Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:37 AM GMT

PDB ID	:	2HOD
Title	:	Crystal Structure of Fragment D from Human Fibrinogen Complexed with Gly-hydroxyPro-Arg-Pro-amide
Authors	:	Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.
Deposited on	:	2006-07-14
Resolution	:	2.90 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

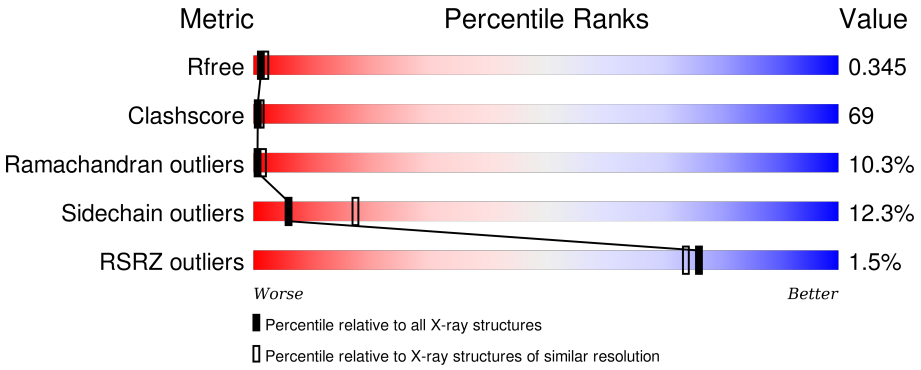
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	87	11% 48% 24% • 15%
1	D	87	25% 46% 10% 18%
1	G	87	2% 15% 53% 16% • 15%
1	J	87	29% 47% 15% 9%
2	B	328	2% 20% 53% 18% • 6%

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Mol	Chain	Length	Quality of chain
2	E	328	32% 50% 11% 7%
2	H	328	% 21% 54% 17% 6%
2	K	328	32% 50% 11% 7%
3	C	323	3% 13% 60% 20% 6%
3	F	323	% 27% 55% 11% 7%
3	I	323	4% 16% 56% 21% 6%
3	L	323	% 28% 55% 10% 7%
4	M	5	20% 60% 20%
4	N	5	60% 20% 20%
4	O	5	20% 60% 20%
4	P	5	40% 60%
4	Q	5	20% 80%
4	R	5	40% 40% 20%
4	S	5	40% 60%
4	T	5	40% 60%

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
4	HYP	S	2	-	-	X	-
7	CA	E	2	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22278 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	71	Total	C	N	O	S	0	0	0
			584	361	112	108	3			
1	G	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	J	79	Total	C	N	O	S	0	0	0
			652	402	126	121	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	E	304	Total	C	N	O	S	0	0	0
			2434	1514	430	468	22			
2	H	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	K	305	Total	C	N	O	S	0	0	0
			2442	1520	431	469	22			

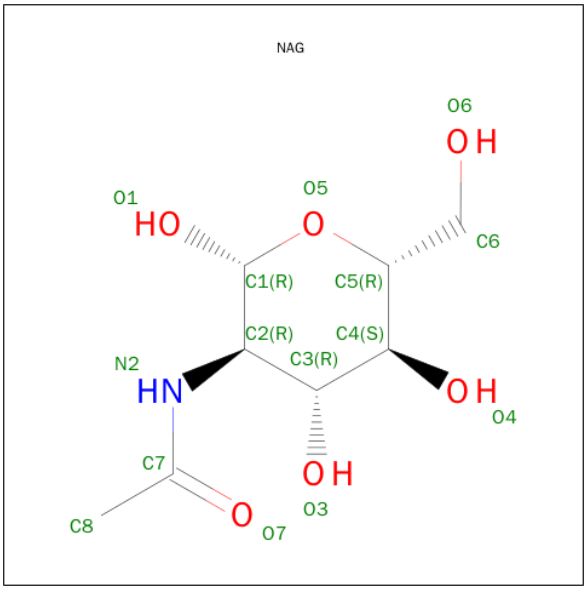
- Molecule 3 is a protein called Fibrinogen, gamma polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2446	1552	410	472	12			
3	F	300	Total	C	N	O	S	0	0	0
			2410	1529	405	464	12			
3	I	305	Total	C	N	O	S	0	0	0
			2446	1552	410	472	12			
3	L	300	Total	C	N	O	S	0	0	0
			2410	1529	405	464	12			

- Molecule 4 is a protein called Gly-hydroxyPro-Arg-Pro-amide peptide ligand.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	M	5	Total C N O 31 18 8 5	0	0	1
4	N	5	Total C N O 31 18 8 5	0	0	1
4	O	5	Total C N O 31 18 8 5	0	0	1
4	P	5	Total C N O 31 18 8 5	0	0	1
4	Q	5	Total C N O 31 18 8 5	0	0	1
4	R	5	Total C N O 31 18 8 5	0	0	1
4	S	5	Total C N O 31 18 8 5	0	0	1
4	T	5	Total C N O 31 18 8 5	0	0	1

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	H	1	Total C N O 14 8 1 5	0	0

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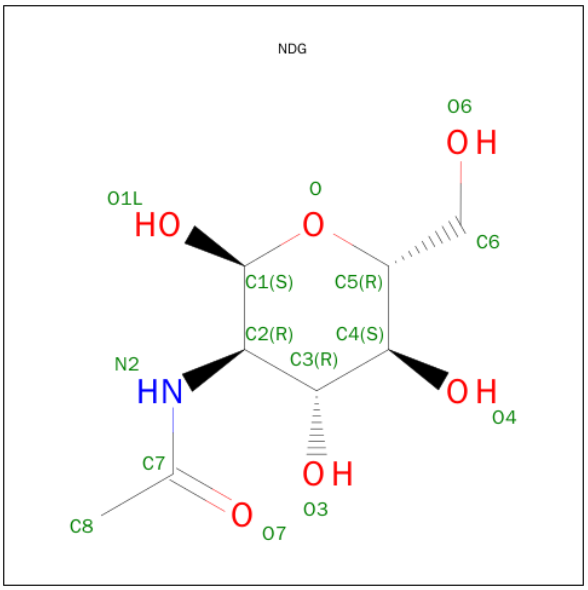
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	K	2	Total Ca 2 2	0	0
7	E	2	Total Ca 2 2	0	0
7	H	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	I	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	L	1	Total Ca 1 1	0	0

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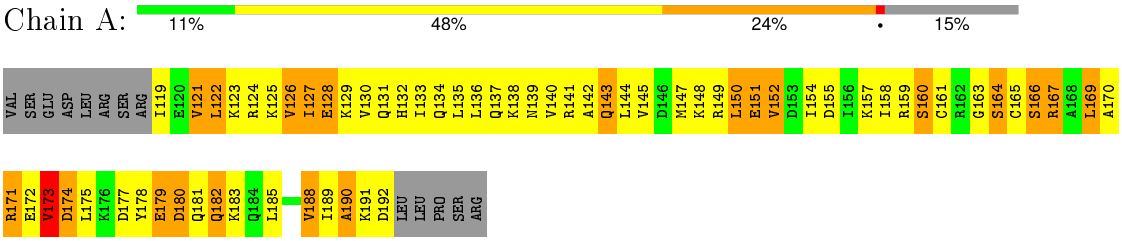
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	F	1	1	1	0	0

3 Residue-property plots (i)

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

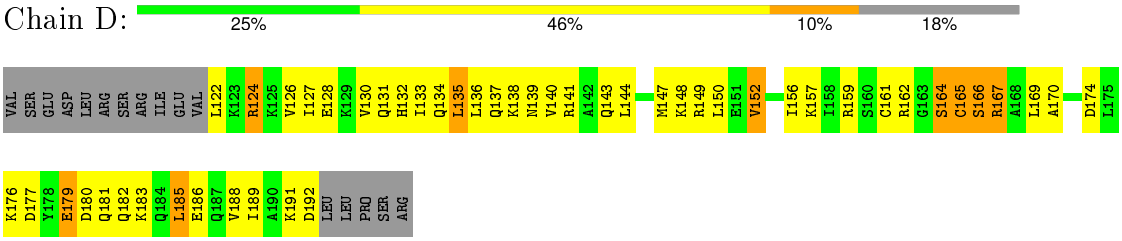
- Molecule 1: Fibrinogen alpha chain

Chain A:



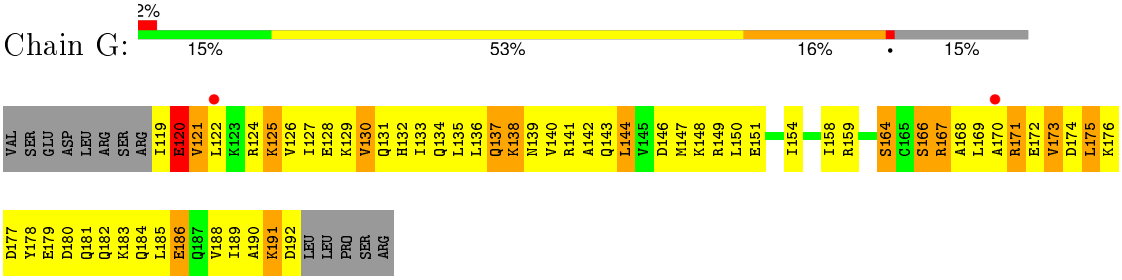
- Molecule 1: Fibrinogen alpha chain

Chain D:



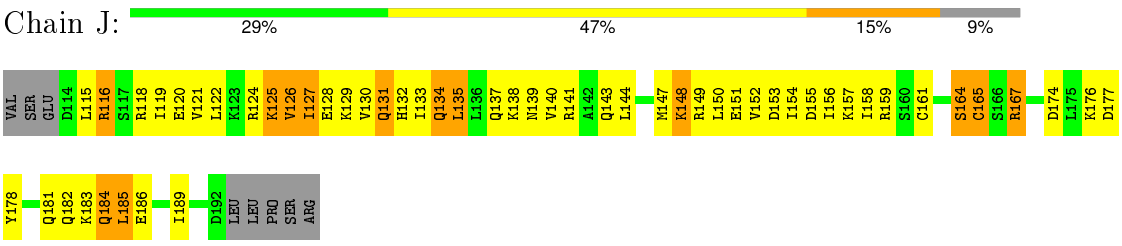
- Molecule 1: Fibrinogen alpha chain

Chain G:



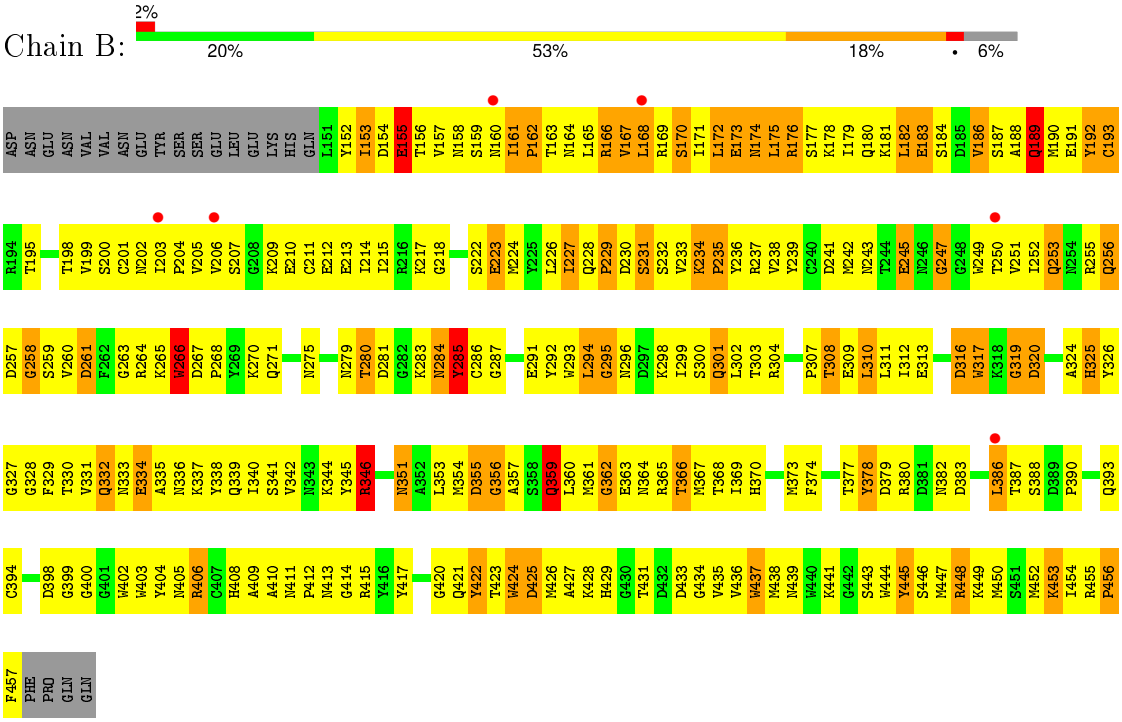
- Molecule 1: Fibrinogen alpha chain

Chain J:



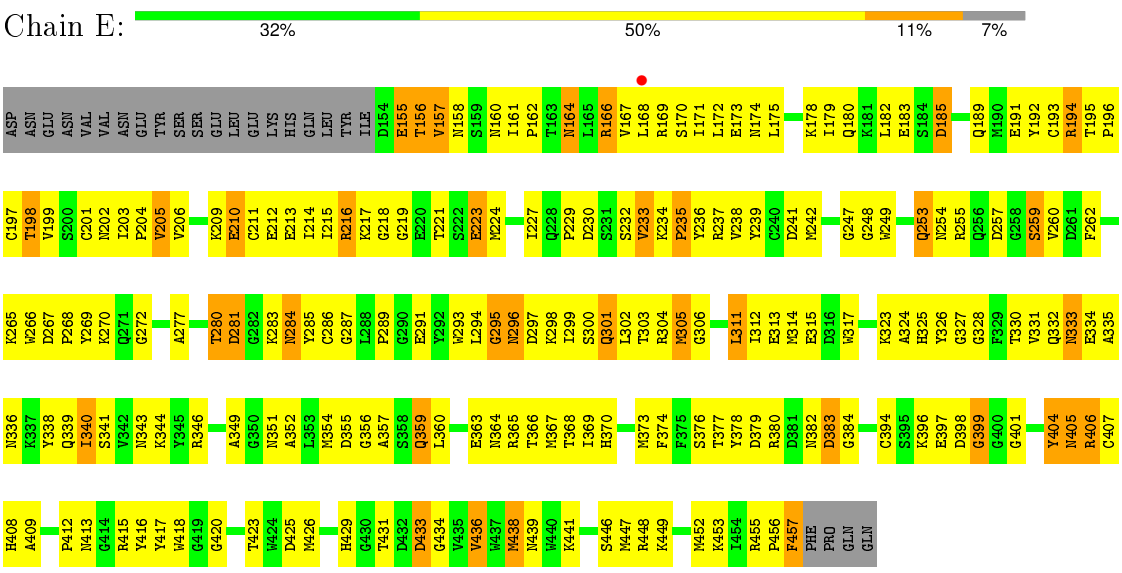
- Molecule 2: Fibrinogen beta chain

Chain B:



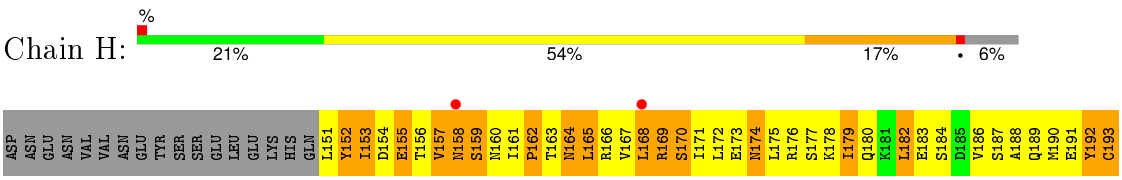
- Molecule 2: Fibrinogen beta chain

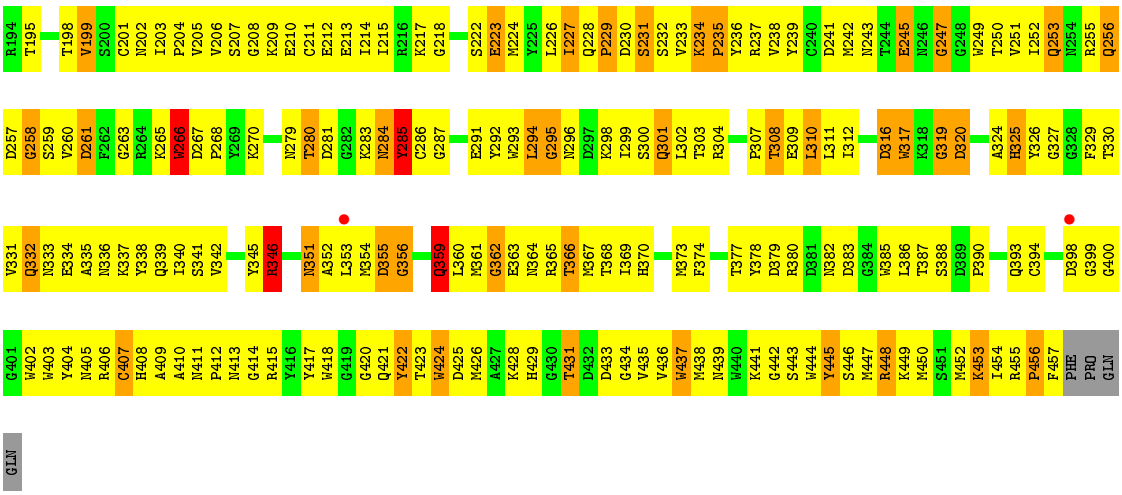
Chain E:



- Molecule 2: Fibrinogen beta chain

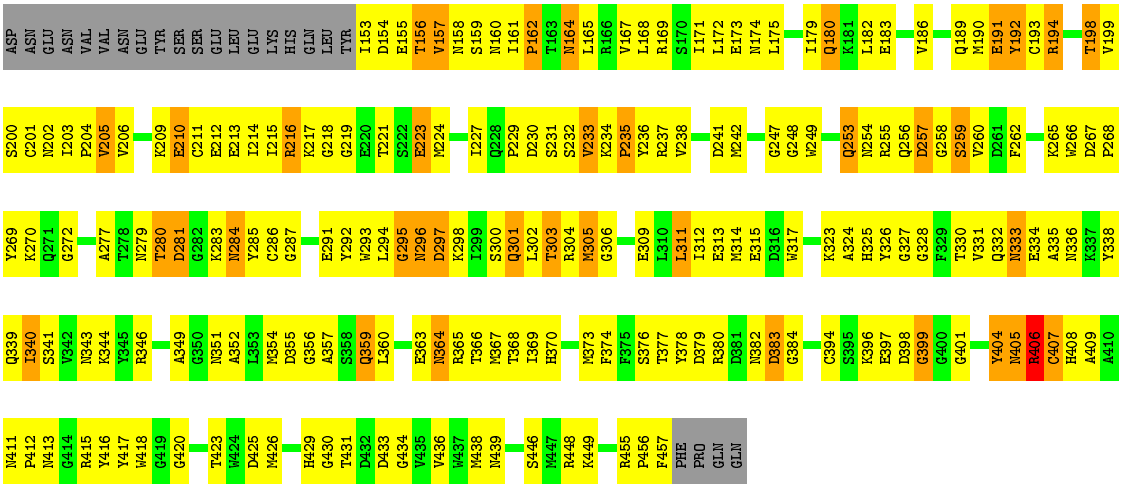
Chain H:





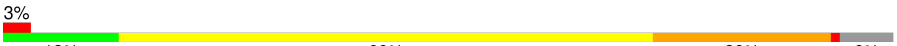
• Molecule 2: Fibrinogen beta chain

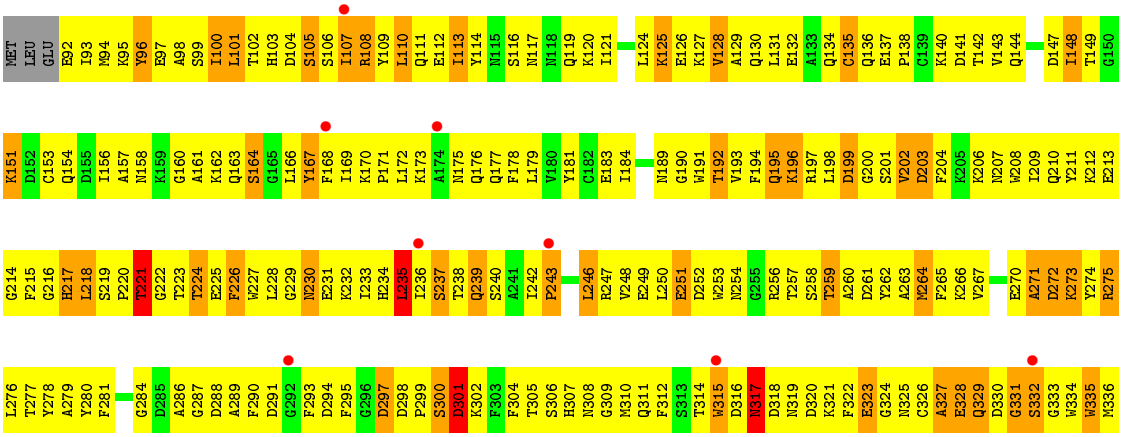
Chain K:

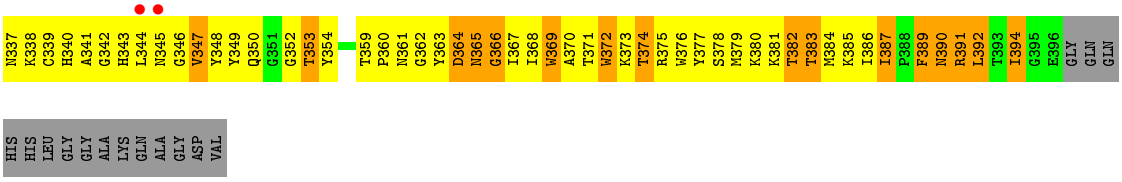


• Molecule 3: Fibrinogen, gamma polypeptide

Chain C:

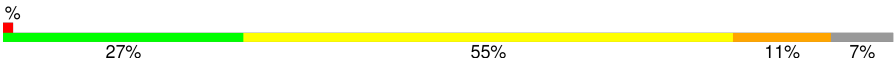


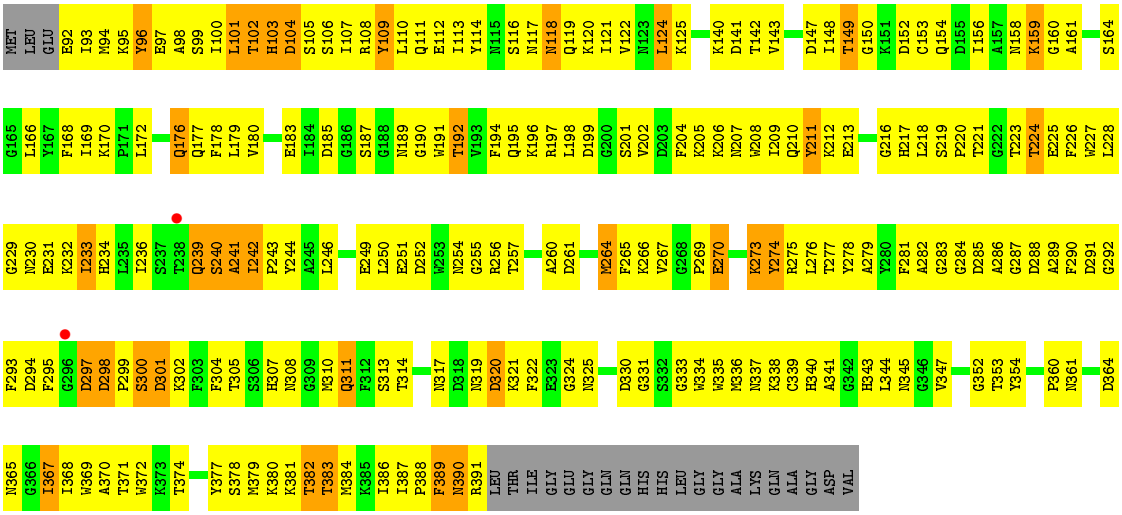




• Molecule 3: Fibrinogen, gamma polypeptide

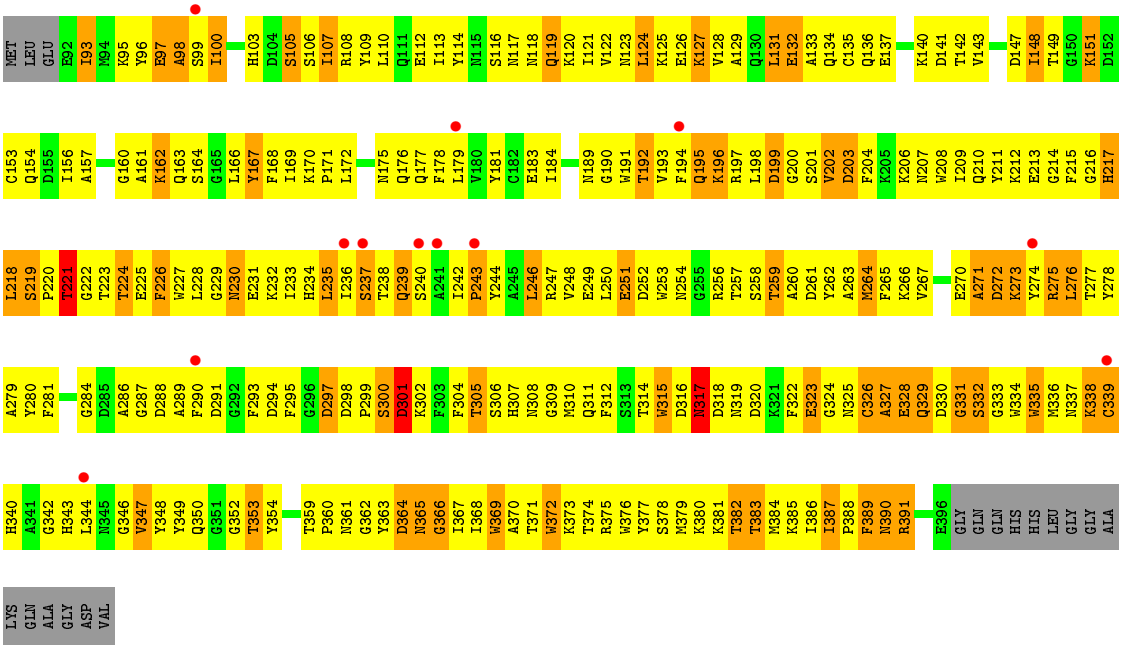
Chain F:





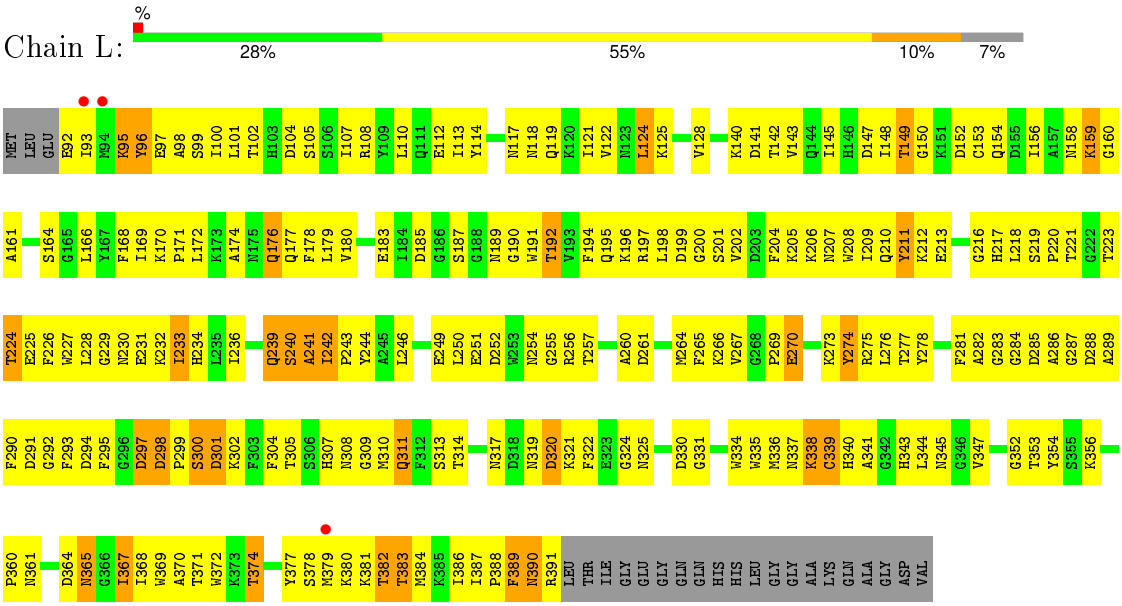
• Molecule 3: Fibrinogen, gamma polypeptide

Chain I:



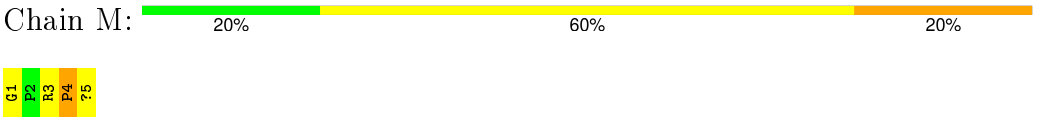
• Molecule 3: Fibrinogen, gamma polypeptide

Chain L:



• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain M:

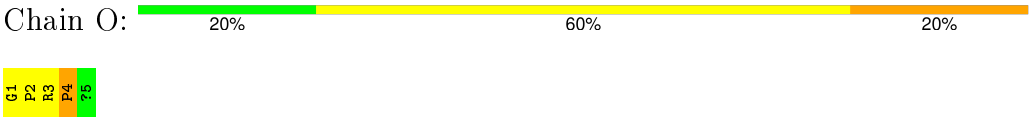


• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain N:

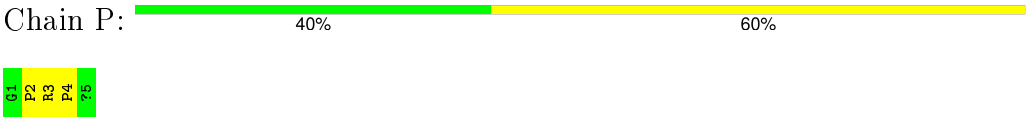
• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain O:



• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain P:

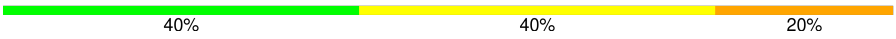


• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain Q:

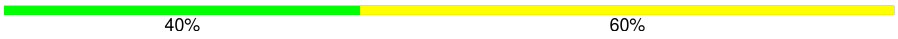
• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain R:



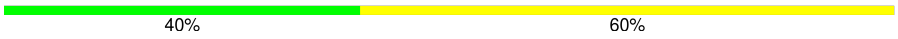
- Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain S:



- Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.65Å 47.07Å 431.46Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 49.22 – 2.79	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-2.90) 85.0 (49.22-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.347 0.265 , 0.345	Depositor DCC
R_{free} test set	3441 reflections (5.45%)	DCC
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 22.1	EDS
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 71011 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22278	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: HYP, CA, NAG, NDG, NH2

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	0.44	0/609	0.76	0/811
1	D	0.47	0/585	0.77	0/778
1	G	0.40	0/609	0.73	0/811
1	J	0.46	0/653	0.76	0/869
2	B	0.44	0/2523	0.77	3/3409 (0.1%)
2	E	0.51	0/2494	0.76	1/3369 (0.0%)
2	H	0.44	0/2523	0.78	3/3409 (0.1%)
2	K	0.52	0/2502	0.79	3/3380 (0.1%)
3	C	0.42	0/2512	0.70	0/3396
3	F	0.45	0/2476	0.72	1/3347 (0.0%)
3	I	0.43	0/2512	0.73	2/3396 (0.1%)
3	L	0.44	0/2476	0.74	3/3347 (0.1%)
4	M	0.66	0/21	0.75	0/25
4	N	0.84	0/21	0.71	0/25
4	O	0.71	0/21	0.56	0/25
4	P	0.51	0/21	0.65	0/25
4	Q	0.58	0/21	0.71	0/25
4	R	0.79	0/21	1.04	0/25
4	S	0.62	0/21	0.53	0/25
4	T	0.62	0/21	0.64	0/25
All	All	0.46	0/22642	0.75	16/30522 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	H	0	1
2	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	406	ARG	C-N-CA	6.48	137.89	121.70
2	H	399	GLY	N-CA-C	6.20	128.59	113.10
2	B	399	GLY	N-CA-C	6.07	128.26	113.10
2	H	437	TRP	N-CA-C	-6.05	94.67	111.00
2	B	437	TRP	N-CA-C	-5.72	95.56	111.00
3	L	338	LYS	N-CA-C	-5.70	95.61	111.00
3	L	274	TYR	N-CA-C	-5.69	95.63	111.00
3	F	274	TYR	N-CA-C	-5.60	95.87	111.00
2	K	406	ARG	CA-C-N	-5.33	105.48	117.20
3	I	338	LYS	C-N-CA	5.32	135.00	121.70
3	L	338	LYS	C-N-CA	5.30	134.95	121.70
3	I	338	LYS	CA-C-N	-5.30	105.55	117.20
2	B	346	ARG	N-CA-C	-5.15	97.09	111.00
2	K	399	GLY	N-CA-C	5.13	125.92	113.10
2	H	346	ARG	N-CA-C	-5.03	97.41	111.00
2	E	399	GLY	N-CA-C	5.01	125.62	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	236	TYR	Sidechain
2	H	152	TYR	Sidechain
2	K	236	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	649	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	584	0	623	74	0
1	G	608	0	649	118	0
1	J	652	0	695	94	0
2	B	2462	0	2327	468	0
2	E	2434	0	2295	248	0
2	H	2462	0	2326	410	0
2	K	2442	0	2307	250	0
3	C	2446	0	2294	480	0
3	F	2410	0	2256	270	0
3	I	2446	0	2294	451	0
3	L	2410	0	2256	256	0
4	M	31	0	32	3	0
4	N	31	0	32	7	0
4	O	31	0	32	10	0
4	P	31	0	32	5	0
4	Q	31	0	32	5	0
4	R	31	0	32	4	0
4	S	31	0	32	12	0
4	T	31	0	32	5	0
5	B	14	0	13	4	0
5	H	14	0	13	3	0
5	K	14	0	13	2	0
6	E	14	0	13	4	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	2	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	K	2	0	0	0	0
7	L	1	0	0	0	0
All	All	22278	0	21279	3017	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 69.

All (3017) 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)
3:F:305:THR:HB	3:F:341:ALA:HB2	1.23	1.17
2:E:355:ASP:HB3	2:E:365:ARG:HH22	1.12	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:245:GLU:HB3	2:H:249:TRP:HE1	1.09	1.15
1:J:127:ILE:HG23	2:K:153:ILE:HG21	1.27	1.15
2:E:191:GLU:HA	2:E:194:ARG:HH21	1.09	1.13
3:L:305:THR:HB	3:L:341:ALA:HB2	1.29	1.13
3:I:330:ASP:HB2	3:I:365:ASN:HB3	1.14	1.12
2:K:355:ASP:HB3	2:K:365:ARG:HH22	1.09	1.11
2:B:245:GLU:HB3	2:B:249:TRP:HE1	1.06	1.11
3:C:330:ASP:HB2	3:C:365:ASN:HB3	1.12	1.09
3:C:105:SER:HA	3:C:108:ARG:HB3	1.31	1.05
2:B:176:ARG:HA	2:B:179:ILE:HD12	1.34	1.04
1:G:148:LYS:NZ	2:H:425:ASP:HB2	1.74	1.02
2:B:204:PRO:HG3	3:C:217:HIS:HB3	1.41	1.01
3:F:148:ILE:HD12	3:F:148:ILE:H	1.25	1.01
2:H:241:ASP:HB3	2:H:249:TRP:HB2	1.39	1.01
3:L:148:ILE:H	3:L:148:ILE:HD12	1.29	0.98
1:D:191:LYS:HG3	1:D:192:ASP:H	1.27	0.97
1:A:133:ILE:HG21	2:B:164:ASN:HD21	1.29	0.97
1:A:169:LEU:HD12	1:A:171:ARG:HG3	1.46	0.97
1:J:167:ARG:NH1	1:J:167:ARG:HB3	1.79	0.96
2:K:398:ASP:HA	2:K:433:ASP:HB3	1.44	0.96
2:H:176:ARG:HA	2:H:179:ILE:HD12	1.44	0.96
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.43	0.96
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.47	0.96
2:K:191:GLU:HA	2:K:194:ARG:HH21	1.26	0.96
2:H:256:GLN:HE21	2:H:449:LYS:HZ1	1.13	0.96
2:H:367:MET:SD	2:H:406:ARG:HG2	2.06	0.96
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.42	0.96
1:J:144:LEU:HD23	1:J:182:GLN:HG2	1.46	0.95
1:A:133:ILE:HG21	2:B:164:ASN:ND2	1.79	0.95
2:H:415:ARG:H	2:H:434:GLY:HA2	1.33	0.94
2:K:352:ALA:HB2	2:K:439:ASN:ND2	1.82	0.94
3:L:240:SER:HB2	3:L:242:ILE:HD11	1.49	0.93
2:B:267:ASP:HB2	2:B:268:PRO:HD3	1.50	0.93
2:H:205:VAL:HG12	3:I:232:LYS:NZ	1.84	0.93
3:I:154:GLN:HE22	3:I:189:ASN:HA	1.33	0.93
1:J:157:LYS:HE2	1:J:157:LYS:HA	1.49	0.93
3:F:194:PHE:HA	3:F:228:LEU:HD12	1.50	0.92
2:E:352:ALA:HB2	2:E:439:ASN:ND2	1.83	0.92
2:B:165:LEU:H	2:B:166:ARG:HH21	1.16	0.92
3:C:221:THR:HG23	3:C:222:GLY:H	1.32	0.92
1:G:132:HIS:C	1:G:133:ILE:HD12	1.89	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLN:HE21	1:A:143:GLN:HA	1.32	0.92
3:I:103:HIS:HA	3:I:106:SER:HB3	1.50	0.92
3:I:221:THR:HG23	3:I:222:GLY:H	1.33	0.91
1:D:167:ARG:CB	1:D:167:ARG:HH11	1.82	0.91
2:B:369:ILE:H	2:B:405:ASN:HD22	1.18	0.91
2:H:169:ARG:HG2	3:I:110:LEU:HD21	1.52	0.91
3:L:194:PHE:HA	3:L:228:LEU:HD12	1.52	0.91
2:H:204:PRO:HG3	3:I:217:HIS:HB3	1.51	0.91
2:H:267:ASP:HB2	2:H:268:PRO:HD3	1.53	0.91
3:L:230:ASN:HA	3:L:233:ILE:HD12	1.53	0.91
2:E:191:GLU:HA	2:E:194:ARG:NH2	1.84	0.91
1:A:148:LYS:HE3	2:B:425:ASP:O	1.70	0.91
2:K:355:ASP:HB3	2:K:365:ARG:NH2	1.85	0.90
2:K:367:MET:HB2	2:K:406:ARG:HB3	1.51	0.90
3:C:154:GLN:HE22	3:C:189:ASN:HA	1.35	0.90
3:C:273:LYS:HE3	3:C:319:ASN:HD21	1.36	0.90
2:B:415:ARG:H	2:B:434:GLY:HA2	1.37	0.90
2:B:245:GLU:HB3	2:B:249:TRP:NE1	1.87	0.90
1:J:140:VAL:HG13	1:J:185:LEU:HD11	1.54	0.90
3:L:208:TRP:HA	3:L:314:THR:HG21	1.54	0.89
2:B:205:VAL:HG12	3:C:232:LYS:NZ	1.87	0.89
2:H:369:ILE:H	2:H:405:ASN:HD22	1.16	0.89
2:H:223:GLU:HB3	2:H:287:GLY:HA2	1.54	0.89
4:S:3:ARG:HG2	4:S:3:ARG:HH21	1.37	0.89
3:I:251:GLU:HG2	3:I:252:ASP:H	1.37	0.89
2:K:327:GLY:HA3	2:K:344:LYS:HB2	1.54	0.89
2:H:367:MET:HB2	2:H:406:ARG:HB3	1.54	0.88
2:B:223:GLU:HB3	2:B:287:GLY:HA2	1.54	0.88
3:F:141:ASP:OD1	3:F:143:VAL:HG22	1.72	0.88
2:E:327:GLY:HA3	2:E:344:LYS:HB2	1.54	0.88
2:E:178:LYS:O	2:E:182:LEU:HD23	1.72	0.88
2:H:245:GLU:HB3	2:H:249:TRP:NE1	1.89	0.87
2:B:165:LEU:H	2:B:166:ARG:NH2	1.72	0.87
2:H:359:GLN:H	2:H:359:GLN:NE2	1.73	0.86
2:K:191:GLU:HA	2:K:194:ARG:NH2	1.90	0.86
3:F:240:SER:HB2	3:F:242:ILE:HD11	1.55	0.86
3:L:340:HIS:O	4:T:1:GLY:HA2	1.75	0.86
2:B:204:PRO:HA	3:C:217:HIS:HA	1.56	0.86
2:B:300:SER:O	2:B:304:ARG:HG2	1.75	0.86
2:B:158:ASN:ND2	3:C:100:ILE:HG21	1.91	0.86
2:B:158:ASN:HD21	3:C:100:ILE:HG21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:214:GLY:HA2	3:I:229:GLY:HA3	1.57	0.85
2:H:300:SER:O	2:H:304:ARG:HG2	1.75	0.85
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.58	0.85
2:K:333:ASN:HB3	2:K:336:ASN:ND2	1.90	0.85
2:E:355:ASP:HB3	2:E:365:ARG:NH2	1.91	0.85
2:B:198:THR:HG22	3:C:140:LYS:HB3	1.59	0.85
3:C:214:GLY:HA2	3:C:229:GLY:HA3	1.58	0.85
3:I:143:VAL:HG12	3:I:220:PRO:HD3	1.57	0.85
2:K:241:ASP:HB3	2:K:249:TRP:HB2	1.58	0.85
1:J:144:LEU:CD2	1:J:182:GLN:HG2	2.06	0.84
2:E:269:TYR:O	2:E:296:ASN:HB2	1.77	0.84
3:C:209:ILE:H	3:C:209:ILE:HD12	1.38	0.84
2:K:269:TYR:O	2:K:296:ASN:HB2	1.76	0.84
2:H:369:ILE:H	2:H:405:ASN:ND2	1.75	0.84
2:E:352:ALA:HB2	2:E:439:ASN:HD22	1.41	0.84
1:G:148:LYS:HZ3	2:H:425:ASP:HB2	1.42	0.84
3:C:169:ILE:HD12	3:C:171:PRO:HD3	1.59	0.84
3:F:208:TRP:HA	3:F:314:THR:HG21	1.59	0.84
1:G:119:ILE:O	1:G:120:GLU:HB2	1.78	0.84
3:I:169:ILE:HD12	3:I:171:PRO:HD3	1.58	0.83
2:H:204:PRO:HA	3:I:217:HIS:HA	1.59	0.83
3:C:246:LEU:HD12	3:C:247:ARG:N	1.93	0.83
2:K:183:GLU:HG2	3:L:124:LEU:HG	1.60	0.83
2:K:412:PRO:O	2:K:413:ASN:HB2	1.77	0.83
1:D:185:LEU:HD22	1:D:189:ILE:HG13	1.60	0.83
3:I:209:ILE:H	3:I:209:ILE:HD12	1.39	0.83
2:B:157:VAL:C	2:B:158:ASN:HD22	1.81	0.83
3:C:330:ASP:HB2	3:C:365:ASN:CB	2.03	0.83
1:A:164:SER:HB3	3:C:137:GLU:O	1.79	0.82
3:L:276:LEU:HD23	3:L:277:THR:N	1.93	0.82
2:E:183:GLU:HG2	3:F:124:LEU:HG	1.59	0.82
2:B:369:ILE:H	2:B:405:ASN:ND2	1.76	0.82
1:G:128:GLU:HA	1:G:131:GLN:HB3	1.59	0.82
3:F:119:GLN:HA	3:F:119:GLN:HE21	1.42	0.82
2:E:333:ASN:HB3	2:E:336:ASN:ND2	1.93	0.82
3:C:172:LEU:HD13	3:C:239:GLN:HE21	1.44	0.82
1:J:137:GLN:NE2	1:J:189:ILE:HA	1.93	0.82
2:B:359:GLN:H	2:B:359:GLN:NE2	1.77	0.82
3:I:330:ASP:HB2	3:I:365:ASN:CB	2.03	0.82
3:I:172:LEU:HD13	3:I:239:GLN:HE21	1.45	0.82
3:I:276:LEU:CD1	3:I:309:GLY:H	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:158:ILE:HG23	2:K:189:GLN:HE21	1.44	0.82
3:I:172:LEU:HD13	3:I:239:GLN:HB2	1.61	0.82
2:K:352:ALA:HB2	2:K:439:ASN:HD22	1.42	0.82
1:G:148:LYS:HZ1	2:H:425:ASP:HB2	1.44	0.82
2:H:293:TRP:HE1	2:H:296:ASN:ND2	1.79	0.81
2:K:175:LEU:O	2:K:179:ILE:HG13	1.79	0.81
1:D:167:ARG:HB2	1:D:167:ARG:HH11	1.45	0.81
1:J:137:GLN:HE22	1:J:189:ILE:HA	1.44	0.81
2:B:167:VAL:HA	2:B:170:SER:HB3	1.61	0.81
2:H:238:VAL:HG21	2:H:250:THR:HG23	1.63	0.81
3:I:235:LEU:HD12	3:I:235:LEU:H	1.43	0.81
2:B:284:ASN:N	2:B:284:ASN:HD22	1.79	0.81
3:F:276:LEU:HD23	3:F:277:THR:N	1.95	0.81
3:F:105:SER:HA	3:F:108:ARG:NH1	1.95	0.81
3:F:148:ILE:HD12	3:F:148:ILE:N	1.96	0.81
2:H:165:LEU:HD11	3:I:106:SER:O	1.81	0.81
2:B:156:THR:HG22	2:B:160:ASN:HD22	1.46	0.81
2:B:202:ASN:HD22	2:B:284:ASN:HB3	1.44	0.81
3:L:229:GLY:O	3:L:233:ILE:HG13	1.80	0.81
3:C:276:LEU:CD1	3:C:309:GLY:H	1.93	0.81
2:B:176:ARG:O	2:B:180:GLN:HG2	1.81	0.81
3:C:251:GLU:HG2	3:C:252:ASP:H	1.43	0.81
2:H:412:PRO:HG3	2:H:450:MET:CE	2.11	0.80
3:C:143:VAL:HG12	3:C:220:PRO:HD3	1.62	0.80
2:K:253:GLN:OE1	2:K:255:ARG:HG2	1.81	0.80
2:H:198:THR:HG22	3:I:140:LYS:HB3	1.64	0.80
2:E:412:PRO:O	2:E:413:ASN:HB2	1.80	0.80
3:C:228:LEU:O	3:C:232:LYS:HD2	1.82	0.80
3:C:271:ALA:C	3:C:273:LYS:H	1.85	0.80
3:C:273:LYS:HE3	3:C:319:ASN:ND2	1.95	0.80
2:K:235:PRO:HG2	3:L:168:PHE:HE1	1.47	0.80
3:I:273:LYS:HE3	3:I:319:ASN:HD21	1.43	0.80
3:C:233:ILE:HA	3:C:236:ILE:HD11	1.63	0.80
2:B:361:MET:HB2	5:B:470:NAG:H81	1.64	0.80
2:E:398:ASP:CA	2:E:433:ASP:HB3	2.11	0.80
2:H:351:ASN:O	2:H:355:ASP:HB2	1.80	0.80
2:B:168:LEU:HD23	3:C:110:LEU:HD21	1.64	0.80
3:L:166:LEU:HD21	3:L:218:LEU:HB3	1.64	0.79
2:B:412:PRO:HG3	2:B:450:MET:CE	2.12	0.79
3:L:141:ASP:OD1	3:L:143:VAL:HG22	1.81	0.79
1:D:137:GLN:NE2	2:E:164:ASN:HD21	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:GLN:HA	3:F:119:GLN:NE2	1.97	0.79
1:A:150:LEU:O	1:A:150:LEU:HD12	1.81	0.79
3:I:246:LEU:HD12	3:I:247:ARG:N	1.98	0.79
3:L:148:ILE:N	3:L:148:ILE:HD12	1.98	0.79
2:E:253:GLN:OE1	2:E:255:ARG:HG2	1.81	0.79
3:C:365:ASN:N	3:C:365:ASN:HD22	1.81	0.79
2:H:176:ARG:HA	2:H:179:ILE:CD1	2.13	0.79
3:F:270:GLU:HB2	3:F:274:TYR:OH	1.82	0.79
3:F:166:LEU:HD21	3:F:218:LEU:HB3	1.65	0.79
3:C:214:GLY:CA	3:C:229:GLY:HA3	2.13	0.79
2:H:284:ASN:HD22	2:H:284:ASN:N	1.81	0.79
2:H:159:SER:C	2:H:162:PRO:HD2	2.02	0.79
3:L:278:TYR:CZ	3:L:308:ASN:HB2	2.18	0.79
2:B:359:GLN:O	2:B:360:LEU:HD23	1.83	0.79
2:H:157:VAL:O	2:H:158:ASN:HB2	1.80	0.78
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.65	0.78
3:F:305:THR:CB	3:F:341:ALA:HB2	2.10	0.78
1:G:130:VAL:O	1:G:134:GLN:HG2	1.82	0.78
2:H:203:ILE:HG21	2:H:226:LEU:HD22	1.66	0.78
2:H:210:GLU:OE1	2:H:212:GLU:N	2.15	0.78
1:G:181:GLN:O	1:G:184:GLN:HG3	1.83	0.78
2:K:212:GLU:HG2	2:K:456:PRO:HG2	1.65	0.78
3:C:235:LEU:HD12	3:C:235:LEU:H	1.46	0.78
2:B:186:VAL:O	2:B:190:MET:HB2	1.83	0.78
3:C:212:LYS:HG2	3:C:231:GLU:HB2	1.65	0.78
3:C:232:LYS:O	3:C:236:ILE:HG12	1.83	0.78
2:H:359:GLN:O	2:H:360:LEU:HD23	1.83	0.78
3:L:391:ARG:HH11	3:L:391:ARG:HB2	1.48	0.78
2:H:214:ILE:HD12	2:H:227:ILE:HG22	1.65	0.78
3:C:228:LEU:HD11	3:C:232:LYS:HD3	1.66	0.78
1:J:178:TYR:O	1:J:182:GLN:HG3	1.82	0.78
1:J:156:ILE:HG21	2:K:415:ARG:NH1	1.99	0.78
3:I:271:ALA:C	3:I:273:LYS:H	1.87	0.78
1:D:124:ARG:HD3	1:D:124:ARG:H	1.47	0.78
2:E:212:GLU:HG2	2:E:456:PRO:HG2	1.65	0.78
3:I:365:ASN:HD22	3:I:365:ASN:N	1.83	0.77
3:F:251:GLU:HA	3:F:257:THR:HG22	1.66	0.77
3:I:298:ASP:O	3:I:301:ASP:HB2	1.84	0.77
2:K:398:ASP:CA	2:K:433:ASP:HB3	2.13	0.77
1:G:144:LEU:HD22	1:G:182:GLN:HB3	1.64	0.77
2:H:301:GLN:HE22	2:H:302:LEU:HD23	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:214:GLY:CA	3:I:229:GLY:HA3	2.15	0.77
2:B:203:ILE:HG21	2:B:226:LEU:HD22	1.66	0.77
3:I:348:TYR:HA	3:I:367:ILE:HD11	1.66	0.77
3:I:252:ASP:HB2	3:I:377:TYR:OH	1.82	0.77
3:I:279:ALA:HB2	3:L:308:ASN:ND2	1.99	0.77
3:L:251:GLU:HA	3:L:257:THR:HG22	1.66	0.77
3:L:270:GLU:HB2	3:L:274:TYR:OH	1.83	0.77
3:C:298:ASP:O	3:C:301:ASP:HB2	1.84	0.77
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.20	0.77
2:H:256:GLN:HE21	2:H:449:LYS:NZ	1.82	0.77
3:C:275:ARG:HB2	3:C:311:GLN:HA	1.66	0.77
3:F:229:GLY:O	3:F:233:ILE:HG13	1.84	0.77
2:E:175:LEU:O	2:E:179:ILE:HG13	1.85	0.77
1:G:189:ILE:HG23	1:G:189:ILE:O	1.85	0.77
3:C:348:TYR:HA	3:C:367:ILE:HD11	1.66	0.76
3:L:227:TRP:HZ2	3:L:230:ASN:HD21	1.32	0.76
2:B:162:PRO:HA	2:B:166:ARG:HD2	1.67	0.76
2:B:214:ILE:HD12	2:B:227:ILE:HG22	1.66	0.76
3:I:93:ILE:N	3:I:93:ILE:HD12	2.01	0.76
2:B:293:TRP:HE1	2:B:296:ASN:ND2	1.84	0.76
3:I:273:LYS:HE3	3:I:319:ASN:ND2	1.99	0.76
2:H:202:ASN:HD22	2:H:284:ASN:HB3	1.49	0.76
3:I:212:LYS:HG2	3:I:231:GLU:HB2	1.67	0.76
3:I:250:LEU:HD21	3:I:379:MET:SD	2.26	0.76
2:B:176:ARG:HH11	2:B:176:ARG:CB	1.99	0.76
3:C:252:ASP:HB2	3:C:377:TYR:OH	1.84	0.76
3:C:250:LEU:HD21	3:C:379:MET:SD	2.26	0.76
3:C:278:TYR:OH	3:C:290:PHE:HB3	1.85	0.76
2:K:210:GLU:OE1	2:K:212:GLU:HB3	1.86	0.76
1:A:147:MET:HG3	2:B:175:LEU:HD21	1.67	0.76
1:G:149:ARG:HH21	2:H:425:ASP:HA	1.51	0.76
3:F:148:ILE:CD1	3:F:148:ILE:H	1.99	0.76
3:L:227:TRP:HZ2	3:L:230:ASN:ND2	1.84	0.75
3:I:278:TYR:OH	3:I:290:PHE:HB3	1.85	0.75
3:C:259:THR:H	3:C:286:ALA:HB2	1.52	0.75
2:E:235:PRO:HG2	3:F:168:PHE:HE1	1.51	0.75
3:I:276:LEU:HD12	3:I:309:GLY:H	1.51	0.75
3:F:391:ARG:HB2	3:F:391:ARG:HH11	1.51	0.75
3:F:322:PHE:CZ	4:P:3:ARG:HD2	2.21	0.75
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.50	0.75
3:I:276:LEU:HD11	3:I:308:ASN:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:327:ALA:HB1	3:I:332:SER:O	1.87	0.74
2:E:360:LEU:HD13	2:E:364:ASN:O	1.86	0.74
1:A:148:LYS:NZ	2:B:425:ASP:HB2	2.02	0.74
3:C:110:LEU:HD23	3:C:111:GLN:N	2.01	0.74
3:I:200:GLY:N	3:I:225:GLU:OE2	2.20	0.74
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.35	0.74
1:A:185:LEU:O	1:A:185:LEU:HD13	1.87	0.74
3:F:153:CYS:HB2	3:F:192:THR:HG22	1.69	0.74
1:J:130:VAL:O	1:J:133:ILE:HG22	1.88	0.74
3:C:103:HIS:O	3:C:107:ILE:HG22	1.86	0.74
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.88	0.74
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.68	0.74
2:K:360:LEU:HD13	2:K:364:ASN:O	1.86	0.74
2:H:351:ASN:C	2:H:351:ASN:HD22	1.91	0.74
3:I:325:ASN:HD21	3:I:327:ALA:HB3	1.52	0.74
2:B:351:ASN:O	2:B:355:ASP:HB2	1.88	0.74
3:I:232:LYS:O	3:I:236:ILE:HG12	1.86	0.74
3:C:105:SER:HA	3:C:108:ARG:CB	2.16	0.74
3:C:327:ALA:HB1	3:C:332:SER:O	1.88	0.74
2:H:351:ASN:HD21	2:H:354:MET:HG2	1.52	0.74
2:B:224:MET:SD	2:B:237:ARG:HB3	2.27	0.73
1:J:167:ARG:O	2:K:192:TYR:HB3	1.88	0.73
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.69	0.73
3:I:228:LEU:O	3:I:232:LYS:HD2	1.87	0.73
3:C:209:ILE:N	3:C:209:ILE:HD12	2.02	0.73
1:G:169:LEU:HD12	1:G:171:ARG:HD2	1.68	0.73
3:I:288:ASP:C	3:I:371:THR:HG21	2.08	0.73
2:E:317:TRP:CZ2	2:E:448:ARG:HG3	2.22	0.73
1:A:144:LEU:HD21	1:A:182:GLN:HA	1.70	0.73
3:I:305:THR:HG21	4:S:2:HYP:HD23	1.70	0.73
3:C:276:LEU:HD12	3:C:309:GLY:H	1.53	0.73
2:K:235:PRO:HG2	3:L:168:PHE:CE1	2.21	0.73
1:J:116:ARG:H	1:J:116:ARG:HD2	1.53	0.73
3:I:157:ALA:HA	3:I:161:ALA:HB3	1.70	0.73
2:H:173:GLU:C	2:H:175:LEU:H	1.91	0.73
3:I:275:ARG:HB2	3:I:311:GLN:HA	1.69	0.73
2:B:213:GLU:HG2	2:B:217:LYS:HE3	1.69	0.73
2:B:184:SER:O	2:B:187:SER:N	2.22	0.73
3:I:197:ARG:NH2	3:I:346:GLY:O	2.22	0.73
3:I:259:THR:H	3:I:286:ALA:HB2	1.54	0.73
3:L:320:ASP:HA	3:L:336:MET:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:305:THR:CB	3:L:341:ALA:HB2	2.16	0.73
1:G:154:ILE:HD13	2:H:186:VAL:HG21	1.68	0.73
2:E:210:GLU:HA	2:E:227:ILE:HG21	1.71	0.73
1:A:140:VAL:HG23	1:A:141:ARG:N	2.04	0.73
3:C:288:ASP:C	3:C:371:THR:HG21	2.09	0.73
3:I:193:VAL:HG12	3:I:195:GLN:H	1.53	0.73
3:L:338:LYS:HG2	4:T:3:ARG:HB2	1.71	0.73
2:B:284:ASN:N	2:B:284:ASN:ND2	2.36	0.73
3:I:228:LEU:HD11	3:I:232:LYS:HD3	1.70	0.73
3:I:337:ASN:C	3:I:339:CYS:H	1.86	0.73
2:B:159:SER:C	2:B:162:PRO:HD2	2.10	0.72
2:B:178:LYS:C	2:B:180:GLN:H	1.89	0.72
2:B:255:ARG:HB2	2:B:450:MET:H	1.54	0.72
3:L:216:GLY:HA3	3:L:226:PHE:HA	1.71	0.72
3:C:365:ASN:H	3:C:365:ASN:HD22	1.37	0.72
3:I:300:SER:C	3:I:302:LYS:H	1.90	0.72
2:B:212:GLU:O	2:B:215:ILE:HG22	1.89	0.72
2:B:253:GLN:HB2	2:B:293:TRP:CE3	2.24	0.72
3:I:233:ILE:HA	3:I:236:ILE:HD11	1.71	0.72
3:L:185:ASP:OD2	3:L:187:SER:HB3	1.90	0.72
3:I:249:GLU:HB2	3:I:383:THR:HG23	1.71	0.72
3:C:178:PHE:HE2	3:C:228:LEU:HD21	1.54	0.72
3:C:193:VAL:HG12	3:C:195:GLN:H	1.53	0.72
3:L:148:ILE:CD1	3:L:148:ILE:H	2.02	0.72
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	1.86	0.72
3:L:196:LYS:HG2	3:L:198:LEU:HD11	1.70	0.72
3:C:276:LEU:HD11	3:C:308:ASN:HA	1.69	0.72
2:K:210:GLU:HA	2:K:227:ILE:HG21	1.72	0.72
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.24	0.72
1:J:167:ARG:CZ	1:J:167:ARG:HB3	2.18	0.72
3:I:195:GLN:HE22	3:I:382:THR:CG2	2.03	0.72
3:L:250:LEU:HG	3:L:379:MET:HG3	1.72	0.72
3:F:149:THR:OG1	3:F:150:GLY:N	2.23	0.72
2:B:253:GLN:HB2	2:B:293:TRP:CZ3	2.25	0.72
2:B:370:HIS:O	2:B:373:MET:HB2	1.89	0.72
2:B:434:GLY:O	2:B:436:VAL:N	2.23	0.72
2:B:317:TRP:HE1	2:B:447:MET:HA	1.54	0.72
2:H:266:TRP:HE1	2:H:380:ARG:NH2	1.87	0.72
2:K:230:ASP:OD2	2:K:232:SER:HB2	1.89	0.72
2:H:212:GLU:O	2:H:215:ILE:HG22	1.90	0.72
3:F:101:LEU:O	3:F:104:ASP:HB3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.24	0.72
3:F:338:LYS:HG2	4:P:3:ARG:HB2	1.70	0.72
1:J:167:ARG:HH11	1:J:167:ARG:HB3	1.54	0.72
2:H:236:TYR:HB2	2:H:298:LYS:NZ	2.05	0.72
3:I:103:HIS:O	3:I:107:ILE:HG12	1.90	0.72
2:B:292:TYR:HE2	2:B:294:LEU:HB2	1.55	0.72
2:K:333:ASN:HB3	2:K:336:ASN:HD22	1.54	0.72
2:K:317:TRP:CZ2	2:K:448:ARG:HG3	2.24	0.72
3:C:279:ALA:HB2	3:F:308:ASN:ND2	2.03	0.72
1:G:132:HIS:O	1:G:133:ILE:HD12	1.89	0.71
3:C:172:LEU:HD13	3:C:239:GLN:HB2	1.72	0.71
2:H:284:ASN:N	2:H:284:ASN:ND2	2.38	0.71
3:I:365:ASN:HD22	3:I:365:ASN:H	1.38	0.71
3:I:178:PHE:HE2	3:I:228:LEU:HD21	1.54	0.71
1:D:140:VAL:HG13	1:D:185:LEU:HD11	1.71	0.71
3:F:196:LYS:HG2	3:F:198:LEU:HD11	1.70	0.71
2:H:205:VAL:HG12	3:I:232:LYS:HZ2	1.52	0.71
3:I:370:ALA:HA	3:I:373:LYS:O	1.90	0.71
2:E:333:ASN:H	2:E:336:ASN:HD22	1.38	0.71
3:I:123:ASN:O	3:I:127:LYS:HD3	1.89	0.71
2:H:345:TYR:CE2	2:H:351:ASN:HB2	2.26	0.71
3:I:172:LEU:H	3:I:172:LEU:HD12	1.55	0.71
2:K:157:VAL:C	2:K:158:ASN:HD22	1.94	0.71
1:G:138:LYS:O	1:G:141:ARG:HG2	1.90	0.71
3:C:300:SER:C	3:C:302:LYS:H	1.91	0.71
3:I:97:GLU:C	3:I:99:SER:H	1.92	0.71
2:B:161:ILE:HG23	2:B:166:ARG:NH2	2.06	0.71
2:H:434:GLY:O	2:H:436:VAL:N	2.24	0.71
3:L:153:CYS:HB2	3:L:192:THR:HG22	1.72	0.71
6:E:470:NDG:C6	4:N:4:PRO:HG3	2.20	0.71
1:A:136:LEU:O	2:B:168:LEU:HD11	1.91	0.71
2:B:193:CYS:HB3	3:C:134:GLN:OE1	1.89	0.71
2:H:253:GLN:HB2	2:H:293:TRP:CZ3	2.26	0.71
3:F:172:LEU:HD13	3:F:240:SER:OG	1.90	0.71
1:A:159:ARG:O	1:A:161:CYS:N	2.23	0.71
1:G:124:ARG:O	1:G:126:VAL:N	2.23	0.71
2:B:301:GLN:HE22	2:B:302:LEU:HD23	1.56	0.71
2:E:230:ASP:O	2:E:233:VAL:HG12	1.91	0.71
3:C:99:SER:C	3:C:101:LEU:H	1.93	0.71
3:F:172:LEU:HD22	3:F:240:SER:OG	1.91	0.70
1:G:120:GLU:CD	1:G:121:VAL:H	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:209:ILE:HD12	3:I:209:ILE:N	2.06	0.70
1:D:131:GLN:HB2	1:D:134:GLN:HE21	1.56	0.70
2:B:351:ASN:C	2:B:351:ASN:HD22	1.92	0.70
2:B:398:ASP:HA	2:B:433:ASP:CB	2.21	0.70
3:L:219:SER:HB3	3:L:224:THR:CG2	2.20	0.70
2:B:204:PRO:CG	3:C:217:HIS:HB3	2.19	0.70
3:F:153:CYS:O	3:F:156:ILE:HB	1.92	0.70
3:L:149:THR:OG1	3:L:150:GLY:N	2.24	0.70
2:H:270:LYS:HG3	2:H:338:TYR:OH	1.91	0.70
2:H:370:HIS:O	2:H:373:MET:HB2	1.91	0.70
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.73	0.70
2:H:213:GLU:HG2	2:H:217:LYS:HE3	1.74	0.70
2:B:284:ASN:H	2:B:284:ASN:ND2	1.89	0.70
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.56	0.70
2:K:242:MET:HA	2:K:247:GLY:HA3	1.73	0.70
3:I:196:LYS:O	3:I:197:ARG:HG2	1.92	0.70
2:B:205:VAL:HG12	3:C:232:LYS:HZ2	1.53	0.70
3:C:256:ARG:HG3	3:C:256:ARG:HH11	1.56	0.70
2:B:434:GLY:O	2:B:436:VAL:HG13	1.92	0.70
3:C:281:PHE:CD1	3:C:288:ASP:HB2	2.26	0.70
3:C:338:LYS:HG2	3:C:338:LYS:O	1.91	0.70
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.27	0.70
2:H:242:MET:HA	2:H:247:GLY:CA	2.22	0.70
2:B:266:TRP:HE1	2:B:380:ARG:NH2	1.89	0.70
3:I:219:SER:HB3	3:I:224:THR:HG21	1.73	0.70
3:F:216:GLY:HA3	3:F:226:PHE:HA	1.74	0.70
3:C:195:GLN:HE22	3:C:382:THR:CG2	2.05	0.70
3:L:389:PHE:O	3:L:391:ARG:N	2.24	0.70
3:C:196:LYS:O	3:C:197:ARG:HG2	1.92	0.70
2:H:224:MET:SD	2:H:237:ARG:HB3	2.31	0.70
1:G:127:ILE:HD12	1:G:128:GLU:N	2.07	0.70
3:C:370:ALA:HA	3:C:373:LYS:O	1.91	0.69
2:H:351:ASN:HD21	2:H:354:MET:H	1.40	0.69
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.24	0.69
3:C:307:HIS:CD2	3:C:334:TRP:HE1	2.11	0.69
3:C:271:ALA:O	3:C:273:LYS:N	2.24	0.69
2:B:367:MET:SD	2:B:406:ARG:HG2	2.31	0.69
1:D:166:SER:HB2	2:E:195:THR:O	1.92	0.69
3:C:230:ASN:HD22	3:C:230:ASN:N	1.90	0.69
3:C:367:ILE:O	3:C:379:MET:HG2	1.93	0.69
2:H:242:MET:HA	2:H:247:GLY:HA3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:214:ILE:HD11	2:K:227:ILE:HG22	1.74	0.69
3:F:219:SER:HB3	3:F:224:THR:CG2	2.22	0.69
3:C:278:TYR:HE2	3:C:290:PHE:HD2	1.39	0.69
3:I:154:GLN:NE2	3:I:189:ASN:HA	2.07	0.69
2:B:210:GLU:OE1	2:B:212:GLU:N	2.19	0.69
2:B:266:TRP:CE3	2:B:266:TRP:HA	2.27	0.69
3:C:103:HIS:HA	3:C:106:SER:HB2	1.74	0.69
2:H:193:CYS:HB3	3:I:134:GLN:OE1	1.92	0.69
3:C:209:ILE:CD1	3:C:209:ILE:H	2.06	0.69
3:I:278:TYR:HE2	3:I:290:PHE:HD2	1.40	0.69
3:C:219:SER:HB3	3:C:224:THR:HG21	1.73	0.69
2:H:168:LEU:HB3	3:I:110:LEU:HD13	1.75	0.69
4:S:3:ARG:HG2	4:S:3:ARG:NH2	2.07	0.69
2:B:236:TYR:HB2	2:B:298:LYS:NZ	2.07	0.69
2:H:238:VAL:HG22	2:H:239:TYR:H	1.57	0.69
2:H:398:ASP:HA	2:H:433:ASP:CB	2.22	0.69
2:H:310:LEU:HD13	2:H:312:ILE:HG13	1.75	0.69
2:H:415:ARG:N	2:H:434:GLY:HA2	2.08	0.69
3:I:166:LEU:HD21	3:I:219:SER:O	1.92	0.69
3:I:256:ARG:HG3	3:I:256:ARG:HH11	1.57	0.69
3:L:251:GLU:HB3	3:L:381:LYS:HB2	1.75	0.69
2:B:209:LYS:HA	2:B:228:GLN:O	1.93	0.69
3:I:293:PHE:N	3:I:302:LYS:HG3	2.08	0.69
1:J:140:VAL:CG1	1:J:185:LEU:HD11	2.23	0.69
2:B:455:ARG:CG	2:B:456:PRO:HD2	2.22	0.68
2:B:165:LEU:N	2:B:166:ARG:HE	1.90	0.68
3:C:344:LEU:HD12	3:C:384:MET:SD	2.33	0.68
2:H:351:ASN:HB3	2:H:355:ASP:HB2	1.75	0.68
2:H:284:ASN:H	2:H:284:ASN:ND2	1.90	0.68
3:I:209:ILE:H	3:I:209:ILE:CD1	2.07	0.68
3:L:205:LYS:HE2	3:L:331:GLY:HA2	1.75	0.68
3:I:353:THR:HG23	3:I:377:TYR:HD1	1.58	0.68
3:F:250:LEU:HG	3:F:379:MET:HG3	1.75	0.68
2:H:249:TRP:HB3	2:H:453:LYS:HB2	1.75	0.68
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.28	0.68
3:I:183:GLU:O	3:I:191:TRP:HD1	1.76	0.68
3:F:242:ILE:HG22	3:F:243:PRO:HD2	1.74	0.68
3:C:200:GLY:N	3:C:225:GLU:OE2	2.26	0.68
3:I:297:ASP:HB2	3:I:301:ASP:OD2	1.93	0.68
2:E:235:PRO:HG2	3:F:168:PHE:CE1	2.26	0.68
3:C:304:PHE:O	3:C:306:SER:N	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:333:ASN:HB3	2:E:336:ASN:HD22	1.58	0.68
2:B:238:VAL:HG22	2:B:239:TYR:H	1.58	0.68
3:F:192:THR:HG23	3:F:386:ILE:O	1.93	0.68
3:I:281:PHE:CD1	3:I:288:ASP:HB2	2.28	0.68
3:L:172:LEU:HD13	3:L:240:SER:OG	1.93	0.68
2:K:230:ASP:O	2:K:233:VAL:HG12	1.94	0.68
1:A:157:LYS:HD3	1:A:160:SER:OG	1.94	0.68
3:I:344:LEU:HD12	3:I:384:MET:SD	2.34	0.68
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.75	0.68
2:E:346:ARG:HH11	2:E:346:ARG:HG2	1.59	0.68
2:K:212:GLU:HG2	2:K:456:PRO:CG	2.22	0.68
3:F:160:GLY:O	3:F:161:ALA:HB3	1.94	0.68
2:H:213:GLU:O	2:H:217:LYS:HG3	1.94	0.68
2:H:317:TRP:HE1	2:H:447:MET:HA	1.59	0.68
1:J:181:GLN:HE22	2:K:174:ASN:HB3	1.58	0.68
3:C:103:HIS:C	3:C:105:SER:H	1.96	0.68
2:H:255:ARG:HB2	2:H:450:MET:H	1.59	0.68
3:I:170:LYS:HB2	3:I:177:GLN:HB3	1.75	0.68
3:C:154:GLN:NE2	3:C:189:ASN:HA	2.09	0.68
3:I:271:ALA:O	3:I:273:LYS:N	2.26	0.68
2:K:326:TYR:OH	2:K:351:ASN:ND2	2.26	0.68
2:H:304:ARG:NH2	2:H:333:ASN:H	1.92	0.67
3:L:334:TRP:CD1	3:L:335:TRP:N	2.63	0.67
3:C:103:HIS:HA	3:C:106:SER:CB	2.23	0.67
2:B:351:ASN:HD21	2:B:354:MET:H	1.42	0.67
2:B:351:ASN:HB3	2:B:355:ASP:HB2	1.76	0.67
2:B:390:PRO:HA	2:B:393:GLN:HE21	1.60	0.67
2:H:253:GLN:HB2	2:H:293:TRP:CE3	2.30	0.67
3:L:265:PHE:O	3:L:266:LYS:HG3	1.93	0.67
3:I:208:TRP:HA	3:I:314:THR:HG21	1.75	0.67
2:B:251:VAL:C	2:B:252:ILE:HD13	2.14	0.67
2:H:434:GLY:O	2:H:436:VAL:HG13	1.95	0.67
2:B:270:LYS:HG3	2:B:338:TYR:OH	1.94	0.67
2:B:152:TYR:C	2:B:154:ASP:H	1.98	0.67
3:F:305:THR:HB	3:F:341:ALA:CB	2.14	0.67
1:J:133:ILE:HD11	2:K:165:LEU:HD13	1.75	0.67
3:I:304:PHE:O	3:I:306:SER:N	2.24	0.67
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.77	0.67
3:L:391:ARG:NH1	3:L:391:ARG:HB2	2.08	0.67
3:L:97:GLU:O	3:L:100:ILE:HG13	1.95	0.67
3:C:172:LEU:H	3:C:172:LEU:HD12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LYS:C	2:H:180:GLN:H	1.98	0.67
2:H:412:PRO:HG3	2:H:450:MET:HE2	1.77	0.67
2:B:233:VAL:HG22	2:B:234:LYS:H	1.60	0.67
2:B:310:LEU:HD13	2:B:312:ILE:HG13	1.74	0.67
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.30	0.67
2:H:266:TRP:CE3	2:H:266:TRP:HA	2.30	0.67
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.94	0.67
2:B:266:TRP:NE1	2:B:380:ARG:NE	2.42	0.67
4:O:3:ARG:HB3	4:O:4:PRO:CD	2.25	0.67
1:J:127:ILE:HA	1:J:130:VAL:HB	1.76	0.67
2:B:245:GLU:HG2	2:B:249:TRP:HZ2	1.60	0.67
3:C:170:LYS:HB2	3:C:177:GLN:HB3	1.77	0.67
3:F:273:LYS:HG3	3:F:311:GLN:HB3	1.76	0.67
2:H:266:TRP:NE1	2:H:380:ARG:NE	2.42	0.67
3:C:208:TRP:HA	3:C:314:THR:HG21	1.75	0.67
3:C:228:LEU:CD1	3:C:232:LYS:HD3	2.24	0.66
2:K:234:LYS:HG2	2:K:235:PRO:HD2	1.76	0.66
2:K:203:ILE:HD12	2:K:203:ILE:N	2.10	0.66
1:G:149:ARG:HG2	2:H:426:MET:O	1.95	0.66
3:C:183:GLU:O	3:C:191:TRP:HD1	1.77	0.66
1:D:191:LYS:O	1:D:192:ASP:HB2	1.95	0.66
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.30	0.66
2:K:215:ILE:HG23	2:K:216:ARG:N	2.11	0.66
2:B:180:GLN:HE21	2:B:180:GLN:HA	1.59	0.66
2:B:304:ARG:NH2	2:B:333:ASN:H	1.93	0.66
3:L:227:TRP:CZ2	3:L:230:ASN:ND2	2.63	0.66
1:D:144:LEU:HD22	1:D:182:GLN:HG3	1.78	0.66
2:B:191:GLU:C	2:B:193:CYS:H	1.98	0.66
3:I:238:THR:HG22	3:I:266:LYS:CG	2.24	0.66
2:E:212:GLU:HG2	2:E:456:PRO:CG	2.24	0.66
2:E:301:GLN:NE2	2:E:302:LEU:HG	2.11	0.66
1:A:149:ARG:HG2	2:B:426:MET:O	1.96	0.66
2:H:266:TRP:HE1	2:H:380:ARG:HH21	1.42	0.66
3:C:147:ASP:O	3:C:149:THR:HG23	1.96	0.66
3:C:197:ARG:NH2	3:C:346:GLY:O	2.28	0.66
3:I:147:ASP:O	3:I:149:THR:HG23	1.95	0.66
3:I:367:ILE:O	3:I:379:MET:HG2	1.96	0.66
3:F:389:PHE:O	3:F:391:ARG:N	2.27	0.66
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.30	0.66
1:D:122:LEU:N	1:D:124:ARG:HE	1.93	0.66
2:K:284:ASN:HD22	2:K:285:TYR:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:209:LYS:HA	2:H:228:GLN:O	1.96	0.66
1:A:125:LYS:O	1:A:129:LYS:HG2	1.95	0.66
2:B:255:ARG:O	2:B:449:LYS:HA	1.96	0.66
3:L:153:CYS:SG	3:L:192:THR:HB	2.36	0.66
3:C:94:MET:C	3:C:96:TYR:H	1.97	0.66
2:B:266:TRP:HE3	2:B:266:TRP:HA	1.60	0.66
3:L:105:SER:HA	3:L:108:ARG:HG2	1.78	0.66
2:H:330:THR:OG1	2:H:341:SER:HB2	1.95	0.66
2:K:363:GLU:O	2:K:367:MET:HG2	1.96	0.66
2:B:161:ILE:HG21	3:C:103:HIS:CD2	2.30	0.66
3:C:198:LEU:O	3:C:348:TYR:OH	2.09	0.66
2:H:255:ARG:O	2:H:449:LYS:HA	1.96	0.66
2:H:369:ILE:N	2:H:405:ASN:HD22	1.91	0.66
3:C:287:GLY:HA3	3:C:371:THR:O	1.96	0.66
2:B:242:MET:HA	2:B:247:GLY:CA	2.26	0.66
3:I:110:LEU:HD23	3:I:113:ILE:HD12	1.78	0.66
3:C:258:SER:OG	3:C:372:TRP:NE1	2.28	0.66
3:I:230:ASN:HD22	3:I:230:ASN:N	1.94	0.66
2:K:333:ASN:H	2:K:336:ASN:HD22	1.44	0.66
3:L:304:PHE:HA	3:L:337:ASN:HD21	1.59	0.66
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.76	0.65
3:C:230:ASN:H	3:C:230:ASN:ND2	1.95	0.65
2:K:194:ARG:HH12	4:P:4:PRO:HB2	1.60	0.65
3:I:198:LEU:O	3:I:348:TYR:OH	2.09	0.65
2:B:230:ASP:O	2:B:233:VAL:HG12	1.96	0.65
2:H:172:LEU:HD21	3:I:113:ILE:O	1.95	0.65
2:B:364:ASN:HD22	5:B:470:NAG:C7	2.08	0.65
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.78	0.65
2:H:152:TYR:O	2:H:154:ASP:N	2.29	0.65
2:E:215:ILE:HG23	2:E:216:ARG:N	2.12	0.65
1:G:143:GLN:HA	1:G:146:ASP:HB3	1.77	0.65
2:H:186:VAL:HG11	3:I:128:VAL:HG22	1.78	0.65
2:H:230:ASP:O	2:H:233:VAL:HG12	1.96	0.65
2:H:202:ASN:HA	3:I:143:VAL:HG11	1.77	0.65
3:F:153:CYS:SG	3:F:192:THR:HB	2.37	0.65
3:L:166:LEU:HD22	3:L:179:LEU:HD11	1.78	0.65
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.77	0.65
4:O:3:ARG:HB3	4:O:4:PRO:HD2	1.77	0.65
3:C:365:ASN:N	3:C:365:ASN:ND2	2.43	0.65
3:C:166:LEU:HD21	3:C:219:SER:O	1.96	0.65
3:F:391:ARG:HB2	3:F:391:ARG:NH1	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:C	1:A:182:GLN:H	1.99	0.65
3:C:93:ILE:HD12	3:C:94:MET:N	2.12	0.65
2:E:203:ILE:N	2:E:203:ILE:HD12	2.11	0.65
2:H:245:GLU:HG2	2:H:249:TRP:HZ2	1.62	0.65
3:I:365:ASN:HD22	3:I:366:GLY:H	1.45	0.65
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.77	0.65
3:C:117:ASN:O	3:C:120:LYS:HB3	1.96	0.65
3:C:197:ARG:HA	3:C:225:GLU:CG	2.26	0.65
1:G:147:MET:HG3	2:H:175:LEU:HD11	1.79	0.65
3:F:104:ASP:O	3:F:107:ILE:HG22	1.96	0.65
2:B:202:ASN:HD22	2:B:284:ASN:CB	2.09	0.65
3:L:236:ILE:O	3:L:239:GLN:HG2	1.96	0.65
2:H:266:TRP:HA	2:H:266:TRP:HE3	1.62	0.65
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.32	0.65
2:B:172:LEU:HD12	2:B:172:LEU:O	1.97	0.65
3:C:238:THR:HG22	3:C:266:LYS:CG	2.26	0.65
3:L:117:ASN:O	3:L:121:ILE:HG13	1.96	0.65
1:G:130:VAL:CA	1:G:133:ILE:HB	2.26	0.65
2:B:210:GLU:OE2	2:B:212:GLU:HB3	1.97	0.65
2:B:256:GLN:HE21	2:B:449:LYS:NZ	1.94	0.65
3:C:297:ASP:HB2	3:C:301:ASP:OD2	1.96	0.65
2:H:394:CYS:SG	2:H:407:CYS:N	2.70	0.65
2:E:191:GLU:HG2	2:E:194:ARG:NH2	2.12	0.65
1:G:176:LYS:O	1:G:180:ASP:HB2	1.97	0.65
1:J:157:LYS:CE	1:J:157:LYS:HA	2.25	0.65
1:A:144:LEU:HG	1:A:182:GLN:CD	2.17	0.65
2:E:203:ILE:HD12	2:E:203:ILE:H	1.61	0.65
3:I:222:GLY:O	3:I:224:THR:HG22	1.96	0.65
2:K:202:ASN:ND2	2:K:284:ASN:HB2	2.12	0.65
2:E:363:GLU:O	2:E:367:MET:HG2	1.97	0.65
3:C:235:LEU:HD12	3:C:235:LEU:N	2.11	0.65
3:F:304:PHE:HA	3:F:337:ASN:HD21	1.61	0.65
3:F:298:ASP:O	3:F:301:ASP:HB2	1.96	0.64
2:K:373:MET:SD	2:K:405:ASN:HB2	2.37	0.64
3:I:197:ARG:HA	3:I:225:GLU:HG2	1.76	0.64
2:B:454:ILE:HD12	2:B:454:ILE:C	2.18	0.64
1:A:148:LYS:CE	2:B:425:ASP:HB2	2.27	0.64
2:H:233:VAL:HG22	2:H:234:LYS:H	1.63	0.64
2:B:324:ALA:O	2:B:325:HIS:HB2	1.98	0.64
3:C:293:PHE:N	3:C:302:LYS:HG3	2.12	0.64
1:D:191:LYS:HG3	1:D:192:ASP:N	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.80	0.64
2:B:267:ASP:HB2	2:B:268:PRO:CD	2.26	0.64
2:H:251:VAL:C	2:H:252:ILE:HD13	2.17	0.64
1:J:154:ILE:HG12	3:L:128:VAL:HG21	1.80	0.64
2:B:310:LEU:HD12	2:B:310:LEU:O	1.98	0.64
2:E:284:ASN:HD22	2:E:285:TYR:H	1.45	0.64
2:H:191:GLU:C	2:H:193:CYS:H	2.00	0.64
2:H:304:ARG:NH2	2:H:333:ASN:N	2.45	0.64
1:J:143:GLN:O	1:J:147:MET:HG2	1.97	0.64
3:L:211:TYR:HE1	3:L:345:ASN:HD22	1.44	0.64
2:E:284:ASN:HD22	2:E:285:TYR:N	1.94	0.64
2:H:324:ALA:O	2:H:325:HIS:HB2	1.98	0.64
2:B:173:GLU:O	2:B:176:ARG:HB3	1.96	0.64
3:C:275:ARG:HB2	3:C:311:GLN:HG2	1.79	0.64
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.33	0.64
2:H:210:GLU:OE2	2:H:212:GLU:HB3	1.98	0.64
3:L:295:PHE:CE2	4:T:2:HYP:HD23	2.32	0.64
2:H:364:ASN:ND2	5:H:470:NAG:H62	2.11	0.64
1:J:133:ILE:O	1:J:133:ILE:HG23	1.96	0.64
2:H:251:VAL:O	2:H:252:ILE:HD13	1.98	0.64
3:I:195:GLN:O	3:I:196:LYS:CB	2.46	0.64
2:B:417:TYR:HB2	2:B:446:SER:CB	2.27	0.64
2:H:417:TYR:HB2	2:H:446:SER:CB	2.27	0.64
2:B:165:LEU:HG	2:B:166:ARG:NH2	2.12	0.64
2:H:345:TYR:CZ	2:H:351:ASN:HB2	2.32	0.64
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.80	0.64
3:F:119:GLN:NE2	3:F:122:VAL:HG21	2.13	0.64
3:I:365:ASN:N	3:I:365:ASN:ND2	2.45	0.64
3:L:242:ILE:HG22	3:L:243:PRO:HD2	1.79	0.64
3:I:307:HIS:CD2	3:I:334:TRP:HE1	2.16	0.64
2:E:242:MET:HA	2:E:247:GLY:HA3	1.80	0.64
3:C:125:LYS:HA	3:C:125:LYS:HE3	1.78	0.64
3:C:168:PHE:CD1	3:C:179:LEU:HD13	2.33	0.64
3:C:334:TRP:O	3:C:336:MET:HG2	1.97	0.64
2:H:199:VAL:O	3:I:142:THR:HG23	1.97	0.64
3:C:390:ASN:O	3:C:391:ARG:HD2	1.98	0.64
3:C:222:GLY:O	3:C:224:THR:HG22	1.99	0.63
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.66	0.63
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.33	0.63
3:C:113:ILE:O	3:C:113:ILE:HG22	1.98	0.63
2:B:455:ARG:HG3	2:B:456:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:VAL:O	3:C:142:THR:HG23	1.97	0.63
1:A:157:LYS:HD2	3:C:132:GLU:HB3	1.81	0.63
1:G:124:ARG:C	1:G:126:VAL:H	2.01	0.63
2:B:369:ILE:N	2:B:405:ASN:HD22	1.92	0.63
2:K:327:GLY:HA3	2:K:344:LYS:HE3	1.79	0.63
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.79	0.63
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.79	0.63
2:H:455:ARG:CG	2:H:456:PRO:HD2	2.28	0.63
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.33	0.63
3:C:195:GLN:O	3:C:196:LYS:CB	2.47	0.63
2:B:242:MET:HA	2:B:247:GLY:HA3	1.79	0.63
3:C:272:ASP:OD2	3:C:275:ARG:NE	2.31	0.63
2:H:238:VAL:HG22	2:H:239:TYR:N	2.14	0.63
3:L:192:THR:HG23	3:L:386:ILE:O	1.99	0.63
3:F:293:PHE:CD2	3:F:370:ALA:HB1	2.34	0.63
5:K:470:NAG:H61	4:R:4:PRO:HG2	1.80	0.63
3:C:178:PHE:CE2	3:C:228:LEU:HD11	2.33	0.63
2:H:408:HIS:CD2	2:H:411:ASN:HB2	2.33	0.63
2:B:373:MET:HE3	2:B:374:PHE:H	1.64	0.63
1:J:126:VAL:O	1:J:129:LYS:N	2.32	0.63
3:C:172:LEU:HD13	3:C:239:GLN:NE2	2.12	0.63
2:H:326:TYR:OH	2:H:351:ASN:ND2	2.32	0.63
3:I:227:TRP:HZ2	3:I:230:ASN:HD21	1.46	0.63
3:I:353:THR:HG23	3:I:377:TYR:CD1	2.34	0.63
2:B:402:TRP:CZ2	2:B:412:PRO:HD2	2.32	0.63
3:F:166:LEU:HD22	3:F:179:LEU:HD11	1.79	0.63
3:F:295:PHE:CE2	4:P:2:HYP:HD23	2.32	0.63
2:K:313:GLU:HG2	2:K:323:LYS:CD	2.28	0.63
2:B:153:ILE:O	2:B:153:ILE:HG12	1.99	0.63
2:H:310:LEU:O	2:H:310:LEU:HD12	1.99	0.63
3:I:172:LEU:CD1	3:I:172:LEU:H	2.11	0.63
2:E:234:LYS:HG2	2:E:235:PRO:HD2	1.80	0.63
1:A:151:GLU:CD	1:A:173:VAL:HG12	2.19	0.63
2:B:205:VAL:HG12	3:C:232:LYS:HZ3	1.64	0.63
2:E:327:GLY:HA3	2:E:344:LYS:CB	2.28	0.63
1:D:126:VAL:O	1:D:130:VAL:HG23	1.97	0.63
3:C:93:ILE:O	3:C:96:TYR:HB3	1.98	0.63
2:E:283:LYS:HB3	2:E:285:TYR:CE2	2.34	0.63
1:J:149:ARG:HH21	2:K:425:ASP:HA	1.64	0.63
1:J:130:VAL:C	1:J:133:ILE:HG22	2.19	0.63
2:K:397:GLU:HB3	2:K:431:THR:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:273:LYS:HG3	3:L:311:GLN:HB3	1.80	0.63
3:L:153:CYS:O	3:L:156:ILE:HB	1.99	0.63
2:K:203:ILE:HD12	2:K:203:ILE:H	1.62	0.63
3:L:295:PHE:HE2	4:T:2:HYP:HD23	1.64	0.63
2:K:266:TRP:HA	2:K:377:THR:HG21	1.81	0.63
2:E:355:ASP:O	2:E:365:ARG:NH1	2.32	0.63
3:C:172:LEU:CD1	3:C:172:LEU:H	2.11	0.63
1:J:182:GLN:O	1:J:186:GLU:HG2	1.98	0.63
3:I:168:PHE:CD1	3:I:179:LEU:HD13	2.33	0.63
3:L:337:ASN:C	3:L:339:CYS:H	2.01	0.63
2:H:228:GLN:HE21	2:H:231:SER:HA	1.63	0.63
2:K:370:HIS:CE1	2:K:408:HIS:HB2	2.34	0.63
2:K:301:GLN:NE2	2:K:302:LEU:HG	2.14	0.63
3:C:264:MET:N	3:C:264:MET:SD	2.71	0.63
1:G:178:TYR:C	1:G:180:ASP:H	2.03	0.62
3:C:315:TRP:HE3	3:C:328:GLU:HG2	1.63	0.62
2:H:180:GLN:C	2:H:182:LEU:H	2.01	0.62
2:H:454:ILE:HD12	2:H:454:ILE:C	2.20	0.62
3:I:258:SER:OG	3:I:372:TRP:NE1	2.31	0.62
2:B:373:MET:SD	2:B:405:ASN:HB2	2.39	0.62
2:B:420:GLY:HA2	2:B:446:SER:O	1.98	0.62
2:B:238:VAL:HG22	2:B:239:TYR:N	2.15	0.62
3:C:271:ALA:C	3:C:273:LYS:N	2.52	0.62
3:F:304:PHE:HA	3:F:337:ASN:ND2	2.14	0.62
1:G:191:LYS:O	1:G:192:ASP:HB3	1.99	0.62
3:F:320:ASP:HA	3:F:336:MET:O	1.99	0.62
1:J:127:ILE:HG23	2:K:153:ILE:CG2	2.18	0.62
2:B:340:ILE:HD12	2:B:403:TRP:CE3	2.34	0.62
2:K:327:GLY:HA3	2:K:344:LYS:CB	2.28	0.62
2:B:326:TYR:OH	2:B:351:ASN:ND2	2.32	0.62
3:C:160:GLY:O	3:C:161:ALA:HB3	1.98	0.62
1:A:123:LYS:O	1:A:126:VAL:HB	2.00	0.62
2:H:166:ARG:NE	2:H:166:ARG:HA	2.14	0.62
2:E:364:ASN:ND2	6:E:470:NDG:C7	2.62	0.62
2:K:183:GLU:CG	3:L:124:LEU:HG	2.29	0.62
3:I:197:ARG:NH2	3:I:348:TYR:HB2	2.14	0.62
3:I:305:THR:CG2	4:S:2:HYP:HD23	2.29	0.62
2:H:359:GLN:HE21	2:H:359:GLN:H	1.44	0.62
3:L:304:PHE:HA	3:L:337:ASN:ND2	2.14	0.62
1:A:121:VAL:HG23	1:A:122:LEU:N	2.13	0.62
2:B:157:VAL:HG23	2:B:158:ASN:ND2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:ND2	2:B:284:ASN:HB3	2.11	0.62
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.82	0.62
3:L:160:GLY:O	3:L:161:ALA:HB3	2.00	0.62
1:D:165:CYS:O	2:E:196:PRO:HA	2.00	0.62
3:L:101:LEU:HD22	3:L:101:LEU:N	2.15	0.62
3:F:265:PHE:O	3:F:266:LYS:HG3	1.99	0.62
3:L:293:PHE:CD2	3:L:370:ALA:HB1	2.35	0.62
3:C:112:GLU:C	3:C:114:TYR:H	2.02	0.62
2:H:292:TYR:HE2	2:H:294:LEU:HB2	1.64	0.62
3:I:334:TRP:O	3:I:336:MET:HG2	1.99	0.62
3:C:189:ASN:OD1	3:C:394:ILE:HD12	1.99	0.62
3:I:275:ARG:HB2	3:I:311:GLN:HG2	1.80	0.62
3:C:365:ASN:HD22	3:C:366:GLY:H	1.48	0.62
3:F:211:TYR:HE1	3:F:345:ASN:HD22	1.47	0.62
2:H:204:PRO:CG	3:I:217:HIS:HB3	2.27	0.62
3:I:315:TRP:HE3	3:I:328:GLU:HG2	1.65	0.62
1:G:130:VAL:N	1:G:133:ILE:HD13	2.14	0.62
3:I:272:ASP:O	3:I:273:LYS:HB2	2.00	0.62
3:I:153:CYS:HB2	3:I:192:THR:HG22	1.81	0.62
2:E:359:GLN:O	2:E:360:LEU:HD23	2.00	0.62
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.82	0.62
2:H:402:TRP:CZ2	2:H:412:PRO:HD2	2.33	0.62
2:K:284:ASN:HD22	2:K:285:TYR:H	1.46	0.62
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.80	0.62
3:I:235:LEU:HD12	3:I:235:LEU:N	2.15	0.62
2:K:215:ILE:CG2	2:K:216:ARG:N	2.63	0.62
1:G:143:GLN:HE22	3:I:117:ASN:HB2	1.65	0.62
2:K:266:TRP:CE3	2:K:380:ARG:HG2	2.35	0.62
3:F:205:LYS:HE2	3:F:331:GLY:HA2	1.82	0.62
3:C:168:PHE:CE1	3:C:179:LEU:HD13	2.34	0.61
1:J:147:MET:HG3	2:K:175:LEU:HD13	1.82	0.61
3:C:273:LYS:CE	3:C:319:ASN:HD21	2.12	0.61
2:E:317:TRP:CH2	2:E:448:ARG:HG3	2.34	0.61
2:H:236:TYR:HB2	2:H:298:LYS:HZ3	1.63	0.61
3:I:228:LEU:CD1	3:I:232:LYS:HD3	2.30	0.61
2:K:242:MET:HA	2:K:247:GLY:CA	2.30	0.61
2:B:330:THR:OG1	2:B:341:SER:HB2	1.99	0.61
2:E:313:GLU:HG2	2:E:323:LYS:HD3	1.80	0.61
2:B:165:LEU:N	2:B:166:ARG:NE	2.47	0.61
3:C:151:LYS:HD2	3:C:172:LEU:HD11	1.83	0.61
3:F:194:PHE:CA	3:F:228:LEU:HD12	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:367:ILE:O	3:I:367:ILE:HG22	2.00	0.61
2:B:253:GLN:HA	2:B:292:TYR:O	2.00	0.61
2:H:210:GLU:HA	2:H:227:ILE:HB	1.82	0.61
2:K:247:GLY:O	2:K:455:ARG:NH1	2.32	0.61
2:K:313:GLU:HG2	2:K:323:LYS:HD3	1.81	0.61
2:H:263:GLY:HA2	2:H:400:GLY:HA2	1.81	0.61
2:E:191:GLU:O	2:E:193:CYS:N	2.34	0.61
2:K:394:CYS:SG	2:K:407:CYS:N	2.73	0.61
1:A:128:GLU:HA	1:A:131:GLN:HG2	1.83	0.61
3:I:197:ARG:HA	3:I:225:GLU:CG	2.30	0.61
3:I:227:TRP:CD1	3:I:229:GLY:HA2	2.35	0.61
1:G:140:VAL:HA	3:I:114:TYR:HE1	1.66	0.61
2:E:313:GLU:HG2	2:E:323:LYS:CD	2.30	0.61
1:A:164:SER:CB	3:C:137:GLU:O	2.46	0.61
3:I:287:GLY:HA3	3:I:371:THR:O	2.00	0.61
2:H:390:PRO:HA	2:H:393:GLN:HE21	1.66	0.61
3:L:199:ASP:OD1	3:L:201:SER:HB3	1.99	0.61
3:L:298:ASP:O	3:L:301:ASP:HB2	1.99	0.61
3:F:334:TRP:CD1	3:F:335:TRP:N	2.69	0.61
3:I:199:ASP:N	3:I:225:GLU:OE2	2.34	0.61
1:G:129:LYS:O	1:G:130:VAL:HG23	1.99	0.61
2:B:256:GLN:HE21	2:B:449:LYS:HZ1	1.46	0.61
2:B:365:ARG:HG2	2:B:366:THR:N	2.16	0.61
1:G:166:SER:HB3	2:H:195:THR:O	2.00	0.61
3:F:209:ILE:O	3:F:213:GLU:HG2	2.00	0.61
2:H:223:GLU:CB	2:H:287:GLY:HA2	2.27	0.61
1:G:125:LYS:O	1:G:125:LYS:HG2	2.00	0.61
3:L:143:VAL:HA	3:L:220:PRO:HG2	1.82	0.61
1:G:167:ARG:C	1:G:167:ARG:HD2	2.20	0.61
1:J:149:ARG:NH2	2:K:425:ASP:HA	2.15	0.61
3:F:185:ASP:OD2	3:F:187:SER:HB3	2.01	0.61
2:K:277:ALA:HB1	2:K:286:CYS:HB3	1.81	0.61
3:C:100:ILE:O	3:C:100:ILE:HG22	2.01	0.61
3:I:230:ASN:ND2	3:I:230:ASN:H	1.98	0.61
3:L:204:PHE:HB3	3:L:211:TYR:OH	2.00	0.61
3:I:279:ALA:HB2	3:L:308:ASN:HD21	1.63	0.61
3:C:97:GLU:C	3:C:99:SER:H	2.04	0.61
3:F:265:PHE:CE2	3:F:267:VAL:HG23	2.36	0.61
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.35	0.61
3:C:107:ILE:O	3:C:107:ILE:HD13	2.01	0.61
3:I:271:ALA:C	3:I:273:LYS:N	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:295:PHE:H	3:C:301:ASP:HB3	1.65	0.61
2:B:205:VAL:HG23	3:C:216:GLY:O	2.01	0.61
2:H:411:ASN:N	2:H:436:VAL:O	2.32	0.61
3:I:251:GLU:HG2	3:I:252:ASP:N	2.14	0.61
3:C:272:ASP:O	3:C:273:LYS:HB2	2.01	0.61
3:I:329:GLN:OE1	3:I:361:ASN:HB2	2.01	0.61
3:L:288:ASP:C	3:L:371:THR:HG21	2.21	0.61
3:I:264:MET:SD	3:I:264:MET:N	2.73	0.61
2:E:191:GLU:CA	2:E:194:ARG:HH21	2.00	0.60
2:B:202:ASN:HA	3:C:143:VAL:HG11	1.82	0.60
3:C:367:ILE:HG22	3:C:379:MET:CG	2.30	0.60
2:E:429:HIS:O	2:E:431:THR:HG23	2.01	0.60
2:H:267:ASP:HB2	2:H:268:PRO:CD	2.29	0.60
3:F:288:ASP:C	3:F:371:THR:HG21	2.21	0.60
3:C:353:THR:HA	3:C:376:TRP:O	2.01	0.60
1:G:154:ILE:HD13	2:H:186:VAL:CG2	2.31	0.60
3:F:343:HIS:O	3:F:367:ILE:HA	2.01	0.60
3:I:167:TYR:N	3:I:167:TYR:CD1	2.69	0.60
2:B:304:ARG:NH2	2:B:333:ASN:N	2.48	0.60
3:I:117:ASN:C	3:I:119:GLN:H	2.04	0.60
3:F:287:GLY:HA3	3:F:371:THR:HB	1.84	0.60
3:I:103:HIS:C	3:I:105:SER:H	2.05	0.60
2:B:236:TYR:HB2	2:B:298:LYS:HZ3	1.64	0.60
1:D:143:GLN:HE21	3:F:118:ASN:ND2	1.99	0.60
2:K:283:LYS:HB3	2:K:285:TYR:CE2	2.36	0.60
3:F:199:ASP:N	3:F:225:GLU:OE2	2.32	0.60
2:B:307:PRO:HB2	2:B:457:PHE:C	2.21	0.60
1:A:143:GLN:NE2	1:A:143:GLN:HA	2.11	0.60
2:B:178:LYS:C	2:B:180:GLN:N	2.52	0.60
3:C:170:LYS:HE2	3:C:177:GLN:HB3	1.84	0.60
2:K:215:ILE:HA	2:K:219:GLY:O	2.01	0.60
3:I:160:GLY:O	3:I:161:ALA:HB3	2.02	0.60
1:G:158:ILE:HD11	2:H:189:GLN:HB3	1.83	0.60
1:A:127:ILE:O	1:A:130:VAL:HG12	2.01	0.60
3:F:231:GLU:O	3:F:234:HIS:HB3	2.02	0.60
2:H:412:PRO:O	2:H:413:ASN:HB2	2.01	0.60
2:H:253:GLN:HA	2:H:292:TYR:O	2.02	0.60
2:H:205:VAL:HG12	3:I:232:LYS:HZ3	1.64	0.60
3:L:304:PHE:CD1	3:L:338:LYS:HB2	2.37	0.60
3:C:353:THR:HG23	3:C:377:TYR:CD1	2.37	0.60
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:340:HIS:ND1	3:L:368:ILE:HD11	2.16	0.60
3:F:104:ASP:HA	3:F:107:ILE:HG22	1.84	0.60
3:C:329:GLN:NE2	4:O:3:ARG:NH1	2.50	0.60
2:E:303:THR:HB	2:E:330:THR:HA	1.83	0.60
1:J:122:LEU:HD13	1:J:122:LEU:C	2.22	0.60
2:H:307:PRO:HB2	2:H:457:PHE:C	2.21	0.60
2:K:357:ALA:HB3	2:K:360:LEU:HD12	1.81	0.60
3:C:197:ARG:NH2	3:C:348:TYR:HB2	2.16	0.60
2:H:187:SER:O	2:H:191:GLU:HB2	2.02	0.60
2:B:412:PRO:HG3	2:B:450:MET:HE3	1.82	0.60
2:K:346:ARG:HH11	2:K:346:ARG:HG2	1.67	0.60
2:K:317:TRP:CH2	2:K:448:ARG:HG3	2.36	0.60
3:I:316:ASP:O	3:I:317:ASN:HB2	2.01	0.60
2:B:409:ALA:O	2:B:438:MET:HB2	2.01	0.60
2:B:161:ILE:O	2:B:166:ARG:CZ	2.50	0.60
3:C:195:GLN:HE21	3:C:384:MET:HG3	1.65	0.60
3:I:259:THR:O	3:I:284:GLY:HA3	2.02	0.60
2:E:352:ALA:CB	2:E:439:ASN:ND2	2.63	0.60
2:B:310:LEU:HD23	2:B:329:PHE:CD2	2.37	0.60
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.67	0.60
2:B:228:GLN:HG3	2:B:235:PRO:HG3	1.84	0.60
2:K:205:VAL:HG12	2:K:206:VAL:N	2.17	0.60
3:C:214:GLY:HA2	3:C:229:GLY:CA	2.29	0.60
3:C:353:THR:HG23	3:C:377:TYR:HD1	1.65	0.60
3:L:194:PHE:CA	3:L:228:LEU:HD12	2.29	0.60
2:E:242:MET:HA	2:E:247:GLY:CA	2.32	0.60
3:L:246:LEU:HD13	3:L:265:PHE:CE1	2.37	0.60
2:B:204:PRO:HA	3:C:217:HIS:CA	2.29	0.60
3:C:178:PHE:CE2	3:C:228:LEU:HD21	2.35	0.60
3:C:248:VAL:O	3:C:259:THR:HA	2.02	0.60
3:I:172:LEU:HD13	3:I:239:GLN:NE2	2.16	0.60
3:I:178:PHE:CE2	3:I:228:LEU:HD21	2.35	0.60
2:E:327:GLY:HA3	2:E:344:LYS:HE3	1.83	0.60
2:E:331:VAL:HA	2:E:339:GLN:O	2.01	0.60
2:B:356:GLY:HA2	2:B:368:THR:O	2.00	0.60
2:E:215:ILE:HA	2:E:219:GLY:O	2.02	0.60
3:L:199:ASP:N	3:L:225:GLU:OE2	2.33	0.60
3:F:199:ASP:OD1	3:F:201:SER:HB3	2.01	0.60
2:B:205:VAL:HG21	3:C:215:PHE:O	2.03	0.59
3:C:293:PHE:CD2	3:C:370:ALA:HB1	2.36	0.59
1:A:169:LEU:HB2	2:B:189:GLN:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:195:GLN:HE21	3:I:384:MET:HG3	1.65	0.59
3:I:251:GLU:HB3	3:I:381:LYS:HB2	1.84	0.59
3:L:204:PHE:C	3:L:206:LYS:H	2.04	0.59
1:G:140:VAL:HG23	1:G:141:ARG:N	2.16	0.59
2:E:205:VAL:HG12	2:E:206:VAL:N	2.17	0.59
2:B:280:THR:O	2:B:281:ASP:OD2	2.19	0.59
1:A:127:ILE:HA	1:A:130:VAL:HG12	1.85	0.59
3:I:300:SER:C	3:I:302:LYS:N	2.56	0.59
2:B:210:GLU:HA	2:B:227:ILE:HB	1.84	0.59
2:B:252:ILE:HG12	2:B:452:MET:O	2.03	0.59
2:H:152:TYR:C	2:H:154:ASP:N	2.54	0.59
3:C:167:TYR:CD1	3:C:167:TYR:N	2.70	0.59
2:H:293:TRP:HE1	2:H:296:ASN:HD21	1.51	0.59
1:A:148:LYS:HE3	2:B:425:ASP:HB2	1.83	0.59
2:B:165:LEU:HD21	3:C:107:ILE:HG12	1.84	0.59
2:B:176:ARG:NH1	2:B:179:ILE:HD12	2.16	0.59
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.03	0.59
2:H:356:GLY:HA2	2:H:368:THR:O	2.01	0.59
3:I:178:PHE:CE2	3:I:228:LEU:HD11	2.37	0.59
3:I:331:GLY:O	3:I:332:SER:HB3	2.03	0.59
3:I:367:ILE:HG21	3:I:379:MET:HB2	1.85	0.59
3:L:195:GLN:OE1	3:L:382:THR:HG22	2.03	0.59
2:K:325:HIS:HB3	2:K:346:ARG:HB3	1.85	0.59
2:E:179:ILE:O	2:E:183:GLU:HG3	2.02	0.59
2:B:228:GLN:HE21	2:B:231:SER:HA	1.67	0.59
3:L:265:PHE:CE2	3:L:267:VAL:HG23	2.38	0.59
2:H:209:LYS:HB3	2:H:209:LYS:HZ2	1.66	0.59
3:L:95:LYS:HG2	3:L:98:ALA:HB3	1.83	0.59
2:E:277:ALA:HB1	2:E:286:CYS:HB3	1.84	0.59
3:C:334:TRP:HZ3	3:C:344:LEU:HB2	1.68	0.59
3:C:293:PHE:CE2	3:C:370:ALA:HB1	2.38	0.59
2:H:373:MET:CG	2:H:405:ASN:HB2	2.32	0.59
3:I:168:PHE:CE1	3:I:179:LEU:HD13	2.37	0.59
3:I:251:GLU:OE1	3:I:381:LYS:HD2	2.02	0.59
3:I:367:ILE:HG22	3:I:379:MET:CG	2.32	0.59
2:H:359:GLN:NE2	2:H:359:GLN:N	2.48	0.59
3:L:322:PHE:CZ	4:T:3:ARG:HD2	2.37	0.59
3:I:117:ASN:N	3:I:117:ASN:HD22	1.99	0.59
2:H:409:ALA:O	2:H:438:MET:HB2	2.02	0.59
2:B:161:ILE:HG22	2:B:162:PRO:HD3	1.84	0.59
3:C:141:ASP:OD2	3:C:143:VAL:HG22	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:278:TYR:CZ	3:I:308:ASN:HB2	2.37	0.59
2:K:301:GLN:NE2	2:K:302:LEU:N	2.51	0.59
1:J:124:ARG:HH11	1:J:124:ARG:HG2	1.68	0.59
2:K:429:HIS:O	2:K:431:THR:HG23	2.01	0.59
3:I:214:GLY:HA2	3:I:229:GLY:CA	2.30	0.59
3:I:353:THR:HA	3:I:376:TRP:O	2.03	0.59
3:L:343:HIS:O	3:L:367:ILE:HA	2.02	0.59
2:K:209:LYS:HG3	2:K:213:GLU:OE1	2.01	0.59
2:E:215:ILE:CG2	2:E:216:ARG:N	2.65	0.59
2:B:266:TRP:HE1	2:B:380:ARG:HH21	1.48	0.59
2:B:152:TYR:O	2:B:154:ASP:N	2.36	0.59
4:N:3:ARG:HH21	4:N:3:ARG:HG2	1.67	0.59
3:C:169:ILE:CD1	3:C:171:PRO:HD3	2.32	0.59
2:H:373:MET:SD	2:H:405:ASN:HB2	2.42	0.59
3:I:103:HIS:HA	3:I:106:SER:CB	2.29	0.59
2:B:365:ARG:O	2:B:368:THR:HG23	2.02	0.59
3:L:97:GLU:C	3:L:99:SER:H	2.06	0.59
1:G:139:ASN:HB3	3:I:114:TYR:CZ	2.37	0.59
3:F:246:LEU:HD22	3:F:265:PHE:CD1	2.38	0.59
3:L:92:GLU:HG2	3:L:93:ILE:N	2.17	0.59
2:K:304:ARG:C	2:K:306:GLY:H	2.05	0.59
2:E:191:GLU:C	2:E:193:CYS:H	2.06	0.59
3:C:198:LEU:HD22	3:C:223:THR:HG23	1.85	0.59
2:H:177:SER:O	2:H:180:GLN:HB2	2.02	0.59
3:F:344:LEU:HD22	3:F:382:THR:OG1	2.03	0.59
3:I:154:GLN:CD	3:I:190:GLY:H	2.06	0.59
3:L:251:GLU:OE1	3:L:381:LYS:HD2	2.02	0.59
3:C:329:GLN:OE1	3:C:361:ASN:HB2	2.02	0.59
3:F:246:LEU:HD13	3:F:265:PHE:CE1	2.38	0.59
1:A:190:ALA:O	1:A:191:LYS:HG3	2.02	0.59
2:H:280:THR:O	2:H:281:ASP:OD2	2.20	0.59
2:K:164:ASN:O	2:K:168:LEU:HD23	2.02	0.59
2:K:356:GLY:HA3	2:K:368:THR:OG1	2.01	0.59
2:H:374:PHE:HB3	2:H:382:ASN:HB3	1.85	0.59
1:J:151:GLU:HG3	1:J:178:TYR:OH	2.03	0.59
2:B:340:ILE:HG23	2:B:340:ILE:O	2.03	0.59
2:E:160:ASN:H	2:E:162:PRO:HD2	1.67	0.59
2:B:180:GLN:HA	2:B:183:GLU:OE1	2.02	0.58
3:L:251:GLU:CD	3:L:381:LYS:HD2	2.23	0.58
2:K:315:GLU:OE2	2:K:448:ARG:NH2	2.35	0.58
2:B:251:VAL:O	2:B:252:ILE:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.18	0.58
2:H:171:ILE:HA	2:H:174:ASN:HB2	1.85	0.58
2:K:303:THR:HB	2:K:330:THR:HG22	1.84	0.58
2:B:176:ARG:HH11	2:B:176:ARG:CA	2.16	0.58
3:F:251:GLU:OE1	3:F:381:LYS:HD2	2.03	0.58
3:I:329:GLN:HE22	3:I:363:TYR:HB2	1.69	0.58
2:B:365:ARG:O	2:B:367:MET:N	2.37	0.58
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.37	0.58
2:B:209:LYS:HZ2	2:B:209:LYS:HB3	1.65	0.58
3:I:181:TYR:CG	3:I:181:TYR:O	2.55	0.58
2:B:218:GLY:CA	3:C:210:GLN:HE21	2.16	0.58
2:B:263:GLY:HA2	2:B:400:GLY:HA2	1.84	0.58
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.03	0.58
3:C:300:SER:C	3:C:302:LYS:N	2.57	0.58
1:D:127:ILE:HG23	1:D:128:GLU:H	1.67	0.58
3:L:246:LEU:HD13	3:L:265:PHE:CD1	2.39	0.58
2:E:303:THR:HB	2:E:330:THR:HG22	1.84	0.58
1:A:119:ILE:O	1:A:119:ILE:HG12	2.02	0.58
1:A:128:GLU:OE1	1:A:129:LYS:HD3	2.02	0.58
3:F:204:PHE:C	3:F:206:LYS:H	2.05	0.58
3:I:198:LEU:HD22	3:I:223:THR:HG23	1.86	0.58
3:L:231:GLU:O	3:L:234:HIS:HB3	2.03	0.58
2:H:420:GLY:HA2	2:H:446:SER:O	2.03	0.58
2:K:199:VAL:O	3:L:142:THR:HG23	2.03	0.58
3:I:312:PHE:CE1	3:I:334:TRP:HA	2.38	0.58
2:K:331:VAL:HA	2:K:339:GLN:O	2.02	0.58
2:K:212:GLU:HG3	2:K:212:GLU:O	2.03	0.58
1:A:140:VAL:HG23	1:A:141:ARG:H	1.67	0.58
3:C:259:THR:O	3:C:284:GLY:HA3	2.04	0.58
3:C:334:TRP:O	3:C:336:MET:N	2.37	0.58
2:H:230:ASP:C	2:H:232:SER:H	2.07	0.58
2:B:412:PRO:HB3	2:B:450:MET:HG2	1.86	0.58
3:F:236:ILE:O	3:F:239:GLN:HG2	2.03	0.58
1:D:137:GLN:OE1	1:D:189:ILE:HA	2.03	0.58
1:J:181:GLN:HE22	2:K:174:ASN:CB	2.17	0.58
3:I:242:ILE:HD12	3:I:242:ILE:N	2.18	0.58
3:L:154:GLN:HA	3:L:190:GLY:HA3	1.85	0.58
3:F:93:ILE:O	3:F:95:LYS:N	2.37	0.58
2:B:223:GLU:CB	2:B:287:GLY:HA2	2.28	0.58
3:C:170:LYS:NZ	3:C:177:GLN:H	2.02	0.58
3:C:316:ASP:O	3:C:317:ASN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:191:GLU:O	2:K:193:CYS:N	2.37	0.58
2:H:202:ASN:HD22	2:H:284:ASN:CB	2.15	0.58
1:J:134:GLN:OE1	1:J:137:GLN:HB2	2.04	0.58
3:F:117:ASN:O	3:F:121:ILE:HG13	2.03	0.58
3:I:272:ASP:OD2	3:I:275:ARG:NE	2.36	0.58
3:F:304:PHE:CD1	3:F:338:LYS:HB3	2.39	0.58
2:K:356:GLY:HA2	2:K:409:ALA:CB	2.33	0.58
1:J:139:ASN:HB3	3:L:114:TYR:CZ	2.39	0.58
2:K:172:LEU:HB3	3:L:113:ILE:HG21	1.85	0.58
2:E:304:ARG:C	2:E:306:GLY:H	2.06	0.58
3:F:154:GLN:HA	3:F:190:GLY:HA3	1.85	0.58
2:B:161:ILE:HG21	3:C:103:HIS:NE2	2.19	0.58
3:I:295:PHE:H	3:I:301:ASP:HB3	1.67	0.58
2:K:270:LYS:HG2	2:K:270:LYS:O	2.04	0.58
2:B:345:TYR:CZ	2:B:351:ASN:HB2	2.38	0.58
2:H:455:ARG:HG3	2:H:456:PRO:HD2	1.85	0.58
2:K:405:ASN:C	2:K:407:CYS:N	2.56	0.58
2:B:171:ILE:O	2:B:175:LEU:HB3	2.03	0.58
3:C:331:GLY:O	3:C:332:SER:HB3	2.04	0.58
3:I:246:LEU:HD11	3:I:248:VAL:HG23	1.85	0.58
1:G:130:VAL:HA	1:G:133:ILE:HB	1.85	0.58
2:B:337:LYS:HG3	2:B:374:PHE:CD2	2.38	0.58
2:B:412:PRO:O	2:B:413:ASN:HB2	2.03	0.58
3:F:250:LEU:HD21	3:F:369:TRP:CD1	2.39	0.58
1:G:174:ASP:OD1	1:G:177:ASP:HB2	2.03	0.58
3:I:141:ASP:OD2	3:I:143:VAL:HG22	2.03	0.57
3:I:293:PHE:CE2	3:I:370:ALA:HB1	2.40	0.57
2:B:310:LEU:HD12	2:B:310:LEU:C	2.25	0.57
3:L:276:LEU:HD21	3:L:278:TYR:HD2	1.69	0.57
3:I:340:HIS:C	4:S:1:GLY:H2	2.07	0.57
1:A:140:VAL:CG2	1:A:141:ARG:N	2.68	0.57
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.50	0.57
2:H:337:LYS:HG3	2:H:374:PHE:CD2	2.38	0.57
2:E:247:GLY:O	2:E:455:ARG:NH1	2.36	0.57
3:L:246:LEU:HD22	3:L:265:PHE:CD1	2.40	0.57
2:B:303:THR:HA	2:B:308:THR:HG21	1.85	0.57
3:C:230:ASN:HD22	3:C:230:ASN:H	1.48	0.57
2:H:204:PRO:HA	3:I:217:HIS:CA	2.32	0.57
2:K:234:LYS:HD3	2:K:235:PRO:N	2.19	0.57
3:C:329:GLN:HE22	3:C:363:TYR:HB2	1.69	0.57
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:355:ASP:O	2:K:365:ARG:NH1	2.37	0.57
2:B:224:MET:CE	2:B:237:ARG:HE	2.17	0.57
3:C:352:GLY:HA2	3:C:378:SER:HB3	1.85	0.57
1:A:158:ILE:CG1	2:B:189:GLN:HG3	2.35	0.57
3:I:170:LYS:HE2	3:I:177:GLN:HB3	1.87	0.57
3:I:151:LYS:HD2	3:I:172:LEU:HD11	1.87	0.57
3:I:248:VAL:O	3:I:259:THR:HA	2.04	0.57
3:I:293:PHE:CD2	3:I:370:ALA:HB1	2.39	0.57
2:K:455:ARG:HG3	2:K:456:PRO:HD2	1.86	0.57
1:A:189:ILE:O	1:A:190:ALA:HB3	2.04	0.57
3:C:181:TYR:O	3:C:181:TYR:CG	2.56	0.57
2:K:169:ARG:HG2	2:K:173:GLU:OE2	2.04	0.57
6:E:470:NDG:O6	4:N:4:PRO:HG3	2.05	0.57
2:B:172:LEU:HD21	3:C:114:TYR:HB2	1.87	0.57
3:F:204:PHE:HB3	3:F:211:TYR:OH	2.03	0.57
2:H:340:ILE:HG12	2:H:342:VAL:HG13	1.87	0.57
2:H:202:ASN:ND2	2:H:284:ASN:HB3	2.17	0.57
3:L:204:PHE:O	3:L:211:TYR:HE2	1.87	0.57
3:C:272:ASP:CG	3:C:275:ARG:HE	2.07	0.57
3:L:340:HIS:CE1	3:L:368:ILE:HD11	2.40	0.57
1:J:156:ILE:HG21	2:K:415:ARG:HH11	1.68	0.57
1:J:116:ARG:O	1:J:120:GLU:HG3	2.05	0.57
2:H:228:GLN:HG3	2:H:235:PRO:HG3	1.87	0.57
3:F:295:PHE:HE2	4:P:2:HYP:HD23	1.69	0.57
1:G:159:ARG:NH1	2:H:418:TRP:CE3	2.73	0.57
1:D:149:ARG:NH2	2:E:425:ASP:HA	2.19	0.57
3:L:299:PRO:O	3:L:301:ASP:N	2.35	0.57
2:B:161:ILE:HG23	2:B:166:ARG:HH22	1.69	0.57
1:A:167:ARG:HH12	1:A:169:LEU:HD22	1.68	0.57
2:B:402:TRP:HB3	2:B:404:TYR:CE1	2.40	0.57
2:E:301:GLN:NE2	2:E:302:LEU:N	2.53	0.57
2:E:203:ILE:CD1	2:E:203:ILE:H	2.18	0.57
3:C:92:GLU:O	3:C:95:LYS:HE3	2.03	0.57
3:I:220:PRO:HG2	3:I:221:THR:H	1.70	0.57
3:I:334:TRP:O	3:I:336:MET:N	2.38	0.57
3:I:334:TRP:HZ3	3:I:344:LEU:HB2	1.69	0.57
2:E:255:ARG:NH1	2:E:255:ARG:HG3	2.20	0.57
2:H:152:TYR:C	2:H:154:ASP:H	2.08	0.57
2:K:158:ASN:HD21	3:L:100:ILE:HD12	1.70	0.57
2:B:173:GLU:C	2:B:175:LEU:H	2.08	0.57
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:251:GLU:OE1	3:C:381:LYS:HD2	2.04	0.57
3:I:326:CYS:HB3	3:I:336:MET:HE2	1.86	0.57
3:I:274:TYR:O	3:I:335:TRP:NE1	2.37	0.57
3:I:337:ASN:C	3:I:339:CYS:N	2.57	0.57
2:B:340:ILE:HG12	2:B:342:VAL:HG13	1.87	0.57
2:B:415:ARG:N	2:B:434:GLY:HA2	2.15	0.57
2:B:213:GLU:O	2:B:217:LYS:HG3	2.05	0.57
1:J:149:ARG:O	1:J:152:VAL:HG22	2.05	0.57
1:G:168:ALA:HA	2:H:189:GLN:OE1	2.04	0.57
1:A:169:LEU:HD13	1:A:170:ALA:N	2.20	0.57
1:A:158:ILE:HD13	1:A:171:ARG:HE	1.70	0.57
3:I:326:CYS:HB3	3:I:336:MET:CE	2.35	0.57
3:I:195:GLN:HE22	3:I:382:THR:HG22	1.69	0.57
1:J:185:LEU:HD22	1:J:189:ILE:HG13	1.86	0.57
2:K:234:LYS:HD3	2:K:234:LYS:C	2.25	0.57
2:K:201:CYS:O	3:L:143:VAL:HG21	2.05	0.57
2:K:160:ASN:O	2:K:161:ILE:C	2.42	0.57
3:C:315:TRP:CE3	3:C:328:GLU:HG2	2.39	0.57
3:I:170:LYS:NZ	3:I:177:GLN:H	2.03	0.57
2:E:265:LYS:O	2:E:268:PRO:HD2	2.05	0.57
1:D:169:LEU:HD13	2:E:185:ASP:OD1	2.05	0.57
2:E:356:GLY:HA3	2:E:368:THR:OG1	2.04	0.57
3:C:110:LEU:HD23	3:C:110:LEU:C	2.24	0.56
2:B:199:VAL:N	3:C:140:LYS:O	2.38	0.56
3:C:367:ILE:HG21	3:C:379:MET:HB2	1.87	0.56
3:F:204:PHE:O	3:F:211:TYR:HE2	1.88	0.56
2:H:205:VAL:HG23	3:I:216:GLY:O	2.05	0.56
2:B:230:ASP:C	2:B:232:SER:H	2.08	0.56
2:B:158:ASN:ND2	3:C:100:ILE:HD13	2.20	0.56
3:C:193:VAL:HG22	3:C:385:LYS:HB3	1.87	0.56
3:C:199:ASP:N	3:C:225:GLU:OE2	2.37	0.56
1:A:155:ASP:O	1:A:158:ILE:HG22	2.05	0.56
1:A:159:ARG:C	1:A:161:CYS:H	2.06	0.56
1:J:154:ILE:HD12	2:K:182:LEU:HD13	1.88	0.56
2:K:255:ARG:NH1	2:K:255:ARG:HG3	2.20	0.56
1:G:186:GLU:HA	1:G:189:ILE:HG22	1.87	0.56
2:B:209:LYS:CB	2:B:209:LYS:NZ	2.68	0.56
2:H:410:ALA:HB1	2:H:437:TRP:CE3	2.39	0.56
2:K:359:GLN:O	2:K:360:LEU:HD23	2.05	0.56
2:B:176:ARG:HH12	2:B:179:ILE:CD1	2.18	0.56
3:F:367:ILE:O	3:F:378:SER:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:PHE:CD2	3:F:384:MET:O	2.58	0.56
3:F:196:LYS:HG2	3:F:198:LEU:CD1	2.36	0.56
2:H:310:LEU:HD23	2:H:329:PHE:CD2	2.41	0.56
1:J:151:GLU:HG3	1:J:178:TYR:CE2	2.41	0.56
1:J:157:LYS:CA	1:J:157:LYS:HE2	2.28	0.56
3:I:97:GLU:O	3:I:99:SER:N	2.38	0.56
2:B:233:VAL:HG22	2:B:234:LYS:N	2.20	0.56
2:B:408:HIS:O	4:M:1:GLY:N	2.37	0.56
3:F:143:VAL:HG23	3:F:143:VAL:O	2.05	0.56
2:K:210:GLU:HA	2:K:227:ILE:CG2	2.35	0.56
2:E:210:GLU:HA	2:E:227:ILE:CG2	2.35	0.56
3:L:289:ALA:HB3	3:L:369:TRP:CZ2	2.40	0.56
2:E:351:ASN:HD21	2:E:354:MET:HB2	1.70	0.56
3:C:153:CYS:HB2	3:C:192:THR:HG22	1.86	0.56
2:B:410:ALA:HB1	2:B:437:TRP:CE3	2.39	0.56
3:C:169:ILE:O	3:C:177:GLN:HB2	2.05	0.56
2:E:211:CYS:HB3	2:E:242:MET:HE1	1.86	0.56
2:E:356:GLY:HA2	2:E:409:ALA:CB	2.35	0.56
3:F:278:TYR:CE2	3:F:308:ASN:HB2	2.40	0.56
2:K:352:ALA:CB	2:K:439:ASN:ND2	2.62	0.56
1:D:127:ILE:HG23	1:D:128:GLU:N	2.20	0.56
3:F:104:ASP:CA	3:F:107:ILE:HG22	2.35	0.56
1:J:116:ARG:H	1:J:116:ARG:CD	2.17	0.56
2:H:218:GLY:CA	3:I:210:GLN:HE21	2.19	0.56
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.40	0.56
3:I:169:ILE:HD11	3:I:178:PHE:CE1	2.41	0.56
3:I:390:ASN:O	3:I:391:ARG:HD2	2.06	0.56
3:C:154:GLN:CD	3:C:190:GLY:H	2.09	0.56
1:D:144:LEU:HD22	1:D:182:GLN:CG	2.36	0.56
2:E:404:TYR:O	2:E:405:ASN:HB2	2.05	0.56
1:A:157:LYS:HZ2	3:C:132:GLU:HB2	1.70	0.56
2:H:402:TRP:HB3	2:H:404:TYR:CE1	2.41	0.56
1:G:128:GLU:O	1:G:133:ILE:HD13	2.05	0.56
3:L:196:LYS:HG2	3:L:198:LEU:CD1	2.36	0.56
2:B:152:TYR:C	2:B:154:ASP:N	2.56	0.56
2:H:279:ASN:C	2:H:281:ASP:H	2.07	0.56
2:E:406:ARG:NH2	4:N:4:PRO:O	2.39	0.56
2:B:176:ARG:HH11	2:B:176:ARG:HA	1.70	0.56
1:G:144:LEU:HD13	1:G:182:GLN:HA	1.88	0.56
3:I:96:TYR:C	3:I:96:TYR:CD1	2.79	0.56
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:322:PHE:CD2	3:C:324:GLY:N	2.74	0.56
2:E:198:THR:HG22	3:F:140:LYS:O	2.06	0.56
3:C:242:ILE:N	3:C:242:ILE:HD12	2.21	0.56
3:C:312:PHE:CZ	3:C:333:GLY:O	2.59	0.56
3:I:304:PHE:CG	3:I:338:LYS:HB3	2.41	0.56
2:B:310:LEU:HB3	2:B:329:PHE:CD2	2.41	0.56
3:L:278:TYR:CE2	3:L:308:ASN:HB2	2.40	0.56
2:B:411:ASN:ND2	2:B:434:GLY:H	2.04	0.56
2:B:359:GLN:HE21	2:B:359:GLN:H	1.50	0.56
1:A:133:ILE:HD13	2:B:164:ASN:HD22	1.69	0.56
3:C:246:LEU:HD12	3:C:247:ARG:H	1.70	0.56
3:C:367:ILE:HG22	3:C:367:ILE:O	2.06	0.56
2:H:173:GLU:O	2:H:175:LEU:N	2.36	0.56
2:H:362:GLY:O	2:H:365:ARG:N	2.39	0.56
3:L:209:ILE:O	3:L:213:GLU:HG2	2.05	0.56
2:K:311:LEU:HD22	2:K:325:HIS:CD2	2.40	0.56
2:K:156:THR:O	2:K:158:ASN:N	2.39	0.56
3:L:267:VAL:HA	3:L:275:ARG:O	2.06	0.56
2:B:181:LYS:C	2:B:183:GLU:H	2.08	0.55
3:C:251:GLU:HG2	3:C:252:ASP:N	2.19	0.55
2:H:176:ARG:HG2	2:H:176:ARG:HH11	1.69	0.55
3:I:195:GLN:O	3:I:196:LYS:HB3	2.06	0.55
3:L:194:PHE:CD2	3:L:384:MET:O	2.59	0.55
2:H:261:ASP:OD2	2:H:261:ASP:C	2.45	0.55
2:K:265:LYS:O	2:K:268:PRO:HD2	2.06	0.55
2:K:407:CYS:HB2	4:R:1:GLY:O	2.06	0.55
2:B:173:GLU:O	2:B:176:ARG:N	2.39	0.55
3:F:196:LYS:O	3:F:197:ARG:HD2	2.05	0.55
2:H:310:LEU:HD12	2:H:310:LEU:C	2.27	0.55
3:L:172:LEU:HD22	3:L:240:SER:OG	2.06	0.55
3:I:169:ILE:O	3:I:177:GLN:HB2	2.06	0.55
1:G:129:LYS:HA	1:G:133:ILE:CD1	2.35	0.55
2:B:229:PRO:HG2	2:B:233:VAL:HG11	1.87	0.55
2:E:340:ILE:HG12	2:E:341:SER:N	2.21	0.55
2:E:366:THR:HA	2:E:369:ILE:CD1	2.36	0.55
3:C:224:THR:HG23	3:C:224:THR:O	2.05	0.55
2:H:175:LEU:O	2:H:179:ILE:HG13	2.07	0.55
3:F:276:LEU:HD11	3:F:290:PHE:CE2	2.42	0.55
3:I:172:LEU:CD1	3:I:239:GLN:HE21	2.17	0.55
2:B:309:GLU:O	2:B:309:GLU:HG3	2.06	0.55
2:B:258:GLY:O	2:B:260:VAL:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ASN:ND2	2:B:354:MET:H	2.04	0.55
2:E:234:LYS:HD3	2:E:235:PRO:N	2.21	0.55
2:K:203:ILE:H	2:K:203:ILE:CD1	2.19	0.55
3:L:108:ARG:O	3:L:112:GLU:HG3	2.06	0.55
3:F:246:LEU:HD13	3:F:265:PHE:CD1	2.42	0.55
2:B:173:GLU:HA	2:B:176:ARG:HB3	1.88	0.55
3:C:318:ASP:OD2	3:C:325:ASN:HB2	2.06	0.55
2:E:394:CYS:O	2:E:397:GLU:O	2.25	0.55
3:L:228:LEU:O	3:L:232:LYS:HD2	2.06	0.55
2:B:412:PRO:HG3	2:B:450:MET:HE2	1.89	0.55
3:F:169:ILE:HD11	3:F:236:ILE:HD11	1.88	0.55
2:K:332:GLN:HB3	2:K:336:ASN:HB2	1.88	0.55
3:I:288:ASP:OD2	3:I:291:ASP:HB2	2.06	0.55
3:F:109:TYR:CD1	3:F:110:LEU:HD23	2.41	0.55
3:C:312:PHE:CE1	3:C:334:TRP:HA	2.41	0.55
3:I:126:GLU:O	3:I:129:ALA:HB3	2.07	0.55
2:H:256:GLN:NE2	2:H:449:LYS:HZ1	1.95	0.55
2:H:312:ILE:HG12	2:H:452:MET:HG2	1.89	0.55
2:H:340:ILE:HD12	2:H:403:TRP:CE3	2.42	0.55
2:B:373:MET:CG	2:B:405:ASN:HB2	2.36	0.55
3:L:270:GLU:HB2	3:L:274:TYR:CZ	2.40	0.55
3:I:276:LEU:O	3:I:276:LEU:HD12	2.07	0.55
2:H:209:LYS:CB	2:H:209:LYS:NZ	2.70	0.55
2:H:156:THR:HG22	2:H:160:ASN:HD22	1.72	0.55
3:F:267:VAL:HA	3:F:275:ARG:O	2.07	0.55
2:E:360:LEU:O	2:E:365:ARG:HD2	2.07	0.55
2:B:176:ARG:HH11	2:B:176:ARG:CG	2.19	0.55
3:C:274:TYR:O	3:C:335:TRP:NE1	2.40	0.55
3:F:212:LYS:HG3	3:F:231:GLU:HB2	1.88	0.55
3:L:344:LEU:HA	3:L:367:ILE:HG23	1.88	0.55
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.42	0.55
3:L:287:GLY:HA3	3:L:371:THR:HB	1.89	0.55
2:B:279:ASN:C	2:B:281:ASP:H	2.08	0.55
1:A:163:GLY:O	3:C:138:PRO:HA	2.07	0.55
3:C:195:GLN:HE22	3:C:382:THR:HG22	1.71	0.55
3:C:256:ARG:HG3	3:C:256:ARG:NH1	2.22	0.55
3:F:211:TYR:HE1	3:F:345:ASN:ND2	2.05	0.55
2:H:233:VAL:HG22	2:H:234:LYS:N	2.22	0.55
2:B:374:PHE:HB3	2:B:382:ASN:HB3	1.89	0.55
2:H:151:LEU:HD23	2:H:152:TYR:N	2.21	0.55
2:K:215:ILE:HD12	2:K:248:GLY:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:415:ARG:O	2:K:434:GLY:HA2	2.06	0.55
2:H:190:MET:O	2:H:190:MET:SD	2.64	0.55
2:B:176:ARG:HA	2:B:179:ILE:CD1	2.23	0.55
3:C:219:SER:CB	3:C:224:THR:HG21	2.36	0.55
3:C:279:ALA:HB2	3:F:308:ASN:HD21	1.71	0.55
2:H:301:GLN:HE21	2:H:302:LEU:N	2.04	0.55
2:H:411:ASN:ND2	2:H:434:GLY:H	2.05	0.55
2:H:199:VAL:HG23	3:I:141:ASP:OD1	2.07	0.55
2:B:369:ILE:O	2:B:405:ASN:HB3	2.06	0.55
2:E:294:LEU:O	2:E:295:GLY:C	2.45	0.55
2:E:234:LYS:C	2:E:234:LYS:HD3	2.26	0.55
1:J:152:VAL:HG23	1:J:153:ASP:N	2.21	0.55
2:E:374:PHE:HB2	2:E:382:ASN:HB3	1.88	0.55
2:E:199:VAL:O	3:F:142:THR:HG23	2.06	0.55
2:B:175:LEU:HD13	2:B:179:ILE:HD11	1.87	0.55
3:C:221:THR:HG23	3:C:222:GLY:N	2.12	0.55
2:H:369:ILE:O	2:H:405:ASN:HB3	2.07	0.55
3:I:170:LYS:HZ3	3:I:177:GLN:N	2.05	0.55
3:I:219:SER:CB	3:I:224:THR:HG21	2.36	0.55
3:I:237:SER:OG	3:I:266:LYS:HA	2.07	0.55
3:I:372:TRP:CE3	3:I:373:LYS:HE3	2.42	0.55
3:C:189:ASN:HB3	3:C:387:ILE:HD11	1.89	0.55
3:F:299:PRO:O	3:F:301:ASP:N	2.37	0.54
3:F:196:LYS:HA	3:F:382:THR:O	2.07	0.54
2:H:365:ARG:O	2:H:367:MET:N	2.41	0.54
3:I:193:VAL:HG22	3:I:385:LYS:HB3	1.87	0.54
2:K:255:ARG:HH11	2:K:255:ARG:HG3	1.72	0.54
3:C:96:TYR:O	3:C:99:SER:N	2.35	0.54
3:F:372:TRP:HZ3	3:F:379:MET:CE	2.20	0.54
1:J:131:GLN:HE21	1:J:132:HIS:H	1.55	0.54
2:E:189:GLN:O	2:E:193:CYS:SG	2.65	0.54
3:I:252:ASP:OD2	3:I:254:ASN:HB2	2.06	0.54
2:B:293:TRP:HE1	2:B:296:ASN:HD21	1.56	0.54
2:E:325:HIS:HB3	2:E:346:ARG:HB3	1.89	0.54
1:D:131:GLN:C	1:D:133:ILE:N	2.60	0.54
3:C:96:TYR:CD1	3:C:96:TYR:C	2.80	0.54
3:F:96:TYR:HD1	3:F:97:GLU:N	2.03	0.54
1:G:180:ASP:O	1:G:183:LYS:HB3	2.06	0.54
3:I:315:TRP:CE3	3:I:328:GLU:HG2	2.41	0.54
3:I:189:ASN:HB3	3:I:387:ILE:HD11	1.89	0.54
3:I:389:PHE:O	3:I:391:ARG:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HG2	2:B:426:MET:C	2.27	0.54
1:D:137:GLN:HE21	2:E:164:ASN:HD21	1.54	0.54
2:E:169:ARG:O	2:E:173:GLU:HG3	2.07	0.54
3:L:288:ASP:OD2	3:L:291:ASP:HB2	2.07	0.54
3:I:322:PHE:CD2	3:I:324:GLY:N	2.76	0.54
2:H:301:GLN:NE2	2:H:302:LEU:N	2.55	0.54
2:H:351:ASN:ND2	2:H:354:MET:H	2.04	0.54
3:C:389:PHE:O	3:C:391:ARG:N	2.35	0.54
1:J:137:GLN:HB3	1:J:189:ILE:HG12	1.88	0.54
1:D:185:LEU:HD22	1:D:189:ILE:CG1	2.36	0.54
2:B:359:GLN:NE2	2:B:359:GLN:N	2.53	0.54
3:I:272:ASP:CG	3:I:275:ARG:HE	2.10	0.54
2:K:158:ASN:HD21	3:L:100:ILE:CD1	2.20	0.54
1:A:163:GLY:CA	2:B:275:ASN:HD21	2.21	0.54
2:B:175:LEU:O	2:B:175:LEU:HD22	2.08	0.54
2:H:412:PRO:HG3	2:H:450:MET:HE3	1.89	0.54
2:H:252:ILE:HG12	2:H:452:MET:O	2.08	0.54
3:L:307:HIS:O	3:L:310:MET:HG2	2.08	0.54
3:C:275:ARG:HB2	3:C:311:GLN:CA	2.34	0.54
2:B:266:TRP:HE1	2:B:380:ARG:CZ	2.21	0.54
3:F:223:THR:HG22	3:F:223:THR:O	2.08	0.54
2:B:163:THR:O	2:B:163:THR:HG22	2.07	0.54
2:B:176:ARG:HH12	2:B:179:ILE:HD12	1.73	0.54
1:A:157:LYS:NZ	3:C:132:GLU:HB2	2.23	0.54
2:H:199:VAL:N	3:I:140:LYS:O	2.41	0.54
3:I:312:PHE:CZ	3:I:333:GLY:O	2.61	0.54
1:G:128:GLU:HA	1:G:131:GLN:CB	2.34	0.54
2:E:332:GLN:HB3	2:E:336:ASN:HB2	1.89	0.54
3:I:276:LEU:HD11	3:I:309:GLY:H	1.72	0.54
2:K:167:VAL:HG23	2:K:168:LEU:HD22	1.90	0.54
2:K:303:THR:HB	2:K:330:THR:HA	1.88	0.54
3:F:96:TYR:C	3:F:98:ALA:H	2.11	0.54
2:E:254:ASN:O	2:E:291:GLU:HA	2.07	0.54
2:B:237:ARG:HH22	3:C:143:VAL:HG21	1.73	0.54
3:C:237:SER:OG	3:C:266:LYS:HA	2.07	0.54
3:C:248:VAL:HB	3:C:260:ALA:HB3	1.90	0.54
2:H:337:LYS:HB3	2:H:382:ASN:OD1	2.08	0.54
3:I:367:ILE:HG22	3:I:379:MET:HG2	1.90	0.54
2:H:168:LEU:HB3	3:I:110:LEU:CD1	2.38	0.54
2:E:166:ARG:HD3	2:E:167:VAL:N	2.22	0.54
2:E:266:TRP:N	2:E:379:ASP:OD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:352:GLY:HA2	3:I:378:SER:HB3	1.88	0.54
6:E:470:NDG:H6C2	4:N:4:PRO:HG3	1.89	0.54
2:B:180:GLN:NE2	2:B:180:GLN:HA	2.22	0.54
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.72	0.54
1:G:130:VAL:H	1:G:133:ILE:HD13	1.72	0.54
3:L:211:TYR:HE1	3:L:345:ASN:ND2	2.06	0.54
3:L:234:HIS:CE1	3:L:269:PRO:HD3	2.41	0.54
2:E:333:ASN:OD1	2:E:334:GLU:N	2.41	0.54
3:C:97:GLU:C	3:C:99:SER:N	2.61	0.54
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.07	0.54
1:D:181:GLN:HE22	2:E:174:ASN:CB	2.21	0.54
1:A:140:VAL:CG2	1:A:141:ARG:H	2.21	0.54
2:H:365:ARG:HG2	2:H:366:THR:N	2.23	0.54
2:H:373:MET:HE3	2:H:374:PHE:H	1.72	0.54
3:C:275:ARG:CB	3:C:311:GLN:HA	2.35	0.54
3:C:276:LEU:HD12	3:C:276:LEU:O	2.07	0.54
1:D:124:ARG:H	1:D:124:ARG:CD	2.10	0.54
1:J:152:VAL:CG2	1:J:153:ASP:N	2.71	0.54
2:E:370:HIS:HE1	2:E:408:HIS:HB2	1.73	0.54
3:I:124:LEU:O	3:I:124:LEU:HG	2.08	0.54
2:K:394:CYS:O	2:K:397:GLU:O	2.25	0.54
3:F:276:LEU:HD21	3:F:278:TYR:HD2	1.73	0.54
3:F:290:PHE:HA	3:F:307:HIS:HD1	1.71	0.54
3:I:221:THR:HG23	3:I:222:GLY:N	2.13	0.54
3:I:208:TRP:HE3	3:I:314:THR:HG23	1.73	0.54
3:L:276:LEU:O	3:L:277:THR:HG23	2.08	0.54
1:J:140:VAL:HG13	1:J:185:LEU:CD1	2.34	0.54
2:H:152:TYR:CD2	2:H:155:GLU:HG2	2.43	0.54
1:D:174:ASP:OD1	1:D:177:ASP:HB2	2.07	0.54
2:E:367:MET:O	2:E:405:ASN:O	2.25	0.53
1:A:136:LEU:HA	1:A:139:ASN:HB2	1.90	0.53
2:B:165:LEU:H	2:B:166:ARG:CZ	2.19	0.53
3:I:208:TRP:CA	3:I:314:THR:HG21	2.38	0.53
3:I:191:TRP:HH2	3:I:247:ARG:HH11	1.54	0.53
3:I:105:SER:HA	3:I:108:ARG:HB3	1.89	0.53
3:F:242:ILE:CG2	3:F:243:PRO:HD2	2.39	0.53
1:D:131:GLN:O	1:D:134:GLN:HG2	2.08	0.53
2:K:215:ILE:CG2	2:K:216:ARG:H	2.22	0.53
3:L:372:TRP:HZ3	3:L:379:MET:CE	2.21	0.53
2:K:156:THR:HG22	2:K:157:VAL:N	2.23	0.53
1:D:164:SER:O	2:E:197:CYS:SG	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ILE:N	3:C:148:ILE:HD12	2.23	0.53
3:L:223:THR:O	3:L:223:THR:HG22	2.08	0.53
2:E:189:GLN:HA	2:E:189:GLN:OE1	2.09	0.53
3:C:111:GLN:O	3:C:114:TYR:HB3	2.07	0.53
2:H:237:ARG:HH22	3:I:143:VAL:HG21	1.73	0.53
3:I:248:VAL:HB	3:I:260:ALA:HB3	1.90	0.53
3:L:367:ILE:O	3:L:378:SER:HA	2.08	0.53
1:D:126:VAL:HG23	1:D:127:ILE:N	2.23	0.53
3:L:281:PHE:HB2	3:L:288:ASP:OD1	2.07	0.53
3:L:380:LYS:O	3:L:381:LYS:HG3	2.08	0.53
2:B:231:SER:HB2	3:C:176:GLN:NE2	2.23	0.53
2:K:204:PRO:HA	3:L:217:HIS:HD2	1.72	0.53
2:K:304:ARG:O	2:K:306:GLY:N	2.42	0.53
2:E:156:THR:HG22	2:E:157:VAL:N	2.22	0.53
2:B:346:ARG:HH11	2:B:346:ARG:HB2	1.72	0.53
2:B:181:LYS:O	2:B:183:GLU:N	2.38	0.53
2:K:191:GLU:C	2:K:193:CYS:H	2.11	0.53
2:H:293:TRP:NE1	2:H:296:ASN:ND2	2.54	0.53
1:J:151:GLU:HG3	1:J:178:TYR:CZ	2.42	0.53
3:I:218:LEU:O	3:I:219:SER:HB3	2.09	0.53
3:I:344:LEU:HD12	3:I:384:MET:HE3	1.91	0.53
2:E:346:ARG:NH1	2:E:346:ARG:HG2	2.22	0.53
2:B:156:THR:HA	2:B:160:ASN:HB2	1.90	0.53
2:E:253:GLN:HB2	2:E:293:TRP:CE3	2.43	0.53
3:C:126:GLU:C	3:C:128:VAL:H	2.10	0.53
3:C:311:GLN:OE1	3:C:319:ASN:HB3	2.09	0.53
3:I:368:ILE:HG21	3:I:375:ARG:C	2.28	0.53
3:C:368:ILE:HG21	3:C:375:ARG:C	2.28	0.53
3:C:202:VAL:HG11	3:C:216:GLY:HA3	1.91	0.53
3:C:246:LEU:HB2	3:C:265:PHE:CE1	2.44	0.53
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.28	0.53
1:G:131:GLN:C	1:G:133:ILE:H	2.12	0.53
1:D:143:GLN:O	1:D:147:MET:HG2	2.09	0.53
2:E:209:LYS:HG3	2:E:213:GLU:OE1	2.08	0.53
2:B:209:LYS:HB3	2:B:209:LYS:NZ	2.23	0.53
1:J:115:LEU:HD13	1:J:115:LEU:C	2.29	0.53
2:B:183:GLU:HG2	2:B:183:GLU:O	2.08	0.53
2:H:237:ARG:HH22	3:I:143:VAL:CG2	2.22	0.53
3:L:307:HIS:O	3:L:308:ASN:C	2.45	0.53
2:B:317:TRP:N	2:B:317:TRP:CD1	2.69	0.53
3:F:249:GLU:O	3:F:250:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:249:TRP:CZ3	2:H:455:ARG:HB2	2.43	0.53
3:I:256:ARG:HG3	3:I:256:ARG:NH1	2.23	0.53
1:J:140:VAL:HG13	1:J:141:ARG:N	2.24	0.53
1:G:191:LYS:O	1:G:192:ASP:CB	2.57	0.53
3:L:360:PRO:O	3:L:361:ASN:ND2	2.42	0.53
3:C:170:LYS:HZ1	3:C:177:GLN:H	1.55	0.53
3:I:128:VAL:O	3:I:129:ALA:C	2.47	0.53
2:H:408:HIS:O	4:Q:1:GLY:N	2.40	0.53
3:I:337:ASN:OD1	3:I:338:LYS:N	2.35	0.53
3:C:276:LEU:HD11	3:C:309:GLY:H	1.73	0.53
1:J:126:VAL:HG12	1:J:127:ILE:N	2.23	0.53
1:A:136:LEU:HD12	3:C:107:ILE:HD11	1.91	0.53
3:I:132:GLU:C	3:I:134:GLN:H	2.11	0.53
2:H:229:PRO:HG2	2:H:233:VAL:HG11	1.90	0.53
3:I:193:VAL:HG12	3:I:195:GLN:N	2.24	0.53
3:L:212:LYS:HG3	3:L:231:GLU:HB2	1.90	0.53
2:B:402:TRP:CH2	2:B:412:PRO:HD2	2.44	0.53
2:E:300:SER:OG	2:E:332:GLN:O	2.27	0.53
2:B:363:GLU:O	2:B:367:MET:HE2	2.07	0.53
2:E:301:GLN:HE22	2:E:302:LEU:HG	1.73	0.53
2:E:204:PRO:HA	3:F:217:HIS:HD2	1.71	0.53
2:K:266:TRP:N	2:K:379:ASP:OD1	2.39	0.53
3:I:354:TYR:OH	3:I:364:ASP:HA	2.08	0.53
3:I:364:ASP:OD2	4:S:1:GLY:N	2.42	0.53
3:C:193:VAL:HG12	3:C:195:GLN:N	2.23	0.53
2:B:191:GLU:O	2:B:193:CYS:N	2.41	0.53
3:I:246:LEU:HB2	3:I:265:PHE:CE1	2.44	0.53
3:I:373:LYS:HG3	3:I:379:MET:HE1	1.91	0.53
2:B:394:CYS:SG	2:B:406:ARG:HA	2.49	0.53
2:K:374:PHE:HB2	2:K:382:ASN:HB3	1.90	0.53
2:H:309:GLU:HG3	2:H:309:GLU:O	2.09	0.53
2:K:198:THR:HG22	3:L:140:LYS:O	2.09	0.53
3:I:365:ASN:HD22	3:I:366:GLY:N	2.05	0.52
3:I:284:GLY:C	3:I:286:ALA:H	2.11	0.52
2:E:166:ARG:O	2:E:169:ARG:HB3	2.09	0.52
2:E:314:MET:HA	2:E:449:LYS:O	2.09	0.52
2:B:213:GLU:CG	2:B:217:LYS:HE3	2.39	0.52
1:G:139:ASN:O	1:G:142:ALA:HB3	2.09	0.52
2:B:202:ASN:O	2:B:204:PRO:HD3	2.10	0.52
3:C:191:TRP:HH2	3:C:247:ARG:HH11	1.55	0.52
3:C:284:GLY:C	3:C:286:ALA:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:179:ILE:O	2:H:179:ILE:HG22	2.09	0.52
3:L:242:ILE:CG2	3:L:243:PRO:HD2	2.39	0.52
2:H:161:ILE:N	2:H:162:PRO:CD	2.73	0.52
2:B:310:LEU:HD23	2:B:329:PHE:CG	2.44	0.52
3:L:311:GLN:O	3:L:335:TRP:HA	2.10	0.52
2:K:270:LYS:HG3	2:K:338:TYR:OH	2.09	0.52
3:L:143:VAL:HG23	3:L:143:VAL:O	2.09	0.52
2:E:212:GLU:HB2	2:E:455:ARG:HG3	1.90	0.52
2:E:234:LYS:HD3	2:E:235:PRO:O	2.09	0.52
2:H:266:TRP:HE1	2:H:380:ARG:CZ	2.23	0.52
2:K:351:ASN:HD21	2:K:354:MET:HB2	1.73	0.52
2:B:388:SER:O	2:B:390:PRO:HD3	2.10	0.52
2:K:294:LEU:O	2:K:295:GLY:C	2.46	0.52
2:B:161:ILE:HG22	2:B:162:PRO:CD	2.39	0.52
3:C:347:VAL:HB	3:C:349:TYR:CE2	2.43	0.52
2:H:411:ASN:HB3	2:H:436:VAL:HG22	1.92	0.52
3:I:170:LYS:HZ3	3:I:177:GLN:H	1.58	0.52
2:K:300:SER:OG	2:K:332:GLN:O	2.27	0.52
2:H:303:THR:HA	2:H:308:THR:HG21	1.91	0.52
2:E:283:LYS:HD2	2:E:283:LYS:N	2.24	0.52
3:F:96:TYR:HD1	3:F:97:GLU:H	1.57	0.52
1:A:181:GLN:NE2	2:B:174:ASN:HB2	2.25	0.52
2:H:249:TRP:CZ2	2:H:455:ARG:CZ	2.92	0.52
3:C:354:TYR:OH	3:C:364:ASP:HA	2.09	0.52
3:C:178:PHE:HE2	3:C:228:LEU:HD11	1.73	0.52
1:G:150:LEU:O	1:G:150:LEU:HD12	2.09	0.52
3:F:234:HIS:CE1	3:F:269:PRO:HD3	2.44	0.52
3:F:307:HIS:O	3:F:308:ASN:C	2.46	0.52
1:G:120:GLU:OE1	1:G:121:VAL:N	2.38	0.52
2:E:333:ASN:N	2:E:336:ASN:HD22	2.05	0.52
2:H:242:MET:HA	2:H:247:GLY:HA2	1.91	0.52
1:J:156:ILE:CG2	2:K:415:ARG:NH1	2.72	0.52
3:C:295:PHE:CD2	4:O:2:HYP:HD23	2.45	0.52
3:C:94:MET:C	3:C:96:TYR:N	2.62	0.52
2:H:213:GLU:CG	2:H:217:LYS:HE3	2.38	0.52
3:F:281:PHE:HB2	3:F:288:ASP:OD1	2.09	0.52
2:E:161:ILE:N	2:E:162:PRO:CD	2.72	0.52
1:J:167:ARG:CZ	1:J:167:ARG:CB	2.87	0.52
3:F:228:LEU:O	3:F:232:LYS:HD2	2.09	0.52
3:F:380:LYS:O	3:F:381:LYS:HG3	2.10	0.52
2:H:255:ARG:NH1	2:H:413:ASN:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:304:ARG:HH22	2:H:333:ASN:H	1.57	0.52
3:I:171:PRO:HB3	3:I:235:LEU:O	2.09	0.52
3:I:93:ILE:CD1	3:I:93:ILE:N	2.72	0.52
3:L:197:ARG:C	3:L:198:LEU:HD12	2.30	0.52
2:H:227:ILE:HD13	2:H:238:VAL:HG11	1.92	0.52
3:F:281:PHE:O	3:F:283:GLY:N	2.43	0.52
2:K:283:LYS:N	2:K:283:LYS:HD2	2.24	0.52
1:A:121:VAL:O	1:A:122:LEU:HB3	2.10	0.52
1:J:119:ILE:HA	1:J:122:LEU:HB3	1.90	0.52
2:H:428:LYS:HG2	2:H:429:HIS:HD2	1.73	0.52
2:E:218:GLY:HA3	3:F:210:GLN:HG2	1.92	0.52
2:B:175:LEU:O	2:B:179:ILE:HG13	2.09	0.52
3:F:195:GLN:HG3	3:F:227:TRP:CZ3	2.44	0.52
3:I:97:GLU:C	3:I:99:SER:N	2.61	0.52
2:B:332:GLN:HB3	2:B:336:ASN:HD22	1.75	0.52
3:L:344:LEU:HD22	3:L:382:THR:OG1	2.10	0.52
2:K:216:ARG:CZ	2:K:216:ARG:HB2	2.39	0.52
2:E:215:ILE:HD12	2:E:248:GLY:N	2.25	0.52
2:K:158:ASN:HD22	2:K:158:ASN:N	2.06	0.52
2:B:303:THR:HB	2:B:330:THR:HA	1.91	0.52
3:I:322:PHE:CG	3:I:323:GLU:N	2.78	0.52
2:K:340:ILE:HG12	2:K:341:SER:N	2.25	0.52
1:G:172:GLU:O	1:G:173:VAL:HG23	2.09	0.52
2:E:373:MET:SD	2:E:405:ASN:HB2	2.50	0.52
2:B:165:LEU:HB2	2:B:166:ARG:CZ	2.40	0.52
2:B:175:LEU:HA	2:B:178:LYS:HG3	1.92	0.52
3:F:310:MET:O	3:F:311:GLN:O	2.28	0.52
2:H:351:ASN:ND2	2:H:351:ASN:C	2.62	0.52
2:H:205:VAL:HG21	3:I:215:PHE:O	2.10	0.52
3:I:304:PHE:C	3:I:306:SER:H	2.11	0.52
2:B:255:ARG:HB2	2:B:450:MET:N	2.24	0.52
1:J:185:LEU:O	1:J:189:ILE:HG13	2.09	0.52
3:F:239:GLN:O	3:F:242:ILE:HD12	2.10	0.52
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.90	0.52
2:K:357:ALA:HB3	2:K:360:LEU:CD1	2.39	0.52
3:L:196:LYS:O	3:L:197:ARG:HD2	2.08	0.52
3:F:153:CYS:SG	3:F:192:THR:HA	2.50	0.52
3:F:297:ASP:O	3:F:298:ASP:CB	2.57	0.52
2:E:369:ILE:O	2:E:405:ASN:ND2	2.38	0.52
3:L:297:ASP:O	3:L:298:ASP:CB	2.57	0.52
2:K:366:THR:HA	2:K:369:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:230:ASP:O	2:H:232:SER:N	2.43	0.52
2:H:310:LEU:HB3	2:H:329:PHE:CD2	2.45	0.52
2:B:337:LYS:HB3	2:B:382:ASN:OD1	2.10	0.52
2:B:411:ASN:N	2:B:436:VAL:O	2.33	0.52
2:E:270:LYS:HA	2:E:296:ASN:CB	2.40	0.52
2:E:266:TRP:HA	2:E:377:THR:HG21	1.92	0.52
3:F:340:HIS:ND1	3:F:368:ILE:HD11	2.25	0.52
3:I:134:GLN:C	3:I:136:GLN:H	2.13	0.52
3:I:131:LEU:O	3:I:134:GLN:HB3	2.10	0.52
2:H:236:TYR:CB	2:H:298:LYS:NZ	2.73	0.52
3:I:329:GLN:HE21	4:S:3:ARG:CZ	2.22	0.52
2:E:255:ARG:HH11	2:E:255:ARG:HG3	1.74	0.52
1:D:122:LEU:N	1:D:124:ARG:NE	2.57	0.52
2:E:215:ILE:CG2	2:E:216:ARG:H	2.23	0.52
1:G:167:ARG:HH22	1:G:169:LEU:HD23	1.75	0.52
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.40	0.51
2:E:397:GLU:O	2:E:398:ASP:HB2	2.10	0.51
2:H:251:VAL:HG12	2:H:252:ILE:N	2.24	0.51
2:H:304:ARG:HH11	2:H:304:ARG:HG3	1.76	0.51
3:I:297:ASP:HB2	3:I:301:ASP:CG	2.31	0.51
3:I:275:ARG:HB2	3:I:311:GLN:CA	2.37	0.51
3:C:170:LYS:NZ	3:C:175:ASN:O	2.42	0.51
1:A:158:ILE:HG12	2:B:189:GLN:HG3	1.91	0.51
2:E:398:ASP:HA	2:E:433:ASP:CB	2.27	0.51
3:F:313:SER:N	3:F:334:TRP:O	2.40	0.51
2:H:365:ARG:O	2:H:368:THR:HG23	2.09	0.51
2:K:255:ARG:HD3	2:K:262:PHE:CZ	2.45	0.51
2:H:189:GLN:HA	2:H:189:GLN:HE21	1.75	0.51
3:I:347:VAL:HB	3:I:349:TYR:CE2	2.44	0.51
2:K:280:THR:O	2:K:281:ASP:C	2.49	0.51
2:H:319:GLY:O	2:H:320:ASP:O	2.29	0.51
1:A:127:ILE:HG22	1:A:128:GLU:N	2.26	0.51
1:A:147:MET:SD	3:C:121:ILE:HD11	2.51	0.51
2:E:332:GLN:HB2	2:E:339:GLN:H	1.75	0.51
2:B:351:ASN:HD21	2:B:354:MET:CG	2.23	0.51
2:B:361:MET:CB	5:B:470:NAG:H81	2.36	0.51
3:L:250:LEU:HD21	3:L:369:TRP:CD1	2.45	0.51
2:B:433:ASP:O	2:B:433:ASP:OD1	2.29	0.51
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.92	0.51
1:G:164:SER:CB	3:I:137:GLU:O	2.58	0.51
3:F:294:ASP:HA	3:F:301:ASP:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:LYS:O	1:J:129:LYS:HG2	2.11	0.51
1:J:128:GLU:O	1:J:131:GLN:NE2	2.43	0.51
1:A:139:ASN:O	3:C:114:TYR:OH	2.28	0.51
3:C:169:ILE:HD11	3:C:178:PHE:CE1	2.46	0.51
3:C:349:TYR:HB2	3:C:378:SER:CB	2.41	0.51
3:F:307:HIS:O	3:F:310:MET:HG2	2.11	0.51
2:H:412:PRO:HB3	2:H:450:MET:HG2	1.93	0.51
3:I:169:ILE:HD11	3:I:178:PHE:HE1	1.76	0.51
3:I:208:TRP:NE1	3:I:270:GLU:OE2	2.43	0.51
3:L:232:LYS:O	3:L:234:HIS:N	2.44	0.51
2:K:270:LYS:HA	2:K:296:ASN:HB3	1.91	0.51
1:A:172:GLU:O	1:A:173:VAL:HG13	2.09	0.51
2:K:324:ALA:HB2	2:K:349:ALA:HB3	1.92	0.51
3:C:340:HIS:O	4:O:1:GLY:HA2	2.10	0.51
3:C:365:ASN:HD22	3:C:366:GLY:N	2.07	0.51
3:C:348:TYR:HA	3:C:367:ILE:CD1	2.40	0.51
3:F:311:GLN:O	3:F:335:TRP:HA	2.11	0.51
3:I:202:VAL:HG11	3:I:216:GLY:HA3	1.93	0.51
2:E:270:LYS:O	2:E:270:LYS:HG2	2.10	0.51
1:D:140:VAL:CG1	1:D:185:LEU:HD11	2.38	0.51
2:B:351:ASN:ND2	2:B:355:ASP:H	2.09	0.51
3:C:101:LEU:HD12	3:C:104:ASP:OD1	2.11	0.51
3:C:304:PHE:C	3:C:306:SER:H	2.12	0.51
2:E:304:ARG:O	2:E:306:GLY:N	2.44	0.51
2:K:280:THR:O	2:K:281:ASP:O	2.28	0.51
2:K:328:GLY:HA3	2:K:343:ASN:OD1	2.11	0.51
3:C:220:PRO:HG2	3:C:221:THR:H	1.76	0.51
2:H:178:LYS:O	2:H:182:LEU:HB3	2.11	0.51
3:F:197:ARG:NH1	3:F:344:LEU:O	2.44	0.51
2:K:210:GLU:OE2	2:K:213:GLU:HB2	2.11	0.51
2:E:216:ARG:HB2	2:E:216:ARG:CZ	2.41	0.51
2:H:209:LYS:HB3	2:H:209:LYS:NZ	2.24	0.51
2:K:356:GLY:HA2	2:K:409:ALA:HB2	1.93	0.51
2:E:356:GLY:HA2	2:E:409:ALA:HB2	1.92	0.51
2:H:346:ARG:HH11	2:H:346:ARG:HB2	1.75	0.51
2:B:168:LEU:C	3:C:110:LEU:HD11	2.31	0.51
3:I:170:LYS:NZ	3:I:175:ASN:O	2.42	0.51
3:C:149:THR:C	3:C:156:ILE:HG12	2.32	0.51
3:C:221:THR:CG2	3:C:222:GLY:H	2.09	0.51
3:I:193:VAL:HG12	3:I:194:PHE:N	2.26	0.51
3:L:196:LYS:HA	3:L:382:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:346:ARG:HG2	2:K:346:ARG:NH1	2.25	0.51
3:L:249:GLU:O	3:L:250:LEU:HD12	2.11	0.51
1:G:189:ILE:CG2	1:G:189:ILE:O	2.58	0.51
1:A:180:ASP:C	1:A:182:GLN:N	2.64	0.51
3:F:374:THR:OG1	3:F:377:TYR:HB2	2.11	0.51
2:E:280:THR:O	2:E:281:ASP:C	2.49	0.51
1:D:156:ILE:HG21	2:E:415:ARG:NH1	2.26	0.51
2:B:155:GLU:C	2:B:157:VAL:N	2.63	0.51
2:H:424:TRP:N	2:H:444:TRP:CZ3	2.79	0.51
3:L:239:GLN:O	3:L:242:ILE:HD12	2.10	0.51
2:B:227:ILE:HD13	2:B:238:VAL:HG11	1.93	0.51
3:L:227:TRP:HZ3	3:L:384:MET:HE2	1.76	0.51
2:K:253:GLN:HB2	2:K:293:TRP:CE3	2.46	0.51
3:I:369:TRP:NE1	3:I:371:THR:OG1	2.44	0.51
1:G:185:LEU:HG	1:G:185:LEU:O	2.11	0.51
2:B:222:SER:HB2	2:B:243:ASN:OD1	2.11	0.51
2:E:423:THR:HG23	2:E:426:MET:HE3	1.91	0.51
2:B:155:GLU:C	2:B:157:VAL:H	2.14	0.51
2:B:224:MET:HE2	2:B:237:ARG:HE	1.75	0.51
3:C:218:LEU:O	3:C:219:SER:HB3	2.11	0.51
3:F:227:TRP:HZ3	3:F:384:MET:HE2	1.76	0.51
1:J:151:GLU:OE2	2:K:182:LEU:HD21	2.09	0.51
2:K:270:LYS:HA	2:K:296:ASN:CB	2.42	0.51
3:I:276:LEU:CD1	3:I:308:ASN:HA	2.38	0.51
2:K:204:PRO:HG2	2:K:224:MET:O	2.11	0.51
2:E:408:HIS:C	2:E:408:HIS:CD2	2.84	0.51
4:R:3:ARG:HH21	4:R:3:ARG:HG2	1.75	0.51
2:B:237:ARG:HH22	3:C:143:VAL:CG2	2.24	0.50
3:C:252:ASP:OD2	3:C:254:ASN:HB2	2.10	0.50
3:F:232:LYS:O	3:F:234:HIS:N	2.44	0.50
3:I:156:ILE:HD11	3:I:169:ILE:HG22	1.92	0.50
2:B:301:GLN:NE2	2:B:302:LEU:N	2.59	0.50
3:L:278:TYR:OH	3:L:308:ASN:HB2	2.10	0.50
2:K:327:GLY:CA	2:K:344:LYS:HB2	2.35	0.50
3:F:153:CYS:HB2	3:F:192:THR:CG2	2.39	0.50
2:K:270:LYS:HE2	2:K:297:ASP:OD2	2.10	0.50
2:H:317:TRP:N	2:H:317:TRP:CD1	2.72	0.50
2:H:388:SER:O	2:H:390:PRO:HD3	2.12	0.50
2:K:303:THR:CG2	2:K:330:THR:HA	2.41	0.50
2:E:404:TYR:O	2:E:405:ASN:CB	2.60	0.50
3:I:166:LEU:C	3:I:167:TYR:CD1	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:CG	1:D:167:ARG:HH11	2.23	0.50
2:B:301:GLN:HE21	2:B:302:LEU:N	2.08	0.50
3:I:275:ARG:CB	3:I:311:GLN:HA	2.40	0.50
3:L:322:PHE:HB2	3:L:338:LYS:HA	1.94	0.50
3:C:148:ILE:HD12	3:C:148:ILE:H	1.77	0.50
2:K:397:GLU:O	2:K:398:ASP:HB2	2.11	0.50
1:A:128:GLU:CA	1:A:131:GLN:HG2	2.42	0.50
1:A:158:ILE:CG2	1:A:159:ARG:N	2.73	0.50
2:H:333:ASN:OD1	2:H:335:ALA:HB3	2.10	0.50
3:I:179:LEU:O	3:I:218:LEU:HD11	2.11	0.50
3:I:93:ILE:H	3:I:93:ILE:HD12	1.74	0.50
3:I:363:TYR:CD2	4:S:3:ARG:HD3	2.46	0.50
2:H:215:ILE:HD13	2:H:242:MET:HB3	1.93	0.50
3:F:179:LEU:HG	3:F:218:LEU:HD12	1.93	0.50
3:I:349:TYR:HB2	3:I:378:SER:CB	2.41	0.50
2:H:316:ASP:OD1	2:H:320:ASP:HB3	2.11	0.50
3:C:116:SER:O	3:C:120:LYS:N	2.40	0.50
3:C:326:CYS:HB3	3:C:336:MET:CE	2.42	0.50
2:B:242:MET:HA	2:B:247:GLY:HA2	1.93	0.50
3:L:276:LEU:HD11	3:L:290:PHE:CE2	2.46	0.50
2:E:212:GLU:O	2:E:212:GLU:HG3	2.11	0.50
2:E:455:ARG:HG3	2:E:456:PRO:HD2	1.93	0.50
2:E:351:ASN:ND2	2:E:354:MET:HB2	2.26	0.50
3:C:208:TRP:CA	3:C:314:THR:HG21	2.40	0.50
3:L:93:ILE:O	3:L:95:LYS:N	2.40	0.50
3:F:158:ASN:O	3:F:159:LYS:HB2	2.11	0.50
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.94	0.50
2:B:158:ASN:HD21	3:C:100:ILE:HD13	1.77	0.50
3:C:125:LYS:HA	3:C:125:LYS:CE	2.41	0.50
3:L:374:THR:OG1	3:L:377:TYR:HB2	2.11	0.50
3:I:194:PHE:HB2	3:I:233:ILE:CD1	2.42	0.50
3:I:326:CYS:O	3:I:327:ALA:C	2.49	0.50
2:B:230:ASP:O	2:B:232:SER:N	2.45	0.50
3:C:275:ARG:CA	3:C:311:GLN:HA	2.42	0.50
1:J:185:LEU:HD22	1:J:189:ILE:CG1	2.41	0.50
2:H:212:GLU:O	2:H:215:ILE:CG2	2.59	0.50
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.12	0.50
1:G:140:VAL:HG23	1:G:185:LEU:HD21	1.93	0.50
3:C:322:PHE:CG	3:C:323:GLU:N	2.80	0.50
3:I:253:TRP:CZ3	3:I:380:LYS:HG3	2.47	0.50
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:NH2	3:C:136:GLN:O	2.38	0.50
2:K:257:ASP:HA	2:K:416:TYR:CE2	2.45	0.50
3:I:359:THR:HB	3:I:362:GLY:C	2.32	0.50
2:B:165:LEU:HD13	3:C:106:SER:O	2.12	0.50
3:C:193:VAL:CG1	3:C:195:GLN:H	2.24	0.50
3:C:204:PHE:HE2	3:C:227:TRP:HB2	1.76	0.50
3:I:224:THR:O	3:I:224:THR:HG23	2.11	0.50
2:B:373:MET:CE	2:B:374:PHE:H	2.24	0.50
3:I:119:GLN:NE2	3:I:120:LYS:N	2.60	0.50
3:L:113:ILE:O	3:L:114:TYR:C	2.50	0.50
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.46	0.50
2:B:261:ASP:OD2	2:B:261:ASP:C	2.50	0.50
2:K:398:ASP:HA	2:K:433:ASP:CB	2.28	0.50
2:B:245:GLU:HG2	2:B:249:TRP:CZ2	2.42	0.50
3:C:193:VAL:HG12	3:C:194:PHE:N	2.26	0.50
3:C:310:MET:O	3:C:335:TRP:HD1	1.93	0.50
3:C:124:LEU:HD12	3:C:127:LYS:HB3	1.94	0.50
2:H:374:PHE:CB	2:H:382:ASN:HB3	2.42	0.50
3:I:197:ARG:HB2	3:I:382:THR:HB	1.94	0.50
2:B:229:PRO:HB2	2:B:301:GLN:OE1	2.12	0.50
3:L:251:GLU:CB	3:L:381:LYS:HB2	2.41	0.50
2:H:266:TRP:HB2	2:H:379:ASP:OD2	2.12	0.50
2:H:407:CYS:SG	4:Q:3:ARG:NH2	2.85	0.50
3:F:185:ASP:C	3:F:187:SER:H	2.14	0.50
2:E:415:ARG:O	2:E:434:GLY:HA2	2.12	0.50
2:B:428:LYS:HG2	2:B:429:HIS:HD2	1.76	0.50
1:J:125:LYS:HE3	1:J:125:LYS:HA	1.94	0.50
3:C:238:THR:HG22	3:C:266:LYS:HG3	1.94	0.50
3:C:251:GLU:HA	3:C:256:ARG:O	2.11	0.50
2:H:178:LYS:C	2:H:180:GLN:N	2.64	0.50
2:H:310:LEU:HD23	2:H:329:PHE:CE2	2.47	0.50
2:B:424:TRP:C	2:B:426:MET:H	2.16	0.50
2:E:201:CYS:O	3:F:143:VAL:HG21	2.11	0.50
3:L:179:LEU:HG	3:L:218:LEU:HD12	1.94	0.50
3:C:207:ASN:ND2	3:C:210:GLN:HG3	2.26	0.50
1:A:160:SER:O	3:C:135:CYS:HB3	2.12	0.49
2:K:189:GLN:O	2:K:193:CYS:SG	2.70	0.49
3:I:310:MET:SD	3:I:337:ASN:ND2	2.85	0.49
2:E:164:ASN:ND2	2:E:164:ASN:O	2.45	0.49
1:D:133:ILE:C	1:D:135:LEU:N	2.64	0.49
2:K:212:GLU:CG	2:K:212:GLU:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:ARG:HH11	1:G:171:ARG:HG2	1.75	0.49
1:G:139:ASN:O	3:I:114:TYR:OH	2.30	0.49
1:J:152:VAL:HG21	2:K:426:MET:O	2.12	0.49
3:L:252:ASP:C	3:L:254:ASN:H	2.15	0.49
2:K:367:MET:O	2:K:405:ASN:O	2.29	0.49
3:C:196:LYS:HD2	3:C:198:LEU:HD11	1.94	0.49
3:C:253:TRP:NE1	3:C:378:SER:O	2.28	0.49
1:A:154:ILE:O	1:A:157:LYS:N	2.46	0.49
3:F:195:GLN:HG3	3:F:227:TRP:CE3	2.48	0.49
3:F:198:LEU:HD23	3:F:381:LYS:HE2	1.92	0.49
2:K:333:ASN:ND2	2:K:335:ALA:HB3	2.27	0.49
2:H:258:GLY:O	2:H:260:VAL:N	2.40	0.49
3:L:305:THR:HB	3:L:341:ALA:CB	2.21	0.49
3:C:195:GLN:O	3:C:196:LYS:HB3	2.12	0.49
3:C:250:LEU:HG	3:C:251:GLU:H	1.76	0.49
2:H:223:GLU:OE2	2:H:285:TYR:HD1	1.96	0.49
3:I:204:PHE:HE2	3:I:227:TRP:HB2	1.77	0.49
3:I:353:THR:HA	3:I:377:TYR:HA	1.94	0.49
2:B:226:LEU:O	2:B:227:ILE:O	2.30	0.49
3:L:194:PHE:CD1	3:L:233:ILE:HD13	2.48	0.49
1:G:136:LEU:O	1:G:140:VAL:HG13	2.11	0.49
2:K:272:GLY:N	2:K:295:GLY:HA2	2.28	0.49
2:K:420:GLY:HA2	2:K:446:SER:O	2.12	0.49
2:B:249:TRP:CZ2	2:B:455:ARG:CZ	2.95	0.49
3:C:103:HIS:C	3:C:105:SER:N	2.64	0.49
1:A:158:ILE:HG21	1:A:171:ARG:HE	1.77	0.49
3:I:169:ILE:CD1	3:I:171:PRO:HD3	2.34	0.49
3:I:194:PHE:CZ	3:I:384:MET:HB3	2.47	0.49
3:I:251:GLU:CG	3:I:252:ASP:H	2.17	0.49
3:I:93:ILE:O	3:I:96:TYR:HD2	1.96	0.49
3:L:249:GLU:HB2	3:L:383:THR:HG23	1.94	0.49
3:C:304:PHE:O	3:C:337:ASN:ND2	2.45	0.49
2:B:265:LYS:HB3	2:B:379:ASP:CG	2.33	0.49
2:K:257:ASP:OD2	2:K:259:SER:OG	2.30	0.49
1:J:130:VAL:O	1:J:133:ILE:CG2	2.60	0.49
2:B:158:ASN:HD22	2:B:158:ASN:N	2.05	0.49
3:C:326:CYS:HB3	3:C:336:MET:HE2	1.93	0.49
1:A:167:ARG:HH22	1:A:169:LEU:HD23	1.78	0.49
2:B:191:GLU:C	2:B:193:CYS:N	2.66	0.49
2:E:417:TYR:HE1	2:E:433:ASP:O	1.95	0.49
3:I:149:THR:C	3:I:156:ILE:HG12	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:VAL:HG12	2:B:252:ILE:N	2.26	0.49
3:L:195:GLN:HG3	3:L:227:TRP:CZ3	2.47	0.49
2:E:327:GLY:CA	2:E:344:LYS:HB2	2.36	0.49
2:B:362:GLY:O	2:B:365:ARG:N	2.45	0.49
1:A:150:LEU:C	1:A:150:LEU:HD12	2.30	0.49
3:F:289:ALA:HB2	3:F:371:THR:OG1	2.13	0.49
1:G:166:SER:CB	2:H:195:THR:O	2.61	0.49
3:C:166:LEU:C	3:C:167:TYR:CD1	2.86	0.49
3:C:350:GLN:C	3:C:352:GLY:H	2.15	0.49
3:L:310:MET:O	3:L:311:GLN:O	2.31	0.49
2:B:424:TRP:N	2:B:444:TRP:CZ3	2.81	0.49
2:E:272:GLY:N	2:E:295:GLY:HA2	2.28	0.49
3:C:208:TRP:NE1	3:C:270:GLU:OE2	2.45	0.49
1:D:183:LYS:O	1:D:186:GLU:HB2	2.12	0.49
3:I:230:ASN:H	3:I:230:ASN:HD22	1.55	0.49
3:I:304:PHE:O	3:I:337:ASN:ND2	2.46	0.49
3:L:313:SER:N	3:L:334:TRP:O	2.38	0.49
2:B:411:ASN:HB3	2:B:436:VAL:HG22	1.95	0.49
3:L:281:PHE:O	3:L:283:GLY:N	2.46	0.49
3:C:208:TRP:HE3	3:C:314:THR:HG23	1.77	0.49
2:H:303:THR:HA	2:H:308:THR:OG1	2.12	0.49
1:A:175:LEU:C	1:A:177:ASP:H	2.16	0.49
2:H:222:SER:HB2	2:H:243:ASN:OD1	2.13	0.49
2:K:417:TYR:HE1	2:K:433:ASP:O	1.95	0.49
3:C:195:GLN:NE2	3:C:384:MET:HG3	2.25	0.49
2:H:351:ASN:ND2	2:H:355:ASP:H	2.11	0.49
3:I:195:GLN:NE2	3:I:384:MET:HG3	2.26	0.49
3:I:250:LEU:O	3:I:257:THR:HB	2.13	0.49
3:I:339:CYS:HB2	4:S:2:HYP:HA	1.93	0.49
2:K:332:GLN:HB2	2:K:339:GLN:H	1.78	0.49
2:K:333:ASN:OD1	2:K:334:GLU:N	2.46	0.49
2:H:211:CYS:O	2:H:242:MET:HE1	2.13	0.49
2:K:351:ASN:ND2	2:K:354:MET:HB2	2.28	0.49
3:I:253:TRP:NE1	3:I:378:SER:O	2.29	0.49
3:F:353:THR:HG23	3:F:377:TYR:CD1	2.47	0.49
3:L:158:ASN:O	3:L:159:LYS:HB2	2.12	0.49
2:K:360:LEU:O	2:K:365:ARG:HD2	2.12	0.49
2:K:367:MET:O	2:K:405:ASN:ND2	2.46	0.49
3:C:194:PHE:CZ	3:C:384:MET:HB3	2.47	0.49
2:H:354:MET:C	2:H:356:GLY:H	2.16	0.49
3:I:238:THR:HG22	3:I:266:LYS:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:HD23	2:B:329:PHE:CE2	2.47	0.49
2:H:245:GLU:HG2	2:H:249:TRP:CZ2	2.45	0.49
3:C:156:ILE:HD11	3:C:169:ILE:HG22	1.94	0.49
3:F:278:TYR:OH	3:F:308:ASN:HB2	2.12	0.49
2:H:310:LEU:HA	2:H:454:ILE:HG22	1.95	0.49
2:B:402:TRP:HB3	2:B:404:TYR:CZ	2.48	0.49
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.95	0.49
2:K:254:ASN:O	2:K:291:GLU:HA	2.12	0.49
2:E:360:LEU:HB3	2:E:364:ASN:O	2.13	0.48
2:B:164:ASN:C	2:B:166:ARG:H	2.17	0.48
1:J:158:ILE:HG23	2:K:189:GLN:NE2	2.21	0.48
3:I:178:PHE:HE2	3:I:228:LEU:HD11	1.77	0.48
2:K:157:VAL:HG23	2:K:158:ASN:ND2	2.28	0.48
3:L:105:SER:CA	3:L:108:ARG:HG2	2.43	0.48
2:B:417:TYR:HB2	2:B:446:SER:HB3	1.92	0.48
2:K:305:MET:O	2:K:305:MET:HG2	2.13	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.96	0.48
3:C:124:LEU:HG	3:C:124:LEU:O	2.13	0.48
2:B:339:GLN:HG2	2:B:340:ILE:N	2.26	0.48
2:B:374:PHE:CB	2:B:382:ASN:HB3	2.43	0.48
1:D:137:GLN:OE1	1:D:189:ILE:HG12	2.13	0.48
3:C:289:ALA:HB2	3:C:371:THR:HG23	1.96	0.48
1:A:183:LYS:HD3	1:A:183:LYS:O	2.13	0.48
3:C:344:LEU:HD12	3:C:384:MET:HE3	1.95	0.48
3:I:193:VAL:CG1	3:I:195:GLN:H	2.26	0.48
1:G:125:LYS:O	1:G:129:LYS:HG2	2.13	0.48
2:B:337:LYS:HG3	2:B:374:PHE:CE2	2.49	0.48
3:L:153:CYS:HB2	3:L:192:THR:CG2	2.42	0.48
3:L:294:ASP:HA	3:L:301:ASP:HB3	1.94	0.48
3:C:179:LEU:O	3:C:218:LEU:HD11	2.14	0.48
3:C:353:THR:HA	3:C:377:TYR:HA	1.95	0.48
2:H:184:SER:O	2:H:188:ALA:N	2.47	0.48
3:F:310:MET:C	3:F:311:GLN:O	2.52	0.48
3:I:163:GLN:O	3:I:167:TYR:OH	2.26	0.48
2:K:234:LYS:HD3	2:K:235:PRO:O	2.14	0.48
2:K:423:THR:HG23	2:K:426:MET:HE3	1.96	0.48
2:B:319:GLY:O	2:B:320:ASP:O	2.32	0.48
2:B:158:ASN:OD1	3:C:100:ILE:HD13	2.13	0.48
3:C:317:ASN:HD22	3:C:317:ASN:C	2.16	0.48
2:H:373:MET:CE	2:H:374:PHE:H	2.26	0.48
2:H:159:SER:H	2:H:162:PRO:CD	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:SER:C	3:C:101:LEU:N	2.62	0.48
3:C:321:LYS:O	3:C:338:LYS:HB2	2.13	0.48
2:H:433:ASP:O	2:H:433:ASP:OD1	2.31	0.48
2:K:408:HIS:C	2:K:408:HIS:CD2	2.87	0.48
3:L:353:THR:HG23	3:L:377:TYR:CD1	2.47	0.48
2:B:455:ARG:HG2	2:B:456:PRO:HD2	1.94	0.48
2:H:236:TYR:OH	2:H:302:LEU:HD11	2.14	0.48
3:F:240:SER:O	3:F:242:ILE:HG13	2.12	0.48
1:G:167:ARG:NH1	1:G:169:LEU:HA	2.28	0.48
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.45	0.48
3:L:219:SER:CB	3:L:224:THR:HG21	2.44	0.48
1:A:189:ILE:O	1:A:190:ALA:CB	2.61	0.48
3:L:365:ASN:HD22	3:L:365:ASN:C	2.16	0.48
2:H:424:TRP:C	2:H:426:MET:H	2.17	0.48
3:C:178:PHE:HD1	3:C:178:PHE:H	1.60	0.48
3:C:367:ILE:HG22	3:C:379:MET:HG2	1.94	0.48
3:I:121:ILE:HG23	3:I:122:VAL:N	2.29	0.48
2:H:229:PRO:HB2	2:H:301:GLN:OE1	2.14	0.48
3:C:386:ILE:O	3:C:387:ILE:HB	2.14	0.48
2:K:269:TYR:CE2	2:K:401:GLY:HA3	2.49	0.48
1:D:147:MET:HG3	2:E:175:LEU:HD13	1.95	0.48
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.28	0.48
2:E:332:GLN:HB3	2:E:336:ASN:CB	2.43	0.48
2:H:153:ILE:HG12	2:H:153:ILE:O	2.12	0.48
1:G:167:ARG:NE	2:H:192:TYR:CD2	2.77	0.48
3:I:117:ASN:N	3:I:117:ASN:ND2	2.61	0.48
2:K:405:ASN:O	2:K:406:ARG:C	2.52	0.48
3:C:169:ILE:HD11	3:C:178:PHE:HE1	1.79	0.48
3:C:312:PHE:HZ	3:C:333:GLY:O	1.96	0.48
1:A:154:ILE:O	1:A:158:ILE:N	2.41	0.48
1:A:157:LYS:HE3	3:C:132:GLU:OE1	2.14	0.48
1:A:161:CYS:HA	3:C:135:CYS:HB3	1.96	0.48
2:B:292:TYR:CE2	2:B:294:LEU:HB2	2.41	0.48
3:F:118:ASN:O	3:F:122:VAL:HG23	2.14	0.48
3:C:276:LEU:CD1	3:C:308:ASN:HA	2.41	0.48
2:K:212:GLU:HB2	2:K:455:ARG:HG3	1.94	0.48
2:B:317:TRP:HD1	2:B:317:TRP:H	1.54	0.48
2:K:448:ARG:O	2:K:449:LYS:HG3	2.14	0.48
1:G:140:VAL:O	1:G:143:GLN:N	2.46	0.48
3:I:116:SER:O	3:I:119:GLN:HB3	2.14	0.48
2:E:378:TYR:HB2	2:E:396:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ASP:OD1	1:J:177:ASP:HB2	2.13	0.48
2:H:439:ASN:HD22	2:H:439:ASN:H	1.62	0.48
2:B:441:LYS:HB3	2:B:445:TYR:HB3	1.96	0.48
3:C:307:HIS:CE1	3:C:341:ALA:H	2.32	0.48
2:H:402:TRP:HB3	2:H:404:TYR:CZ	2.49	0.48
2:H:236:TYR:HB2	2:H:298:LYS:HZ1	1.77	0.48
2:H:224:MET:CE	2:H:237:ARG:HE	2.27	0.48
2:E:311:LEU:HD22	2:E:325:HIS:CD2	2.49	0.48
1:D:131:GLN:HG3	1:D:132:HIS:N	2.29	0.48
3:F:102:THR:O	3:F:104:ASP:N	2.46	0.48
2:H:189:GLN:HA	2:H:189:GLN:NE2	2.28	0.48
3:I:316:ASP:O	3:I:317:ASN:CB	2.61	0.48
3:C:280:TYR:N	3:C:280:TYR:CD1	2.82	0.48
2:H:337:LYS:HG3	2:H:374:PHE:CE2	2.49	0.48
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.94	0.48
3:I:386:ILE:O	3:I:387:ILE:HB	2.14	0.48
2:H:161:ILE:HG21	3:I:103:HIS:CE1	2.48	0.48
1:D:185:LEU:CD2	1:D:189:ILE:HG13	2.39	0.48
2:E:332:GLN:HG3	2:E:339:GLN:HB3	1.96	0.48
2:K:211:CYS:HB3	2:K:242:MET:HE1	1.95	0.48
1:G:135:LEU:O	1:G:138:LYS:HB3	2.13	0.48
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.13	0.48
2:H:176:ARG:HA	2:H:179:ILE:CG1	2.44	0.47
3:I:96:TYR:O	3:I:98:ALA:N	2.47	0.47
2:B:293:TRP:NE1	2:B:296:ASN:ND2	2.59	0.47
3:L:153:CYS:SG	3:L:192:THR:HA	2.54	0.47
3:F:92:GLU:HG2	3:F:93:ILE:N	2.29	0.47
2:E:359:GLN:OE1	2:E:438:MET:HB3	2.14	0.47
2:B:177:SER:HA	2:B:180:GLN:CG	2.43	0.47
3:C:196:LYS:CD	3:C:198:LEU:HD11	2.43	0.47
3:C:373:LYS:HG3	3:C:379:MET:HE1	1.96	0.47
2:B:191:GLU:HG3	2:B:192:TYR:N	2.28	0.47
2:B:186:VAL:HG12	3:C:127:LYS:HE2	1.96	0.47
2:H:253:GLN:HE21	2:H:253:GLN:HB3	1.53	0.47
2:H:293:TRP:O	2:H:295:GLY:N	2.47	0.47
2:H:340:ILE:HG23	2:H:340:ILE:O	2.14	0.47
2:B:296:ASN:O	2:B:299:ILE:N	2.47	0.47
3:L:344:LEU:HB3	3:L:382:THR:HG21	1.96	0.47
3:F:103:HIS:N	3:F:103:HIS:HD1	2.11	0.47
2:H:441:LYS:HB3	2:H:445:TYR:HB3	1.96	0.47
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:298:ASP:OD2	3:L:300:SER:HB2	2.14	0.47
2:K:364:ASN:ND2	5:K:470:NAG:O7	2.46	0.47
3:C:178:PHE:CD2	3:C:228:LEU:HD11	2.49	0.47
3:C:171:PRO:HB3	3:C:235:LEU:O	2.13	0.47
3:C:334:TRP:CH2	3:C:344:LEU:HG	2.50	0.47
2:H:252:ILE:HD11	2:H:454:ILE:HG13	1.96	0.47
2:B:253:GLN:HB3	2:B:253:GLN:HE21	1.54	0.47
3:L:197:ARG:NH1	3:L:344:LEU:O	2.47	0.47
3:L:185:ASP:C	3:L:187:SER:H	2.16	0.47
2:K:224:MET:SD	2:K:237:ARG:HD3	2.53	0.47
2:K:313:GLU:OE2	2:K:323:LYS:NZ	2.43	0.47
2:E:223:GLU:CB	2:E:287:GLY:HA2	2.44	0.47
2:K:312:ILE:HB	2:K:324:ALA:HB3	1.96	0.47
1:A:137:GLN:HA	1:A:140:VAL:HG22	1.96	0.47
2:H:296:ASN:O	2:H:299:ILE:N	2.47	0.47
2:H:310:LEU:CB	2:H:454:ILE:HG22	2.44	0.47
3:I:373:LYS:HG3	3:I:377:TYR:CD2	2.49	0.47
2:B:310:LEU:HA	2:B:454:ILE:HG22	1.97	0.47
2:E:332:GLN:CG	2:E:339:GLN:HB3	2.43	0.47
1:G:143:GLN:NE2	3:I:117:ASN:HB2	2.30	0.47
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.15	0.47
3:F:372:TRP:HZ3	3:F:379:MET:HE1	1.77	0.47
2:H:303:THR:HB	2:H:330:THR:HA	1.96	0.47
4:N:3:ARG:HG2	4:N:3:ARG:NH2	2.29	0.47
2:B:161:ILE:HD13	3:C:103:HIS:CD2	2.49	0.47
2:B:164:ASN:H	2:B:166:ARG:HE	1.62	0.47
2:H:353:LEU:HA	2:H:370:HIS:HD2	1.80	0.47
3:I:325:ASN:ND2	3:I:327:ALA:HB3	2.24	0.47
2:B:161:ILE:O	2:B:166:ARG:NE	2.48	0.47
3:C:202:VAL:HG22	3:C:217:HIS:CE1	2.49	0.47
3:C:350:GLN:C	3:C:352:GLY:N	2.67	0.47
3:F:230:ASN:CA	3:F:233:ILE:HD12	2.31	0.47
2:H:383:ASP:HA	2:H:404:TYR:O	2.15	0.47
3:I:280:TYR:CD1	3:I:280:TYR:N	2.82	0.47
2:B:156:THR:HG22	2:B:160:ASN:ND2	2.23	0.47
3:L:145:ILE:HD13	3:L:168:PHE:HE2	1.80	0.47
2:B:367:MET:O	2:B:406:ARG:O	2.31	0.47
2:K:214:ILE:HD11	2:K:227:ILE:CG2	2.44	0.47
3:L:322:PHE:CE2	3:L:324:GLY:HA3	2.50	0.47
3:L:246:LEU:HD22	3:L:265:PHE:HD1	1.79	0.47
2:H:361:MET:HB2	5:H:470:NAG:O7	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.79	0.47
1:D:157:LYS:HA	1:D:157:LYS:CE	2.45	0.47
3:I:354:TYR:CE1	3:I:366:GLY:HA3	2.49	0.47
2:K:363:GLU:C	2:K:365:ARG:H	2.18	0.47
1:A:127:ILE:CG2	1:A:128:GLU:N	2.78	0.47
3:C:231:GLU:O	3:C:234:HIS:HB3	2.15	0.47
2:B:223:GLU:OE2	2:B:285:TYR:HD1	1.98	0.47
2:B:199:VAL:HG23	3:C:141:ASP:OD1	2.15	0.47
2:H:294:LEU:O	2:H:295:GLY:O	2.33	0.47
1:J:144:LEU:HD21	1:J:182:GLN:HG2	1.94	0.47
3:I:300:SER:O	3:I:302:LYS:N	2.47	0.47
3:I:143:VAL:HG12	3:I:220:PRO:CD	2.36	0.47
3:I:377:TYR:HD2	3:I:379:MET:CE	2.28	0.47
2:B:304:ARG:HH22	2:B:333:ASN:H	1.60	0.47
2:B:212:GLU:O	2:B:215:ILE:CG2	2.60	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.96	0.47
2:B:383:ASP:HA	2:B:404:TYR:O	2.15	0.47
2:E:164:ASN:O	2:E:168:LEU:HD12	2.15	0.47
1:D:188:VAL:HB	2:E:164:ASN:OD1	2.15	0.47
3:F:179:LEU:HG	3:F:218:LEU:CD1	2.45	0.47
3:L:372:TRP:HZ3	3:L:379:MET:HE1	1.78	0.47
3:C:297:ASP:HB2	3:C:301:ASP:CG	2.35	0.47
1:G:142:ALA:O	1:G:146:ASP:N	2.47	0.47
2:B:303:THR:HA	2:B:308:THR:OG1	2.14	0.47
1:A:188:VAL:O	1:A:189:ILE:HG13	2.15	0.47
3:C:128:VAL:C	3:C:130:GLN:N	2.67	0.47
1:J:164:SER:C	1:J:165:CYS:O	2.53	0.47
1:A:139:ASN:O	1:A:142:ALA:HB3	2.15	0.47
2:B:164:ASN:HB3	2:B:166:ARG:HH21	1.78	0.47
2:B:178:LYS:O	2:B:180:GLN:N	2.48	0.47
2:B:179:ILE:CD1	3:C:117:ASN:ND2	2.78	0.47
2:B:223:GLU:OE1	2:B:224:MET:O	2.33	0.47
3:C:195:GLN:CD	3:C:196:LYS:H	2.18	0.47
3:I:251:GLU:HA	3:I:256:ARG:O	2.14	0.47
3:I:318:ASP:OD2	3:I:325:ASN:HB2	2.15	0.47
2:B:211:CYS:O	2:B:242:MET:HE1	2.15	0.47
2:H:172:LEU:CD2	3:I:113:ILE:HG22	2.45	0.47
2:E:269:TYR:CE2	2:E:401:GLY:HA3	2.50	0.47
2:E:255:ARG:HD3	2:E:262:PHE:CZ	2.50	0.47
3:L:179:LEU:HG	3:L:218:LEU:CD1	2.45	0.47
2:B:280:THR:O	2:B:281:ASP:CG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:GLU:O	3:C:232:LYS:HE3	2.14	0.47
3:C:326:CYS:O	3:C:327:ALA:C	2.52	0.47
2:H:223:GLU:OE1	2:H:224:MET:O	2.33	0.47
3:L:330:ASP:HB3	3:L:343:HIS:HE1	1.79	0.47
2:K:333:ASN:N	2:K:336:ASN:HD22	2.10	0.47
2:H:155:GLU:C	2:H:157:VAL:N	2.66	0.47
2:E:210:GLU:OE2	2:E:213:GLU:HB2	2.15	0.47
3:C:99:SER:O	3:C:102:THR:HG23	2.15	0.47
1:G:158:ILE:HG13	2:H:189:GLN:HG2	1.96	0.47
2:E:239:TYR:OH	2:E:287:GLY:O	2.23	0.47
3:I:350:GLN:C	3:I:352:GLY:H	2.18	0.47
2:B:429:HIS:C	2:B:431:THR:H	2.19	0.47
3:I:203:ASP:O	3:I:206:LYS:HE3	2.15	0.47
2:H:249:TRP:CE3	2:H:455:ARG:HB2	2.50	0.47
3:I:134:GLN:O	3:I:136:GLN:N	2.43	0.47
2:H:339:GLN:HG2	2:H:340:ILE:N	2.29	0.47
1:J:183:LYS:O	1:J:186:GLU:HB2	2.15	0.47
2:E:270:LYS:HA	2:E:296:ASN:HB3	1.96	0.47
2:E:270:LYS:HG3	2:E:338:TYR:OH	2.15	0.47
1:G:171:ARG:HH11	1:G:171:ARG:CG	2.28	0.47
3:I:262:TYR:OH	3:I:288:ASP:OD1	2.23	0.47
2:E:157:VAL:HG23	2:E:158:ASN:N	2.30	0.47
2:E:280:THR:O	2:E:281:ASP:O	2.32	0.47
3:F:360:PRO:O	3:F:361:ASN:ND2	2.48	0.47
2:K:218:GLY:HA3	3:L:210:GLN:HG2	1.97	0.47
1:G:149:ARG:NH2	2:H:425:ASP:HA	2.24	0.46
3:C:316:ASP:O	3:C:317:ASN:CB	2.62	0.46
3:I:172:LEU:N	3:I:172:LEU:HD12	2.27	0.46
2:B:252:ILE:HD11	2:B:454:ILE:HG13	1.96	0.46
1:A:149:ARG:HD3	2:B:427:ALA:O	2.14	0.46
2:B:266:TRP:HB2	2:B:379:ASP:OD2	2.15	0.46
3:F:246:LEU:HD22	3:F:265:PHE:HD1	1.79	0.46
3:I:263:ALA:O	3:I:264:MET:C	2.52	0.46
1:D:169:LEU:CD1	2:E:185:ASP:OD1	2.63	0.46
3:C:322:PHE:C	3:C:324:GLY:H	2.18	0.46
2:B:249:TRP:CZ3	2:B:455:ARG:HB2	2.50	0.46
3:C:310:MET:O	3:C:335:TRP:CD1	2.68	0.46
3:I:167:TYR:N	3:I:167:TYR:HD1	2.11	0.46
3:I:196:LYS:HA	3:I:382:THR:O	2.16	0.46
2:B:207:SER:O	2:B:214:ILE:HG12	2.13	0.46
2:B:270:LYS:HD2	2:B:334:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:290:PHE:HA	3:L:307:HIS:HD1	1.78	0.46
1:A:148:LYS:HZ2	2:B:425:ASP:HB2	1.79	0.46
2:H:226:LEU:O	2:H:227:ILE:O	2.33	0.46
3:C:262:TYR:OH	3:C:288:ASP:OD1	2.25	0.46
2:B:354:MET:C	2:B:356:GLY:H	2.17	0.46
3:C:96:TYR:C	3:C:98:ALA:N	2.67	0.46
2:K:301:GLN:HE22	2:K:302:LEU:HG	1.77	0.46
2:K:374:PHE:CB	2:K:382:ASN:HB3	2.45	0.46
2:E:328:GLY:HA3	2:E:343:ASN:OD1	2.15	0.46
3:I:340:HIS:O	4:S:1:GLY:N	2.43	0.46
2:B:177:SER:HA	2:B:180:GLN:HG3	1.98	0.46
2:H:421:GLN:NE2	2:H:444:TRP:O	2.48	0.46
3:C:170:LYS:CE	3:C:177:GLN:HB3	2.44	0.46
3:C:212:LYS:CG	3:C:231:GLU:HB2	2.40	0.46
3:C:131:LEU:C	3:C:131:LEU:HD23	2.35	0.46
3:L:388:PRO:O	3:L:389:PHE:C	2.54	0.46
2:K:233:VAL:HG13	2:K:233:VAL:O	2.14	0.46
3:L:96:TYR:N	3:L:96:TYR:CD2	2.79	0.46
3:L:219:SER:CB	3:L:224:THR:CG2	2.91	0.46
1:J:122:LEU:HD21	3:L:98:ALA:HA	1.98	0.46
2:B:257:ASP:O	2:B:291:GLU:OE2	2.33	0.46
3:C:109:TYR:O	3:C:110:LEU:C	2.53	0.46
3:C:219:SER:HB2	3:C:220:PRO:HD2	1.97	0.46
3:C:233:ILE:HA	3:C:236:ILE:CD1	2.42	0.46
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.97	0.46
2:H:363:GLU:O	2:H:367:MET:HE2	2.14	0.46
3:I:191:TRP:HH2	3:I:247:ARG:NH1	2.13	0.46
3:I:344:LEU:HD12	3:I:384:MET:CE	2.45	0.46
1:D:143:GLN:HE21	3:F:118:ASN:HD22	1.64	0.46
2:H:214:ILE:CD1	2:H:227:ILE:HG22	2.41	0.46
3:C:354:TYR:CE1	3:C:366:GLY:HA3	2.50	0.46
3:C:372:TRP:CE3	3:C:373:LYS:HE3	2.50	0.46
1:G:133:ILE:HD12	1:G:133:ILE:N	2.29	0.46
3:C:189:ASN:OD1	3:C:391:ARG:NE	2.39	0.46
3:F:160:GLY:O	3:F:161:ALA:CB	2.61	0.46
3:F:240:SER:O	3:F:241:ALA:C	2.54	0.46
2:K:370:HIS:HE1	2:K:408:HIS:HB2	1.77	0.46
1:D:164:SER:O	1:D:165:CYS:O	2.34	0.46
1:D:159:ARG:HB3	1:D:159:ARG:HH11	1.81	0.46
3:F:100:ILE:HG22	3:F:100:ILE:O	2.16	0.46
1:G:150:LEU:HD13	3:I:125:LYS:HZ3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:365:ARG:O	2:H:368:THR:N	2.49	0.46
3:I:195:GLN:CD	3:I:196:LYS:H	2.19	0.46
3:I:213:GLU:O	3:I:232:LYS:HE3	2.15	0.46
3:I:312:PHE:HZ	3:I:333:GLY:O	1.98	0.46
3:I:154:GLN:NE2	3:I:190:GLY:H	2.14	0.46
2:B:215:ILE:HB	2:B:242:MET:CE	2.45	0.46
3:F:103:HIS:H	3:F:103:HIS:HD1	1.64	0.46
2:E:224:MET:SD	2:E:237:ARG:HD3	2.55	0.46
1:G:164:SER:HA	3:I:137:GLU:O	2.15	0.46
1:A:128:GLU:OE1	1:A:129:LYS:CD	2.63	0.46
2:B:283:LYS:HB3	2:B:285:TYR:CE2	2.51	0.46
3:C:197:ARG:HA	3:C:225:GLU:HG3	1.96	0.46
2:H:202:ASN:O	2:H:204:PRO:HD3	2.15	0.46
3:I:250:LEU:HD23	3:I:372:TRP:CE3	2.51	0.46
3:I:208:TRP:HZ2	3:I:270:GLU:HG3	1.80	0.46
3:I:334:TRP:CH2	3:I:344:LEU:HG	2.51	0.46
3:I:367:ILE:HB	3:I:379:MET:N	2.30	0.46
3:I:93:ILE:O	3:I:96:TYR:CD2	2.69	0.46
2:B:353:LEU:HA	2:B:370:HIS:HD2	1.81	0.46
3:L:391:ARG:HH11	3:L:391:ARG:CB	2.24	0.46
3:L:372:TRP:CZ3	3:L:379:MET:HE1	2.50	0.46
3:C:160:GLY:O	3:C:161:ALA:CB	2.63	0.46
3:I:317:ASN:HD22	3:I:317:ASN:C	2.19	0.46
3:L:152:ASP:OD1	3:L:154:GLN:N	2.48	0.46
2:K:161:ILE:HB	2:K:162:PRO:HD3	1.98	0.46
3:F:109:TYR:HA	3:F:112:GLU:OE1	2.16	0.46
1:J:159:ARG:HD3	2:K:418:TRP:HZ3	1.80	0.46
2:K:369:ILE:O	2:K:405:ASN:ND2	2.46	0.46
3:C:246:LEU:HD11	3:C:248:VAL:HG23	1.97	0.46
2:H:301:GLN:O	2:H:304:ARG:HB2	2.16	0.46
2:H:332:GLN:HB3	2:H:336:ASN:HD22	1.80	0.46
2:H:201:CYS:O	3:I:143:VAL:HG21	2.16	0.46
3:I:318:ASP:HB2	3:I:320:ASP:OD1	2.15	0.46
3:I:325:ASN:HD21	3:I:327:ALA:CB	2.27	0.46
2:B:215:ILE:HD13	2:B:242:MET:HB3	1.98	0.46
3:L:334:TRP:CG	3:L:335:TRP:N	2.83	0.46
3:F:119:GLN:CA	3:F:119:GLN:HE21	2.13	0.46
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.51	0.46
3:F:352:GLY:O	3:F:377:TYR:HA	2.15	0.46
3:L:170:LYS:HE2	3:L:176:GLN:C	2.36	0.46
3:I:184:ILE:N	3:I:184:ILE:HD12	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:284:GLY:C	3:C:286:ALA:N	2.67	0.46
1:A:157:LYS:HD2	3:C:132:GLU:CB	2.45	0.46
2:B:184:SER:O	2:B:188:ALA:N	2.46	0.46
2:H:198:THR:HA	3:I:140:LYS:O	2.15	0.46
3:I:219:SER:HB2	3:I:220:PRO:HD2	1.97	0.46
3:I:284:GLY:C	3:I:286:ALA:N	2.67	0.46
2:H:162:PRO:C	2:H:164:ASN:N	2.69	0.46
2:E:255:ARG:HH11	2:E:255:ARG:CG	2.28	0.46
2:B:365:ARG:O	2:B:368:THR:N	2.49	0.46
2:B:406:ARG:O	2:B:406:ARG:CG	2.62	0.46
2:H:377:THR:O	2:H:379:ASP:N	2.47	0.46
3:F:372:TRP:CZ3	3:F:379:MET:HE1	2.51	0.46
2:H:364:ASN:ND2	5:H:470:NAG:C6	2.78	0.46
3:F:95:LYS:HD2	3:F:98:ALA:CB	2.46	0.46
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.97	0.46
3:F:252:ASP:C	3:F:254:ASN:H	2.18	0.46
2:H:311:LEU:HB3	2:H:453:LYS:O	2.16	0.46
2:B:311:LEU:HB3	2:B:453:LYS:O	2.16	0.46
3:C:253:TRP:CZ3	3:C:380:LYS:HG3	2.51	0.46
3:C:367:ILE:HB	3:C:379:MET:N	2.31	0.46
1:A:165:CYS:HB3	2:B:193:CYS:HA	1.97	0.46
1:G:154:ILE:CD1	2:H:186:VAL:HG21	2.44	0.46
3:F:333:GLY:O	3:F:334:TRP:HB2	2.16	0.46
3:I:170:LYS:CE	3:I:177:GLN:HB3	2.45	0.46
2:B:214:ILE:CD1	2:B:227:ILE:HG22	2.41	0.46
2:B:310:LEU:CB	2:B:454:ILE:HG22	2.46	0.46
3:L:310:MET:C	3:L:311:GLN:O	2.54	0.46
2:K:255:ARG:HH11	2:K:255:ARG:CG	2.27	0.46
1:D:136:LEU:HD23	2:E:168:LEU:HD22	1.96	0.46
2:H:152:TYR:HE2	2:H:155:GLU:OE2	1.98	0.46
2:H:398:ASP:HA	2:H:433:ASP:HA	1.98	0.46
2:K:161:ILE:N	2:K:162:PRO:CD	2.79	0.46
3:C:242:ILE:HA	3:C:243:PRO:HD2	1.72	0.46
4:R:3:ARG:NH2	4:R:3:ARG:HG2	2.31	0.46
3:C:197:ARG:NH1	3:C:204:PHE:CD1	2.84	0.45
3:C:250:LEU:O	3:C:257:THR:HB	2.16	0.45
3:C:131:LEU:HD23	3:C:132:GLU:N	2.32	0.45
1:D:147:MET:SD	3:F:121:ILE:HD11	2.56	0.45
3:F:104:ASP:O	3:F:108:ARG:N	2.39	0.45
2:E:363:GLU:C	2:E:365:ARG:H	2.20	0.45
2:B:201:CYS:O	3:C:143:VAL:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:PHE:CE2	3:C:232:LYS:HB3	2.51	0.45
3:C:250:LEU:HD23	3:C:372:TRP:CE3	2.52	0.45
2:H:229:PRO:O	2:H:230:ASP:C	2.53	0.45
3:L:169:ILE:HD11	3:L:236:ILE:HD11	1.97	0.45
3:L:240:SER:O	3:L:241:ALA:C	2.55	0.45
3:I:178:PHE:H	3:I:178:PHE:HD1	1.63	0.45
2:B:329:PHE:HD1	2:B:342:VAL:HG12	1.81	0.45
1:A:145:VAL:HG13	1:A:148:LYS:HE2	1.99	0.45
2:H:359:GLN:O	2:H:359:GLN:HG2	2.17	0.45
2:H:210:GLU:OE1	2:H:212:GLU:CB	2.64	0.45
3:I:342:GLY:HA2	3:I:368:ILE:O	2.17	0.45
3:L:219:SER:HB3	3:L:224:THR:HG21	1.96	0.45
2:B:377:THR:O	2:B:379:ASP:N	2.46	0.45
2:E:155:GLU:O	2:E:156:THR:C	2.54	0.45
2:K:223:GLU:CB	2:K:287:GLY:HA2	2.46	0.45
2:K:359:GLN:OE1	2:K:438:MET:HB3	2.16	0.45
3:C:103:HIS:HA	3:C:106:SER:OG	2.17	0.45
2:H:184:SER:O	2:H:187:SER:N	2.41	0.45
3:I:123:ASN:C	3:I:125:LYS:H	2.19	0.45
2:H:310:LEU:HB3	2:H:454:ILE:HG22	1.98	0.45
2:H:283:LYS:HB3	2:H:285:TYR:CE2	2.51	0.45
3:I:301:ASP:HA	4:S:2:HYP:OD1	2.16	0.45
3:I:304:PHE:HB3	3:I:338:LYS:HB3	1.98	0.45
3:I:189:ASN:OD1	3:I:391:ARG:NE	2.40	0.45
2:B:207:SER:C	2:B:214:ILE:HG12	2.37	0.45
2:B:256:GLN:HB3	2:B:449:LYS:HZ3	1.82	0.45
3:F:304:PHE:O	3:F:337:ASN:ND2	2.46	0.45
2:B:398:ASP:HA	2:B:433:ASP:CA	2.45	0.45
3:C:337:ASN:OD1	3:C:338:LYS:N	2.47	0.45
2:E:204:PRO:HG2	2:E:224:MET:O	2.17	0.45
3:I:242:ILE:HA	3:I:243:PRO:HD2	1.71	0.45
3:C:243:PRO:HG3	3:F:279:ALA:HB1	1.99	0.45
3:L:317:ASN:ND2	3:L:319:ASN:OD1	2.49	0.45
2:E:420:GLY:HA2	2:E:446:SER:O	2.17	0.45
1:J:131:GLN:NE2	1:J:132:HIS:N	2.64	0.45
1:G:150:LEU:HD22	3:I:121:ILE:HD11	1.98	0.45
2:H:182:LEU:O	2:H:182:LEU:HD23	2.15	0.45
2:H:292:TYR:CE2	2:H:294:LEU:HB2	2.49	0.45
3:I:304:PHE:CE2	3:I:338:LYS:HD3	2.51	0.45
3:L:195:GLN:HG3	3:L:227:TRP:CE3	2.52	0.45
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:215:ILE:HB	2:H:242:MET:CE	2.46	0.45
1:D:132:HIS:O	1:D:135:LEU:HB3	2.15	0.45
2:B:351:ASN:ND2	2:B:354:MET:HG2	2.25	0.45
3:C:301:ASP:OD2	4:O:2:HYP:OD1	2.23	0.45
3:L:100:ILE:C	3:L:102:THR:H	2.19	0.45
2:H:398:ASP:HA	2:H:433:ASP:CA	2.45	0.45
2:K:313:GLU:HG2	2:K:323:LYS:HD2	1.98	0.45
3:F:152:ASP:OD1	3:F:154:GLN:N	2.48	0.45
2:K:378:TYR:HB2	2:K:396:LYS:HG2	1.98	0.45
4:M:3:ARG:O	4:M:5:NH2:N	2.50	0.45
3:C:359:THR:HB	3:C:362:GLY:C	2.37	0.45
1:J:121:VAL:HG12	1:J:121:VAL:O	2.16	0.45
3:C:196:LYS:HD2	3:C:198:LEU:CD1	2.46	0.45
2:H:252:ILE:HG22	2:H:299:ILE:HD11	1.99	0.45
3:I:334:TRP:O	3:I:335:TRP:C	2.55	0.45
2:K:327:GLY:CA	2:K:344:LYS:HE3	2.45	0.45
1:A:151:GLU:HB2	2:B:182:LEU:HD13	1.98	0.45
2:H:280:THR:O	2:H:281:ASP:CG	2.55	0.45
3:I:350:GLN:C	3:I:352:GLY:N	2.69	0.45
2:E:257:ASP:HA	2:E:416:TYR:CE2	2.51	0.45
2:E:406:ARG:O	2:E:406:ARG:HG2	2.16	0.45
2:B:176:ARG:HA	2:B:176:ARG:NH1	2.31	0.45
3:C:377:TYR:HD2	3:C:379:MET:CE	2.29	0.45
3:I:191:TRP:CG	3:I:385:LYS:HD2	2.52	0.45
1:G:127:ILE:O	1:G:131:GLN:N	2.49	0.45
2:B:236:TYR:CB	2:B:298:LYS:NZ	2.76	0.45
3:L:204:PHE:C	3:L:206:LYS:N	2.70	0.45
3:L:304:PHE:CD1	3:L:338:LYS:CB	2.99	0.45
3:L:183:GLU:HB3	3:L:191:TRP:HB2	1.99	0.45
1:A:119:ILE:HD11	3:C:95:LYS:HZ3	1.81	0.45
2:E:382:ASN:O	2:E:383:ASP:O	2.34	0.45
3:L:352:GLY:O	3:L:377:TYR:HA	2.16	0.45
3:L:118:ASN:O	3:L:122:VAL:HG23	2.16	0.45
2:E:305:MET:HG2	2:E:305:MET:O	2.16	0.45
2:B:166:ARG:N	2:B:166:ARG:CD	2.80	0.45
3:C:112:GLU:C	3:C:114:TYR:N	2.69	0.45
3:C:197:ARG:HD3	3:C:204:PHE:CE1	2.52	0.45
3:C:226:PHE:HE2	3:C:228:LEU:HB2	1.82	0.45
2:H:176:ARG:HB3	2:H:176:ARG:CZ	2.46	0.45
3:I:129:ALA:O	3:I:132:GLU:HB3	2.16	0.45
3:F:344:LEU:HA	3:F:367:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:326:TYR:OH	2:H:353:LEU:HB2	2.17	0.45
3:I:250:LEU:HG	3:I:251:GLU:H	1.80	0.45
3:I:270:GLU:HB2	3:I:274:TYR:OH	2.16	0.45
3:I:208:TRP:HE3	3:I:314:THR:CG2	2.28	0.45
2:B:294:LEU:O	2:B:295:GLY:O	2.35	0.45
1:A:149:ARG:HA	1:A:152:VAL:HG23	1.99	0.45
3:F:119:GLN:O	3:F:122:VAL:HB	2.17	0.45
1:A:144:LEU:HG	1:A:182:GLN:OE1	2.16	0.45
3:C:263:ALA:O	3:C:264:MET:C	2.54	0.45
1:A:191:LYS:O	1:A:192:ASP:OD2	2.34	0.45
2:E:160:ASN:N	2:E:162:PRO:HD2	2.31	0.45
1:G:159:ARG:HG2	2:H:258:GLY:HA3	1.99	0.45
2:K:160:ASN:C	2:K:162:PRO:HD2	2.37	0.45
1:A:183:LYS:HD3	1:A:183:LYS:C	2.37	0.45
2:E:191:GLU:C	2:E:193:CYS:N	2.69	0.45
3:L:292:GLY:C	3:L:302:LYS:HD2	2.37	0.45
1:A:133:ILE:HG22	1:A:137:GLN:OE1	2.17	0.45
2:H:423:THR:HA	2:H:444:TRP:CE3	2.52	0.45
2:B:205:VAL:CG1	3:C:232:LYS:HZ3	2.29	0.45
3:F:251:GLU:CB	3:F:381:LYS:HB2	2.46	0.45
2:H:351:ASN:ND2	2:H:354:MET:HG2	2.25	0.45
2:B:226:LEU:O	2:B:227:ILE:C	2.55	0.45
2:H:207:SER:C	2:H:214:ILE:HG12	2.38	0.45
3:F:321:LYS:N	3:F:337:ASN:O	2.38	0.45
1:J:149:ARG:O	1:J:150:LEU:C	2.54	0.45
2:K:168:LEU:HB3	3:L:110:LEU:HD13	1.99	0.45
2:H:257:ASP:O	2:H:291:GLU:OE2	2.34	0.45
3:L:293:PHE:N	3:L:305:THR:OG1	2.50	0.45
3:C:214:GLY:HA3	3:C:228:LEU:O	2.17	0.45
1:G:129:LYS:HA	1:G:133:ILE:HD13	1.99	0.45
3:I:95:LYS:C	3:I:97:GLU:N	2.70	0.45
3:F:118:ASN:HA	3:F:118:ASN:HD22	1.66	0.45
1:D:122:LEU:N	1:D:124:ARG:HG2	2.31	0.45
3:F:219:SER:CB	3:F:224:THR:HG21	2.46	0.45
3:I:207:ASN:ND2	3:I:210:GLN:HG3	2.31	0.45
2:E:257:ASP:OD2	2:E:259:SER:OG	2.34	0.45
1:J:176:LYS:HE3	1:J:176:LYS:HB2	1.68	0.45
3:C:340:HIS:O	4:O:1:GLY:CA	2.65	0.45
2:B:158:ASN:CG	3:C:100:ILE:HD13	2.37	0.45
3:C:212:LYS:C	3:C:214:GLY:H	2.19	0.45
3:C:173:LYS:HE3	3:C:238:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:127:LYS:O	3:I:128:VAL:C	2.55	0.45
3:I:223:THR:O	3:I:224:THR:HB	2.17	0.45
3:I:367:ILE:CG2	3:I:379:MET:HB2	2.46	0.45
3:L:207:ASN:OD1	3:L:208:TRP:N	2.50	0.45
3:L:166:LEU:HD22	3:L:179:LEU:CD1	2.45	0.45
2:H:153:ILE:HG23	2:H:154:ASP:OD2	2.17	0.45
2:E:367:MET:O	2:E:405:ASN:ND2	2.50	0.44
3:I:226:PHE:HE2	3:I:228:LEU:HB2	1.82	0.44
2:H:210:GLU:CD	2:H:212:GLU:HB3	2.38	0.44
2:E:172:LEU:HG	3:F:113:ILE:CG2	2.47	0.44
3:I:275:ARG:CA	3:I:311:GLN:HA	2.48	0.44
3:L:97:GLU:HA	3:L:100:ILE:CD1	2.47	0.44
2:K:203:ILE:HA	2:K:204:PRO:HD3	1.77	0.44
3:L:284:GLY:C	3:L:286:ALA:H	2.20	0.44
3:C:184:ILE:HD12	3:C:184:ILE:N	2.32	0.44
2:H:455:ARG:HG2	2:H:456:PRO:HD2	1.97	0.44
3:L:293:PHE:O	3:L:301:ASP:O	2.35	0.44
3:C:167:TYR:HD1	3:C:167:TYR:N	2.12	0.44
1:A:167:ARG:NE	2:B:192:TYR:CD2	2.73	0.44
3:C:124:LEU:CG	3:C:124:LEU:O	2.65	0.44
3:F:197:ARG:C	3:F:198:LEU:HD12	2.38	0.44
3:I:178:PHE:CD2	3:I:228:LEU:HD11	2.53	0.44
2:B:214:ILE:O	2:B:214:ILE:HG22	2.17	0.44
1:D:131:GLN:HA	1:D:134:GLN:HG2	1.99	0.44
2:B:398:ASP:HA	2:B:433:ASP:HA	1.99	0.44
3:L:105:SER:O	3:L:108:ARG:HG2	2.18	0.44
2:E:170:SER:O	2:E:171:ILE:C	2.55	0.44
3:F:293:PHE:N	3:F:305:THR:OG1	2.50	0.44
2:K:405:ASN:O	2:K:407:CYS:N	2.50	0.44
2:B:161:ILE:HG23	2:B:166:ARG:CZ	2.47	0.44
2:B:167:VAL:O	2:B:171:ILE:HG12	2.17	0.44
3:C:191:TRP:HH2	3:C:247:ARG:NH1	2.14	0.44
3:C:253:TRP:CZ2	3:C:349:TYR:O	2.70	0.44
3:F:148:ILE:CD1	3:F:148:ILE:N	2.68	0.44
3:L:121:ILE:O	3:L:125:LYS:HG2	2.18	0.44
3:I:196:LYS:CD	3:I:198:LEU:HD11	2.47	0.44
1:G:124:ARG:C	1:G:126:VAL:N	2.68	0.44
1:G:129:LYS:HA	1:G:133:ILE:HD11	1.99	0.44
2:B:329:PHE:CZ	2:B:331:VAL:HG23	2.52	0.44
3:L:229:GLY:O	3:L:230:ASN:C	2.55	0.44
2:B:411:ASN:HD22	2:B:434:GLY:H	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:408:HIS:CE1	2:K:411:ASN:HB2	2.51	0.44
2:E:415:ARG:H	2:E:434:GLY:HA2	1.82	0.44
3:F:298:ASP:OD2	3:F:300:SER:HB2	2.17	0.44
1:J:130:VAL:CA	1:J:133:ILE:HG22	2.47	0.44
3:I:340:HIS:CE1	3:I:364:ASP:OD2	2.70	0.44
3:C:143:VAL:O	3:C:144:GLN:HG3	2.17	0.44
3:C:367:ILE:CG2	3:C:379:MET:HB2	2.47	0.44
2:H:193:CYS:O	3:I:134:GLN:OE1	2.36	0.44
2:H:301:GLN:HE22	2:H:302:LEU:CD2	2.24	0.44
3:I:154:GLN:OE1	3:I:190:GLY:N	2.49	0.44
2:B:293:TRP:O	2:B:295:GLY:N	2.50	0.44
3:L:197:ARG:NE	3:L:204:PHE:CE1	2.85	0.44
3:L:307:HIS:HA	3:L:310:MET:HG2	1.98	0.44
2:H:206:VAL:HG22	2:H:214:ILE:HG23	1.99	0.44
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.99	0.44
2:B:265:LYS:HE3	2:B:378:TYR:CE1	2.53	0.44
1:J:181:GLN:HE21	2:K:171:ILE:HA	1.82	0.44
2:E:303:THR:CB	2:E:330:THR:HA	2.46	0.44
2:E:407:CYS:HB2	4:N:3:ARG:HH22	1.81	0.44
3:C:207:ASN:CG	3:C:210:GLN:HG3	2.38	0.44
1:A:119:ILE:O	1:A:119:ILE:HG23	2.18	0.44
3:F:284:GLY:C	3:F:286:ALA:H	2.21	0.44
3:F:293:PHE:O	3:F:301:ASP:O	2.36	0.44
2:K:366:THR:HA	2:K:369:ILE:HG13	1.99	0.44
2:B:164:ASN:H	2:B:166:ARG:NE	2.15	0.44
2:B:165:LEU:CG	2:B:166:ARG:NH2	2.80	0.44
3:C:169:ILE:HD12	3:C:171:PRO:CD	2.38	0.44
3:C:251:GLU:HA	3:C:257:THR:HA	1.99	0.44
1:G:154:ILE:HD12	2:H:182:LEU:CD2	2.47	0.44
2:H:180:GLN:C	2:H:182:LEU:N	2.69	0.44
3:F:204:PHE:C	3:F:206:LYS:N	2.70	0.44
2:K:191:GLU:C	2:K:193:CYS:N	2.71	0.44
2:H:236:TYR:O	2:H:236:TYR:CD1	2.70	0.44
2:H:310:LEU:HD23	2:H:329:PHE:CG	2.52	0.44
3:I:310:MET:O	3:I:335:TRP:HD1	1.99	0.44
1:G:125:LYS:HG2	1:G:129:LYS:HE2	1.98	0.44
1:D:140:VAL:HG13	1:D:141:ARG:N	2.32	0.44
3:I:316:ASP:OD2	3:I:316:ASP:O	2.35	0.44
1:A:119:ILE:HD11	3:C:95:LYS:NZ	2.31	0.44
3:C:163:GLN:O	3:C:167:TYR:OH	2.30	0.44
3:C:191:TRP:CG	3:C:385:LYS:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:290:PHE:CD1	3:F:307:HIS:ND1	2.86	0.44
2:H:402:TRP:CH2	2:H:412:PRO:HD2	2.52	0.44
2:H:351:ASN:OD1	2:H:354:MET:HG3	2.18	0.44
2:K:309:GLU:HB2	2:K:325:HIS:HE1	1.82	0.44
1:D:135:LEU:CD2	1:D:139:ASN:HD21	2.31	0.44
3:C:369:TRP:NE1	3:C:371:THR:OG1	2.51	0.44
2:E:366:THR:HA	2:E:369:ILE:HG13	2.00	0.44
1:A:131:GLN:C	1:A:133:ILE:H	2.21	0.44
2:B:155:GLU:O	2:B:159:SER:N	2.49	0.44
3:C:171:PRO:O	3:C:172:LEU:C	2.55	0.44
3:I:169:ILE:HD12	3:I:171:PRO:CD	2.39	0.44
3:I:212:LYS:CG	3:I:231:GLU:HB2	2.43	0.44
3:I:251:GLU:HA	3:I:257:THR:HA	1.99	0.44
3:I:295:PHE:HB2	3:I:301:ASP:OD2	2.18	0.44
2:E:327:GLY:CA	2:E:344:LYS:HE3	2.46	0.44
2:K:332:GLN:CG	2:K:339:GLN:HB3	2.47	0.44
1:G:120:GLU:CD	1:G:121:VAL:N	2.68	0.44
2:E:253:GLN:HB2	2:E:293:TRP:CZ3	2.53	0.44
2:B:390:PRO:O	2:B:393:GLN:NE2	2.51	0.44
2:E:434:GLY:O	2:E:436:VAL:HG13	2.18	0.44
2:E:324:ALA:HB2	2:E:349:ALA:HB3	1.98	0.44
2:E:360:LEU:CD1	2:E:364:ASN:O	2.62	0.44
2:B:198:THR:HA	3:C:140:LYS:O	2.18	0.44
1:J:167:ARG:NH1	2:K:192:TYR:CZ	2.86	0.44
2:H:170:SER:O	2:H:173:GLU:HB2	2.18	0.44
2:H:191:GLU:O	2:H:193:CYS:N	2.49	0.44
2:E:433:ASP:O	2:E:433:ASP:OD1	2.36	0.44
2:H:326:TYR:O	2:H:327:GLY:C	2.56	0.44
3:L:384:MET:HE3	3:L:384:MET:HB2	1.81	0.44
1:D:133:ILE:HG13	3:F:107:ILE:HD12	1.99	0.44
3:L:250:LEU:HD23	3:L:372:TRP:HE3	1.83	0.44
3:L:96:TYR:O	3:L:99:SER:HB2	2.18	0.44
2:H:228:GLN:NE2	2:H:231:SER:OG	2.51	0.44
2:K:382:ASN:O	2:K:383:ASP:O	2.35	0.44
1:J:124:ARG:O	1:J:128:GLU:HB2	2.17	0.44
2:B:159:SER:CA	2:B:162:PRO:HD2	2.48	0.44
3:C:143:VAL:HG12	3:C:220:PRO:CD	2.40	0.44
3:C:204:PHE:CE2	3:C:227:TRP:HB2	2.53	0.44
1:A:166:SER:CB	2:B:195:THR:O	2.66	0.44
2:B:184:SER:C	2:B:186:VAL:N	2.71	0.44
2:H:329:PHE:CZ	2:H:331:VAL:HG23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:178:PHE:CE2	3:I:232:LYS:HB3	2.53	0.44
3:I:195:GLN:HE21	3:I:195:GLN:HB3	1.64	0.44
3:I:239:GLN:O	3:I:240:SER:HB3	2.17	0.44
3:I:331:GLY:O	3:I:332:SER:CB	2.65	0.44
2:B:236:TYR:HB2	2:B:298:LYS:HZ1	1.80	0.44
2:K:332:GLN:HB3	2:K:336:ASN:CB	2.47	0.44
1:D:147:MET:O	1:D:148:LYS:C	2.56	0.44
2:H:207:SER:O	2:H:214:ILE:HG12	2.16	0.44
1:D:126:VAL:O	1:D:127:ILE:C	2.55	0.44
3:C:276:LEU:HD12	3:C:276:LEU:C	2.38	0.44
2:E:214:ILE:HD11	2:E:227:ILE:CG2	2.47	0.44
3:I:322:PHE:C	3:I:324:GLY:H	2.21	0.44
1:A:137:GLN:CA	1:A:140:VAL:HG22	2.48	0.43
2:B:165:LEU:N	2:B:166:ARG:CZ	2.81	0.43
3:C:211:TYR:HD1	3:C:227:TRP:NE1	2.16	0.43
3:F:204:PHE:O	3:F:206:LYS:N	2.48	0.43
2:H:337:LYS:O	2:H:338:TYR:HB2	2.18	0.43
3:I:231:GLU:O	3:I:234:HIS:HB3	2.18	0.43
2:B:210:GLU:CD	2:B:212:GLU:HB3	2.39	0.43
3:C:273:LYS:HG3	3:C:319:ASN:ND2	2.33	0.43
3:F:189:ASN:ND2	3:F:391:ARG:HG2	2.33	0.43
2:E:270:LYS:HE2	2:E:297:ASP:OD2	2.17	0.43
3:I:289:ALA:HB2	3:I:371:THR:HG23	2.00	0.43
3:F:250:LEU:HD21	3:F:369:TRP:CG	2.53	0.43
3:C:208:TRP:HZ2	3:C:270:GLU:HG3	1.83	0.43
2:B:303:THR:O	2:B:308:THR:OG1	2.35	0.43
1:G:188:VAL:HG21	2:H:167:VAL:HG21	1.99	0.43
2:H:167:VAL:O	2:H:171:ILE:HG12	2.18	0.43
1:J:159:ARG:HG2	2:K:258:GLY:HA3	2.00	0.43
3:I:365:ASN:ND2	3:I:366:GLY:N	2.66	0.43
3:C:234:HIS:HA	3:C:267:VAL:HG12	2.00	0.43
1:A:165:CYS:O	1:A:166:SER:O	2.36	0.43
3:I:348:TYR:HA	3:I:367:ILE:CD1	2.41	0.43
2:B:229:PRO:O	2:B:230:ASP:C	2.54	0.43
3:L:269:PRO:C	3:L:273:LYS:O	2.56	0.43
1:D:133:ILE:HG22	1:D:134:GLN:N	2.33	0.43
2:E:304:ARG:HH11	2:E:304:ARG:HB3	1.83	0.43
2:K:257:ASP:HA	2:K:416:TYR:CZ	2.54	0.43
1:G:178:TYR:C	1:G:180:ASP:N	2.69	0.43
2:H:251:VAL:CG1	2:H:252:ILE:N	2.81	0.43
2:H:351:ASN:HB3	2:H:355:ASP:CB	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:GLN:HE22	2:B:302:LEU:CD2	2.28	0.43
2:E:241:ASP:N	2:E:249:TRP:O	2.46	0.43
3:C:278:TYR:OH	3:C:308:ASN:HB2	2.18	0.43
1:G:136:LEU:HA	1:G:139:ASN:HB2	2.01	0.43
2:H:317:TRP:CE3	2:H:448:ARG:HD2	2.52	0.43
3:C:329:GLN:NE2	4:O:3:ARG:HH11	2.14	0.43
3:C:322:PHE:C	3:C:324:GLY:N	2.72	0.43
2:E:374:PHE:CB	2:E:382:ASN:HB3	2.47	0.43
2:K:256:GLN:O	2:K:257:ASP:HB3	2.18	0.43
3:L:260:ALA:HB2	3:L:286:ALA:HB3	2.00	0.43
3:F:354:TYR:OH	3:F:364:ASP:HB2	2.18	0.43
2:B:313:GLU:HB2	2:B:453:LYS:NZ	2.33	0.43
2:H:173:GLU:C	2:H:175:LEU:N	2.62	0.43
3:F:195:GLN:CG	3:F:227:TRP:CE3	3.02	0.43
3:F:234:HIS:HE1	3:F:269:PRO:HD3	1.81	0.43
3:I:220:PRO:HG2	3:I:221:THR:N	2.30	0.43
2:B:326:TYR:O	2:B:327:GLY:C	2.56	0.43
1:A:178:TYR:O	1:A:180:ASP:N	2.42	0.43
2:K:186:VAL:O	2:K:190:MET:HG3	2.18	0.43
3:C:340:HIS:CE1	3:C:364:ASP:OD2	2.71	0.43
3:C:194:PHE:HB2	3:C:233:ILE:CD1	2.48	0.43
3:C:267:VAL:O	3:C:267:VAL:HG13	2.17	0.43
2:B:190:MET:SD	2:B:190:MET:O	2.76	0.43
3:F:269:PRO:C	3:F:273:LYS:O	2.56	0.43
3:F:307:HIS:HA	3:F:310:MET:HG2	1.99	0.43
2:H:253:GLN:HB2	2:H:293:TRP:HZ3	1.80	0.43
2:H:301:GLN:NE2	2:H:301:GLN:C	2.72	0.43
3:I:214:GLY:HA3	3:I:228:LEU:O	2.19	0.43
3:I:172:LEU:CD1	3:I:239:GLN:NE2	2.78	0.43
3:F:124:LEU:O	3:F:125:LYS:C	2.55	0.43
2:H:214:ILE:HG22	2:H:214:ILE:O	2.18	0.43
3:F:108:ARG:O	3:F:111:GLN:HB3	2.18	0.43
3:C:281:PHE:CG	3:C:288:ASP:HB2	2.53	0.43
2:B:351:ASN:OD1	2:B:354:MET:HG3	2.19	0.43
1:D:124:ARG:HD3	1:D:124:ARG:N	2.24	0.43
3:C:157:ALA:HA	3:C:161:ALA:CB	2.42	0.43
3:F:219:SER:CB	3:F:224:THR:CG2	2.95	0.43
3:L:205:LYS:HG2	3:L:331:GLY:C	2.38	0.43
3:F:250:LEU:HD23	3:F:372:TRP:HE3	1.84	0.43
2:H:390:PRO:O	2:H:393:GLN:NE2	2.52	0.43
3:F:109:TYR:CE1	3:F:110:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:429:HIS:C	2:H:431:THR:H	2.22	0.43
3:L:252:ASP:OD1	3:L:255:GLY:N	2.51	0.43
3:F:170:LYS:HE2	3:F:176:GLN:C	2.38	0.43
1:A:124:ARG:N	1:A:124:ARG:HD2	2.32	0.43
1:J:126:VAL:C	1:J:128:GLU:N	2.72	0.43
3:C:172:LEU:CD1	3:C:239:GLN:HE21	2.23	0.43
2:E:398:ASP:C	2:E:433:ASP:HB3	2.39	0.43
3:I:171:PRO:O	3:I:172:LEU:C	2.56	0.43
3:I:204:PHE:CE2	3:I:227:TRP:HB2	2.53	0.43
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.84	0.43
2:B:423:THR:HA	2:B:444:TRP:CE3	2.54	0.43
3:C:278:TYR:HE2	3:C:290:PHE:CD2	2.27	0.43
3:I:273:LYS:CE	3:I:319:ASN:HD21	2.20	0.43
3:F:219:SER:HB3	3:F:224:THR:HG21	1.97	0.43
3:C:329:GLN:NE2	3:C:363:TYR:HB2	2.31	0.43
2:E:303:THR:CG2	2:E:330:THR:HA	2.48	0.43
2:K:303:THR:CB	2:K:330:THR:HA	2.47	0.43
2:K:303:THR:HG21	2:K:330:THR:HA	2.00	0.43
3:I:253:TRP:CZ2	3:I:349:TYR:O	2.71	0.43
3:C:196:LYS:C	3:C:197:ARG:HG2	2.38	0.43
3:C:251:GLU:CG	3:C:252:ASP:H	2.21	0.43
3:F:334:TRP:CG	3:F:335:TRP:N	2.86	0.43
3:I:196:LYS:HD2	3:I:198:LEU:HD11	2.00	0.43
1:A:149:ARG:HA	1:A:152:VAL:CG2	2.48	0.43
2:E:456:PRO:O	2:E:457:PHE:C	2.57	0.43
2:H:266:TRP:NE1	2:H:380:ARG:NH2	2.59	0.43
3:L:156:ILE:O	3:L:160:GLY:O	2.36	0.43
3:F:109:TYR:CD1	3:F:109:TYR:C	2.92	0.43
3:C:126:GLU:HA	3:C:129:ALA:HB3	2.00	0.43
2:B:165:LEU:HD13	3:C:106:SER:C	2.39	0.43
1:G:148:LYS:CE	1:G:182:GLN:HE22	2.31	0.43
3:C:344:LEU:HD12	3:C:384:MET:CE	2.49	0.43
3:F:229:GLY:O	3:F:230:ASN:C	2.57	0.43
3:C:154:GLN:HE21	3:C:158:ASN:HD21	1.67	0.43
1:D:150:LEU:HD13	3:F:125:LYS:HE2	1.99	0.43
2:B:359:GLN:HG2	2:B:359:GLN:O	2.19	0.43
3:I:276:LEU:HD11	3:I:309:GLY:N	2.34	0.43
2:E:212:GLU:CG	2:E:212:GLU:O	2.67	0.43
3:I:281:PHE:CG	3:I:288:ASP:HB2	2.53	0.43
2:K:301:GLN:HE21	2:K:302:LEU:N	2.16	0.43
3:F:205:LYS:HG2	3:F:331:GLY:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:321:LYS:HA	3:L:321:LYS:HD3	1.88	0.43
2:K:365:ARG:O	2:K:365:ARG:HG2	2.18	0.43
3:I:131:LEU:HD23	3:I:132:GLU:N	2.34	0.43
3:I:234:HIS:HA	3:I:267:VAL:HG12	2.00	0.43
2:B:250:THR:O	2:B:252:ILE:HD11	2.19	0.43
3:L:198:LEU:HD12	3:L:198:LEU:N	2.33	0.43
2:B:423:THR:O	2:B:426:MET:HG3	2.19	0.43
3:F:178:PHE:CZ	3:F:236:ILE:HD11	2.54	0.43
3:F:391:ARG:HH11	3:F:391:ARG:CB	2.27	0.43
2:K:332:GLN:HG3	2:K:339:GLN:HB3	2.01	0.43
3:L:250:LEU:O	3:L:257:THR:HG22	2.19	0.43
3:L:289:ALA:HB2	3:L:371:THR:OG1	2.19	0.43
2:B:317:TRP:CE3	2:B:448:ARG:HD2	2.53	0.43
3:L:275:ARG:NH1	3:L:309:GLY:O	2.47	0.43
1:A:175:LEU:O	1:A:179:GLU:N	2.51	0.43
2:H:316:ASP:HB2	2:H:445:TYR:OH	2.18	0.43
2:B:429:HIS:O	2:B:431:THR:N	2.46	0.43
3:C:203:ASP:O	3:C:206:LYS:HE3	2.19	0.43
2:K:384:GLY:H	2:K:405:ASN:HA	1.84	0.43
3:C:279:ALA:CB	3:C:280:TYR:CD1	3.02	0.43
2:H:199:VAL:HG23	3:I:141:ASP:HA	2.01	0.43
2:B:236:TYR:OH	2:B:302:LEU:HD11	2.19	0.43
2:B:333:ASN:OD1	2:B:335:ALA:HB3	2.18	0.43
3:L:208:TRP:CA	3:L:314:THR:HG21	2.38	0.43
2:K:241:ASP:N	2:K:249:TRP:O	2.48	0.43
3:I:276:LEU:C	3:I:276:LEU:HD12	2.39	0.43
3:L:97:GLU:C	3:L:99:SER:N	2.70	0.43
3:C:99:SER:O	3:C:102:THR:CG2	2.67	0.43
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.79	0.43
2:B:346:ARG:HH11	2:B:346:ARG:CB	2.32	0.43
3:F:252:ASP:OD1	3:F:255:GLY:N	2.51	0.43
2:B:223:GLU:HB2	2:B:286:CYS:O	2.18	0.42
3:C:220:PRO:HG2	3:C:221:THR:N	2.34	0.42
3:C:300:SER:O	3:C:302:LYS:N	2.51	0.42
2:H:310:LEU:CA	2:H:454:ILE:HG22	2.49	0.42
3:I:377:TYR:CD2	3:I:379:MET:HE1	2.54	0.42
2:B:210:GLU:OE1	2:B:212:GLU:CB	2.67	0.42
2:B:304:ARG:HH22	2:B:333:ASN:ND2	2.17	0.42
3:C:154:GLN:NE2	3:C:190:GLY:H	2.17	0.42
1:D:131:GLN:C	1:D:133:ILE:H	2.22	0.42
3:I:288:ASP:O	3:I:371:THR:HG21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLN:NE2	2:B:231:SER:OG	2.52	0.42
2:H:231:SER:HB2	3:I:176:GLN:NE2	2.34	0.42
3:F:170:LYS:HE3	3:F:177:GLN:HB3	2.00	0.42
2:B:161:ILE:C	2:B:163:THR:H	2.23	0.42
3:C:108:ARG:O	3:C:111:GLN:HB3	2.18	0.42
2:H:442:GLY:O	2:H:444:TRP:N	2.52	0.42
3:C:235:LEU:CD1	3:C:235:LEU:H	2.12	0.42
3:C:318:ASP:HB2	3:C:320:ASP:OD1	2.18	0.42
2:H:176:ARG:HH11	2:H:176:ARG:CG	2.32	0.42
3:I:148:ILE:N	3:I:148:ILE:HD12	2.34	0.42
2:B:206:VAL:HG22	2:B:214:ILE:HG23	2.01	0.42
2:B:271:GLN:O	2:B:295:GLY:HA3	2.19	0.42
3:F:236:ILE:HG21	3:F:386:ILE:HD11	2.01	0.42
2:K:249:TRP:CZ2	2:K:311:LEU:HD23	2.54	0.42
3:L:250:LEU:HD21	3:L:369:TRP:CG	2.54	0.42
3:C:295:PHE:HB2	3:C:301:ASP:OD2	2.18	0.42
2:H:265:LYS:HB3	2:H:379:ASP:CG	2.40	0.42
3:L:205:LYS:HG2	3:L:331:GLY:O	2.19	0.42
2:E:284:ASN:N	2:E:284:ASN:ND2	2.67	0.42
3:L:101:LEU:CD2	3:L:101:LEU:N	2.81	0.42
2:E:160:ASN:O	2:E:161:ILE:C	2.57	0.42
1:D:176:LYS:HB2	1:D:176:LYS:HE2	1.85	0.42
3:C:227:TRP:CZ3	3:C:345:ASN:OD1	2.73	0.42
2:B:190:MET:CB	3:C:131:LEU:HD12	2.50	0.42
1:G:150:LEU:HD13	3:I:125:LYS:NZ	2.35	0.42
1:G:150:LEU:HD22	3:I:125:LYS:HZ3	1.85	0.42
3:F:276:LEU:O	3:F:277:THR:HG23	2.20	0.42
3:I:197:ARG:HD3	3:I:204:PHE:CE1	2.55	0.42
3:I:107:ILE:C	3:I:109:TYR:N	2.72	0.42
1:D:167:ARG:CG	1:D:167:ARG:NH1	2.82	0.42
2:B:373:MET:HG3	2:B:405:ASN:HB2	2.01	0.42
3:L:270:GLU:HA	3:L:273:LYS:O	2.19	0.42
2:B:412:PRO:HB3	2:B:450:MET:CG	2.47	0.42
4:S:3:ARG:CG	4:S:3:ARG:NH2	2.75	0.42
3:F:207:ASN:OD1	3:F:208:TRP:N	2.53	0.42
3:I:342:GLY:HA2	3:I:369:TRP:HA	2.02	0.42
3:I:114:TYR:C	3:I:116:SER:N	2.72	0.42
3:I:117:ASN:C	3:I:119:GLN:N	2.72	0.42
2:H:317:TRP:CZ3	2:H:448:ARG:HD2	2.54	0.42
3:F:95:LYS:HD2	3:F:98:ALA:HB2	2.00	0.42
3:C:128:VAL:O	3:C:130:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ILE:C	1:A:135:LEU:N	2.73	0.42
2:B:176:ARG:HH11	2:B:176:ARG:HB2	1.80	0.42
3:C:170:LYS:HZ1	3:C:177:GLN:HG2	1.85	0.42
3:C:223:THR:O	3:C:224:THR:HB	2.19	0.42
3:C:239:GLN:O	3:C:240:SER:HB3	2.19	0.42
3:C:327:ALA:O	3:C:328:GLU:C	2.56	0.42
1:G:150:LEU:HD22	3:I:125:LYS:NZ	2.34	0.42
1:J:147:MET:O	1:J:148:LYS:C	2.56	0.42
1:J:183:LYS:O	1:J:184:GLN:C	2.57	0.42
3:I:195:GLN:HE22	3:I:382:THR:HG23	1.83	0.42
3:I:196:LYS:HE2	3:I:198:LEU:HD11	2.01	0.42
2:H:207:SER:OG	2:H:208:GLY:N	2.53	0.42
2:H:226:LEU:O	2:H:227:ILE:C	2.57	0.42
3:C:276:LEU:HD11	3:C:309:GLY:N	2.34	0.42
3:L:288:ASP:OD2	3:L:291:ASP:CB	2.67	0.42
3:C:368:ILE:HB	3:C:374:THR:O	2.20	0.42
1:D:159:ARG:CB	1:D:159:ARG:HH11	2.32	0.42
2:E:257:ASP:HA	2:E:416:TYR:CZ	2.55	0.42
2:B:249:TRP:CE3	2:B:455:ARG:HB2	2.54	0.42
2:B:161:ILE:O	2:B:163:THR:N	2.45	0.42
2:B:180:GLN:O	2:B:183:GLU:HB3	2.20	0.42
3:C:112:GLU:O	3:C:114:TYR:N	2.51	0.42
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.30	0.42
1:A:159:ARG:HB3	2:B:258:GLY:HA3	2.02	0.42
3:F:197:ARG:NE	3:F:204:PHE:CE1	2.87	0.42
3:F:195:GLN:CG	3:F:227:TRP:HE3	2.32	0.42
2:K:191:GLU:CA	2:K:194:ARG:HH21	2.14	0.42
2:H:329:PHE:HD1	2:H:342:VAL:HG12	1.84	0.42
3:L:178:PHE:CZ	3:L:236:ILE:HD11	2.54	0.42
3:I:147:ASP:O	3:I:148:ILE:C	2.57	0.42
3:I:96:TYR:CD1	3:I:97:GLU:N	2.86	0.42
3:C:154:GLN:OE1	3:C:190:GLY:N	2.51	0.42
3:I:329:GLN:NE2	3:I:363:TYR:HB2	2.32	0.42
2:E:333:ASN:CG	2:E:334:GLU:N	2.73	0.42
3:F:113:ILE:O	3:F:114:TYR:C	2.56	0.42
3:L:252:ASP:HB2	3:L:254:ASN:ND2	2.34	0.42
2:K:200:SER:H	2:K:279:ASN:HD21	1.67	0.42
3:F:292:GLY:C	3:F:302:LYS:HD2	2.40	0.42
1:J:127:ILE:O	1:J:131:GLN:HG3	2.19	0.42
2:B:175:LEU:C	2:B:175:LEU:HD13	2.39	0.42
2:B:179:ILE:HG13	2:B:179:ILE:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:TYR:O	1:G:180:ASP:N	2.45	0.42
3:C:173:LYS:CE	3:C:239:GLN:HA	2.49	0.42
3:C:373:LYS:HG3	3:C:377:TYR:CD2	2.54	0.42
3:F:276:LEU:C	3:F:276:LEU:HD23	2.39	0.42
2:H:367:MET:HB2	2:H:406:ARG:CB	2.37	0.42
3:I:197:ARG:NH1	3:I:204:PHE:CD1	2.87	0.42
2:H:162:PRO:O	2:H:164:ASN:N	2.52	0.42
2:B:301:GLN:C	2:B:301:GLN:NE2	2.73	0.42
2:B:405:ASN:CG	2:B:405:ASN:O	2.57	0.42
3:L:204:PHE:O	3:L:206:LYS:N	2.50	0.42
3:F:388:PRO:O	3:F:389:PHE:C	2.58	0.42
2:E:297:ASP:O	2:E:299:ILE:N	2.52	0.42
3:L:289:ALA:HA	3:L:371:THR:HG23	2.02	0.42
3:I:120:LYS:HB2	3:I:120:LYS:HE3	1.86	0.42
3:C:99:SER:O	3:C:101:LEU:N	2.52	0.42
3:C:337:ASN:HB3	3:C:339:CYS:O	2.20	0.42
1:J:150:LEU:HA	1:J:150:LEU:HD12	1.77	0.42
1:G:159:ARG:NH1	2:H:418:TRP:CD2	2.88	0.42
2:B:429:HIS:O	2:B:431:THR:HG23	2.18	0.42
2:E:441:LYS:CG	2:E:447:MET:HE1	2.49	0.42
3:I:365:ASN:ND2	3:I:366:GLY:H	2.14	0.42
2:B:158:ASN:O	2:B:162:PRO:HG2	2.19	0.42
3:C:202:VAL:HG21	3:C:225:GLU:O	2.20	0.42
2:H:191:GLU:C	2:H:193:CYS:N	2.69	0.42
3:F:384:MET:HB2	3:F:384:MET:HE3	1.84	0.42
2:H:411:ASN:HD22	2:H:434:GLY:H	1.66	0.42
2:H:223:GLU:HB2	2:H:286:CYS:O	2.19	0.42
2:B:252:ILE:HG22	2:B:299:ILE:HD11	2.02	0.42
2:B:336:ASN:C	2:B:338:TYR:N	2.72	0.42
2:E:253:GLN:H	2:E:452:MET:HB2	1.84	0.42
2:E:255:ARG:HH12	2:E:413:ASN:N	2.18	0.42
3:L:160:GLY:O	3:L:161:ALA:CB	2.66	0.42
3:F:289:ALA:HB3	3:F:369:TRP:CZ2	2.54	0.42
2:E:313:GLU:OE1	2:E:453:LYS:HE2	2.19	0.42
4:M:3:ARG:HA	4:M:4:PRO:HD3	1.95	0.42
1:A:128:GLU:OE1	1:A:129:LYS:CE	2.67	0.42
2:B:169:ARG:O	2:B:173:GLU:HB2	2.19	0.42
2:B:200:SER:OG	3:C:142:THR:HG21	2.20	0.42
3:C:170:LYS:HE2	3:C:177:GLN:OE1	2.20	0.42
3:C:195:GLN:HB3	3:C:195:GLN:HE21	1.66	0.42
3:F:264:MET:O	3:F:278:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:202:VAL:HG22	3:I:217:HIS:CE1	2.55	0.42
3:I:202:VAL:HG21	3:I:225:GLU:O	2.19	0.42
2:B:421:GLN:NE2	2:B:444:TRP:O	2.53	0.42
2:E:295:GLY:O	2:E:299:ILE:HG13	2.20	0.42
2:E:172:LEU:HG	3:F:113:ILE:HG22	2.01	0.42
2:B:364:ASN:HA	2:B:367:MET:HE3	2.01	0.42
2:K:215:ILE:C	2:K:217:LYS:H	2.22	0.42
2:K:314:MET:HA	2:K:449:LYS:O	2.20	0.42
1:G:140:VAL:CG2	1:G:141:ARG:N	2.82	0.42
4:Q:3:ARG:O	4:Q:5:NH2:N	2.53	0.42
1:G:158:ILE:CD1	2:H:189:GLN:HB3	2.50	0.42
3:I:242:ILE:CD1	3:I:242:ILE:N	2.83	0.42
3:C:128:VAL:O	3:C:129:ALA:C	2.56	0.42
3:C:392:LEU:HG	3:C:392:LEU:O	2.20	0.42
1:D:179:GLU:O	1:D:180:ASP:C	2.57	0.42
3:C:334:TRP:O	3:C:335:TRP:C	2.58	0.42
2:H:295:GLY:O	2:H:299:ILE:HG13	2.19	0.42
3:I:196:LYS:C	3:I:197:ARG:HG2	2.40	0.42
3:I:267:VAL:O	3:I:267:VAL:HG13	2.19	0.42
2:B:251:VAL:CG1	2:B:252:ILE:N	2.83	0.42
3:L:204:PHE:O	3:L:211:TYR:CE2	2.70	0.42
3:L:230:ASN:HA	3:L:233:ILE:CD1	2.38	0.42
3:L:382:THR:HG22	3:L:382:THR:O	2.19	0.42
3:F:99:SER:O	3:F:101:LEU:HG	2.20	0.42
2:H:152:TYR:HD2	2:H:155:GLU:HG2	1.84	0.42
3:F:338:LYS:N	3:F:339:CYS:HA	2.34	0.42
2:K:317:TRP:CE2	2:K:448:ARG:HB2	2.55	0.42
2:B:266:TRP:NE1	2:B:380:ARG:NH2	2.60	0.42
2:H:317:TRP:H	2:H:317:TRP:HD1	1.59	0.42
3:L:92:GLU:HG2	3:L:93:ILE:H	1.85	0.42
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.55	0.42
3:F:95:LYS:O	3:F:98:ALA:HB3	2.19	0.42
2:K:433:ASP:O	2:K:433:ASP:OD1	2.38	0.42
1:A:147:MET:SD	3:C:121:ILE:CD1	3.08	0.42
2:B:175:LEU:HA	2:B:178:LYS:CG	2.49	0.42
3:C:172:LEU:HD12	3:C:172:LEU:N	2.29	0.42
3:C:172:LEU:CD1	3:C:239:GLN:NE2	2.81	0.42
3:C:267:VAL:O	3:C:267:VAL:CG1	2.68	0.42
2:H:336:ASN:C	2:H:338:TYR:N	2.73	0.42
2:H:351:ASN:OD1	2:H:354:MET:CG	2.68	0.42
2:B:301:GLN:O	2:B:304:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:278:TYR:HE2	3:I:290:PHE:CD2	2.28	0.42
2:K:213:GLU:O	2:K:217:LYS:HG3	2.20	0.42
2:E:215:ILE:C	2:E:217:LYS:H	2.23	0.42
2:H:398:ASP:CA	2:H:433:ASP:CB	2.97	0.42
3:F:288:ASP:O	3:F:371:THR:HG21	2.19	0.42
2:E:370:HIS:HE1	2:E:408:HIS:CB	2.33	0.42
3:L:365:ASN:ND2	3:L:365:ASN:C	2.73	0.42
3:F:252:ASP:HB2	3:F:254:ASN:ND2	2.34	0.42
3:L:171:PRO:HD2	3:L:174:ALA:HB2	2.02	0.42
1:J:130:VAL:HA	1:J:133:ILE:HG22	2.02	0.41
3:C:316:ASP:OD2	3:C:316:ASP:O	2.38	0.41
1:A:167:ARG:C	1:A:167:ARG:HD2	2.40	0.41
3:I:310:MET:O	3:I:335:TRP:CD1	2.73	0.41
1:G:126:VAL:O	1:G:129:LYS:N	2.53	0.41
2:B:236:TYR:O	2:B:236:TYR:CD1	2.72	0.41
3:C:298:ASP:CG	3:C:299:PRO:HD2	2.40	0.41
2:H:385:TRP:CE2	4:Q:3:ARG:HG3	2.55	0.41
1:G:191:LYS:HE2	2:H:160:ASN:ND2	2.35	0.41
3:L:119:GLN:HA	3:L:122:VAL:HG23	2.02	0.41
3:L:356:LYS:HE3	3:L:356:LYS:HB3	1.88	0.41
2:K:363:GLU:HB3	2:K:367:MET:HE2	2.01	0.41
3:I:234:HIS:CE1	3:I:238:THR:OG1	2.73	0.41
1:G:122:LEU:C	1:G:124:ARG:H	2.23	0.41
2:E:255:ARG:HH12	2:E:413:ASN:H	1.68	0.41
3:I:311:GLN:HB2	3:I:319:ASN:HB2	2.02	0.41
2:K:242:MET:SD	2:K:248:GLY:HA2	2.60	0.41
3:C:298:ASP:O	3:C:301:ASP:CB	2.63	0.41
3:F:321:LYS:HA	3:F:321:LYS:HD3	1.88	0.41
2:K:158:ASN:ND2	2:K:158:ASN:N	2.67	0.41
2:E:158:ASN:N	2:E:158:ASN:HD22	2.17	0.41
1:A:124:ARG:H	1:A:124:ARG:HD2	1.85	0.41
3:I:100:ILE:O	3:I:100:ILE:HG13	2.19	0.41
3:C:173:LYS:HE3	3:C:239:GLN:HA	2.02	0.41
3:C:193:VAL:CG1	3:C:194:PHE:N	2.83	0.41
3:C:253:TRP:O	3:C:254:ASN:OD1	2.38	0.41
1:J:167:ARG:NH1	2:K:192:TYR:CE1	2.88	0.41
3:I:298:ASP:CG	3:I:299:PRO:HD2	2.41	0.41
3:I:304:PHE:O	3:I:337:ASN:CG	2.58	0.41
3:I:377:TYR:HD2	3:I:379:MET:HE1	1.85	0.41
2:H:159:SER:H	2:H:162:PRO:HD3	1.84	0.41
2:B:454:ILE:CD1	2:B:454:ILE:C	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:275:ARG:HA	3:I:311:GLN:HA	2.01	0.41
2:E:242:MET:SD	2:E:248:GLY:HA2	2.60	0.41
1:G:140:VAL:HG23	1:G:141:ARG:H	1.83	0.41
1:D:159:ARG:CB	1:D:159:ARG:NH1	2.83	0.41
3:F:116:SER:O	3:F:120:LYS:HG3	2.20	0.41
3:F:204:PHE:O	3:F:211:TYR:CE2	2.71	0.41
2:H:256:GLN:NE2	2:H:449:LYS:NZ	2.58	0.41
2:H:224:MET:HB2	2:H:286:CYS:HB2	2.02	0.41
2:B:312:ILE:HG12	2:B:452:MET:HG2	2.03	0.41
2:K:253:GLN:HA	2:K:292:TYR:O	2.19	0.41
2:E:167:VAL:HG23	2:E:168:LEU:N	2.35	0.41
3:L:189:ASN:ND2	3:L:391:ARG:HG2	2.35	0.41
2:E:233:VAL:HG13	2:E:233:VAL:O	2.19	0.41
3:F:293:PHE:N	3:F:302:LYS:HD2	2.36	0.41
2:K:404:TYR:O	2:K:405:ASN:HB2	2.21	0.41
1:A:128:GLU:C	1:A:131:GLN:HG2	2.40	0.41
2:B:164:ASN:N	2:B:166:ARG:HE	2.18	0.41
2:H:236:TYR:CE1	2:H:294:LEU:HD21	2.55	0.41
3:I:223:THR:O	3:I:224:THR:CB	2.68	0.41
3:I:297:ASP:HB2	3:I:301:ASP:OD1	2.20	0.41
2:B:229:PRO:HG2	2:B:233:VAL:CG1	2.51	0.41
3:I:276:LEU:HD11	3:I:308:ASN:CA	2.43	0.41
2:H:238:VAL:CG2	2:H:250:THR:HG23	2.44	0.41
1:D:126:VAL:C	1:D:130:VAL:HG23	2.41	0.41
3:F:103:HIS:O	3:F:104:ASP:HB2	2.20	0.41
2:B:366:THR:C	2:B:368:THR:H	2.22	0.41
2:H:385:TRP:CH2	4:Q:3:ARG:NE	2.88	0.41
1:G:164:SER:HB3	3:I:137:GLU:O	2.20	0.41
2:H:346:ARG:HH11	2:H:346:ARG:CB	2.34	0.41
1:G:151:GLU:OE1	2:H:182:LEU:HD11	2.21	0.41
2:H:230:ASP:C	2:H:232:SER:N	2.74	0.41
3:I:194:PHE:HB2	3:I:233:ILE:HD11	2.03	0.41
3:I:304:PHE:CB	3:I:338:LYS:HB3	2.50	0.41
1:G:128:GLU:OE2	1:G:129:LYS:NZ	2.46	0.41
1:G:133:ILE:O	1:G:133:ILE:HG22	2.20	0.41
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.56	0.41
2:H:261:ASP:OD2	2:H:263:GLY:N	2.53	0.41
3:I:322:PHE:HB3	3:I:324:GLY:O	2.20	0.41
3:F:353:THR:HG23	3:F:377:TYR:CE1	2.55	0.41
2:K:180:GLN:NE2	2:K:180:GLN:C	2.74	0.41
2:B:456:PRO:HB2	2:B:457:PHE:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:GLN:O	2:H:183:GLU:N	2.54	0.41
1:J:148:LYS:HG3	1:J:178:TYR:CG	2.56	0.41
3:L:240:SER:O	3:L:242:ILE:HG13	2.20	0.41
2:B:337:LYS:O	2:B:338:TYR:HB2	2.21	0.41
2:B:411:ASN:C	2:B:412:PRO:O	2.56	0.41
3:F:156:ILE:O	3:F:160:GLY:O	2.38	0.41
1:G:137:GLN:OE1	1:G:189:ILE:HG13	2.20	0.41
3:L:97:GLU:HA	3:L:100:ILE:HD11	2.03	0.41
2:K:266:TRP:H	2:K:379:ASP:CG	2.23	0.41
1:G:158:ILE:CG1	2:H:189:GLN:HB3	2.51	0.41
2:B:218:GLY:HA3	3:C:210:GLN:HE21	1.86	0.41
1:A:175:LEU:C	1:A:177:ASP:N	2.74	0.41
1:J:124:ARG:HG2	1:J:124:ARG:NH1	2.36	0.41
1:J:132:HIS:O	1:J:135:LEU:HB3	2.20	0.41
3:L:293:PHE:N	3:L:302:LYS:HD2	2.36	0.41
3:C:340:HIS:O	4:O:1:GLY:N	2.54	0.41
3:C:212:LYS:C	3:C:214:GLY:N	2.74	0.41
2:B:296:ASN:HA	2:B:299:ILE:HD12	2.03	0.41
1:D:130:VAL:O	1:D:133:ILE:HB	2.21	0.41
1:G:186:GLU:HA	1:G:189:ILE:CG2	2.51	0.41
2:B:317:TRP:HE1	2:B:447:MET:CA	2.27	0.41
2:B:307:PRO:HB2	2:B:457:PHE:O	2.20	0.41
3:C:365:ASN:ND2	3:C:366:GLY:N	2.68	0.41
2:B:161:ILE:O	2:B:164:ASN:N	2.50	0.41
2:B:176:ARG:CG	2:B:176:ARG:NH1	2.79	0.41
2:B:169:ARG:HB2	3:C:110:LEU:HD12	2.02	0.41
3:C:171:PRO:HG3	3:C:236:ILE:HG22	2.01	0.41
3:C:352:GLY:O	3:C:353:THR:C	2.59	0.41
3:C:197:ARG:N	3:C:382:THR:O	2.54	0.41
3:C:164:SER:HB2	3:C:183:GLU:HA	2.03	0.41
3:C:315:TRP:CD1	3:C:316:ASP:N	2.88	0.41
2:H:256:GLN:HB3	2:H:449:LYS:HG2	2.02	0.41
2:H:255:ARG:HH11	2:H:413:ASN:HA	1.84	0.41
1:J:154:ILE:O	1:J:155:ASP:C	2.59	0.41
3:I:156:ILE:HG13	3:I:156:ILE:H	1.74	0.41
3:I:232:LYS:O	3:I:235:LEU:HD12	2.21	0.41
3:I:334:TRP:CZ3	3:I:344:LEU:HB2	2.53	0.41
3:I:170:LYS:HE2	3:I:177:GLN:OE1	2.21	0.41
3:I:267:VAL:O	3:I:267:VAL:CG1	2.69	0.41
1:G:122:LEU:HD11	3:I:98:ALA:HB2	2.02	0.41
1:G:128:GLU:CA	1:G:131:GLN:HB3	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:LYS:O	1:G:125:LYS:CG	2.69	0.41
2:B:215:ILE:HB	2:B:242:MET:HE1	2.02	0.41
3:L:276:LEU:HD23	3:L:276:LEU:C	2.40	0.41
3:I:279:ALA:CB	3:I:280:TYR:CD1	3.04	0.41
3:L:347:VAL:O	3:L:367:ILE:HG13	2.21	0.41
3:C:311:GLN:HB2	3:C:319:ASN:HB2	2.02	0.41
3:F:243:PRO:O	3:F:389:PHE:N	2.53	0.41
1:D:148:LYS:O	1:D:152:VAL:HG12	2.21	0.41
3:F:105:SER:HA	3:F:108:ARG:CZ	2.49	0.41
3:F:166:LEU:HD22	3:F:179:LEU:CD1	2.49	0.41
3:F:304:PHE:CD1	3:F:338:LYS:HD2	2.56	0.41
2:E:266:TRP:H	2:E:379:ASP:CG	2.23	0.41
2:B:303:THR:HA	2:B:308:THR:CG2	2.50	0.41
1:G:158:ILE:HD12	1:G:158:ILE:HA	1.84	0.41
2:H:352:ALA:O	2:H:409:ALA:HB3	2.21	0.41
2:K:304:ARG:C	2:K:306:GLY:N	2.73	0.41
2:H:279:ASN:O	2:H:281:ASP:N	2.53	0.41
3:L:170:LYS:HE3	3:L:177:GLN:HB3	2.02	0.41
2:B:386:LEU:HD22	2:B:386:LEU:HA	1.80	0.41
1:G:178:TYR:O	1:G:182:GLN:HG2	2.21	0.41
3:F:233:ILE:H	3:F:233:ILE:HG13	1.54	0.41
3:I:96:TYR:C	3:I:98:ALA:N	2.74	0.41
2:B:304:ARG:HH21	2:B:332:GLN:HA	1.85	0.41
2:B:423:THR:O	2:B:425:ASP:N	2.54	0.41
1:J:140:VAL:CG1	1:J:141:ARG:N	2.83	0.41
2:K:253:GLN:HB2	2:K:293:TRP:CZ3	2.56	0.41
2:B:361:MET:HB2	5:B:470:NAG:C8	2.43	0.41
2:H:152:TYR:O	2:H:153:ILE:C	2.59	0.41
3:F:250:LEU:HD23	3:F:372:TRP:CE3	2.56	0.41
1:D:169:LEU:HD23	1:D:170:ALA:N	2.36	0.41
2:E:218:GLY:CA	3:F:210:GLN:HG2	2.50	0.41
1:D:159:ARG:NE	2:E:418:TRP:CE3	2.88	0.41
2:H:422:TYR:HE1	2:H:444:TRP:HA	1.84	0.40
3:C:234:HIS:CE1	3:C:238:THR:OG1	2.74	0.40
3:C:196:LYS:HA	3:C:382:THR:O	2.21	0.40
2:H:366:THR:C	2:H:368:THR:H	2.24	0.40
3:I:193:VAL:CG1	3:I:194:PHE:N	2.84	0.40
3:L:207:ASN:OD1	3:L:209:ILE:N	2.54	0.40
1:D:140:VAL:O	1:D:144:LEU:HB2	2.21	0.40
3:C:262:TYR:OH	3:C:290:PHE:HB2	2.21	0.40
2:B:351:ASN:HB3	2:B:355:ASP:CB	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:LEU:HD13	1:G:170:ALA:N	2.36	0.40
3:I:157:ALA:HA	3:I:161:ALA:CB	2.46	0.40
3:F:281:PHE:C	3:F:283:GLY:H	2.24	0.40
3:F:205:LYS:HG2	3:F:331:GLY:O	2.21	0.40
3:I:322:PHE:C	3:I:324:GLY:N	2.75	0.40
1:A:181:GLN:HE22	2:B:174:ASN:HB2	1.86	0.40
3:I:112:GLU:OE1	3:I:112:GLU:HA	2.21	0.40
2:E:384:GLY:H	2:E:405:ASN:HA	1.87	0.40
2:B:171:ILE:HG13	2:B:172:LEU:N	2.35	0.40
3:C:212:LYS:O	3:C:231:GLU:HB3	2.21	0.40
3:C:132:GLU:C	3:C:134:GLN:H	2.24	0.40
2:H:175:LEU:O	2:H:178:LYS:HB2	2.21	0.40
3:L:242:ILE:N	3:L:242:ILE:HD12	2.36	0.40
2:E:249:TRP:CZ2	2:E:311:LEU:HD23	2.57	0.40
1:A:185:LEU:HD13	1:A:185:LEU:C	2.39	0.40
2:B:398:ASP:C	2:B:433:ASP:HB2	2.42	0.40
2:H:303:THR:O	2:H:308:THR:OG1	2.39	0.40
2:E:223:GLU:HB2	2:E:286:CYS:O	2.21	0.40
3:I:162:LYS:HA	3:I:184:ILE:HG21	2.03	0.40
2:H:456:PRO:HB2	2:H:457:PHE:H	1.68	0.40
2:B:165:LEU:CD2	3:C:107:ILE:HG12	2.51	0.40
1:A:158:ILE:HD13	1:A:171:ARG:NE	2.35	0.40
3:F:347:VAL:O	3:F:367:ILE:HG13	2.21	0.40
2:H:252:ILE:CG2	2:H:299:ILE:HG12	2.51	0.40
2:H:298:LYS:O	2:H:302:LEU:HG	2.21	0.40
3:L:124:LEU:O	3:L:125:LYS:C	2.59	0.40
3:I:200:GLY:H	3:I:225:GLU:CD	2.20	0.40
2:H:205:VAL:CG1	3:I:232:LYS:NZ	2.70	0.40
3:I:265:PHE:CD2	3:I:266:LYS:N	2.89	0.40
3:I:251:GLU:CD	3:I:381:LYS:HD2	2.42	0.40
2:B:238:VAL:CG2	2:B:239:TYR:N	2.84	0.40
2:B:252:ILE:CG2	2:B:299:ILE:HG12	2.51	0.40
3:L:269:PRO:O	3:L:273:LYS:O	2.40	0.40
3:C:329:GLN:HE21	4:O:3:ARG:CZ	2.33	0.40
2:H:189:GLN:HG3	2:H:189:GLN:O	2.21	0.40
3:C:148:ILE:CD1	3:C:148:ILE:H	2.29	0.40
2:B:200:SER:OG	3:C:142:THR:CG2	2.69	0.40
2:H:353:LEU:O	2:H:370:HIS:N	2.44	0.40
1:G:126:VAL:O	1:G:127:ILE:C	2.59	0.40
2:B:300:SER:O	2:B:304:ARG:CG	2.59	0.40
2:B:300:SER:HA	2:B:331:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ARG:HG2	2:B:450:MET:O	2.22	0.40
2:E:448:ARG:O	2:E:449:LYS:HG3	2.22	0.40
2:K:448:ARG:O	2:K:448:ARG:HG2	2.21	0.40
1:G:143:GLN:O	1:G:146:ASP:N	2.53	0.40
2:H:317:TRP:CZ3	2:H:448:ARG:CD	3.05	0.40
1:G:175:LEU:C	1:G:177:ASP:H	2.25	0.40
2:E:157:VAL:C	2:E:158:ASN:HD22	2.25	0.40
3:L:354:TYR:OH	3:L:364:ASP:HB2	2.21	0.40
3:I:244:TYR:CE2	3:I:388:PRO:HG3	2.56	0.40
1:A:140:VAL:O	1:A:143:GLN:N	2.54	0.40
1:G:148:LYS:NZ	2:H:425:ASP:O	2.49	0.40
2:H:369:ILE:O	2:H:405:ASN:CB	2.68	0.40
1:J:147:MET:SD	3:L:121:ILE:HD11	2.61	0.40
2:H:224:MET:HE2	2:H:237:ARG:HE	1.85	0.40
3:I:212:LYS:C	3:I:214:GLY:H	2.25	0.40
3:I:327:ALA:O	3:I:328:GLU:C	2.59	0.40
2:B:310:LEU:CA	2:B:454:ILE:HG22	2.51	0.40
3:C:154:GLN:HG3	3:C:158:ASN:ND2	2.36	0.40
2:K:262:PHE:O	2:K:269:TYR:OH	2.31	0.40
3:C:242:ILE:N	3:C:242:ILE:CD1	2.85	0.40
3:C:342:GLY:HA2	3:C:368:ILE:O	2.22	0.40
2:B:328:GLY:H	2:B:344:LYS:HB2	1.86	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	72/87 (83%)	43 (60%)	17 (24%)	12 (17%)	0 0
1	D	69/87 (79%)	47 (68%)	19 (28%)	3 (4%)	3 13
1	G	72/87 (83%)	43 (60%)	19 (26%)	10 (14%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	77/87 (88%)	58 (75%)	15 (20%)	4 (5%)	2 8
2	B	305/328 (93%)	195 (64%)	70 (23%)	40 (13%)	0 1
2	E	302/328 (92%)	229 (76%)	53 (18%)	20 (7%)	1 4
2	H	305/328 (93%)	191 (63%)	70 (23%)	44 (14%)	0 0
2	K	303/328 (92%)	230 (76%)	47 (16%)	26 (9%)	1 2
3	C	303/323 (94%)	168 (55%)	96 (32%)	39 (13%)	0 1
3	F	298/323 (92%)	210 (70%)	70 (24%)	18 (6%)	2 6
3	I	303/323 (94%)	175 (58%)	85 (28%)	43 (14%)	0 0
3	L	298/323 (92%)	215 (72%)	66 (22%)	17 (6%)	2 6
4	M	2/5 (40%)	1 (50%)	0	1 (50%)	0 0
4	N	2/5 (40%)	1 (50%)	0	1 (50%)	0 0
4	O	2/5 (40%)	0	1 (50%)	1 (50%)	0 0
4	P	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
4	Q	2/5 (40%)	1 (50%)	0	1 (50%)	0 0
4	R	2/5 (40%)	1 (50%)	0	1 (50%)	0 0
4	S	2/5 (40%)	2 (100%)	0	0	100 100
4	T	2/5 (40%)	2 (100%)	0	0	100 100
All	All	2723/2992 (91%)	1813 (67%)	629 (23%)	281 (10%)	1 1

All (281) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL
1	A	122	LEU
1	A	160	SER
1	A	166	SER
2	B	170	SER
2	B	189	GLN
2	B	227	ILE
2	B	285	TYR
2	B	295	GLY
2	B	320	ASP
2	B	366	THR
2	B	435	VAL
3	C	151	LYS
3	C	162	LYS

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Mol	Chain	Res	Type
3	C	196	LYS
3	C	201	SER
3	C	224	THR
3	C	271	ALA
3	C	272	ASP
3	C	305	THR
3	C	317	ASN
3	C	335	TRP
3	C	353	THR
1	D	165	CYS
2	E	192	TYR
2	E	205	VAL
2	E	229	PRO
2	E	233	VAL
2	E	259	SER
2	E	281	ASP
2	E	399	GLY
2	E	405	ASN
3	F	104	ASP
3	F	159	LYS
3	F	282	ALA
3	F	298	ASP
3	F	311	GLN
3	F	390	ASN
1	G	120	GLU
1	G	121	VAL
1	G	125	LYS
1	G	130	VAL
1	G	166	SER
2	H	158	ASN
2	H	174	ASN
2	H	227	ILE
2	H	285	TYR
2	H	295	GLY
2	H	320	ASP
2	H	435	VAL
3	I	98	ALA
3	I	151	LYS
3	I	162	LYS
3	I	196	LYS
3	I	201	SER
3	I	224	THR

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Mol	Chain	Res	Type
3	I	271	ALA
3	I	305	THR
3	I	317	ASN
3	I	335	TRP
3	I	353	THR
2	K	156	THR
2	K	157	VAL
2	K	205	VAL
2	K	229	PRO
2	K	233	VAL
2	K	259	SER
2	K	281	ASP
2	K	405	ASN
3	L	159	LYS
3	L	256	ARG
3	L	298	ASP
3	L	311	GLN
3	L	390	ASN
4	M	4	PRO
1	A	173	VAL
1	A	190	ALA
2	B	153	ILE
2	B	182	LEU
2	B	231	SER
2	B	258	GLY
2	B	280	THR
2	B	332	GLN
2	B	359	GLN
2	B	362	GLY
2	B	378	TYR
2	B	424	TRP
2	B	443	SER
2	B	456	PRO
3	C	100	ILE
3	C	164	SER
3	C	218	LEU
3	C	237	SER
3	C	243	PRO
3	C	331	GLY
3	C	360	PRO
1	D	164	SER
2	E	156	THR

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Mol	Chain	Res	Type
2	E	157	VAL
2	E	295	GLY
2	E	305	MET
2	E	383	ASP
3	F	233	ILE
3	F	240	SER
3	F	241	ALA
3	F	256	ARG
3	F	270	GLU
3	F	285	ASP
1	G	191	LYS
2	H	153	ILE
2	H	159	SER
2	H	170	SER
2	H	231	SER
2	H	258	GLY
2	H	280	THR
2	H	359	GLN
2	H	362	GLY
2	H	366	THR
2	H	378	TYR
2	H	407	CYS
2	H	424	TRP
2	H	443	SER
2	H	456	PRO
3	I	97	GLU
3	I	105	SER
3	I	164	SER
3	I	218	LEU
3	I	237	SER
3	I	243	PRO
3	I	272	ASP
3	I	327	ALA
3	I	331	GLY
3	I	332	SER
3	I	339	CYS
3	I	360	PRO
3	I	366	GLY
3	I	390	ASN
1	J	165	CYS
2	K	192	TYR
2	K	295	GLY

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Mol	Chain	Res	Type
2	K	305	MET
2	K	399	GLY
3	L	233	ILE
3	L	240	SER
3	L	241	ALA
3	L	270	GLU
3	L	282	ALA
3	L	285	ASP
3	L	300	SER
3	L	339	CYS
4	N	4	PRO
1	A	164	SER
2	B	155	GLU
2	B	247	GLY
2	B	259	SER
2	B	266	TRP
2	B	317	TRP
2	B	325	HIS
2	B	334	GLU
2	B	355	ASP
3	C	113	ILE
3	C	251	GLU
3	C	273	LYS
3	C	327	ALA
3	C	332	SER
3	C	374	THR
3	C	389	PHE
3	C	390	ASN
1	D	166	SER
2	E	216	ARG
2	E	298	LYS
2	E	404	TYR
2	E	406	ARG
3	F	94	MET
3	F	102	THR
3	F	300	SER
3	F	367	ILE
3	F	389	PHE
2	H	182	LEU
2	H	247	GLY
2	H	259	SER
2	H	294	LEU

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Mol	Chain	Res	Type
2	H	317	TRP
2	H	325	HIS
2	H	332	GLN
2	H	334	GLU
2	H	355	ASP
2	H	356	GLY
3	I	135	CYS
3	I	221	THR
3	I	251	GLU
3	I	273	LYS
3	I	301	ASP
3	I	374	THR
2	K	162	PRO
2	K	216	ARG
2	K	298	LYS
2	K	364	ASN
2	K	383	ASP
2	K	407	CYS
3	L	389	PHE
4	Q	4	PRO
4	R	4	PRO
1	A	180	ASP
2	B	174	ASN
2	B	192	TYR
2	B	229	PRO
2	B	356	GLY
3	C	105	SER
3	C	128	VAL
3	C	221	THR
3	C	259	THR
3	C	301	ASP
3	C	366	GLY
2	E	223	GLU
1	G	179	GLU
2	H	192	TYR
2	H	229	PRO
2	H	266	TRP
3	I	118	ASN
3	I	133	ALA
3	I	369	TRP
3	I	389	PHE
1	J	164	SER

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Mol	Chain	Res	Type
2	K	159	SER
2	K	164	ASN
2	K	223	GLU
1	A	174	ASP
1	A	179	GLU
1	A	188	VAL
2	B	256	GLN
2	B	294	LEU
2	B	406	ARG
2	B	425	ASP
3	C	135	CYS
3	C	202	VAL
3	C	235	LEU
3	C	369	TRP
2	E	438	MET
1	G	164	SER
1	G	173	VAL
1	G	190	ALA
2	H	162	PRO
2	H	163	THR
2	H	256	GLN
2	H	431	THR
3	I	100	ILE
3	I	124	LEU
3	I	202	VAL
3	I	259	THR
1	J	184	GLN
3	L	367	ILE
3	L	374	THR
2	B	162	PRO
3	C	387	ILE
3	F	273	LYS
2	H	179	ILE
3	I	387	ILE
2	K	257	ASP
2	K	404	TYR
2	K	406	ARG
2	B	235	PRO
1	A	126	VAL
2	B	414	GLY
2	E	235	PRO
2	H	414	GLY

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Mol	Chain	Res	Type
3	I	107	ILE
2	K	235	PRO
2	K	430	GLY
2	H	235	PRO
3	I	219	SER
3	I	347	VAL
4	O	4	PRO
3	C	394	ILE
2	H	157	VAL
2	H	199	VAL
1	J	126	VAL
2	B	319	GLY
3	C	347	VAL
2	H	319	GLY
3	L	200	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	69/82 (84%)	56 (81%)	13 (19%)	2 6
1	D	66/82 (80%)	57 (86%)	9 (14%)	5 13
1	G	69/82 (84%)	61 (88%)	8 (12%)	7 20
1	J	74/82 (90%)	62 (84%)	12 (16%)	3 9
2	B	265/286 (93%)	231 (87%)	34 (13%)	5 16
2	E	262/286 (92%)	238 (91%)	24 (9%)	11 33
2	H	265/286 (93%)	238 (90%)	27 (10%)	9 27
2	K	263/286 (92%)	238 (90%)	25 (10%)	11 31
3	C	257/269 (96%)	216 (84%)	41 (16%)	3 9
3	F	253/269 (94%)	223 (88%)	30 (12%)	6 19
3	I	257/269 (96%)	216 (84%)	41 (16%)	3 9
3	L	253/269 (94%)	225 (89%)	28 (11%)	8 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	M	2/2 (100%)	2 (100%)	0	100 100
4	N	2/2 (100%)	2 (100%)	0	100 100
4	O	2/2 (100%)	2 (100%)	0	100 100
4	P	2/2 (100%)	2 (100%)	0	100 100
4	Q	2/2 (100%)	2 (100%)	0	100 100
4	R	2/2 (100%)	2 (100%)	0	100 100
4	S	2/2 (100%)	2 (100%)	0	100 100
4	T	2/2 (100%)	2 (100%)	0	100 100
All	All	2369/2564 (92%)	2077 (88%)	292 (12%)	6 17

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	128	GLU
1	A	132	HIS
1	A	138	LYS
1	A	143	GLN
1	A	150	LEU
1	A	151	GLU
1	A	152	VAL
1	A	167	ARG
1	A	169	LEU
1	A	171	ARG
1	A	173	VAL
1	A	182	GLN
2	B	155	GLU
2	B	161	ILE
2	B	166	ARG
2	B	167	VAL
2	B	168	LEU
2	B	172	LEU
2	B	173	GLU
2	B	175	LEU
2	B	176	ARG
2	B	183	GLU
2	B	186	VAL
2	B	189	GLN
2	B	193	CYS

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Mol	Chain	Res	Type
2	B	223	GLU
2	B	234	LYS
2	B	245	GLU
2	B	253	GLN
2	B	261	ASP
2	B	266	TRP
2	B	284	ASN
2	B	285	TYR
2	B	301	GLN
2	B	308	THR
2	B	310	LEU
2	B	316	ASP
2	B	346	ARG
2	B	351	ASN
2	B	359	GLN
2	B	386	LEU
2	B	387	THR
2	B	422	TYR
2	B	445	TYR
2	B	448	ARG
2	B	453	LYS
3	C	96	TYR
3	C	101	LEU
3	C	107	ILE
3	C	108	ARG
3	C	110	LEU
3	C	119	GLN
3	C	125	LYS
3	C	148	ILE
3	C	167	TYR
3	C	192	THR
3	C	195	GLN
3	C	199	ASP
3	C	203	ASP
3	C	217	HIS
3	C	221	THR
3	C	226	PHE
3	C	230	ASN
3	C	235	LEU
3	C	239	GLN
3	C	246	LEU
3	C	261	ASP

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Mol	Chain	Res	Type
3	C	264	MET
3	C	275	ARG
3	C	277	THR
3	C	294	ASP
3	C	297	ASP
3	C	300	SER
3	C	301	ASP
3	C	315	TRP
3	C	317	ASN
3	C	323	GLU
3	C	328	GLU
3	C	329	GLN
3	C	343	HIS
3	C	364	ASP
3	C	365	ASN
3	C	372	TRP
3	C	382	THR
3	C	383	THR
3	C	391	ARG
3	C	392	LEU
1	D	124	ARG
1	D	135	LEU
1	D	138	LYS
1	D	152	VAL
1	D	161	CYS
1	D	162	ARG
1	D	167	ARG
1	D	179	GLU
1	D	185	LEU
2	E	155	GLU
2	E	164	ASN
2	E	166	ARG
2	E	180	GLN
2	E	185	ASP
2	E	194	ARG
2	E	198	THR
2	E	210	GLU
2	E	221	THR
2	E	238	VAL
2	E	253	GLN
2	E	260	VAL
2	E	280	THR

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Mol	Chain	Res	Type
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	311	LEU
2	E	333	ASN
2	E	340	ILE
2	E	359	GLN
2	E	376	SER
2	E	433	ASP
2	E	436	VAL
2	E	457	PHE
3	F	96	TYR
3	F	101	LEU
3	F	103	HIS
3	F	106	SER
3	F	109	TYR
3	F	118	ASN
3	F	124	LEU
3	F	147	ASP
3	F	149	THR
3	F	164	SER
3	F	176	GLN
3	F	180	VAL
3	F	192	THR
3	F	202	VAL
3	F	211	TYR
3	F	221	THR
3	F	224	THR
3	F	239	GLN
3	F	242	ILE
3	F	244	TYR
3	F	261	ASP
3	F	264	MET
3	F	297	ASP
3	F	301	ASP
3	F	320	ASP
3	F	325	ASN
3	F	365	ASN
3	F	382	THR
3	F	383	THR
3	F	390	ASN
1	G	120	GLU

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Mol	Chain	Res	Type
1	G	137	GLN
1	G	138	LYS
1	G	144	LEU
1	G	167	ARG
1	G	171	ARG
1	G	175	LEU
1	G	186	GLU
2	H	155	GLU
2	H	164	ASN
2	H	165	LEU
2	H	168	LEU
2	H	169	ARG
2	H	193	CYS
2	H	223	GLU
2	H	234	LYS
2	H	245	GLU
2	H	253	GLN
2	H	261	ASP
2	H	266	TRP
2	H	284	ASN
2	H	285	TYR
2	H	301	GLN
2	H	308	THR
2	H	310	LEU
2	H	316	ASP
2	H	346	ARG
2	H	351	ASN
2	H	359	GLN
2	H	386	LEU
2	H	387	THR
2	H	422	TYR
2	H	445	TYR
2	H	448	ARG
2	H	453	LYS
3	I	93	ILE
3	I	119	GLN
3	I	127	LYS
3	I	131	LEU
3	I	132	GLU
3	I	148	ILE
3	I	167	TYR
3	I	192	THR

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Mol	Chain	Res	Type
3	I	195	GLN
3	I	199	ASP
3	I	203	ASP
3	I	211	TYR
3	I	217	HIS
3	I	221	THR
3	I	226	PHE
3	I	230	ASN
3	I	235	LEU
3	I	239	GLN
3	I	246	LEU
3	I	261	ASP
3	I	264	MET
3	I	275	ARG
3	I	276	LEU
3	I	277	THR
3	I	294	ASP
3	I	297	ASP
3	I	300	SER
3	I	301	ASP
3	I	315	TRP
3	I	317	ASN
3	I	323	GLU
3	I	326	CYS
3	I	328	GLU
3	I	329	GLN
3	I	343	HIS
3	I	364	ASP
3	I	365	ASN
3	I	372	TRP
3	I	382	THR
3	I	383	THR
3	I	391	ARG
1	J	116	ARG
1	J	118	ARG
1	J	125	LYS
1	J	127	ILE
1	J	131	GLN
1	J	134	GLN
1	J	135	LEU
1	J	138	LYS
1	J	148	LYS

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Mol	Chain	Res	Type
1	J	161	CYS
1	J	167	ARG
1	J	185	LEU
2	K	154	ASP
2	K	155	GLU
2	K	180	GLN
2	K	191	GLU
2	K	194	ARG
2	K	198	THR
2	K	210	GLU
2	K	221	THR
2	K	231	SER
2	K	238	VAL
2	K	253	GLN
2	K	260	VAL
2	K	280	THR
2	K	284	ASN
2	K	296	ASN
2	K	297	ASP
2	K	301	GLN
2	K	303	THR
2	K	311	LEU
2	K	333	ASN
2	K	340	ILE
2	K	359	GLN
2	K	376	SER
2	K	436	VAL
2	K	457	PHE
3	L	95	LYS
3	L	96	TYR
3	L	104	ASP
3	L	107	ILE
3	L	124	LEU
3	L	147	ASP
3	L	149	THR
3	L	164	SER
3	L	176	GLN
3	L	180	VAL
3	L	192	THR
3	L	202	VAL
3	L	211	TYR
3	L	221	THR

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Mol	Chain	Res	Type
3	L	224	THR
3	L	239	GLN
3	L	242	ILE
3	L	244	TYR
3	L	261	ASP
3	L	264	MET
3	L	297	ASP
3	L	301	ASP
3	L	320	ASP
3	L	325	ASN
3	L	365	ASN
3	L	382	THR
3	L	383	THR
3	L	390	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (165) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	180	GLN
2	B	202	ASN
2	B	228	GLN
2	B	253	GLN
2	B	256	GLN
2	B	279	ASN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	336	ASN
2	B	351	ASN
2	B	359	GLN
2	B	393	GLN
2	B	405	ASN
2	B	408	HIS
2	B	411	ASN
2	B	421	GLN

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Mol	Chain	Res	Type
2	B	429	HIS
2	B	439	ASN
3	C	130	GLN
3	C	136	GLN
3	C	158	ASN
3	C	176	GLN
3	C	195	GLN
3	C	210	GLN
3	C	217	HIS
3	C	230	ASN
3	C	234	HIS
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	317	ASN
3	C	319	ASN
3	C	329	GLN
3	C	365	ASN
1	D	134	GLN
1	D	139	ASN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	158	ASN
2	E	164	ASN
2	E	180	GLN
2	E	202	ASN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	336	ASN
2	E	351	ASN
2	E	359	GLN
2	E	382	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	118	ASN

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Mol	Chain	Res	Type
3	F	119	GLN
3	F	134	GLN
3	F	136	GLN
3	F	144	GLN
3	F	163	GLN
3	F	189	ASN
3	F	217	HIS
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN
3	F	308	ASN
3	F	325	ASN
3	F	337	ASN
3	F	361	ASN
3	F	365	ASN
1	G	181	GLN
2	H	160	ASN
2	H	164	ASN
2	H	174	ASN
2	H	189	GLN
2	H	202	ASN
2	H	228	GLN
2	H	253	GLN
2	H	254	ASN
2	H	256	GLN
2	H	279	ASN
2	H	284	ASN
2	H	296	ASN
2	H	301	GLN
2	H	336	ASN
2	H	351	ASN
2	H	359	GLN
2	H	393	GLN
2	H	405	ASN
2	H	408	HIS
2	H	411	ASN
2	H	421	GLN
2	H	429	HIS
2	H	439	ASN
3	I	103	HIS
3	I	111	GLN
3	I	117	ASN

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Mol	Chain	Res	Type
3	I	119	GLN
3	I	123	ASN
3	I	136	GLN
3	I	158	ASN
3	I	176	GLN
3	I	195	GLN
3	I	210	GLN
3	I	217	HIS
3	I	230	ASN
3	I	234	HIS
3	I	239	GLN
3	I	254	ASN
3	I	307	HIS
3	I	317	ASN
3	I	319	ASN
3	I	329	GLN
3	I	345	ASN
3	I	365	ASN
1	J	131	GLN
1	J	137	GLN
1	J	139	ASN
1	J	181	GLN
1	J	182	GLN
1	J	187	GLN
2	K	158	ASN
2	K	160	ASN
2	K	180	GLN
2	K	189	GLN
2	K	202	ASN
2	K	256	GLN
2	K	271	GLN
2	K	284	ASN
2	K	296	ASN
2	K	301	GLN
2	K	325	HIS
2	K	336	ASN
2	K	351	ASN
2	K	382	ASN
2	K	408	HIS
2	K	421	GLN
2	K	439	ASN
3	L	111	GLN

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Mol	Chain	Res	Type
3	L	115	ASN
3	L	117	ASN
3	L	136	GLN
3	L	144	GLN
3	L	163	GLN
3	L	189	ASN
3	L	217	HIS
3	L	230	ASN
3	L	239	GLN
3	L	254	ASN
3	L	308	ASN
3	L	325	ASN
3	L	337	ASN
3	L	361	ASN
3	L	365	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HYP	M	2	4	7,8,9	0.95	0	5,10,12	1.27	1 (20%)
4	HYP	N	2	4	7,8,9	0.72	0	5,10,12	1.58	1 (20%)
4	HYP	O	2	4	7,8,9	0.55	0	5,10,12	1.84	2 (40%)
4	HYP	P	2	4	7,8,9	0.80	0	5,10,12	1.09	0
4	HYP	Q	2	4	7,8,9	0.85	0	5,10,12	1.33	0
4	HYP	R	2	4	7,8,9	0.72	0	5,10,12	1.97	1 (20%)
4	HYP	S	2	4	7,8,9	0.83	0	5,10,12	1.17	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HYP	T	2	4	7,8,9	0.65	0	5,10,12	1.13	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
4	HYP	M	2	4	-	0/0/11/13	0/1/1/1
4	HYP	N	2	4	-	0/0/11/13	0/1/1/1
4	HYP	O	2	4	-	0/0/11/13	0/1/1/1
4	HYP	P	2	4	-	0/0/11/13	0/1/1/1
4	HYP	Q	2	4	-	0/0/11/13	0/1/1/1
4	HYP	R	2	4	-	0/0/11/13	0/1/1/1
4	HYP	S	2	4	-	0/0/11/13	0/1/1/1
4	HYP	T	2	4	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	2	HYP	CG-CB-CA	-3.28	99.20	103.90
4	N	2	HYP	CG-CB-CA	-2.79	99.91	103.90
4	O	2	HYP	CG-CB-CA	-2.65	100.10	103.90
4	O	2	HYP	CB-CG-CD	-2.17	100.45	103.14
4	M	2	HYP	CG-CB-CA	-2.08	100.91	103.90
4	S	2	HYP	CG-CB-CA	-2.03	100.98	103.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	2	HYP	2	0
4	P	2	HYP	2	0
4	S	2	HYP	4	0
4	T	2	HYP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	NAG	B	470	2	14,14,15	0.62	0	15,19,21	0.93	1 (6%)
6	NDG	E	470	2	14,14,15	0.77	1 (7%)	15,19,21	0.81	0
5	NAG	H	470	2	14,14,15	0.74	0	15,19,21	0.90	1 (6%)
5	NAG	K	470	2	14,14,15	0.61	0	15,19,21	1.02	1 (6%)

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
5	NAG	B	470	2	-	0/6/23/26	0/1/1/1
6	NDG	E	470	2	-	2/6/23/26	0/1/1/1
5	NAG	H	470	2	-	0/6/23/26	0/1/1/1
5	NAG	K	470	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	470	NDG	C1-C2	2.21	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	470	NAG	C2-N2-C7	-3.19	118.94	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	470	NAG	C2-N2-C7	-2.98	119.20	123.04
5	H	470	NAG	C2-N2-C7	-2.38	119.98	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	470	NDG	C8-C7-N2-C2
6	E	470	NDG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	4	0
6	E	470	NDG	4	0
5	H	470	NAG	3	0
5	K	470	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	74/87 (85%)	-0.19	0 100 100	61, 81, 96, 116	0
1	D	71/87 (81%)	-0.36	0 100 100	36, 59, 88, 90	0
1	G	74/87 (85%)	-0.18	2 (2%) 58 52	56, 82, 101, 110	0
1	J	79/87 (90%)	-0.39	0 100 100	37, 60, 102, 108	0
2	B	307/328 (93%)	-0.24	6 (1%) 68 64	49, 78, 102, 115	0
2	E	304/328 (92%)	-0.40	1 (0%) 94 94	30, 52, 82, 104	0
2	H	307/328 (93%)	-0.22	4 (1%) 79 78	49, 78, 101, 115	0
2	K	305/328 (92%)	-0.46	0 100 100	29, 52, 83, 105	0
3	C	305/323 (94%)	-0.09	10 (3%) 50 42	49, 85, 110, 121	0
3	F	300/323 (92%)	-0.33	2 (0%) 89 88	35, 70, 93, 123	0
3	I	305/323 (94%)	-0.02	12 (3%) 43 36	47, 85, 108, 123	0
3	L	300/323 (92%)	-0.32	3 (1%) 84 82	38, 70, 92, 113	0
4	M	3/5 (60%)	0.12	0 100 100	70, 70, 73, 91	0
4	N	3/5 (60%)	-0.31	0 100 100	57, 57, 66, 83	0
4	O	3/5 (60%)	0.58	0 100 100	94, 94, 110, 115	0
4	P	3/5 (60%)	-0.26	0 100 100	67, 67, 70, 99	0
4	Q	3/5 (60%)	0.15	0 100 100	66, 66, 67, 87	0
4	R	3/5 (60%)	-0.00	0 100 100	51, 51, 63, 77	0
4	S	3/5 (60%)	-0.24	0 100 100	89, 89, 98, 123	0
4	T	3/5 (60%)	0.06	0 100 100	65, 65, 69, 91	0
All	All	2755/2992 (92%)	-0.26	40 (1%) 76 74	29, 73, 102, 123	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	168	LEU	5.6
3	C	236	ILE	5.5
2	B	206	VAL	5.3
3	C	344	LEU	4.8
3	I	243	PRO	4.3
3	I	179	LEU	4.0
2	B	168	LEU	3.6
3	C	315	TRP	3.3
2	B	160	ASN	3.3
3	I	344	LEU	3.2
2	B	250	THR	3.1
3	I	241	ALA	3.1
1	G	122	LEU	3.0
2	H	158	ASN	3.0
3	I	339	CYS	3.0
3	I	274	TYR	2.8
2	H	353	LEU	2.8
3	I	237	SER	2.7
3	F	296	GLY	2.7
3	C	292	GLY	2.7
1	G	170	ALA	2.6
3	I	194	PHE	2.4
3	I	290	PHE	2.4
2	B	386	LEU	2.4
3	C	168	PHE	2.4
3	L	94	MET	2.4
3	F	238	THR	2.4
2	E	168	LEU	2.3
3	L	93	ILE	2.3
3	C	174	ALA	2.2
3	I	240	SER	2.2
2	H	398	ASP	2.2
3	C	243	PRO	2.2
3	I	236	ILE	2.1
3	C	107	ILE	2.1
3	C	332	SER	2.1
3	I	99	SER	2.1
3	C	345	ASN	2.1
3	L	379	MET	2.0
2	B	203	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	HYP	M	2	8/9	0.96	0.14	-	70,73,74,74	0
4	HYP	N	2	8/9	0.96	0.13	-	49,56,63,64	0
4	HYP	O	2	8/9	0.68	0.20	-	97,105,109,110	0
4	HYP	P	2	8/9	0.94	0.14	-	72,76,81,85	0
4	HYP	Q	2	8/9	0.94	0.14	-	70,72,73,76	0
4	HYP	R	2	8/9	0.95	0.15	-	43,49,56,59	0
4	HYP	S	2	8/9	0.82	0.25	-	90,94,98,103	0
4	HYP	T	2	8/9	0.93	0.16	-	73,75,76,79	0

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, 95^{th} 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
7	CA	E	2	1/1	0.94	0.26	2.45	60,60,60,60	0
6	NDG	E	470	14/15	0.92	0.14	-0.41	66,77,88,93	0
7	CA	C	1	1/1	0.95	0.14	-0.54	70,70,70,70	0
7	CA	E	3	1/1	0.72	0.12	-0.73	88,88,88,88	0
7	CA	H	2	1/1	0.78	0.17	-0.80	87,87,87,87	0
7	CA	B	2	1/1	0.94	0.09	-1.17	86,86,86,86	0
7	CA	K	2	1/1	0.96	0.11	-1.30	60,60,60,60	0
7	CA	F	1	1/1	0.94	0.09	-1.41	64,64,64,64	0
7	CA	I	1	1/1	0.96	0.05	-1.69	69,69,69,69	0
7	CA	K	3	1/1	0.84	0.12	-1.74	94,94,94,94	0
7	CA	L	1	1/1	0.92	0.09	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	NAG	K	470	14/15	0.80	0.22	-	65,89,100,103	0
5	NAG	B	470	14/15	0.82	0.15	-	85,88,92,100	0
5	NAG	H	470	14/15	0.90	0.19	-	82,95,103,105	0

6.5 Other polymers (i)

There are no such residues in this entry.