:HA	1.77	0.42
1:C:430:THR:HG22	1:I:300:VAL:HG11	2.01	0.42
1:K:115:ILE:O	1:K:118:GLU:HB2	2.20	0.42
1:E:136:PHE:HE2	1:E:194:GLN:HB2	1.81	0.42
1:F:224:LYS:HD2	1:F:225:HIS:CD2	2.55	0.42
1:A:273:HIS:NE2	1:A:361:LYS:HA	2.33	0.42
1:H:248:LEU:HD21	1:H:347:LEU:HD11	2.00	0.42
1:B:274:PHE:O	1:B:278:ILE:HD13	2.20	0.42
1:A:216:LEU:HA	1:A:216:LEU:HD12	1.75	0.42
1:G:421:LYS:CD	1:G:424:GLU:OE2	2.66	0.42
1:I:426:ASP:OD1	1:I:429:ARG:NH1	2.52	0.42
1:G:20:TYR:HB3	1:G:89:VAL:HG22	2.01	0.42
1:A:341:ALA:HB1	1:A:346:ALA:HB2	2.02	0.42
1:A:264:ASP:C	1:A:265:LEU:HD12	2.40	0.42
1:J:258:PHE:HZ	1:J:274:PHE:CD1	2.37	0.42
1:G:417:PHE:O	1:G:418:ILE:C	2.58	0.42
1:E:30:GLY:CA	1:E:342:ASN:ND2	2.83	0.42
1:B:137:LEU:HD23	1:B:229:ALA:HA	2.02	0.42
1:L:19:LYS:HA	1:L:39:VAL:CG1	2.49	0.42
1:A:13:VAL:HG11	1:A:42:LEU:HD22	2.01	0.42
1:E:9:ILE:HG13	1:E:74:LEU:CD1	2.29	0.42
1:C:372:ILE:O	1:C:380:ARG:HD3	2.20	0.42
1:F:9:ILE:HD12	1:F:77:PHE:CG	2.55	0.42
1:B:62:ARG:O	1:B:62:ARG:HG3	2.20	0.42
1:B:150:LEU:CD1	1:B:192:PRO:HB2	2.50	0.42
1:B:282:ALA:HA	1:B:285:PHE:CE1	2.55	0.42
1:J:208:CYS:HA	1:J:211:ILE:HD12	2.01	0.42
1:J:368:ILE:HD11	1:J:384:GLY:O	2.20	0.42
1:F:22:ARG:NH1	1:F:22:ARG:HG2	2.34	0.42
1:L:399:PHE:CE1	1:L:405:MET:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:PHE:CA	1:H:271:ALA:HB2	2.50	0.42
1:K:169:ARG:HG3	1:K:169:ARG:NH2	2.34	0.42
1:E:12:LEU:HA	1:E:15:GLU:OE1	2.19	0.42
1:L:35:VAL:O	1:L:35:VAL:HG23	2.20	0.42
1:B:253:ASN:O	1:B:255:VAL:HG23	2.20	0.42
1:C:209:ASP:O	1:C:212:GLN:HB2	2.20	0.42
1:J:267:LEU:CD2	1:J:326:ARG:HH12	2.33	0.42
1:B:28:ILE:HD11	1:B:417:PHE:HB2	2.02	0.42
1:E:53:ASP:OD1	1:E:65:GLU:HG3	2.20	0.42
1:C:206:ARG:HG3	4:C:604:HOH:O	2.19	0.42
1:L:32:ILE:CD1	1:L:216:LEU:HD22	2.50	0.42
1:I:137:LEU:HD23	1:I:229:ALA:HA	2.02	0.42
1:B:317:SER:HB2	1:B:335:ARG:HH22	1.84	0.42
1:E:431:GLN:HG2	1:K:435:TRP:CD1	2.54	0.42
1:A:383:ASN:C	1:A:385:ILE:H	2.22	0.42
1:K:315:ASN:HD22	1:K:315:ASN:HA	1.58	0.42
1:J:191:ALA:HB3	1:J:194:GLN:NE2	2.34	0.42
1:C:39:VAL:C	1:C:41:GLN:H	2.23	0.42
1:K:112:LEU:HD12	1:K:205:VAL:HG22	2.02	0.42
1:H:380:ARG:CZ	1:H:380:ARG:HB2	2.50	0.42
1:L:437:ARG:HD2	4:L:622:HOH:O	2.18	0.42
1:A:129:LEU:HD22	1:A:130:GLY:N	2.34	0.42
1:I:223:ARG:O	1:I:226:GLY:N	2.53	0.42
1:E:259:PHE:CE2	1:E:326:ARG:HD3	2.55	0.42
1:C:52:PHE:CZ	1:C:54:GLY:HA2	2.54	0.42
1:K:264:ASP:C	1:K:266:GLN:N	2.74	0.42
1:A:52:PHE:HZ	1:A:57:ILE:HD11	1.85	0.42
1:K:37:ILE:HD12	1:K:38:PRO:O	2.20	0.42
1:E:67:ASP:C	1:E:68:MET:HG2	2.40	0.42
1:E:441:MET:HG3	1:E:441:MET:O	2.19	0.42
1:D:11:LYS:CG	1:D:15:GLU:OE2	2.67	0.42
1:G:137:LEU:O	1:G:151:ASN:HB3	2.19	0.42
1:A:167:ASN:C	1:A:167:ASN:HD22	2.22	0.42
1:J:260:ASP:OD1	1:J:263:ALA:HB2	2.20	0.42
1:C:300:VAL:HG21	1:I:430:THR:HG22	2.01	0.42
1:L:163:ASP:HA	1:L:167:ASN:HD22	1.85	0.42
1:F:108:PRO:O	1:F:111:ASN:N	2.53	0.42
1:B:52:PHE:CD1	1:B:70:LEU:HD13	2.55	0.42
1:B:141:ASP:OD2	1:B:141:ASP:C	2.59	0.42
1:I:183:ILE:HD13	1:I:197:ILE:CG2	2.50	0.41
1:G:250:LEU:HB3	1:G:257:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:LYS:HB2	1:H:75:ASN:OD1	2.20	0.41
1:F:4:TYR:CB	1:F:9:ILE:HD11	2.47	0.41
1:I:285:PHE:HB3	1:I:405:MET:SD	2.60	0.41
1:E:141:ASP:OD2	1:E:144:GLY:N	2.53	0.41
1:K:360:ASN:N	1:K:360:ASN:ND2	2.68	0.41
1:F:175:GLU:O	1:F:179:MET:HG3	2.20	0.41
1:B:155:GLY:H	1:B:158:ASP:CG	2.23	0.41
1:J:131:PRO:HG2	1:J:211:ILE:CG1	2.50	0.41
1:D:146:PRO:CG	1:D:228:HIS:CD2	3.03	0.41
1:C:78:VAL:HB	1:C:91:ARG:HG3	2.02	0.41
1:L:311:TRP:CG	1:L:311:TRP:O	2.73	0.41
1:E:34:ASN:OD1	1:E:35:VAL:N	2.53	0.41
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.55	0.41
1:K:98:ASN:HB3	1:K:100:ASP:OD2	2.19	0.41
1:K:380:ARG:CB	1:K:385:ILE:HD12	2.48	0.41
1:C:9:ILE:HD11	1:C:74:LEU:HB3	2.01	0.41
1:A:354:GLY:O	1:A:358:ILE:HG12	2.20	0.41
1:A:58:GLU:H	1:A:58:GLU:HG2	1.66	0.41
1:F:52:PHE:CE2	1:F:54:GLY:HA2	2.54	0.41
1:E:380:ARG:HB3	1:E:380:ARG:HH11	1.85	0.41
1:B:373:TYR:N	1:B:373:TYR:CD2	2.88	0.41
1:C:283:THR:HG21	1:C:386:VAL:HG12	2.02	0.41
1:C:137:LEU:HD12	1:C:195:HIS:HE2	1.85	0.41
1:J:312:SER:HB3	1:J:315:ASN:HB2	2.02	0.41
1:F:296:TYR:HB3	1:F:390:ALA:O	2.19	0.41
1:F:143:LYS:HE3	1:F:143:LYS:HB2	1.88	0.41
1:A:83:THR:HG23	1:A:83:THR:O	2.20	0.41
1:L:175:GLU:HA	1:L:175:GLU:OE2	2.20	0.41
1:I:116:LEU:HA	1:I:116:LEU:HD23	1.93	0.41
1:J:9:ILE:O	1:J:13:VAL:HG23	2.19	0.41
1:F:133:PRO:HG2	1:F:199:PHE:CE1	2.55	0.41
1:B:309:VAL:CG2	1:B:386:VAL:HG13	2.50	0.41
1:C:164:LEU:HD23	1:C:164:LEU:C	2.40	0.41
1:D:259:PHE:HB2	1:D:330:THR:OG1	2.20	0.41
1:H:112:LEU:HD12	1:H:344:TYR:HA	2.02	0.41
1:L:368:ILE:HG21	1:L:372:ILE:HG21	2.01	0.41
1:C:360:ASN:O	1:C:361:LYS:C	2.57	0.41
1:H:328:ILE:N	1:H:328:ILE:CD1	2.81	0.41
1:L:276:ALA:O	1:L:279:VAL:HB	2.20	0.41
1:H:86:LYS:HG3	1:I:174:LEU:HB3	2.02	0.41
1:J:139:LYS:HA	1:J:227:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ASN:CB	1:F:345:LEU:HD12	2.50	0.41
1:B:103:PRO:HB3	1:B:110:ASN:ND2	2.35	0.41
1:J:16:GLU:HA	1:J:16:GLU:OE2	2.20	0.41
1:J:291:PRO:O	1:J:392:LEU:HD13	2.20	0.41
1:I:293:VAL:HG11	1:I:428:PHE:CG	2.54	0.41
1:K:27:ASP:HA	1:K:57:ILE:HG23	2.02	0.41
1:C:370:ARG:HB3	1:C:371:ASN:H	1.63	0.41
1:J:393:ALA:HB2	1:J:425:TRP:CE2	2.56	0.41
1:E:85:GLU:H	1:E:85:GLU:CD	2.16	0.41
1:F:133:PRO:CG	1:F:199:PHE:HE1	2.33	0.41
1:F:200:LYS:O	1:F:201:TYR:C	2.58	0.41
1:F:129:LEU:O	1:F:201:TYR:HA	2.21	0.41
1:B:405:MET:O	1:B:406:VAL:C	2.58	0.41
1:L:172:ILE:O	1:L:176:LEU:HG	2.20	0.41
1:K:116:LEU:HD23	1:K:116:LEU:HA	1.90	0.41
1:E:80:PHE:HD2	1:E:82:TRP:CZ3	2.38	0.41
1:D:248:LEU:HD11	1:D:350:LEU:HD13	2.02	0.41
1:A:234:LYS:HE3	1:A:239:VAL:O	2.20	0.41
1:D:289:THR:C	1:D:290:ASN:ND2	2.73	0.41
1:A:119:MET:CE	1:A:127:PHE:HB2	2.50	0.41
1:F:36:GLU:H	1:F:36:GLU:HG2	1.67	0.41
1:C:338:ASP:OD2	1:C:340:ALA:HB3	2.20	0.41
1:A:274:PHE:CE2	1:A:278:ILE:HD11	2.55	0.41
1:L:282:ALA:HA	1:L:285:PHE:CE1	2.56	0.41
1:A:86:LYS:HG3	1:F:174:LEU:HB3	2.01	0.41
1:G:211:ILE:HG22	1:G:215:LYS:HE3	2.03	0.41
1:A:230:THR:OG1	1:A:232:MET:HB2	2.20	0.41
1:D:378:GLU:OE2	1:D:381:MET:HE3	2.21	0.41
1:E:150:LEU:HD13	1:E:192:PRO:HG2	2.02	0.41
1:C:364:ALA:HB1	1:C:365:PRO:HD2	2.03	0.41
1:L:314:GLN:HA	1:L:314:GLN:HE21	1.85	0.41
1:E:405:MET:O	1:E:408:ALA:N	2.47	0.41
1:H:137:LEU:HD12	1:H:195:HIS:NE2	2.35	0.41
1:H:310:ALA:HB1	1:H:368:ILE:CG1	2.47	0.41
1:E:73:ASP:OD2	1:E:76:THR:HG23	2.20	0.41
1:B:309:VAL:HG21	1:B:386:VAL:HG13	2.02	0.41
1:F:80:PHE:HB3	1:F:82:TRP:CE3	2.55	0.41
1:A:300:VAL:HG22	1:G:429:ARG:NH1	2.33	0.41
1:E:297:LYS:HD3	1:K:429:ARG:O	2.19	0.41
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.55	0.41
1:E:23:LEU:HB3	1:E:70:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:LEU:CD1	1:F:336:SER:HB3	2.47	0.41
1:K:289:THR:C	1:K:290:ASN:ND2	2.74	0.41
1:B:436:GLU:CD	1:H:297:LYS:HE3	2.40	0.41
1:C:189:GLU:HA	1:C:189:GLU:OE2	2.18	0.41
1:A:286:THR:HG21	1:A:389:PRO:HD2	2.03	0.41
1:J:271:ALA:O	1:J:274:PHE:HB3	2.21	0.41
1:D:381:MET:HG2	4:D:605:HOH:O	2.20	0.41
1:L:141:ASP:OD2	1:L:144:GLY:N	2.53	0.41
1:H:418:ILE:O	1:H:422:GLU:HG3	2.21	0.41
1:A:440:TYR:OH	1:G:293:VAL:HG23	2.21	0.41
1:L:105:GLU:OE1	1:L:105:GLU:O	2.37	0.41
1:J:404:VAL:O	1:J:408:ALA:N	2.52	0.41
1:K:33:LYS:HA	1:L:158:ASP:CA	2.38	0.41
1:F:279:VAL:HG13	1:F:309:VAL:HG12	2.02	0.41
1:D:169:ARG:O	1:D:170:ARG:C	2.58	0.41
1:J:319:LEU:HD23	1:J:320:ILE:HG12	2.02	0.41
1:K:247:ASN:HB3	1:K:331:ARG:CG	2.47	0.41
1:G:23:LEU:O	1:G:35:VAL:HG12	2.20	0.41
1:A:234:LYS:HB3	1:A:294:ASN:ND2	2.35	0.41
1:E:439:GLN:HB2	1:E:440:TYR:H	1.72	0.41
1:C:232:MET:HA	1:C:233:PRO:HD3	1.86	0.41
1:F:281:HIS:HE1	1:F:356:ASP:OD2	2.04	0.41
1:C:321:ARG:HB2	1:C:335:ARG:HD2	2.03	0.41
1:D:71:TYR:C	1:D:94:CYS:HB3	2.41	0.41
1:K:252:LYS:O	1:K:252:LYS:HD2	2.20	0.41
1:C:345:LEU:CD2	1:C:413:LEU:HD13	2.50	0.41
1:D:164:LEU:HD11	1:E:224:LYS:NZ	2.35	0.41
1:D:163:ASP:OD1	1:E:89:VAL:HG21	2.20	0.41
1:L:186:SER:O	1:L:187:HIS:HB3	2.20	0.41
1:D:6:ARG:O	1:D:6:ARG:HD3	2.21	0.41
1:B:280:LYS:HD2	1:B:362:LEU:CD2	2.51	0.41
1:J:250:LEU:HB2	1:J:258:PHE:CZ	2.56	0.41
1:C:291:PRO:O	1:C:392:LEU:HD13	2.20	0.41
1:B:30:GLY:H	1:B:342:ASN:HD22	1.69	0.41
1:B:260:ASP:HB2	1:B:268:SER:HA	2.01	0.41
1:K:73:ASP:O	1:K:74:LEU:C	2.58	0.41
1:K:72:PRO:HA	1:K:94:CYS:HB3	2.03	0.41
1:K:143:LYS:O	1:K:144:GLY:C	2.57	0.41
1:A:296:TYR:HB3	1:A:390:ALA:O	2.20	0.41
1:J:102:THR:HA	1:J:103:PRO:HD3	1.92	0.41
1:F:146:PRO:HG3	1:F:228:HIS:HD2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ILE:HG21	1:G:216:LEU:CD1	2.51	0.41
1:J:135:PHE:N	1:J:135:PHE:CD1	2.88	0.41
1:J:319:LEU:O	1:J:320:ILE:HD13	2.20	0.41
1:G:131:PRO:HG2	1:G:199:PHE:CE1	2.55	0.41
1:F:221:ILE:O	1:F:225:HIS:CD2	2.73	0.41
1:I:9:ILE:CG1	1:I:74:LEU:HD12	2.50	0.41
1:C:129:LEU:HD23	1:C:130:GLY:N	2.36	0.41
1:F:82:TRP:HH2	1:F:217:VAL:HG22	1.85	0.41
1:K:67:ASP:N	1:K:67:ASP:OD2	2.53	0.41
1:A:119:MET:HG2	1:A:124:PHE:HB2	2.01	0.41
1:L:320:ILE:HG22	1:L:321:ARG:N	2.35	0.41
1:K:58:GLU:OE1	1:K:416:HIS:NE2	2.53	0.41
1:F:41:GLN:HB3	1:F:41:GLN:HE21	1.59	0.41
1:D:65:GLU:HG3	1:D:65:GLU:O	2.20	0.41
1:F:150:LEU:HD22	1:F:192:PRO:O	2.21	0.41
1:A:327:GLY:C	1:A:329:SER:H	2.23	0.41
1:B:351:LEU:HD22	1:B:355:LEU:HG	2.02	0.41
1:C:377:LYS:O	1:C:381:MET:HE2	2.20	0.41
1:J:85:GLU:O	1:J:87:GLY:N	2.43	0.41
1:F:170:ARG:HG2	1:F:170:ARG:HH11	1.85	0.41
1:I:212:GLN:OE1	1:I:212:GLN:HA	2.21	0.41
1:J:114:ARG:NH1	1:J:115:ILE:HD11	2.35	0.41
1:I:248:LEU:HD13	1:I:332:VAL:HG23	2.02	0.41
1:E:96:ILE:HD13	1:E:107:ASP:OD1	2.21	0.41
1:E:91:ARG:CZ	1:E:93:ILE:HD11	2.51	0.41
1:A:117:LYS:C	1:A:119:MET:N	2.74	0.41
1:L:129:LEU:HD22	1:L:131:PRO:HD3	2.02	0.41
1:K:46:LEU:C	1:K:48:ASN:H	2.24	0.41
1:G:306:PRO:HG2	1:G:335:ARG:HB2	2.02	0.41
1:K:423:ILE:O	1:K:427:MET:HG3	2.20	0.41
1:E:151:ASN:HD22	1:E:166:GLU:CD	2.24	0.41
1:D:383:ASN:HD22	1:D:383:ASN:HA	1.60	0.41
1:B:315:ASN:OD1	1:B:371:ASN:HA	2.21	0.41
1:J:4:TYR:HB3	1:J:9:ILE:HD11	2.02	0.41
1:E:176:LEU:HD11	1:E:214:PHE:CD1	2.56	0.41
1:G:199:PHE:N	1:G:199:PHE:CD1	2.85	0.41
1:K:120:GLU:HA	1:K:124:PHE:O	2.19	0.41
1:I:223:ARG:O	1:I:225:HIS:N	2.54	0.41
1:I:140:LEU:HD12	1:I:227:LEU:N	2.36	0.41
1:C:24:GLN:HE22	1:C:91:ARG:HH11	1.64	0.41
1:G:55:SER:CB	1:G:62:ARG:HE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:MET:CG	1:C:294:ASN:HD22	2.34	0.41
1:F:205:VAL:HG13	1:F:206:ARG:H	1.85	0.41
1:E:169:ARG:O	1:E:171:ASP:N	2.54	0.41
1:B:214:PHE:O	1:B:218:VAL:HG23	2.21	0.41
1:I:321:ARG:HE	1:I:321:ARG:HB3	1.75	0.41
1:J:134:GLU:HG2	1:J:196:GLU:HB2	2.01	0.41
1:G:112:LEU:HD12	1:G:344:TYR:CD2	2.56	0.41
1:J:58:GLU:O	1:J:59:GLY:C	2.58	0.41
1:H:346:ALA:O	1:H:350:LEU:HB2	2.20	0.41
1:G:44:LYS:HE3	1:G:49:LYS:O	2.21	0.41
1:H:186:SER:HB2	1:H:197:ILE:HG12	2.02	0.41
1:G:116:LEU:CD1	1:G:205:VAL:HG23	2.50	0.41
1:C:378:GLU:OE1	1:C:378:GLU:N	2.48	0.41
1:E:306:PRO:CB	1:E:319:LEU:HA	2.47	0.41
1:J:64:GLU:HG2	1:K:315:ASN:C	2.42	0.41
1:K:20:TYR:C	1:K:21:ILE:HD12	2.40	0.41
1:H:3:LYS:HD3	1:H:4:TYR:HE1	1.86	0.41
1:I:20:TYR:OH	1:I:36:GLU:HG3	2.20	0.41
1:E:399:PHE:CE1	1:E:405:MET:HB3	2.56	0.41
1:L:20:TYR:CZ	1:L:36:GLU:HB3	2.56	0.41
1:F:275:ILE:O	1:F:279:VAL:HG23	2.20	0.41
1:D:170:ARG:O	1:D:174:LEU:HG	2.21	0.41
1:E:225:HIS:O	1:E:227:LEU:HG	2.21	0.41
1:G:13:VAL:HG21	1:G:42:LEU:CD2	2.51	0.41
1:L:91:ARG:CD	1:L:91:ARG:C	2.83	0.41
1:J:207:SER:O	1:J:209:ASP:N	2.53	0.41
1:J:343:PRO:O	1:J:347:LEU:HB2	2.21	0.41
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.87	0.41
1:E:371:ASN:HB3	1:E:375:MET:CG	2.51	0.41
1:A:429:ARG:HG3	1:A:429:ARG:HH11	1.86	0.41
1:D:288:VAL:HG22	1:D:417:PHE:CE2	2.56	0.41
1:A:407:LYS:O	1:A:408:ALA:C	2.59	0.41
1:D:21:ILE:HD11	1:D:39:VAL:HA	2.03	0.41
1:B:68:MET:SD	1:B:96:ILE:HG22	2.60	0.41
1:C:248:LEU:HB2	1:C:332:VAL:CG1	2.51	0.41
1:D:203:GLY:O	1:D:205:VAL:N	2.54	0.41
1:H:124:PHE:CD2	1:H:250:LEU:HD13	2.56	0.41
1:F:241:GLY:HA3	1:F:298:ARG:CG	2.50	0.41
1:H:397:GLU:HA	1:H:400:LYS:NZ	2.36	0.41
1:F:245:HIS:CD2	1:F:335:ARG:HA	2.56	0.41
1:G:20:TYR:OH	1:G:36:GLU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ALA:O	1:L:186:SER:HB2	2.19	0.41
1:H:135:PHE:HB3	1:H:231:PHE:CE1	2.54	0.41
1:K:28:ILE:HD11	1:K:417:PHE:N	2.36	0.41
1:B:109:ARG:O	1:B:112:LEU:HB3	2.21	0.41
1:B:112:LEU:O	1:B:116:LEU:HG	2.21	0.41
1:I:396:LEU:HD11	1:I:421:LYS:CB	2.51	0.41
1:J:19:LYS:HD2	1:J:86:LYS:O	2.21	0.41
1:I:418:ILE:O	1:I:419:GLU:C	2.59	0.41
1:A:399:PHE:HZ	1:A:409:LEU:CD1	2.33	0.41
1:I:151:ASN:HD22	1:I:166:GLU:CD	2.23	0.41
1:K:141:ASP:HB3	1:K:147:THR:CG2	2.51	0.41
1:A:421:LYS:HD3	1:A:421:LYS:HA	1.89	0.41
1:F:343:PRO:O	1:F:347:LEU:HD23	2.21	0.41
1:J:36:GLU:H	1:J:36:GLU:HG2	1.67	0.41
1:K:186:SER:HB2	1:K:196:GLU:O	2.21	0.41
1:L:132:GLU:HG2	1:L:198:ASP:OD1	2.20	0.41
1:G:41:GLN:NE2	1:G:44:LYS:HD3	2.36	0.41
1:I:152:ASP:OD2	1:I:188:HIS:NE2	2.39	0.41
1:B:32:ILE:HD13	1:B:216:LEU:HD12	2.02	0.41
1:J:27:ASP:C	1:J:27:ASP:OD2	2.59	0.41
1:D:296:TYR:N	1:D:296:TYR:CD1	2.89	0.41
1:L:152:ASP:OD2	1:L:188:HIS:NE2	2.40	0.41
1:H:393:ALA:HB2	1:H:425:TRP:CD2	2.55	0.41
1:F:378:GLU:O	1:F:381:MET:HG2	2.21	0.41
1:I:393:ALA:HB2	1:I:425:TRP:CE2	2.56	0.41
1:B:175:GLU:O	1:B:179:MET:HG3	2.21	0.41
1:F:112:LEU:O	1:F:116:LEU:HG	2.21	0.41
1:E:182:GLU:HA	1:E:182:GLU:OE1	2.21	0.41
1:I:283:THR:HG22	1:I:388:LEU:HD23	2.02	0.41
1:J:78:VAL:HG11	1:J:179:MET:CE	2.51	0.41
1:E:172:ILE:HD11	1:E:221:ILE:HB	2.03	0.41
1:A:156:TYR:CE2	1:B:62:ARG:NH1	2.89	0.41
1:J:306:PRO:HB3	1:J:319:LEU:HA	2.02	0.41
1:C:169:ARG:O	1:C:172:ILE:HB	2.21	0.41
1:L:138:PHE:CZ	1:L:150:LEU:HD23	2.55	0.41
1:I:97:TYR:HE2	1:I:101:GLY:O	2.04	0.41
1:C:129:LEU:HD23	1:C:130:GLY:H	1.86	0.41
1:L:331:ARG:HH11	1:L:331:ARG:HG2	1.86	0.41
1:E:436:GLU:OE1	1:K:297:LYS:NZ	2.54	0.41
1:I:170:ARG:NH1	1:I:171:ASP:OD2	2.54	0.41
1:B:256:ASN:O	1:B:258:PHE:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:GLU:CB	1:I:62:ARG:HB2	2.51	0.41
1:C:74:LEU:HA	1:C:92:PHE:CE2	2.56	0.41
1:H:355:LEU:HA	1:H:355:LEU:HD23	1.86	0.41
1:H:125:SER:HB2	1:H:251:PHE:HB3	2.03	0.41
1:L:214:PHE:O	1:L:215:LYS:C	2.57	0.41
1:L:282:ALA:C	1:L:284:SER:H	2.25	0.41
1:K:141:ASP:OD1	1:K:145:GLU:HB2	2.21	0.41
1:G:98:ASN:HD21	1:G:104:PHE:HA	1.86	0.41
1:D:443:GLN:HA	1:D:443:GLN:NE2	2.36	0.41
1:C:286:THR:O	1:C:290:ASN:HB2	2.21	0.41
1:G:410:GLY:O	1:G:411:GLU:C	2.59	0.41
1:F:113:LYS:O	1:F:116:LEU:HB2	2.21	0.41
1:F:262:ASN:O	1:F:263:ALA:HB2	2.21	0.41
1:C:301:PRO:HB3	1:C:308:TYR:OH	2.21	0.41
1:A:28:ILE:CG2	1:A:29:LEU:N	2.83	0.41
1:K:60:PHE:HZ	1:K:420:ALA:O	2.03	0.41
1:K:33:LYS:HA	1:L:159:LEU:H	1.86	0.40
1:B:371:ASN:O	1:B:374:VAL:HG22	2.21	0.40
1:G:156:TYR:O	1:G:158:ASP:N	2.54	0.40
1:K:320:ILE:HG22	1:K:321:ARG:N	2.36	0.40
1:A:231:PHE:HB2	1:G:444:TYR:OXT	2.21	0.40
1:B:281:HIS:CD2	1:B:404:VAL:HG21	2.56	0.40
1:H:370:ARG:NH1	1:H:370:ARG:CG	2.84	0.40
1:K:322:ILE:HA	1:K:323:PRO:HD2	1.95	0.40
1:J:116:LEU:HD23	1:J:351:LEU:CD1	2.51	0.40
1:A:234:LYS:HB3	1:A:294:ASN:HD21	1.86	0.40
1:B:441:MET:O	1:H:228:HIS:CE1	2.66	0.40
1:C:52:PHE:HE1	1:C:70:LEU:HD13	1.79	0.40
1:K:264:ASP:C	1:K:266:GLN:H	2.25	0.40
1:D:139:LYS:O	1:D:147:THR:HG23	2.21	0.40
1:E:338:ASP:HB2	1:E:339:PRO:CD	2.50	0.40
1:D:184:GLU:OE2	1:D:200:LYS:NZ	2.50	0.40
1:K:258:PHE:CB	1:K:271:ALA:HB2	2.51	0.40
1:L:203:GLY:O	1:L:205:VAL:N	2.54	0.40
1:I:258:PHE:HA	1:I:271:ALA:HB2	2.03	0.40
1:J:37:ILE:HG22	1:K:185:ALA:HB2	2.03	0.40
1:B:115:ILE:HD11	1:B:408:ALA:HA	2.04	0.40
1:G:150:LEU:HD13	1:G:192:PRO:O	2.21	0.40
1:D:81:PRO:HA	4:D:619:HOH:O	2.21	0.40
1:I:53:ASP:C	1:I:53:ASP:OD2	2.60	0.40
1:E:262:ASN:HA	1:E:262:ASN:HD22	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ASN:HA	1:E:110:ASN:HD22	1.71	0.40
1:G:375:MET:CE	1:G:385:ILE:HG13	2.51	0.40
1:G:250:LEU:CB	1:G:258:PHE:CZ	2.98	0.40
1:I:127:PHE:CE2	1:I:347:LEU:HD11	2.56	0.40
1:J:389:PRO:HG3	1:J:395:ALA:HB2	2.03	0.40
1:E:273:HIS:NE2	1:E:361:LYS:CB	2.85	0.40
1:J:129:LEU:HD22	1:J:131:PRO:HD3	2.02	0.40
1:B:377:LYS:HD3	1:B:387:ASP:OD2	2.20	0.40
1:G:183:ILE:HG21	1:G:197:ILE:HG22	2.03	0.40
1:G:78:VAL:HG11	1:G:91:ARG:NH2	2.36	0.40
1:E:440:TYR:HD1	1:E:444:TYR:CE2	2.38	0.40
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.56	0.40
1:C:106:GLY:O	1:C:413:LEU:HD21	2.21	0.40
1:D:45:ALA:HA	1:D:50:VAL:CG2	2.50	0.40
1:C:112:LEU:HD12	1:C:344:TYR:CD2	2.51	0.40
1:K:377:LYS:HA	1:K:380:ARG:CZ	2.52	0.40
1:H:404:VAL:HG13	1:H:405:MET:HE2	2.02	0.40
1:D:54:GLY:C	1:D:56:SER:N	2.74	0.40
1:E:409:LEU:HB3	1:E:413:LEU:HB2	2.03	0.40
1:G:167:ASN:HD22	1:G:170:ARG:NH1	2.18	0.40
1:L:374:VAL:HG12	1:L:374:VAL:O	2.21	0.40
1:A:260:ASP:O	1:A:266:GLN:HA	2.20	0.40
1:D:293:VAL:HG11	1:D:428:PHE:CD2	2.56	0.40
1:K:60:PHE:CD1	1:K:60:PHE:C	2.93	0.40
1:K:133:PRO:HD2	1:K:197:ILE:O	2.21	0.40
1:L:110:ASN:HA	1:L:110:ASN:HD22	1.66	0.40
1:I:129:LEU:HD23	1:I:130:GLY:N	2.36	0.40
1:L:156:TYR:C	1:L:158:ASP:H	2.24	0.40
1:E:274:PHE:CE2	1:E:278:ILE:HD11	2.56	0.40
1:G:34:ASN:CG	1:H:159:LEU:HG	2.41	0.40
1:L:380:ARG:NH1	1:L:380:ARG:CB	2.85	0.40
1:L:296:TYR:CE1	1:L:392:LEU:HA	2.56	0.40
1:C:159:LEU:HA	1:C:159:LEU:HD12	1.95	0.40
1:H:243:GLY:HA2	1:H:338:ASP:HA	2.03	0.40
1:B:338:ASP:HB2	1:B:339:PRO:CD	2.47	0.40
1:C:416:HIS:O	1:C:417:PHE:C	2.60	0.40
1:F:122:LEU:HD12	1:F:355:LEU:HD13	2.02	0.40
1:F:351:LEU:CD2	1:F:355:LEU:HG	2.51	0.40
1:G:285:PHE:CD1	1:G:285:PHE:C	2.95	0.40
1:I:203:GLY:O	1:I:204:ALA:C	2.60	0.40
1:D:103:PRO:HB2	1:D:110:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.90	0.40
1:D:378:GLU:OE1	1:D:382:GLU:HG3	2.21	0.40
1:G:370:ARG:HH22	1:G:383:ASN:ND2	2.19	0.40
1:I:259:PHE:CD1	1:I:260:ASP:N	2.89	0.40
1:G:258:PHE:O	1:G:330:THR:HG21	2.22	0.40
1:I:129:LEU:O	1:I:131:PRO:HD3	2.21	0.40
1:E:282:ALA:C	1:E:284:SER:N	2.73	0.40
1:G:351:LEU:CD2	1:G:355:LEU:HG	2.51	0.40
1:L:351:LEU:O	1:L:355:LEU:N	2.43	0.40
1:K:124:PHE:CZ	1:K:358:ILE:HG21	2.56	0.40
1:K:207:SER:O	1:K:211:ILE:HG13	2.21	0.40
1:F:82:TRP:CH2	1:F:217:VAL:HG22	2.56	0.40
1:D:289:THR:HG22	1:D:337:VAL:HG13	2.03	0.40
1:C:232:MET:HG3	1:C:294:ASN:HD22	1.87	0.40
1:F:109:ARG:HE	1:F:205:VAL:CG2	2.34	0.40
1:B:18:VAL:HG22	1:B:88:LYS:HB2	2.04	0.40
1:L:115:ILE:H	1:L:115:ILE:HD12	1.87	0.40
1:I:174:LEU:HD12	1:I:174:LEU:HA	1.90	0.40
1:J:273:HIS:CE1	1:J:361:LYS:HB3	2.57	0.40
1:A:402:ASN:HD21	1:A:404:VAL:HG12	1.87	0.40
1:J:274:PHE:C	1:J:274:PHE:CD2	2.95	0.40
1:L:337:VAL:HG12	1:L:338:ASP:N	2.36	0.40
1:C:155:GLY:O	1:C:158:ASP:HB2	2.21	0.40
1:H:83:THR:O	1:H:83:THR:HG23	2.22	0.40
1:G:258:PHE:HA	1:G:268:SER:OG	2.22	0.40
1:L:308:TYR:OH	1:L:373:TYR:HA	2.21	0.40
1:E:324:ALA:O	1:E:325:SER:C	2.60	0.40
1:A:252:LYS:O	1:A:253:ASN:HB2	2.21	0.40
1:B:159:LEU:HD11	1:C:22:ARG:NH1	2.34	0.40
1:C:22:ARG:HB3	1:C:34:ASN:HD22	1.86	0.40
1:A:129:LEU:CD2	1:A:130:GLY:N	2.85	0.40
1:B:343:PRO:O	1:B:347:LEU:HB2	2.21	0.40
1:I:68:MET:CE	1:I:104:PHE:HB2	2.51	0.40
1:I:355:LEU:O	1:I:357:GLY:N	2.54	0.40
1:G:183:ILE:CG2	1:G:197:ILE:HG22	2.52	0.40
1:K:406:VAL:HG22	1:K:414:PHE:CZ	2.56	0.40
1:E:429:ARG:HH11	1:E:429:ARG:HG3	1.87	0.40
1:D:13:VAL:HG21	1:D:42:LEU:HD22	2.02	0.40
1:H:20:TYR:OH	1:H:36:GLU:CB	2.69	0.40
1:C:282:ALA:HA	1:C:285:PHE:CZ	2.57	0.40
1:A:142:GLU:N	1:A:142:GLU:CD	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD23	1:B:351:LEU:HD11	2.03	0.40
1:K:345:LEU:O	1:K:349:VAL:HG22	2.21	0.40
1:J:19:LYS:HA	1:J:39:VAL:HB	2.02	0.40
1:F:288:VAL:O	1:F:291:PRO:HD3	2.22	0.40
1:I:360:ASN:O	1:I:361:LYS:C	2.60	0.40
1:A:203:GLY:O	1:A:204:ALA:C	2.60	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	435/443 (98%)	358 (82%)	63 (14%)	14 (3%)	5	26
1	B	435/443 (98%)	367 (84%)	52 (12%)	16 (4%)	4	23
1	C	434/443 (98%)	341 (79%)	67 (15%)	26 (6%)	2	11
1	D	435/443 (98%)	347 (80%)	72 (17%)	16 (4%)	4	23
1	E	434/443 (98%)	344 (79%)	66 (15%)	24 (6%)	2	13
1	F	433/443 (98%)	345 (80%)	69 (16%)	19 (4%)	3	18
1	G	434/443 (98%)	353 (81%)	58 (13%)	23 (5%)	2	14
1	H	433/443 (98%)	356 (82%)	58 (13%)	19 (4%)	3	18
1	I	432/443 (98%)	364 (84%)	45 (10%)	23 (5%)	2	14
1	J	434/443 (98%)	342 (79%)	69 (16%)	23 (5%)	2	14
1	K	434/443 (98%)	356 (82%)	56 (13%)	22 (5%)	2	15
1	L	436/443 (98%)	346 (79%)	66 (15%)	24 (6%)	2	13
All	All	5209/5316 (98%)	4219 (81%)	741 (14%)	249 (5%)	3	17

All (249) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	161	PRO
1	A	166	GLU
1	A	325	SER
1	A	411	GLU
1	B	3	LYS
1	B	166	GLU
1	B	325	SER
1	C	101	GLY
1	C	166	GLU
1	C	314	GLN
1	C	369	ASP
1	D	161	PRO
1	D	163	ASP
1	D	371	ASN
1	E	166	GLU
1	E	361	LYS
1	E	369	ASP
1	E	411	GLU
1	F	84	ALA
1	F	101	GLY
1	F	161	PRO
1	F	166	GLU
1	F	190	VAL
1	F	316	ARG
1	G	3	LYS
1	G	63	ILE
1	G	78	VAL
1	G	156	TYR
1	G	166	GLU
1	G	325	SER
1	G	369	ASP
1	G	411	GLU
1	G	441	MET
1	H	125	SER
1	H	167	ASN
1	H	190	VAL
1	I	100	ASP
1	I	158	ASP
1	I	201	TYR
1	I	325	SER
1	J	3	LYS
1	J	161	PRO

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Mol	Chain	Res	Type
1	J	163	ASP
1	J	325	SER
1	J	368	ILE
1	K	156	TYR
1	K	161	PRO
1	K	162	THR
1	K	166	GLU
1	K	312	SER
1	L	82	TRP
1	L	167	ASN
1	L	386	VAL
1	A	101	GLY
1	A	157	PHE
1	A	164	LEU
1	A	201	TYR
1	A	204	ALA
1	A	314	GLN
1	A	410	GLY
1	B	256	ASN
1	B	292	THR
1	C	161	PRO
1	C	163	ASP
1	C	283	THR
1	C	365	PRO
1	D	85	GLU
1	D	204	ALA
1	D	412	HIS
1	E	161	PRO
1	E	163	ASP
1	E	170	ARG
1	E	325	SER
1	E	329	SER
1	F	67	ASP
1	F	157	PHE
1	F	260	ASP
1	G	58	GLU
1	G	157	PHE
1	G	161	PRO
1	G	256	ASN
1	G	257	ALA
1	G	268	SER
1	G	361	LYS

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Mol	Chain	Res	Type
1	H	163	ASP
1	H	260	ASP
1	H	325	SER
1	H	371	ASN
1	I	3	LYS
1	I	157	PHE
1	I	161	PRO
1	I	166	GLU
1	I	167	ASN
1	I	260	ASP
1	I	283	THR
1	I	361	LYS
1	I	372	ILE
1	I	376	SER
1	I	441	MET
1	J	81	PRO
1	J	190	VAL
1	J	268	SER
1	J	291	PRO
1	J	292	THR
1	K	85	GLU
1	K	368	ILE
1	L	74	LEU
1	L	83	THR
1	L	101	GLY
1	L	157	PHE
1	L	166	GLU
1	L	204	ALA
1	L	325	SER
1	L	368	ILE
1	B	121	ASP
1	B	124	PHE
1	B	161	PRO
1	B	204	ALA
1	B	257	ALA
1	B	291	PRO
1	C	3	LYS
1	C	86	LYS
1	C	204	ALA
1	C	312	SER
1	C	348	SER
1	D	158	ASP

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Mol	Chain	Res	Type
1	D	360	ASN
1	D	361	LYS
1	E	143	LYS
1	E	148	LEU
1	E	224	LYS
1	F	310	ALA
1	F	361	LYS
1	G	329	SER
1	H	3	LYS
1	H	6	ARG
1	H	101	GLY
1	H	161	PRO
1	H	261	GLU
1	J	55	SER
1	J	164	LEU
1	J	207	SER
1	J	283	THR
1	J	376	SER
1	K	148	LEU
1	K	169	ARG
1	K	313	ALA
1	L	13	VAL
1	L	159	LEU
1	L	163	ASP
1	L	220	THR
1	L	371	ASN
1	B	39	VAL
1	C	6	ARG
1	C	139	LYS
1	C	160	ALA
1	C	261	GLU
1	C	325	SER
1	C	368	ILE
1	D	74	LEU
1	D	166	GLU
1	D	315	ASN
1	D	370	ARG
1	D	411	GLU
1	E	57	ILE
1	E	157	PHE
1	E	200	LYS
1	E	202	ALA

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Mol	Chain	Res	Type
1	E	262	ASN
1	E	268	SER
1	E	291	PRO
1	E	412	HIS
1	F	58	GLU
1	F	348	SER
1	F	412	HIS
1	G	85	GLU
1	G	163	ASP
1	G	224	LYS
1	G	238	GLY
1	H	100	ASP
1	H	160	ALA
1	H	224	LYS
1	H	372	ILE
1	H	375	MET
1	I	17	ASN
1	I	268	SER
1	I	329	SER
1	I	419	GLU
1	J	181	PHE
1	J	208	CYS
1	J	361	LYS
1	K	74	LEU
1	K	99	PRO
1	L	148	LEU
1	L	291	PRO
1	L	412	HIS
1	A	169	ARG
1	B	282	ALA
1	C	220	THR
1	D	169	ARG
1	E	144	GLY
1	E	376	SER
1	F	3	LYS
1	F	201	TYR
1	G	101	GLY
1	G	204	ALA
1	H	58	GLU
1	H	283	THR
1	I	162	THR
1	I	204	ALA

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Mol	Chain	Res	Type
1	J	85	GLU
1	J	261	GLU
1	J	329	SER
1	K	75	ASN
1	K	83	THR
1	K	373	TYR
1	K	376	SER
1	K	411	GLU
1	L	29	LEU
1	L	190	VAL
1	L	276	ALA
1	L	369	ASP
1	A	17	ASN
1	B	283	THR
1	B	368	ILE
1	C	157	PHE
1	C	291	PRO
1	C	349	VAL
1	C	370	ARG
1	F	220	THR
1	J	58	GLU
1	L	324	ALA
1	B	101	GLY
1	F	386	VAL
1	C	337	VAL
1	E	101	GLY
1	I	368	ILE
1	K	367	PRO
1	K	374	VAL
1	C	190	VAL
1	F	160	ALA
1	K	160	ALA
1	K	337	VAL
1	J	101	GLY
1	D	385	ILE
1	E	372	ILE
1	I	160	ALA
1	K	190	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	380/382 (100%)	341 (90%)	39 (10%)	9	32
1	B	380/382 (100%)	353 (93%)	27 (7%)	18	54
1	C	379/382 (99%)	345 (91%)	34 (9%)	12	41
1	D	380/382 (100%)	347 (91%)	33 (9%)	13	44
1	E	379/382 (99%)	340 (90%)	39 (10%)	9	32
1	F	378/382 (99%)	338 (89%)	40 (11%)	8	31
1	G	379/382 (99%)	340 (90%)	39 (10%)	9	32
1	H	378/382 (99%)	344 (91%)	34 (9%)	12	41
1	I	377/382 (99%)	334 (89%)	43 (11%)	7	28
1	J	379/382 (99%)	338 (89%)	41 (11%)	8	30
1	K	379/382 (99%)	338 (89%)	41 (11%)	8	30
1	L	380/382 (100%)	347 (91%)	33 (9%)	13	44
All	All	4548/4584 (99%)	4105 (90%)	443 (10%)	10	36

All (443) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	34	ASN
1	A	36	GLU
1	A	37	ILE
1	A	70	LEU
1	A	78	VAL
1	A	85	GLU
1	A	91	ARG
1	A	94	CYS
1	A	102	THR
1	A	105	GLU
1	A	112	LEU
1	A	129	LEU
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	161	PRO
1	A	164	LEU
1	A	167	ASN
1	A	169	ARG
1	A	186	SER
1	A	206	ARG
1	A	252	LYS
1	A	262	ASN
1	A	273	HIS
1	A	285	PHE
1	A	294	ASN
1	A	308	TYR
1	A	314	GLN
1	A	347	LEU
1	A	359	LYS
1	A	363	GLU
1	A	369	ASP
1	A	371	ASN
1	A	373	TYR
1	A	375	MET
1	A	380	ARG
1	A	401	SER
1	A	431	GLN
1	A	441	MET
1	B	7	GLU
1	B	12	LEU
1	B	32	ILE
1	B	49	LYS
1	B	67	ASP
1	B	82	TRP
1	B	91	ARG
1	B	122	LEU
1	B	124	PHE
1	B	129	LEU
1	B	153	LYS
1	B	186	SER
1	B	201	TYR
1	B	236	LEU
1	B	285	PHE
1	B	286	THR
1	B	294	ASN

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Mol	Chain	Res	Type
1	B	331	ARG
1	B	347	LEU
1	B	349	VAL
1	B	369	ASP
1	B	370	ARG
1	B	371	ASN
1	B	372	ILE
1	B	380	ARG
1	B	387	ASP
1	B	429	ARG
1	C	34	ASN
1	C	36	GLU
1	C	41	GLN
1	C	48	ASN
1	C	49	LYS
1	C	61	VAL
1	C	73	ASP
1	C	75	ASN
1	C	91	ARG
1	C	105	GLU
1	C	112	LEU
1	C	120	GLU
1	C	129	LEU
1	C	153	LYS
1	C	161	PRO
1	C	163	ASP
1	C	183	ILE
1	C	194	GLN
1	C	201	TYR
1	C	206	ARG
1	C	252	LYS
1	C	264	ASP
1	C	286	THR
1	C	297	LYS
1	C	308	TYR
1	C	312	SER
1	C	347	LEU
1	C	371	ASN
1	C	373	TYR
1	C	382	GLU
1	C	409	LEU
1	C	429	ARG

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Mol	Chain	Res	Type
1	C	431	GLN
1	C	441	MET
1	D	5	THR
1	D	6	ARG
1	D	28	ILE
1	D	34	ASN
1	D	35	VAL
1	D	40	SER
1	D	70	LEU
1	D	82	TRP
1	D	91	ARG
1	D	94	CYS
1	D	112	LEU
1	D	129	LEU
1	D	145	GLU
1	D	151	ASN
1	D	159	LEU
1	D	161	PRO
1	D	163	ASP
1	D	164	LEU
1	D	177	GLU
1	D	183	ILE
1	D	207	SER
1	D	295	SER
1	D	308	TYR
1	D	314	GLN
1	D	319	LEU
1	D	326	ARG
1	D	328	ILE
1	D	331	ARG
1	D	338	ASP
1	D	383	ASN
1	D	387	ASP
1	D	394	GLU
1	D	443	GLN
1	E	5	THR
1	E	7	GLU
1	E	8	ASP
1	E	11	LYS
1	E	16	GLU
1	E	51	MET
1	E	61	VAL

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Mol	Chain	Res	Type
1	E	62	ARG
1	E	82	TRP
1	E	91	ARG
1	E	105	GLU
1	E	109	ARG
1	E	110	ASN
1	E	126	ASP
1	E	129	LEU
1	E	148	LEU
1	E	149	GLU
1	E	161	PRO
1	E	164	LEU
1	E	183	ILE
1	E	201	TYR
1	E	223	ARG
1	E	230	THR
1	E	262	ASN
1	E	264	ASP
1	E	273	HIS
1	E	285	PHE
1	E	289	THR
1	E	294	ASN
1	E	326	ARG
1	E	328	ILE
1	E	349	VAL
1	E	369	ASP
1	E	370	ARG
1	E	373	TYR
1	E	381	MET
1	E	391	THR
1	E	412	HIS
1	E	436	GLU
1	F	14	LYS
1	F	28	ILE
1	F	29	LEU
1	F	31	THR
1	F	34	ASN
1	F	36	GLU
1	F	40	SER
1	F	41	GLN
1	F	61	VAL
1	F	70	LEU

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Mol	Chain	Res	Type
1	F	82	TRP
1	F	91	ARG
1	F	98	ASN
1	F	100	ASP
1	F	105	GLU
1	F	112	LEU
1	F	126	ASP
1	F	129	LEU
1	F	148	LEU
1	F	150	LEU
1	F	159	LEU
1	F	161	PRO
1	F	189	GLU
1	F	201	TYR
1	F	206	ARG
1	F	219	LYS
1	F	236	LEU
1	F	285	PHE
1	F	308	TYR
1	F	328	ILE
1	F	342	ASN
1	F	349	VAL
1	F	351	LEU
1	F	370	ARG
1	F	378	GLU
1	F	387	ASP
1	F	398	GLU
1	F	423	ILE
1	F	437	ARG
1	F	439	GLN
1	G	6	ARG
1	G	25	PHE
1	G	34	ASN
1	G	41	GLN
1	G	63	ILE
1	G	64	GLU
1	G	70	LEU
1	G	91	ARG
1	G	95	ASP
1	G	117	LYS
1	G	122	LEU
1	G	152	ASP

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Mol	Chain	Res	Type
1	G	156	TYR
1	G	158	ASP
1	G	161	PRO
1	G	168	CYS
1	G	169	ARG
1	G	177	GLU
1	G	183	ILE
1	G	198	ASP
1	G	199	PHE
1	G	201	TYR
1	G	216	LEU
1	G	223	ARG
1	G	250	LEU
1	G	251	PHE
1	G	258	PHE
1	G	285	PHE
1	G	316	ARG
1	G	331	ARG
1	G	335	ARG
1	G	342	ASN
1	G	350	LEU
1	G	351	LEU
1	G	370	ARG
1	G	373	TYR
1	G	385	ILE
1	G	409	LEU
1	G	442	SER
1	H	7	GLU
1	H	19	LYS
1	H	21	ILE
1	H	34	ASN
1	H	74	LEU
1	H	82	TRP
1	H	91	ARG
1	H	94	CYS
1	H	105	GLU
1	H	112	LEU
1	H	126	ASP
1	H	143	LYS
1	H	158	ASP
1	H	159	LEU
1	H	161	PRO

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Mol	Chain	Res	Type
1	H	166	GLU
1	H	171	ASP
1	H	201	TYR
1	H	223	ARG
1	H	240	ASN
1	H	264	ASP
1	H	273	HIS
1	H	321	ARG
1	H	328	ILE
1	H	351	LEU
1	H	359	LYS
1	H	362	LEU
1	H	370	ARG
1	H	372	ILE
1	H	378	GLU
1	H	381	MET
1	H	387	ASP
1	H	401	SER
1	H	419	GLU
1	I	7	GLU
1	I	8	ASP
1	I	28	ILE
1	I	34	ASN
1	I	40	SER
1	I	58	GLU
1	I	62	ARG
1	I	70	LEU
1	I	86	LYS
1	I	91	ARG
1	I	94	CYS
1	I	100	ASP
1	I	109	ARG
1	I	110	ASN
1	I	112	LEU
1	I	114	ARG
1	I	129	LEU
1	I	158	ASP
1	I	159	LEU
1	I	161	PRO
1	I	164	LEU
1	I	169	ARG
1	I	174	LEU

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Mol	Chain	Res	Type
1	I	199	PHE
1	I	201	TYR
1	I	206	ARG
1	I	207	SER
1	I	216	LEU
1	I	239	VAL
1	I	248	LEU
1	I	261	GLU
1	I	285	PHE
1	I	328	ILE
1	I	331	ARG
1	I	349	VAL
1	I	351	LEU
1	I	370	ARG
1	I	372	ILE
1	I	373	TYR
1	I	391	THR
1	I	409	LEU
1	I	434	PRO
1	I	441	MET
1	J	5	THR
1	J	12	LEU
1	J	34	ASN
1	J	36	GLU
1	J	37	ILE
1	J	49	LYS
1	J	66	SER
1	J	85	GLU
1	J	91	ARG
1	J	94	CYS
1	J	112	LEU
1	J	117	LYS
1	J	125	SER
1	J	126	ASP
1	J	129	LEU
1	J	142	GLU
1	J	161	PRO
1	J	167	ASN
1	J	169	ARG
1	J	200	LYS
1	J	201	TYR
1	J	206	ARG

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Mol	Chain	Res	Type
1	J	212	GLN
1	J	216	LEU
1	J	223	ARG
1	J	250	LEU
1	J	262	ASN
1	J	265	LEU
1	J	270	THR
1	J	272	LYS
1	J	285	PHE
1	J	286	THR
1	J	294	ASN
1	J	308	TYR
1	J	326	ARG
1	J	331	ARG
1	J	347	LEU
1	J	349	VAL
1	J	363	GLU
1	J	373	TYR
1	J	387	ASP
1	K	7	GLU
1	K	24	GLN
1	K	34	ASN
1	K	36	GLU
1	K	65	GLU
1	K	91	ARG
1	K	94	CYS
1	K	109	ARG
1	K	142	GLU
1	K	153	LYS
1	K	156	TYR
1	K	159	LEU
1	K	166	GLU
1	K	169	ARG
1	K	174	LEU
1	K	197	ILE
1	K	199	PHE
1	K	223	ARG
1	K	239	VAL
1	K	252	LYS
1	K	270	THR
1	K	273	HIS
1	K	283	THR

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Mol	Chain	Res	Type
1	K	285	PHE
1	K	298	ARG
1	K	315	ASN
1	K	316	ARG
1	K	326	ARG
1	K	331	ARG
1	K	337	VAL
1	K	360	ASN
1	K	363	GLU
1	K	373	TYR
1	K	374	VAL
1	K	375	MET
1	K	382	GLU
1	K	391	THR
1	K	411	GLU
1	K	426	ASP
1	K	439	GLN
1	K	442	SER
1	L	11	LYS
1	L	14	LYS
1	L	21	ILE
1	L	34	ASN
1	L	40	SER
1	L	75	ASN
1	L	91	ARG
1	L	102	THR
1	L	105	GLU
1	L	109	ARG
1	L	122	LEU
1	L	129	LEU
1	L	149	GLU
1	L	162	THR
1	L	164	LEU
1	L	167	ASN
1	L	174	LEU
1	L	183	ILE
1	L	189	GLU
1	L	194	GLN
1	L	201	TYR
1	L	236	LEU
1	L	262	ASN
1	L	285	PHE

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Mol	Chain	Res	Type
1	L	321	ARG
1	L	325	SER
1	L	349	VAL
1	L	351	LEU
1	L	363	GLU
1	L	372	ILE
1	L	378	GLU
1	L	402	ASN
1	L	443	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (170) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	98	ASN
1	A	128	ASN
1	A	167	ASN
1	A	194	GLN
1	A	253	ASN
1	A	281	HIS
1	A	315	ASN
1	A	383	ASN
1	A	431	GLN
1	A	443	GLN
1	B	41	GLN
1	B	128	ASN
1	B	167	ASN
1	B	194	GLN
1	B	225	HIS
1	B	245	HIS
1	B	262	ASN
1	B	266	GLN
1	B	281	HIS
1	B	290	ASN
1	B	294	ASN
1	B	315	ASN
1	B	342	ASN
1	B	371	ASN
1	B	383	ASN
1	B	431	GLN
1	C	17	ASN
1	C	24	GLN

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Mol	Chain	Res	Type
1	C	34	ASN
1	C	98	ASN
1	C	110	ASN
1	C	225	HIS
1	C	228	HIS
1	C	245	HIS
1	C	266	GLN
1	C	290	ASN
1	C	294	ASN
1	C	314	GLN
1	C	416	HIS
1	C	431	GLN
1	C	439	GLN
1	C	443	GLN
1	D	110	ASN
1	D	111	ASN
1	D	128	ASN
1	D	187	HIS
1	D	194	GLN
1	D	225	HIS
1	D	228	HIS
1	D	262	ASN
1	D	273	HIS
1	D	281	HIS
1	D	290	ASN
1	D	314	GLN
1	D	383	ASN
1	D	433	HIS
1	D	443	GLN
1	E	41	GLN
1	E	110	ASN
1	E	151	ASN
1	E	187	HIS
1	E	195	HIS
1	E	225	HIS
1	E	228	HIS
1	E	247	ASN
1	E	262	ASN
1	E	281	HIS
1	E	290	ASN
1	E	314	GLN
1	E	342	ASN

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Mol	Chain	Res	Type
1	E	431	GLN
1	F	17	ASN
1	F	24	GLN
1	F	41	GLN
1	F	98	ASN
1	F	151	ASN
1	F	167	ASN
1	F	187	HIS
1	F	194	GLN
1	F	225	HIS
1	F	228	HIS
1	F	266	GLN
1	F	290	ASN
1	F	314	GLN
1	F	360	ASN
1	F	371	ASN
1	F	383	ASN
1	F	439	GLN
1	F	443	GLN
1	G	98	ASN
1	G	151	ASN
1	G	167	ASN
1	G	194	GLN
1	G	225	HIS
1	G	228	HIS
1	G	247	ASN
1	G	253	ASN
1	G	266	GLN
1	G	281	HIS
1	G	314	GLN
1	G	342	ASN
1	G	360	ASN
1	G	383	ASN
1	G	431	GLN
1	G	443	GLN
1	H	17	ASN
1	H	41	GLN
1	H	98	ASN
1	H	128	ASN
1	H	194	GLN
1	H	228	HIS
1	H	240	ASN

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Mol	Chain	Res	Type
1	H	245	HIS
1	H	281	HIS
1	H	290	ASN
1	H	315	ASN
1	H	383	ASN
1	H	431	GLN
1	I	110	ASN
1	I	128	ASN
1	I	151	ASN
1	I	194	GLN
1	I	240	ASN
1	I	253	ASN
1	I	266	GLN
1	I	290	ASN
1	I	416	HIS
1	I	431	GLN
1	I	433	HIS
1	I	439	GLN
1	J	17	ASN
1	J	34	ASN
1	J	98	ASN
1	J	110	ASN
1	J	111	ASN
1	J	128	ASN
1	J	194	GLN
1	J	225	HIS
1	J	245	HIS
1	J	281	HIS
1	J	371	ASN
1	K	17	ASN
1	K	98	ASN
1	K	128	ASN
1	K	194	GLN
1	K	212	GLN
1	K	245	HIS
1	K	262	ASN
1	K	281	HIS
1	K	290	ASN
1	K	315	ASN
1	K	360	ASN
1	K	383	ASN
1	K	431	GLN

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Mol	Chain	Res	Type
1	K	443	GLN
1	L	24	GLN
1	L	98	ASN
1	L	110	ASN
1	L	111	ASN
1	L	128	ASN
1	L	151	ASN
1	L	167	ASN
1	L	194	GLN
1	L	228	HIS
1	L	266	GLN
1	L	281	HIS
1	L	290	ASN
1	L	402	ASN
1	L	431	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 25 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	D	504	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	E	503	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	F	503	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	H	501	-	4,4,4	0.17	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	501	-	-	0/0/0/0	0/0/0/0
3	SO4	D	504	-	-	0/0/0/0	0/0/0/0
3	SO4	E	503	-	-	0/0/0/0	0/0/0/0
3	SO4	F	503	-	-	0/0/0/0	0/0/0/0
3	SO4	H	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	439/443 (99%)	-0.33	5 (1%)	82 66	38, 61, 115, 125	0
1	B	439/443 (99%)	-0.31	7 (1%)	74 55	34, 61, 114, 124	0
1	C	438/443 (98%)	-0.35	6 (1%)	78 60	31, 61, 114, 126	0
1	D	439/443 (99%)	-0.30	9 (2%)	67 44	38, 63, 116, 130	0
1	E	438/443 (98%)	-0.34	6 (1%)	78 60	39, 64, 118, 126	0
1	F	437/443 (98%)	-0.36	7 (1%)	74 55	40, 60, 114, 130	0
1	G	438/443 (98%)	-0.40	5 (1%)	82 66	35, 60, 116, 124	0
1	H	437/443 (98%)	-0.38	3 (0%)	89 78	35, 60, 115, 127	0
1	I	436/443 (98%)	-0.34	6 (1%)	78 60	39, 62, 118, 132	0
1	J	438/443 (98%)	-0.32	5 (1%)	82 66	40, 63, 118, 126	0
1	K	438/443 (98%)	-0.37	4 (0%)	85 72	39, 63, 116, 127	0
1	L	440/443 (99%)	-0.34	6 (1%)	78 60	32, 59, 116, 126	0
All	All	5257/5316 (98%)	-0.35	69 (1%)	79 62	31, 62, 116, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	307	CYS	7.7
1	J	306	PRO	7.5
1	C	307	CYS	6.2
1	I	2	ALA	5.4
1	A	306	PRO	5.2
1	H	312	SER	5.1
1	C	312	SER	5.0
1	H	307	CYS	4.8
1	H	369	ASP	4.4
1	F	312	SER	4.2
1	D	315	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	312	SER	4.1
1	B	313	ALA	4.0
1	B	312	SER	3.8
1	F	307	CYS	3.7
1	K	371	ASN	3.7
1	D	314	GLN	3.5
1	D	385	ILE	3.5
1	L	306	PRO	3.4
1	A	307	CYS	3.2
1	D	306	PRO	3.2
1	F	315	ASN	3.2
1	E	311	TRP	3.2
1	B	307	CYS	3.2
1	G	307	CYS	3.1
1	J	371	ASN	3.1
1	K	365	PRO	3.0
1	J	312	SER	3.0
1	I	315	ASN	2.9
1	C	315	ASN	2.9
1	C	311	TRP	2.9
1	F	369	ASP	2.8
1	A	312	SER	2.8
1	L	307	CYS	2.8
1	F	368	ILE	2.7
1	I	312	SER	2.7
1	E	369	ASP	2.7
1	L	315	ASN	2.6
1	L	365	PRO	2.5
1	E	367	PRO	2.4
1	A	311	TRP	2.4
1	C	313	ALA	2.4
1	B	306	PRO	2.4
1	E	306	PRO	2.3
1	B	61	VAL	2.3
1	F	370	ARG	2.3
1	L	314	GLN	2.3
1	K	306	PRO	2.3
1	D	316	ARG	2.2
1	D	380	ARG	2.2
1	C	372	ILE	2.2
1	J	61	VAL	2.2
1	I	370	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	366	ALA	2.2
1	K	311	TRP	2.1
1	B	314	GLN	2.1
1	G	314	GLN	2.1
1	I	313	ALA	2.1
1	A	301	PRO	2.1
1	E	307	CYS	2.1
1	I	372	ILE	2.1
1	D	309	VAL	2.1
1	G	312	SER	2.1
1	B	309	VAL	2.1
1	D	372	ILE	2.0
1	E	386	VAL	2.0
1	D	307	CYS	2.0
1	G	315	ASN	2.0
1	G	2	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	D	501	5/5	0.76	0.33	3.07	131,131,132,132	0
3	SO4	F	503	5/5	0.79	0.24	2.92	181,181,182,182	0
2	MG	C	501	1/1	0.96	0.22	2.15	27,27,27,27	0
2	MG	H	502	1/1	0.96	0.20	1.90	16,16,16,16	0
2	MG	L	501	1/1	0.88	0.22	1.88	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	E	503	5/5	0.81	0.19	1.72	158,159,159,159	0
2	MG	B	501	1/1	0.99	0.20	1.14	21,21,21,21	0
3	SO4	H	501	5/5	0.84	0.21	1.03	169,169,169,169	0
2	MG	I	501	1/1	0.95	0.20	0.91	18,18,18,18	0
2	MG	H	503	1/1	0.97	0.18	0.81	35,35,35,35	0
2	MG	K	501	1/1	0.96	0.20	0.66	13,13,13,13	0
2	MG	K	502	1/1	0.96	0.19	0.29	39,39,39,39	0
2	MG	J	501	1/1	0.95	0.19	0.26	30,30,30,30	0
2	MG	F	501	1/1	0.88	0.19	0.01	32,32,32,32	0
2	MG	D	503	1/1	0.94	0.18	-0.38	32,32,32,32	0
2	MG	L	502	1/1	0.97	0.17	-0.83	29,29,29,29	0
2	MG	I	502	1/1	0.95	0.13	-1.47	39,39,39,39	0
2	MG	E	502	1/1	0.93	0.14	-1.56	39,39,39,39	0
2	MG	A	501	1/1	0.96	0.15	-1.80	10,10,10,10	0
2	MG	F	502	1/1	0.92	0.14	-5.86	22,22,22,22	0
2	MG	B	503	1/1	0.51	0.39	-	92,92,92,92	0
2	MG	E	501	1/1	0.95	0.22	-	22,22,22,22	0
2	MG	G	501	1/1	0.97	0.17	-	24,24,24,24	0
2	MG	C	502	1/1	0.98	0.27	-	34,34,34,34	0
2	MG	B	502	1/1	0.96	0.19	-	23,23,23,23	0
2	MG	A	502	1/1	0.97	0.15	-	19,19,19,19	0
2	MG	D	502	1/1	1.00	0.16	-	7,7,7,7	0
3	SO4	D	504	5/5	0.90	0.13	-	154,154,154,155	0
2	MG	J	502	1/1	0.98	0.34	-	27,27,27,27	0
2	MG	G	502	1/1	0.97	0.22	-	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.