



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:30 am BST

PDB ID : 3IKO
Title : Crystal structure of the heterotrimeric Sec13-Nup145C-Nup84 nucleoporin complex
Authors : Nagy, V.; Hsia, K.-C.; Debler, E.W.; Davenport, A.; Blobel, G.; Hoelz, A.
Deposited on : 2009-08-06
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

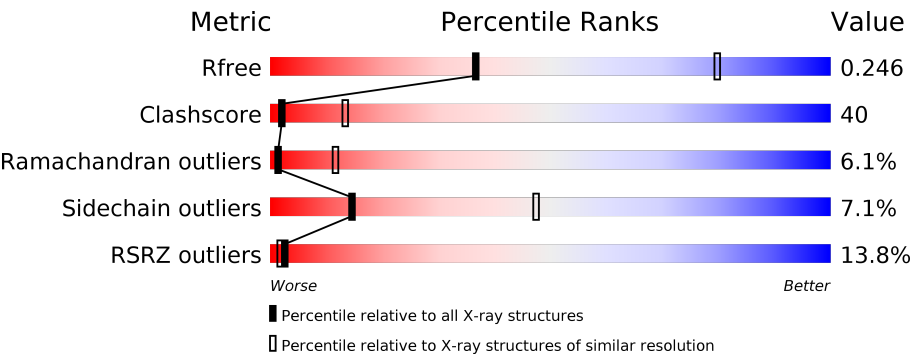
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	<div><div>30%</div><div><div></div><div></div><div></div><div></div></div><div>32%54%6%8%</div></div>
1	D	297	<div><div>32%</div><div><div></div><div></div><div></div><div></div></div><div>34%52%7%8%</div></div>
1	G	297	<div><div>38%</div><div><div></div><div></div><div></div><div></div></div><div>31%54%7%8%</div></div>
2	B	442	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>43%46%8%..</div></div>
2	E	442	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>43%44%8%..</div></div>
2	H	442	<div><div>17%</div><div><div></div><div></div><div></div><div></div></div><div>42%43%9%5%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	460	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div></div>
3	F	460	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>4%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div></div>
3	I	460	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>44%</div><div>38%</div><div>7%</div><div>10%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27032 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	D	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	G	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	9	0	0
			3528	2254	587	675	12			
2	E	423	Total	C	N	O	S	9	0	0
			3438	2201	570	656	11			
2	H	420	Total	C	N	O	S	9	0	0
			3409	2182	566	650	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	EXPRESSION TAG	UNP P49687
B	112	GLY	-	EXPRESSION TAG	UNP P49687
B	113	SER	-	EXPRESSION TAG	UNP P49687
B	114	SER	-	EXPRESSION TAG	UNP P49687
B	115	HIS	-	EXPRESSION TAG	UNP P49687
B	116	HIS	-	EXPRESSION TAG	UNP P49687
B	117	HIS	-	EXPRESSION TAG	UNP P49687
B	118	HIS	-	EXPRESSION TAG	UNP P49687
B	119	HIS	-	EXPRESSION TAG	UNP P49687
B	120	HIS	-	EXPRESSION TAG	UNP P49687
B	121	SER	-	EXPRESSION TAG	UNP P49687
B	122	GLN	-	EXPRESSION TAG	UNP P49687

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Chain	Residue	Modelled	Actual	Comment	Reference
B	123	ASP	-	EXPRESSION TAG	UNP P49687
B	124	PRO	-	EXPRESSION TAG	UNP P49687
E	111	MET	-	EXPRESSION TAG	UNP P49687
E	112	GLY	-	EXPRESSION TAG	UNP P49687
E	113	SER	-	EXPRESSION TAG	UNP P49687
E	114	SER	-	EXPRESSION TAG	UNP P49687
E	115	HIS	-	EXPRESSION TAG	UNP P49687
E	116	HIS	-	EXPRESSION TAG	UNP P49687
E	117	HIS	-	EXPRESSION TAG	UNP P49687
E	118	HIS	-	EXPRESSION TAG	UNP P49687
E	119	HIS	-	EXPRESSION TAG	UNP P49687
E	120	HIS	-	EXPRESSION TAG	UNP P49687
E	121	SER	-	EXPRESSION TAG	UNP P49687
E	122	GLN	-	EXPRESSION TAG	UNP P49687
E	123	ASP	-	EXPRESSION TAG	UNP P49687
E	124	PRO	-	EXPRESSION TAG	UNP P49687
H	111	MET	-	EXPRESSION TAG	UNP P49687
H	112	GLY	-	EXPRESSION TAG	UNP P49687
H	113	SER	-	EXPRESSION TAG	UNP P49687
H	114	SER	-	EXPRESSION TAG	UNP P49687
H	115	HIS	-	EXPRESSION TAG	UNP P49687
H	116	HIS	-	EXPRESSION TAG	UNP P49687
H	117	HIS	-	EXPRESSION TAG	UNP P49687
H	118	HIS	-	EXPRESSION TAG	UNP P49687
H	119	HIS	-	EXPRESSION TAG	UNP P49687
H	120	HIS	-	EXPRESSION TAG	UNP P49687
H	121	SER	-	EXPRESSION TAG	UNP P49687
H	122	GLN	-	EXPRESSION TAG	UNP P49687
H	123	ASP	-	EXPRESSION TAG	UNP P49687
H	124	PRO	-	EXPRESSION TAG	UNP P49687

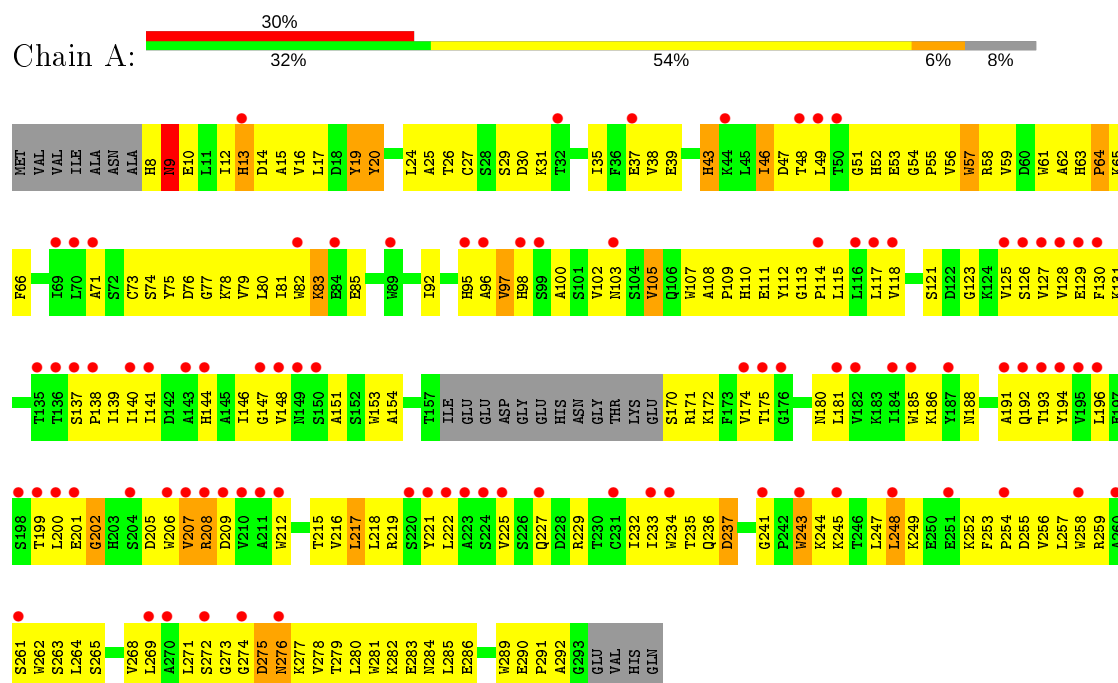
- Molecule 3 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			
3	F	419	Total	C	N	O	S	0	0	0
			3404	2178	558	656	12			
3	I	414	Total	C	N	O	S	0	0	0
			3369	2155	554	649	11			

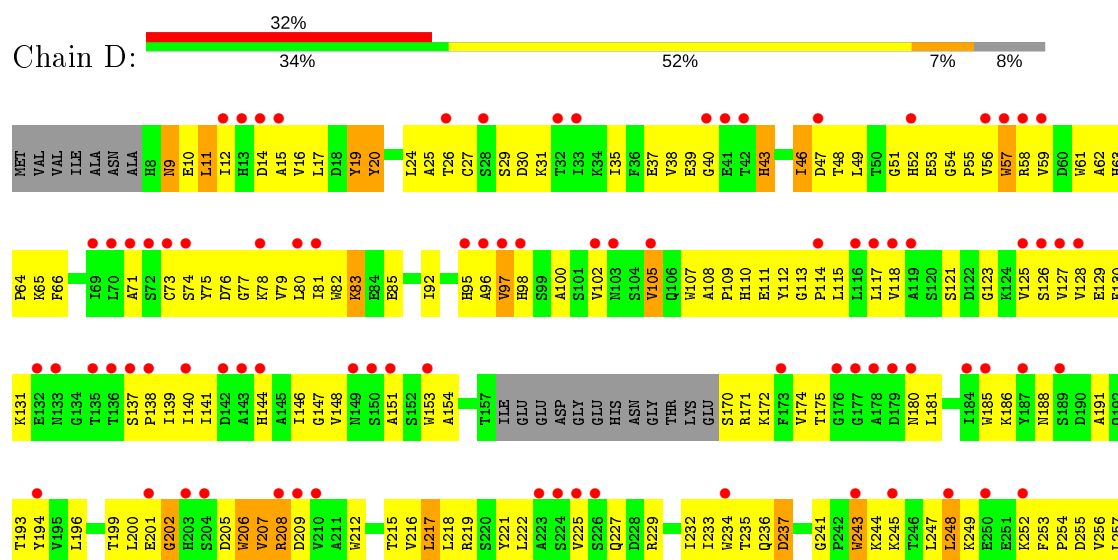
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Protein transport protein SEC13

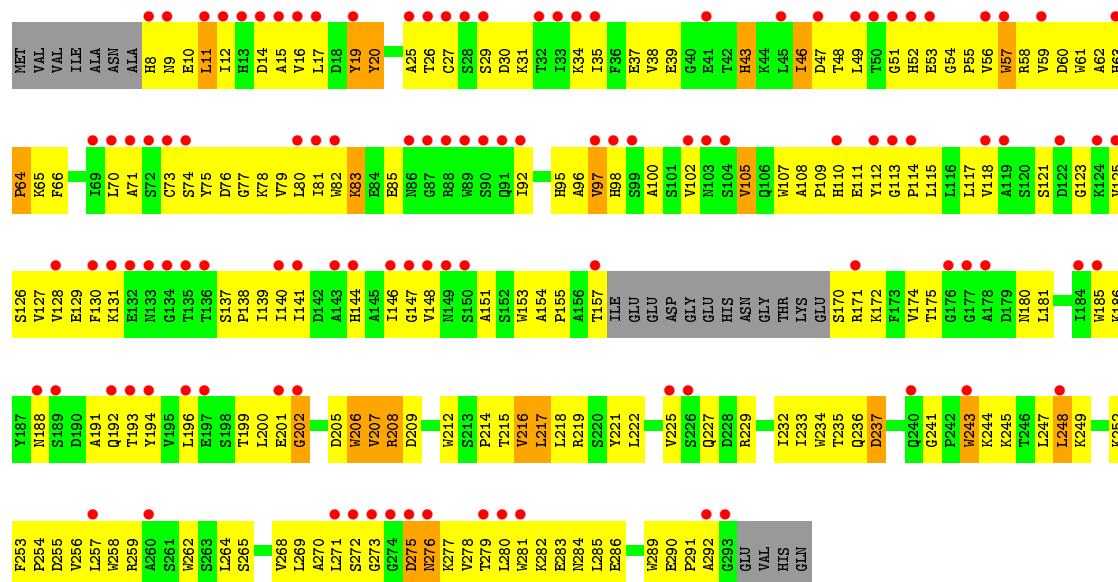


• Molecule 1: Protein transport protein SEC13

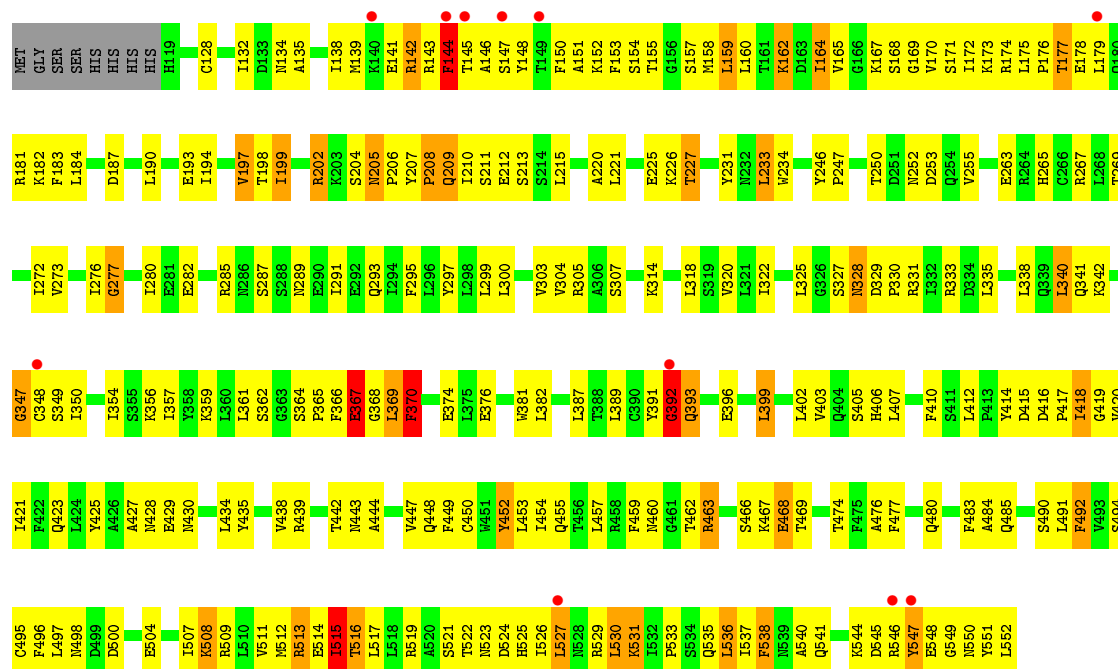
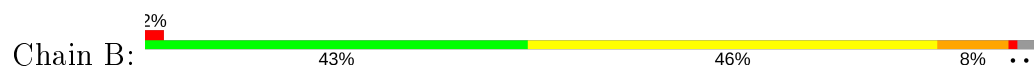




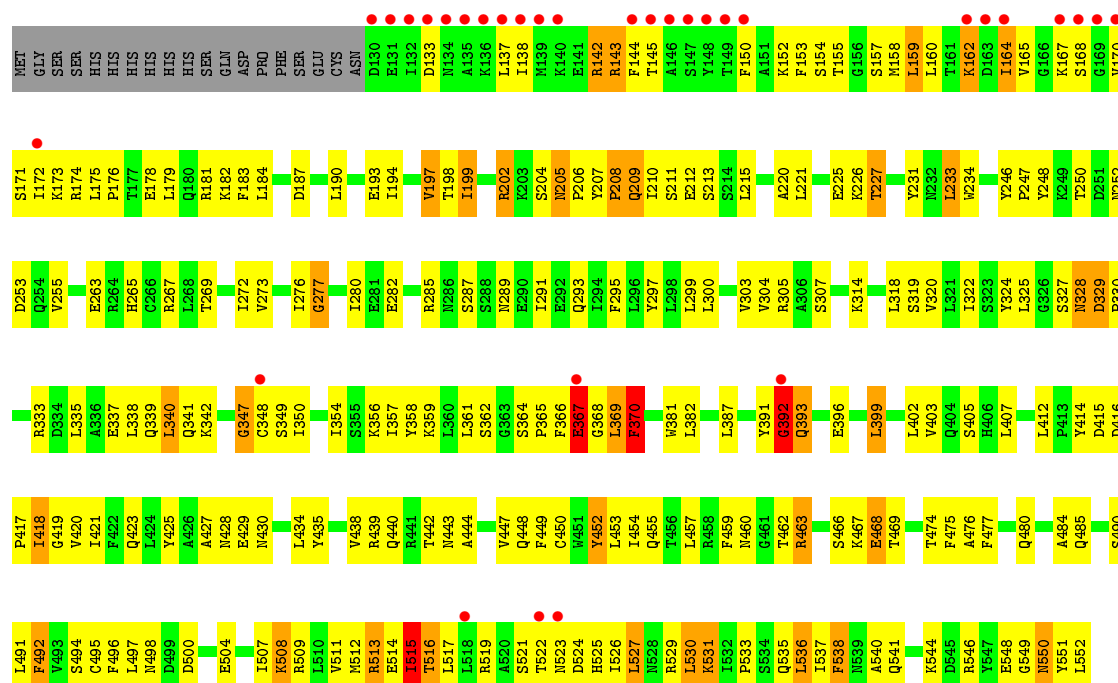
• Molecule 1: Protein transport protein SEC13



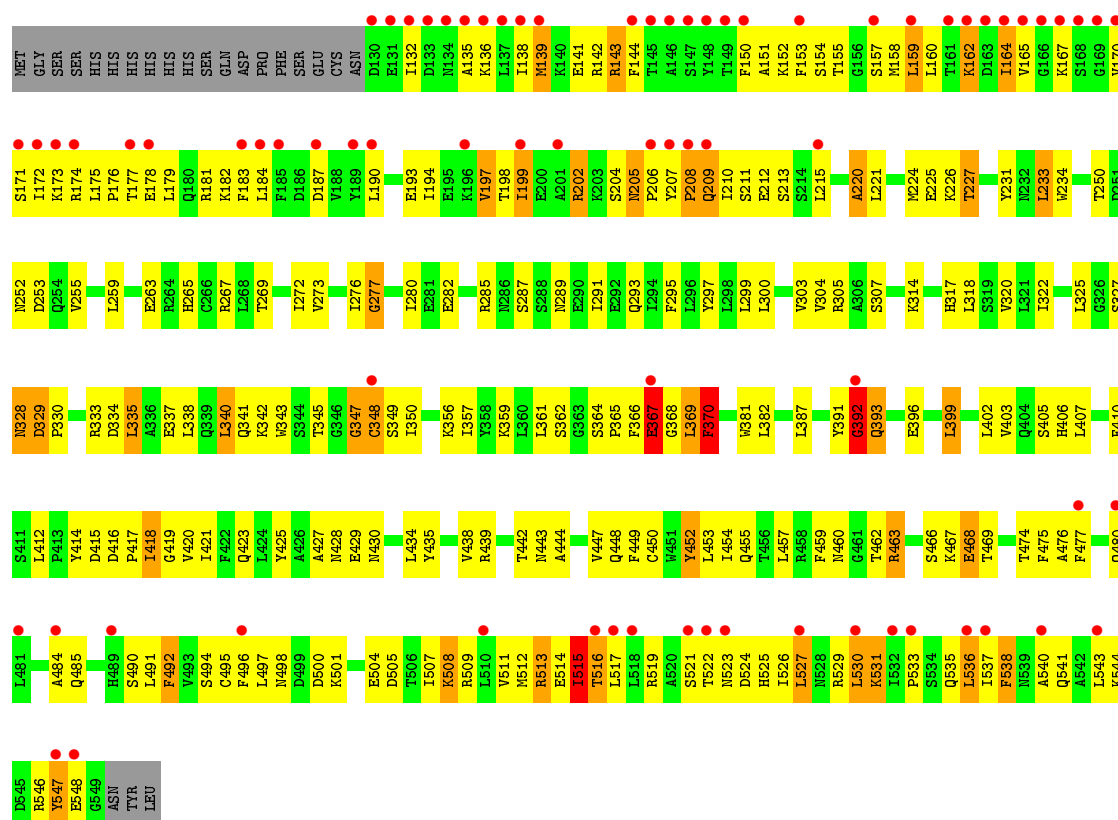
• Molecule 2: Nucleoporin NUP145C



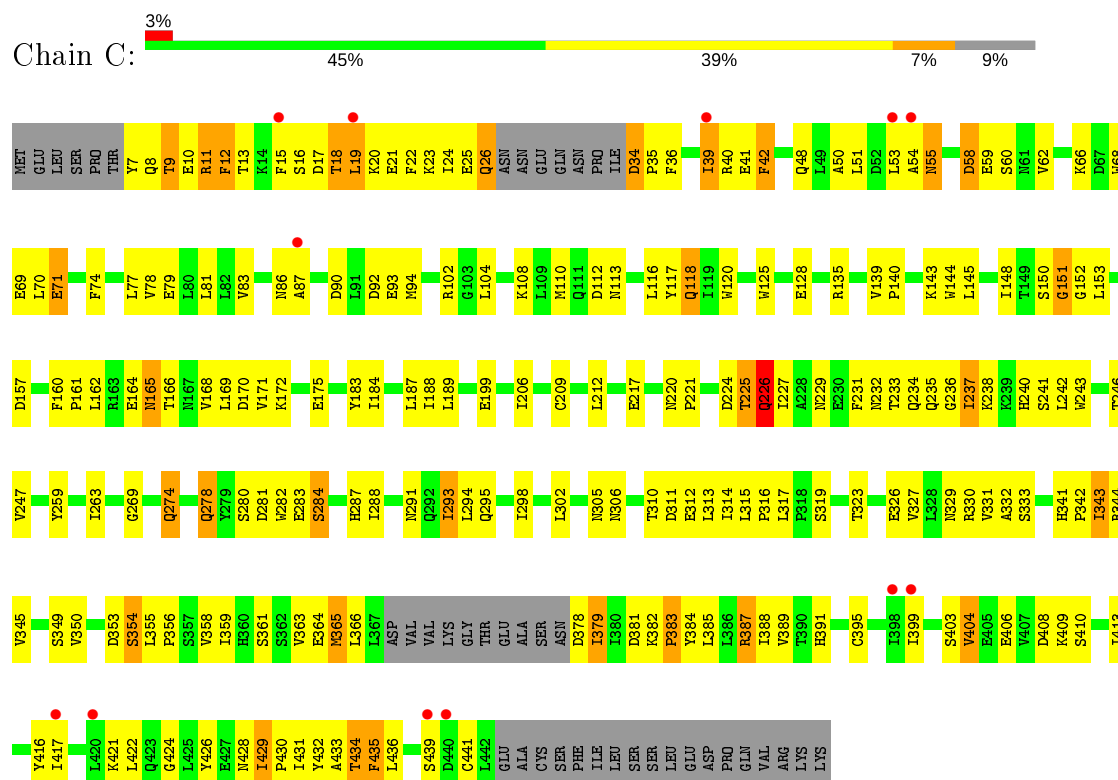
• Molecule 2: Nucleoporin NUP145C



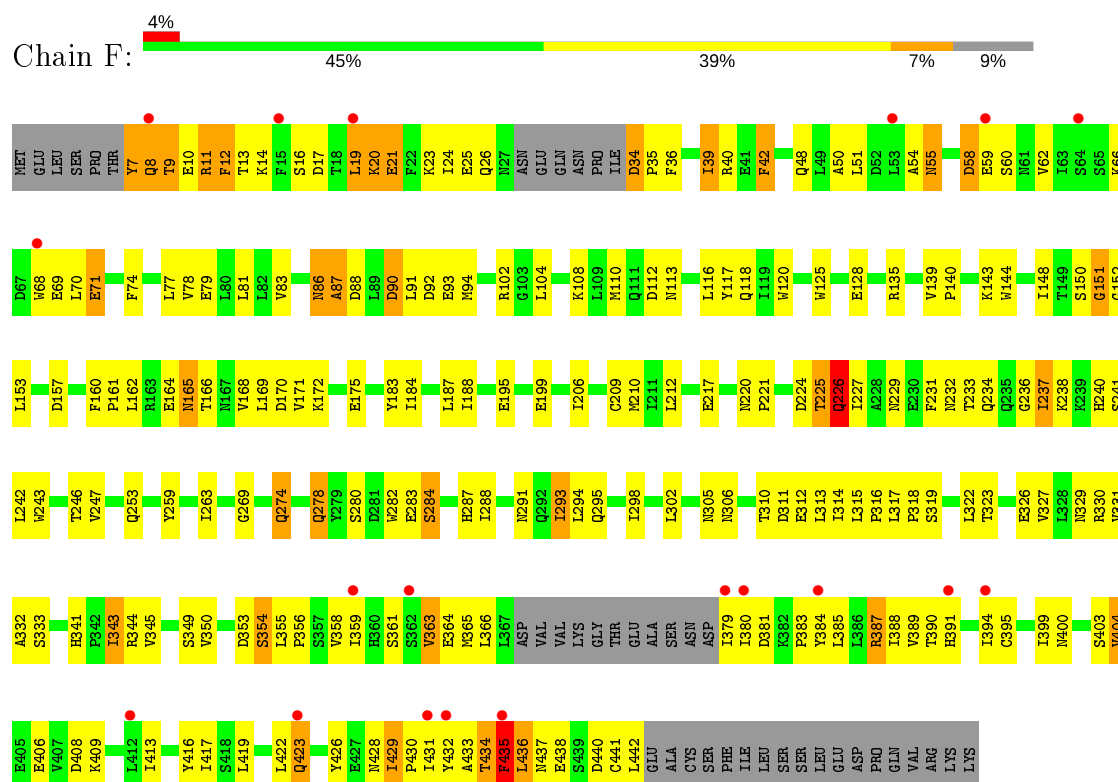
• Molecule 2: Nucleoporin NUP145C



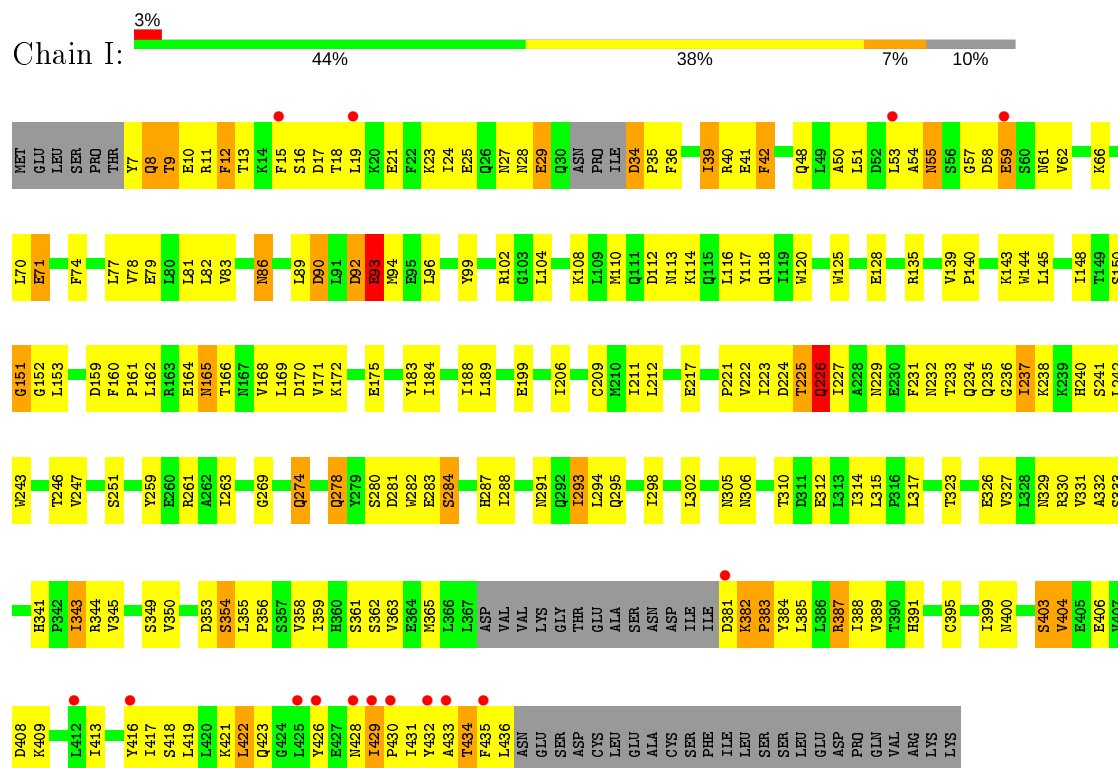
- Molecule 3: Nucleoporin NUP84



- Molecule 3: Nucleoporin NUP84



- Molecule 3: Nucleoporin NUP84



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.40Å 194.05Å 327.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 48.79 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.20) 96.2 (48.79-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.234 , 0.273 0.243 , 0.246	Depositor DCC
R_{free} test set	5253 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27032	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/2220	0.68	1/3028 (0.0%)
1	D	0.47	0/2220	0.67	0/3028
1	G	0.47	0/2220	0.67	0/3028
2	B	0.55	0/3598	0.74	1/4856 (0.0%)
2	E	0.57	0/3504	0.75	1/4728 (0.0%)
2	H	0.56	0/3474	0.74	1/4688 (0.0%)
3	C	0.63	0/3472	0.76	0/4714
3	F	0.63	0/3472	0.77	3/4714 (0.1%)
3	I	0.62	0/3437	0.76	0/4666
All	All	0.57	0/27617	0.74	7/37450 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	392	GLY	N-CA-C	5.99	128.08	113.10
2	H	392	GLY	N-CA-C	5.98	128.05	113.10
2	B	392	GLY	N-CA-C	5.96	128.01	113.10
3	F	435	PHE	N-CA-C	5.71	126.41	111.00
3	F	436	LEU	N-CA-C	5.29	125.28	111.00
1	A	9	ASN	CA-C-N	-5.09	105.99	117.20
3	F	436	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	435	PHE	Mainchain
3	F	435	PHE	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2160	0	2096	239	0
1	D	2160	0	2096	228	0
1	G	2160	0	2096	226	0
2	B	3528	0	3521	301	0
2	E	3438	0	3452	293	0
2	H	3409	0	3426	313	0
3	C	3404	0	3378	249	0
3	F	3404	0	3380	246	0
3	I	3369	0	3341	243	0
All	All	27032	0	26786	2165	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 40.

All (2165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:369:LEU:O	2:E:369:LEU:HG	1.36	1.13
2:E:208:PRO:HB3	2:E:531:LYS:HB2	1.32	1.10
1:A:131:LYS:HE3	1:A:137:SER:HB2	1.38	1.06
2:H:208:PRO:HB3	2:H:531:LYS:HB2	1.32	1.06
2:B:208:PRO:HB3	2:B:531:LYS:HB2	1.32	1.05
2:H:139:MET:HG2	2:H:144:PHE:O	1.56	1.05
1:A:126:SER:HB3	1:A:140:ILE:HG13	1.38	1.04
1:D:131:LYS:HE3	1:D:137:SER:HB2	1.38	1.04
3:C:70:LEU:HD22	3:C:343:ILE:HD11	1.35	1.03
1:G:131:LYS:HE3	1:G:137:SER:HB2	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:LYS:HA	2:H:139:MET:HB3	1.40	1.02
2:H:202:ARG:HG2	2:H:209:GLN:NE2	1.75	1.02
2:E:202:ARG:HG2	2:E:209:GLN:NE2	1.75	1.02
1:A:13:HIS:CE1	2:B:144:PHE:CZ	2.47	1.01
2:B:202:ARG:HG2	2:B:209:GLN:NE2	1.75	1.01
1:A:259:ARG:NH1	2:B:150:PHE:HB2	1.76	1.00
1:D:126:SER:HB3	1:D:140:ILE:HG13	1.38	1.00
1:G:126:SER:HB3	1:G:140:ILE:HG13	1.38	1.00
3:F:70:LEU:HD22	3:F:343:ILE:HD11	1.44	0.99
3:I:8:GLN:NE2	3:I:53:LEU:HG	1.77	0.99
3:F:13:THR:O	3:F:17:ASP:HB2	1.63	0.99
2:B:198:THR:HB	2:B:212:GLU:HB2	1.44	0.98
1:G:212:TRP:HA	1:G:222:LEU:CD2	1.94	0.98
1:G:229:ARG:HH11	1:G:229:ARG:HB2	1.29	0.98
1:D:212:TRP:HA	1:D:222:LEU:CD2	1.94	0.98
1:D:229:ARG:HH11	1:D:229:ARG:HB2	1.29	0.97
1:A:212:TRP:HA	1:A:222:LEU:CD2	1.94	0.97
2:H:320:VAL:HA	3:I:246:THR:HG21	1.45	0.97
2:H:198:THR:HB	2:H:212:GLU:HB2	1.44	0.96
1:A:229:ARG:HB2	1:A:229:ARG:HH11	1.29	0.96
2:E:198:THR:HB	2:E:212:GLU:HB2	1.45	0.96
3:I:384:TYR:HA	3:I:387:ARG:HH12	1.31	0.95
3:F:341:HIS:HE1	3:F:343:ILE:HG23	1.32	0.95
3:C:341:HIS:HE1	3:C:343:ILE:HG23	1.32	0.94
3:F:384:TYR:HA	3:F:387:ARG:HH12	1.31	0.94
3:I:341:HIS:HE1	3:I:343:ILE:HG23	1.32	0.94
1:G:227:GLN:HA	1:G:256:VAL:HG13	1.50	0.94
3:C:384:TYR:HA	3:C:387:ARG:HH12	1.30	0.93
2:B:524:ASP:HA	2:B:527:LEU:HD12	1.51	0.93
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.50	0.93
1:D:229:ARG:HH12	1:D:252:LYS:HD3	1.34	0.93
1:G:229:ARG:HH12	1:G:252:LYS:HD3	1.34	0.93
1:D:227:GLN:HA	1:D:256:VAL:HG13	1.50	0.92
2:H:524:ASP:HA	2:H:527:LEU:HD12	1.51	0.92
2:E:524:ASP:HA	2:E:527:LEU:HD12	1.50	0.92
1:D:49:LEU:HB3	1:D:82:TRP:CZ3	2.05	0.92
1:G:64:PRO:HB2	2:H:543:LEU:HD11	1.50	0.92
2:E:320:VAL:HA	3:F:246:THR:HG21	1.52	0.92
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.06	0.92
3:F:314:ILE:HG22	3:F:315:LEU:HG	1.52	0.91
3:I:8:GLN:HE22	3:I:53:LEU:HG	1.31	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:LEU:HB3	1:G:82:TRP:CZ3	2.05	0.91
1:A:261:SER:HB2	2:B:152:LYS:HG2	1.51	0.91
1:A:20:TYR:CE2	2:B:544:LYS:HD3	2.06	0.90
3:C:314:ILE:HG22	3:C:315:LEU:HG	1.51	0.90
2:H:155:THR:HG22	2:H:513:ARG:HG3	1.52	0.90
1:A:229:ARG:HH12	1:A:252:LYS:HD3	1.34	0.90
1:A:229:ARG:HB2	1:A:229:ARG:NH1	1.87	0.90
3:I:89:LEU:HD13	3:I:114:LYS:HZ3	1.37	0.89
3:C:34:ASP:HB3	3:C:35:PRO:HD3	1.54	0.89
3:C:16:SER:HA	3:C:19:LEU:HD12	1.55	0.89
3:I:314:ILE:HG22	3:I:315:LEU:HG	1.51	0.89
1:G:229:ARG:HB2	1:G:229:ARG:NH1	1.87	0.89
1:D:229:ARG:NH1	1:D:229:ARG:HB2	1.87	0.89
3:I:34:ASP:HB3	3:I:35:PRO:HD3	1.54	0.88
2:E:181:ARG:HD2	2:E:448:GLN:OE1	1.74	0.88
3:F:280:SER:HB2	3:F:284:SER:HB3	1.56	0.88
3:F:34:ASP:HB3	3:F:35:PRO:HD3	1.55	0.88
1:D:229:ARG:NH1	1:D:252:LYS:HD3	1.88	0.87
1:A:229:ARG:NH1	1:A:252:LYS:HD3	1.88	0.87
3:C:280:SER:HB2	3:C:284:SER:HB3	1.56	0.87
1:G:229:ARG:NH1	1:G:252:LYS:HD3	1.88	0.87
2:H:181:ARG:HD2	2:H:448:GLN:OE1	1.74	0.87
3:I:70:LEU:HD22	3:I:343:ILE:HD11	1.56	0.87
1:D:17:LEU:HD12	2:E:154:SER:HA	1.54	0.87
1:G:232:ILE:HG12	1:G:247:LEU:HD23	1.56	0.87
2:H:291:ILE:H	2:H:291:ILE:HD12	1.40	0.87
2:B:524:ASP:O	2:B:527:LEU:HB2	1.75	0.86
2:E:524:ASP:O	2:E:527:LEU:HB2	1.75	0.86
3:I:341:HIS:CE1	3:I:343:ILE:HG23	2.10	0.86
1:A:13:HIS:CE1	2:B:144:PHE:CE1	2.63	0.86
3:F:341:HIS:CE1	3:F:343:ILE:HG23	2.10	0.86
1:D:232:ILE:HG12	1:D:247:LEU:HD23	1.56	0.86
2:H:524:ASP:O	2:H:527:LEU:HB2	1.75	0.86
2:B:181:ARG:HD2	2:B:448:GLN:OE1	1.75	0.85
1:A:64:PRO:HB3	2:B:547:TYR:HB2	1.57	0.85
3:F:437:ASN:O	3:F:440:ASP:HB2	1.77	0.85
3:I:280:SER:HB2	3:I:284:SER:HB3	1.56	0.85
1:A:20:TYR:HE2	2:B:544:LYS:HD3	1.35	0.85
3:C:341:HIS:CE1	3:C:343:ILE:HG23	2.10	0.85
1:A:261:SER:CB	2:B:152:LYS:HA	2.07	0.85
2:B:291:ILE:HD12	2:B:291:ILE:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:291:ILE:H	2:E:291:ILE:HD12	1.41	0.84
1:A:232:ILE:HG12	1:A:247:LEU:HD23	1.56	0.84
2:B:320:VAL:HA	3:C:246:THR:HG21	1.60	0.84
1:D:57:TRP:HE1	2:E:142:ARG:NH2	1.75	0.83
3:C:20:LYS:O	3:C:24:ILE:HG12	1.79	0.83
2:E:434:LEU:O	2:E:438:VAL:HG23	1.78	0.83
2:H:210:ILE:HD12	2:H:210:ILE:H	1.43	0.83
2:B:434:LEU:O	2:B:438:VAL:HG23	1.78	0.83
3:I:416:TYR:HE2	3:I:432:TYR:CE2	1.97	0.83
3:I:8:GLN:C	3:I:10:GLU:H	1.82	0.82
2:B:210:ILE:H	2:B:210:ILE:HD12	1.43	0.82
1:G:64:PRO:HB2	2:H:543:LEU:CD1	2.09	0.82
1:D:25:ALA:O	1:D:59:VAL:HG21	1.79	0.82
3:C:83:VAL:O	3:C:87:ALA:HB3	1.80	0.82
1:G:25:ALA:O	1:G:59:VAL:HG21	1.79	0.82
2:H:434:LEU:O	2:H:438:VAL:HG23	1.78	0.81
3:I:13:THR:HG22	3:I:17:ASP:OD2	1.81	0.81
2:H:175:LEU:HD12	2:H:176:PRO:HD2	1.63	0.81
2:E:512:MET:HG2	2:E:540:ALA:HB2	1.62	0.81
1:G:212:TRP:HA	1:G:222:LEU:HD23	1.62	0.81
1:A:78:LYS:HA	1:A:96:ALA:HB2	1.62	0.81
3:C:13:THR:O	3:C:17:ASP:HB2	1.78	0.81
1:D:78:LYS:HA	1:D:96:ALA:HB2	1.62	0.81
2:E:340:LEU:CD2	2:E:370:PHE:CD1	2.64	0.81
2:B:190:LEU:O	2:B:194:ILE:HG13	1.81	0.81
2:B:175:LEU:HD12	2:B:176:PRO:HD2	1.63	0.81
1:A:25:ALA:O	1:A:59:VAL:HG21	1.79	0.80
1:G:217:LEU:HD22	1:G:218:LEU:H	1.46	0.80
3:I:89:LEU:HD13	3:I:114:LYS:CE	2.11	0.80
1:D:217:LEU:HD22	1:D:218:LEU:H	1.47	0.80
1:G:19:TYR:HD2	1:G:20:TYR:CE1	1.99	0.80
3:I:237:ILE:HD12	3:I:237:ILE:C	2.02	0.80
3:I:8:GLN:HE22	3:I:53:LEU:CG	1.93	0.80
1:A:12:ILE:HD12	2:B:169:GLY:HA3	1.62	0.80
2:H:340:LEU:CD2	2:H:370:PHE:CD1	2.64	0.80
2:H:512:MET:HG2	2:H:540:ALA:HB2	1.61	0.80
1:A:19:TYR:HD2	1:A:20:TYR:CE1	1.98	0.80
2:B:442:THR:HG22	2:B:444:ALA:H	1.46	0.80
2:H:136:LYS:HA	2:H:139:MET:CB	2.11	0.80
1:G:78:LYS:HA	1:G:96:ALA:HB2	1.62	0.80
2:H:442:THR:HG22	2:H:444:ALA:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:THR:O	2:H:513:ARG:HD2	1.80	0.80
3:I:59:GLU:HA	3:I:62:VAL:HG23	1.62	0.80
1:D:19:TYR:HD2	1:D:20:TYR:CE1	1.99	0.80
2:E:175:LEU:HD12	2:E:176:PRO:HD2	1.63	0.79
3:F:237:ILE:C	3:F:237:ILE:HD12	2.03	0.79
2:E:210:ILE:H	2:E:210:ILE:HD12	1.43	0.79
2:B:512:MET:HG2	2:B:540:ALA:HB2	1.61	0.79
3:F:94:MET:HE2	3:F:108:LYS:HB2	1.64	0.79
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.12	0.79
2:H:190:LEU:O	2:H:194:ILE:HG13	1.81	0.79
3:C:237:ILE:HD12	3:C:237:ILE:C	2.03	0.79
2:H:210:ILE:CD1	2:H:495:CYS:HB2	2.12	0.79
3:I:89:LEU:HD13	3:I:114:LYS:NZ	1.96	0.79
1:G:65:LYS:HA	2:H:546:ARG:NH2	1.97	0.79
2:E:210:ILE:CD1	2:E:495:CYS:HB2	2.12	0.79
2:E:442:THR:HG22	2:E:444:ALA:H	1.46	0.79
1:D:212:TRP:HA	1:D:222:LEU:HD23	1.62	0.79
2:H:265:HIS:HB2	2:H:399:LEU:HD21	1.64	0.79
1:G:278:VAL:HG21	2:H:151:ALA:HB3	1.64	0.78
3:I:416:TYR:CE2	3:I:432:TYR:CE2	2.71	0.78
2:E:190:LEU:O	2:E:194:ILE:HG13	1.81	0.78
2:E:265:HIS:HB2	2:E:399:LEU:HD21	1.65	0.78
3:F:416:TYR:CE2	3:F:432:TYR:CE2	2.71	0.78
3:I:419:LEU:HD23	3:I:422:LEU:HD12	1.65	0.78
3:C:20:LYS:HG2	3:C:431:ILE:CG1	2.14	0.78
2:E:320:VAL:HG22	3:F:246:THR:HG22	1.65	0.78
1:A:217:LEU:HD22	1:A:218:LEU:H	1.47	0.78
1:A:29:SER:HA	1:A:55:PRO:HB3	1.66	0.78
3:F:108:LYS:HE3	3:F:112:ASP:OD2	1.83	0.78
3:C:108:LYS:HE3	3:C:112:ASP:OD2	1.84	0.77
2:H:320:VAL:HG22	3:I:246:THR:HG22	1.64	0.77
1:G:29:SER:HA	1:G:55:PRO:HB3	1.66	0.77
2:B:265:HIS:HB2	2:B:399:LEU:HD21	1.64	0.77
1:D:29:SER:HA	1:D:55:PRO:HB3	1.66	0.77
1:A:63:HIS:HD2	1:A:65:LYS:HB2	1.50	0.77
3:C:74:PHE:O	3:C:78:VAL:HG23	1.85	0.77
2:H:524:ASP:HA	2:H:527:LEU:CD1	2.15	0.77
2:B:522:THR:HA	2:B:525:HIS:HB2	1.66	0.77
1:G:131:LYS:CE	1:G:137:SER:HB2	2.15	0.77
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.62	0.77
2:B:524:ASP:HA	2:B:527:LEU:CD1	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:74:PHE:O	3:F:78:VAL:HG23	1.84	0.76
3:I:108:LYS:HE3	3:I:112:ASP:OD2	1.83	0.76
1:A:131:LYS:CE	1:A:137:SER:HB2	2.15	0.76
2:E:524:ASP:HA	2:E:527:LEU:CD1	2.15	0.76
3:F:416:TYR:HE2	3:F:432:TYR:CE2	2.02	0.76
2:H:522:THR:HA	2:H:525:HIS:HB2	1.66	0.76
2:E:522:THR:HA	2:E:525:HIS:HB2	1.66	0.76
3:I:74:PHE:O	3:I:78:VAL:HG23	1.85	0.76
1:A:225:VAL:HG13	1:A:257:LEU:HB2	1.67	0.75
3:C:116:LEU:HD21	3:C:294:LEU:HD11	1.69	0.75
1:A:208:ARG:NH2	2:B:143:ARG:HB2	2.01	0.75
1:D:131:LYS:CE	1:D:137:SER:HB2	2.15	0.75
3:C:18:THR:HG23	3:C:41:GLU:OE1	1.86	0.75
3:I:269:GLY:HA3	3:I:295:GLN:HG2	1.68	0.75
3:C:269:GLY:HA3	3:C:295:GLN:HG2	1.68	0.74
1:D:275:ASP:O	1:D:276:ASN:HB2	1.86	0.74
1:G:259:ARG:HD2	2:H:152:LYS:HE3	1.69	0.74
2:B:165:VAL:O	2:B:165:VAL:HG12	1.84	0.74
3:F:269:GLY:HA3	3:F:295:GLN:HG2	1.69	0.74
2:B:155:THR:HG22	2:B:513:ARG:HD2	1.69	0.74
2:H:523:ASN:O	2:H:527:LEU:HG	1.87	0.74
3:I:116:LEU:HD21	3:I:294:LEU:HD11	1.69	0.74
2:E:340:LEU:HD22	2:E:370:PHE:CD1	2.23	0.74
1:D:225:VAL:HG13	1:D:257:LEU:HB2	1.67	0.74
1:G:10:GLU:O	1:G:11:LEU:HG	1.88	0.74
1:G:285:LEU:HD12	1:G:285:LEU:H	1.53	0.74
3:C:11:ARG:CG	3:C:12:PHE:N	2.50	0.74
1:D:24:LEU:CD2	2:E:170:VAL:HG21	2.18	0.74
2:E:207:TYR:CE1	2:E:504:GLU:HG3	2.23	0.74
2:E:369:LEU:CG	2:E:369:LEU:O	2.23	0.74
2:H:207:TYR:CE1	2:H:504:GLU:HG3	2.23	0.74
1:A:285:LEU:H	1:A:285:LEU:HD12	1.53	0.74
1:D:10:GLU:O	1:D:11:LEU:HG	1.88	0.74
2:E:523:ASN:O	2:E:527:LEU:HG	1.88	0.74
1:A:275:ASP:O	1:A:276:ASN:HB2	1.86	0.73
1:D:285:LEU:HD12	1:D:285:LEU:H	1.53	0.73
1:G:225:VAL:HG13	1:G:257:LEU:HB2	1.67	0.73
1:G:275:ASP:O	1:G:276:ASN:HB2	1.86	0.73
1:G:265:SER:HB2	2:H:509:ARG:HH22	1.52	0.73
3:I:293:ILE:HD11	3:I:327:VAL:HG21	1.70	0.73
1:D:57:TRP:NE1	2:E:142:ARG:NH2	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:MET:HA	2:B:540:ALA:HB1	1.69	0.73
3:C:384:TYR:HA	3:C:387:ARG:NH1	2.04	0.73
2:H:512:MET:HA	2:H:540:ALA:HB1	1.69	0.73
2:B:207:TYR:CE1	2:B:504:GLU:HG3	2.23	0.73
2:H:530:LEU:O	2:H:531:LYS:HG2	1.89	0.73
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.71	0.73
3:F:116:LEU:HD21	3:F:294:LEU:HD11	1.68	0.73
1:G:17:LEU:HD12	2:H:154:SER:HA	1.70	0.73
2:H:340:LEU:HD23	2:H:370:PHE:CD1	2.24	0.73
2:B:442:THR:HG22	2:B:443:ASN:N	2.04	0.73
2:B:523:ASN:O	2:B:527:LEU:HG	1.88	0.73
3:F:293:ILE:HD11	3:F:327:VAL:HG21	1.70	0.73
1:G:180:ASN:HA	1:G:207:VAL:HG23	1.71	0.73
2:B:530:LEU:O	2:B:531:LYS:HG2	1.89	0.72
2:E:512:MET:HA	2:E:540:ALA:HB1	1.69	0.72
2:H:167:LYS:HD3	2:H:167:LYS:O	1.89	0.72
3:C:11:ARG:HG2	3:C:12:PHE:H	1.54	0.72
3:C:8:GLN:C	3:C:10:GLU:H	1.92	0.72
2:E:320:VAL:CA	3:F:246:THR:HG21	2.19	0.72
2:B:167:LYS:O	2:B:167:LYS:HD3	1.89	0.72
2:E:507:ILE:O	2:E:511:VAL:HG23	1.90	0.72
3:C:139:VAL:HG13	3:C:140:PRO:HD2	1.72	0.72
2:H:136:LYS:CA	2:H:139:MET:HB3	2.18	0.72
2:H:162:LYS:CE	2:H:164:ILE:HD11	2.20	0.72
1:A:103:ASN:OD1	2:B:142:ARG:NH2	2.22	0.72
2:E:162:LYS:CE	2:E:164:ILE:HD11	2.20	0.72
2:E:167:LYS:O	2:E:167:LYS:HD3	1.89	0.72
2:E:530:LEU:O	2:E:531:LYS:HG2	1.90	0.72
1:G:138:PRO:HB2	1:G:140:ILE:HD11	1.72	0.72
1:A:261:SER:HB3	2:B:152:LYS:HA	1.72	0.72
3:C:20:LYS:HG2	3:C:431:ILE:HG12	1.70	0.72
3:C:293:ILE:HD11	3:C:327:VAL:HG21	1.71	0.72
2:E:442:THR:HG22	2:E:443:ASN:N	2.04	0.72
3:F:406:GLU:HA	3:F:409:LYS:HE3	1.72	0.72
2:B:187:ASP:HB3	2:B:523:ASN:ND2	2.05	0.71
3:C:8:GLN:O	3:C:10:GLU:N	2.23	0.71
3:I:384:TYR:HA	3:I:387:ARG:NH1	2.04	0.71
1:D:180:ASN:HA	1:D:207:VAL:HG23	1.71	0.71
2:E:494:SER:O	2:E:497:LEU:HD13	1.90	0.71
3:I:406:GLU:HA	3:I:409:LYS:HE3	1.72	0.71
3:I:89:LEU:HD13	3:I:114:LYS:HE2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:TYR:O	3:F:9:THR:N	2.23	0.71
2:B:204:SER:O	2:B:205:ASN:HB3	1.91	0.71
2:B:507:ILE:O	2:B:511:VAL:HG23	1.90	0.71
3:C:20:LYS:NZ	3:C:428:ASN:OD1	2.23	0.71
2:E:187:ASP:HB3	2:E:523:ASN:ND2	2.05	0.71
3:C:8:GLN:HE22	3:C:53:LEU:HG	1.54	0.71
2:E:160:LEU:HD23	2:E:171:SER:O	1.91	0.71
3:F:139:VAL:HG13	3:F:140:PRO:HD2	1.72	0.71
3:F:384:TYR:HA	3:F:387:ARG:NH1	2.04	0.71
2:H:442:THR:HG22	2:H:443:ASN:N	2.04	0.71
2:H:507:ILE:O	2:H:511:VAL:HG23	1.90	0.71
3:I:139:VAL:HG13	3:I:140:PRO:HD2	1.72	0.71
3:I:385:LEU:O	3:I:389:VAL:HG23	1.91	0.71
3:F:350:VAL:HG22	3:F:355:LEU:HD22	1.73	0.71
2:H:187:ASP:HB3	2:H:523:ASN:ND2	2.05	0.71
1:A:259:ARG:HH12	2:B:150:PHE:HB2	1.55	0.71
3:C:93:GLU:HG3	3:C:94:MET:N	2.06	0.71
1:G:57:TRP:HE1	2:H:142:ARG:HH21	1.37	0.71
3:I:11:ARG:HG3	3:I:12:PHE:CD1	2.26	0.71
2:B:158:MET:HB2	2:B:173:LYS:O	1.91	0.71
2:E:159:LEU:HD13	2:E:160:LEU:H	1.56	0.71
3:C:350:VAL:HG22	3:C:355:LEU:HD22	1.73	0.70
1:D:138:PRO:HB2	1:D:140:ILE:HD11	1.72	0.70
1:G:126:SER:CB	1:G:140:ILE:HG13	2.20	0.70
2:H:204:SER:O	2:H:205:ASN:HB3	1.91	0.70
1:D:17:LEU:HD21	2:E:160:LEU:HD11	1.72	0.70
2:H:494:SER:O	2:H:497:LEU:HD13	1.91	0.70
3:I:409:LYS:O	3:I:413:ILE:HG13	1.91	0.70
1:A:83:LYS:HD3	1:A:92:ILE:HD12	1.73	0.70
2:B:494:SER:O	2:B:497:LEU:HD13	1.90	0.70
2:B:160:LEU:HD23	2:B:171:SER:O	1.91	0.70
1:D:217:LEU:HD13	1:D:218:LEU:N	2.07	0.70
3:I:350:VAL:HG22	3:I:355:LEU:HD22	1.73	0.70
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.72	0.70
2:E:521:SER:O	2:E:524:ASP:HB2	1.92	0.70
3:F:327:VAL:O	3:F:331:VAL:HG23	1.92	0.70
2:H:158:MET:HB2	2:H:173:LYS:O	1.91	0.70
3:I:293:ILE:HD11	3:I:327:VAL:CG2	2.21	0.70
3:I:23:LYS:HZ3	3:I:431:ILE:HA	1.54	0.70
2:B:521:SER:O	2:B:524:ASP:HB2	1.92	0.70
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:70:LEU:HD21	3:I:344:ARG:NH1	2.05	0.70
3:C:11:ARG:CG	3:C:12:PHE:H	2.04	0.70
3:C:406:GLU:HA	3:C:409:LYS:HE3	1.72	0.70
3:C:435:PHE:O	3:C:436:LEU:HD23	1.92	0.70
2:E:204:SER:O	2:E:205:ASN:HB3	1.91	0.70
3:C:385:LEU:O	3:C:389:VAL:HG23	1.91	0.70
2:E:391:TYR:O	2:E:393:GLN:N	2.25	0.70
2:E:327:SER:OG	3:F:238:LYS:HG3	1.91	0.70
1:G:217:LEU:HD13	1:G:218:LEU:N	2.07	0.70
3:I:434:THR:O	3:I:434:THR:HG22	1.91	0.70
1:A:126:SER:CB	1:A:140:ILE:HG13	2.21	0.70
2:B:159:LEU:HD13	2:B:160:LEU:H	1.56	0.70
3:C:409:LYS:O	3:C:413:ILE:HG13	1.91	0.70
2:H:533:PRO:O	2:H:537:ILE:HG13	1.92	0.70
3:I:327:VAL:O	3:I:331:VAL:HG23	1.92	0.70
2:E:267:ARG:HH11	2:E:267:ARG:HG3	1.56	0.69
2:E:299:LEU:HD23	2:E:387:LEU:HD21	1.74	0.69
2:E:544:LYS:O	2:E:548:GLU:HG3	1.92	0.69
3:F:293:ILE:HD11	3:F:327:VAL:CG2	2.22	0.69
2:H:521:SER:O	2:H:524:ASP:HB2	1.92	0.69
1:A:20:TYR:HD2	2:B:544:LYS:HZ2	1.38	0.69
1:A:217:LEU:HD13	1:A:218:LEU:N	2.07	0.69
2:B:533:PRO:O	2:B:537:ILE:HG13	1.92	0.69
3:C:382:LYS:HD3	3:C:384:TYR:OH	1.92	0.69
2:E:158:MET:HB2	2:E:173:LYS:O	1.91	0.69
3:F:409:LYS:O	3:F:413:ILE:HG13	1.91	0.69
3:F:385:LEU:O	3:F:389:VAL:HG23	1.91	0.69
2:H:159:LEU:HD13	2:H:160:LEU:H	1.56	0.69
2:H:544:LYS:O	2:H:548:GLU:HG3	1.92	0.69
1:A:262:TRP:O	2:B:153:PHE:HB2	1.92	0.69
1:A:12:ILE:HD13	2:B:168:SER:O	1.92	0.69
2:H:155:THR:HG22	2:H:513:ARG:CG	2.22	0.69
3:C:327:VAL:O	3:C:331:VAL:HG23	1.91	0.69
1:G:83:LYS:HD3	1:G:92:ILE:HD12	1.73	0.69
1:A:24:LEU:HD21	2:B:170:VAL:HG21	1.73	0.69
3:C:70:LEU:CD2	3:C:343:ILE:HD11	2.20	0.69
2:H:160:LEU:HD23	2:H:171:SER:O	1.91	0.69
1:D:83:LYS:HD3	1:D:92:ILE:HD12	1.73	0.69
2:E:533:PRO:O	2:E:537:ILE:HG13	1.92	0.69
1:G:77:GLY:HA2	1:G:100:ALA:O	1.93	0.69
3:F:363:VAL:HG11	3:F:408:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:434:THR:HG22	3:F:434:THR:O	1.92	0.69
3:I:21:GLU:HB3	3:I:25:GLU:OE1	1.93	0.69
2:B:544:LYS:O	2:B:548:GLU:HG3	1.92	0.69
3:C:434:THR:O	3:C:434:THR:HG22	1.92	0.69
1:A:77:GLY:HA2	1:A:100:ALA:O	1.93	0.68
2:B:491:LEU:HD11	2:B:507:ILE:HG23	1.75	0.68
2:H:287:SER:OG	2:H:293:GLN:HG2	1.93	0.68
2:H:299:LEU:HD23	2:H:387:LEU:HD21	1.74	0.68
2:H:457:LEU:HD13	2:H:463:ARG:HB2	1.76	0.68
3:I:102:ARG:HD3	3:I:302:LEU:HD13	1.76	0.68
3:C:227:ILE:C	3:C:229:ASN:H	1.96	0.68
2:E:457:LEU:HD13	2:E:463:ARG:HB2	1.75	0.68
1:G:35:ILE:HB	1:G:47:ASP:HB2	1.75	0.68
2:H:391:TYR:O	2:H:393:GLN:N	2.26	0.68
3:I:435:PHE:O	3:I:436:LEU:HG	1.92	0.68
2:B:267:ARG:HG3	2:B:267:ARG:HH11	1.56	0.68
2:B:457:LEU:HD13	2:B:463:ARG:HB2	1.76	0.68
3:C:293:ILE:HD11	3:C:327:VAL:CG2	2.22	0.68
2:E:491:LEU:HD11	2:E:507:ILE:HG23	1.75	0.68
1:D:35:ILE:HB	1:D:47:ASP:HB2	1.75	0.68
1:D:77:GLY:HA2	1:D:100:ALA:O	1.93	0.68
2:E:329:ASP:OD2	3:F:236:GLY:N	2.25	0.68
3:F:319:SER:OG	2:H:337:GLU:HG2	1.94	0.68
2:B:287:SER:OG	2:B:293:GLN:HG2	1.93	0.68
2:B:314:LYS:HG2	3:C:162:LEU:O	1.94	0.68
1:G:20:TYR:CE2	2:H:544:LYS:HD3	2.29	0.68
2:B:391:TYR:O	2:B:393:GLN:N	2.26	0.67
2:H:418:ILE:H	2:H:418:ILE:HD13	1.59	0.67
3:C:8:GLN:NE2	3:C:53:LEU:HG	2.10	0.67
3:I:23:LYS:NZ	3:I:434:THR:OG1	2.25	0.67
3:F:102:ARG:HD3	3:F:302:LEU:HD13	1.76	0.67
2:E:202:ARG:HG3	2:E:500:ASP:OD1	1.95	0.67
3:F:227:ILE:C	3:F:229:ASN:H	1.96	0.67
1:A:63:HIS:HD2	1:A:65:LYS:CB	2.08	0.67
2:B:299:LEU:HD23	2:B:387:LEU:HD21	1.75	0.67
2:B:418:ILE:H	2:B:418:ILE:HD13	1.60	0.67
2:E:287:SER:OG	2:E:293:GLN:HG2	1.93	0.67
3:F:438:GLU:HA	3:F:438:GLU:OE1	1.94	0.67
2:H:340:LEU:HD22	2:H:370:PHE:CD1	2.29	0.67
3:I:227:ILE:C	3:I:229:ASN:H	1.96	0.67
3:C:171:VAL:O	3:C:175:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:LEU:HD13	1:G:234:TRP:CE3	2.30	0.67
3:I:417:ILE:HG23	3:I:429:ILE:HG23	1.76	0.67
3:I:89:LEU:HD22	3:I:114:LYS:HZ1	1.59	0.67
3:F:91:LEU:HG	3:F:92:ASP:H	1.60	0.66
2:H:320:VAL:CA	3:I:246:THR:HG21	2.23	0.66
1:A:35:ILE:HB	1:A:47:ASP:HB2	1.75	0.66
2:B:153:PHE:HA	2:B:159:LEU:HD22	1.77	0.66
2:B:320:VAL:HG22	3:C:246:THR:HG22	1.76	0.66
3:C:83:VAL:O	3:C:87:ALA:CB	2.43	0.66
1:D:200:LEU:HD13	1:D:234:TRP:CE3	2.30	0.66
2:E:549:GLY:O	2:E:551:TYR:N	2.28	0.66
3:F:171:VAL:O	3:F:175:GLU:HG3	1.95	0.66
2:B:202:ARG:HG3	2:B:500:ASP:OD1	1.94	0.66
1:G:78:LYS:HA	1:G:96:ALA:CB	2.25	0.66
1:A:200:LEU:HD13	1:A:234:TRP:CE3	2.30	0.66
2:B:476:ALA:O	2:B:480:GLN:HG2	1.95	0.66
1:D:38:VAL:O	1:D:39:GLU:HG3	1.95	0.66
2:H:491:LEU:HD11	2:H:507:ILE:HG23	1.75	0.66
3:C:24:ILE:HG22	3:C:24:ILE:O	1.94	0.66
2:E:418:ILE:H	2:E:418:ILE:HD13	1.59	0.66
2:H:442:THR:HG22	2:H:443:ASN:H	1.60	0.66
2:H:476:ALA:O	2:H:480:GLN:HG2	1.95	0.66
3:I:77:LEU:HD12	3:I:125:TRP:CH2	2.31	0.66
1:G:217:LEU:HD13	1:G:218:LEU:H	1.61	0.66
1:A:217:LEU:HD13	1:A:218:LEU:H	1.61	0.66
2:B:327:SER:O	2:B:329:ASP:N	2.29	0.66
2:B:416:ASP:O	2:B:420:VAL:HG23	1.95	0.66
2:B:178:GLU:HB2	2:B:480:GLN:OE1	1.95	0.66
2:H:202:ARG:HG3	2:H:500:ASP:OD1	1.95	0.66
2:H:347:GLY:O	2:H:349:SER:N	2.29	0.66
2:H:416:ASP:O	2:H:420:VAL:HG23	1.95	0.66
2:E:175:LEU:HD12	2:E:176:PRO:CD	2.26	0.66
2:E:327:SER:HA	3:F:238:LYS:HE3	1.76	0.66
3:F:34:ASP:HB3	3:F:35:PRO:CD	2.26	0.66
2:H:178:GLU:HB2	2:H:480:GLN:OE1	1.95	0.66
2:E:442:THR:HG22	2:E:443:ASN:H	1.61	0.66
1:G:38:VAL:O	1:G:39:GLU:HG3	1.95	0.66
2:H:155:THR:CG2	2:H:513:ARG:HG3	2.25	0.66
2:H:159:LEU:CD1	2:H:160:LEU:H	2.09	0.66
3:I:171:VAL:O	3:I:175:GLU:HG3	1.94	0.66
3:I:382:LYS:N	3:I:383:PRO:CD	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HD3	1:A:92:ILE:CD1	2.26	0.65
3:C:102:ARG:HD3	3:C:302:LEU:HD13	1.77	0.65
1:G:284:ASN:OD1	1:G:286:GLU:HB2	1.96	0.65
2:H:136:LYS:HE3	2:H:139:MET:SD	2.36	0.65
2:H:162:LYS:HE2	2:H:164:ILE:HD11	1.78	0.65
2:B:347:GLY:O	2:B:349:SER:N	2.29	0.65
2:E:314:LYS:HG3	3:F:162:LEU:HB3	1.78	0.65
2:E:347:GLY:O	2:E:349:SER:N	2.29	0.65
1:A:284:ASN:OD1	1:A:286:GLU:HB2	1.96	0.65
2:B:159:LEU:CD1	2:B:160:LEU:H	2.09	0.65
2:B:512:MET:O	2:B:514:GLU:N	2.29	0.65
1:D:78:LYS:HA	1:D:96:ALA:CB	2.25	0.65
1:D:57:TRP:HE1	2:E:142:ARG:HH21	1.43	0.65
2:E:178:GLU:HB2	2:E:480:GLN:OE1	1.95	0.65
1:G:229:ARG:HH12	1:G:252:LYS:CD	2.09	0.65
2:H:153:PHE:HA	2:H:159:LEU:HD22	1.77	0.65
3:I:34:ASP:HB3	3:I:35:PRO:CD	2.25	0.65
1:A:78:LYS:HA	1:A:96:ALA:CB	2.25	0.65
2:B:442:THR:HG22	2:B:443:ASN:H	1.61	0.65
2:E:476:ALA:O	2:E:480:GLN:HG2	1.95	0.65
1:A:38:VAL:O	1:A:39:GLU:HG3	1.95	0.65
1:G:20:TYR:HE2	2:H:544:LYS:HD3	1.62	0.65
1:D:284:ASN:OD1	1:D:286:GLU:HB2	1.96	0.65
1:G:265:SER:HB2	2:H:509:ARG:NH2	2.11	0.65
2:H:512:MET:O	2:H:514:GLU:N	2.29	0.65
3:C:11:ARG:HG2	3:C:12:PHE:CD1	2.32	0.65
1:D:49:LEU:HD13	1:D:82:TRP:CE3	2.32	0.65
2:E:159:LEU:CD1	2:E:160:LEU:H	2.09	0.65
2:H:175:LEU:HD12	2:H:176:PRO:CD	2.26	0.65
1:D:83:LYS:HD3	1:D:92:ILE:CD1	2.26	0.65
3:F:8:GLN:C	3:F:10:GLU:H	2.00	0.65
1:G:49:LEU:HD13	1:G:82:TRP:CE3	2.32	0.65
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.79	0.65
1:D:229:ARG:HH12	1:D:252:LYS:CD	2.09	0.65
2:E:512:MET:O	2:E:514:GLU:N	2.29	0.64
1:G:83:LYS:HD3	1:G:92:ILE:CD1	2.27	0.64
2:H:392:GLY:O	2:H:393:GLN:CB	2.45	0.64
1:A:229:ARG:HH12	1:A:252:LYS:CD	2.10	0.64
2:B:177:THR:HG21	2:B:484:ALA:HB2	1.79	0.64
2:B:392:GLY:O	2:B:393:GLN:CB	2.46	0.64
1:D:24:LEU:HD21	2:E:170:VAL:HG21	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:416:TYR:CE2	3:F:432:TYR:HE2	2.15	0.64
3:C:429:ILE:N	3:C:430:PRO:CD	2.60	0.64
2:E:327:SER:O	2:E:329:ASP:N	2.29	0.64
2:E:416:ASP:O	2:E:420:VAL:HG23	1.96	0.64
3:I:429:ILE:N	3:I:430:PRO:CD	2.59	0.64
3:I:58:ASP:HB3	3:I:61:ASN:OD1	1.97	0.64
1:D:217:LEU:HD22	1:D:218:LEU:N	2.12	0.64
1:D:57:TRP:CZ2	2:E:142:ARG:HG2	2.32	0.64
2:E:153:PHE:HA	2:E:159:LEU:HD22	1.77	0.64
2:E:320:VAL:CG2	3:F:246:THR:HG22	2.26	0.64
3:F:429:ILE:N	3:F:430:PRO:CD	2.60	0.64
2:E:392:GLY:O	2:E:393:GLN:CB	2.46	0.64
3:F:20:LYS:HE2	3:F:431:ILE:HD11	1.79	0.64
1:A:140:ILE:HG22	1:A:141:ILE:N	2.13	0.64
2:B:175:LEU:HD12	2:B:176:PRO:CD	2.26	0.64
2:H:259:LEU:HD11	3:I:99:TYR:CD1	2.33	0.64
3:C:77:LEU:O	3:C:77:LEU:HD23	1.98	0.64
1:D:140:ILE:HG22	1:D:141:ILE:N	2.13	0.64
3:F:437:ASN:O	3:F:440:ASP:CB	2.45	0.64
1:A:229:ARG:CB	1:A:229:ARG:HH11	2.09	0.64
2:B:221:LEU:HD22	2:B:231:TYR:CE1	2.32	0.64
1:D:208:ARG:NH2	2:E:143:ARG:HG3	2.12	0.64
3:F:431:ILE:H	3:F:431:ILE:CD1	2.11	0.64
3:I:431:ILE:N	3:I:431:ILE:HD12	2.13	0.64
1:A:49:LEU:HD13	1:A:82:TRP:CE3	2.32	0.64
2:E:162:LYS:HE2	2:E:164:ILE:HD11	1.78	0.64
1:G:140:ILE:HG22	1:G:141:ILE:N	2.13	0.64
2:H:252:ASN:OD1	2:H:253:ASP:N	2.31	0.64
2:H:320:VAL:HA	3:I:246:THR:CG2	2.23	0.64
1:A:144:HIS:HB2	1:A:148:VAL:HG22	1.80	0.64
1:A:17:LEU:HD21	2:B:160:LEU:HD11	1.79	0.64
3:C:431:ILE:N	3:C:431:ILE:HD12	2.13	0.64
3:I:8:GLN:HE22	3:I:53:LEU:CD2	2.11	0.64
1:D:126:SER:CB	1:D:140:ILE:HG13	2.20	0.63
1:D:286:GLU:HG2	2:E:440:GLN:OE1	1.97	0.63
2:H:327:SER:O	2:H:329:ASP:N	2.29	0.63
2:E:221:LEU:HD22	2:E:231:TYR:CE1	2.33	0.63
2:E:210:ILE:HD11	2:E:495:CYS:HB2	1.79	0.63
2:H:202:ARG:HG2	2:H:209:GLN:HE22	1.63	0.63
1:D:205:ASP:HB3	1:D:227:GLN:HB3	1.79	0.63
3:C:20:LYS:HG2	3:C:431:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:GLN:OE1	1:D:256:VAL:HG11	1.99	0.63
3:F:77:LEU:O	3:F:77:LEU:HD23	1.98	0.63
1:G:65:LYS:HA	2:H:546:ARG:HH21	1.64	0.63
3:I:62:VAL:HG12	3:I:66:LYS:HE3	1.80	0.63
2:E:252:ASN:OD1	2:E:253:ASP:N	2.31	0.63
1:G:105:VAL:O	1:G:105:VAL:HG13	1.99	0.63
1:G:205:ASP:HB3	1:G:227:GLN:HB3	1.79	0.63
3:I:431:ILE:CD1	3:I:431:ILE:H	2.11	0.63
3:C:62:VAL:HG12	3:C:66:LYS:HE3	1.80	0.63
2:E:521:SER:HB2	2:E:523:ASN:OD1	1.99	0.63
2:H:259:LEU:HD23	3:I:223:ILE:HD13	1.80	0.63
3:I:387:ARG:HH11	3:I:387:ARG:HB3	1.63	0.63
1:A:217:LEU:HD22	1:A:218:LEU:N	2.12	0.63
3:C:116:LEU:HD21	3:C:294:LEU:CD1	2.29	0.63
3:C:431:ILE:CD1	3:C:431:ILE:H	2.11	0.63
3:C:416:TYR:HE2	3:C:432:TYR:CE2	2.17	0.63
1:D:217:LEU:HD13	1:D:218:LEU:H	1.60	0.63
3:F:431:ILE:N	3:F:431:ILE:HD12	2.13	0.63
2:H:210:ILE:HD11	2:H:495:CYS:HB2	1.80	0.63
3:I:416:TYR:CE2	3:I:432:TYR:HE2	2.16	0.63
3:I:77:LEU:O	3:I:77:LEU:HD23	1.98	0.63
2:E:202:ARG:HG2	2:E:209:GLN:HE22	1.63	0.63
3:F:387:ARG:HH11	3:F:387:ARG:HB3	1.64	0.63
1:G:55:PRO:HB2	1:G:57:TRP:CZ3	2.34	0.63
2:H:221:LEU:HD22	2:H:231:TYR:CE1	2.33	0.63
2:H:521:SER:HB2	2:H:523:ASN:OD1	1.99	0.63
3:C:20:LYS:HE2	3:C:431:ILE:CD1	2.29	0.63
1:D:105:VAL:HG13	1:D:105:VAL:O	1.99	0.63
1:A:55:PRO:HB2	1:A:57:TRP:CZ3	2.34	0.62
1:A:73:CYS:HB2	1:A:102:VAL:HG12	1.81	0.62
3:C:387:ARG:HB3	3:C:387:ARG:HH11	1.63	0.62
3:F:102:ARG:HD2	3:F:217:GLU:OE2	1.99	0.62
1:G:73:CYS:HB2	1:G:102:VAL:HG12	1.81	0.62
1:G:227:GLN:OE1	1:G:256:VAL:HG11	1.99	0.62
2:B:252:ASN:OD1	2:B:253:ASP:N	2.31	0.62
1:D:55:PRO:HB2	1:D:57:TRP:CZ3	2.34	0.62
1:G:144:HIS:HB2	1:G:148:VAL:HG22	1.80	0.62
1:G:282:LYS:HE2	1:G:292:ALA:HB2	1.80	0.62
2:B:521:SER:HB2	2:B:523:ASN:OD1	1.99	0.62
1:G:217:LEU:HD22	1:G:218:LEU:N	2.12	0.62
1:G:278:VAL:HG21	2:H:151:ALA:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:PRO:CB	2:H:543:LEU:HD11	2.29	0.62
1:A:259:ARG:NH1	2:B:150:PHE:CB	2.60	0.62
3:C:70:LEU:HB3	3:C:343:ILE:CD1	2.30	0.62
1:D:217:LEU:CD2	1:D:218:LEU:H	2.13	0.62
3:F:62:VAL:HG12	3:F:66:LYS:HE3	1.80	0.62
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.80	0.62
3:F:116:LEU:HD21	3:F:294:LEU:CD1	2.29	0.62
1:G:229:ARG:HH11	1:G:229:ARG:CB	2.09	0.62
3:I:363:VAL:HG11	3:I:408:ASP:OD1	1.99	0.62
1:A:8:HIS:O	1:A:9:ASN:HB2	1.97	0.62
2:B:314:LYS:HG3	3:C:162:LEU:HB3	1.80	0.62
3:C:102:ARG:HD2	3:C:217:GLU:OE2	1.99	0.62
3:F:93:GLU:HG2	3:F:94:MET:H	1.65	0.62
3:I:10:GLU:O	3:I:13:THR:HB	1.99	0.62
3:I:426:TYR:HA	3:I:429:ILE:HG13	1.81	0.62
3:C:20:LYS:HE2	3:C:431:ILE:HG12	1.82	0.62
1:A:227:GLN:OE1	1:A:256:VAL:HG11	1.99	0.62
1:A:13:HIS:NE2	2:B:144:PHE:CE1	2.68	0.62
1:D:73:CYS:HB2	1:D:102:VAL:HG12	1.81	0.62
1:D:229:ARG:HH11	1:D:229:ARG:CB	2.09	0.62
1:A:217:LEU:CD2	1:A:218:LEU:H	2.13	0.62
1:A:282:LYS:HE2	1:A:292:ALA:HB2	1.80	0.62
3:C:426:TYR:HA	3:C:429:ILE:HG13	1.81	0.62
2:E:142:ARG:C	2:E:143:ARG:HG2	2.19	0.62
3:F:8:GLN:O	3:F:10:GLU:N	2.32	0.62
3:F:11:ARG:HB2	3:F:12:PHE:CD1	2.35	0.62
3:F:12:PHE:CD1	3:F:12:PHE:N	2.63	0.62
3:I:102:ARG:HD2	3:I:217:GLU:OE2	1.99	0.62
1:A:13:HIS:HE1	2:B:144:PHE:CE2	2.18	0.62
2:B:202:ARG:HG2	2:B:209:GLN:HE22	1.62	0.62
2:B:179:LEU:HD11	2:B:477:PHE:HE1	1.65	0.62
2:E:354:ILE:HD13	3:F:157:ASP:CG	2.20	0.62
3:I:79:GLU:O	3:I:83:VAL:HG23	2.00	0.62
1:D:144:HIS:HB2	1:D:148:VAL:HG22	1.80	0.61
3:F:426:TYR:HA	3:F:429:ILE:HG13	1.81	0.61
3:C:11:ARG:HG3	3:C:12:PHE:N	2.15	0.61
2:E:340:LEU:HD23	2:E:370:PHE:CD1	2.35	0.61
1:A:105:VAL:O	1:A:105:VAL:HG13	1.98	0.61
3:F:438:GLU:C	3:F:440:ASP:H	2.00	0.61
2:H:179:LEU:HD21	2:H:184:LEU:HD13	1.82	0.61
2:H:179:LEU:HD11	2:H:477:PHE:HE1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:116:LEU:HD21	3:I:294:LEU:CD1	2.30	0.61
2:B:267:ARG:HG3	2:B:267:ARG:NH1	2.15	0.61
3:C:34:ASP:HB3	3:C:35:PRO:CD	2.25	0.61
2:H:325:LEU:CD2	2:H:361:LEU:HD23	2.30	0.61
3:C:20:LYS:HZ3	3:C:428:ASN:CG	2.02	0.61
3:F:21:GLU:O	3:F:25:GLU:HG3	2.01	0.61
3:I:417:ILE:HG23	3:I:429:ILE:CG2	2.30	0.61
2:E:325:LEU:CD2	2:E:361:LEU:HD23	2.29	0.61
2:H:547:TYR:CE2	2:H:548:GLU:HG2	2.36	0.61
3:F:16:SER:HA	3:F:19:LEU:HD12	1.83	0.61
2:B:226:LYS:HA	2:B:231:TYR:CD2	2.36	0.61
3:C:79:GLU:O	3:C:83:VAL:HG23	2.00	0.61
1:G:227:GLN:HA	1:G:256:VAL:CG1	2.28	0.61
3:C:310:THR:HG23	3:C:311:ASP:N	2.15	0.61
2:H:226:LYS:HA	2:H:231:TYR:CD2	2.36	0.60
2:E:226:LYS:HA	2:E:231:TYR:CD2	2.36	0.60
1:G:19:TYR:O	2:H:155:THR:HG21	2.01	0.60
3:I:387:ARG:NH1	3:I:387:ARG:HB3	2.17	0.60
3:C:431:ILE:H	3:C:431:ILE:HD12	1.66	0.60
1:D:282:LYS:HE2	1:D:292:ALA:HB2	1.80	0.60
2:H:210:ILE:HD12	2:H:495:CYS:HB2	1.84	0.60
1:G:264:LEU:HD22	2:H:509:ARG:HD2	1.83	0.60
3:C:387:ARG:HB3	3:C:387:ARG:NH1	2.17	0.60
2:E:280:ILE:HG21	2:E:300:LEU:HG	1.83	0.60
1:G:282:LYS:CE	1:G:292:ALA:HB2	2.32	0.60
3:I:431:ILE:HD12	3:I:431:ILE:H	1.66	0.60
1:A:79:VAL:HG22	1:A:102:VAL:HG11	1.82	0.60
3:C:341:HIS:O	3:C:345:VAL:HG23	2.02	0.60
2:E:179:LEU:HD11	2:E:477:PHE:HE1	1.65	0.60
3:F:431:ILE:H	3:F:431:ILE:HD12	1.66	0.60
3:F:77:LEU:HD12	3:F:125:TRP:CH2	2.37	0.60
3:I:341:HIS:O	3:I:345:VAL:HG23	2.02	0.60
1:D:285:LEU:HD12	1:D:285:LEU:N	2.17	0.60
2:H:267:ARG:HG3	2:H:267:ARG:NH1	2.15	0.60
2:E:142:ARG:HH11	2:E:142:ARG:HG3	1.67	0.60
3:I:89:LEU:HD22	3:I:114:LYS:NZ	2.17	0.60
3:I:34:ASP:CB	3:I:35:PRO:HD3	2.29	0.60
1:A:146:ILE:O	1:A:146:ILE:HG22	2.02	0.60
1:D:140:ILE:H	1:D:140:ILE:HD12	1.67	0.60
3:F:341:HIS:O	3:F:345:VAL:HG23	2.02	0.60
3:F:79:GLU:O	3:F:83:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:LEU:CD2	1:G:218:LEU:H	2.13	0.60
2:B:314:LYS:HE3	3:C:162:LEU:HB3	1.84	0.60
1:D:282:LYS:CE	1:D:292:ALA:HB2	2.32	0.60
2:E:402:LEU:O	2:E:405:SER:HB3	2.02	0.60
1:G:79:VAL:HG22	1:G:102:VAL:HG11	1.82	0.60
1:A:140:ILE:H	1:A:140:ILE:HD12	1.67	0.59
1:A:285:LEU:N	1:A:285:LEU:HD12	2.17	0.59
1:A:264:LEU:HD12	2:B:155:THR:O	2.01	0.59
2:B:179:LEU:HD21	2:B:184:LEU:HD13	1.83	0.59
2:B:280:ILE:HG21	2:B:300:LEU:HG	1.84	0.59
3:C:34:ASP:CB	3:C:35:PRO:HD3	2.29	0.59
3:C:364:GLU:C	3:C:366:LEU:H	2.05	0.59
1:D:259:ARG:HD2	2:E:152:LYS:HE3	1.84	0.59
2:E:466:SER:HB2	2:E:469:THR:H	1.67	0.59
1:G:146:ILE:O	1:G:146:ILE:HG22	2.02	0.59
2:H:402:LEU:O	2:H:405:SER:HB3	2.02	0.59
3:I:70:LEU:HB3	3:I:343:ILE:CD1	2.32	0.59
1:A:227:GLN:HA	1:A:256:VAL:CG1	2.28	0.59
3:F:387:ARG:HB3	3:F:387:ARG:NH1	2.17	0.59
3:I:15:PHE:CD1	3:I:387:ARG:HD3	2.36	0.59
1:A:282:LYS:CE	1:A:292:ALA:HB2	2.32	0.59
1:D:79:VAL:HG22	1:D:102:VAL:HG11	1.83	0.59
1:A:259:ARG:HH11	2:B:150:PHE:HB2	1.61	0.59
3:C:349:SER:OG	3:C:358:VAL:HG21	2.02	0.59
2:E:179:LEU:HD21	2:E:184:LEU:HD13	1.83	0.59
3:I:11:ARG:HG3	3:I:12:PHE:CE1	2.37	0.59
1:D:57:TRP:HE1	2:E:142:ARG:CZ	2.14	0.59
3:C:417:ILE:HG23	3:C:429:ILE:HD13	1.84	0.59
3:F:438:GLU:C	3:F:440:ASP:N	2.54	0.59
3:I:349:SER:OG	3:I:358:VAL:HG21	2.02	0.59
2:B:466:SER:HB2	2:B:469:THR:H	1.67	0.59
3:C:319:SER:OG	2:E:337:GLU:HG2	2.03	0.59
1:D:227:GLN:NE2	2:E:143:ARG:HH12	2.01	0.59
2:B:402:LEU:O	2:B:405:SER:HB3	2.02	0.59
1:D:146:ILE:HG22	1:D:146:ILE:O	2.02	0.59
1:D:212:TRP:CG	1:D:222:LEU:HD21	2.37	0.59
2:E:210:ILE:HD12	2:E:495:CYS:HB2	1.84	0.59
1:D:15:ALA:HB2	1:D:26:THR:HG22	1.84	0.59
2:H:138:ILE:HA	2:H:141:GLU:HG2	1.84	0.59
2:H:466:SER:HB2	2:H:469:THR:H	1.67	0.59
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TRP:CG	1:A:222:LEU:HD21	2.38	0.59
1:A:63:HIS:CD2	1:A:65:LYS:HB2	2.36	0.59
3:C:11:ARG:O	3:C:13:THR:N	2.36	0.59
1:D:200:LEU:HD11	1:D:243:TRP:CD1	2.38	0.58
3:F:349:SER:OG	3:F:358:VAL:HG21	2.02	0.58
1:D:17:LEU:HD12	2:E:154:SER:CA	2.32	0.58
1:A:272:SER:OG	2:B:151:ALA:HB3	2.03	0.58
2:H:304:VAL:HG13	3:I:314:ILE:HD11	1.83	0.58
2:H:177:THR:HG21	2:H:484:ALA:HB2	1.85	0.58
3:I:406:GLU:HG2	3:I:409:LYS:NZ	2.18	0.58
3:C:11:ARG:C	3:C:13:THR:N	2.55	0.58
2:E:515:ILE:HD13	2:E:540:ALA:C	2.23	0.58
3:F:366:LEU:HB2	3:F:379:ILE:HG21	1.85	0.58
1:G:15:ALA:HB2	1:G:26:THR:HG22	1.84	0.58
2:H:280:ILE:HG21	2:H:300:LEU:HG	1.84	0.58
3:C:406:GLU:HG2	3:C:409:LYS:NZ	2.18	0.58
2:E:269:THR:O	2:E:273:VAL:HG23	2.04	0.58
1:G:157:THR:HG21	2:H:501:LYS:NZ	2.19	0.58
1:G:200:LEU:HD11	1:G:243:TRP:CD1	2.38	0.58
1:A:20:TYR:HD2	2:B:544:LYS:NZ	2.01	0.58
1:A:15:ALA:HB2	1:A:26:THR:HG22	1.84	0.58
2:B:515:ILE:HD13	2:B:540:ALA:C	2.23	0.58
3:F:359:ILE:HG21	3:F:404:VAL:HG11	1.85	0.58
2:H:285:ARG:HG3	2:H:285:ARG:HH11	1.68	0.58
1:A:37:GLU:HG2	1:A:46:ILE:HD12	1.86	0.58
2:B:269:THR:O	2:B:273:VAL:HG23	2.04	0.58
1:D:9:ASN:H	1:D:9:ASN:HD22	1.52	0.58
1:G:140:ILE:H	1:G:140:ILE:HD12	1.67	0.58
2:H:515:ILE:HD13	2:H:540:ALA:C	2.24	0.58
3:I:8:GLN:CD	3:I:53:LEU:HG	2.22	0.58
1:A:258:TRP:NE1	2:B:148:TYR:HA	2.18	0.58
2:B:213:SER:HB3	2:B:459:PHE:CG	2.39	0.58
2:B:250:THR:HG21	2:B:255:VAL:HB	1.86	0.58
2:E:425:TYR:O	2:E:463:ARG:NH2	2.37	0.58
1:G:212:TRP:CG	1:G:222:LEU:HD21	2.38	0.58
1:A:12:ILE:CD1	2:B:168:SER:O	2.52	0.57
2:B:285:ARG:HG3	2:B:285:ARG:HH11	1.68	0.57
2:E:285:ARG:HH11	2:E:285:ARG:HG3	1.69	0.57
1:G:285:LEU:HD12	1:G:285:LEU:N	2.17	0.57
2:H:340:LEU:CD2	2:H:370:PHE:CG	2.87	0.57
1:D:181:LEU:HD22	1:D:199:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:HIS:CD2	2:E:168:SER:HB3	2.39	0.57
3:F:34:ASP:CB	3:F:35:PRO:HD3	2.30	0.57
3:F:91:LEU:CG	3:F:92:ASP:H	2.17	0.57
2:H:250:THR:HG21	2:H:255:VAL:HB	1.86	0.57
2:H:425:TYR:O	2:H:463:ARG:NH2	2.38	0.57
1:D:37:GLU:HG2	1:D:46:ILE:HD12	1.86	0.57
2:E:267:ARG:HG3	2:E:267:ARG:NH1	2.15	0.57
3:F:406:GLU:HG2	3:F:409:LYS:NZ	2.18	0.57
2:H:259:LEU:CD2	3:I:223:ILE:HD13	2.34	0.57
1:A:181:LEU:HD22	1:A:199:THR:CG2	2.35	0.57
2:H:291:ILE:CD1	2:H:291:ILE:H	2.16	0.57
1:A:13:HIS:CE1	2:B:144:PHE:CE2	2.90	0.57
1:A:153:TRP:HH2	1:A:194:TYR:HH	1.52	0.57
2:B:198:THR:CB	2:B:212:GLU:HB2	2.29	0.57
2:H:213:SER:HB3	2:H:459:PHE:CG	2.39	0.57
3:I:94:MET:HE3	3:I:96:LEU:HD21	1.85	0.57
2:B:165:VAL:CG1	2:B:165:VAL:O	2.52	0.57
1:A:20:TYR:CE2	2:B:544:LYS:CD	2.84	0.57
1:D:73:CYS:HB2	1:D:102:VAL:CG1	2.35	0.57
2:B:202:ARG:CG	2:B:209:GLN:NE2	2.60	0.57
2:B:210:ILE:HD12	2:B:495:CYS:HB2	1.84	0.57
2:B:425:TYR:O	2:B:463:ARG:NH2	2.37	0.57
3:C:22:PHE:C	3:C:24:ILE:H	2.08	0.57
3:I:418:SER:O	3:I:422:LEU:HG	2.03	0.57
2:E:133:ASP:O	2:E:137:LEU:HG	2.05	0.57
1:D:181:LEU:HD22	1:D:199:THR:CG2	2.35	0.57
2:H:202:ARG:CG	2:H:209:GLN:NE2	2.60	0.57
2:H:269:THR:O	2:H:273:VAL:HG23	2.04	0.57
1:A:73:CYS:HB2	1:A:102:VAL:CG1	2.35	0.57
1:A:16:VAL:HG21	1:A:59:VAL:O	2.05	0.57
2:B:160:LEU:HA	2:B:171:SER:O	2.05	0.57
2:E:205:ASN:OD1	2:E:207:TYR:HB2	2.05	0.57
2:E:213:SER:HB3	2:E:459:PHE:CG	2.40	0.57
3:F:50:ALA:HB1	3:F:69:GLU:HG2	1.86	0.57
1:G:227:GLN:O	1:G:256:VAL:HG22	2.05	0.57
1:D:112:TYR:HA	1:D:171:ARG:NH2	2.19	0.56
2:E:198:THR:CB	2:E:212:GLU:HB2	2.29	0.56
3:F:116:LEU:CD2	3:F:294:LEU:HD11	2.35	0.56
3:I:160:PHE:CE2	3:I:168:VAL:HG11	2.40	0.56
1:D:227:GLN:O	1:D:256:VAL:HG22	2.05	0.56
3:I:416:TYR:HE2	3:I:432:TYR:HE2	1.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:VAL:HG21	1:D:59:VAL:O	2.05	0.56
2:H:369:LEU:O	2:H:370:PHE:HB2	2.05	0.56
1:A:141:ILE:HD12	1:A:185:TRP:CE3	2.40	0.56
3:F:379:ILE:HG13	3:F:385:LEU:HG	1.87	0.56
1:A:96:ALA:C	1:A:98:HIS:H	2.09	0.56
3:C:116:LEU:CD2	3:C:294:LEU:HD11	2.35	0.56
1:D:10:GLU:O	1:D:11:LEU:CG	2.54	0.56
2:E:358:TYR:HE2	3:F:210:MET:HE1	1.70	0.56
3:F:326:GLU:O	3:F:330:ARG:HG3	2.06	0.56
1:G:181:LEU:HD22	1:G:199:THR:HG22	1.86	0.56
2:H:340:LEU:HD22	2:H:370:PHE:CG	2.40	0.56
2:H:320:VAL:CG2	3:I:246:THR:HG22	2.35	0.56
1:A:227:GLN:O	1:A:256:VAL:HG22	2.05	0.56
1:A:261:SER:CB	2:B:152:LYS:HG2	2.32	0.56
1:D:227:GLN:HA	1:D:256:VAL:CG1	2.28	0.56
2:E:325:LEU:HD23	2:E:361:LEU:HD23	1.88	0.56
1:G:37:GLU:HG2	1:G:46:ILE:HD12	1.86	0.56
1:G:16:VAL:HG21	1:G:59:VAL:O	2.05	0.56
1:G:96:ALA:C	1:G:98:HIS:H	2.09	0.56
2:H:138:ILE:HA	2:H:141:GLU:CG	2.35	0.56
2:B:512:MET:C	2:B:514:GLU:H	2.09	0.56
2:E:324:TYR:CE2	3:F:237:ILE:HG21	2.39	0.56
1:G:181:LEU:HD22	1:G:199:THR:CG2	2.35	0.56
1:G:20:TYR:CE2	2:H:544:LYS:HA	2.41	0.56
3:I:70:LEU:HB3	3:I:343:ILE:HD11	1.87	0.56
1:A:181:LEU:HD22	1:A:199:THR:HG22	1.87	0.56
2:B:205:ASN:OD1	2:B:207:TYR:HB2	2.05	0.56
2:B:291:ILE:CD1	2:B:291:ILE:H	2.16	0.56
3:C:387:ARG:HG2	3:C:391:HIS:CE1	2.41	0.56
3:F:160:PHE:CE2	3:F:168:VAL:HG11	2.40	0.56
3:F:387:ARG:HG2	3:F:391:HIS:CE1	2.41	0.56
3:F:441:CYS:O	3:F:442:LEU:HG	2.06	0.56
1:G:237:ASP:OD1	1:G:244:LYS:HE3	2.06	0.56
2:H:205:ASN:OD1	2:H:207:TYR:HB2	2.05	0.56
1:A:12:ILE:CD1	2:B:169:GLY:HA3	2.35	0.56
3:F:23:LYS:O	3:F:26:GLN:HB2	2.06	0.56
2:H:512:MET:C	2:H:514:GLU:H	2.09	0.56
1:A:13:HIS:ND1	2:B:148:TYR:CE2	2.74	0.56
3:C:160:PHE:CE2	3:C:168:VAL:HG11	2.40	0.56
3:C:326:GLU:O	3:C:330:ARG:HG3	2.06	0.56
3:C:50:ALA:HB1	3:C:69:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:LYS:HE3	2:E:164:ILE:HD11	1.88	0.56
1:G:233:ILE:HD11	1:G:248:LEU:HD13	1.88	0.56
3:I:116:LEU:CD2	3:I:294:LEU:HD11	2.35	0.56
2:E:202:ARG:NE	2:E:202:ARG:HA	2.21	0.55
2:E:250:THR:HG21	2:E:255:VAL:HB	1.86	0.55
2:H:325:LEU:HD23	2:H:361:LEU:HD23	1.89	0.55
1:D:138:PRO:HB2	1:D:140:ILE:CD1	2.37	0.55
1:D:221:TYR:O	1:D:222:LEU:HD23	2.06	0.55
1:D:209:ASP:OD1	1:D:259:ARG:HD3	2.06	0.55
2:E:202:ARG:CG	2:E:209:GLN:NE2	2.61	0.55
2:E:512:MET:C	2:E:514:GLU:H	2.09	0.55
1:G:221:TYR:O	1:G:222:LEU:HD23	2.06	0.55
1:G:209:ASP:OD1	1:G:259:ARG:HD3	2.06	0.55
3:I:326:GLU:O	3:I:330:ARG:HG3	2.07	0.55
3:I:387:ARG:HG2	3:I:391:HIS:CE1	2.41	0.55
3:C:11:ARG:C	3:C:13:THR:H	2.09	0.55
1:D:19:TYR:O	2:E:155:THR:HG21	2.06	0.55
1:D:9:ASN:ND2	1:D:9:ASN:N	2.54	0.55
3:F:94:MET:CE	3:F:108:LYS:HB2	2.35	0.55
1:G:109:PRO:HD2	1:G:112:TYR:CD1	2.42	0.55
1:G:105:VAL:HA	1:G:117:LEU:O	2.07	0.55
2:H:160:LEU:HA	2:H:171:SER:O	2.05	0.55
1:G:73:CYS:HB2	1:G:102:VAL:CG1	2.35	0.55
3:I:110:MET:SD	3:I:116:LEU:HD22	2.47	0.55
2:E:160:LEU:HA	2:E:171:SER:O	2.05	0.55
2:H:162:LYS:HE3	2:H:164:ILE:HD11	1.88	0.55
1:A:109:PRO:HD2	1:A:112:TYR:CD1	2.42	0.55
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.72	0.55
1:A:127:VAL:HG21	1:A:194:TYR:CE1	2.41	0.55
2:B:155:THR:HG22	2:B:513:ARG:CD	2.37	0.55
2:B:207:TYR:HE2	2:B:536:LEU:HD22	1.72	0.55
2:B:320:VAL:CA	3:C:246:THR:HG21	2.35	0.55
1:D:96:ALA:C	1:D:98:HIS:H	2.09	0.55
1:G:10:GLU:O	1:G:11:LEU:CG	2.54	0.55
1:D:139:ILE:HG22	1:D:139:ILE:O	2.07	0.55
1:D:57:TRP:NE1	2:E:142:ARG:CZ	2.70	0.55
2:E:303:VAL:HG13	2:E:322:ILE:HG22	1.89	0.55
2:E:369:LEU:O	2:E:370:PHE:HB2	2.07	0.55
3:F:16:SER:O	3:F:19:LEU:HB2	2.07	0.55
1:A:112:TYR:HA	1:A:171:ARG:NH2	2.22	0.55
1:A:237:ASP:OD1	1:A:244:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASP:OD1	1:A:259:ARG:HD3	2.06	0.55
2:B:150:PHE:CE2	2:B:162:LYS:HB2	2.41	0.55
2:E:291:ILE:CD1	2:E:291:ILE:H	2.17	0.55
3:F:143:LYS:HE3	3:F:144:TRP:NE1	2.22	0.55
1:G:138:PRO:HB2	1:G:140:ILE:CD1	2.37	0.55
2:H:207:TYR:HE2	2:H:536:LEU:HD22	1.72	0.55
3:I:143:LYS:HE3	3:I:144:TRP:NE1	2.22	0.55
3:I:8:GLN:C	3:I:10:GLU:N	2.53	0.55
1:A:139:ILE:O	1:A:139:ILE:HG22	2.07	0.55
1:D:109:PRO:HD2	1:D:112:TYR:CD1	2.42	0.55
1:D:105:VAL:HA	1:D:117:LEU:O	2.07	0.55
2:E:339:GLN:HB2	3:F:206:ILE:HG21	1.89	0.55
3:I:7:TYR:HB3	3:I:10:GLU:OE1	2.06	0.55
1:A:138:PRO:HB2	1:A:140:ILE:CD1	2.37	0.55
1:A:233:ILE:HD11	1:A:248:LEU:HD13	1.88	0.55
2:B:202:ARG:NE	2:B:202:ARG:HA	2.21	0.55
2:B:303:VAL:HG13	2:B:322:ILE:HG22	1.89	0.55
3:C:110:MET:SD	3:C:116:LEU:HD22	2.47	0.55
3:C:184:ILE:O	3:C:188:ILE:HG13	2.07	0.55
1:D:117:LEU:HB2	1:D:153:TRP:HE1	1.72	0.55
1:D:19:TYR:CD2	1:D:20:TYR:CE1	2.88	0.55
1:D:237:ASP:OD1	1:D:244:LYS:HE3	2.06	0.55
3:F:16:SER:HA	3:F:19:LEU:CD1	2.36	0.55
1:A:221:TYR:O	1:A:222:LEU:HD23	2.06	0.54
2:E:207:TYR:HE2	2:E:536:LEU:HD22	1.72	0.54
3:F:20:LYS:O	3:F:23:LYS:N	2.40	0.54
1:G:19:TYR:CD2	1:G:20:TYR:CE1	2.89	0.54
2:H:202:ARG:HA	2:H:202:ARG:NE	2.21	0.54
2:H:474:THR:HG21	2:H:497:LEU:HD12	1.89	0.54
1:G:217:LEU:HG	2:H:475:PHE:CE1	2.42	0.54
3:I:89:LEU:CD1	3:I:114:LYS:HZ3	2.13	0.54
1:G:140:ILE:HD12	1:G:140:ILE:N	2.23	0.54
3:I:206:ILE:O	3:I:209:CYS:HB3	2.08	0.54
1:G:117:LEU:HB2	1:G:153:TRP:HE1	1.72	0.54
3:I:184:ILE:O	3:I:188:ILE:HG13	2.08	0.54
3:C:143:LYS:HE3	3:C:144:TRP:NE1	2.22	0.54
3:C:206:ILE:O	3:C:209:CYS:HB3	2.07	0.54
1:D:233:ILE:HD11	1:D:248:LEU:HD13	1.88	0.54
3:F:110:MET:SD	3:F:116:LEU:HD22	2.47	0.54
1:G:279:THR:CB	1:G:281:TRP:HE1	2.21	0.54
3:I:421:LYS:C	3:I:423:GLN:H	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:LEU:HB3	2:B:231:TYR:HE1	1.73	0.54
2:E:342:LYS:HD2	3:F:206:ILE:HD11	1.90	0.54
3:F:416:TYR:CD2	3:F:432:TYR:CE2	2.95	0.54
2:H:303:VAL:HG13	2:H:322:ILE:HG22	1.89	0.54
1:A:105:VAL:HA	1:A:117:LEU:O	2.07	0.54
1:A:140:ILE:N	1:A:140:ILE:HD12	2.23	0.54
2:B:484:ALA:O	2:B:485:GLN:HB2	2.08	0.54
1:G:139:ILE:O	1:G:139:ILE:HG22	2.07	0.54
1:G:153:TRP:HH2	1:G:194:TYR:HH	1.56	0.54
1:D:279:THR:HB	1:D:281:TRP:HE1	1.73	0.54
2:E:509:ARG:HH11	2:E:509:ARG:HG2	1.72	0.54
1:G:109:PRO:HD2	1:G:112:TYR:CE1	2.43	0.54
1:G:31:LYS:HG2	1:G:54:GLY:O	2.08	0.54
3:I:70:LEU:HD11	3:I:344:ARG:NH2	2.23	0.54
1:D:140:ILE:N	1:D:140:ILE:HD12	2.23	0.54
1:D:279:THR:CB	1:D:281:TRP:HE1	2.21	0.54
1:D:9:ASN:N	1:D:9:ASN:HD22	2.05	0.54
3:F:23:LYS:HA	3:F:26:GLN:OE1	2.07	0.54
1:G:247:LEU:O	1:G:248:LEU:C	2.46	0.54
2:H:509:ARG:HH11	2:H:509:ARG:HG2	1.72	0.54
3:I:160:PHE:HE2	3:I:168:VAL:HG11	1.73	0.54
1:A:279:THR:HB	1:A:281:TRP:HE1	1.73	0.54
2:B:474:THR:HG21	2:B:497:LEU:HD12	1.90	0.54
3:C:384:TYR:CD1	3:C:385:LEU:N	2.76	0.54
1:D:138:PRO:C	1:D:139:ILE:HD12	2.29	0.54
1:A:31:LYS:HG2	1:A:54:GLY:O	2.08	0.53
2:B:233:LEU:HD21	2:B:421:ILE:HD11	1.90	0.53
2:E:546:ARG:HB2	2:E:551:TYR:CE1	2.42	0.53
2:H:233:LEU:HD21	2:H:421:ILE:HD11	1.90	0.53
3:C:227:ILE:C	3:C:229:ASN:N	2.61	0.53
1:D:95:HIS:CE1	1:D:97:VAL:HG22	2.43	0.53
3:F:227:ILE:C	3:F:229:ASN:N	2.61	0.53
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.38	0.53
2:B:145:THR:HG22	2:B:147:SER:H	1.72	0.53
2:B:442:THR:CG2	2:B:443:ASN:N	2.72	0.53
2:B:449:PHE:CE2	2:B:453:LEU:HD12	2.43	0.53
1:D:109:PRO:HD2	1:D:112:TYR:CE1	2.43	0.53
1:G:138:PRO:C	1:G:139:ILE:HD12	2.29	0.53
1:G:225:VAL:HG21	1:G:271:LEU:HD22	1.91	0.53
1:G:95:HIS:CE1	1:G:97:VAL:HG22	2.43	0.53
2:H:207:TYR:CE2	2:H:536:LEU:HD22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:102:ARG:NH2	3:I:241:SER:H	2.06	0.53
1:A:247:LEU:O	1:A:248:LEU:C	2.46	0.53
1:D:262:TRP:CZ3	1:D:269:LEU:HB2	2.44	0.53
1:D:31:LYS:HG2	1:D:54:GLY:O	2.08	0.53
2:E:150:PHE:CE2	2:E:162:LYS:HB2	2.44	0.53
2:E:207:TYR:CE2	2:E:536:LEU:HD22	2.43	0.53
2:E:484:ALA:O	2:E:485:GLN:HB2	2.09	0.53
3:F:160:PHE:HE2	3:F:168:VAL:HG11	1.74	0.53
3:F:184:ILE:O	3:F:188:ILE:HG13	2.08	0.53
3:I:148:ILE:CD1	3:I:153:LEU:HD12	2.39	0.53
1:A:138:PRO:C	1:A:139:ILE:HD12	2.29	0.53
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.43	0.53
1:A:103:ASN:HD21	2:B:142:ARG:HH22	1.57	0.53
3:C:77:LEU:CD2	3:C:81:LEU:HD12	2.39	0.53
1:G:112:TYR:HA	1:G:171:ARG:NH2	2.23	0.53
2:H:449:PHE:CE2	2:H:453:LEU:HD12	2.43	0.53
2:H:515:ILE:CD1	2:H:544:LYS:HB2	2.38	0.53
3:I:77:LEU:CD2	3:I:81:LEU:HD12	2.39	0.53
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.91	0.53
2:E:221:LEU:HB3	2:E:231:TYR:HE1	1.73	0.53
2:E:474:THR:HG21	2:E:497:LEU:HD12	1.90	0.53
3:F:384:TYR:CD1	3:F:385:LEU:N	2.76	0.53
1:G:225:VAL:CG2	1:G:271:LEU:HD22	2.38	0.53
3:I:23:LYS:HA	3:I:27:ASN:OD1	2.09	0.53
3:C:148:ILE:CD1	3:C:153:LEU:HD12	2.39	0.53
3:C:160:PHE:HE2	3:C:168:VAL:HG11	1.73	0.53
1:D:225:VAL:CG2	1:D:271:LEU:HD22	2.38	0.53
3:F:117:TYR:O	3:F:120:TRP:HB3	2.09	0.53
3:F:70:LEU:HB3	3:F:343:ILE:CD1	2.38	0.53
3:F:83:VAL:O	3:F:87:ALA:HB3	2.09	0.53
2:H:538:PHE:C	2:H:538:PHE:CD1	2.82	0.53
3:I:227:ILE:C	3:I:229:ASN:N	2.61	0.53
1:A:225:VAL:HG21	1:A:271:LEU:HD22	1.91	0.53
1:A:279:THR:CB	1:A:281:TRP:HE1	2.21	0.53
2:B:509:ARG:HH11	2:B:509:ARG:HG2	1.72	0.53
3:C:35:PRO:HB2	3:C:399:ILE:HG12	1.90	0.53
1:G:262:TRP:CZ3	1:G:269:LEU:HB2	2.44	0.53
2:H:221:LEU:HB3	2:H:231:TYR:HE1	1.73	0.53
2:H:297:TYR:CE2	2:H:305:ARG:HD2	2.44	0.53
1:A:262:TRP:CZ3	1:A:269:LEU:HB2	2.44	0.53
1:A:265:SER:O	2:B:483:PHE:CE2	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:MET:HB3	3:C:379:ILE:CG2	2.39	0.53
1:D:181:LEU:HD23	1:D:201:GLU:HG2	1.91	0.53
2:E:515:ILE:CD1	2:E:544:LYS:HB2	2.39	0.53
3:F:77:LEU:CD2	3:F:81:LEU:HD12	2.38	0.53
2:H:484:ALA:O	2:H:485:GLN:HB2	2.08	0.53
1:A:121:SER:O	1:A:147:GLY:HA2	2.09	0.53
1:A:261:SER:HB2	2:B:152:LYS:CG	2.33	0.53
2:B:138:ILE:O	2:B:141:GLU:HG2	2.09	0.53
2:B:538:PHE:CD1	2:B:538:PHE:C	2.82	0.53
3:C:102:ARG:NH2	3:C:241:SER:H	2.06	0.53
1:D:225:VAL:HG13	1:D:257:LEU:CB	2.39	0.53
1:D:225:VAL:HG21	1:D:271:LEU:HD22	1.91	0.53
1:D:27:CYS:HB2	1:D:56:VAL:HB	1.91	0.53
2:E:538:PHE:CD1	2:E:538:PHE:C	2.82	0.53
3:F:86:ASN:C	3:F:88:ASP:H	2.13	0.53
2:H:415:ASP:HA	2:H:442:THR:HG21	1.91	0.53
1:A:191:ALA:C	1:A:193:THR:H	2.13	0.52
1:D:217:LEU:CD1	1:D:218:LEU:H	2.22	0.52
2:E:297:TYR:CE2	2:E:305:ARG:HD2	2.44	0.52
2:E:415:ASP:HA	2:E:442:THR:HG21	1.91	0.52
2:E:442:THR:CG2	2:E:443:ASN:N	2.72	0.52
3:F:102:ARG:NH2	3:F:241:SER:H	2.07	0.52
3:F:428:ASN:C	3:F:430:PRO:HD2	2.29	0.52
3:I:86:ASN:ND2	3:I:86:ASN:O	2.42	0.52
2:B:207:TYR:CE2	2:B:536:LEU:HD22	2.43	0.52
1:D:191:ALA:C	1:D:193:THR:H	2.13	0.52
2:E:233:LEU:HD21	2:E:421:ILE:HD11	1.90	0.52
2:E:551:TYR:CD2	2:E:552:LEU:HG	2.44	0.52
3:F:206:ILE:O	3:F:209:CYS:HB3	2.07	0.52
1:G:181:LEU:HD23	1:G:201:GLU:HG2	1.91	0.52
1:G:29:SER:C	1:G:31:LYS:H	2.13	0.52
3:I:160:PHE:HB3	3:I:161:PRO:HD3	1.92	0.52
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.92	0.52
3:C:416:TYR:CE2	3:C:432:TYR:CE2	2.98	0.52
1:D:29:SER:C	1:D:31:LYS:H	2.13	0.52
1:D:9:ASN:OD1	1:D:12:ILE:HD11	2.10	0.52
2:H:442:THR:CG2	2:H:443:ASN:N	2.72	0.52
3:I:117:TYR:O	3:I:120:TRP:HB3	2.10	0.52
2:H:335:LEU:HD12	3:I:206:ILE:HG23	1.92	0.52
3:I:243:TRP:O	3:I:247:VAL:HG23	2.09	0.52
3:C:117:TYR:O	3:C:120:TRP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:LYS:NZ	3:C:428:ASN:CG	2.62	0.52
3:C:431:ILE:CD1	3:C:431:ILE:N	2.72	0.52
2:E:449:PHE:CE2	2:E:453:LEU:HD12	2.44	0.52
2:H:150:PHE:CE2	2:H:162:LYS:HB2	2.44	0.52
1:A:29:SER:C	1:A:31:LYS:H	2.13	0.52
3:C:143:LYS:HG3	3:C:144:TRP:N	2.25	0.52
3:C:342:PRO:HG2	3:C:382:LYS:CD	2.39	0.52
1:D:40:GLY:O	2:E:172:ILE:HD13	2.09	0.52
2:E:448:GLN:HG3	2:E:477:PHE:CZ	2.45	0.52
1:G:191:ALA:C	1:G:193:THR:H	2.13	0.52
3:C:20:LYS:HE2	3:C:431:ILE:CG1	2.39	0.52
3:C:428:ASN:C	3:C:430:PRO:HD2	2.30	0.52
1:D:259:ARG:HB2	1:D:272:SER:HB2	1.91	0.52
2:E:320:VAL:HA	3:F:246:THR:CG2	2.34	0.52
1:A:109:PRO:HD2	1:A:112:TYR:CE1	2.43	0.52
2:B:369:LEU:O	2:B:370:PHE:HB2	2.10	0.52
2:B:415:ASP:HA	2:B:442:THR:HG21	1.91	0.52
2:B:551:TYR:CD2	2:B:552:LEU:HG	2.44	0.52
1:D:121:SER:O	1:D:147:GLY:HA2	2.09	0.52
1:D:247:LEU:O	1:D:248:LEU:C	2.46	0.52
2:B:515:ILE:CD1	2:B:544:LYS:HB2	2.39	0.52
1:D:118:VAL:O	1:D:125:VAL:HA	2.10	0.52
2:E:142:ARG:HB3	2:E:144:PHE:CD1	2.44	0.52
2:E:442:THR:HG22	2:E:444:ALA:N	2.21	0.52
3:F:148:ILE:CD1	3:F:153:LEU:HD12	2.39	0.52
2:H:527:LEU:HA	2:H:530:LEU:HD13	1.92	0.52
1:A:118:VAL:O	1:A:125:VAL:HA	2.10	0.52
2:B:442:THR:HG22	2:B:444:ALA:N	2.21	0.52
2:B:525:HIS:C	2:B:527:LEU:N	2.62	0.52
3:C:77:LEU:HD12	3:C:125:TRP:CH2	2.45	0.52
2:H:448:GLN:HG3	2:H:477:PHE:CZ	2.45	0.52
2:B:297:TYR:CE2	2:B:305:ARG:HD2	2.44	0.52
2:B:327:SER:C	2:B:329:ASP:H	2.13	0.52
2:B:448:GLN:HG3	2:B:477:PHE:CZ	2.45	0.52
3:C:243:TRP:O	3:C:247:VAL:HG23	2.10	0.52
1:D:283:GLU:HB2	1:D:289:TRP:CZ3	2.45	0.52
3:F:243:TRP:O	3:F:247:VAL:HG23	2.09	0.52
3:I:35:PRO:HB2	3:I:399:ILE:HG12	1.92	0.52
1:A:19:TYR:CD2	1:A:20:TYR:CE1	2.88	0.51
1:G:121:SER:O	1:G:147:GLY:HA2	2.10	0.51
1:G:279:THR:HB	1:G:281:TRP:HE1	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:CYS:HB2	1:G:56:VAL:HB	1.91	0.51
2:H:442:THR:HG22	2:H:444:ALA:N	2.21	0.51
3:I:77:LEU:HB2	3:I:125:TRP:CE2	2.45	0.51
1:A:24:LEU:HD21	2:B:170:VAL:CG2	2.38	0.51
1:A:283:GLU:HB2	1:A:289:TRP:CZ3	2.46	0.51
2:B:289:ASN:O	2:B:293:GLN:HG3	2.11	0.51
3:C:20:LYS:CG	3:C:431:ILE:HG12	2.39	0.51
3:C:70:LEU:HB3	3:C:343:ILE:HD11	1.91	0.51
2:E:320:VAL:HG22	3:F:246:THR:CG2	2.38	0.51
3:I:428:ASN:C	3:I:430:PRO:HD2	2.30	0.51
1:A:15:ALA:CB	2:B:170:VAL:HG11	2.41	0.51
3:C:363:VAL:HG11	3:C:408:ASP:OD1	2.09	0.51
1:G:217:LEU:CD1	1:G:218:LEU:H	2.22	0.51
1:G:268:VAL:HG12	1:G:269:LEU:N	2.25	0.51
1:G:62:ALA:HB2	1:G:107:TRP:CE2	2.45	0.51
3:I:166:THR:O	3:I:166:THR:HG22	2.10	0.51
3:I:384:TYR:CD1	3:I:385:LEU:N	2.78	0.51
1:A:151:ALA:HB2	1:A:175:THR:HG22	1.91	0.51
2:B:511:VAL:HG21	2:B:536:LEU:HD21	1.93	0.51
3:C:160:PHE:HB3	3:C:161:PRO:HD3	1.92	0.51
2:E:152:LYS:O	2:E:159:LEU:HD13	2.11	0.51
2:E:225:GLU:C	2:E:227:THR:H	2.14	0.51
1:D:217:LEU:HG	2:E:475:PHE:CE1	2.45	0.51
2:E:358:TYR:HE2	3:F:210:MET:CE	2.24	0.51
1:G:57:TRP:HE1	2:H:142:ARG:NH2	2.07	0.51
2:H:141:GLU:HG3	2:H:142:ARG:N	2.26	0.51
1:A:103:ASN:HD21	2:B:142:ARG:NH2	2.08	0.51
1:A:229:ARG:HD2	1:A:253:PHE:O	2.11	0.51
2:B:152:LYS:N	2:B:159:LEU:HD11	2.26	0.51
1:D:229:ARG:HD2	1:D:253:PHE:O	2.11	0.51
1:D:268:VAL:HG12	1:D:269:LEU:N	2.25	0.51
3:F:143:LYS:HG3	3:F:144:TRP:N	2.25	0.51
3:F:160:PHE:HB3	3:F:161:PRO:HD3	1.93	0.51
1:G:118:VAL:O	1:G:125:VAL:HA	2.10	0.51
1:G:225:VAL:HG13	1:G:257:LEU:CB	2.39	0.51
2:H:525:HIS:C	2:H:527:LEU:N	2.62	0.51
3:I:18:THR:HG23	3:I:41:GLU:OE1	2.10	0.51
3:I:359:ILE:HG21	3:I:404:VAL:CG1	2.40	0.51
2:B:202:ARG:NH2	2:B:209:GLN:O	2.44	0.51
1:D:54:GLY:HA3	1:D:75:TYR:HB3	1.93	0.51
2:E:511:VAL:HG21	2:E:536:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ARG:HD2	1:G:253:PHE:O	2.11	0.51
1:G:54:GLY:HA3	1:G:75:TYR:HB3	1.93	0.51
2:H:512:MET:HA	2:H:540:ALA:CB	2.41	0.51
3:I:235:GLN:HG2	3:I:236:GLY:N	2.25	0.51
3:I:294:LEU:O	3:I:298:ILE:CD1	2.58	0.51
1:D:63:HIS:C	1:D:65:LYS:H	2.14	0.51
3:F:384:TYR:CA	3:F:387:ARG:HH12	2.15	0.51
1:G:180:ASN:ND2	1:G:205:ASP:N	2.59	0.51
1:G:283:GLU:HB2	1:G:289:TRP:CZ3	2.46	0.51
2:H:152:LYS:N	2:H:159:LEU:HD11	2.26	0.51
2:H:255:VAL:HG22	3:I:222:VAL:O	2.11	0.51
1:A:54:GLY:HA3	1:A:75:TYR:HB3	1.93	0.51
2:B:225:GLU:C	2:B:227:THR:H	2.14	0.51
2:E:152:LYS:N	2:E:159:LEU:HD11	2.26	0.51
2:E:314:LYS:NZ	3:F:253:GLN:HB3	2.26	0.51
3:F:71:GLU:O	3:F:74:PHE:HB3	2.11	0.51
1:G:63:HIS:C	1:G:65:LYS:H	2.14	0.51
1:G:8:HIS:O	1:G:9:ASN:ND2	2.43	0.51
2:H:198:THR:CB	2:H:212:GLU:HB2	2.29	0.51
2:H:547:TYR:CD2	2:H:548:GLU:HG2	2.46	0.51
3:I:400:ASN:HB2	3:I:403:SER:OG	2.10	0.51
3:I:359:ILE:HG21	3:I:404:VAL:HG11	1.92	0.51
3:I:431:ILE:N	3:I:431:ILE:CD1	2.72	0.51
3:C:226:GLN:CD	3:C:226:GLN:H	2.14	0.51
2:E:272:ILE:HG23	2:E:382:LEU:HG	1.93	0.51
2:E:525:HIS:C	2:E:527:LEU:N	2.62	0.51
3:F:417:ILE:HG23	3:F:429:ILE:HG23	1.93	0.51
1:A:27:CYS:HB2	1:A:56:VAL:HB	1.91	0.51
1:A:63:HIS:C	1:A:65:LYS:H	2.15	0.51
1:D:180:ASN:ND2	1:D:205:ASP:N	2.59	0.51
2:E:289:ASN:O	2:E:293:GLN:HG3	2.11	0.51
2:B:522:THR:HA	2:B:525:HIS:CB	2.39	0.50
2:B:527:LEU:HA	2:B:530:LEU:HD13	1.92	0.50
1:D:62:ALA:HB2	1:D:107:TRP:CE2	2.45	0.50
2:E:138:ILE:HG22	2:E:138:ILE:O	2.11	0.50
1:G:259:ARG:HB2	1:G:272:SER:HB2	1.92	0.50
2:H:202:ARG:NH2	2:H:209:GLN:O	2.44	0.50
2:H:327:SER:C	2:H:329:ASP:H	2.13	0.50
2:H:453:LEU:C	2:H:453:LEU:HD23	2.32	0.50
3:I:71:GLU:O	3:I:74:PHE:HB3	2.11	0.50
1:A:180:ASN:ND2	1:A:205:ASP:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LYS:O	2:B:159:LEU:HD13	2.11	0.50
2:B:272:ILE:HG23	2:B:382:LEU:HG	1.93	0.50
1:D:153:TRP:HH2	1:D:194:TYR:HH	1.59	0.50
2:E:142:ARG:HG2	2:E:144:PHE:HE1	1.77	0.50
2:E:172:ILE:HD12	2:E:172:ILE:N	2.27	0.50
3:F:166:THR:HG22	3:F:166:THR:O	2.10	0.50
2:H:289:ASN:O	2:H:293:GLN:HG3	2.11	0.50
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.46	0.50
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.45	0.50
3:C:342:PRO:HG2	3:C:382:LYS:HD2	1.92	0.50
2:E:453:LEU:HD23	2:E:453:LEU:C	2.32	0.50
3:F:294:LEU:O	3:F:298:ILE:CD1	2.59	0.50
3:F:70:LEU:CD2	3:F:343:ILE:HD11	2.30	0.50
1:A:217:LEU:CD1	1:A:218:LEU:H	2.23	0.50
1:A:225:VAL:HG13	1:A:257:LEU:CB	2.39	0.50
1:A:268:VAL:HG12	1:A:269:LEU:N	2.25	0.50
3:C:24:ILE:CG2	3:C:24:ILE:O	2.60	0.50
2:E:427:ALA:O	2:E:429:GLU:N	2.45	0.50
2:B:354:ILE:HD13	3:C:157:ASP:CG	2.32	0.50
3:C:25:GLU:O	3:C:25:GLU:HG2	2.12	0.50
2:E:202:ARG:NH2	2:E:209:GLN:O	2.44	0.50
2:E:527:LEU:HA	2:E:530:LEU:HD13	1.92	0.50
1:G:53:GLU:HB2	1:G:76:ASP:CB	2.42	0.50
2:H:142:ARG:O	2:H:143:ARG:HB2	2.12	0.50
2:H:546:ARG:CG	2:H:546:ARG:O	2.60	0.50
2:B:142:ARG:HH11	2:B:142:ARG:HA	1.77	0.50
1:A:263:SER:HB3	2:B:153:PHE:CE1	2.47	0.50
1:D:236:GLN:HB2	1:D:243:TRP:CE3	2.46	0.50
1:A:249:LYS:HE2	1:A:253:PHE:CE2	2.47	0.50
2:B:427:ALA:O	2:B:429:GLU:N	2.45	0.50
2:B:435:TYR:CE2	2:B:454:ILE:HD11	2.47	0.50
2:B:453:LEU:HD23	2:B:453:LEU:C	2.32	0.50
1:D:271:LEU:C	1:D:278:VAL:HG13	2.32	0.50
1:G:154:ALA:HB2	1:G:212:TRP:CE3	2.46	0.50
2:H:442:THR:CG2	2:H:443:ASN:H	2.25	0.50
3:I:143:LYS:HG3	3:I:144:TRP:N	2.25	0.50
3:I:237:ILE:HD12	3:I:237:ILE:O	2.12	0.50
3:I:382:LYS:N	3:I:383:PRO:HD2	2.26	0.50
1:A:140:ILE:HG22	1:A:141:ILE:H	1.77	0.50
2:B:512:MET:HA	2:B:540:ALA:CB	2.41	0.50
3:C:166:THR:O	3:C:166:THR:HG22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:VAL:HG13	3:C:314:ILE:HD11	1.94	0.50
2:E:165:VAL:O	2:E:165:VAL:HG12	2.11	0.50
3:F:380:ILE:O	3:F:380:ILE:HG22	2.12	0.50
3:F:9:THR:O	3:F:9:THR:HG22	2.11	0.50
1:G:236:GLN:HB2	1:G:243:TRP:CE3	2.47	0.50
1:G:249:LYS:HE2	1:G:253:PHE:CE2	2.47	0.50
2:H:152:LYS:O	2:H:159:LEU:HD13	2.11	0.50
2:H:272:ILE:HG23	2:H:382:LEU:HG	1.93	0.50
2:B:172:ILE:HD12	2:B:172:ILE:N	2.27	0.50
3:C:20:LYS:HE2	3:C:431:ILE:HD11	1.94	0.50
3:C:71:GLU:O	3:C:74:PHE:HB3	2.11	0.50
2:E:320:VAL:N	3:F:246:THR:HG21	2.26	0.50
2:E:512:MET:HA	2:E:540:ALA:CB	2.41	0.50
2:H:511:VAL:HG21	2:H:536:LEU:HD21	1.93	0.50
3:I:421:LYS:C	3:I:423:GLN:N	2.66	0.50
1:D:249:LYS:HE2	1:D:253:PHE:CE2	2.47	0.49
1:D:53:GLU:HB2	1:D:76:ASP:CB	2.42	0.49
2:E:435:TYR:CE2	2:E:454:ILE:HD11	2.47	0.49
3:F:8:GLN:C	3:F:10:GLU:N	2.65	0.49
2:H:165:VAL:O	2:H:165:VAL:HG12	2.11	0.49
2:H:427:ALA:O	2:H:429:GLU:N	2.45	0.49
3:C:93:GLU:HG3	3:C:94:MET:H	1.76	0.49
2:E:442:THR:CG2	2:E:443:ASN:H	2.25	0.49
3:F:431:ILE:N	3:F:431:ILE:CD1	2.72	0.49
2:H:225:GLU:C	2:H:227:THR:H	2.14	0.49
1:A:14:ASP:HB3	1:A:58:ARG:HA	1.95	0.49
3:C:294:LEU:O	3:C:298:ILE:CD1	2.59	0.49
2:E:159:LEU:O	2:E:173:LYS:HB2	2.12	0.49
1:G:129:GLU:HG2	1:G:130:PHE:N	2.27	0.49
2:H:419:GLY:O	2:H:423:GLN:HG3	2.12	0.49
3:I:350:VAL:HG22	3:I:355:LEU:CD2	2.41	0.49
2:B:320:VAL:HA	3:C:246:THR:CG2	2.38	0.49
3:C:237:ILE:HD12	3:C:237:ILE:O	2.12	0.49
2:B:327:SER:OG	3:C:238:LYS:HG3	2.13	0.49
2:E:327:SER:C	2:E:329:ASP:H	2.13	0.49
2:E:546:ARG:O	2:E:546:ARG:CG	2.59	0.49
2:B:159:LEU:O	2:B:173:LYS:HB2	2.12	0.49
2:B:466:SER:HB3	2:B:468:GLU:HG2	1.94	0.49
1:D:154:ALA:HB2	1:D:212:TRP:CE3	2.48	0.49
2:E:530:LEU:O	2:E:531:LYS:CG	2.59	0.49
3:F:387:ARG:HG2	3:F:391:HIS:ND1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:ILE:HG22	1:G:141:ILE:H	1.77	0.49
2:H:466:SER:HB3	2:H:468:GLU:HG2	1.95	0.49
3:I:387:ARG:HG2	3:I:391:HIS:ND1	2.28	0.49
3:I:384:TYR:O	3:I:388:ILE:HG13	2.13	0.49
1:A:271:LEU:C	1:A:278:VAL:HG13	2.32	0.49
2:B:419:GLY:O	2:B:423:GLN:HG3	2.13	0.49
2:B:546:ARG:CG	2:B:546:ARG:O	2.60	0.49
3:F:353:ASP:O	3:F:355:LEU:N	2.43	0.49
1:G:271:LEU:C	1:G:278:VAL:HG13	2.32	0.49
3:I:226:GLN:CD	3:I:226:GLN:H	2.14	0.49
3:I:381:ASP:N	3:I:383:PRO:HD2	2.27	0.49
1:A:53:GLU:HB2	1:A:76:ASP:CB	2.42	0.49
3:C:282:TRP:HE3	3:C:283:GLU:OE2	1.96	0.49
3:F:226:GLN:CD	3:F:226:GLN:H	2.13	0.49
3:F:237:ILE:O	3:F:237:ILE:HD12	2.12	0.49
2:H:435:TYR:CE2	2:H:454:ILE:HD11	2.47	0.49
3:I:23:LYS:NZ	3:I:431:ILE:HA	2.26	0.49
1:A:48:THR:O	1:A:49:LEU:HD23	2.13	0.49
2:B:442:THR:CG2	2:B:443:ASN:H	2.25	0.49
2:B:512:MET:C	2:B:514:GLU:N	2.66	0.49
3:C:77:LEU:HD21	3:C:81:LEU:HD12	1.95	0.49
2:H:172:ILE:HD12	2:H:172:ILE:N	2.27	0.49
2:H:304:VAL:CG1	3:I:314:ILE:HD11	2.43	0.49
3:I:353:ASP:O	3:I:355:LEU:N	2.44	0.49
2:B:197:VAL:HG12	2:B:210:ILE:HG23	1.94	0.49
3:C:387:ARG:HG2	3:C:391:HIS:ND1	2.28	0.49
3:C:410:SER:HA	3:C:436:LEU:HD11	1.94	0.49
1:D:112:TYR:CZ	1:D:171:ARG:HG2	2.48	0.49
1:D:259:ARG:HH11	1:D:259:ARG:HG3	1.78	0.49
1:G:31:LYS:HD3	1:G:52:HIS:O	2.13	0.49
2:H:522:THR:HA	2:H:525:HIS:CB	2.39	0.49
3:I:92:ASP:O	3:I:93:GLU:C	2.51	0.49
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.78	0.49
1:A:57:TRP:HE3	1:A:57:TRP:HA	1.78	0.49
2:B:530:LEU:O	2:B:531:LYS:CG	2.59	0.49
2:E:197:VAL:HG12	2:E:210:ILE:HG23	1.94	0.49
3:F:50:ALA:HB1	3:F:69:GLU:CG	2.42	0.49
1:G:11:LEU:HD23	2:H:162:LYS:NZ	2.28	0.49
1:G:259:ARG:HG3	1:G:259:ARG:HH11	1.78	0.49
2:H:524:ASP:CA	2:H:527:LEU:HD12	2.35	0.49
3:I:12:PHE:HD1	3:I:12:PHE:H	1.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:434:THR:O	3:C:434:THR:CG2	2.61	0.48
3:C:433:ALA:O	3:C:435:PHE:N	2.46	0.48
1:D:48:THR:O	1:D:49:LEU:HD23	2.13	0.48
2:E:419:GLY:O	2:E:423:GLN:HG3	2.13	0.48
2:H:159:LEU:O	2:H:173:LYS:HB2	2.12	0.48
2:H:155:THR:HG22	2:H:513:ARG:CD	2.43	0.48
3:I:237:ILE:HD11	3:I:240:HIS:HA	1.95	0.48
3:C:384:TYR:CA	3:C:387:ARG:HH12	2.15	0.48
1:D:205:ASP:CB	1:D:227:GLN:HB3	2.44	0.48
2:E:508:LYS:HG2	2:E:509:ARG:N	2.28	0.48
2:B:145:THR:O	2:B:147:SER:N	2.46	0.48
3:C:365:MET:HB3	3:C:379:ILE:HG22	1.94	0.48
2:E:160:LEU:HD23	2:E:172:ILE:HA	1.96	0.48
3:F:148:ILE:HD13	3:F:153:LEU:HD12	1.95	0.48
2:H:530:LEU:O	2:H:531:LYS:CG	2.59	0.48
1:D:202:GLY:HA2	1:D:245:LYS:NZ	2.29	0.48
1:A:129:GLU:HG2	1:A:130:PHE:N	2.27	0.48
3:C:148:ILE:HD13	3:C:153:LEU:HD12	1.95	0.48
3:C:350:VAL:HG22	3:C:355:LEU:CD2	2.41	0.48
1:D:129:GLU:HG2	1:D:130:PHE:N	2.27	0.48
1:D:140:ILE:HG22	1:D:141:ILE:H	1.77	0.48
2:E:399:LEU:HB3	2:E:425:TYR:OH	2.14	0.48
3:F:77:LEU:HD21	3:F:81:LEU:HD12	1.95	0.48
1:G:57:TRP:HA	1:G:57:TRP:HE3	1.78	0.48
2:H:197:VAL:HG12	2:H:210:ILE:HG23	1.94	0.48
3:I:282:TRP:HE3	3:I:283:GLU:OE2	1.97	0.48
2:B:172:ILE:H	2:B:172:ILE:HD12	1.79	0.48
3:C:11:ARG:HG2	3:C:12:PHE:HD1	1.78	0.48
1:D:270:ALA:HB2	2:E:153:PHE:CE1	2.49	0.48
2:E:154:SER:HB3	2:E:158:MET:H	1.79	0.48
2:E:449:PHE:HE2	2:E:453:LEU:HD12	1.79	0.48
2:E:466:SER:HB3	2:E:468:GLU:HG2	1.94	0.48
3:F:282:TRP:HE3	3:F:283:GLU:OE2	1.96	0.48
3:F:416:TYR:HE2	3:F:432:TYR:CZ	2.32	0.48
2:H:449:PHE:HE2	2:H:453:LEU:HD12	1.78	0.48
3:I:433:ALA:O	3:I:435:PHE:N	2.46	0.48
1:A:31:LYS:HD3	1:A:52:HIS:O	2.13	0.48
3:C:355:LEU:N	3:C:356:PRO:HD2	2.29	0.48
3:C:7:TYR:C	3:C:7:TYR:CD1	2.87	0.48
2:E:491:LEU:HD12	2:E:507:ILE:HD13	1.95	0.48
2:E:522:THR:HA	2:E:525:HIS:CB	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:ALA:O	2:B:138:ILE:N	2.46	0.48
2:B:174:ARG:O	2:B:175:LEU:C	2.52	0.48
2:B:508:LYS:HG2	2:B:509:ARG:N	2.29	0.48
3:C:237:ILE:HD11	3:C:240:HIS:HA	1.95	0.48
2:E:327:SER:OG	3:F:238:LYS:CG	2.62	0.48
3:F:237:ILE:HD11	3:F:240:HIS:HA	1.95	0.48
3:F:355:LEU:N	3:F:356:PRO:HD2	2.29	0.48
1:G:117:LEU:HB2	1:G:153:TRP:NE1	2.29	0.48
1:G:157:THR:HG21	2:H:501:LYS:HZ2	1.79	0.48
1:G:20:TYR:CE2	2:H:544:LYS:CD	2.97	0.48
1:G:52:HIS:CE1	1:G:80:LEU:HD12	2.49	0.48
2:H:314:LYS:HE3	3:I:162:LEU:HB3	1.95	0.48
3:I:189:LEU:HA	3:I:189:LEU:HD23	1.71	0.48
1:A:280:LEU:HB2	1:A:292:ALA:O	2.14	0.48
3:C:8:GLN:C	3:C:10:GLU:N	2.60	0.48
1:D:31:LYS:HD3	1:D:52:HIS:O	2.13	0.48
2:E:392:GLY:O	2:E:393:GLN:HB2	2.14	0.48
3:F:113:ASN:OD1	3:F:113:ASN:C	2.52	0.48
3:F:406:GLU:HG2	3:F:409:LYS:HZ1	1.78	0.48
1:G:48:THR:O	1:G:49:LEU:HD23	2.13	0.48
1:A:171:ARG:O	1:A:172:LYS:HG3	2.14	0.48
3:F:355:LEU:H	3:F:356:PRO:HD2	1.79	0.48
3:F:433:ALA:O	3:F:435:PHE:N	2.45	0.48
1:G:171:ARG:O	1:G:172:LYS:HG3	2.14	0.48
2:H:392:GLY:O	2:H:393:GLN:HB2	2.14	0.48
3:I:86:ASN:OD1	3:I:399:ILE:HG22	2.14	0.48
1:A:205:ASP:CB	1:A:227:GLN:HB3	2.43	0.47
1:A:273:GLY:C	1:A:275:ASP:H	2.17	0.47
2:B:508:LYS:HA	2:B:536:LEU:HD11	1.96	0.47
1:D:273:GLY:C	1:D:275:ASP:H	2.17	0.47
2:E:515:ILE:HD12	2:E:544:LYS:HB2	1.95	0.47
2:H:172:ILE:H	2:H:172:ILE:HD12	1.79	0.47
3:I:104:LEU:CD1	3:I:224:ASP:HB3	2.44	0.47
1:G:127:VAL:HG21	1:G:194:TYR:CE1	2.49	0.47
1:G:253:PHE:O	1:G:255:ASP:N	2.48	0.47
1:A:290:GLU:HG3	1:A:291:PRO:HD2	1.96	0.47
3:C:170:ASP:OD1	3:C:172:LYS:N	2.47	0.47
3:C:355:LEU:H	3:C:356:PRO:HD2	1.79	0.47
3:F:437:ASN:O	3:F:437:ASN:OD1	2.33	0.47
1:G:280:LEU:HB2	1:G:292:ALA:O	2.14	0.47
2:H:508:LYS:HG2	2:H:509:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:148:ILE:HD13	3:I:153:LEU:HD12	1.96	0.47
2:B:154:SER:HB3	2:B:158:MET:H	1.79	0.47
2:B:515:ILE:O	2:B:519:ARG:HG3	2.15	0.47
1:D:253:PHE:O	1:D:255:ASP:N	2.48	0.47
1:D:57:TRP:HA	1:D:57:TRP:HE3	1.78	0.47
3:F:242:LEU:HB2	3:F:312:GLU:HG2	1.96	0.47
3:F:341:HIS:CE1	3:F:343:ILE:HD12	2.50	0.47
2:H:160:LEU:HD23	2:H:172:ILE:HA	1.96	0.47
3:I:355:LEU:N	3:I:356:PRO:HD2	2.30	0.47
3:I:77:LEU:HD21	3:I:81:LEU:HD12	1.95	0.47
1:A:202:GLY:HA2	1:A:245:LYS:NZ	2.29	0.47
1:A:253:PHE:O	1:A:255:ASP:N	2.48	0.47
2:B:160:LEU:HD23	2:B:172:ILE:HA	1.95	0.47
2:B:491:LEU:HD12	2:B:507:ILE:HD13	1.95	0.47
1:D:117:LEU:HB2	1:D:153:TRP:NE1	2.29	0.47
3:F:10:GLU:O	3:F:11:ARG:C	2.52	0.47
3:F:350:VAL:HG22	3:F:355:LEU:CD2	2.41	0.47
1:G:57:TRP:HA	1:G:57:TRP:CE3	2.49	0.47
2:H:210:ILE:H	2:H:210:ILE:CD1	2.21	0.47
2:H:515:ILE:HD12	2:H:544:LYS:HB2	1.94	0.47
3:I:355:LEU:H	3:I:356:PRO:HD2	1.80	0.47
3:I:434:THR:O	3:I:434:THR:CG2	2.61	0.47
2:B:515:ILE:HD12	2:B:544:LYS:HB2	1.95	0.47
1:D:14:ASP:HB3	1:D:58:ARG:HA	1.95	0.47
2:E:324:TYR:CD2	3:F:237:ILE:HG21	2.48	0.47
1:G:202:GLY:HA2	1:G:245:LYS:NZ	2.29	0.47
2:H:221:LEU:HD22	2:H:231:TYR:CD1	2.49	0.47
2:H:522:THR:O	2:H:526:ILE:HG13	2.15	0.47
2:B:392:GLY:O	2:B:393:GLN:HB2	2.14	0.47
2:B:449:PHE:HE2	2:B:453:LEU:HD12	1.78	0.47
2:B:522:THR:O	2:B:526:ILE:HG13	2.15	0.47
3:C:104:LEU:CD1	3:C:224:ASP:HB3	2.44	0.47
1:D:140:ILE:CG2	1:D:141:ILE:N	2.78	0.47
1:D:280:LEU:HB2	1:D:292:ALA:O	2.14	0.47
1:D:290:GLU:HG3	1:D:291:PRO:HD2	1.97	0.47
1:D:57:TRP:HA	1:D:57:TRP:CE3	2.49	0.47
1:D:52:HIS:CE1	1:D:80:LEU:HD12	2.49	0.47
3:F:104:LEU:CD1	3:F:224:ASP:HB3	2.44	0.47
2:H:154:SER:HB3	2:H:158:MET:H	1.79	0.47
2:H:491:LEU:HD12	2:H:507:ILE:HD13	1.96	0.47
3:I:113:ASN:C	3:I:113:ASN:OD1	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:24:ILE:HG22	3:I:25:GLU:N	2.28	0.47
3:I:317:LEU:HD23	3:I:317:LEU:HA	1.59	0.47
1:A:215:THR:O	1:A:215:THR:HG23	2.15	0.47
2:B:366:PHE:O	2:B:368:GLY:N	2.43	0.47
3:C:235:GLN:HG2	3:C:236:GLY:N	2.30	0.47
1:G:273:GLY:C	1:G:275:ASP:H	2.17	0.47
1:G:14:ASP:HB3	1:G:58:ARG:HA	1.95	0.47
2:H:250:THR:HG23	3:I:99:TYR:OH	2.13	0.47
2:H:399:LEU:HB3	2:H:425:TYR:OH	2.14	0.47
2:H:512:MET:C	2:H:514:GLU:N	2.66	0.47
3:C:16:SER:HB2	3:C:432:TYR:HE1	1.79	0.47
1:D:11:LEU:HD23	2:E:162:LYS:NZ	2.29	0.47
1:D:208:ARG:HH21	2:E:143:ARG:HG3	1.80	0.47
1:D:217:LEU:CG	1:D:218:LEU:H	2.28	0.47
3:C:313:LEU:HD13	2:E:341:GLN:HB3	1.97	0.47
2:E:341:GLN:O	2:E:342:LYS:C	2.53	0.47
2:E:512:MET:C	2:E:514:GLU:N	2.66	0.47
2:E:508:LYS:HA	2:E:536:LEU:HD11	1.97	0.47
1:G:205:ASP:CB	1:G:227:GLN:HB3	2.44	0.47
1:G:57:TRP:NE1	2:H:142:ARG:NH2	2.62	0.47
1:G:74:SER:HB3	1:G:76:ASP:OD1	2.15	0.47
3:I:242:LEU:HB2	3:I:312:GLU:HG2	1.96	0.47
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.49	0.47
3:C:11:ARG:CG	3:C:12:PHE:CD1	2.97	0.47
1:D:215:THR:O	1:D:215:THR:HG23	2.15	0.47
1:G:102:VAL:HG13	1:G:118:VAL:HG13	1.97	0.47
1:G:141:ILE:HD12	1:G:185:TRP:CE3	2.50	0.47
1:G:43:HIS:N	1:G:43:HIS:ND1	2.63	0.47
2:H:435:TYR:OH	2:H:450:CYS:HB3	2.15	0.47
3:I:7:TYR:O	3:I:9:THR:N	2.47	0.47
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.29	0.47
1:A:217:LEU:CG	1:A:218:LEU:H	2.28	0.47
1:A:57:TRP:CE3	1:A:57:TRP:HA	2.49	0.47
2:B:399:LEU:HB3	2:B:425:TYR:OH	2.14	0.47
3:C:113:ASN:OD1	3:C:113:ASN:C	2.53	0.47
2:E:172:ILE:H	2:E:172:ILE:HD12	1.79	0.47
2:H:364:SER:HB3	2:H:367:GLU:HB2	1.97	0.47
2:H:515:ILE:O	2:H:519:ARG:HG3	2.14	0.47
3:C:274:GLN:O	3:C:278:GLN:HB3	2.15	0.46
3:C:284:SER:O	3:C:287:HIS:HB3	2.15	0.46
3:C:341:HIS:CE1	3:C:343:ILE:HD12	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ARG:O	1:D:172:LYS:HG3	2.14	0.46
2:E:142:ARG:O	2:E:143:ARG:HG2	2.14	0.46
2:E:333:ARG:HG2	2:E:362:SER:O	2.15	0.46
3:F:58:ASP:C	3:F:60:SER:N	2.69	0.46
2:H:174:ARG:O	2:H:175:LEU:C	2.52	0.46
1:A:43:HIS:ND1	1:A:43:HIS:N	2.63	0.46
3:C:139:VAL:CG1	3:C:140:PRO:HD2	2.43	0.46
3:C:310:THR:CG2	3:C:311:ASP:N	2.78	0.46
2:E:174:ARG:O	2:E:175:LEU:C	2.53	0.46
2:E:206:PRO:O	2:E:533:PRO:HG3	2.15	0.46
2:E:515:ILE:O	2:E:519:ARG:HG3	2.15	0.46
2:E:522:THR:O	2:E:526:ILE:HG13	2.15	0.46
3:F:274:GLN:O	3:F:278:GLN:HB3	2.15	0.46
3:C:439:SER:C	3:C:441:CYS:H	2.18	0.46
2:E:221:LEU:HD22	2:E:231:TYR:CD1	2.50	0.46
3:F:12:PHE:HD2	3:F:416:TYR:HH	1.62	0.46
3:I:170:ASP:OD1	3:I:172:LYS:N	2.48	0.46
3:I:341:HIS:CE1	3:I:343:ILE:HD12	2.50	0.46
2:B:134:ASN:O	2:B:138:ILE:HG13	2.15	0.46
2:B:221:LEU:HD22	2:B:231:TYR:CD1	2.49	0.46
1:D:63:HIS:O	1:D:65:LYS:N	2.49	0.46
2:E:340:LEU:HD22	2:E:370:PHE:CG	2.50	0.46
3:F:170:ASP:OD1	3:F:172:LYS:N	2.48	0.46
1:G:215:THR:HG23	1:G:215:THR:O	2.15	0.46
2:H:508:LYS:HA	2:H:536:LEU:HD11	1.96	0.46
1:G:65:LYS:CA	2:H:546:ARG:NH2	2.73	0.46
3:I:274:GLN:O	3:I:278:GLN:HB3	2.15	0.46
2:B:206:PRO:O	2:B:533:PRO:HG3	2.15	0.46
2:B:435:TYR:OH	2:B:450:CYS:HB3	2.15	0.46
1:G:37:GLU:CG	1:G:46:ILE:HD12	2.45	0.46
1:G:53:GLU:HB2	1:G:76:ASP:HB3	1.98	0.46
2:H:333:ARG:HG2	2:H:362:SER:O	2.15	0.46
3:F:313:LEU:HB3	2:H:338:LEU:HD11	1.98	0.46
1:A:151:ALA:CB	1:A:175:THR:HG22	2.46	0.46
1:A:53:GLU:HB2	1:A:76:ASP:HB3	1.98	0.46
1:A:61:TRP:O	1:A:107:TRP:CD1	2.69	0.46
2:B:460:ASN:C	2:B:462:THR:H	2.19	0.46
2:B:526:ILE:O	2:B:529:ARG:HB2	2.16	0.46
1:D:229:ARG:HH11	1:D:252:LYS:HB3	1.81	0.46
2:E:250:THR:CG2	2:E:255:VAL:HB	2.45	0.46
2:E:546:ARG:O	2:E:546:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:441:CYS:SG	3:F:441:CYS:O	2.74	0.46
1:G:290:GLU:HG3	1:G:291:PRO:HD2	1.97	0.46
2:H:206:PRO:O	2:H:533:PRO:HG3	2.15	0.46
2:H:546:ARG:O	2:H:546:ARG:HG2	2.15	0.46
3:I:54:ALA:O	3:I:55:ASN:C	2.53	0.46
1:A:37:GLU:CG	1:A:46:ILE:HD12	2.45	0.46
2:B:327:SER:HA	3:C:238:LYS:HE3	1.98	0.46
1:D:37:GLU:CG	1:D:46:ILE:HD12	2.45	0.46
2:E:514:GLU:O	2:E:516:THR:N	2.49	0.46
3:F:59:GLU:HA	3:F:62:VAL:HG23	1.98	0.46
3:F:7:TYR:CD1	3:F:7:TYR:N	2.84	0.46
2:H:348:CYS:O	2:H:349:SER:OG	2.30	0.46
3:I:36:PHE:HB3	3:I:40:ARG:HH21	1.81	0.46
2:H:259:LEU:HD11	3:I:99:TYR:CG	2.50	0.46
1:A:63:HIS:O	1:A:65:LYS:N	2.49	0.46
1:A:78:LYS:CA	1:A:96:ALA:HB2	2.41	0.46
2:B:452:TYR:O	2:B:452:TYR:HD2	1.98	0.46
3:C:104:LEU:HD23	3:C:104:LEU:HA	1.72	0.46
2:E:142:ARG:HG3	2:E:142:ARG:NH1	2.31	0.46
3:F:10:GLU:HG3	3:F:11:ARG:N	2.31	0.46
3:F:36:PHE:HB3	3:F:40:ARG:HH21	1.80	0.46
3:F:434:THR:O	3:F:434:THR:CG2	2.61	0.46
1:G:229:ARG:HH11	1:G:252:LYS:HB3	1.80	0.46
1:A:261:SER:HB2	2:B:152:LYS:HA	1.91	0.46
2:B:417:PRO:HG2	2:B:418:ILE:HD13	1.98	0.46
1:D:57:TRP:CH2	2:E:144:PHE:CE1	3.04	0.46
2:E:435:TYR:OH	2:E:450:CYS:HB3	2.15	0.46
2:E:234:TRP:CH2	2:E:452:TYR:CD1	3.04	0.46
3:F:68:TRP:CH2	3:F:387:ARG:NH2	2.84	0.46
2:H:452:TYR:O	2:H:452:TYR:HD2	1.99	0.46
2:H:526:ILE:O	2:H:529:ARG:HB2	2.16	0.46
2:B:164:ILE:HG13	2:B:164:ILE:O	2.15	0.46
3:C:406:GLU:HA	3:C:409:LYS:CE	2.45	0.46
2:E:210:ILE:HD12	2:E:495:CYS:CB	2.46	0.46
2:E:318:LEU:HD23	2:E:318:LEU:O	2.16	0.46
3:F:13:THR:O	3:F:17:ASP:CB	2.51	0.46
2:H:250:THR:CG2	2:H:255:VAL:HB	2.45	0.46
2:H:338:LEU:O	2:H:342:LYS:HG3	2.16	0.46
2:H:417:PRO:HG2	2:H:418:ILE:HD13	1.98	0.46
1:A:102:VAL:HG13	1:A:118:VAL:HG13	1.98	0.45
1:A:140:ILE:CG2	1:A:141:ILE:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:THR:CG2	2:B:255:VAL:HB	2.45	0.45
2:B:333:ARG:HG2	2:B:362:SER:O	2.16	0.45
2:B:338:LEU:O	2:B:342:LYS:HG3	2.16	0.45
2:B:420:VAL:CG1	2:B:438:VAL:HG11	2.46	0.45
2:B:546:ARG:HG2	2:B:546:ARG:O	2.15	0.45
3:C:242:LEU:HB2	3:C:312:GLU:HG2	1.97	0.45
1:D:10:GLU:N	1:D:10:GLU:OE1	2.45	0.45
2:E:460:ASN:C	2:E:462:THR:H	2.19	0.45
3:F:139:VAL:CG1	3:F:140:PRO:HD2	2.43	0.45
3:F:77:LEU:C	3:F:77:LEU:HD23	2.36	0.45
1:G:140:ILE:CG2	1:G:141:ILE:N	2.78	0.45
2:H:234:TRP:CH2	2:H:452:TYR:CD1	3.04	0.45
2:H:460:ASN:C	2:H:462:THR:H	2.19	0.45
3:I:139:VAL:CG1	3:I:140:PRO:HD2	2.42	0.45
3:I:284:SER:O	3:I:287:HIS:HB3	2.16	0.45
1:A:151:ALA:HA	1:A:174:VAL:O	2.16	0.45
1:A:8:HIS:O	1:A:9:ASN:CB	2.65	0.45
1:D:102:VAL:HG13	1:D:118:VAL:HG13	1.97	0.45
1:D:61:TRP:O	1:D:107:TRP:CD1	2.69	0.45
2:E:338:LEU:O	2:E:342:LYS:HG3	2.16	0.45
2:E:342:LYS:HD2	3:F:206:ILE:CD1	2.47	0.45
3:F:284:SER:O	3:F:287:HIS:HB3	2.16	0.45
1:G:217:LEU:CG	1:G:218:LEU:H	2.28	0.45
2:H:318:LEU:O	2:H:318:LEU:HD23	2.16	0.45
3:I:294:LEU:O	3:I:298:ILE:HD12	2.17	0.45
3:C:269:GLY:HA3	3:C:295:GLN:CG	2.42	0.45
3:C:36:PHE:HB3	3:C:40:ARG:HH21	1.81	0.45
3:C:54:ALA:O	3:C:55:ASN:C	2.55	0.45
1:G:61:TRP:O	1:G:107:TRP:CD1	2.69	0.45
2:H:225:GLU:O	2:H:231:TYR:HB2	2.15	0.45
3:I:413:ILE:O	3:I:417:ILE:HG13	2.17	0.45
2:B:210:ILE:HD12	2:B:495:CYS:CB	2.46	0.45
3:C:144:TRP:O	3:C:148:ILE:HG12	2.17	0.45
3:C:23:LYS:O	3:C:26:GLN:OE1	2.34	0.45
3:C:413:ILE:O	3:C:417:ILE:HG13	2.17	0.45
2:E:225:GLU:O	2:E:231:TYR:HB2	2.16	0.45
2:E:366:PHE:O	2:E:368:GLY:N	2.44	0.45
2:E:417:PRO:HG2	2:E:418:ILE:HD13	1.98	0.45
3:F:233:THR:HG22	3:F:234:GLN:O	2.17	0.45
3:F:406:GLU:HA	3:F:409:LYS:CE	2.45	0.45
2:B:246:TYR:HA	2:B:247:PRO:HD2	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:TYR:CE2	3:C:199:GLU:HG3	2.52	0.45
3:I:77:LEU:C	3:I:77:LEU:HD23	2.36	0.45
2:B:210:ILE:CD1	2:B:210:ILE:H	2.22	0.45
2:B:364:SER:HB3	2:B:367:GLU:HB2	1.98	0.45
2:B:529:ARG:O	2:B:530:LEU:C	2.55	0.45
2:E:265:HIS:HB2	2:E:399:LEU:CD2	2.42	0.45
2:E:526:ILE:O	2:E:529:ARG:HB2	2.16	0.45
3:F:294:LEU:O	3:F:298:ILE:HD12	2.17	0.45
2:H:210:ILE:HD12	2:H:495:CYS:CB	2.46	0.45
1:A:126:SER:HB3	1:A:140:ILE:CG1	2.28	0.45
3:C:189:LEU:HD23	3:C:189:LEU:HA	1.70	0.45
3:C:227:ILE:HD12	3:C:227:ILE:C	2.37	0.45
1:D:43:HIS:N	1:D:43:HIS:ND1	2.63	0.45
1:D:74:SER:HB3	1:D:76:ASP:OD1	2.16	0.45
3:F:144:TRP:O	3:F:148:ILE:HG12	2.17	0.45
3:F:42:PHE:CZ	3:F:391:HIS:HB3	2.52	0.45
3:F:58:ASP:C	3:F:60:SER:H	2.20	0.45
1:G:63:HIS:O	1:G:65:LYS:N	2.49	0.45
2:H:215:LEU:HB3	2:H:452:TYR:CE2	2.52	0.45
1:A:74:SER:HB3	1:A:76:ASP:OD1	2.15	0.45
2:B:215:LEU:HB3	2:B:452:TYR:CE2	2.52	0.45
3:C:206:ILE:HD12	3:C:206:ILE:H	1.82	0.45
3:C:353:ASP:O	3:C:355:LEU:N	2.44	0.45
1:D:232:ILE:HG12	1:D:247:LEU:CD2	2.38	0.45
2:E:340:LEU:CD2	2:E:370:PHE:CG	2.99	0.45
2:E:420:VAL:CG1	2:E:438:VAL:HG11	2.46	0.45
2:H:420:VAL:CG1	2:H:438:VAL:HG11	2.46	0.45
3:I:144:TRP:O	3:I:148:ILE:HG12	2.17	0.45
3:I:102:ARG:NH2	3:I:241:SER:OG	2.45	0.45
1:A:229:ARG:HH11	1:A:252:LYS:HB3	1.81	0.45
2:B:234:TRP:CH2	2:B:452:TYR:CD1	3.04	0.45
2:B:514:GLU:O	2:B:516:THR:N	2.50	0.45
3:C:135:ARG:HG3	3:C:183:TYR:CE2	2.52	0.45
3:C:22:PHE:C	3:C:24:ILE:N	2.69	0.45
1:D:217:LEU:HD13	1:D:218:LEU:HB2	1.99	0.45
2:E:197:VAL:HG11	2:E:210:ILE:CG1	2.47	0.45
3:C:313:LEU:O	2:E:342:LYS:HE2	2.17	0.45
2:E:215:LEU:HB3	2:E:452:TYR:CE2	2.52	0.45
2:E:452:TYR:HD2	2:E:452:TYR:O	1.98	0.45
2:E:526:ILE:C	2:E:529:ARG:HB2	2.37	0.45
3:F:54:ALA:O	3:F:55:ASN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:ALA:HB2	1:G:175:THR:HG22	1.99	0.45
2:H:142:ARG:O	2:H:143:ARG:CB	2.65	0.45
3:F:319:SER:CB	2:H:337:GLU:HG2	2.47	0.45
2:B:327:SER:OG	3:C:238:LYS:N	2.33	0.45
3:C:58:ASP:C	3:C:60:SER:H	2.20	0.45
3:C:77:LEU:HD23	3:C:77:LEU:C	2.37	0.45
1:D:127:VAL:HG21	1:D:194:TYR:CE1	2.52	0.45
2:E:233:LEU:HD21	2:E:421:ILE:CD1	2.47	0.45
3:F:413:ILE:O	3:F:417:ILE:HG13	2.17	0.45
3:F:48:GLN:HA	3:F:51:LEU:HD12	1.99	0.45
1:G:10:GLU:N	1:G:10:GLU:OE1	2.45	0.45
1:G:9:ASN:HD21	1:G:34:LYS:HE3	1.81	0.45
1:D:17:LEU:HD21	2:E:160:LEU:CD1	2.43	0.44
1:D:53:GLU:HB2	1:D:76:ASP:HB3	1.98	0.44
2:E:529:ARG:O	2:E:530:LEU:C	2.55	0.44
3:F:77:LEU:HD12	3:F:125:TRP:CZ2	2.52	0.44
3:F:183:TYR:CE2	3:F:199:GLU:HG3	2.52	0.44
3:F:329:ASN:O	3:F:332:ALA:HB3	2.17	0.44
3:F:70:LEU:HB3	3:F:343:ILE:HD11	1.99	0.44
1:G:58:ARG:NH2	1:G:259:ARG:HE	2.14	0.44
3:I:227:ILE:HD12	3:I:227:ILE:C	2.37	0.44
1:A:217:LEU:HD13	1:A:218:LEU:HB2	1.99	0.44
2:B:318:LEU:O	2:B:318:LEU:HD23	2.16	0.44
2:B:155:THR:HG22	2:B:513:ARG:CG	2.48	0.44
3:C:12:PHE:H	3:C:12:PHE:HD1	1.61	0.44
3:F:135:ARG:HG3	3:F:183:TYR:CE2	2.52	0.44
2:H:153:PHE:HA	2:H:159:LEU:CD2	2.46	0.44
2:H:341:GLN:O	2:H:342:LYS:C	2.52	0.44
2:H:366:PHE:O	2:H:368:GLY:N	2.47	0.44
2:H:514:GLU:O	2:H:516:THR:N	2.50	0.44
2:H:526:ILE:C	2:H:529:ARG:HB2	2.37	0.44
2:H:529:ARG:O	2:H:530:LEU:C	2.55	0.44
2:H:538:PHE:O	2:H:541:GLN:HB3	2.17	0.44
3:I:11:ARG:C	3:I:13:THR:N	2.71	0.44
3:I:183:TYR:CE2	3:I:199:GLU:HG3	2.52	0.44
3:I:329:ASN:O	3:I:332:ALA:HB3	2.17	0.44
2:B:197:VAL:HG11	2:B:210:ILE:CG1	2.47	0.44
2:B:225:GLU:O	2:B:231:TYR:HB2	2.16	0.44
1:D:151:ALA:HB2	1:D:175:THR:HG22	1.99	0.44
1:D:208:ARG:HD3	1:D:208:ARG:HA	1.81	0.44
2:E:538:PHE:O	2:E:541:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:184:LEU:HA	2:H:184:LEU:HD23	1.85	0.44
2:H:233:LEU:HD21	2:H:421:ILE:CD1	2.48	0.44
1:G:19:TYR:CD2	2:H:543:LEU:HD21	2.52	0.44
1:A:232:ILE:HG12	1:A:247:LEU:CD2	2.38	0.44
2:B:142:ARG:HG3	2:B:142:ARG:NH1	2.33	0.44
2:B:175:LEU:CD1	2:B:176:PRO:HD2	2.42	0.44
2:B:263:GLU:HA	2:B:263:GLU:OE1	2.17	0.44
3:C:225:THR:HG22	3:C:226:GLN:N	2.32	0.44
3:C:39:ILE:HD11	3:C:399:ILE:HD11	1.99	0.44
1:G:126:SER:HB3	1:G:140:ILE:CG1	2.28	0.44
1:G:281:TRP:CD1	1:G:281:TRP:N	2.86	0.44
1:A:38:VAL:HG12	1:A:39:GLU:N	2.33	0.44
3:C:34:ASP:CB	3:C:35:PRO:CD	2.93	0.44
3:C:358:VAL:O	3:C:361:SER:HB3	2.18	0.44
1:D:273:GLY:O	1:D:275:ASP:N	2.46	0.44
3:F:317:LEU:HD23	3:F:317:LEU:HA	1.58	0.44
2:H:174:ARG:HE	2:H:174:ARG:HA	1.82	0.44
2:H:263:GLU:OE1	2:H:263:GLU:HA	2.18	0.44
2:H:255:VAL:HG13	3:I:223:ILE:HA	1.99	0.44
3:I:23:LYS:CE	3:I:434:THR:OG1	2.65	0.44
3:I:384:TYR:CA	3:I:387:ARG:HH12	2.15	0.44
1:A:66:PHE:CZ	1:A:113:GLY:O	2.71	0.44
3:C:233:THR:HG22	3:C:234:GLN:O	2.17	0.44
2:E:159:LEU:CD1	2:E:160:LEU:N	2.79	0.44
2:E:304:VAL:HG21	3:F:311:ASP:HB3	1.99	0.44
1:G:78:LYS:CA	1:G:96:ALA:HB2	2.41	0.44
2:H:265:HIS:CB	2:H:399:LEU:HD21	2.42	0.44
3:I:135:ARG:HG3	3:I:183:TYR:CE2	2.52	0.44
3:I:77:LEU:HD12	3:I:125:TRP:CZ3	2.52	0.44
1:A:109:PRO:O	1:A:111:GLU:N	2.51	0.44
1:A:279:THR:HB	1:A:281:TRP:NE1	2.33	0.44
2:B:516:THR:OG1	2:B:544:LYS:HE2	2.18	0.44
3:C:382:LYS:HA	3:C:383:PRO:HD3	1.47	0.44
3:C:7:TYR:O	3:C:10:GLU:HB2	2.18	0.44
2:E:299:LEU:CD2	2:E:387:LEU:HD21	2.46	0.44
3:F:227:ILE:C	3:F:227:ILE:HD12	2.37	0.44
1:G:95:HIS:ND1	1:G:128:VAL:HG21	2.33	0.44
1:A:10:GLU:OE1	1:A:10:GLU:HA	2.18	0.44
1:A:95:HIS:ND1	1:A:128:VAL:HG21	2.33	0.44
1:A:9:ASN:HA	1:A:9:ASN:HD22	1.49	0.44
2:B:381:TRP:CD2	2:B:412:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:HIS:CB	2:B:399:LEU:HD21	2.42	0.44
3:C:16:SER:O	3:C:19:LEU:HB2	2.18	0.44
3:C:116:LEU:CD2	3:C:294:LEU:CD1	2.95	0.44
1:D:66:PHE:CZ	1:D:113:GLY:O	2.71	0.44
1:D:58:ARG:NH2	1:D:259:ARG:HE	2.16	0.44
3:F:269:GLY:HA3	3:F:295:GLN:CG	2.42	0.44
3:F:298:ILE:HD12	3:F:298:ILE:N	2.33	0.44
1:G:217:LEU:HD13	1:G:218:LEU:HB2	1.99	0.44
2:H:381:TRP:CD2	2:H:412:LEU:HD22	2.53	0.44
2:H:399:LEU:O	2:H:403:VAL:HG23	2.18	0.44
3:I:144:TRP:CZ2	3:I:169:LEU:HD11	2.53	0.44
3:I:48:GLN:HA	3:I:51:LEU:HD12	1.99	0.44
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.53	0.44
3:C:164:GLU:O	3:C:165:ASN:O	2.36	0.44
3:C:294:LEU:HG	3:C:298:ILE:HD11	1.99	0.44
3:C:329:ASN:O	3:C:332:ALA:HB3	2.18	0.44
1:D:236:GLN:HG3	1:D:241:GLY:O	2.18	0.44
2:E:153:PHE:HA	2:E:159:LEU:CD2	2.46	0.44
2:E:193:GLU:HG3	2:E:215:LEU:HD11	2.00	0.44
3:F:358:VAL:O	3:F:361:SER:HB3	2.18	0.44
1:G:38:VAL:HG12	1:G:39:GLU:N	2.33	0.44
2:H:197:VAL:HG11	2:H:210:ILE:CG1	2.47	0.44
3:I:416:TYR:CD2	3:I:432:TYR:CE2	3.06	0.44
1:A:12:ILE:HG21	1:A:26:THR:HB	2.00	0.43
1:A:273:GLY:O	1:A:275:ASP:N	2.47	0.43
2:B:193:GLU:HG3	2:B:215:LEU:HD11	2.00	0.43
3:C:406:GLU:HG2	3:C:409:LYS:HZ1	1.83	0.43
1:D:95:HIS:ND1	1:D:128:VAL:HG21	2.33	0.43
2:E:263:GLU:OE1	2:E:263:GLU:HA	2.17	0.43
3:F:144:TRP:CZ2	3:F:169:LEU:HD11	2.53	0.43
3:F:212:LEU:HA	3:F:212:LEU:HD23	1.74	0.43
3:F:436:LEU:HB3	3:F:437:ASN:H	1.46	0.43
1:G:57:TRP:CH2	2:H:144:PHE:CE1	3.05	0.43
2:H:340:LEU:HD23	2:H:370:PHE:CE1	2.53	0.43
2:H:340:LEU:HD22	2:H:370:PHE:CB	2.48	0.43
3:I:164:GLU:O	3:I:165:ASN:O	2.36	0.43
3:I:419:LEU:O	3:I:423:GLN:HB2	2.18	0.43
3:C:9:THR:O	3:C:9:THR:HG22	2.17	0.43
2:E:174:ARG:HE	2:E:174:ARG:HA	1.82	0.43
2:E:393:GLN:HG2	2:E:396:GLU:HB2	2.00	0.43
1:G:112:TYR:CZ	1:G:171:ARG:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:SER:HA	1:G:186:LYS:HE3	2.00	0.43
1:G:20:TYR:N	1:G:20:TYR:CD1	2.86	0.43
1:G:233:ILE:HD11	1:G:248:LEU:CD1	2.48	0.43
2:H:135:ALA:O	2:H:139:MET:HB2	2.18	0.43
2:H:150:PHE:CZ	2:H:170:VAL:HG12	2.53	0.43
2:H:150:PHE:HZ	2:H:170:VAL:HG12	1.83	0.43
3:I:104:LEU:HA	3:I:104:LEU:HD23	1.72	0.43
3:I:294:LEU:HG	3:I:298:ILE:HD11	1.99	0.43
1:A:20:TYR:N	1:A:20:TYR:CD1	2.87	0.43
1:A:219:ARG:HB2	1:A:236:GLN:O	2.19	0.43
2:B:145:THR:C	2:B:147:SER:H	2.22	0.43
2:B:174:ARG:HE	2:B:174:ARG:HA	1.82	0.43
2:B:527:LEU:C	2:B:529:ARG:N	2.72	0.43
3:C:317:LEU:HA	3:C:317:LEU:HD23	1.58	0.43
3:C:354:SER:O	3:C:358:VAL:HG23	2.19	0.43
1:D:38:VAL:HG12	1:D:39:GLU:N	2.33	0.43
2:E:150:PHE:HZ	2:E:170:VAL:HG12	1.83	0.43
3:C:316:PRO:HB3	2:E:338:LEU:HB2	1.99	0.43
2:E:381:TRP:CD2	2:E:412:LEU:HD22	2.53	0.43
3:F:298:ILE:H	3:F:298:ILE:HD12	1.83	0.43
3:F:305:ASN:O	3:F:306:ASN:C	2.56	0.43
3:F:384:TYR:O	3:F:388:ILE:HG13	2.18	0.43
1:G:219:ARG:HB2	1:G:236:GLN:O	2.19	0.43
2:H:393:GLN:HG2	2:H:396:GLU:HB2	2.00	0.43
3:I:206:ILE:HD12	3:I:206:ILE:H	1.84	0.43
3:I:354:SER:O	3:I:358:VAL:HG23	2.19	0.43
1:A:274:GLY:O	2:B:147:SER:HB2	2.19	0.43
2:B:265:HIS:HB2	2:B:399:LEU:CD2	2.42	0.43
2:B:341:GLN:O	2:B:342:LYS:C	2.52	0.43
2:B:526:ILE:C	2:B:529:ARG:HB2	2.37	0.43
2:B:538:PHE:O	2:B:541:GLN:HB3	2.18	0.43
3:C:144:TRP:CZ2	3:C:169:LEU:HD11	2.54	0.43
3:C:294:LEU:O	3:C:298:ILE:HD13	2.18	0.43
3:C:364:GLU:C	3:C:366:LEU:N	2.69	0.43
1:D:233:ILE:HD11	1:D:248:LEU:CD1	2.48	0.43
3:F:24:ILE:HD13	3:F:24:ILE:N	2.34	0.43
3:F:343:ILE:HD13	3:F:344:ARG:N	2.34	0.43
1:G:227:GLN:C	1:G:229:ARG:H	2.22	0.43
2:H:330:PRO:HA	2:H:333:ARG:HB2	2.00	0.43
2:H:467:LYS:HD2	2:H:498:ASN:HB3	2.01	0.43
2:H:527:LEU:C	2:H:529:ARG:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:516:THR:OG1	2:H:544:LYS:HE2	2.18	0.43
3:I:233:THR:HG22	3:I:234:GLN:O	2.17	0.43
1:A:185:TRP:CE2	1:A:196:LEU:HD13	2.54	0.43
1:A:281:TRP:CD1	1:A:281:TRP:N	2.86	0.43
1:D:170:SER:HA	1:D:186:LYS:HE3	2.00	0.43
1:D:232:ILE:HG21	1:D:234:TRP:CZ2	2.53	0.43
3:F:102:ARG:NH2	3:F:241:SER:OG	2.45	0.43
3:F:294:LEU:HD12	3:F:294:LEU:HA	1.81	0.43
1:G:66:PHE:CZ	1:G:113:GLY:O	2.71	0.43
2:H:314:LYS:HG2	3:I:162:LEU:O	2.19	0.43
3:I:225:THR:HG22	3:I:226:GLN:N	2.33	0.43
3:I:298:ILE:N	3:I:298:ILE:HD12	2.33	0.43
3:I:343:ILE:HD13	3:I:344:ARG:N	2.34	0.43
3:I:421:LYS:O	3:I:423:GLN:N	2.52	0.43
2:B:202:ARG:HE	2:B:209:GLN:HB2	1.84	0.43
3:C:298:ILE:N	3:C:298:ILE:HD12	2.34	0.43
3:C:384:TYR:O	3:C:388:ILE:HG13	2.19	0.43
3:C:94:MET:HE3	3:C:104:LEU:HD22	2.01	0.43
1:D:185:TRP:CE2	1:D:196:LEU:HD13	2.54	0.43
1:D:208:ARG:HE	1:D:258:TRP:HZ3	1.67	0.43
1:D:264:LEU:HD12	2:E:155:THR:O	2.19	0.43
2:E:297:TYR:HE2	2:E:305:ARG:HH11	1.67	0.43
2:E:399:LEU:O	2:E:403:VAL:HG23	2.19	0.43
3:F:104:LEU:HA	3:F:104:LEU:HD23	1.72	0.43
1:G:279:THR:HB	1:G:281:TRP:NE1	2.33	0.43
1:G:289:TRP:CD1	1:G:289:TRP:N	2.87	0.43
2:H:193:GLU:HG3	2:H:215:LEU:HD11	2.00	0.43
2:H:318:LEU:HD11	2:H:357:ILE:HD12	2.00	0.43
1:A:103:ASN:ND2	2:B:142:ARG:NH2	2.66	0.43
3:C:16:SER:HB3	3:C:432:TYR:OH	2.17	0.43
3:C:212:LEU:HD23	3:C:212:LEU:HA	1.75	0.43
2:E:150:PHE:CZ	2:E:170:VAL:HG12	2.53	0.43
2:E:246:TYR:HA	2:E:247:PRO:HD2	1.76	0.43
2:E:468:GLU:N	2:E:468:GLU:OE1	2.47	0.43
3:F:206:ILE:HD12	3:F:206:ILE:H	1.83	0.43
3:F:294:LEU:HG	3:F:298:ILE:HD11	2.00	0.43
1:G:232:ILE:HG21	1:G:234:TRP:CZ2	2.54	0.43
3:I:143:LYS:HE3	3:I:144:TRP:CD1	2.54	0.43
3:I:305:ASN:O	3:I:306:ASN:C	2.56	0.43
3:I:435:PHE:O	3:I:436:LEU:CG	2.65	0.43
1:A:102:VAL:CG1	1:A:118:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HD3	1:A:208:ARG:HA	1.81	0.43
1:A:227:GLN:C	1:A:229:ARG:H	2.22	0.43
2:B:142:ARG:O	2:B:143:ARG:CB	2.66	0.43
2:B:150:PHE:HZ	2:B:170:VAL:HG12	1.83	0.43
2:B:340:LEU:HA	2:B:340:LEU:HD12	1.80	0.43
2:B:325:LEU:CD2	2:B:361:LEU:HD23	2.49	0.43
2:B:467:LYS:HD2	2:B:498:ASN:HB3	2.01	0.43
3:C:143:LYS:HE3	3:C:144:TRP:CD1	2.54	0.43
3:C:428:ASN:C	3:C:430:PRO:CD	2.87	0.43
3:F:164:GLU:O	3:F:165:ASN:O	2.36	0.43
3:F:225:THR:HG22	3:F:226:GLN:N	2.32	0.43
3:F:34:ASP:CB	3:F:35:PRO:CD	2.93	0.43
2:H:285:ARG:HG3	2:H:285:ARG:NH1	2.33	0.43
3:I:116:LEU:CD2	3:I:294:LEU:CD1	2.96	0.43
2:B:318:LEU:HD11	2:B:357:ILE:HD12	2.01	0.43
2:B:233:LEU:HD21	2:B:421:ILE:CD1	2.47	0.43
3:F:428:ASN:C	3:F:430:PRO:CD	2.87	0.43
1:G:236:GLN:HG3	1:G:241:GLY:O	2.18	0.43
1:G:273:GLY:O	1:G:275:ASP:N	2.46	0.43
2:H:327:SER:OG	3:I:238:LYS:HG3	2.19	0.43
3:I:294:LEU:O	3:I:298:ILE:HD13	2.19	0.43
2:B:159:LEU:CD1	2:B:160:LEU:N	2.79	0.43
2:B:314:LYS:HE3	3:C:162:LEU:CB	2.47	0.43
2:B:393:GLN:HG2	2:B:396:GLU:HB2	2.00	0.43
3:C:48:GLN:HA	3:C:51:LEU:HD12	1.99	0.43
1:D:102:VAL:CG1	1:D:118:VAL:HG13	2.49	0.43
1:D:121:SER:C	1:D:123:GLY:H	2.22	0.43
1:D:219:ARG:HB2	1:D:236:GLN:O	2.19	0.43
1:D:279:THR:HB	1:D:281:TRP:NE1	2.33	0.43
1:D:281:TRP:CD1	1:D:281:TRP:N	2.86	0.43
2:E:524:ASP:CA	2:E:527:LEU:HD12	2.35	0.43
1:G:102:VAL:CG1	1:G:118:VAL:HG13	2.49	0.43
1:G:108:ALA:HB1	1:G:112:TYR:HD1	1.84	0.43
2:H:138:ILE:HG23	2:H:141:GLU:OE2	2.18	0.43
1:G:264:LEU:HB3	2:H:509:ARG:NH1	2.33	0.43
3:C:294:LEU:O	3:C:298:ILE:HD12	2.18	0.42
1:D:108:ALA:HB1	1:D:112:TYR:HD1	1.84	0.42
1:D:229:ARG:NH1	1:D:252:LYS:HB3	2.34	0.42
2:E:197:VAL:HG11	2:E:210:ILE:HG12	2.01	0.42
2:E:516:THR:OG1	2:E:544:LYS:HE2	2.18	0.42
1:G:208:ARG:HE	1:G:258:TRP:HZ3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ARG:NH1	1:G:252:LYS:HB3	2.34	0.42
2:H:297:TYR:HE2	2:H:305:ARG:HH11	1.67	0.42
2:H:359:LYS:HG3	2:H:365:PRO:HA	2.01	0.42
2:B:396:GLU:N	2:B:396:GLU:OE1	2.51	0.42
2:B:177:THR:CG2	2:B:484:ALA:HB2	2.45	0.42
3:C:11:ARG:HD2	3:C:12:PHE:CE1	2.54	0.42
3:C:343:ILE:HD13	3:C:344:ARG:N	2.34	0.42
1:D:227:GLN:C	1:D:229:ARG:H	2.22	0.42
1:D:57:TRP:CH2	2:E:144:PHE:HE1	2.37	0.42
1:G:185:TRP:CE2	1:G:196:LEU:HD13	2.53	0.42
1:G:12:ILE:HG21	1:G:26:THR:HB	2.01	0.42
3:F:316:PRO:HB2	2:H:334:ASP:HB3	2.00	0.42
3:I:21:GLU:HG2	3:I:25:GLU:OE2	2.18	0.42
3:I:269:GLY:HA3	3:I:295:GLN:CG	2.42	0.42
3:I:358:VAL:O	3:I:361:SER:HB3	2.18	0.42
3:I:59:GLU:HA	3:I:62:VAL:CG2	2.42	0.42
1:A:108:ALA:HB1	1:A:112:TYR:HD1	1.85	0.42
1:A:229:ARG:NH1	1:A:252:LYS:HB3	2.34	0.42
2:B:153:PHE:HA	2:B:159:LEU:CD2	2.46	0.42
2:B:198:THR:O	2:B:211:SER:HB3	2.19	0.42
2:B:330:PRO:HA	2:B:333:ARG:HB2	2.02	0.42
2:B:399:LEU:O	2:B:403:VAL:HG23	2.19	0.42
3:C:42:PHE:CZ	3:C:391:HIS:HB3	2.55	0.42
1:D:217:LEU:CD2	2:E:475:PHE:HE1	2.31	0.42
2:E:202:ARG:HE	2:E:209:GLN:HB2	1.84	0.42
2:H:136:LYS:HB3	2:H:136:LYS:HE2	1.82	0.42
2:H:295:PHE:CE1	2:H:356:LYS:HB3	2.55	0.42
2:H:495:CYS:C	2:H:497:LEU:H	2.23	0.42
3:I:16:SER:O	3:I:19:LEU:HB2	2.20	0.42
2:H:320:VAL:HG11	3:I:211:ILE:HD13	2.02	0.42
1:A:100:ALA:CB	1:A:121:SER:HB2	2.50	0.42
1:A:233:ILE:HD11	1:A:248:LEU:CD1	2.48	0.42
1:A:236:GLN:HG3	1:A:241:GLY:O	2.18	0.42
2:B:142:ARG:O	2:B:143:ARG:HB2	2.19	0.42
2:B:150:PHE:CZ	2:B:170:VAL:HG12	2.54	0.42
2:B:314:LYS:HE3	3:C:162:LEU:HD22	2.01	0.42
2:E:495:CYS:C	2:E:497:LEU:H	2.23	0.42
3:F:10:GLU:O	3:F:12:PHE:N	2.52	0.42
3:F:150:SER:O	3:F:151:GLY:O	2.37	0.42
3:F:294:LEU:O	3:F:298:ILE:HD13	2.20	0.42
3:F:354:SER:O	3:F:358:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:364:GLU:C	3:F:366:LEU:H	2.23	0.42
1:G:109:PRO:O	1:G:111:GLU:N	2.52	0.42
1:G:100:ALA:CB	1:G:121:SER:HB2	2.49	0.42
3:I:28:ASN:O	3:I:29:GLU:O	2.38	0.42
3:I:53:LEU:O	3:I:61:ASN:HB3	2.20	0.42
1:A:121:SER:C	1:A:123:GLY:H	2.22	0.42
2:B:295:PHE:CE1	2:B:356:LYS:HB3	2.54	0.42
3:C:220:ASN:HA	3:C:221:PRO:HD3	1.88	0.42
1:D:212:TRP:HA	1:D:222:LEU:HD22	1.92	0.42
2:E:330:PRO:HA	2:E:333:ARG:HB2	2.01	0.42
3:F:221:PRO:HG3	3:F:231:PHE:HB2	2.01	0.42
3:F:93:GLU:CG	3:F:94:MET:H	2.31	0.42
2:H:250:THR:HG23	3:I:99:TYR:CZ	2.55	0.42
2:H:396:GLU:OE1	2:H:396:GLU:N	2.52	0.42
3:I:428:ASN:C	3:I:430:PRO:CD	2.87	0.42
1:A:232:ILE:HG21	1:A:234:TRP:CZ2	2.53	0.42
2:B:527:LEU:O	2:B:530:LEU:HB2	2.20	0.42
3:C:227:ILE:O	3:C:229:ASN:N	2.53	0.42
3:C:298:ILE:H	3:C:298:ILE:HD12	1.85	0.42
1:D:109:PRO:O	1:D:111:GLU:N	2.52	0.42
1:D:141:ILE:HD12	1:D:185:TRP:CE3	2.54	0.42
1:D:15:ALA:CB	1:D:26:THR:HG22	2.49	0.42
1:D:61:TRP:N	1:D:61:TRP:CD1	2.87	0.42
1:G:15:ALA:CB	1:G:26:THR:HG22	2.49	0.42
2:H:175:LEU:CD1	2:H:176:PRO:HD2	2.42	0.42
2:H:197:VAL:HG21	2:H:492:PHE:CZ	2.55	0.42
3:I:8:GLN:O	3:I:10:GLU:N	2.52	0.42
3:I:355:LEU:HA	3:I:355:LEU:HD12	1.84	0.42
3:I:82:LEU:HA	3:I:82:LEU:HD23	1.80	0.42
3:I:9:THR:HG22	3:I:423:GLN:OE1	2.20	0.42
1:A:289:TRP:CD1	1:A:289:TRP:N	2.87	0.42
2:B:208:PRO:HB3	2:B:531:LYS:CB	2.24	0.42
2:B:491:LEU:O	2:B:494:SER:HB2	2.19	0.42
3:C:305:ASN:O	3:C:306:ASN:C	2.56	0.42
3:C:355:LEU:HD12	3:C:355:LEU:HA	1.83	0.42
3:C:7:TYR:O	3:C:7:TYR:CD1	2.72	0.42
1:D:100:ALA:CB	1:D:121:SER:HB2	2.49	0.42
1:D:12:ILE:HG21	1:D:26:THR:HB	2.01	0.42
2:E:234:TRP:CZ3	2:E:452:TYR:CD1	3.08	0.42
2:E:467:LYS:HD2	2:E:498:ASN:HB3	2.01	0.42
1:G:121:SER:C	1:G:123:GLY:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ARG:CG	1:G:256:VAL:HA	2.50	0.42
1:G:61:TRP:N	1:G:61:TRP:CD1	2.87	0.42
2:H:225:GLU:C	2:H:227:THR:N	2.73	0.42
3:I:237:ILE:CD1	3:I:237:ILE:C	2.75	0.42
1:A:170:SER:HA	1:A:186:LYS:HE3	2.00	0.42
2:B:202:ARG:CG	2:B:500:ASP:OD1	2.67	0.42
3:C:206:ILE:N	3:C:206:ILE:HD12	2.35	0.42
1:D:20:TYR:CD1	1:D:20:TYR:N	2.87	0.42
1:D:289:TRP:CD1	1:D:289:TRP:N	2.87	0.42
2:E:175:LEU:CD1	2:E:176:PRO:HD2	2.42	0.42
2:E:265:HIS:CB	2:E:399:LEU:HD21	2.42	0.42
2:E:197:VAL:HG21	2:E:492:PHE:CZ	2.55	0.42
3:F:35:PRO:HB2	3:F:399:ILE:HG12	2.00	0.42
3:I:150:SER:O	3:I:151:GLY:O	2.37	0.42
1:A:141:ILE:HD12	1:A:185:TRP:CZ3	2.54	0.42
1:A:205:ASP:CG	1:A:227:GLN:HB3	2.40	0.42
2:B:197:VAL:HG11	2:B:210:ILE:HG12	2.02	0.42
2:B:495:CYS:C	2:B:497:LEU:H	2.23	0.42
3:C:221:PRO:HG3	3:C:231:PHE:HB2	2.01	0.42
2:E:276:ILE:O	2:E:277:GLY:C	2.58	0.42
2:E:318:LEU:HD11	2:E:357:ILE:HD12	2.01	0.42
2:E:359:LYS:HG3	2:E:365:PRO:HA	2.01	0.42
1:G:79:VAL:CG2	1:G:102:VAL:HG11	2.49	0.42
1:G:205:ASP:CG	1:G:227:GLN:HB3	2.40	0.42
1:G:282:LYS:NZ	2:H:178:GLU:OE2	2.53	0.42
1:A:112:TYR:CZ	1:A:171:ARG:HG2	2.54	0.42
1:A:202:GLY:HA3	1:A:245:LYS:HE3	2.02	0.42
1:A:277:LYS:HG3	1:A:278:VAL:N	2.35	0.42
1:A:285:LEU:CD1	1:A:285:LEU:H	2.27	0.42
1:A:282:LYS:CD	1:A:292:ALA:HB2	2.50	0.42
2:B:128:CYS:O	2:B:132:ILE:HG13	2.20	0.42
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.79	0.42
3:C:42:PHE:HD2	3:C:42:PHE:HA	1.76	0.42
1:D:229:ARG:CG	1:D:256:VAL:HA	2.50	0.42
1:D:55:PRO:HD3	2:E:138:ILE:HD13	2.00	0.42
3:F:125:TRP:O	3:F:128:GLU:HB3	2.20	0.42
3:F:195:GLU:OE2	3:F:195:GLU:N	2.44	0.42
3:F:17:ASP:O	3:F:20:LYS:HB2	2.20	0.42
3:F:20:LYS:O	3:F:24:ILE:HG12	2.20	0.42
3:F:116:LEU:CD2	3:F:294:LEU:CD1	2.95	0.42
3:F:419:LEU:HA	3:F:422:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:LEU:CD1	1:G:285:LEU:H	2.27	0.42
2:H:202:ARG:HE	2:H:209:GLN:HB2	1.84	0.42
1:G:216:VAL:HG23	2:H:505:ASP:OD2	2.20	0.42
2:H:317:HIS:ND1	3:I:159:ASP:OD1	2.53	0.42
2:B:297:TYR:HE2	2:B:305:ARG:HH11	1.67	0.41
2:B:197:VAL:HG21	2:B:492:PHE:CZ	2.55	0.41
3:C:187:LEU:HD23	3:C:187:LEU:HA	1.93	0.41
3:C:102:ARG:HH22	3:C:241:SER:H	1.68	0.41
3:C:378:ASP:HB3	3:C:381:ASP:OD2	2.19	0.41
3:C:439:SER:C	3:C:441:CYS:N	2.73	0.41
2:E:198:THR:O	2:E:211:SER:HB3	2.19	0.41
2:E:295:PHE:CE1	2:E:356:LYS:HB3	2.55	0.41
3:F:259:TYR:O	3:F:263:ILE:HG13	2.20	0.41
2:H:291:ILE:HD12	2:H:291:ILE:N	2.20	0.41
2:H:491:LEU:O	2:H:494:SER:HB2	2.20	0.41
2:H:527:LEU:O	2:H:530:LEU:HB2	2.20	0.41
3:I:235:GLN:HG2	3:I:236:GLY:H	1.85	0.41
3:I:8:GLN:O	3:I:11:ARG:HG2	2.21	0.41
1:A:200:LEU:HD11	1:A:243:TRP:CG	2.55	0.41
1:A:229:ARG:CG	1:A:256:VAL:HA	2.50	0.41
2:B:142:ARG:HH11	2:B:142:ARG:HG3	1.84	0.41
2:B:187:ASP:HB3	2:B:523:ASN:HD22	1.82	0.41
2:B:359:LYS:HG3	2:B:365:PRO:HA	2.01	0.41
3:C:125:TRP:O	3:C:128:GLU:HB3	2.20	0.41
3:C:150:SER:O	3:C:151:GLY:O	2.37	0.41
3:C:323:THR:O	3:C:327:VAL:HG23	2.20	0.41
3:C:341:HIS:HA	3:C:342:PRO:HD3	1.90	0.41
3:C:359:ILE:HG21	3:C:404:VAL:HG11	2.03	0.41
1:D:205:ASP:CG	1:D:227:GLN:HB3	2.40	0.41
1:D:282:LYS:CD	1:D:292:ALA:HB2	2.50	0.41
2:E:527:LEU:O	2:E:530:LEU:HB2	2.19	0.41
3:F:288:ILE:O	3:F:291:ASN:HB3	2.21	0.41
1:G:200:LEU:HD11	1:G:243:TRP:CG	2.55	0.41
2:H:198:THR:O	2:H:211:SER:HB3	2.19	0.41
3:I:227:ILE:O	3:I:229:ASN:N	2.53	0.41
1:A:140:ILE:CG2	1:A:141:ILE:H	2.33	0.41
2:B:225:GLU:C	2:B:227:THR:N	2.73	0.41
2:B:276:ILE:O	2:B:277:GLY:C	2.59	0.41
2:B:359:LYS:HA	2:B:359:LYS:HD2	1.80	0.41
2:B:468:GLU:OE1	2:B:468:GLU:N	2.47	0.41
3:C:39:ILE:HA	3:C:42:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ILE:HG22	1:D:235:THR:HG23	2.03	0.41
2:E:527:LEU:C	2:E:529:ARG:N	2.71	0.41
3:F:322:LEU:HA	3:F:322:LEU:HD23	1.77	0.41
3:F:39:ILE:HA	3:F:42:PHE:HB2	2.02	0.41
1:G:151:ALA:HA	1:G:174:VAL:O	2.20	0.41
1:G:277:LYS:HG3	1:G:278:VAL:N	2.35	0.41
2:H:139:MET:CG	2:H:144:PHE:O	2.47	0.41
2:H:155:THR:C	2:H:513:ARG:HD2	2.38	0.41
3:I:125:TRP:O	3:I:128:GLU:HB3	2.20	0.41
3:I:12:PHE:CD1	3:I:12:PHE:N	2.70	0.41
3:I:298:ILE:H	3:I:298:ILE:HD12	1.84	0.41
3:I:39:ILE:HA	3:I:42:PHE:HB2	2.02	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.21	0.41
2:B:512:MET:O	2:B:515:ILE:HG12	2.20	0.41
3:C:50:ALA:HB1	3:C:69:GLU:CG	2.49	0.41
3:C:68:TRP:CH2	3:C:387:ARG:NH2	2.89	0.41
1:D:79:VAL:CG2	1:D:102:VAL:HG11	2.49	0.41
1:D:277:LYS:HG3	1:D:278:VAL:N	2.35	0.41
2:E:197:VAL:CG1	2:E:210:ILE:HG23	2.51	0.41
2:H:159:LEU:CD1	2:H:160:LEU:N	2.79	0.41
2:H:208:PRO:HB3	2:H:531:LYS:CB	2.25	0.41
2:H:208:PRO:O	2:H:209:GLN:CB	2.68	0.41
3:I:281:ASP:O	3:I:282:TRP:C	2.59	0.41
1:A:208:ARG:HE	1:A:258:TRP:HZ3	1.67	0.41
1:A:283:GLU:HB2	1:A:289:TRP:CH2	2.56	0.41
3:C:288:ILE:O	3:C:291:ASN:HB3	2.21	0.41
3:C:421:LYS:O	3:C:424:GLY:N	2.44	0.41
1:D:200:LEU:HD11	1:D:243:TRP:CG	2.55	0.41
1:D:283:GLU:HB2	1:D:289:TRP:CH2	2.56	0.41
2:E:291:ILE:N	2:E:291:ILE:HD12	2.21	0.41
3:F:143:LYS:HE3	3:F:144:TRP:CD1	2.54	0.41
3:F:323:THR:O	3:F:327:VAL:HG23	2.20	0.41
3:F:432:TYR:O	3:F:435:PHE:HD1	2.04	0.41
1:G:212:TRP:HA	1:G:222:LEU:HD22	1.92	0.41
1:G:233:ILE:HG22	1:G:235:THR:HG23	2.03	0.41
2:H:198:THR:HG22	2:H:198:THR:O	2.20	0.41
2:H:276:ILE:O	2:H:277:GLY:C	2.59	0.41
2:H:359:LYS:HD2	2:H:359:LYS:HA	1.80	0.41
3:I:102:ARG:HH22	3:I:241:SER:H	1.68	0.41
3:I:259:TYR:O	3:I:263:ILE:HG13	2.20	0.41
1:A:253:PHE:C	1:A:255:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:ASP:OD1	2:B:331:ARG:HB2	2.20	0.41
2:B:545:ASP:O	2:B:549:GLY:N	2.49	0.41
3:C:15:PHE:H	3:C:15:PHE:HD1	1.68	0.41
2:B:320:VAL:CG2	3:C:246:THR:HG22	2.45	0.41
1:D:202:GLY:HA3	1:D:245:LYS:HE3	2.02	0.41
1:D:63:HIS:C	1:D:65:LYS:N	2.74	0.41
2:E:248:TYR:CD2	2:E:248:TYR:N	2.88	0.41
2:E:319:SER:OG	3:F:246:THR:HG23	2.21	0.41
2:E:202:ARG:CG	2:E:500:ASP:OD1	2.67	0.41
3:F:227:ILE:O	3:F:229:ASN:N	2.53	0.41
3:F:363:VAL:HG12	3:F:364:GLU:N	2.35	0.41
1:G:202:GLY:HA3	1:G:245:LYS:HE3	2.02	0.41
1:G:63:HIS:C	1:G:65:LYS:N	2.74	0.41
2:H:197:VAL:HG11	2:H:210:ILE:HG12	2.02	0.41
2:H:406:HIS:CE1	2:H:410:PHE:CE1	3.09	0.41
1:G:19:TYR:CD2	2:H:543:LEU:CD2	3.03	0.41
3:I:21:GLU:HA	3:I:25:GLU:HG3	2.02	0.41
1:A:63:HIS:C	1:A:65:LYS:N	2.74	0.41
2:B:197:VAL:CG1	2:B:210:ILE:HG23	2.51	0.41
3:C:259:TYR:O	3:C:263:ILE:HG13	2.20	0.41
3:C:432:TYR:O	3:C:435:PHE:HD1	2.03	0.41
3:C:50:ALA:O	3:C:54:ALA:HB2	2.21	0.41
2:E:364:SER:HB3	2:E:367:GLU:HB2	2.02	0.41
2:E:491:LEU:O	2:E:494:SER:HB2	2.19	0.41
3:F:317:LEU:HA	3:F:318:PRO:HD2	1.90	0.41
3:F:379:ILE:C	3:F:381:ASP:H	2.23	0.41
3:F:50:ALA:O	3:F:54:ALA:HB2	2.21	0.41
1:G:282:LYS:CD	1:G:292:ALA:HB2	2.50	0.41
1:G:31:LYS:HA	1:G:56:VAL:HG23	2.03	0.41
2:H:197:VAL:CG1	2:H:210:ILE:HG23	2.51	0.41
2:H:234:TRP:CZ3	2:H:452:TYR:CD1	3.08	0.41
2:H:468:GLU:OE1	2:H:468:GLU:N	2.46	0.41
2:H:513:ARG:HG2	2:H:513:ARG:O	2.21	0.41
3:I:21:GLU:HB3	3:I:25:GLU:CD	2.40	0.41
3:I:221:PRO:HG3	3:I:231:PHE:HB2	2.01	0.41
3:I:50:ALA:O	3:I:54:ALA:HB2	2.21	0.41
2:B:160:LEU:CD2	2:B:172:ILE:HA	2.50	0.41
2:B:406:HIS:CE1	2:B:410:PHE:CE1	3.09	0.41
1:D:118:VAL:O	1:D:125:VAL:HG13	2.21	0.41
2:E:225:GLU:C	2:E:227:THR:N	2.73	0.41
2:H:160:LEU:CD2	2:H:172:ILE:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:ASP:HB3	2:H:523:ASN:HD22	1.82	0.41
1:A:118:VAL:O	1:A:125:VAL:HG13	2.21	0.41
1:A:233:ILE:HG22	1:A:235:THR:HG23	2.03	0.41
1:A:96:ALA:O	1:A:98:HIS:N	2.52	0.41
3:C:280:SER:CB	3:C:284:SER:HB3	2.41	0.41
1:D:78:LYS:CA	1:D:96:ALA:HB2	2.42	0.41
2:E:198:THR:HG22	2:E:198:THR:O	2.20	0.41
2:E:495:CYS:O	2:E:497:LEU:N	2.54	0.41
2:E:512:MET:O	2:E:515:ILE:HG12	2.21	0.41
2:E:513:ARG:HG2	2:E:513:ARG:O	2.21	0.41
3:F:14:LYS:O	3:F:17:ASP:HB3	2.21	0.41
3:F:220:ASN:HA	3:F:221:PRO:HD3	1.87	0.41
1:G:270:ALA:HB2	2:H:153:PHE:CE1	2.55	0.41
2:H:299:LEU:CD2	2:H:387:LEU:HD21	2.46	0.41
2:H:512:MET:O	2:H:515:ILE:HG12	2.20	0.41
3:I:145:LEU:HD12	3:I:145:LEU:HA	1.75	0.41
3:I:323:THR:O	3:I:327:VAL:HG23	2.20	0.41
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.21	0.41
2:B:198:THR:HG22	2:B:198:THR:O	2.20	0.41
1:A:265:SER:O	2:B:483:PHE:CZ	2.74	0.41
2:B:495:CYS:O	2:B:497:LEU:N	2.54	0.41
3:C:145:LEU:HA	3:C:145:LEU:HD12	1.75	0.41
1:D:77:GLY:CA	1:D:100:ALA:O	2.67	0.41
1:D:271:LEU:O	1:D:278:VAL:HG13	2.21	0.41
1:D:31:LYS:HA	1:D:56:VAL:HG23	2.03	0.41
2:E:199:ILE:HG22	2:E:209:GLN:H	1.86	0.41
2:E:208:PRO:O	2:E:209:GLN:CB	2.68	0.41
2:E:342:LYS:CD	3:F:206:ILE:HD11	2.51	0.41
3:F:187:LEU:HA	3:F:187:LEU:HD23	1.92	0.41
1:G:283:GLU:HB2	1:G:289:TRP:CH2	2.55	0.41
2:H:250:THR:HG21	2:H:255:VAL:CB	2.50	0.41
2:H:265:HIS:HB2	2:H:399:LEU:CD2	2.42	0.41
1:A:61:TRP:CD1	1:A:61:TRP:N	2.87	0.41
2:B:162:LYS:HE2	2:B:164:ILE:CG2	2.51	0.41
2:B:234:TRP:CZ3	2:B:452:TYR:CD1	3.08	0.41
2:B:250:THR:HG21	2:B:255:VAL:CB	2.50	0.41
2:B:392:GLY:O	2:B:393:GLN:HB3	2.19	0.41
2:B:513:ARG:HG2	2:B:513:ARG:O	2.21	0.41
3:C:281:ASP:O	3:C:282:TRP:C	2.60	0.41
1:D:253:PHE:C	1:D:255:ASP:H	2.24	0.41
2:E:314:LYS:HG2	3:F:162:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:355:LEU:HD12	3:F:355:LEU:HA	1.84	0.41
3:F:419:LEU:O	3:F:423:GLN:HB2	2.21	0.41
3:F:58:ASP:HB2	3:F:60:SER:H	1.85	0.41
1:G:60:ASP:H	1:G:70:LEU:CD1	2.34	0.41
2:H:199:ILE:HG22	2:H:209:GLN:H	1.86	0.41
2:H:343:TRP:C	2:H:345:THR:H	2.24	0.41
3:I:288:ILE:O	3:I:291:ASN:HB3	2.21	0.41
3:I:362:SER:O	3:I:365:MET:HB3	2.21	0.41
1:A:79:VAL:CG2	1:A:102:VAL:HG11	2.49	0.40
2:B:199:ILE:HG22	2:B:209:GLN:H	1.86	0.40
2:B:389:LEU:HA	2:B:389:LEU:HD23	1.86	0.40
3:C:48:GLN:O	3:C:51:LEU:HB2	2.21	0.40
1:D:151:ALA:HA	1:D:174:VAL:O	2.20	0.40
2:E:525:HIS:O	2:E:527:LEU:N	2.54	0.40
3:F:88:ASP:O	3:F:90:ASP:N	2.54	0.40
2:H:153:PHE:HE2	2:H:175:LEU:HD22	1.86	0.40
3:I:432:TYR:O	3:I:435:PHE:HD1	2.04	0.40
1:A:71:ALA:HB2	1:A:107:TRP:CZ2	2.57	0.40
2:B:208:PRO:O	2:B:209:GLN:CB	2.69	0.40
1:D:95:HIS:CG	1:D:128:VAL:HG21	2.57	0.40
1:D:151:ALA:CB	1:D:175:THR:HG22	2.51	0.40
1:D:285:LEU:CD1	1:D:285:LEU:H	2.27	0.40
2:E:142:ARG:HG2	2:E:144:PHE:CE1	2.54	0.40
2:E:202:ARG:HD2	2:E:500:ASP:OD1	2.21	0.40
2:E:517:LEU:HD12	2:E:517:LEU:N	2.36	0.40
1:G:155:PRO:HG3	1:G:214:PRO:HA	2.02	0.40
1:G:71:ALA:HB2	1:G:107:TRP:CZ2	2.56	0.40
2:H:138:ILE:O	2:H:142:ARG:HB2	2.20	0.40
2:H:495:CYS:O	2:H:497:LEU:N	2.54	0.40
3:I:23:LYS:O	3:I:27:ASN:HB2	2.21	0.40
2:B:202:ARG:HD2	2:B:500:ASP:OD1	2.21	0.40
1:D:80:LEU:O	1:D:82:TRP:CD1	2.75	0.40
2:E:160:LEU:CD2	2:E:172:ILE:HA	2.50	0.40
2:E:285:ARG:NH1	2:E:285:ARG:HG3	2.33	0.40
2:E:392:GLY:O	2:E:393:GLN:HB3	2.19	0.40
1:G:253:PHE:C	1:G:255:ASP:H	2.24	0.40
2:H:220:ALA:O	2:H:224:MET:HG3	2.22	0.40
2:H:190:LEU:CD1	2:H:492:PHE:HD1	2.35	0.40
1:G:264:LEU:HB3	2:H:509:ARG:CZ	2.51	0.40
2:H:515:ILE:HD11	2:H:544:LYS:HB2	2.04	0.40
3:I:10:GLU:O	3:I:10:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:HD23	2:B:361:LEU:HD23	2.03	0.40
2:B:517:LEU:N	2:B:517:LEU:HD12	2.37	0.40
3:C:81:LEU:CD2	3:C:118:GLN:HG2	2.51	0.40
3:C:18:THR:O	3:C:19:LEU:C	2.59	0.40
1:D:205:ASP:O	1:D:206:TRP:C	2.60	0.40
1:D:71:ALA:HB2	1:D:107:TRP:CZ2	2.56	0.40
1:D:81:ILE:HG12	1:D:130:PHE:HZ	1.86	0.40
3:F:390:THR:O	3:F:394:ILE:HG12	2.22	0.40
1:G:205:ASP:O	1:G:206:TRP:C	2.60	0.40
3:I:251:SER:O	3:I:261:ARG:HD2	2.21	0.40
3:I:90:ASP:OD1	3:I:90:ASP:N	2.54	0.40
1:A:81:ILE:HG12	1:A:130:PHE:HZ	1.86	0.40
1:A:271:LEU:O	1:A:278:VAL:HG13	2.21	0.40
2:B:374:GLU:C	2:B:376:GLU:H	2.25	0.40
2:B:525:HIS:O	2:B:527:LEU:N	2.54	0.40
1:D:57:TRP:HD1	1:D:102:VAL:O	2.05	0.40
2:E:153:PHE:HE2	2:E:175:LEU:HD22	1.86	0.40
3:F:206:ILE:HD12	3:F:206:ILE:N	2.36	0.40
3:F:102:ARG:HH22	3:F:241:SER:H	1.68	0.40
1:G:118:VAL:O	1:G:125:VAL:HG13	2.21	0.40
1:G:81:ILE:HG12	1:G:130:PHE:HZ	1.86	0.40
2:H:517:LEU:N	2:H:517:LEU:HD12	2.37	0.40
3:I:212:LEU:HA	3:I:212:LEU:HD23	1.76	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	270/297 (91%)	199 (74%)	51 (19%)	20 (7%)	1 7
1	D	270/297 (91%)	200 (74%)	51 (19%)	19 (7%)	1 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	270/297 (91%)	200 (74%)	50 (18%)	20 (7%)	1	7
2	B	432/442 (98%)	346 (80%)	55 (13%)	31 (7%)	1	7
2	E	421/442 (95%)	343 (82%)	48 (11%)	30 (7%)	1	8
2	H	418/442 (95%)	339 (81%)	49 (12%)	30 (7%)	1	7
3	C	413/460 (90%)	341 (83%)	55 (13%)	17 (4%)	3	21
3	F	413/460 (90%)	343 (83%)	53 (13%)	17 (4%)	3	21
3	I	408/460 (89%)	334 (82%)	56 (14%)	18 (4%)	2	19
All	All	3315/3597 (92%)	2645 (80%)	468 (14%)	202 (6%)	1	12

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	254	PRO
2	B	209	GLN
2	B	348	CYS
2	B	367	GLU
2	B	370	PHE
2	B	392	GLY
2	B	393	GLN
2	B	428	ASN
2	B	513	ARG
3	C	9	THR
3	C	11	ARG
3	C	55	ASN
3	C	90	ASP
3	C	165	ASN
3	C	434	THR
1	D	254	PRO
2	E	209	GLN
2	E	348	CYS
2	E	367	GLU
2	E	370	PHE
2	E	392	GLY
2	E	393	GLN
2	E	428	ASN
2	E	513	ARG
2	E	550	ASN
3	F	8	GLN
3	F	9	THR

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Mol	Chain	Res	Type
3	F	11	ARG
3	F	55	ASN
3	F	165	ASN
3	F	434	THR
1	G	254	PRO
2	H	209	GLN
2	H	348	CYS
2	H	367	GLU
2	H	370	PHE
2	H	392	GLY
2	H	393	GLN
2	H	428	ASN
2	H	513	ARG
3	I	8	GLN
3	I	29	GLU
3	I	165	ASN
3	I	434	THR
1	A	97	VAL
1	A	110	HIS
1	A	248	LEU
2	B	139	MET
2	B	146	ALA
2	B	157	SER
2	B	182	LYS
2	B	183	PHE
2	B	205	ASN
2	B	220	ALA
2	B	277	GLY
2	B	328	ASN
2	B	347	GLY
2	B	515	ILE
2	B	531	LYS
2	B	535	GLN
3	C	151	GLY
3	C	226	GLN
1	D	97	VAL
1	D	110	HIS
1	D	248	LEU
2	E	157	SER
2	E	182	LYS
2	E	183	PHE
2	E	205	ASN

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Mol	Chain	Res	Type
2	E	220	ALA
2	E	277	GLY
2	E	328	ASN
2	E	347	GLY
2	E	515	ILE
2	E	531	LYS
2	E	535	GLN
3	F	90	ASP
3	F	151	GLY
3	F	226	GLN
1	G	97	VAL
1	G	110	HIS
1	G	248	LEU
2	H	143	ARG
2	H	157	SER
2	H	182	LYS
2	H	183	PHE
2	H	205	ASN
2	H	220	ALA
2	H	277	GLY
2	H	328	ASN
2	H	347	GLY
2	H	515	ILE
2	H	531	LYS
2	H	535	GLN
3	I	55	ASN
3	I	59	GLU
3	I	151	GLY
3	I	226	GLN
1	A	19	TYR
1	A	51	GLY
1	A	105	VAL
1	A	115	LEU
1	A	202	GLY
1	A	206	TRP
1	A	207	VAL
1	A	208	ARG
2	B	162	LYS
2	B	530	LEU
2	B	536	LEU
3	C	12	PHE
3	C	19	LEU

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Mol	Chain	Res	Type
1	D	19	TYR
1	D	51	GLY
1	D	105	VAL
1	D	115	LEU
1	D	202	GLY
1	D	206	TRP
1	D	207	VAL
1	D	208	ARG
2	E	162	LYS
2	E	530	LEU
2	E	536	LEU
3	F	21	GLU
3	F	87	ALA
1	G	19	TYR
1	G	51	GLY
1	G	105	VAL
1	G	115	LEU
1	G	202	GLY
1	G	206	TRP
1	G	207	VAL
1	G	208	ARG
2	H	162	LYS
2	H	530	LEU
2	H	536	LEU
3	I	57	GLY
3	I	93	GLU
3	I	383	PRO
2	B	144	PHE
2	B	164	ILE
2	B	496	PHE
2	B	508	LYS
2	B	516	THR
2	B	527	LEU
3	C	21	GLU
3	C	59	GLU
3	C	403	SER
1	D	11	LEU
2	E	164	ILE
2	E	496	PHE
2	E	508	LYS
2	E	516	THR
2	E	527	LEU

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Mol	Chain	Res	Type
3	F	403	SER
1	G	11	LEU
2	H	164	ILE
2	H	496	PHE
2	H	508	LYS
2	H	516	THR
2	H	527	LEU
3	I	92	ASP
3	I	403	SER
1	A	114	PRO
3	C	152	GLY
3	C	354	SER
1	D	114	PRO
3	F	20	LYS
3	F	152	GLY
3	F	354	SER
1	G	114	PRO
3	I	152	GLY
3	I	354	SER
3	I	422	LEU
1	A	64	PRO
1	A	83	LYS
1	A	192	GLN
1	A	243	TRP
1	A	276	ASN
3	C	333	SER
1	D	64	PRO
1	D	83	LYS
1	D	243	TRP
1	D	276	ASN
3	F	333	SER
1	G	64	PRO
1	G	83	LYS
1	G	192	GLN
1	G	243	TRP
1	G	276	ASN
3	I	333	SER
1	A	216	VAL
1	D	216	VAL
3	F	383	PRO
1	G	216	VAL
2	B	208	PRO

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Mol	Chain	Res	Type
2	E	208	PRO
2	H	208	PRO
2	E	329	ASP
2	H	329	ASP
3	C	383	PRO
3	I	382	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/252 (92%)	221 (95%)	12 (5%)	23	59
1	D	233/252 (92%)	222 (95%)	11 (5%)	26	62
1	G	233/252 (92%)	223 (96%)	10 (4%)	29	64
2	B	397/404 (98%)	362 (91%)	35 (9%)	10	36
2	E	386/404 (96%)	352 (91%)	34 (9%)	10	36
2	H	383/404 (95%)	350 (91%)	33 (9%)	10	38
3	C	387/425 (91%)	361 (93%)	26 (7%)	16	50
3	F	387/425 (91%)	359 (93%)	28 (7%)	14	47
3	I	382/425 (90%)	358 (94%)	24 (6%)	18	52
All	All	3021/3243 (93%)	2808 (93%)	213 (7%)	14	47

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	HIS
1	A	20	TYR
1	A	30	ASP
1	A	43	HIS
1	A	46	ILE
1	A	57	TRP
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	217	LEU
1	A	237	ASP
1	A	275	ASP
2	B	142	ARG
2	B	144	PHE
2	B	159	LEU
2	B	177	THR
2	B	197	VAL
2	B	199	ILE
2	B	202	ARG
2	B	227	THR
2	B	233	LEU
2	B	282	GLU
2	B	307	SER
2	B	328	ASN
2	B	335	LEU
2	B	340	LEU
2	B	350	ILE
2	B	367	GLU
2	B	369	LEU
2	B	370	PHE
2	B	399	LEU
2	B	407	LEU
2	B	414	TYR
2	B	418	ILE
2	B	430	ASN
2	B	439	ARG
2	B	447	VAL
2	B	452	TYR
2	B	455	GLN
2	B	463	ARG
2	B	468	GLU
2	B	490	SER
2	B	492	PHE
2	B	515	ILE
2	B	538	PHE
2	B	547	TYR
2	B	550	ASN
3	C	18	THR
3	C	26	GLN
3	C	34	ASP

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Mol	Chain	Res	Type
3	C	39	ILE
3	C	42	PHE
3	C	58	ASP
3	C	71	GLU
3	C	86	ASN
3	C	92	ASP
3	C	118	GLN
3	C	225	THR
3	C	226	GLN
3	C	232	ASN
3	C	237	ILE
3	C	274	GLN
3	C	278	GLN
3	C	284	SER
3	C	293	ILE
3	C	343	ILE
3	C	365	MET
3	C	379	ILE
3	C	387	ARG
3	C	395	CYS
3	C	404	VAL
3	C	422	LEU
3	C	429	ILE
1	D	9	ASN
1	D	20	TYR
1	D	30	ASP
1	D	43	HIS
1	D	46	ILE
1	D	57	TRP
1	D	85	GLU
1	D	188	ASN
1	D	217	LEU
1	D	237	ASP
1	D	275	ASP
2	E	142	ARG
2	E	143	ARG
2	E	145	THR
2	E	159	LEU
2	E	197	VAL
2	E	199	ILE
2	E	202	ARG
2	E	227	THR

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Mol	Chain	Res	Type
2	E	233	LEU
2	E	282	GLU
2	E	307	SER
2	E	328	ASN
2	E	335	LEU
2	E	340	LEU
2	E	350	ILE
2	E	367	GLU
2	E	369	LEU
2	E	370	PHE
2	E	399	LEU
2	E	407	LEU
2	E	414	TYR
2	E	418	ILE
2	E	430	ASN
2	E	439	ARG
2	E	447	VAL
2	E	452	TYR
2	E	455	GLN
2	E	463	ARG
2	E	468	GLU
2	E	490	SER
2	E	492	PHE
2	E	515	ILE
2	E	538	PHE
2	E	550	ASN
3	F	7	TYR
3	F	12	PHE
3	F	19	LEU
3	F	34	ASP
3	F	39	ILE
3	F	42	PHE
3	F	58	ASP
3	F	71	GLU
3	F	86	ASN
3	F	118	GLN
3	F	225	THR
3	F	226	GLN
3	F	232	ASN
3	F	237	ILE
3	F	274	GLN
3	F	278	GLN

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Mol	Chain	Res	Type
3	F	284	SER
3	F	293	ILE
3	F	310	THR
3	F	343	ILE
3	F	363	VAL
3	F	365	MET
3	F	387	ARG
3	F	395	CYS
3	F	400	ASN
3	F	404	VAL
3	F	423	GLN
3	F	429	ILE
1	G	20	TYR
1	G	30	ASP
1	G	43	HIS
1	G	46	ILE
1	G	57	TRP
1	G	85	GLU
1	G	188	ASN
1	G	217	LEU
1	G	237	ASP
1	G	275	ASP
2	H	132	ILE
2	H	139	MET
2	H	159	LEU
2	H	197	VAL
2	H	199	ILE
2	H	202	ARG
2	H	227	THR
2	H	233	LEU
2	H	282	GLU
2	H	307	SER
2	H	328	ASN
2	H	335	LEU
2	H	340	LEU
2	H	350	ILE
2	H	367	GLU
2	H	369	LEU
2	H	370	PHE
2	H	399	LEU
2	H	407	LEU
2	H	414	TYR

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Mol	Chain	Res	Type
2	H	418	ILE
2	H	430	ASN
2	H	439	ARG
2	H	447	VAL
2	H	452	TYR
2	H	455	GLN
2	H	463	ARG
2	H	468	GLU
2	H	490	SER
2	H	492	PHE
2	H	515	ILE
2	H	538	PHE
2	H	547	TYR
3	I	9	THR
3	I	12	PHE
3	I	34	ASP
3	I	39	ILE
3	I	42	PHE
3	I	71	GLU
3	I	86	ASN
3	I	90	ASP
3	I	93	GLU
3	I	118	GLN
3	I	225	THR
3	I	226	GLN
3	I	232	ASN
3	I	237	ILE
3	I	274	GLN
3	I	278	GLN
3	I	284	SER
3	I	293	ILE
3	I	310	THR
3	I	343	ILE
3	I	387	ARG
3	I	395	CYS
3	I	404	VAL
3	I	429	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

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Mol	Chain	Res	Type
1	A	13	HIS
1	A	63	HIS
3	C	235	GLN
1	D	9	ASN
1	D	149	ASN
2	E	328	ASN
3	F	300	ASN
1	G	9	ASN
2	H	328	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/297 (92%)	1.65	90 (32%) 0 0	103, 167, 201, 202	0
1	D	274/297 (92%)	1.78	95 (34%) 0 0	101, 185, 202, 202	0
1	G	274/297 (92%)	1.90	113 (41%) 0 0	127, 193, 202, 202	0
2	B	434/442 (98%)	0.18	11 (2%) 57 43	44, 102, 181, 202	2 (0%)
2	E	423/442 (95%)	0.40	32 (7%) 13 7	49, 94, 192, 202	2 (0%)
2	H	420/442 (95%)	0.83	76 (18%) 1 1	46, 122, 200, 202	2 (0%)
3	C	419/460 (91%)	0.12	12 (2%) 51 36	9, 95, 175, 202	19 (4%)
3	F	419/460 (91%)	0.19	19 (4%) 33 21	11, 96, 178, 201	19 (4%)
3	I	414/460 (90%)	0.11	15 (3%) 42 27	48, 95, 181, 202	0
All	All	3351/3597 (93%)	0.67	463 (13%) 2 2	9, 124, 201, 202	44 (1%)

All (463) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	148	VAL	10.6
1	D	73	CYS	10.5
1	D	41	GLU	10.2
1	D	136	THR	9.6
2	E	138	ILE	9.3
1	A	223	ALA	9.2
1	A	127	VAL	9.0
2	E	134	ASN	9.0
2	H	132	ILE	8.7
2	H	133	ASP	8.6
1	D	223	ALA	8.6
1	D	272	SER	8.5
1	D	72	SER	8.3
1	A	194	TYR	8.2
1	G	272	SER	8.2

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Mol	Chain	Res	Type	RSRZ
2	H	170	VAL	8.0
1	G	133	ASN	7.7
2	H	523	ASN	7.7
2	H	145	THR	7.6
1	A	128	VAL	7.5
1	D	273	GLY	7.5
1	G	134	GLY	7.4
1	G	72	SER	7.2
1	D	224	SER	7.1
2	E	133	ASP	7.0
2	H	172	ILE	6.9
1	G	273	GLY	6.9
1	A	136	THR	6.9
1	D	118	VAL	6.8
1	D	117	LEU	6.8
2	E	136	LYS	6.7
1	A	185	TRP	6.6
1	G	112	TYR	6.6
1	A	126	SER	6.6
1	A	70	LEU	6.5
1	G	201	GLU	6.5
2	H	134	ASN	6.4
1	G	144	HIS	6.4
2	H	135	ALA	6.4
1	A	138	PRO	6.3
2	H	150	PHE	6.3
2	E	130	ASP	6.3
2	H	547	TYR	6.2
1	G	147	GLY	6.1
1	G	41	GLU	6.1
1	D	135	THR	6.1
1	D	40	GLY	6.0
2	H	169	GLY	5.9
1	G	149	ASN	5.9
1	A	95	HIS	5.9
1	G	177	GLY	5.9
1	D	210	VAL	5.8
1	D	143	ALA	5.8
1	A	200	LEU	5.8
1	G	143	ALA	5.8
2	H	149	THR	5.8
1	D	74	SER	5.8

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Mol	Chain	Res	Type	RSRZ
2	E	144	PHE	5.8
2	H	162	LYS	5.7
1	G	89	TRP	5.6
1	G	82	TRP	5.6
1	D	32	THR	5.5
2	H	532	ILE	5.5
1	G	135	THR	5.5
2	E	139	MET	5.4
1	G	73	CYS	5.4
2	E	135	ALA	5.4
1	D	225	VAL	5.3
2	H	208	PRO	5.3
2	E	131	GLU	5.2
1	A	50	THR	5.2
1	G	98	HIS	5.2
1	A	193	THR	5.1
2	H	161	THR	5.1
3	F	432	TYR	5.1
2	E	168	SER	5.0
1	D	248	LEU	5.0
1	D	126	SER	4.9
2	H	163	ASP	4.9
2	H	537	ILE	4.9
1	G	33	ILE	4.9
2	E	132	ILE	4.9
1	A	260	ALA	4.8
1	D	271	LEU	4.8
1	G	119	ALA	4.8
2	E	145	THR	4.8
3	F	53	LEU	4.8
2	H	489	HIS	4.7
1	G	29	SER	4.7
2	H	171	SER	4.7
1	D	138	PRO	4.7
1	A	125	VAL	4.7
1	G	70	LEU	4.7
1	D	201	GLU	4.7
3	I	432	TYR	4.7
2	E	167	LYS	4.6
1	D	176	GLY	4.6
1	G	178	ALA	4.5
2	H	131	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	4.5
1	G	132	GLU	4.5
2	H	527	LEU	4.5
1	A	182	VAL	4.5
2	H	543	LEU	4.5
1	G	16	VAL	4.4
3	C	15	PHE	4.4
1	G	125	VAL	4.4
1	G	185	TRP	4.4
1	G	12	ILE	4.4
1	A	231	CYS	4.4
2	H	146	ALA	4.4
1	G	271	LEU	4.4
2	H	148	TYR	4.3
2	H	130	ASP	4.3
1	D	187	TYR	4.3
1	D	59	VAL	4.3
1	A	221	TYR	4.3
1	G	13	HIS	4.3
1	D	15	ALA	4.3
1	A	135	THR	4.3
1	A	195	VAL	4.2
1	G	90	SER	4.2
1	A	71	ALA	4.2
1	D	270	ALA	4.2
1	D	209	ASP	4.2
1	A	44	LYS	4.2
1	D	289	TRP	4.2
1	G	281	TRP	4.2
1	G	59	VAL	4.2
1	G	118	VAL	4.1
1	D	208	ARG	4.1
1	A	98	HIS	4.1
1	D	96	ALA	4.1
2	E	146	ALA	4.1
1	A	32	THR	4.0
1	D	151	ALA	4.0
1	G	56	VAL	4.0
1	A	144	HIS	4.0
1	G	103	ASN	4.0
3	F	15	PHE	4.0
2	H	136	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	28	SER	4.0
1	A	206	TRP	3.9
1	G	136	THR	3.9
1	A	270	ALA	3.9
1	D	13	HIS	3.9
1	D	279	THR	3.9
1	D	98	HIS	3.9
1	D	125	VAL	3.9
2	H	536	LEU	3.8
2	H	189	TYR	3.8
1	A	149	ASN	3.8
2	H	348	CYS	3.8
1	A	147	GLY	3.8
1	A	272	SER	3.8
2	H	147	SER	3.8
1	G	69	ILE	3.8
2	E	170	VAL	3.8
1	G	141	ILE	3.8
2	E	149	THR	3.7
1	D	102	VAL	3.7
1	D	173	PHE	3.7
2	E	148	TYR	3.7
1	D	33	ILE	3.7
1	G	243	TRP	3.6
2	E	137	LEU	3.6
3	C	53	LEU	3.6
1	G	8	HIS	3.6
1	A	148	VAL	3.6
1	D	275	ASP	3.6
2	H	183	PHE	3.6
1	A	196	LEU	3.6
1	G	274	GLY	3.6
2	H	166	GLY	3.5
1	A	141	ILE	3.5
2	B	145	THR	3.5
1	A	254	PRO	3.5
1	D	226	SER	3.5
2	E	147	SER	3.5
1	D	274	GLY	3.5
3	C	440	ASP	3.4
2	E	163	ASP	3.4
2	H	533	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	149	ASN	3.4
1	A	234	TRP	3.4
1	G	52	HIS	3.4
1	G	11	LEU	3.4
1	D	116	LEU	3.4
1	G	176	GLY	3.4
1	D	26	THR	3.4
1	G	92	ILE	3.4
1	D	114	PRO	3.4
1	A	243	TRP	3.3
2	H	206	PRO	3.3
1	A	199	THR	3.3
2	H	477	PHE	3.3
1	D	127	VAL	3.3
2	B	144	PHE	3.3
1	D	119	ALA	3.3
1	A	69	ILE	3.3
1	A	103	ASN	3.3
2	H	510	LEU	3.3
2	E	172	ILE	3.2
1	A	248	LEU	3.2
2	H	518	LEU	3.2
2	E	523	ASN	3.2
1	G	260	ALA	3.2
1	A	274	GLY	3.2
1	D	140	ILE	3.2
3	I	15	PHE	3.2
1	D	259	ARG	3.2
1	A	150	SER	3.2
1	A	208	ARG	3.2
1	A	201	GLU	3.2
1	G	87	GLY	3.1
2	H	165	VAL	3.1
1	D	12	ILE	3.1
1	D	80	LEU	3.1
1	D	281	TRP	3.1
2	H	173	LYS	3.1
1	D	177	GLY	3.1
1	A	118	VAL	3.1
1	G	26	THR	3.1
1	G	102	VAL	3.1
1	G	197	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	140	ILE	3.1
1	D	185	TRP	3.1
1	G	71	ALA	3.1
2	B	149	THR	3.1
3	I	430	PRO	3.0
3	C	87	ALA	3.0
3	I	433	ALA	3.0
2	E	140	LYS	3.0
1	A	181	LEU	3.0
1	D	52	HIS	3.0
1	D	69	ILE	3.0
1	G	113	GLY	3.0
1	D	97	VAL	3.0
2	B	527	LEU	3.0
2	E	150	PHE	3.0
1	G	86	ASN	3.0
2	H	196	LYS	3.0
1	A	37	GLU	3.0
2	H	164	ILE	2.9
2	H	137	LEU	2.9
1	D	250	GLU	2.9
1	D	56	VAL	2.9
1	D	81	ILE	2.9
1	A	241	GLY	2.9
3	I	59	GLU	2.9
1	G	248	LEU	2.9
1	A	129	GLU	2.9
3	F	8	GLN	2.9
2	H	178	GLU	2.9
3	I	435	PHE	2.9
1	D	133	ASN	2.9
1	G	193	THR	2.9
2	H	157	SER	2.9
1	D	78	LYS	2.9
1	D	153	TRP	2.9
1	A	176	GLY	2.9
1	G	25	ALA	2.9
2	E	348	CYS	2.8
2	H	177	THR	2.8
1	A	225	VAL	2.8
1	G	35	ILE	2.8
1	D	189	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	15	ALA	2.8
3	F	379	ILE	2.8
1	D	204	SER	2.8
1	G	194	TYR	2.8
1	G	189	SER	2.8
1	G	276	ASN	2.8
2	H	207	TYR	2.8
1	G	50	THR	2.8
2	B	546	ARG	2.8
3	C	420	LEU	2.8
1	D	194	TYR	2.8
1	G	293	GLY	2.8
1	D	58	ARG	2.8
2	H	199	ILE	2.8
2	H	144	PHE	2.8
2	H	139	MET	2.8
1	A	209	ASP	2.8
1	D	128	VAL	2.7
1	A	175	THR	2.7
1	G	47	ASP	2.7
3	F	423	GLN	2.7
1	G	226	SER	2.7
1	A	224	SER	2.7
1	D	28	SER	2.7
1	G	51	GLY	2.7
3	F	380	ILE	2.7
1	D	95	HIS	2.7
2	H	168	SER	2.7
2	H	548	GLU	2.7
1	G	88	ARG	2.7
1	G	257	LEU	2.6
2	H	484	ALA	2.6
1	A	192	GLN	2.6
1	A	276	ASN	2.6
1	G	9	ASN	2.6
2	B	547	TYR	2.6
1	G	188	ASN	2.6
1	A	210	VAL	2.6
1	A	269	LEU	2.6
1	G	45	LEU	2.6
3	C	39	ILE	2.6
1	D	137	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	180	ASN	2.6
1	G	150	SER	2.6
3	F	64	SER	2.6
1	G	192	GLN	2.6
2	B	179	LEU	2.6
3	C	19	LEU	2.6
3	F	59	GLU	2.5
3	F	394	ILE	2.5
2	E	162	LYS	2.5
3	I	416	TYR	2.5
2	H	517	LEU	2.5
1	G	57	TRP	2.5
1	G	34	LYS	2.5
1	G	91	GLN	2.5
1	A	207	VAL	2.5
1	D	103	ASN	2.5
1	A	96	ALA	2.5
1	G	80	LEU	2.5
2	E	392	GLY	2.5
1	A	99	SER	2.5
3	F	431	ILE	2.5
2	E	518	LEU	2.5
1	D	144	HIS	2.5
1	G	104	SER	2.5
3	I	425	LEU	2.5
3	I	381	ASP	2.5
1	A	222	LEU	2.4
1	G	49	LEU	2.4
1	G	279	THR	2.4
1	A	212	TRP	2.4
1	G	202	GLY	2.4
1	G	157	THR	2.4
1	A	261	SER	2.4
1	G	97	VAL	2.4
1	G	110	HIS	2.4
1	G	275	ASP	2.4
1	D	252	LYS	2.4
2	E	164	ILE	2.4
2	H	215	LEU	2.4
3	I	53	LEU	2.4
1	G	122	ASP	2.4
1	A	89	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	435	PHE	2.4
2	H	201	ALA	2.4
1	D	203	HIS	2.4
3	I	412	LEU	2.4
1	A	198	SER	2.4
2	H	167	LYS	2.4
3	C	54	ALA	2.4
1	G	128	VAL	2.3
1	A	49	LEU	2.3
1	D	47	ASP	2.3
2	H	174	ARG	2.3
3	F	412	LEU	2.3
3	I	428	ASN	2.3
3	C	398	ILE	2.3
1	A	116	LEU	2.3
1	A	233	ILE	2.3
2	H	138	ILE	2.3
1	A	114	PRO	2.3
1	G	225	VAL	2.3
3	C	439	SER	2.3
1	D	179	ASP	2.3
1	A	245	LYS	2.3
2	H	480	GLN	2.3
1	G	140	ILE	2.3
3	F	384	TYR	2.3
1	D	243	TRP	2.3
1	A	187	TYR	2.3
1	D	105	VAL	2.3
1	D	71	ALA	2.3
2	H	522	THR	2.3
1	A	204	SER	2.3
1	A	227	GLN	2.3
1	A	174	VAL	2.3
1	D	142	ASP	2.3
2	H	516	THR	2.3
2	H	530	LEU	2.3
1	A	13	HIS	2.3
2	H	496	PHE	2.3
1	G	280	LEU	2.3
1	G	53	GLU	2.2
1	D	184	ILE	2.2
2	H	190	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	417	ILE	2.2
1	D	178	ALA	2.2
1	G	124	LYS	2.2
2	H	481	LEU	2.2
1	G	146	ILE	2.2
1	D	132	GLU	2.2
1	A	137	SER	2.2
1	D	150	SER	2.2
2	H	185	PHE	2.2
1	G	240	GLN	2.2
2	E	169	GLY	2.2
1	A	258	TRP	2.2
1	D	70	LEU	2.2
1	G	99	SER	2.2
3	F	68	TRP	2.2
1	D	42	THR	2.2
3	F	391	HIS	2.2
1	G	74	SER	2.2
2	E	522	THR	2.2
3	F	19	LEU	2.2
3	I	19	LEU	2.2
1	A	130	PHE	2.2
1	A	251	GLU	2.2
2	B	140	LYS	2.2
2	H	153	PHE	2.2
1	D	57	TRP	2.2
2	H	159	LEU	2.2
1	G	131	LYS	2.2
2	H	367	GLU	2.2
1	D	269	LEU	2.2
1	A	82	TRP	2.2
3	I	426	TYR	2.2
1	A	220	SER	2.2
3	I	429	ILE	2.2
1	G	63	HIS	2.2
2	H	540	ALA	2.1
1	A	48	THR	2.1
1	G	196	LEU	2.1
1	A	191	ALA	2.1
1	D	278	VAL	2.1
2	B	147	SER	2.1
1	G	17	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	14	ASP	2.1
1	G	171	ARG	2.1
1	D	234	TRP	2.1
1	G	81	ILE	2.1
2	H	209	GLN	2.1
1	G	32	THR	2.1
3	F	359	ILE	2.1
2	B	392	GLY	2.1
1	A	211	ALA	2.1
2	H	392	GLY	2.1
3	F	362	SER	2.1
1	D	245	LYS	2.1
1	G	14	ASP	2.1
1	G	27	CYS	2.1
2	H	184	LEU	2.1
2	H	187	ASP	2.1
1	G	130	PHE	2.1
1	G	19	TYR	2.1
1	A	184	ILE	2.1
1	G	184	ILE	2.0
3	C	399	ILE	2.0
2	B	348	CYS	2.0
2	E	367	GLU	2.0
1	A	117	LEU	2.0
2	H	521	SER	2.0
1	G	292	ALA	2.0
1	G	114	PRO	2.0
1	A	84	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.