Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 05:04 pm GMT

PDB ID	:	4AQ9
EMDB ID	:	EMD-2072
Title	:	Gating movement in acetylcholine receptor analysed by time- resolved electron cryo-microscopy (open class)
Authors	:	Unwin, N.; Fujiyoshi, Y.
Deposited on	:	2012-04-13
Resolution	:	6.20 Å(reported)
Based on initial model	:	2BG9

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

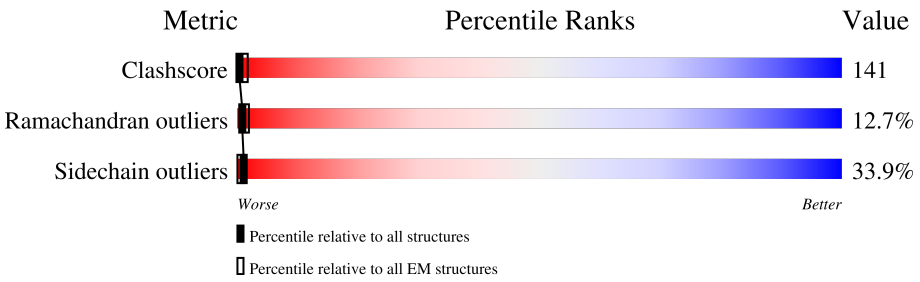
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	25%; • 24% 30% 23% 20%
1	D	461	21%; 5% 21% 30% 24% 20%
2	B	493	25%; 5% 21% 27% 23% 25%
3	C	522	25%; • 19% 26% 23% 29%
4	E	488	19%; • 21% 28% 24% 24%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14924 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	370	2991	1954	478	540	19	0	0
1	D	370	2991	1954	478	540	19	0	0

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR BETA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	370	2972	1938	465	554	15	0	0

- Molecule 3 is a protein called ACETYLCHOLINE RECEPTOR DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	370	2983	1944	489	536	14	0	1

- Molecule 4 is a protein called ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT.

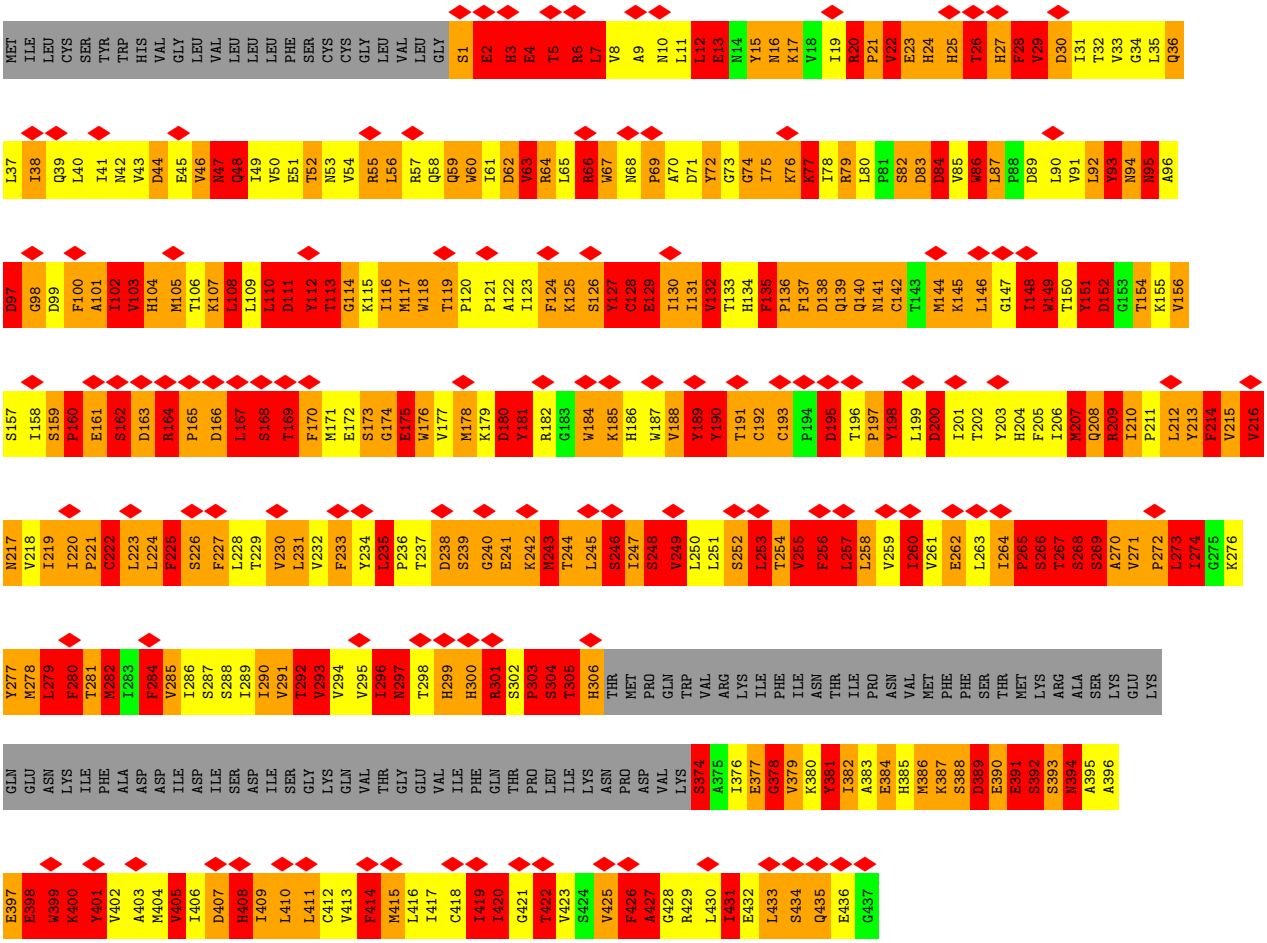
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	371	2987	1948	478	551	10	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

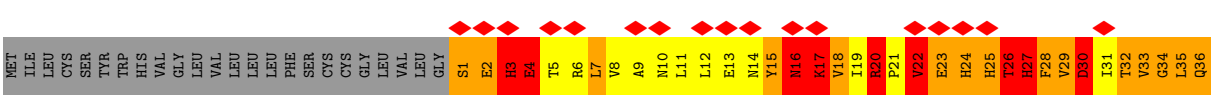
• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

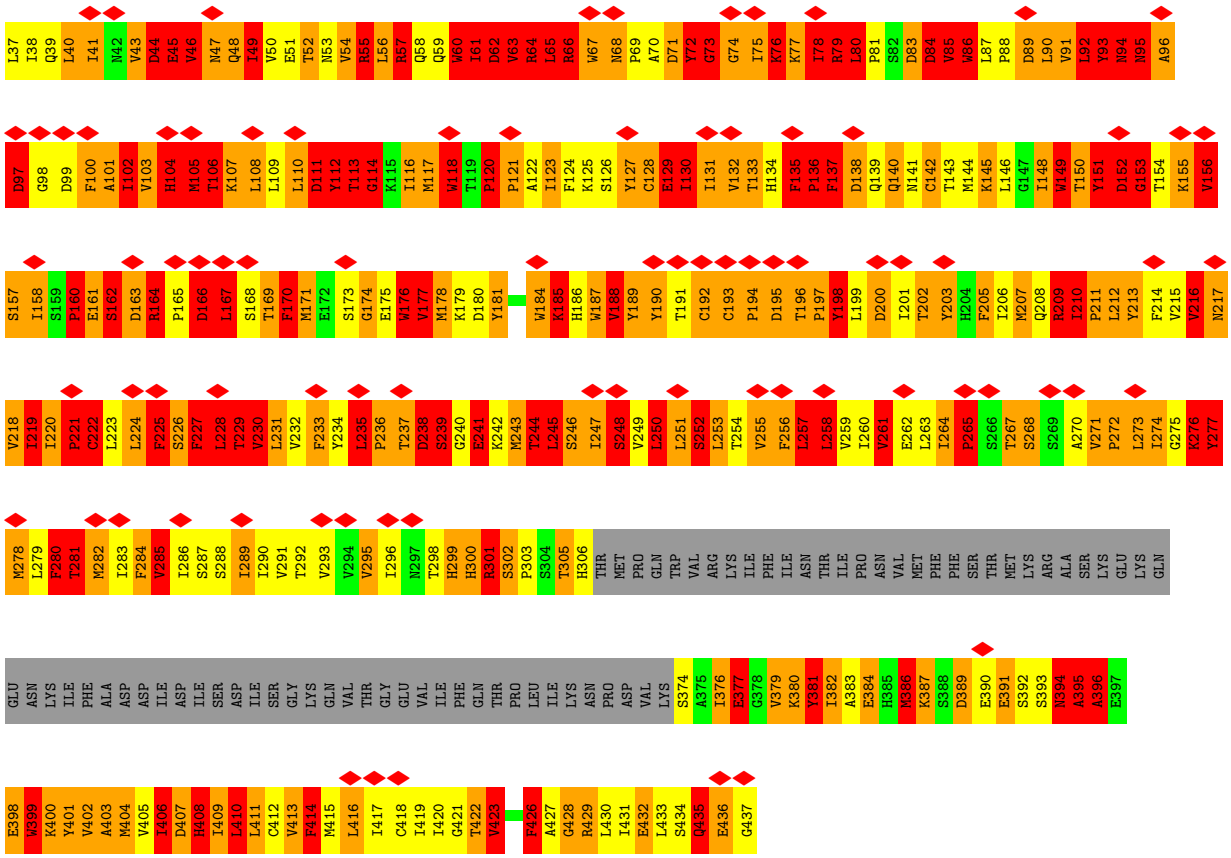
Chain A:



• Molecule 1: ACETYLCHOLINE RECEPTOR SUBUNIT ALPHA

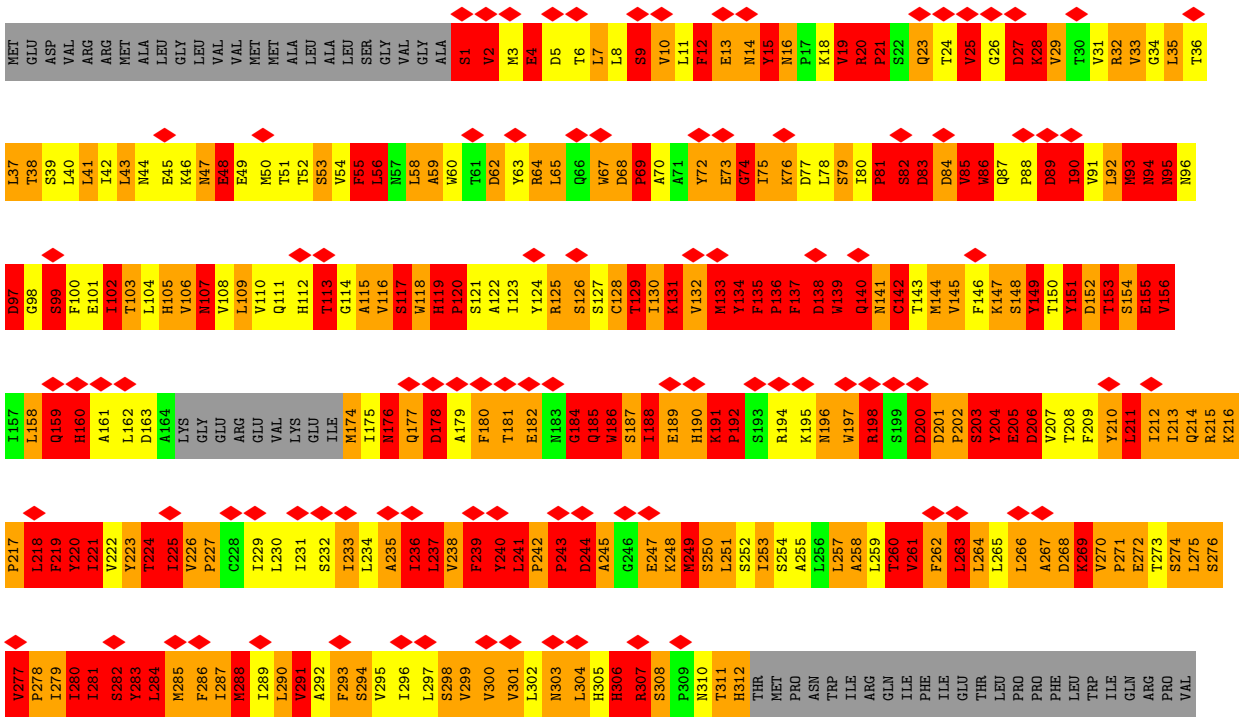
Chain D:

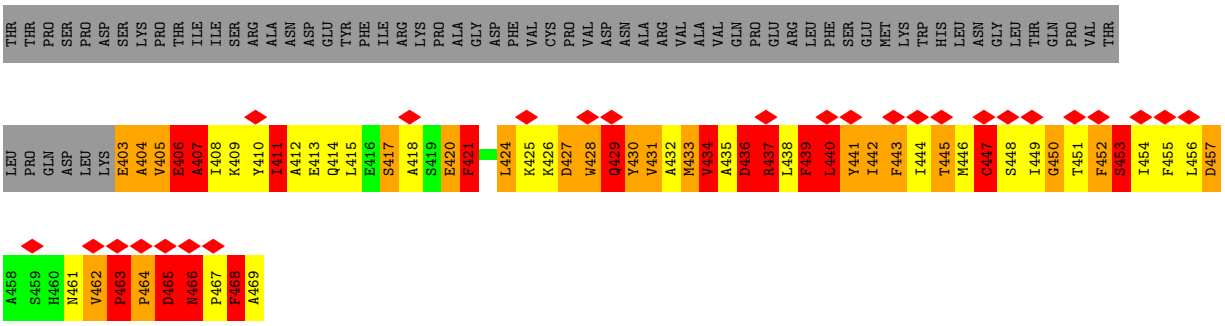




• Molecule 2: ACETYLCHOLINE RECEPTOR BETA SUBUNIT

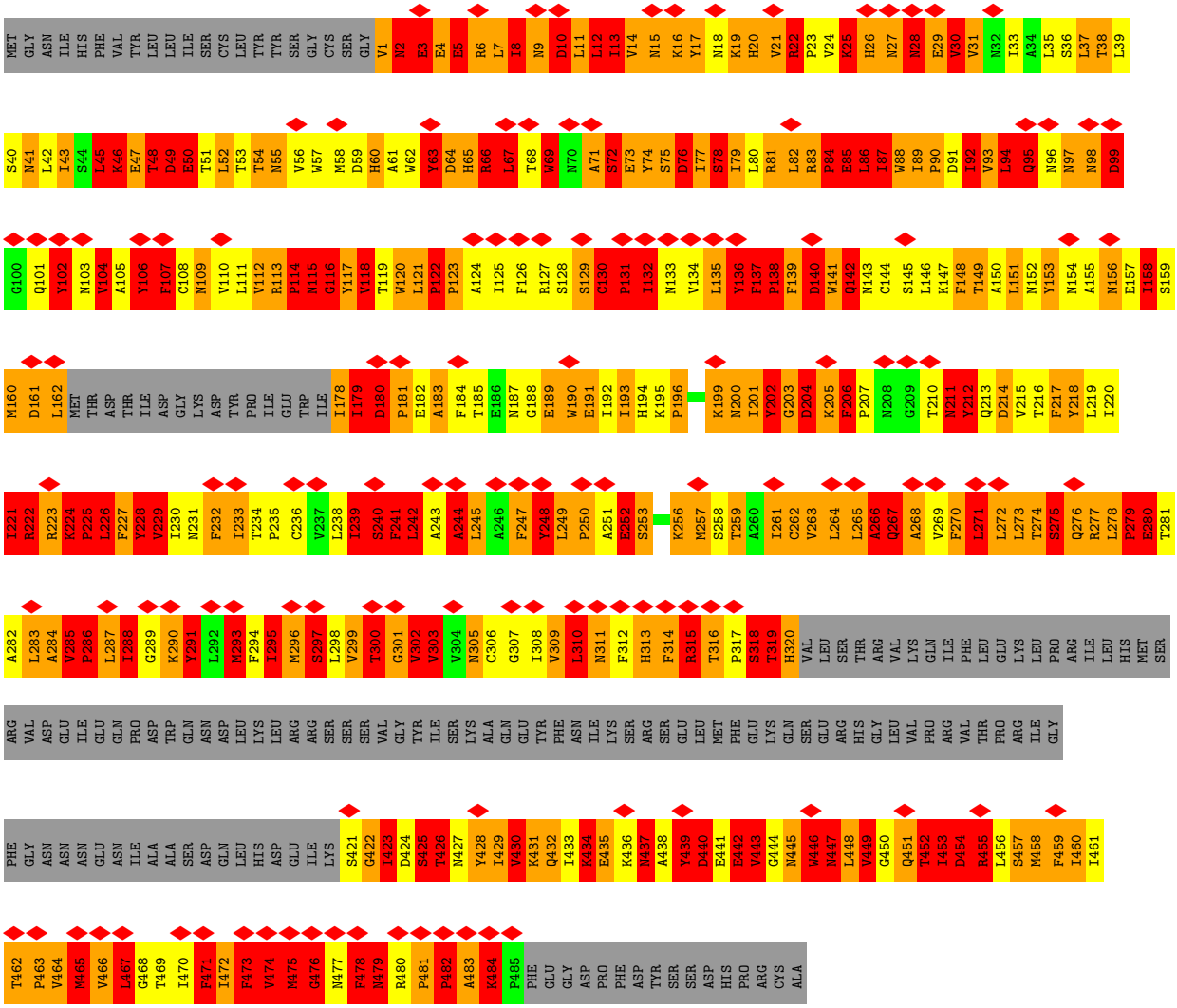
Chain B: 25% 5% 21% 27% 23% 25%





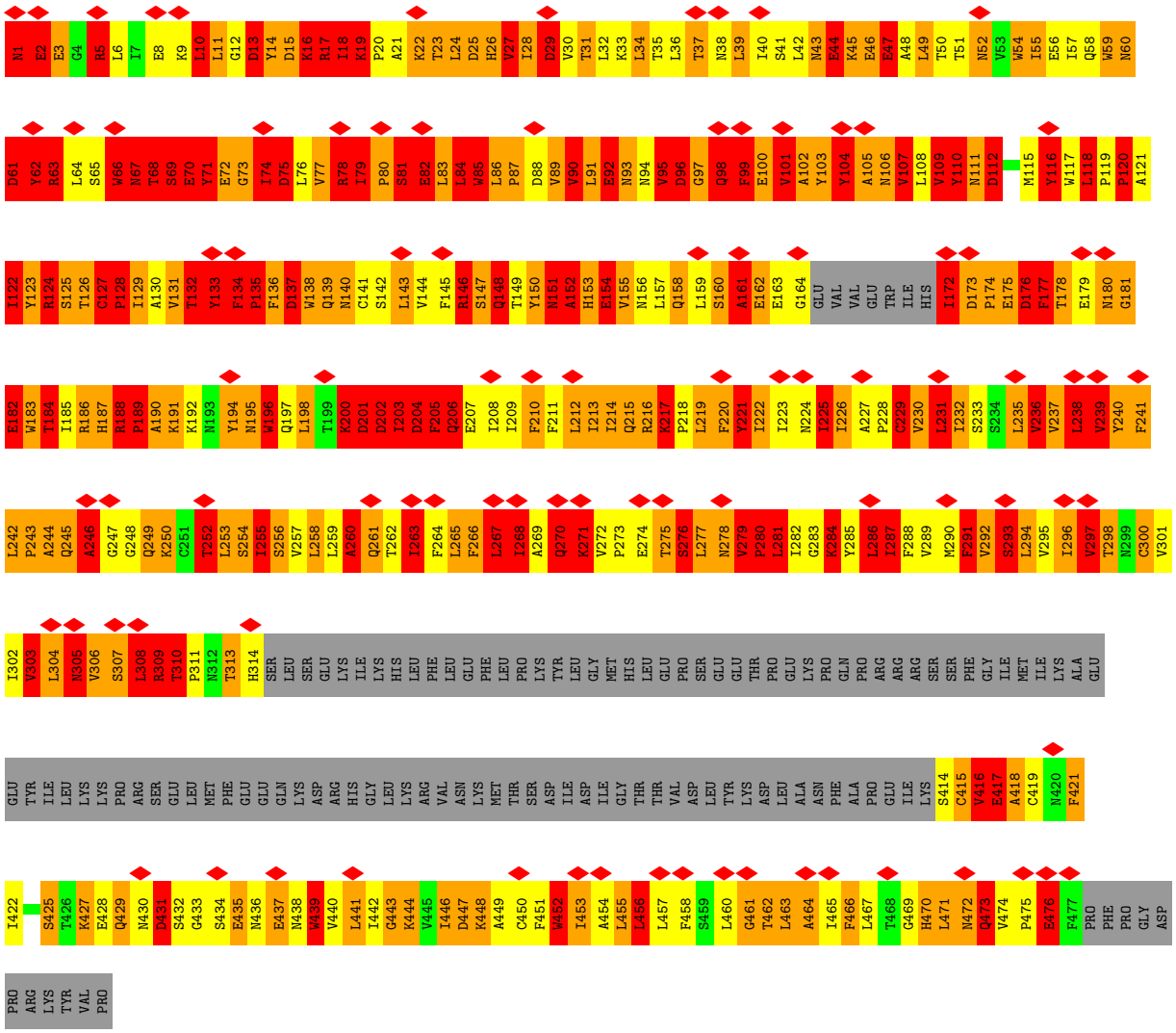
- Molecule 3: ACETYLCHOLINE RECEPTOR DELTA SUBUNIT

Chain C:



- Molecule 4: ACETYLCHOLINE RECEPTOR GAMMA SUBUNIT

Chain E:


N1 E2 E3 G4 R5 L6 I7 E8 K9 L10 L11 G12 D13 Y14 D15 K16 R17 I18 K19 P20 A21 K22 T23 L24 D25 H26 V27 I28 D29 V30 T31 L32 K33 L34 T35 L36 T37 N38 L39 I40 S41 L42 N43 E44 K45 E46 E47 A48 L49 T50 T51 N52 V53 W54 I55 E56 I57 Q58 W59 N60
D61 Y62 R63 L64 S65 W66 N67 T68 S69 E70 Y71 E72 G73 I74 D75 L76 V77 R78 I79 P80 S81 E82 L83 L84 W85 L86 P87 D88 V89 V90 L91 E92 N93 N94 V95 D96 G97 Q98 F99 E100 V101 A102 Y103 Y104 A105 N106 V107 L108 V109 Y110 N111 D112 M115 Y116 W117 L118 P119 P120 A121
I122 Y123 R124 S125 T126 C127 P128 I129 A130 V131 T132 Y133 F134 P135 F136 D137 W138 Q139 N140 C141 S142 L143 V144 F145 R146 S147 Q148 T149 Y150 N151 A152 H153 E154 V155 N156 L157 Q158 L159 S160 A161 E162 E163 G164 GLU VAL VAL GLU TRP ILE HIS I172 D173 P174 E175 D176 F177 T178 E179 N180 G181
E182 W183 T184 I185 R186 H187 R188 P189 A190 K191 K192 N193 Y194 N195 W196 Q197 L198 T199 K200 D201 D202 I203 D204 F205 Q206 E207 I208 I209 F210 F211 L212 I213 I214 Q215 R216 K217 P218 L219 F220 Y221 I222 I223 N224 I225 I226 A227 P228 C229 V230 L231 I232 S233 S234 L235 V236 V237 L238 V239 Y240 F241
L242 P243 A244 Q245 A246 G247 G248 Q249 K250 C251 T252 L253 S254 I255 S256 V257 L258 L259 A260 Q261 T262 I263 F264 L265 F266 L267 I268 A269 Q270 K271 V272 P273 E274 T275 S276 L277 N278 V279 P280 L281 I282 G283 K284 Y285 L286 I287 F288 V289 M290 F291 V292 S293 L294 V295 I296 V297 T298 N299 C300 V301
I302 W303 L304 N305 V306 S307 L308 R309 T310 P311 N312 T313 H314 SER LEU SER GLU LYS ILE LYS HIS LEU PHE LEU GLU PHE LEU PRO LYS TYR LEU GLY MET HIS LEU GLU PRO SER GLU GLU THR PRO GLU LYS PRO GLN PRO ARG ARG ARG SER SER PHE GLY ILE MET ILE LYS ALA GLU
GLU TYR ILE LEU LYS LYS PRO ARG SER GLU LEU MET PHE GLU GLU GLN LYS ASP ARG HIS GLY LEU LYS ARG VAL ASN LYS MET THR SER ASP ILE ASP ILE GLY THR THR VAL ASP LEU TYR LYS ASP LEU ALA ASN PHE ALA PRO GLU ILE LYS S414 C415 V416 E417 A418 C419 N420 F421
I422 S425 T426 K427 E428 Q429 N430 D431 S432 G433 S434 E435 N436 E437 N438 W439 V440 L441 I442 G443 K444 V445 I446 D447 K448 A449 C450 F451 W452 I453 A454 L455 L456 L457 F458 S459 L460 G461 T462 L463 A464 I465 F466 L467 T468 G469 H470 L471 N472 Q473 V474 P475 E476 F477 PRO PHE PRO GLY ASP
PRO ARG LYS TYR VAL PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	EACH TUBE IMAGE	Depositor
Microscope	JEOL 3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	38500	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	5.148	Depositor
Minimum map value	-3.483	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	128.0, 128.0, 168.0	wwPDB
Map dimensions	128, 128, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.68	15/3069 (0.5%)	2.74	258/4186 (6.2%)
1	D	1.68	10/3069 (0.3%)	2.84	300/4186 (7.2%)
2	B	1.68	13/3048 (0.4%)	2.82	301/4162 (7.2%)
3	C	1.69	10/3059 (0.3%)	2.80	285/4175 (6.8%)
4	E	1.69	12/3057 (0.4%)	2.85	295/4174 (7.1%)
All	All	1.68	60/15302 (0.4%)	2.81	1439/20883 (6.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	6	122
1	D	5	120
2	B	11	128
3	C	5	120
4	E	9	118
All	All	36	608

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	GLN	C-N	9.62	1.56	1.34
2	B	129	THR	C-N	-9.40	1.12	1.34
4	E	311	PRO	N-CD	8.91	1.60	1.47
1	A	118	TRP	CB-CG	8.41	1.65	1.50
1	A	222	CYS	CB-SG	-8.07	1.68	1.82
1	D	161	GLU	CD-OE1	7.45	1.33	1.25
2	B	159	GLN	C-N	6.63	1.49	1.34
3	C	130	CYS	C-N	6.61	1.46	1.34
1	D	176	TRP	NE1-CE2	-6.37	1.29	1.37
1	A	391	GLU	CB-CG	6.29	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	439	TYR	CG-CD1	6.26	1.47	1.39
4	E	309	ARG	C-N	-6.22	1.19	1.34
1	A	198	TYR	CG-CD1	6.21	1.47	1.39
4	E	126	THR	C-N	-6.15	1.19	1.34
1	A	401	TYR	CB-CG	6.10	1.60	1.51
1	D	45	GLU	CD-OE1	-6.08	1.19	1.25
1	A	391	GLU	CG-CD	6.02	1.60	1.51
2	B	294	SER	CA-CB	5.94	1.61	1.52
1	A	118	TRP	CG-CD1	5.92	1.45	1.36
2	B	453	SER	CA-CB	5.84	1.61	1.52
1	A	392	SER	CA-CB	5.83	1.61	1.52
1	A	149	TRP	CD2-CE2	5.80	1.48	1.41
2	B	301	VAL	CB-CG2	-5.79	1.40	1.52
1	D	104	HIS	CB-CG	5.79	1.60	1.50
4	E	300	CYS	CB-SG	5.76	1.92	1.82
2	B	413	GLU	CB-CG	5.76	1.63	1.52
1	A	277	TYR	CG-CD1	5.61	1.46	1.39
3	C	182	GLU	CG-CD	5.60	1.60	1.51
1	A	398	GLU	CD-OE1	-5.60	1.19	1.25
4	E	138	TRP	NE1-CE2	-5.59	1.30	1.37
4	E	8	GLU	CG-CD	5.58	1.60	1.51
1	A	180	ASP	C-O	-5.52	1.12	1.23
4	E	182	GLU	C-N	5.51	1.46	1.34
3	C	74	TYR	CG-CD2	5.50	1.46	1.39
2	B	220	TYR	CG-CD1	5.44	1.46	1.39
3	C	190	TRP	CZ3-CH2	-5.41	1.31	1.40
3	C	85	GLU	CD-OE1	-5.40	1.19	1.25
1	D	97	ASP	C-O	5.40	1.33	1.23
2	B	144	MET	C-N	5.40	1.46	1.34
4	E	104	TYR	CG-CD1	5.37	1.46	1.39
4	E	14	TYR	CG-CD1	5.36	1.46	1.39
3	C	97	ASN	C-O	5.35	1.33	1.23
3	C	442	GLU	CB-CG	5.34	1.62	1.52
1	D	239	SER	CB-OG	5.33	1.49	1.42
2	B	420	GLU	CB-CG	5.32	1.62	1.52
2	B	220	TYR	CE1-CZ	5.31	1.45	1.38
4	E	240	TYR	CG-CD2	5.25	1.46	1.39
1	D	55	ARG	NE-CZ	5.18	1.39	1.33
4	E	71	TYR	CB-CG	5.12	1.59	1.51
2	B	205	GLU	CD-OE1	-5.12	1.20	1.25
1	D	140	GLN	C-N	-5.12	1.22	1.34
2	B	428	TRP	CE2-CZ2	5.12	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	280	GLU	CD-OE1	5.12	1.31	1.25
1	A	209	ARG	NE-CZ	5.10	1.39	1.33
3	C	106	TYR	CG-CD1	5.09	1.45	1.39
4	E	476	GLU	CD-OE2	5.08	1.31	1.25
1	A	384	GLU	CD-OE1	-5.08	1.20	1.25
1	D	156	VAL	CA-CB	5.04	1.65	1.54
2	B	225	ILE	CA-CB	5.01	1.66	1.54
1	A	184	TRP	CE3-CZ3	5.01	1.47	1.38

All (1439) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	63	ARG	NE-CZ-NH1	22.18	131.39	120.30
4	E	17	ARG	NE-CZ-NH2	-21.30	109.65	120.30
1	A	190	TYR	CB-CG-CD2	-18.56	109.87	121.00
1	D	164	ARG	NE-CZ-NH1	18.36	129.48	120.30
1	A	209	ARG	NE-CZ-NH2	17.98	129.29	120.30
3	C	223	ARG	NE-CZ-NH2	17.32	128.96	120.30
3	C	66	ARG	NE-CZ-NH2	-16.93	111.83	120.30
3	C	455	ARG	NE-CZ-NH1	16.33	128.47	120.30
1	D	151	TYR	CB-CG-CD1	16.13	130.68	121.00
3	C	22	ARG	NE-CZ-NH2	15.98	128.29	120.30
1	D	284	PHE	CB-CG-CD1	15.67	131.77	120.80
3	C	153	TYR	CB-CG-CD1	-15.30	111.82	121.00
3	C	17	TYR	CB-CG-CD1	-15.22	111.86	121.00
1	A	164	ARG	NE-CZ-NH1	-15.10	112.75	120.30
2	B	441	TYR	CB-CG-CD2	-14.68	112.19	121.00
2	B	457	ASP	CB-CG-OD1	14.59	131.43	118.30
4	E	71	TYR	CG-CD1-CE1	14.56	132.94	121.30
1	D	138	ASP	CB-CG-OD1	14.19	131.07	118.30
1	D	137	PHE	CB-CG-CD1	14.04	130.62	120.80
1	A	277	TYR	CB-CG-CD2	14.00	129.40	121.00
2	B	180	PHE	CB-CG-CD2	-13.99	111.00	120.80
4	E	5	ARG	NE-CZ-NH2	13.97	127.28	120.30
2	B	151	TYR	CB-CG-CD2	13.86	129.31	121.00
1	D	15	TYR	CB-CG-CD1	-13.55	112.87	121.00
1	A	170	PHE	CB-CG-CD1	13.47	130.23	120.80
2	B	220	TYR	CB-CG-CD2	13.41	129.04	121.00
2	B	283	TYR	CB-CG-CD1	13.37	129.02	121.00
4	E	5	ARG	CD-NE-CZ	13.38	142.32	123.60
2	B	215	ARG	NE-CZ-NH1	13.37	126.99	120.30
1	A	79	ARG	NE-CZ-NH2	13.23	126.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	294	PHE	CB-CG-CD1	-13.21	111.55	120.80
1	D	6	ARG	NE-CZ-NH1	13.18	126.89	120.30
4	E	78	ARG	NE-CZ-NH1	-13.18	113.71	120.30
2	B	441	TYR	CG-CD2-CE2	-12.94	110.94	121.30
4	E	62	TYR	CG-CD1-CE1	12.87	131.60	121.30
3	C	473	PHE	CB-CG-CD1	12.82	129.77	120.80
2	B	220	TYR	CZ-CE2-CD2	12.79	131.31	119.80
1	D	66	ARG	NE-CZ-NH1	-12.79	113.91	120.30
2	B	307	ARG	NE-CZ-NH1	-12.79	113.91	120.30
2	B	437	ARG	NE-CZ-NH2	-12.71	113.94	120.30
2	B	20	ARG	NE-CZ-NH2	-12.68	113.96	120.30
3	C	222	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	A	15	TYR	CG-CD2-CE2	-12.45	111.34	121.30
2	B	125	ARG	NE-CZ-NH1	12.43	126.51	120.30
1	A	112	TYR	CB-CG-CD2	12.42	128.45	121.00
2	B	200	ASP	CB-CG-OD1	-12.36	107.18	118.30
1	D	234	TYR	CB-CG-CD1	12.28	128.37	121.00
1	A	66	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	D	111	ASP	CB-CG-OD1	12.15	129.24	118.30
1	D	225	PHE	CB-CG-CD1	12.15	129.31	120.80
4	E	71	TYR	CZ-CE2-CD2	12.12	130.71	119.80
1	D	377	GLU	OE1-CD-OE2	12.12	137.84	123.30
2	B	468	PHE	CB-CG-CD1	12.09	129.26	120.80
1	A	20	ARG	NE-CZ-NH1	12.09	126.34	120.30
4	E	99	PHE	CB-CG-CD2	-12.05	112.37	120.80
3	C	232	PHE	CB-CG-CD1	11.92	129.15	120.80
1	D	55	ARG	NE-CZ-NH1	-11.87	114.36	120.30
3	C	99	ASP	CB-CG-OD1	11.83	128.94	118.30
1	D	401	TYR	CB-CG-CD1	11.73	128.04	121.00
1	A	172	GLU	OE1-CD-OE2	11.71	137.36	123.30
2	B	421	PHE	CB-CG-CD1	-11.71	112.60	120.80
1	A	284	PHE	CB-CG-CD2	11.67	128.97	120.80
1	A	429	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	D	277	TYR	CB-CG-CD1	-11.52	114.09	121.00
1	A	190	TYR	CB-CG-CD1	11.37	127.82	121.00
3	C	140	ASP	CB-CG-OD1	11.34	128.50	118.30
2	B	32	ARG	CD-NE-CZ	11.29	139.41	123.60
3	C	6	ARG	NE-CZ-NH2	-11.15	114.72	120.30
1	D	57	ARG	NE-CZ-NH2	11.11	125.86	120.30
4	E	63	ARG	NH1-CZ-NH2	-11.00	107.30	119.40
3	C	204	ASP	CB-CG-OD2	10.99	128.19	118.30
4	E	439	TRP	NE1-CE2-CD2	10.98	118.28	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	137	PHE	CB-CG-CD2	10.97	128.48	120.80
4	E	204	ASP	CB-CG-OD1	10.82	128.04	118.30
1	D	64	ARG	NE-CZ-NH2	-10.79	114.91	120.30
3	C	66	ARG	NE-CZ-NH1	10.77	125.68	120.30
2	B	100	PHE	CB-CG-CD2	-10.76	113.27	120.80
1	A	213	TYR	CB-CG-CD1	-10.73	114.56	121.00
2	B	204	TYR	CB-CG-CD1	10.66	127.40	121.00
4	E	71	TYR	CG-CD2-CE2	-10.66	112.77	121.30
2	B	20	ARG	NE-CZ-NH1	-10.64	114.98	120.30
1	D	195	ASP	CB-CG-OD1	10.62	127.86	118.30
2	B	20	ARG	NH1-CZ-NH2	10.60	131.06	119.40
3	C	83	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	B	194	ARG	NE-CZ-NH2	10.58	125.59	120.30
1	D	79	ARG	NE-CZ-NH1	-10.55	115.02	120.30
1	A	6	ARG	NE-CZ-NH2	10.52	125.56	120.30
4	E	29	ASP	CB-CG-OD2	10.50	127.75	118.30
2	B	72	TYR	CB-CG-CD1	-10.50	114.70	121.00
1	A	234	TYR	CB-CG-CD1	10.47	127.28	121.00
1	A	277	TYR	CG-CD2-CE2	10.47	129.67	121.30
1	D	280	PHE	CG-CD1-CE1	10.44	132.29	120.80
1	A	64	ARG	NE-CZ-NH2	10.34	125.47	120.30
1	D	401	TYR	CG-CD1-CE1	10.32	129.56	121.30
3	C	228	TYR	CB-CG-CD2	10.30	127.18	121.00
1	A	101	ALA	C-N-CA	10.29	147.42	121.70
2	B	94	ASN	C-N-CA	10.26	147.34	121.70
1	A	214	PHE	CB-CG-CD2	-10.25	113.62	120.80
4	E	116	TYR	CB-CG-CD2	-10.23	114.86	121.00
4	E	177	PHE	CB-CG-CD1	10.21	127.95	120.80
3	C	30	VAL	O-C-N	-10.12	106.51	122.70
1	D	238	ASP	CB-CG-OD2	10.11	127.40	118.30
2	B	455	PHE	CZ-CE2-CD2	10.10	132.22	120.10
1	D	164	ARG	NE-CZ-NH2	-10.10	115.25	120.30
3	C	49	ASP	CB-CG-OD1	10.03	127.33	118.30
3	C	266	ALA	N-CA-CB	10.01	124.12	110.10
4	E	439	TRP	CE2-CD2-CG	-10.01	99.30	107.30
2	B	163	ASP	CB-CG-OD1	9.96	127.27	118.30
2	B	468	PHE	CG-CD1-CE1	9.96	131.76	120.80
4	E	447	ASP	CB-CG-OD1	-9.96	109.33	118.30
2	B	240	TYR	CB-CG-CD2	-9.93	115.04	121.00
1	A	177	VAL	CG1-CB-CG2	9.90	126.74	110.90
1	D	89	ASP	CB-CG-OD1	-9.85	109.44	118.30
1	A	234	TYR	CG-CD1-CE1	9.81	129.15	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	14	TYR	CB-CG-CD2	-9.77	115.14	121.00
4	E	146	ARG	NE-CZ-NH1	9.76	125.18	120.30
4	E	164	GLY	CA-C-O	9.72	138.10	120.60
4	E	133	TYR	CG-CD2-CE2	9.69	129.06	121.30
2	B	430	TYR	CB-CG-CD1	-9.69	115.19	121.00
1	D	251	LEU	O-C-N	9.66	138.16	122.70
4	E	133	TYR	CB-CG-CD1	9.66	126.79	121.00
2	B	186	TRP	CH2-CZ2-CE2	9.65	127.06	117.40
2	B	210	TYR	CB-CG-CD2	9.65	126.79	121.00
3	C	153	TYR	CB-CG-CD2	9.65	126.79	121.00
1	D	100	PHE	CB-CG-CD2	-9.62	114.07	120.80
1	D	137	PHE	CG-CD1-CE1	9.61	131.37	120.80
1	A	84	ASP	CB-CG-OD2	9.59	126.93	118.30
1	D	284	PHE	CB-CG-CD2	-9.51	114.15	120.80
1	A	163	ASP	CB-CG-OD1	9.47	126.82	118.30
3	C	474	VAL	O-C-N	-9.46	107.57	122.70
4	E	183	TRP	CG-CD2-CE3	9.42	142.38	133.90
1	A	79	ARG	NE-CZ-NH1	-9.41	115.59	120.30
4	E	219	LEU	O-C-N	9.40	137.75	122.70
3	C	204	ASP	CB-CG-OD1	-9.34	109.89	118.30
4	E	260	ALA	C-N-CA	9.34	145.06	121.70
2	B	455	PHE	CG-CD1-CE1	9.32	131.06	120.80
3	C	265	LEU	O-C-N	9.28	137.55	122.70
4	E	220	PHE	CB-CG-CD1	9.28	127.30	120.80
1	A	55	ARG	NE-CZ-NH1	9.28	124.94	120.30
4	E	103	TYR	CB-CG-CD2	-9.24	115.46	121.00
4	E	309	ARG	NE-CZ-NH2	9.21	124.90	120.30
1	D	280	PHE	CD1-CE1-CZ	-9.20	109.06	120.10
4	E	186	ARG	NE-CZ-NH2	-9.19	115.70	120.30
3	C	92	ILE	O-C-N	9.18	137.39	122.70
2	B	283	TYR	CG-CD1-CE1	9.16	128.63	121.30
3	C	439	TYR	CB-CG-CD2	-9.16	115.50	121.00
2	B	410	TYR	CZ-CE2-CD2	9.15	128.03	119.80
1	D	176	TRP	CB-CG-CD1	9.13	138.87	127.00
1	D	79	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	D	410	LEU	CA-CB-CG	9.10	136.22	115.30
1	A	93	TYR	CB-CG-CD2	-9.09	115.54	121.00
1	D	151	TYR	CG-CD2-CE2	9.09	128.57	121.30
4	E	458	PHE	CG-CD2-CE2	9.05	130.76	120.80
1	A	174	GLY	C-N-CA	9.05	144.32	121.70
1	D	277	TYR	CD1-CG-CD2	9.03	127.83	117.90
3	C	232	PHE	CG-CD1-CE1	9.03	130.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	104	VAL	CA-CB-CG1	9.02	124.43	110.90
2	B	462	VAL	CB-CA-C	9.02	128.53	111.40
4	E	66	TRP	CD2-CE2-CZ2	8.98	133.08	122.30
1	D	163	ASP	CB-CG-OD2	8.98	126.38	118.30
3	C	139	PHE	CB-CG-CD2	-8.95	114.54	120.80
1	D	79	ARG	NH1-CZ-NH2	8.94	129.24	119.40
1	D	200	ASP	CB-CG-OD1	8.93	126.34	118.30
3	C	222	ARG	NH1-CZ-NH2	-8.91	109.60	119.40
1	D	84	ASP	CB-CG-OD1	8.90	126.31	118.30
3	C	137	PHE	CG-CD1-CE1	-8.87	111.05	120.80
1	A	257	LEU	CB-CG-CD1	-8.86	95.93	111.00
4	E	17	ARG	NH1-CZ-NH2	8.86	129.14	119.40
3	C	64	ASP	CB-CG-OD1	8.85	126.26	118.30
1	D	209	ARG	NE-CZ-NH1	8.85	124.72	120.30
3	C	268	ALA	O-C-N	-8.82	108.58	122.70
2	B	4	GLU	OE1-CD-OE2	-8.80	112.74	123.30
1	D	20	ARG	NE-CZ-NH1	8.79	124.70	120.30
4	E	176	ASP	CB-CG-OD1	-8.77	110.41	118.30
2	B	220	TYR	CG-CD1-CE1	8.76	128.31	121.30
1	A	248	SER	O-C-N	-8.76	108.69	122.70
4	E	183	TRP	CD1-CG-CD2	8.74	113.29	106.30
3	C	314	PHE	CG-CD1-CE1	8.72	130.40	120.80
1	A	198	TYR	CD1-CE1-CZ	8.70	127.63	119.80
1	A	93	TYR	CG-CD2-CE2	-8.70	114.34	121.30
4	E	84	LEU	CA-CB-CG	8.67	135.23	115.30
4	E	221	TYR	CB-CG-CD1	8.65	126.19	121.00
4	E	244	ALA	N-CA-CB	8.64	122.20	110.10
1	D	426	PHE	CB-CG-CD2	8.64	126.85	120.80
3	C	136	TYR	CA-CB-CG	8.64	129.81	113.40
1	D	209	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	D	86	TRP	NE1-CE2-CZ2	8.60	139.86	130.40
2	B	428	TRP	CB-CG-CD2	8.59	137.77	126.60
3	C	141	TRP	CB-CG-CD1	8.59	138.16	127.00
1	A	277	TYR	CZ-CE2-CD2	-8.57	112.08	119.80
3	C	448	LEU	CB-CG-CD1	-8.57	96.43	111.00
2	B	149	TYR	CB-CG-CD1	-8.55	115.87	121.00
1	A	267	THR	N-CA-CB	8.55	126.54	110.30
4	E	67	ASN	C-N-CA	8.52	143.00	121.70
4	E	466	PHE	CB-CG-CD1	8.51	126.76	120.80
4	E	15	ASP	CB-CG-OD1	-8.48	110.67	118.30
3	C	67	LEU	CB-CG-CD1	8.48	125.41	111.00
1	D	250	LEU	CB-CA-C	8.45	126.25	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	134	TYR	CD1-CE1-CZ	8.44	127.39	119.80
1	D	140	GLN	OE1-CD-NE2	-8.42	102.53	121.90
1	A	152	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	D	127	TYR	CZ-CE2-CD2	-8.38	112.26	119.80
4	E	150	TYR	CG-CD2-CE2	8.38	128.00	121.30
4	E	194	TYR	CZ-CE2-CD2	8.37	127.33	119.80
4	E	204	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	301	ARG	NE-CZ-NH1	8.34	124.47	120.30
2	B	138	ASP	CB-CG-OD1	8.33	125.79	118.30
4	E	103	TYR	CG-CD2-CE2	-8.33	114.64	121.30
3	C	241	PHE	CB-CG-CD1	8.31	126.61	120.80
2	B	240	TYR	CG-CD2-CE2	-8.30	114.66	121.30
4	E	198	LEU	CA-CB-CG	8.30	134.38	115.30
2	B	220	TYR	CA-CB-CG	8.28	129.14	113.40
2	B	226	VAL	CG1-CB-CG2	8.28	124.14	110.90
3	C	74	TYR	CB-CG-CD1	8.27	125.96	121.00
4	E	146	ARG	O-C-N	-8.26	109.49	122.70
4	E	214	ILE	C-N-CA	8.26	142.35	121.70
2	B	307	ARG	N-CA-C	8.26	133.29	111.00
1	D	4	GLU	OE1-CD-OE2	-8.25	113.39	123.30
1	D	64	ARG	CD-NE-CZ	8.25	135.15	123.60
3	C	217	PHE	CD1-CE1-CZ	-8.24	110.22	120.10
1	D	401	TYR	CB-CG-CD2	-8.24	116.06	121.00
1	D	401	TYR	CD1-CE1-CZ	-8.23	112.40	119.80
2	B	139	TRP	CH2-CZ2-CE2	8.20	125.60	117.40
1	D	15	TYR	CB-CG-CD2	8.19	125.92	121.00
2	B	215	ARG	NH1-CZ-NH2	-8.18	110.40	119.40
3	C	227	PHE	CB-CG-CD2	8.18	126.53	120.80
1	A	280	PHE	CB-CG-CD2	-8.16	115.08	120.80
3	C	228	TYR	CA-CB-CG	8.14	128.87	113.40
1	A	127	TYR	CB-CG-CD1	8.14	125.88	121.00
1	A	407	ASP	CB-CG-OD2	-8.14	110.98	118.30
3	C	76	ASP	CB-CG-OD1	8.13	125.61	118.30
1	D	151	TYR	CA-CB-CG	8.11	128.81	113.40
1	A	381	TYR	CB-CG-CD2	-8.10	116.14	121.00
3	C	22	ARG	NH1-CZ-NH2	-8.09	110.50	119.40
3	C	206	PHE	CB-CG-CD1	-8.08	115.14	120.80
4	E	240	TYR	CB-CG-CD1	8.07	125.84	121.00
3	C	217	PHE	CB-CG-CD2	-8.05	115.16	120.80
1	D	234	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	D	57	ARG	CD-NE-CZ	8.05	134.87	123.60
4	E	439	TRP	NE1-CE2-CZ2	-8.04	121.55	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	285	VAL	CA-CB-CG1	8.04	122.96	110.90
2	B	63	TYR	CZ-CE2-CD2	8.03	127.03	119.80
3	C	106	TYR	CZ-CE2-CD2	8.03	127.02	119.80
2	B	72	TYR	CA-CB-CG	8.02	128.64	113.40
3	C	224	LYS	N-CA-CB	8.02	125.03	110.60
1	A	64	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	A	21	PRO	O-C-N	7.97	135.45	122.70
3	C	73	GLU	OE1-CD-OE2	-7.97	113.74	123.30
2	B	180	PHE	CG-CD1-CE1	-7.96	112.04	120.80
2	B	215	ARG	CB-CA-C	7.96	126.32	110.40
1	D	112	TYR	CB-CG-CD1	-7.94	116.23	121.00
1	D	209	ARG	NH1-CZ-NH2	-7.94	110.66	119.40
2	B	427	ASP	CB-CG-OD2	7.93	125.44	118.30
3	C	161	ASP	CB-CG-OD2	7.92	125.43	118.30
3	C	117	TYR	CB-CG-CD1	-7.91	116.25	121.00
2	B	97	ASP	CB-CG-OD1	-7.88	111.20	118.30
2	B	135	PHE	O-C-N	7.87	136.06	121.10
4	E	452	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	A	101	ALA	O-C-N	7.85	135.26	122.70
3	C	313	HIS	CA-CB-CG	7.85	126.95	113.60
3	C	247	PHE	CD1-CG-CD2	7.85	128.50	118.30
1	D	72	TYR	CB-CG-CD1	-7.84	116.30	121.00
2	B	210	TYR	CG-CD1-CE1	7.83	127.57	121.30
4	E	98	GLN	OE1-CD-NE2	-7.83	103.89	121.90
2	B	25	VAL	O-C-N	-7.83	109.89	123.20
4	E	161	ALA	N-CA-CB	7.83	121.06	110.10
1	A	390	GLU	OE1-CD-OE2	-7.82	113.91	123.30
2	B	406	GLU	OE1-CD-OE2	-7.82	113.92	123.30
4	E	447	ASP	CB-CG-OD2	7.82	125.34	118.30
3	C	314	PHE	CB-CG-CD2	7.82	126.27	120.80
4	E	116	TYR	CB-CG-CD1	7.81	125.69	121.00
1	D	429	ARG	NE-CZ-NH2	-7.78	116.41	120.30
3	C	247	PHE	CB-CG-CD2	-7.78	115.36	120.80
1	D	65	LEU	CA-CB-CG	7.75	133.13	115.30
2	B	15	TYR	CB-CG-CD1	7.75	125.65	121.00
1	D	198	TYR	CB-CG-CD2	-7.74	116.35	121.00
3	C	113	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	A	209	ARG	NH1-CZ-NH2	-7.71	110.92	119.40
4	E	188	ARG	NE-CZ-NH2	-7.70	116.45	120.30
4	E	25	ASP	CB-CG-OD2	7.70	125.23	118.30
3	C	294	PHE	CG-CD1-CE1	-7.68	112.35	120.80
4	E	194	TYR	CG-CD1-CE1	7.68	127.44	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	72	TYR	CG-CD1-CE1	-7.67	115.16	121.30
1	D	18	VAL	CB-CA-C	-7.66	96.85	111.40
1	A	149	TRP	CB-CA-C	7.64	125.69	110.40
1	A	181	TYR	CB-CG-CD1	7.64	125.58	121.00
3	C	139	PHE	CG-CD2-CE2	-7.64	112.39	120.80
3	C	137	PHE	CD1-CE1-CZ	7.63	129.26	120.10
4	E	44	GLU	OE1-CD-OE2	7.61	132.43	123.30
1	D	248	SER	N-CA-CB	7.60	121.91	110.50
1	A	86	TRP	CE2-CD2-CE3	7.60	127.82	118.70
1	D	265	PRO	CA-N-CD	-7.60	100.86	111.50
4	E	131	VAL	CA-CB-CG1	7.60	122.30	110.90
1	D	129	GLU	OE1-CD-OE2	7.59	132.41	123.30
1	D	55	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	D	244	THR	CA-CB-CG2	-7.58	101.79	112.40
1	D	426	PHE	CB-CG-CD1	-7.58	115.49	120.80
4	E	215	GLN	CG-CD-NE2	7.58	134.90	116.70
1	D	127	TYR	CG-CD2-CE2	7.55	127.34	121.30
1	D	198	TYR	CZ-CE2-CD2	-7.54	113.02	119.80
4	E	62	TYR	CB-CG-CD1	7.53	125.52	121.00
2	B	430	TYR	CB-CG-CD2	7.53	125.52	121.00
1	D	89	ASP	N-CA-CB	7.52	124.14	110.60
4	E	72	GLU	O-C-N	-7.51	110.43	123.20
1	A	426	PHE	CD1-CE1-CZ	-7.50	111.10	120.10
2	B	220	TYR	CG-CD2-CE2	-7.49	115.31	121.30
2	B	219	PHE	CB-CG-CD1	7.49	126.04	120.80
1	D	6	ARG	NH1-CZ-NH2	-7.48	111.17	119.40
2	B	194	ARG	NE-CZ-NH1	-7.47	116.56	120.30
3	C	69	TRP	CD1-CG-CD2	-7.47	100.32	106.30
3	C	184	PHE	CG-CD1-CE1	7.47	129.02	120.80
3	C	129	SER	N-CA-CB	7.47	121.71	110.50
2	B	99	SER	O-C-N	-7.47	110.75	122.70
1	A	407	ASP	O-C-N	-7.47	110.75	122.70
1	D	112	TYR	CG-CD2-CE2	-7.47	115.33	121.30
3	C	312	PHE	CB-CG-CD2	-7.46	115.58	120.80
4	E	81	SER	N-CA-CB	-7.45	99.32	110.50
2	B	156	VAL	CA-CB-CG1	-7.45	99.73	110.90
1	A	135	PHE	CG-CD1-CE1	7.44	128.99	120.80
3	C	69	TRP	N-CA-CB	7.44	124.00	110.60
4	E	238	LEU	N-CA-C	-7.44	90.92	111.00
3	C	185	THR	N-CA-CB	7.43	124.42	110.30
1	A	101	ALA	N-CA-CB	7.43	120.50	110.10
4	E	85	TRP	CE3-CZ3-CH2	-7.43	113.03	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	478	PHE	CB-CG-CD1	-7.43	115.60	120.80
2	B	65	LEU	CA-CB-CG	7.42	132.37	115.30
2	B	413	GLU	OE1-CD-OE2	-7.41	114.40	123.30
2	B	118	TRP	C-N-CA	7.41	140.23	121.70
1	A	52	THR	C-N-CA	7.41	140.22	121.70
3	C	474	VAL	CG1-CB-CG2	7.38	122.71	110.90
1	D	57	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	D	151	TYR	CD1-CG-CD2	-7.38	109.78	117.90
1	A	189	TYR	CB-CG-CD1	-7.38	116.57	121.00
4	E	5	ARG	NE-CZ-NH1	-7.38	116.61	120.30
4	E	124	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	B	178	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	182	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	A	429	ARG	NH1-CZ-NH2	7.36	127.49	119.40
4	E	126	THR	N-CA-CB	7.35	124.27	110.30
2	B	270	VAL	CA-CB-CG2	7.34	121.91	110.90
1	D	94	ASN	N-CA-CB	7.34	123.81	110.60
4	E	476	GLU	OE1-CD-OE2	-7.34	114.49	123.30
2	B	27	ASP	CB-CG-OD2	7.33	124.90	118.30
3	C	244	ALA	O-C-N	-7.33	110.97	122.70
3	C	315	ARG	NE-CZ-NH2	7.33	123.96	120.30
4	E	307	SER	CA-C-N	-7.31	101.12	117.20
3	C	449	VAL	CG1-CB-CG2	-7.31	99.21	110.90
3	C	467	LEU	CA-CB-CG	7.31	132.11	115.30
1	D	381	TYR	CZ-CE2-CD2	7.30	126.38	119.80
3	C	222	ARG	O-C-N	-7.30	111.02	122.70
4	E	238	LEU	CB-CG-CD1	-7.30	98.58	111.00
1	D	105	MET	O-C-N	-7.30	111.02	122.70
4	E	136	PHE	CG-CD1-CE1	7.29	128.82	120.80
3	C	243	ALA	O-C-N	7.29	134.37	122.70
1	A	273	LEU	CA-CB-CG	7.29	132.07	115.30
1	D	55	ARG	O-C-N	-7.29	111.04	122.70
4	E	134	PHE	CB-CG-CD2	7.28	125.90	120.80
4	E	110	TYR	CG-CD1-CE1	7.28	127.12	121.30
1	A	64	ARG	CD-NE-CZ	7.27	133.78	123.60
1	D	168	SER	N-CA-CB	7.27	121.41	110.50
4	E	252	THR	N-CA-CB	7.27	124.12	110.30
1	A	7	LEU	CA-CB-CG	7.27	132.02	115.30
3	C	180	ASP	CB-CG-OD2	-7.25	111.77	118.30
4	E	46	GLU	OE1-CD-OE2	-7.24	114.62	123.30
1	A	86	TRP	CD2-CE3-CZ3	-7.23	109.40	118.80
2	B	288	MET	CA-CB-CG	7.22	125.58	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	ASN	N-CA-C	-7.22	91.50	111.00
1	D	429	ARG	NE-CZ-NH1	7.21	123.91	120.30
4	E	240	TYR	CB-CG-CD2	-7.21	116.67	121.00
1	A	399	TRP	CE3-CZ3-CH2	-7.21	113.27	121.20
1	A	189	TYR	CD1-CG-CD2	7.20	125.82	117.90
3	C	123	PRO	CA-N-CD	-7.20	101.42	111.50
1	A	248	SER	CB-CA-C	7.19	123.77	110.10
1	A	198	TYR	CG-CD2-CE2	7.19	127.05	121.30
1	D	83	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	414	PHE	CB-CG-CD1	-7.19	115.77	120.80
1	A	86	TRP	NE1-CE2-CD2	7.18	114.48	107.30
4	E	308	LEU	CA-CB-CG	7.18	131.81	115.30
4	E	138	TRP	CD2-CE3-CZ3	-7.17	109.48	118.80
1	D	67	TRP	CD1-NE1-CE2	7.16	115.44	109.00
1	D	178	MET	CG-SD-CE	7.15	111.64	100.20
1	D	380	LYS	CD-CE-NZ	7.15	128.14	111.70
1	A	86	TRP	CG-CD2-CE3	-7.15	127.47	133.90
1	D	114	GLY	CA-C-O	-7.14	107.75	120.60
1	D	406	ILE	CG1-CB-CG2	7.14	127.10	111.40
2	B	205	GLU	N-CA-C	7.13	130.26	111.00
4	E	198	LEU	CB-CG-CD2	7.13	123.12	111.00
2	B	465	ASP	CB-CG-OD2	7.11	124.70	118.30
4	E	130	ALA	CB-CA-C	7.11	120.77	110.10
1	A	269	SER	C-N-CA	7.11	139.47	121.70
2	B	19	VAL	C-N-CA	7.11	139.47	121.70
1	A	89	ASP	CB-CG-OD1	7.11	124.69	118.30
1	A	426	PHE	CB-CG-CD2	-7.10	115.83	120.80
1	D	408	HIS	N-CA-CB	7.10	123.38	110.60
3	C	138	PRO	O-C-N	-7.08	111.37	122.70
1	A	274	ILE	CA-CB-CG2	7.08	125.06	110.90
1	A	180	ASP	CB-CG-OD2	7.07	124.67	118.30
3	C	63	TYR	CB-CG-CD2	-7.07	116.76	121.00
4	E	196	TRP	CB-CG-CD1	-7.06	117.82	127.00
4	E	196	TRP	CD2-CE3-CZ3	-7.05	109.63	118.80
2	B	118	TRP	CB-CA-C	7.05	124.50	110.40
1	A	391	GLU	CB-CA-C	7.04	124.49	110.40
1	A	97	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	195	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	397	GLU	OE1-CD-OE2	7.04	131.74	123.30
1	A	151	TYR	CG-CD1-CE1	-7.03	115.68	121.30
4	E	196	TRP	CE3-CZ3-CH2	7.03	128.93	121.20
1	D	195	ASP	OD1-CG-OD2	-7.03	109.95	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	81	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	D	184	TRP	CA-CB-CG	7.01	127.02	113.70
1	A	223	LEU	CB-CG-CD2	7.01	122.91	111.00
3	C	312	PHE	CD1-CG-CD2	7.00	127.40	118.30
4	E	177	PHE	CD1-CG-CD2	-6.99	109.21	118.30
2	B	284	LEU	CA-CB-CG	6.99	131.38	115.30
2	B	404	ALA	N-CA-CB	6.99	119.88	110.10
1	D	198	TYR	CD1-CG-CD2	6.98	125.58	117.90
4	E	416	VAL	O-C-N	-6.98	111.53	122.70
2	B	12	PHE	CD1-CG-CD2	-6.98	109.23	118.30
4	E	205	PHE	N-CA-CB	6.97	123.15	110.60
4	E	103	TYR	CD1-CG-CD2	6.97	125.56	117.90
1	D	93	TYR	CZ-CE2-CD2	-6.96	113.53	119.80
1	D	190	TYR	CG-CD1-CE1	-6.96	115.73	121.30
3	C	184	PHE	CB-CG-CD1	6.96	125.67	120.80
1	D	160	PRO	O-C-N	6.96	133.83	122.70
3	C	247	PHE	CG-CD1-CE1	-6.94	113.16	120.80
4	E	150	TYR	CB-CG-CD1	6.94	125.16	121.00
3	C	222	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	D	127	TYR	CD1-CE1-CZ	6.94	126.04	119.80
1	A	253	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	A	112	TYR	CD1-CG-CD2	-6.93	110.28	117.90
1	A	44	ASP	N-CA-CB	6.93	123.07	110.60
2	B	83	ASP	O-C-N	-6.93	111.62	122.70
4	E	100	GLU	CG-CD-OE2	6.93	132.15	118.30
1	A	44	ASP	CB-CG-OD2	-6.92	112.07	118.30
3	C	102	TYR	CG-CD2-CE2	6.92	126.84	121.30
3	C	113	ARG	NE-CZ-NH1	-6.92	116.84	120.30
3	C	202	TYR	CB-CG-CD2	6.92	125.15	121.00
4	E	133	TYR	C-N-CA	6.92	138.99	121.70
3	C	424	ASP	CB-CG-OD2	-6.91	112.08	118.30
3	C	202	TYR	CZ-CE2-CD2	6.91	126.02	119.80
1	D	127	TYR	CG-CD1-CE1	-6.90	115.78	121.30
1	D	213	TYR	O-C-N	6.90	133.74	122.70
1	A	176	TRP	CA-CB-CG	6.90	126.80	113.70
3	C	453	ILE	O-C-N	-6.89	111.67	122.70
2	B	137	PHE	CD1-CG-CD2	6.89	127.25	118.30
2	B	280	ILE	N-CA-CB	6.89	126.64	110.80
4	E	243	PRO	O-C-N	-6.88	111.70	122.70
1	D	112	TYR	CD1-CG-CD2	6.87	125.46	117.90
1	D	211	PRO	CA-C-O	-6.87	103.71	120.20
3	C	428	TYR	O-C-N	-6.86	111.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	69	PRO	N-CA-C	6.86	129.94	112.10
2	B	285	MET	CA-CB-CG	6.86	124.96	113.30
1	D	162	SER	CA-C-N	-6.85	102.13	117.20
1	D	128	CYS	O-C-N	-6.84	111.75	122.70
1	A	67	TRP	CD1-NE1-CE2	6.84	115.16	109.00
2	B	67	TRP	CH2-CZ2-CE2	6.84	124.24	117.40
2	B	441	TYR	CZ-CE2-CD2	6.84	125.95	119.80
3	C	79	ILE	CB-CA-C	-6.84	97.93	111.60
3	C	225	PRO	O-C-N	6.83	133.64	122.70
4	E	421	PHE	CB-CG-CD2	6.83	125.58	120.80
1	D	209	ARG	C-N-CA	6.83	138.78	121.70
1	A	151	TYR	CB-CG-CD1	-6.82	116.91	121.00
2	B	21	PRO	CA-N-CD	-6.82	101.95	111.50
2	B	140	GLN	O-C-N	-6.82	111.79	122.70
4	E	118	LEU	N-CA-C	6.81	129.40	111.00
3	C	455	ARG	NE-CZ-NH2	-6.81	116.89	120.30
3	C	63	TYR	CG-CD1-CE1	-6.81	115.85	121.30
2	B	204	TYR	CA-C-O	-6.81	105.81	120.10
3	C	30	VAL	CA-C-O	6.80	134.39	120.10
2	B	62	ASP	CB-CG-OD1	6.80	124.42	118.30
3	C	6	ARG	NH1-CZ-NH2	6.79	126.87	119.40
4	E	133	TYR	CZ-CE2-CD2	-6.78	113.70	119.80
3	C	142	GLN	C-N-CA	6.77	138.64	121.70
2	B	62	ASP	CB-CG-OD2	6.77	124.39	118.30
3	C	295	ILE	O-C-N	6.77	133.53	122.70
2	B	12	PHE	CB-CG-CD2	6.77	125.54	120.80
3	C	67	LEU	CA-CB-CG	6.76	130.85	115.30
4	E	203	ILE	N-CA-C	-6.75	92.76	111.00
4	E	8	GLU	OE1-CD-OE2	-6.75	115.20	123.30
2	B	137	PHE	CB-CG-CD2	-6.75	116.08	120.80
1	D	399	TRP	CD1-CG-CD2	-6.75	100.90	106.30
1	A	389	ASP	O-C-N	-6.74	111.91	122.70
2	B	138	ASP	OD1-CG-OD2	-6.74	110.50	123.30
1	D	64	ARG	NH1-CZ-NH2	6.73	126.80	119.40
4	E	132	THR	C-N-CA	6.73	138.52	121.70
4	E	68	THR	N-CA-CB	6.72	123.08	110.30
1	A	15	TYR	CD1-CE1-CZ	-6.72	113.75	119.80
2	B	465	ASP	CB-CG-OD1	-6.72	112.25	118.30
2	B	421	PHE	CZ-CE2-CD2	-6.72	112.04	120.10
4	E	104	TYR	CD1-CE1-CZ	-6.72	113.75	119.80
2	B	5	ASP	C-N-CA	6.72	138.49	121.70
1	A	166	ASP	CB-CG-OD1	6.70	124.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	379	VAL	CG1-CB-CG2	6.70	121.62	110.90
4	E	151	ASN	C-N-CA	6.70	138.44	121.70
1	A	47	ASN	O-C-N	-6.70	111.98	122.70
2	B	77	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	4	GLU	OE1-CD-OE2	-6.69	115.27	123.30
2	B	161	ALA	O-C-N	-6.69	112.00	122.70
1	D	301	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	66	ARG	NH1-CZ-NH2	6.68	126.75	119.40
3	C	31	VAL	C-N-CA	6.68	138.40	121.70
4	E	62	TYR	CD1-CE1-CZ	-6.68	113.79	119.80
1	A	303	PRO	CA-N-CD	-6.68	102.15	111.50
1	D	106	THR	CA-CB-CG2	6.67	121.75	112.40
2	B	441	TYR	CD1-CG-CD2	6.67	125.23	117.90
1	D	414	PHE	O-C-N	-6.67	112.03	122.70
4	E	61	ASP	O-C-N	-6.67	112.03	122.70
2	B	403	GLU	OE1-CD-OE2	6.66	131.29	123.30
3	C	247	PHE	CB-CG-CD1	-6.66	116.14	120.80
2	B	445	THR	O-C-N	6.65	133.34	122.70
1	D	170	PHE	CB-CG-CD1	-6.64	116.15	120.80
4	E	46	GLU	C-N-CA	6.64	138.31	121.70
4	E	99	PHE	CG-CD2-CE2	-6.64	113.49	120.80
2	B	131	LYS	O-C-N	-6.64	112.08	122.70
4	E	110	TYR	CZ-CE2-CD2	6.64	125.78	119.80
2	B	234	LEU	CB-CG-CD1	-6.64	99.72	111.00
3	C	206	PHE	CB-CG-CD2	6.63	125.44	120.80
4	E	220	PHE	CA-C-O	6.63	134.03	120.10
1	A	213	TYR	CD1-CG-CD2	6.63	125.19	117.90
2	B	220	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	A	411	LEU	CA-CB-CG	6.61	130.51	115.30
4	E	138	TRP	CE2-CD2-CE3	6.61	126.63	118.70
4	E	138	TRP	NE1-CE2-CD2	6.61	113.91	107.30
1	A	249	VAL	N-CA-CB	6.61	126.03	111.50
1	D	176	TRP	CB-CG-CD2	-6.60	118.02	126.60
1	D	44	ASP	CB-CG-OD2	-6.60	112.36	118.30
2	B	448	SER	CB-CA-C	6.60	122.64	110.10
1	D	138	ASP	CB-CG-OD2	-6.60	112.36	118.30
2	B	239	PHE	CG-CD2-CE2	-6.59	113.55	120.80
4	E	78	ARG	NE-CZ-NH2	6.59	123.59	120.30
3	C	275	SER	O-C-N	-6.58	112.17	122.70
2	B	434	VAL	CB-CA-C	-6.58	98.89	111.40
1	A	148	ILE	O-C-N	-6.58	112.17	122.70
3	C	17	TYR	CB-CG-CD2	6.58	124.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	114	PRO	CA-CB-CG	-6.58	91.51	104.00
1	A	198	TYR	CG-CD1-CE1	-6.57	116.04	121.30
2	B	421	PHE	CG-CD1-CE1	-6.57	113.57	120.80
3	C	449	VAL	O-C-N	-6.57	112.03	123.20
1	A	255	VAL	CA-CB-CG2	-6.56	101.06	110.90
1	D	46	VAL	CG1-CB-CG2	6.56	121.39	110.90
1	A	213	TYR	CG-CD1-CE1	-6.55	116.06	121.30
4	E	97	GLY	O-C-N	-6.55	112.22	122.70
4	E	54	TRP	CG-CD1-NE1	6.55	116.65	110.10
3	C	422	GLY	O-C-N	-6.55	112.23	122.70
1	D	250	LEU	CA-CB-CG	-6.54	100.25	115.30
4	E	417	GLU	O-C-N	-6.54	112.23	122.70
1	D	161	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	D	261	VAL	CA-CB-CG1	6.54	120.70	110.90
4	E	134	PHE	CD1-CG-CD2	-6.54	109.81	118.30
2	B	410	TYR	CG-CD2-CE2	-6.53	116.07	121.30
1	A	20	ARG	CA-C-O	-6.52	106.41	120.10
2	B	257	LEU	CA-C-N	-6.52	102.86	117.20
3	C	13	ILE	C-N-CA	6.51	137.97	121.70
3	C	151	LEU	CA-CB-CG	6.50	130.26	115.30
3	C	426	THR	O-C-N	-6.50	112.29	122.70
1	D	381	TYR	CA-C-O	-6.50	106.44	120.10
2	B	219	PHE	CG-CD1-CE1	6.50	127.95	120.80
4	E	138	TRP	CE2-CD2-CG	-6.50	102.10	107.30
2	B	85	VAL	CB-CA-C	-6.49	99.07	111.40
3	C	300	THR	C-N-CA	6.49	135.93	122.30
1	D	93	TYR	CB-CG-CD2	-6.49	117.11	121.00
4	E	280	PRO	O-C-N	-6.49	112.32	122.70
4	E	285	TYR	CG-CD2-CE2	-6.49	116.11	121.30
1	D	136	PRO	CB-CA-C	6.49	128.22	112.00
4	E	304	LEU	CB-CG-CD2	-6.48	99.98	111.00
2	B	272	GLU	O-C-N	-6.48	112.33	122.70
3	C	286	PRO	O-C-N	-6.47	112.34	122.70
1	D	277	TYR	CG-CD2-CE2	-6.47	116.12	121.30
3	C	127	ARG	NE-CZ-NH1	6.47	123.54	120.30
4	E	62	TYR	CD1-CG-CD2	-6.47	110.78	117.90
2	B	198	ARG	NE-CZ-NH2	6.46	123.53	120.30
3	C	4	GLU	OE1-CD-OE2	-6.46	115.54	123.30
2	B	14	ASN	O-C-N	-6.46	112.36	122.70
1	A	170	PHE	CD1-CG-CD2	-6.46	109.91	118.30
3	C	430	VAL	CA-CB-CG2	-6.46	101.22	110.90
2	B	192	PRO	N-CD-CG	-6.45	93.52	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	305	ASN	C-N-CA	6.45	137.84	121.70
3	C	107	PHE	CD1-CE1-CZ	6.45	127.84	120.10
2	B	180	PHE	CD1-CG-CD2	6.45	126.68	118.30
1	D	86	TRP	CD1-NE1-CE2	6.45	114.80	109.00
2	B	100	PHE	CG-CD2-CE2	-6.45	113.71	120.80
3	C	140	ASP	OD1-CG-OD2	-6.44	111.06	123.30
1	D	177	VAL	CG1-CB-CG2	6.44	121.20	110.90
3	C	314	PHE	CD1-CG-CD2	-6.44	109.93	118.30
4	E	61	ASP	CB-CG-OD1	6.44	124.09	118.30
2	B	64	ARG	NE-CZ-NH2	-6.44	117.08	120.30
4	E	66	TRP	NE1-CE2-CZ2	-6.44	123.32	130.40
4	E	451	PHE	CB-CG-CD1	-6.44	116.30	120.80
2	B	155	GLU	OE1-CD-OE2	6.43	131.02	123.30
1	A	22	VAL	CA-CB-CG2	6.43	120.55	110.90
1	A	270	ALA	N-CA-CB	6.42	119.09	110.10
4	E	431	ASP	CB-CG-OD2	-6.42	112.52	118.30
3	C	19	LYS	N-CA-CB	6.42	122.16	110.60
2	B	239	PHE	CD1-CE1-CZ	-6.42	112.40	120.10
1	A	128	CYS	CA-CB-SG	6.41	125.54	114.00
4	E	14	TYR	CG-CD1-CE1	-6.41	116.17	121.30
4	E	96	ASP	CB-CG-OD1	-6.41	112.53	118.30
3	C	10	ASP	CB-CG-OD1	6.41	124.07	118.30
4	E	194	TYR	CB-CG-CD1	6.40	124.84	121.00
1	A	97	ASP	O-C-N	-6.40	112.32	123.20
1	A	195	ASP	CB-CG-OD2	6.40	124.06	118.30
4	E	11	LEU	O-C-N	-6.40	112.33	123.20
2	B	267	ALA	N-CA-CB	-6.39	101.15	110.10
2	B	452	PHE	CB-CG-CD2	6.39	125.28	120.80
2	B	205	GLU	C-N-CA	6.39	137.68	121.70
4	E	313	THR	N-CA-CB	6.39	122.45	110.30
4	E	189	PRO	O-C-N	-6.39	112.48	122.70
1	A	427	ALA	CB-CA-C	6.39	119.68	110.10
1	A	374	SER	O-C-N	-6.38	112.48	122.70
3	C	63	TYR	CA-CB-CG	6.38	125.53	113.40
2	B	62	ASP	OD1-CG-OD2	-6.38	111.18	123.30
2	B	133	MET	CA-CB-CG	6.38	124.14	113.30
3	C	74	TYR	CG-CD2-CE2	6.38	126.40	121.30
4	E	452	TRP	CD1-CG-CD2	6.37	111.40	106.30
2	B	447	CYS	CA-CB-SG	-6.36	102.55	114.00
4	E	66	TRP	CA-CB-CG	6.36	125.78	113.70
3	C	462	THR	CA-CB-CG2	6.36	121.30	112.40
2	B	2	VAL	CA-CB-CG1	-6.35	101.38	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	229	VAL	CA-CB-CG1	6.35	120.42	110.90
2	B	468	PHE	N-CA-CB	6.35	122.02	110.60
4	E	183	TRP	CE2-CD2-CG	-6.34	102.23	107.30
2	B	12	PHE	CB-CG-CD1	6.34	125.23	120.80
4	E	85	TRP	CZ3-CH2-CZ2	6.34	129.20	121.60
2	B	141	ASN	N-CA-CB	6.33	122.00	110.60
3	C	83	ARG	NH1-CZ-NH2	6.33	126.37	119.40
1	D	391	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	D	233	PHE	CG-CD1-CE1	6.32	127.75	120.80
2	B	72	TYR	CD1-CE1-CZ	6.32	125.48	119.80
1	A	195	ASP	OD1-CG-OD2	-6.31	111.31	123.30
3	C	221	ILE	C-N-CA	6.31	137.48	121.70
1	A	108	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	198	TYR	CB-CG-CD1	6.31	124.78	121.00
1	A	377	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	A	6	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
1	D	176	TRP	CA-CB-CG	6.30	125.68	113.70
3	C	426	THR	N-CA-CB	6.29	122.26	110.30
2	B	283	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	D	62	ASP	CB-CA-C	6.29	122.98	110.40
4	E	441	LEU	O-C-N	-6.29	112.64	122.70
1	D	406	ILE	CB-CA-C	6.29	124.17	111.60
4	E	70	GLU	CG-CD-OE2	6.29	130.87	118.30
2	B	134	TYR	CG-CD1-CE1	-6.29	116.27	121.30
2	B	445	THR	CA-CB-CG2	-6.29	103.60	112.40
1	D	411	LEU	C-N-CA	6.29	137.41	121.70
3	C	473	PHE	CD1-CG-CD2	-6.28	110.13	118.30
3	C	95	GLN	CA-CB-CG	6.28	127.21	113.40
3	C	265	LEU	CA-C-N	-6.27	103.40	117.20
2	B	291	VAL	CA-CB-CG1	6.27	120.31	110.90
2	B	428	TRP	CE3-CZ3-CH2	-6.27	114.30	121.20
4	E	99	PHE	CD1-CG-CD2	6.27	126.45	118.30
3	C	88	TRP	CH2-CZ2-CE2	6.26	123.66	117.40
1	D	198	TYR	CE1-CZ-CE2	6.26	129.82	119.80
4	E	448	LYS	N-CA-CB	-6.26	99.33	110.60
3	C	464	VAL	CG1-CB-CG2	-6.26	100.89	110.90
4	E	137	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	394	ASN	N-CA-CB	6.26	121.86	110.60
2	B	407	ALA	O-C-N	-6.25	112.69	122.70
4	E	260	ALA	O-C-N	-6.25	112.70	122.70
2	B	293	PHE	CD1-CE1-CZ	-6.25	112.60	120.10
3	C	22	ARG	CG-CD-NE	-6.25	98.68	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	284	PHE	CB-CA-C	-6.25	97.90	110.40
4	E	244	ALA	CB-CA-C	6.25	119.47	110.10
1	A	280	PHE	CB-CG-CD1	6.25	125.17	120.80
1	A	151	TYR	CA-CB-CG	6.24	125.26	113.40
2	B	436	ASP	CB-CG-OD1	6.24	123.92	118.30
3	C	252	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	D	241	GLU	OE1-CD-OE2	-6.24	115.81	123.30
2	B	247	GLU	OE1-CD-OE2	-6.23	115.82	123.30
4	E	128	PRO	O-C-N	-6.23	112.73	122.70
1	D	189	TYR	CB-CG-CD2	6.23	124.74	121.00
1	D	79	ARG	CG-CD-NE	-6.22	98.73	111.80
1	D	233	PHE	CZ-CE2-CD2	6.22	127.57	120.10
4	E	229	CYS	O-C-N	-6.22	112.75	122.70
1	A	225	PHE	CD1-CG-CD2	-6.22	110.22	118.30
2	B	156	VAL	CB-CA-C	-6.21	99.60	111.40
4	E	266	PHE	N-CA-CB	6.21	121.78	110.60
4	E	462	THR	CA-CB-CG2	6.21	121.09	112.40
1	A	159	SER	O-C-N	6.20	132.89	121.10
4	E	110	TYR	N-CA-CB	6.20	121.77	110.60
2	B	431	VAL	CB-CA-C	-6.20	99.62	111.40
2	B	198	ARG	NE-CZ-NH1	-6.20	117.20	120.30
4	E	154	GLU	OE1-CD-OE2	6.20	130.74	123.30
4	E	98	GLN	CG-CD-OE1	6.19	133.99	121.60
4	E	220	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	D	166	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	427	ALA	C-N-CA	6.19	135.29	122.30
1	A	189	TYR	CG-CD1-CE1	-6.18	116.35	121.30
3	C	223	ARG	CD-NE-CZ	6.18	132.26	123.60
4	E	439	TRP	CD1-NE1-CE2	-6.18	103.44	109.00
4	E	176	ASP	OD1-CG-OD2	6.18	135.04	123.30
1	D	43	VAL	CA-CB-CG1	6.18	120.17	110.90
4	E	188	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	15	TYR	CG-CD2-CE2	6.17	126.24	121.30
1	D	60	TRP	CB-CA-C	6.17	122.75	110.40
4	E	261	GLN	O-C-N	6.17	132.57	122.70
3	C	454	ASP	N-CA-CB	6.17	121.70	110.60
4	E	71	TYR	CD1-CE1-CZ	-6.17	114.25	119.80
2	B	90	ILE	CA-C-O	6.17	133.05	120.10
2	B	306	HIS	N-CA-C	6.17	127.66	111.00
1	D	12	LEU	CB-CG-CD2	-6.17	100.52	111.00
1	D	252	SER	N-CA-CB	6.16	119.74	110.50
4	E	12	GLY	O-C-N	6.16	132.56	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	TRP	CB-CG-CD1	-6.15	119.00	127.00
2	B	468	PHE	CD1-CE1-CZ	-6.15	112.72	120.10
3	C	283	LEU	O-C-N	-6.15	112.86	122.70
4	E	267	LEU	O-C-N	-6.15	112.86	122.70
1	A	109	LEU	O-C-N	6.15	132.53	122.70
4	E	109	VAL	O-C-N	6.14	132.52	122.70
1	D	190	TYR	CD1-CG-CD2	6.14	124.65	117.90
4	E	110	TYR	CB-CG-CD2	6.14	124.68	121.00
4	E	92	GLU	OE1-CD-OE2	6.13	130.66	123.30
3	C	71	ALA	O-C-N	-6.13	112.89	122.70
1	D	24	HIS	CB-CA-C	6.13	122.66	110.40
4	E	201	ASP	CB-CG-OD1	-6.13	112.78	118.30
2	B	44	ASN	O-C-N	6.13	132.50	122.70
1	D	228	LEU	CB-CG-CD1	6.12	121.41	111.00
1	D	151	TYR	CG-CD1-CE1	6.12	126.20	121.30
1	D	55	ARG	CD-NE-CZ	6.12	132.17	123.60
4	E	136	PHE	CD1-CE1-CZ	-6.12	112.75	120.10
4	E	172	ILE	N-CA-CB	6.12	124.87	110.80
4	E	452	TRP	CZ3-CH2-CZ2	-6.12	114.26	121.60
4	E	66	TRP	CH2-CZ2-CE2	-6.11	111.29	117.40
1	A	15	TYR	CZ-CE2-CD2	6.10	125.29	119.80
2	B	224	THR	O-C-N	-6.09	112.95	122.70
2	B	119	HIS	CA-CB-CG	6.09	123.96	113.60
1	D	189	TYR	CD1-CG-CD2	-6.09	111.20	117.90
2	B	303	ASN	N-CA-CB	6.09	121.56	110.60
1	D	299	HIS	CB-CA-C	6.09	122.57	110.40
4	E	439	TRP	CB-CG-CD1	-6.09	119.09	127.00
4	E	268	ILE	CG1-CB-CG2	-6.08	98.02	111.40
1	A	137	PHE	CB-CG-CD1	-6.08	116.54	120.80
2	B	86	TRP	CZ3-CH2-CZ2	6.08	128.90	121.60
3	C	447	ASN	CB-CG-OD1	6.08	133.76	121.60
2	B	154	SER	N-CA-CB	6.08	119.62	110.50
1	A	129	GLU	CA-C-O	-6.08	107.33	120.10
2	B	74	GLY	C-N-CA	6.08	136.89	121.70
3	C	25	LYS	O-C-N	6.08	132.42	122.70
4	E	415	CYS	C-N-CA	6.07	136.88	121.70
2	B	63	TYR	CG-CD2-CE2	-6.07	116.44	121.30
2	B	306	HIS	N-CA-CB	6.07	121.53	110.60
1	D	225	PHE	CD1-CG-CD2	-6.07	110.41	118.30
4	E	230	VAL	CA-CB-CG2	6.07	120.00	110.90
1	D	231	LEU	O-C-N	6.06	132.40	122.70
3	C	17	TYR	CG-CD1-CE1	-6.06	116.45	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	26	THR	C-N-CA	6.06	136.85	121.70
1	A	422	THR	CA-CB-CG2	6.05	120.87	112.40
2	B	25	VAL	CA-CB-CG2	6.05	119.98	110.90
1	D	153	GLY	O-C-N	-6.05	113.02	122.70
1	A	112	TYR	CG-CD2-CE2	6.05	126.14	121.30
1	D	52	THR	CA-CB-CG2	-6.05	103.93	112.40
1	A	213	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
2	B	307	ARG	O-C-N	-6.04	113.03	122.70
3	C	459	PHE	O-C-N	6.04	132.36	122.70
1	A	225	PHE	CB-CG-CD2	6.04	125.03	120.80
1	D	229	THR	CA-CB-CG2	-6.04	103.95	112.40
3	C	71	ALA	N-CA-CB	6.03	118.55	110.10
1	A	149	TRP	CH2-CZ2-CE2	6.03	123.43	117.40
1	D	414	PHE	CD1-CE1-CZ	6.03	127.33	120.10
1	A	212	LEU	N-CA-C	6.02	127.26	111.00
1	A	399	TRP	C-N-CA	6.02	136.75	121.70
2	B	235	ALA	N-CA-CB	-6.02	101.67	110.10
3	C	118	VAL	CG1-CB-CG2	-6.02	101.27	110.90
3	C	225	PRO	CA-N-CD	-6.02	103.07	111.50
2	B	56	LEU	O-C-N	-6.01	113.08	122.70
1	A	164	ARG	NE-CZ-NH2	6.01	123.30	120.30
3	C	240	SER	N-CA-CB	6.01	119.51	110.50
1	D	15	TYR	CD1-CE1-CZ	-6.01	114.39	119.80
2	B	153	THR	O-C-N	-6.00	113.09	122.70
2	B	138	ASP	CB-CG-OD2	6.00	123.70	118.30
3	C	425	SER	N-CA-CB	6.00	119.50	110.50
4	E	266	PHE	CZ-CE2-CD2	6.00	127.30	120.10
1	A	230	VAL	CG1-CB-CG2	6.00	120.50	110.90
2	B	277	VAL	CB-CA-C	5.99	122.79	111.40
2	B	286	PHE	CB-CG-CD1	5.99	125.00	120.80
1	D	95	ASN	CA-CB-CG	5.99	126.58	113.40
1	A	169	THR	CA-C-O	-5.99	107.53	120.10
2	B	139	TRP	CB-CG-CD1	-5.98	119.23	127.00
3	C	183	ALA	CB-CA-C	5.98	119.07	110.10
1	A	384	GLU	OE1-CD-OE2	5.98	130.47	123.30
1	D	192	CYS	CA-CB-SG	5.98	124.76	114.00
2	B	434	VAL	O-C-N	-5.98	113.14	122.70
3	C	202	TYR	N-CA-C	5.97	127.13	111.00
1	D	132	VAL	CA-C-O	5.97	132.64	120.10
1	A	301	ARG	CD-NE-CZ	5.96	131.95	123.60
3	C	19	LYS	CB-CA-C	5.96	122.33	110.40
4	E	148	GLN	N-CA-CB	5.96	121.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	77	VAL	O-C-N	5.96	132.24	122.70
3	C	72	SER	O-C-N	-5.96	113.16	122.70
3	C	455	ARG	N-CA-CB	5.96	121.33	110.60
2	B	176	ASN	OD1-CG-ND2	5.95	135.59	121.90
4	E	106	ASN	O-C-N	5.95	132.23	122.70
2	B	211	LEU	CB-CG-CD2	-5.95	100.89	111.00
4	E	458	PHE	CB-CG-CD1	5.94	124.96	120.80
1	A	151	TYR	CD1-CE1-CZ	5.94	125.14	119.80
3	C	102	TYR	CD1-CG-CD2	-5.94	111.37	117.90
1	A	279	LEU	CA-CB-CG	5.93	128.95	115.30
1	D	408	HIS	CG-ND1-CE1	5.93	116.51	108.20
4	E	66	TRP	CE3-CZ3-CH2	5.93	127.73	121.20
4	E	458	PHE	CD1-CE1-CZ	5.93	127.22	120.10
2	B	28	LYS	N-CA-CB	-5.93	99.92	110.60
3	C	74	TYR	CA-CB-CG	5.93	124.67	113.40
1	D	213	TYR	CZ-CE2-CD2	-5.93	114.47	119.80
1	A	13	GLU	OE1-CD-OE2	5.92	130.41	123.30
1	A	188	VAL	CA-CB-CG1	5.92	119.79	110.90
4	E	297	VAL	CB-CA-C	-5.92	100.16	111.40
4	E	430	ASN	N-CA-CB	-5.92	99.95	110.60
4	E	138	TRP	NE1-CE2-CZ2	-5.92	123.89	130.40
2	B	219	PHE	CD1-CG-CD2	-5.91	110.61	118.30
2	B	15	TYR	CA-CB-CG	5.91	124.63	113.40
2	B	126	SER	O-C-N	-5.91	113.24	122.70
2	B	211	LEU	CA-C-O	-5.91	107.69	120.10
3	C	291	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	A	2	GLU	N-CA-CB	5.90	121.22	110.60
1	A	301	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	B	210	TYR	CD1-CG-CD2	-5.90	111.41	117.90
2	B	137	PHE	CB-CG-CD1	-5.90	116.67	120.80
2	B	198	ARG	C-N-CA	5.89	136.43	121.70
3	C	204	ASP	C-N-CA	5.89	136.44	121.70
2	B	135	PHE	CG-CD1-CE1	5.89	127.28	120.80
3	C	87	ILE	N-CA-CB	5.89	124.35	110.80
3	C	102	TYR	CB-CG-CD2	5.89	124.54	121.00
1	A	102	ILE	C-N-CA	5.89	136.43	121.70
3	C	101	GLN	O-C-N	5.89	132.13	122.70
2	B	139	TRP	CB-CG-CD2	5.89	134.26	126.60
2	B	428	TRP	NE1-CE2-CD2	5.89	113.19	107.30
2	B	307	ARG	CD-NE-CZ	-5.88	115.36	123.60
2	B	137	PHE	CG-CD2-CE2	-5.88	114.33	120.80
4	E	116	TYR	N-CA-CB	-5.88	100.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	200	ASP	C-N-CA	5.88	136.40	121.70
1	D	222	CYS	CB-CA-C	5.88	122.16	110.40
2	B	27	ASP	OD1-CG-OD2	-5.88	112.13	123.30
1	D	230	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	A	151	TYR	CG-CD2-CE2	5.87	126.00	121.30
4	E	25	ASP	N-CA-CB	5.87	121.17	110.60
3	C	86	LEU	CB-CA-C	5.87	121.35	110.20
2	B	65	LEU	CB-CG-CD1	5.86	120.96	111.00
2	B	86	TRP	CE3-CZ3-CH2	-5.86	114.75	121.20
1	A	103	VAL	CG1-CB-CG2	-5.86	101.53	110.90
3	C	69	TRP	CH2-CZ2-CE2	-5.86	111.54	117.40
1	A	135	PHE	CD1-CE1-CZ	-5.86	113.07	120.10
3	C	67	LEU	CB-CG-CD2	5.86	120.95	111.00
3	C	86	LEU	C-N-CA	5.86	136.34	121.70
1	D	257	LEU	O-C-N	-5.85	113.33	122.70
2	B	100	PHE	CB-CG-CD1	5.85	124.90	120.80
2	B	197	TRP	CD1-NE1-CE2	5.85	114.27	109.00
1	A	399	TRP	CD2-CE3-CZ3	5.85	126.40	118.80
3	C	137	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	D	99	ASP	N-CA-CB	5.84	121.12	110.60
4	E	2	GLU	OE1-CD-OE2	-5.84	116.29	123.30
3	C	92	ILE	CA-C-N	-5.84	104.36	117.20
2	B	466	ASN	N-CA-C	5.83	126.75	111.00
1	D	414	PHE	CG-CD1-CE1	-5.83	114.39	120.80
1	D	218	VAL	CA-CB-CG1	-5.83	102.16	110.90
4	E	152	ALA	N-CA-C	5.83	126.73	111.00
1	A	47	ASN	C-N-CA	5.82	136.26	121.70
1	A	401	TYR	CZ-CE2-CD2	-5.82	114.56	119.80
2	B	113	THR	O-C-N	5.82	133.10	123.20
3	C	156	ASN	CB-CA-C	5.82	122.05	110.40
2	B	306	HIS	CA-CB-CG	-5.82	103.70	113.60
1	D	67	TRP	NE1-CE2-CD2	-5.82	101.48	107.30
2	B	239	PHE	CB-CG-CD2	-5.82	116.73	120.80
1	D	381	TYR	CG-CD2-CE2	-5.81	116.65	121.30
1	A	162	SER	N-CA-C	5.81	126.69	111.00
2	B	128	CYS	C-N-CA	5.81	136.23	121.70
2	B	64	ARG	CB-CG-CD	5.81	126.70	111.60
4	E	215	GLN	CG-CD-OE1	-5.81	109.98	121.60
1	D	192	CYS	C-N-CA	5.81	136.21	121.70
4	E	286	LEU	CA-CB-CG	5.80	128.65	115.30
4	E	85	TRP	CB-CG-CD1	-5.80	119.46	127.00
1	A	212	LEU	CA-CB-CG	5.80	128.64	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	283	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
3	C	180	ASP	N-CA-CB	5.80	121.04	110.60
3	C	439	TYR	C-N-CA	5.80	136.20	121.70
3	C	232	PHE	CD1-CG-CD2	-5.80	110.76	118.30
1	A	176	TRP	CE3-CZ3-CH2	-5.79	114.83	121.20
2	B	95	ASN	N-CA-CB	5.79	121.02	110.60
2	B	429	GLN	CG-CD-OE1	-5.79	110.02	121.60
3	C	76	ASP	C-N-CA	5.79	136.17	121.70
1	D	102	ILE	N-CA-CB	5.79	124.11	110.80
1	D	238	ASP	OD1-CG-OD2	-5.78	112.31	123.30
1	A	284	PHE	CG-CD2-CE2	5.78	127.15	120.80
1	D	102	ILE	CA-CB-CG1	5.78	121.97	111.00
2	B	257	LEU	CB-CG-CD1	5.77	120.81	111.00
4	E	100	GLU	C-N-CA	5.77	136.13	121.70
1	D	160	PRO	CA-N-CD	-5.77	103.43	111.50
2	B	196	ASN	CB-CG-OD1	5.76	133.13	121.60
1	A	60	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	A	305	THR	OG1-CB-CG2	5.76	123.25	110.00
2	B	293	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	A	277	TYR	CD1-CG-CD2	-5.76	111.57	117.90
1	A	378	GLY	O-C-N	-5.76	113.49	122.70
1	A	192	CYS	CA-CB-SG	5.75	124.36	114.00
2	B	294	SER	O-C-N	-5.75	113.49	122.70
3	C	141	TRP	C-N-CA	5.75	136.08	121.70
1	D	190	TYR	CB-CG-CD2	-5.75	117.55	121.00
4	E	43	ASN	N-CA-CB	5.75	120.95	110.60
1	D	167	LEU	C-N-CA	5.75	136.06	121.70
3	C	93	VAL	CG1-CB-CG2	-5.74	101.71	110.90
1	D	112	TYR	C-N-CA	5.74	136.06	121.70
1	D	118	TRP	O-C-N	5.74	131.89	122.70
4	E	71	TYR	CB-CG-CD1	5.74	124.45	121.00
2	B	10	VAL	O-C-N	-5.74	113.51	122.70
1	A	209	ARG	CD-NE-CZ	5.74	131.63	123.60
2	B	204	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	175	GLU	O-C-N	-5.74	113.52	122.70
2	B	187	SER	C-N-CA	5.74	136.05	121.70
1	D	176	TRP	NE1-CE2-CZ2	-5.74	124.09	130.40
2	B	89	ASP	O-C-N	-5.73	113.53	122.70
2	B	268	ASP	CB-CG-OD2	5.73	123.45	118.30
1	D	211	PRO	O-C-N	5.73	131.87	122.70
4	E	148	GLN	O-C-N	-5.73	113.54	122.70
1	A	146	LEU	CB-CG-CD2	-5.72	101.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	37	THR	CA-CB-CG2	5.72	120.42	112.40
3	C	38	THR	CA-CB-CG2	-5.72	104.39	112.40
1	D	241	GLU	CG-CD-OE1	5.72	129.75	118.30
4	E	150	TYR	CZ-CE2-CD2	-5.72	114.65	119.80
4	E	178	THR	N-CA-C	5.72	126.45	111.00
1	A	284	PHE	CB-CG-CD1	-5.72	116.80	120.80
4	E	452	TRP	CH2-CZ2-CE2	5.71	123.11	117.40
1	A	3	HIS	C-N-CA	5.71	135.98	121.70
3	C	473	PHE	N-CA-C	-5.71	95.58	111.00
4	E	476	GLU	N-CA-CB	5.71	120.88	110.60
2	B	244	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	268	SER	CA-C-O	5.71	132.09	120.10
2	B	200	ASP	CB-CG-OD2	5.70	123.43	118.30
3	C	302	VAL	CA-CB-CG1	5.70	119.45	110.90
1	A	20	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
4	E	100	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	D	433	LEU	CB-CA-C	5.70	121.02	110.20
3	C	268	ALA	CB-CA-C	5.70	118.64	110.10
3	C	294	PHE	CB-CG-CD2	5.69	124.79	120.80
2	B	149	TYR	CG-CD1-CE1	-5.69	116.75	121.30
3	C	94	LEU	CB-CA-C	5.69	121.01	110.20
3	C	257	MET	CG-SD-CE	5.69	109.31	100.20
4	E	246	ALA	N-CA-C	5.69	126.35	111.00
2	B	292	ALA	O-C-N	5.68	131.79	122.70
1	A	394	ASN	CA-CB-CG	5.68	125.90	113.40
2	B	197	TRP	CZ3-CH2-CZ2	5.68	128.42	121.60
1	D	112	TYR	O-C-N	5.68	131.78	122.70
1	A	392	SER	CA-C-O	5.67	132.02	120.10
4	E	54	TRP	CD1-CG-CD2	-5.67	101.76	106.30
1	D	73	GLY	C-N-CA	5.67	134.21	122.30
1	D	166	ASP	CB-CG-OD2	-5.67	113.19	118.30
4	E	107	VAL	CG1-CB-CG2	-5.67	101.83	110.90
4	E	304	LEU	CA-CB-CG	-5.67	102.25	115.30
1	A	135	PHE	O-C-N	5.67	131.87	121.10
3	C	471	PHE	CD1-CE1-CZ	-5.67	113.30	120.10
2	B	271	PRO	O-C-N	5.67	131.76	122.70
1	A	189	TYR	CB-CG-CD2	-5.66	117.60	121.00
2	B	85	VAL	O-C-N	5.66	131.76	122.70
3	C	67	LEU	O-C-N	-5.66	113.64	122.70
1	A	170	PHE	CG-CD2-CE2	5.66	127.02	120.80
1	A	98	GLY	O-C-N	-5.66	113.65	122.70
1	D	161	GLU	CG-CD-OE2	5.65	129.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	PHE	CB-CG-CD1	5.65	124.76	120.80
3	C	63	TYR	CB-CG-CD1	5.65	124.39	121.00
4	E	134	PHE	CG-CD2-CE2	5.65	127.01	120.80
4	E	309	ARG	N-CA-C	5.65	126.25	111.00
3	C	103	ASN	O-C-N	5.64	131.73	122.70
4	E	240	TYR	CD1-CE1-CZ	5.64	124.88	119.80
2	B	218	LEU	N-CA-CB	5.64	121.68	110.40
4	E	240	TYR	CG-CD1-CE1	-5.64	116.79	121.30
1	A	381	TYR	CB-CG-CD1	5.64	124.38	121.00
2	B	134	TYR	CA-CB-CG	5.63	124.11	113.40
1	D	34	GLY	CA-C-N	-5.63	104.81	117.20
1	A	112	TYR	CE1-CZ-CE2	-5.63	110.79	119.80
2	B	151	TYR	CZ-CE2-CD2	5.63	124.87	119.80
1	A	62	ASP	CB-CG-OD2	5.63	123.36	118.30
4	E	1	ASN	N-CA-CB	-5.62	100.48	110.60
1	A	118	TRP	CD1-CG-CD2	-5.62	101.80	106.30
2	B	35	LEU	N-CA-CB	5.62	121.64	110.40
1	D	221	PRO	N-CA-CB	-5.62	96.42	102.60
4	E	221	TYR	CD1-CG-CD2	-5.62	111.72	117.90
1	D	225	PHE	CG-CD1-CE1	5.62	126.98	120.80
1	D	256	PHE	CG-CD2-CE2	5.62	126.98	120.80
1	A	414	PHE	CG-CD1-CE1	-5.61	114.63	120.80
3	C	141	TRP	CB-CG-CD2	-5.61	119.31	126.60
2	B	154	SER	CA-C-O	-5.61	108.32	120.10
3	C	191	GLU	O-C-N	5.61	131.67	122.70
1	D	289	ILE	CA-CB-CG1	-5.61	100.35	111.00
2	B	10	VAL	CA-CB-CG1	5.60	119.30	110.90
3	C	228	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	D	235	LEU	CB-CA-C	5.59	120.83	110.20
1	A	213	TYR	O-C-N	-5.59	113.75	122.70
1	A	393	SER	CA-C-O	-5.59	108.36	120.10
1	D	181	TYR	CZ-CE2-CD2	-5.59	114.77	119.80
4	E	124	ARG	O-C-N	5.59	131.64	122.70
2	B	428	TRP	CA-CB-CG	5.59	124.32	113.70
4	E	19	LYS	CB-CA-C	5.59	121.57	110.40
2	B	431	VAL	N-CA-C	5.58	126.07	111.00
2	B	463	PRO	N-CA-C	5.58	126.61	112.10
2	B	430	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
1	D	23	GLU	O-C-N	-5.57	113.78	122.70
1	D	198	TYR	CD1-CE1-CZ	-5.57	114.78	119.80
4	E	136	PHE	CB-CG-CD1	5.57	124.70	120.80
3	C	20	HIS	CA-CB-CG	-5.57	104.13	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	258	LEU	N-CA-CB	5.57	121.54	110.40
3	C	320	HIS	CG-ND1-CE1	5.57	116.00	108.20
4	E	224	ASN	CA-C-N	-5.57	104.95	117.20
2	B	428	TRP	CB-CA-C	5.57	121.53	110.40
4	E	183	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	D	139	GLN	N-CA-C	5.57	126.03	111.00
1	D	403	ALA	C-N-CA	5.57	135.61	121.70
1	A	82	SER	C-N-CA	5.56	135.61	121.70
1	A	93	TYR	CD1-CE1-CZ	-5.56	114.80	119.80
4	E	221	TYR	CG-CD2-CE2	5.56	125.75	121.30
2	B	242	PRO	CA-N-CD	-5.56	103.72	111.50
1	D	389	ASP	CB-CG-OD2	-5.56	113.30	118.30
3	C	447	ASN	O-C-N	-5.55	113.81	122.70
1	D	130	ILE	O-C-N	5.55	131.59	122.70
4	E	175	GLU	O-C-N	5.55	131.59	122.70
4	E	421	PHE	CG-CD1-CE1	5.55	126.91	120.80
3	C	81	ARG	NE-CZ-NH1	-5.55	117.53	120.30
3	C	132	ILE	CA-CB-CG2	5.55	122.00	110.90
4	E	418	ALA	N-CA-CB	5.55	117.87	110.10
2	B	125	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
3	C	223	ARG	NE-CZ-NH1	-5.55	117.53	120.30
3	C	252	GLU	O-C-N	-5.54	113.83	122.70
1	D	185	LYS	O-C-N	5.54	131.57	122.70
4	E	309	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	A	30	ASP	CB-CA-C	-5.54	99.32	110.40
2	B	1	SER	CB-CA-C	-5.54	99.58	110.10
2	B	132	VAL	C-N-CA	5.54	135.55	121.70
4	E	225	ILE	CA-CB-CG1	-5.54	100.48	111.00
1	A	405	VAL	O-C-N	-5.54	113.84	122.70
2	B	468	PHE	CD1-CG-CD2	-5.54	111.10	118.30
3	C	290	LYS	CD-CE-NZ	5.54	124.43	111.70
1	D	386	MET	CA-CB-CG	5.54	122.71	113.30
1	D	198	TYR	CG-CD1-CE1	-5.53	116.87	121.30
4	E	104	TYR	CB-CG-CD2	5.53	124.32	121.00
3	C	69	TRP	CD2-CE2-CZ2	5.53	128.94	122.30
1	D	230	VAL	O-C-N	-5.53	113.85	122.70
1	A	258	LEU	CB-CG-CD2	5.53	120.39	111.00
1	A	297	ASN	O-C-N	5.53	131.54	122.70
3	C	241	PHE	CD1-CE1-CZ	-5.53	113.47	120.10
2	B	124	TYR	CA-CB-CG	5.52	123.89	113.40
2	B	9	SER	O-C-N	-5.52	113.87	122.70
3	C	297	SER	N-CA-CB	-5.52	102.22	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	21	ALA	O-C-N	5.52	131.53	122.70
1	A	112	TYR	CZ-CE2-CD2	5.51	124.76	119.80
1	D	284	PHE	CD1-CE1-CZ	5.51	126.72	120.10
4	E	435	GLU	OE1-CD-OE2	-5.51	116.68	123.30
2	B	182	GLU	O-C-N	5.51	131.52	122.70
2	B	200	ASP	C-N-CA	5.51	135.47	121.70
1	A	23	GLU	O-C-N	5.51	131.51	122.70
4	E	104	TYR	CA-CB-CG	5.51	123.86	113.40
1	D	256	PHE	CZ-CE2-CD2	-5.50	113.49	120.10
2	B	140	GLN	C-N-CA	5.50	135.45	121.70
1	D	237	THR	N-CA-CB	5.50	120.75	110.30
2	B	284	LEU	CB-CA-C	5.50	120.65	110.20
2	B	463	PRO	O-C-N	-5.50	110.65	121.10
3	C	104	VAL	CA-CB-CG2	5.50	119.15	110.90
3	C	439	TYR	CB-CG-CD1	5.50	124.30	121.00
1	D	45	GLU	O-C-N	-5.50	113.90	122.70
2	B	258	ALA	O-C-N	-5.49	113.91	122.70
1	D	376	ILE	C-N-CA	5.49	135.44	121.70
1	A	181	TYR	CG-CD1-CE1	5.49	125.69	121.30
1	A	240	GLY	O-C-N	-5.49	113.92	122.70
2	B	198	ARG	N-CA-CB	5.49	120.48	110.60
2	B	302	LEU	CB-CA-C	5.49	120.63	110.20
3	C	88	TRP	CD2-CE3-CZ3	5.49	125.93	118.80
1	D	49	ILE	CB-CA-C	-5.48	100.64	111.60
1	A	149	TRP	O-C-N	-5.48	113.93	122.70
2	B	160	HIS	O-C-N	-5.47	113.94	122.70
3	C	287	LEU	CA-C-O	-5.47	108.60	120.10
3	C	109	ASN	O-C-N	5.47	131.46	122.70
4	E	136	PHE	C-N-CA	5.47	135.38	121.70
1	A	257	LEU	CB-CA-C	-5.47	99.81	110.20
1	D	85	VAL	CB-CA-C	-5.47	101.01	111.40
1	A	262	GLU	CA-C-N	-5.47	105.17	117.20
1	A	5	THR	CA-CB-CG2	-5.46	104.75	112.40
1	A	176	TRP	CD1-NE1-CE2	5.46	113.92	109.00
2	B	93	MET	CA-C-O	-5.46	108.63	120.10
3	C	316	THR	N-CA-CB	5.46	120.68	110.30
4	E	246	ALA	N-CA-CB	-5.46	102.45	110.10
4	E	205	PHE	CZ-CE2-CD2	5.46	126.65	120.10
3	C	443	VAL	C-N-CA	5.46	133.76	122.30
1	D	26	THR	N-CA-CB	5.46	120.67	110.30
4	E	134	PHE	C-N-CD	5.46	139.86	128.40
3	C	191	GLU	C-N-CA	5.46	135.34	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	18	VAL	CA-CB-CG2	5.45	119.08	110.90
3	C	277	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	84	ASP	C-N-CA	5.45	135.32	121.70
1	D	61	ILE	O-C-N	-5.45	113.98	122.70
1	D	60	TRP	CG-CD2-CE3	-5.45	129.00	133.90
4	E	219	LEU	CA-C-N	-5.45	105.22	117.20
1	D	280	PHE	CB-CG-CD2	5.44	124.61	120.80
3	C	236	CYS	CB-CA-C	5.44	121.29	110.40
1	D	170	PHE	CG-CD2-CE2	-5.44	114.81	120.80
3	C	22	ARG	CB-CA-C	5.44	121.28	110.40
1	D	67	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	A	249	VAL	CA-CB-CG2	-5.44	102.74	110.90
4	E	239	VAL	CA-CB-CG1	5.44	119.06	110.90
1	A	426	PHE	CG-CD1-CE1	5.44	126.78	120.80
3	C	287	LEU	O-C-N	5.44	131.40	122.70
3	C	116	GLY	N-CA-C	5.43	126.69	113.10
3	C	449	VAL	CA-CB-CG2	5.43	119.05	110.90
4	E	466	PHE	CB-CG-CD2	-5.43	117.00	120.80
3	C	74	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	86	TRP	CD1-NE1-CE2	-5.43	104.11	109.00
3	C	300	THR	CA-CB-CG2	-5.43	104.80	112.40
4	E	25	ASP	OD1-CG-OD2	-5.43	112.99	123.30
4	E	252	THR	O-C-N	-5.43	114.02	122.70
3	C	202	TYR	CE1-CZ-CE2	-5.42	111.12	119.80
4	E	263	ILE	CB-CA-C	-5.42	100.76	111.60
1	D	25	HIS	O-C-N	5.42	131.37	122.70
3	C	69	TRP	CE2-CD2-CE3	-5.41	112.20	118.70
3	C	318	SER	O-C-N	-5.41	114.04	122.70
4	E	91	LEU	CA-CB-CG	5.41	127.75	115.30
3	C	270	PHE	CE1-CZ-CE2	-5.41	110.26	120.00
1	A	301	ARG	N-CA-C	5.41	125.60	111.00
4	E	220	PHE	CA-C-N	-5.41	105.30	117.20
3	C	109	ASN	CA-C-O	-5.41	108.75	120.10
4	E	266	PHE	CB-CG-CD2	-5.41	117.02	120.80
1	A	300	HIS	CA-CB-CG	-5.40	104.42	113.60
2	B	428	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	152	ASP	N-CA-CB	-5.40	100.88	110.60
3	C	312	PHE	CB-CG-CD1	-5.40	117.02	120.80
2	B	48	GLU	N-CA-CB	5.39	120.31	110.60
4	E	476	GLU	O-C-N	-5.39	114.07	122.70
3	C	137	PHE	CZ-CE2-CD2	-5.39	113.63	120.10
4	E	2	GLU	CG-CD-OE2	5.39	129.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	434	LYS	N-CA-CB	5.39	120.30	110.60
3	C	297	SER	O-C-N	5.38	131.31	122.70
4	E	34	LEU	O-C-N	5.38	131.32	122.70
2	B	215	ARG	CA-CB-CG	5.38	125.24	113.40
3	C	482	PRO	CA-N-CD	-5.38	103.97	111.50
2	B	82	SER	CB-CA-C	5.38	120.32	110.10
2	B	203	SER	N-CA-CB	-5.38	102.43	110.50
1	D	15	TYR	CE1-CZ-CE2	5.38	128.41	119.80
1	D	49	ILE	CA-CB-CG1	-5.38	100.78	111.00
3	C	12	LEU	CB-CG-CD1	5.38	120.14	111.00
1	A	136	PRO	CA-N-CD	5.37	119.22	111.70
3	C	14	VAL	CG1-CB-CG2	5.37	119.49	110.90
1	A	190	TYR	CG-CD2-CE2	-5.37	117.01	121.30
3	C	8	ILE	CA-CB-CG2	-5.37	100.17	110.90
4	E	241	PHE	CB-CG-CD1	5.37	124.56	120.80
2	B	239	PHE	CZ-CE2-CD2	5.37	126.54	120.10
1	A	112	TYR	CG-CD1-CE1	5.36	125.59	121.30
1	D	129	GLU	CA-C-N	-5.36	105.40	117.20
1	A	209	ARG	N-CA-C	5.36	125.48	111.00
4	E	281	LEU	O-C-N	-5.36	114.12	122.70
3	C	182	GLU	CG-CD-OE1	5.36	129.01	118.30
3	C	223	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
4	E	202	ASP	CB-CG-OD2	-5.35	113.48	118.30
3	C	431	LYS	CA-CB-CG	5.35	125.17	113.40
3	C	437	ASN	OD1-CG-ND2	5.35	134.20	121.90
3	C	475	MET	CA-CB-CG	5.35	122.39	113.30
1	D	227	PHE	CG-CD1-CE1	5.34	126.68	120.80
3	C	271	LEU	O-C-N	-5.34	114.15	122.70
1	D	176	TRP	NE1-CE2-CD2	5.34	112.64	107.30
1	A	160	PRO	CA-N-CD	-5.34	104.02	111.50
2	B	27	ASP	N-CA-CB	5.34	120.21	110.60
3	C	104	VAL	O-C-N	5.34	131.24	122.70
3	C	189	GLU	OE1-CD-OE2	-5.34	116.90	123.30
3	C	250	PRO	C-N-CA	5.34	135.04	121.70
4	E	77	VAL	C-N-CA	5.34	135.04	121.70
2	B	440	LEU	CA-CB-CG	-5.33	103.03	115.30
2	B	263	LEU	O-C-N	5.33	131.24	122.70
1	D	252	SER	C-N-CA	5.33	135.03	121.70
1	D	184	TRP	CH2-CZ2-CE2	-5.33	112.07	117.40
1	D	190	TYR	CB-CG-CD1	-5.33	117.80	121.00
4	E	451	PHE	CG-CD1-CE1	-5.33	114.94	120.80
1	D	248	SER	O-C-N	5.33	131.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	149	TRP	CD1-CG-CD2	5.33	110.56	106.30
1	D	157	SER	O-C-N	-5.33	114.18	122.70
1	D	149	TRP	CE3-CZ3-CH2	5.32	127.06	121.20
1	D	166	ASP	CA-C-N	-5.32	105.51	117.20
4	E	15	ASP	C-N-CA	5.32	134.99	121.70
4	E	216	ARG	N-CA-CB	5.31	120.17	110.60
1	D	20	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	D	61	ILE	CA-C-O	5.31	131.26	120.10
4	E	443	GLY	CA-C-O	-5.31	111.04	120.60
1	D	277	TYR	N-CA-C	5.31	125.34	111.00
3	C	248	TYR	CB-CG-CD1	5.31	124.19	121.00
2	B	151	TYR	CB-CG-CD1	-5.31	117.81	121.00
2	B	237	LEU	CB-CG-CD1	5.31	120.02	111.00
3	C	446	TRP	C-N-CA	5.31	134.97	121.70
3	C	66	ARG	CD-NE-CZ	5.30	131.02	123.60
3	C	316	THR	CA-CB-CG2	-5.30	104.98	112.40
4	E	78	ARG	CA-CB-CG	5.30	125.06	113.40
2	B	139	TRP	CA-CB-CG	-5.29	103.64	113.70
1	D	63	VAL	CB-CA-C	-5.29	101.34	111.40
4	E	470	HIS	CB-CA-C	-5.29	99.82	110.40
1	D	221	PRO	N-CD-CG	-5.28	95.27	103.20
4	E	292	VAL	O-C-N	5.28	131.15	122.70
1	A	414	PHE	C-N-CA	5.28	134.90	121.70
1	D	71	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	D	135	PHE	CB-CG-CD1	-5.28	117.11	120.80
3	C	28	ASN	O-C-N	-5.27	114.26	122.70
1	D	218	VAL	CA-CB-CG2	5.27	118.81	110.90
4	E	293	SER	O-C-N	-5.27	114.26	122.70
1	A	22	VAL	CG1-CB-CG2	5.27	119.33	110.90
1	D	86	TRP	NE1-CE2-CD2	-5.27	102.03	107.30
3	C	45	LEU	CA-CB-CG	5.27	127.41	115.30
1	D	86	TRP	CH2-CZ2-CE2	5.27	122.67	117.40
2	B	403	GLU	N-CA-CB	5.26	120.08	110.60
3	C	84	PRO	O-C-N	-5.26	114.28	122.70
3	C	101	GLN	OE1-CD-NE2	-5.26	109.80	121.90
1	A	427	ALA	O-C-N	-5.26	114.25	123.20
3	C	288	ILE	CA-C-N	-5.26	105.68	116.20
1	D	152	ASP	N-CA-CB	-5.26	101.14	110.60
4	E	72	GLU	OE1-CD-OE2	-5.25	116.99	123.30
3	C	82	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	136	PRO	CB-CA-C	5.25	125.13	112.00
3	C	226	LEU	CB-CA-C	5.25	120.17	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	76	LYS	CD-CE-NZ	5.25	123.77	111.70
1	D	127	TYR	O-C-N	-5.25	114.31	122.70
2	B	244	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	421	GLY	N-CA-C	-5.25	99.99	113.10
4	E	286	LEU	CA-C-N	-5.25	105.66	117.20
3	C	10	ASP	OD1-CG-OD2	-5.24	113.34	123.30
2	B	44	ASN	N-CA-CB	5.24	120.03	110.60
3	C	69	TRP	CZ3-CH2-CZ2	5.24	127.89	121.60
2	B	240	TYR	CD1-CG-CD2	5.24	123.66	117.90
1	A	60	TRP	CD1-CG-CD2	5.24	110.49	106.30
1	A	419	ILE	CA-C-O	-5.24	109.10	120.10
2	B	282	SER	N-CA-CB	-5.24	102.64	110.50
1	A	381	TYR	CD1-CE1-CZ	5.24	124.51	119.80
1	D	76	LYS	C-N-CA	5.24	134.79	121.70
2	B	197	TRP	CD1-CG-CD2	5.23	110.49	106.30
3	C	99	ASP	CB-CG-OD2	-5.23	113.59	118.30
4	E	122	ILE	N-CA-C	-5.23	96.87	111.00
1	A	379	VAL	CB-CA-C	-5.23	101.46	111.40
2	B	117	SER	CA-C-O	-5.23	109.11	120.10
1	A	284	PHE	CD1-CE1-CZ	5.23	126.38	120.10
4	E	81	SER	C-N-CA	5.23	134.78	121.70
4	E	266	PHE	CG-CD2-CE2	-5.23	115.05	120.80
2	B	302	LEU	CB-CG-CD2	-5.23	102.11	111.00
3	C	37	LEU	N-CA-CB	5.23	120.86	110.40
3	C	315	ARG	CB-CA-C	-5.23	99.94	110.40
1	D	95	ASN	N-CA-CB	5.23	120.01	110.60
4	E	231	LEU	CA-CB-CG	-5.23	103.28	115.30
3	C	74	TYR	N-CA-CB	-5.22	101.19	110.60
4	E	150	TYR	CD1-CG-CD2	-5.22	112.16	117.90
4	E	265	LEU	CB-CA-C	-5.22	100.28	110.20
2	B	139	TRP	CZ3-CH2-CZ2	-5.22	115.34	121.60
3	C	12	LEU	O-C-N	-5.22	114.35	122.70
3	C	118	VAL	O-C-N	-5.22	114.35	122.70
1	D	13	GLU	OE1-CD-OE2	5.22	129.56	123.30
1	D	279	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	D	301	ARG	N-CA-C	5.22	125.08	111.00
1	A	66	ARG	NH1-CZ-NH2	5.21	125.14	119.40
2	B	149	TYR	CD1-CE1-CZ	5.21	124.49	119.80
1	D	117	MET	CB-CG-SD	5.21	128.04	112.40
4	E	152	ALA	C-N-CA	5.21	134.73	121.70
2	B	89	ASP	CB-CG-OD1	5.21	122.99	118.30
4	E	138	TRP	CD1-CG-CD2	5.21	110.47	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	122	PRO	CA-N-CD	-5.21	104.21	111.50
1	A	422	THR	O-C-N	-5.21	114.37	122.70
1	D	27	HIS	N-CA-C	5.21	125.06	111.00
2	B	439	PHE	CB-CG-CD2	5.21	124.44	120.80
3	C	190	TRP	O-C-N	5.21	131.03	122.70
3	C	423	ILE	O-C-N	-5.21	114.37	122.70
2	B	67	TRP	CD2-CE2-CZ2	-5.20	116.06	122.30
3	C	426	THR	CA-C-O	-5.20	109.17	120.10
1	A	99	ASP	C-N-CA	5.20	134.70	121.70
1	D	2	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	D	250	LEU	O-C-N	-5.20	114.38	122.70
1	A	20	ARG	O-C-N	5.20	130.98	121.10
1	A	415	MET	O-C-N	5.20	131.01	122.70
1	A	225	PHE	CG-CD2-CE2	5.20	126.52	120.80
4	E	92	GLU	CG-CD-OE1	-5.20	107.91	118.30
1	A	29	VAL	O-C-N	-5.19	114.39	122.70
1	A	220	ILE	O-C-N	5.19	130.97	121.10
1	D	398	GLU	CG-CD-OE2	5.19	128.69	118.30
1	A	12	LEU	CB-CA-C	-5.19	100.34	110.20
1	A	95	ASN	CB-CA-C	5.19	120.78	110.40
1	A	265	PRO	CA-CB-CG	-5.19	94.14	104.00
3	C	279	PRO	N-CD-CG	-5.19	95.41	103.20
3	C	3	GLU	OE1-CD-OE2	5.19	129.53	123.30
3	C	27	ASN	CA-C-N	-5.19	105.78	117.20
2	B	86	TRP	CH2-CZ2-CE2	-5.19	112.21	117.40
2	B	176	ASN	O-C-N	-5.19	114.40	122.70
1	D	130	ILE	CG1-CB-CG2	5.19	122.81	111.40
1	D	227	PHE	CB-CG-CD2	5.19	124.43	120.80
2	B	27	ASP	CB-CG-OD1	5.18	122.97	118.30
4	E	87	PRO	N-CD-CG	-5.18	95.42	103.20
1	D	162	SER	O-C-N	5.18	130.99	122.70
4	E	112	ASP	CB-CG-OD2	5.18	122.96	118.30
3	C	120	TRP	CD1-NE1-CE2	5.18	113.66	109.00
2	B	420	GLU	N-CA-CB	5.18	119.92	110.60
2	B	424	LEU	O-C-N	5.17	130.98	122.70
1	D	22	VAL	O-C-N	5.17	130.98	122.70
1	A	432	GLU	O-C-N	-5.17	114.42	122.70
2	B	238	VAL	CG1-CB-CG2	-5.17	102.63	110.90
2	B	417	SER	O-C-N	5.17	130.98	122.70
1	D	396	ALA	CB-CA-C	-5.17	102.34	110.10
1	A	113	THR	CA-CB-CG2	-5.17	105.16	112.40
3	C	319	THR	OG1-CB-CG2	-5.17	98.12	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	255	ILE	CB-CA-C	-5.17	101.27	111.60
3	C	102	TYR	CB-CG-CD1	5.16	124.10	121.00
1	D	67	TRP	O-C-N	5.16	130.96	122.70
1	A	7	LEU	N-CA-CB	5.16	120.72	110.40
2	B	214	GLN	O-C-N	-5.16	114.44	122.70
1	D	277	TYR	CG-CD1-CE1	-5.16	117.17	121.30
4	E	461	GLY	CA-C-O	5.16	129.89	120.60
1	A	383	ALA	O-C-N	-5.16	114.45	122.70
1	D	5	THR	O-C-N	-5.16	114.45	122.70
4	E	10	LEU	CB-CG-CD1	-5.16	102.23	111.00
4	E	85	TRP	CD1-CG-CD2	5.16	110.43	106.30
3	C	212	TYR	CA-C-N	-5.16	105.86	117.20
4	E	126	THR	N-CA-C	5.16	124.92	111.00
3	C	139	PHE	CB-CG-CD1	5.15	124.41	120.80
1	D	213	TYR	CB-CG-CD2	5.15	124.09	121.00
4	E	154	GLU	O-C-N	-5.15	114.46	122.70
1	A	67	TRP	N-CA-C	5.15	124.91	111.00
2	B	64	ARG	N-CA-CB	5.15	119.87	110.60
1	D	5	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	257	LEU	O-C-N	-5.15	114.47	122.70
1	D	14	ASN	O-C-N	5.15	130.93	122.70
1	A	82	SER	CA-C-O	5.14	130.90	120.10
1	D	184	TRP	CD1-CG-CD2	-5.14	102.19	106.30
1	A	140	GLN	CG-CD-NE2	5.14	129.04	116.70
1	D	194	PRO	C-N-CA	5.14	134.55	121.70
2	B	244	ASP	OD1-CG-OD2	-5.14	113.54	123.30
2	B	243	PRO	N-CA-CB	5.13	109.46	103.30
1	D	171	MET	CA-C-O	-5.13	109.32	120.10
3	C	478	PHE	CG-CD2-CE2	-5.13	115.15	120.80
1	A	427	ALA	CA-C-N	5.13	126.46	116.20
4	E	136	PHE	CB-CA-C	5.13	120.66	110.40
3	C	120	TRP	NE1-CE2-CZ2	5.13	136.04	130.40
1	D	95	ASN	OD1-CG-ND2	-5.13	110.10	121.90
1	D	410	LEU	N-CA-CB	5.13	120.66	110.40
1	A	129	GLU	OE1-CD-OE2	-5.13	117.15	123.30
3	C	46	LYS	N-CA-C	-5.13	97.15	111.00
3	C	481	PRO	N-CA-C	5.13	125.43	112.10
1	D	245	LEU	CB-CG-CD1	-5.13	102.28	111.00
4	E	439	TRP	CB-CG-CD2	5.13	133.27	126.60
1	A	28	PHE	C-N-CA	-5.13	108.89	121.70
1	A	408	HIS	CG-ND1-CE1	5.13	115.38	108.20
2	B	260	THR	CA-CB-CG2	-5.13	105.22	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	476	GLY	O-C-N	-5.13	114.50	122.70
1	D	234	TYR	CG-CD2-CE2	5.12	125.40	121.30
4	E	183	TRP	CB-CG-CD2	-5.12	119.94	126.60
4	E	236	VAL	CA-C-O	-5.12	109.35	120.10
2	B	206	ASP	N-CA-C	5.12	124.81	111.00
2	B	7	LEU	CB-CG-CD1	-5.12	102.31	111.00
4	E	70	GLU	OE1-CD-OE2	-5.12	117.16	123.30
3	C	101	GLN	CA-C-N	-5.11	105.95	117.20
4	E	291	PHE	CB-CA-C	5.11	120.63	110.40
4	E	427	LYS	CA-CB-CG	5.11	124.65	113.40
1	D	162	SER	N-CA-CB	5.11	118.17	110.50
2	B	156	VAL	O-C-N	-5.11	114.53	122.70
2	B	287	ILE	CG1-CB-CG2	5.11	122.64	111.40
4	E	68	THR	O-C-N	-5.11	114.53	122.70
1	D	276	LYS	N-CA-CB	5.10	119.79	110.60
1	A	67	TRP	CG-CD1-NE1	-5.10	105.00	110.10
2	B	153	THR	CA-C-N	5.10	128.43	117.20
3	C	455	ARG	CD-NE-CZ	5.10	130.74	123.60
1	D	189	TYR	CB-CG-CD1	5.10	124.06	121.00
1	A	10	ASN	C-N-CA	5.10	134.44	121.70
3	C	84	PRO	N-CA-C	5.10	125.36	112.10
4	E	90	VAL	CB-CA-C	-5.10	101.72	111.40
4	E	3	GLU	C-N-CA	5.09	133.00	122.30
2	B	462	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	D	301	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
4	E	153	HIS	CB-CA-C	5.09	120.58	110.40
1	D	399	TRP	CB-CG-CD2	5.09	133.21	126.60
1	D	13	GLU	CA-C-O	-5.08	109.42	120.10
1	A	117	MET	O-C-N	5.08	130.83	122.70
3	C	152	ASN	N-CA-C	5.08	124.72	111.00
4	E	103	TYR	CZ-CE2-CD2	5.08	124.37	119.80
2	B	15	TYR	CD1-CG-CD2	-5.08	112.31	117.90
3	C	75	SER	N-CA-CB	5.08	118.12	110.50
4	E	470	HIS	N-CA-CB	5.08	119.75	110.60
1	A	126	SER	O-C-N	5.08	130.82	122.70
2	B	235	ALA	CB-CA-C	5.08	117.72	110.10
4	E	47	GLU	CA-CB-CG	5.08	124.56	113.40
2	B	142	CYS	C-N-CA	5.07	134.38	121.70
1	D	7	LEU	CA-C-O	-5.07	109.45	120.10
4	E	205	PHE	CB-CG-CD2	5.07	124.35	120.80
1	A	299	HIS	N-CA-CB	-5.07	101.47	110.60
1	D	211	PRO	CB-CA-C	-5.07	99.32	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	463	PRO	CA-N-CD	-5.07	104.40	111.50
1	D	160	PRO	CA-C-N	-5.07	106.05	117.20
1	A	168	SER	CA-C-O	5.07	130.74	120.10
4	E	200	LYS	N-CA-C	5.07	124.68	111.00
1	D	84	ASP	O-C-N	-5.06	114.60	122.70
1	D	160	PRO	N-CA-C	-5.06	98.94	112.10
2	B	428	TRP	CD1-CG-CD2	-5.06	102.25	106.30
1	D	62	ASP	CB-CG-OD2	-5.06	113.75	118.30
4	E	73	GLY	C-N-CA	5.06	134.35	121.70
1	D	130	ILE	CA-CB-CG1	5.06	120.61	111.00
1	A	189	TYR	CG-CD2-CE2	-5.06	117.25	121.30
2	B	13	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	D	196	THR	N-CA-CB	-5.06	100.69	110.30
1	A	426	PHE	CB-CG-CD1	5.05	124.34	120.80
3	C	218	TYR	CG-CD2-CE2	5.05	125.34	121.30
1	A	262	GLU	OE1-CD-OE2	-5.05	117.24	123.30
2	B	455	PHE	CG-CD2-CE2	-5.05	115.24	120.80
1	D	205	PHE	CD1-CE1-CZ	5.05	126.16	120.10
1	D	198	TYR	N-CA-CB	-5.05	101.52	110.60
1	D	130	ILE	CB-CG1-CD1	5.04	128.02	113.90
1	D	187	TRP	O-C-N	5.04	130.77	122.70
1	D	127	TYR	CA-C-N	5.04	128.29	117.20
1	D	395	ALA	CB-CA-C	5.04	117.66	110.10
1	D	433	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	278	MET	N-CA-CB	-5.04	101.53	110.60
2	B	427	ASP	N-CA-CB	5.04	119.67	110.60
1	A	408	HIS	O-C-N	-5.04	114.64	122.70
2	B	428	TRP	CG-CD2-CE3	-5.04	129.37	133.90
1	D	65	LEU	O-C-N	-5.04	114.64	122.70
4	E	241	PHE	CD1-CG-CD2	-5.04	111.75	118.30
1	A	21	PRO	CA-C-N	-5.03	106.12	117.20
1	A	168	SER	O-C-N	-5.03	114.64	122.70
2	B	44	ASN	CB-CG-OD1	5.03	131.66	121.60
2	B	440	LEU	CB-CG-CD1	5.03	119.55	111.00
1	A	256	PHE	N-CA-CB	5.03	119.65	110.60
4	E	437	GLU	O-C-N	5.03	130.74	122.70
3	C	203	GLY	CA-C-O	-5.03	111.55	120.60
3	C	483	ALA	N-CA-CB	5.03	117.14	110.10
2	B	35	LEU	CD1-CG-CD2	5.02	125.57	110.50
2	B	89	ASP	N-CA-CB	5.02	119.64	110.60
4	E	12	GLY	CA-C-O	-5.02	111.56	120.60
4	E	46	GLU	CG-CD-OE2	5.02	128.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	46	LYS	CA-C-N	-5.02	106.16	117.20
1	D	155	LYS	N-CA-C	5.02	124.56	111.00
4	E	29	ASP	C-N-CA	5.02	134.25	121.70
3	C	440	ASP	O-C-N	-5.02	114.67	122.70
1	D	379	VAL	CB-CA-C	-5.02	101.87	111.40
4	E	28	ILE	O-C-N	-5.02	114.67	122.70
4	E	75	ASP	CB-CG-OD2	5.02	122.82	118.30
4	E	103	TYR	O-C-N	-5.02	114.67	122.70
3	C	293	MET	CA-CB-CG	5.02	121.83	113.30
1	A	400	LYS	N-CA-CB	5.01	119.63	110.60
3	C	81	ARG	CD-NE-CZ	5.01	130.62	123.60
1	D	102	ILE	CB-CG1-CD1	5.01	127.94	113.90
4	E	442	ILE	N-CA-CB	5.01	122.33	110.80
1	A	63	VAL	CA-CB-CG1	-5.01	103.39	110.90
1	A	110	LEU	CB-CG-CD1	5.01	119.52	111.00
3	C	228	TYR	CG-CD2-CE2	5.01	125.31	121.30
1	D	103	VAL	CB-CA-C	-5.01	101.88	111.40
1	D	22	VAL	CA-C-N	-5.01	106.19	117.20
3	C	439	TYR	CA-C-N	5.00	128.21	117.20
4	E	131	VAL	O-C-N	-5.00	114.69	122.70
2	B	184	GLY	N-CA-C	5.00	125.60	113.10
2	B	298	SER	O-C-N	5.00	130.70	122.70
2	B	443	PHE	CB-CG-CD1	-5.00	117.30	120.80

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	SER	CA
1	A	149	TRP	CA
1	A	162	SER	CA
1	A	267	THR	CB
1	A	304	SER	CA
1	A	305	THR	CB
2	B	84	ASP	CA
2	B	89	ASP	CA
2	B	95	ASN	CA
2	B	141	ASN	CA
2	B	188	ILE	CA
2	B	198	ARG	CA
2	B	215	ARG	CA
2	B	277	VAL	CA
2	B	280	ILE	CA

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Mol	Chain	Res	Type	Atom
2	B	307	ARG	CA
2	B	403	GLU	CA
3	C	19	LYS	CA
3	C	162	LEU	CA
3	C	180	ASP	CA
3	C	224	LYS	CA
3	C	421	SER	CA
1	D	26	THR	CA
1	D	102	ILE	CB
1	D	106	THR	CA,CB
1	D	130	ILE	CB
4	E	68	THR	CA,CB
4	E	110	TYR	CA
4	E	118	LEU	CA
4	E	126	THR	CA
4	E	148	GLN	CA
4	E	173	ASP	CA
4	E	244	ALA	CA
4	E	414	SER	CA

All (608) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Mainchain
1	A	104	HIS	Mainchain
1	A	110	LEU	Mainchain
1	A	111	ASP	Mainchain
1	A	112	TYR	Mainchain
1	A	113	THR	Mainchain
1	A	114	GLY	Mainchain
1	A	115	LYS	Mainchain
1	A	119	THR	Mainchain
1	A	127	TYR	Mainchain
1	A	128	CYS	Mainchain
1	A	129	GLU	Mainchain
1	A	132	VAL	Mainchain
1	A	135	PHE	Peptide
1	A	138	ASP	Mainchain
1	A	148	ILE	Mainchain
1	A	150	THR	Mainchain
1	A	151	TYR	Mainchain
1	A	152	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	154	THR	Mainchain
1	A	16	ASN	Mainchain
1	A	160	PRO	Mainchain
1	A	161	GLU	Mainchain,Peptide
1	A	162	SER	Mainchain
1	A	165	PRO	Mainchain
1	A	167	LEU	Mainchain
1	A	169	THR	Mainchain
1	A	175	GLU	Mainchain,Peptide
1	A	178	MET	Mainchain
1	A	191	THR	Mainchain
1	A	197	PRO	Mainchain
1	A	198	TYR	Mainchain
1	A	20	ARG	Mainchain
1	A	207	MET	Mainchain
1	A	208	GLN	Mainchain
1	A	209	ARG	Peptide
1	A	214	PHE	Peptide
1	A	216	VAL	Mainchain
1	A	217	ASN	Mainchain
1	A	219	ILE	Mainchain
1	A	22	VAL	Mainchain
1	A	221	PRO	Mainchain
1	A	222	CYS	Mainchain
1	A	226	SER	Mainchain
1	A	23	GLU	Mainchain
1	A	231	LEU	Mainchain
1	A	233	PHE	Mainchain
1	A	235	LEU	Mainchain
1	A	238	ASP	Mainchain
1	A	240	GLY	Mainchain
1	A	241	GLU	Mainchain
1	A	242	LYS	Mainchain
1	A	243	MET	Mainchain
1	A	244	THR	Mainchain
1	A	245	LEU	Mainchain
1	A	246	SER	Mainchain
1	A	248	SER	Mainchain,Peptide
1	A	252	SER	Mainchain
1	A	253	LEU	Mainchain
1	A	255	VAL	Mainchain
1	A	260	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	264	ILE	Mainchain
1	A	265	PRO	Mainchain
1	A	266	SER	Mainchain
1	A	267	THR	Mainchain
1	A	268	SER	Mainchain
1	A	269	SER	Mainchain
1	A	272	PRO	Mainchain
1	A	274	ILE	Mainchain
1	A	28	PHE	Mainchain
1	A	281	THR	Mainchain
1	A	282	MET	Mainchain
1	A	284	PHE	Mainchain
1	A	285	VAL	Mainchain
1	A	291	VAL	Mainchain
1	A	292	THR	Peptide
1	A	296	ILE	Mainchain
1	A	297	ASN	Mainchain
1	A	300	HIS	Peptide
1	A	301	ARG	Mainchain
1	A	303	PRO	Mainchain
1	A	304	SER	Peptide
1	A	305	THR	Mainchain
1	A	374	SER	Mainchain
1	A	378	GLY	Mainchain
1	A	38	ILE	Mainchain
1	A	386	MET	Mainchain
1	A	388	SER	Mainchain
1	A	389	ASP	Mainchain
1	A	394	ASN	Mainchain
1	A	398	GLU	Mainchain
1	A	400	LYS	Mainchain
1	A	403	ALA	Mainchain
1	A	404	MET	Mainchain
1	A	407	ASP	Mainchain
1	A	408	HIS	Mainchain
1	A	411	LEU	Mainchain
1	A	418	CYS	Mainchain
1	A	419	ILE	Mainchain
1	A	420	ILE	Mainchain
1	A	422	THR	Mainchain
1	A	427	ALA	Mainchain
1	A	431	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	434	SER	Mainchain
1	A	44	ASP	Mainchain
1	A	47	ASN	Mainchain
1	A	48	GLN	Mainchain
1	A	5	THR	Mainchain
1	A	59	GLN	Mainchain
1	A	6	ARG	Peptide
1	A	66	ARG	Mainchain
1	A	69	PRO	Mainchain
1	A	74	GLY	Mainchain
1	A	77	LYS	Mainchain
1	A	84	ASP	Mainchain
1	A	86	TRP	Mainchain
1	A	97	ASP	Mainchain,Peptide
1	A	98	GLY	Mainchain
2	B	1	SER	Mainchain
2	B	103	THR	Mainchain
2	B	105	HIS	Mainchain
2	B	106	VAL	Mainchain
2	B	109	LEU	Mainchain
2	B	113	THR	Mainchain
2	B	115	ALA	Mainchain
2	B	116	VAL	Mainchain
2	B	117	SER	Mainchain
2	B	119	HIS	Mainchain
2	B	12	PHE	Mainchain
2	B	130	ILE	Mainchain
2	B	131	LYS	Mainchain
2	B	133	MET	Mainchain
2	B	136	PRO	Mainchain
2	B	14	ASN	Mainchain
2	B	140	GLN	Mainchain,Peptide
2	B	142	CYS	Mainchain
2	B	148	SER	Mainchain
2	B	149	TYR	Mainchain
2	B	151	TYR	Mainchain
2	B	152	ASP	Mainchain
2	B	154	SER	Mainchain
2	B	155	GLU	Peptide
2	B	16	ASN	Mainchain
2	B	160	HIS	Mainchain
2	B	174	MET	Mainchain

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Mol	Chain	Res	Type	Group
2	B	176	ASN	Mainchain
2	B	177	GLN	Mainchain
2	B	178	ASP	Mainchain
2	B	184	GLY	Peptide
2	B	185	GLN	Mainchain
2	B	186	TRP	Mainchain
2	B	188	ILE	Mainchain
2	B	190	HIS	Mainchain
2	B	191	LYS	Mainchain
2	B	192	PRO	Mainchain
2	B	2	VAL	Mainchain
2	B	200	ASP	Mainchain
2	B	203	SER	Mainchain
2	B	204	TYR	Mainchain
2	B	205	GLU	Peptide
2	B	211	LEU	Mainchain
2	B	212	ILE	Mainchain
2	B	214	GLN	Mainchain
2	B	217	PRO	Mainchain
2	B	218	LEU	Mainchain
2	B	219	PHE	Mainchain
2	B	221	ILE	Mainchain
2	B	223	TYR	Mainchain
2	B	224	THR	Mainchain
2	B	225	ILE	Mainchain
2	B	227	PRO	Mainchain
2	B	229	ILE	Mainchain
2	B	237	LEU	Mainchain
2	B	239	PHE	Mainchain
2	B	240	TYR	Mainchain
2	B	241	LEU	Mainchain
2	B	243	PRO	Mainchain
2	B	244	ASP	Mainchain
2	B	245	ALA	Mainchain
2	B	25	VAL	Mainchain
2	B	250	SER	Mainchain
2	B	26	GLY	Peptide
2	B	260	THR	Mainchain
2	B	261	VAL	Mainchain
2	B	262	PHE	Mainchain
2	B	263	LEU	Mainchain
2	B	264	LEU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	266	LEU	Mainchain
2	B	269	LYS	Mainchain
2	B	27	ASP	Mainchain
2	B	274	SER	Mainchain
2	B	276	SER	Peptide
2	B	278	PRO	Mainchain
2	B	279	ILE	Peptide
2	B	28	LYS	Mainchain
2	B	280	ILE	Mainchain
2	B	281	ILE	Mainchain
2	B	282	SER	Mainchain
2	B	288	MET	Mainchain
2	B	290	LEU	Mainchain
2	B	294	SER	Mainchain
2	B	299	VAL	Mainchain
2	B	300	VAL	Mainchain
2	B	303	ASN	Mainchain
2	B	305	HIS	Mainchain
2	B	306	HIS	Peptide
2	B	307	ARG	Mainchain
2	B	308	SER	Mainchain
2	B	38	THR	Mainchain
2	B	4	GLU	Mainchain
2	B	404	ALA	Mainchain
2	B	405	VAL	Mainchain
2	B	406	GLU	Mainchain
2	B	407	ALA	Mainchain
2	B	411	ILE	Mainchain
2	B	412	ALA	Mainchain
2	B	429	GLN	Mainchain
2	B	433	MET	Mainchain
2	B	434	VAL	Mainchain
2	B	439	PHE	Mainchain
2	B	447	CYS	Mainchain
2	B	450	GLY	Mainchain
2	B	453	SER	Mainchain
2	B	457	ASP	Mainchain
2	B	461	ASN	Mainchain
2	B	463	PRO	Mainchain
2	B	465	ASP	Mainchain
2	B	467	PRO	Mainchain
2	B	47	ASN	Mainchain

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Mol	Chain	Res	Type	Group
2	B	55	PHE	Mainchain
2	B	56	LEU	Mainchain
2	B	59	ALA	Mainchain
2	B	62	ASP	Mainchain
2	B	74	GLY	Mainchain
2	B	81	PRO	Mainchain
2	B	83	ASP	Mainchain
2	B	84	ASP	Mainchain
2	B	85	VAL	Peptide
2	B	88	PRO	Peptide
2	B	89	ASP	Mainchain
2	B	9	SER	Mainchain
2	B	92	LEU	Mainchain
2	B	94	ASN	Peptide
2	B	95	ASN	Mainchain
2	B	99	SER	Mainchain
3	C	1	VAL	Peptide
3	C	10	ASP	Mainchain
3	C	106	TYR	Mainchain
3	C	108	CYS	Mainchain
3	C	11	LEU	Mainchain
3	C	112	VAL	Mainchain
3	C	114	PRO	Mainchain
3	C	118	VAL	Mainchain
3	C	12	LEU	Mainchain
3	C	13	ILE	Mainchain
3	C	130	CYS	Mainchain
3	C	131	PRO	Mainchain
3	C	135	LEU	Mainchain
3	C	142	GLN	Mainchain
3	C	158	ILE	Mainchain
3	C	178	ILE	Mainchain
3	C	179	ILE	Peptide
3	C	180	ASP	Mainchain
3	C	181	PRO	Mainchain
3	C	183	ALA	Mainchain
3	C	187	ASN	Mainchain,Peptide
3	C	188	GLY	Mainchain
3	C	189	GLU	Mainchain
3	C	193	ILE	Mainchain
3	C	196	PRO	Mainchain
3	C	203	GLY	Mainchain

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Mol	Chain	Res	Type	Group
3	C	204	ASP	Mainchain
3	C	21	VAL	Mainchain
3	C	211	ASN	Mainchain
3	C	212	TYR	Mainchain
3	C	221	ILE	Mainchain
3	C	222	ARG	Mainchain
3	C	224	LYS	Mainchain
3	C	226	LEU	Mainchain
3	C	23	PRO	Mainchain
3	C	239	ILE	Mainchain
3	C	242	LEU	Mainchain
3	C	244	ALA	Mainchain
3	C	248	TYR	Mainchain
3	C	252	GLU	Mainchain
3	C	26	HIS	Mainchain
3	C	261	ILE	Mainchain
3	C	263	VAL	Mainchain
3	C	266	ALA	Mainchain
3	C	267	GLN	Mainchain
3	C	268	ALA	Mainchain
3	C	273	LEU	Mainchain
3	C	275	SER	Mainchain
3	C	277	ARG	Mainchain
3	C	284	ALA	Mainchain
3	C	285	VAL	Mainchain
3	C	286	PRO	Mainchain
3	C	288	ILE	Mainchain
3	C	29	GLU	Mainchain
3	C	291	TYR	Mainchain
3	C	298	LEU	Mainchain
3	C	3	GLU	Mainchain
3	C	30	VAL	Mainchain
3	C	300	THR	Mainchain,Peptide
3	C	301	GLY	Mainchain
3	C	302	VAL	Mainchain,Peptide
3	C	305	ASN	Mainchain
3	C	311	ASN	Mainchain
3	C	315	ARG	Mainchain
3	C	319	THR	Mainchain
3	C	422	GLY	Mainchain
3	C	425	SER	Mainchain
3	C	426	THR	Mainchain

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Mol	Chain	Res	Type	Group
3	C	435	GLU	Mainchain
3	C	437	ASN	Mainchain
3	C	439	TYR	Mainchain
3	C	440	ASP	Mainchain
3	C	443	VAL	Mainchain
3	C	445	ASN	Mainchain
3	C	447	ASN	Mainchain
3	C	450	GLY	Mainchain
3	C	451	GLN	Mainchain
3	C	452	THR	Mainchain
3	C	453	ILE	Mainchain
3	C	454	ASP	Mainchain
3	C	455	ARG	Mainchain
3	C	457	SER	Mainchain,Peptide
3	C	46	LYS	Mainchain
3	C	463	PRO	Mainchain
3	C	465	MET	Mainchain
3	C	466	VAL	Mainchain
3	C	467	LEU	Mainchain
3	C	47	GLU	Mainchain
3	C	474	VAL	Mainchain
3	C	475	MET	Mainchain
3	C	476	GLY	Mainchain
3	C	478	PHE	Mainchain
3	C	479	ASN	Mainchain
3	C	48	THR	Mainchain
3	C	481	PRO	Mainchain
3	C	482	PRO	Mainchain
3	C	484	LYS	Mainchain
3	C	49	ASP	Mainchain
3	C	5	GLU	Mainchain
3	C	50	GLU	Mainchain
3	C	67	LEU	Peptide
3	C	75	SER	Mainchain
3	C	78	SER	Mainchain
3	C	8	ILE	Mainchain
3	C	84	PRO	Mainchain
3	C	85	GLU	Mainchain
3	C	86	LEU	Mainchain,Peptide
3	C	87	ILE	Mainchain
3	C	89	ILE	Mainchain
3	C	9	ASN	Mainchain

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Mol	Chain	Res	Type	Group
3	C	90	PRO	Mainchain
3	C	94	LEU	Mainchain
3	C	95	GLN	Mainchain
3	C	97	ASN	Mainchain
3	C	98	ASN	Peptide
1	D	1	SER	Mainchain
1	D	101	ALA	Mainchain,Peptide
1	D	104	HIS	Peptide
1	D	105	MET	Mainchain
1	D	110	LEU	Mainchain
1	D	111	ASP	Mainchain
1	D	113	THR	Mainchain,Peptide
1	D	114	GLY	Mainchain
1	D	118	TRP	Mainchain
1	D	128	CYS	Mainchain
1	D	129	GLU	Mainchain
1	D	135	PHE	Peptide
1	D	137	PHE	Mainchain
1	D	138	ASP	Mainchain
1	D	148	ILE	Mainchain
1	D	150	THR	Mainchain
1	D	16	ASN	Mainchain
1	D	160	PRO	Mainchain
1	D	161	GLU	Peptide
1	D	162	SER	Mainchain
1	D	163	ASP	Mainchain
1	D	165	PRO	Mainchain
1	D	166	ASP	Mainchain
1	D	169	THR	Mainchain
1	D	17	LYS	Mainchain
1	D	173	SER	Peptide
1	D	188	VAL	Mainchain
1	D	194	PRO	Mainchain
1	D	195	ASP	Mainchain
1	D	197	PRO	Peptide
1	D	209	ARG	Mainchain
1	D	212	LEU	Mainchain
1	D	216	VAL	Mainchain
1	D	217	ASN	Mainchain
1	D	219	ILE	Mainchain
1	D	22	VAL	Mainchain
1	D	224	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	228	LEU	Mainchain
1	D	229	THR	Mainchain
1	D	23	GLU	Mainchain
1	D	235	LEU	Mainchain
1	D	238	ASP	Mainchain,Peptide
1	D	244	THR	Mainchain
1	D	246	SER	Mainchain
1	D	252	SER	Mainchain
1	D	255	VAL	Mainchain
1	D	258	LEU	Mainchain
1	D	26	THR	Peptide
1	D	261	VAL	Mainchain
1	D	265	PRO	Mainchain
1	D	268	SER	Mainchain
1	D	275	GLY	Mainchain
1	D	276	LYS	Mainchain
1	D	277	TYR	Mainchain
1	D	281	THR	Mainchain
1	D	285	VAL	Mainchain
1	D	29	VAL	Mainchain
1	D	300	HIS	Mainchain
1	D	302	SER	Mainchain
1	D	303	PRO	Mainchain
1	D	305	THR	Mainchain
1	D	32	THR	Mainchain
1	D	33	VAL	Mainchain
1	D	34	GLY	Mainchain,Peptide
1	D	35	LEU	Mainchain
1	D	374	SER	Peptide
1	D	381	TYR	Mainchain
1	D	384	GLU	Mainchain
1	D	386	MET	Mainchain
1	D	394	ASN	Mainchain
1	D	395	ALA	Mainchain
1	D	396	ALA	Mainchain
1	D	4	GLU	Mainchain
1	D	402	VAL	Mainchain
1	D	404	MET	Mainchain
1	D	410	LEU	Mainchain
1	D	413	VAL	Mainchain
1	D	414	PHE	Mainchain
1	D	416	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	D	423	VAL	Mainchain
1	D	428	GLY	Mainchain
1	D	432	GLU	Mainchain
1	D	434	SER	Mainchain
1	D	435	GLN	Mainchain
1	D	436	GLU	Mainchain
1	D	44	ASP	Peptide
1	D	46	VAL	Mainchain
1	D	47	ASN	Mainchain
1	D	48	GLN	Mainchain
1	D	49	ILE	Mainchain
1	D	55	ARG	Mainchain
1	D	57	ARG	Mainchain
1	D	62	ASP	Mainchain
1	D	63	VAL	Mainchain
1	D	65	LEU	Mainchain
1	D	72	TYR	Mainchain
1	D	73	GLY	Mainchain,Peptide
1	D	74	GLY	Mainchain
1	D	76	LYS	Mainchain
1	D	77	LYS	Mainchain
1	D	78	ILE	Mainchain
1	D	79	ARG	Mainchain
1	D	80	LEU	Mainchain
1	D	81	PRO	Mainchain
1	D	83	ASP	Mainchain
1	D	84	ASP	Mainchain
1	D	85	VAL	Mainchain
1	D	9	ALA	Mainchain
1	D	90	LEU	Mainchain
1	D	92	LEU	Mainchain
1	D	93	TYR	Mainchain
1	D	94	ASN	Mainchain
1	D	96	ALA	Peptide
1	D	97	ASP	Mainchain
1	D	98	GLY	Peptide
4	E	1	ASN	Mainchain
4	E	10	LEU	Mainchain
4	E	101	VAL	Mainchain
4	E	102	ALA	Mainchain
4	E	104	TYR	Mainchain
4	E	105	ALA	Mainchain

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Mol	Chain	Res	Type	Group
4	E	109	VAL	Peptide
4	E	11	LEU	Mainchain
4	E	110	TYR	Mainchain
4	E	111	ASN	Mainchain
4	E	112	ASP	Mainchain
4	E	118	LEU	Mainchain,Peptide
4	E	122	ILE	Mainchain
4	E	127	CYS	Mainchain
4	E	128	PRO	Mainchain
4	E	132	THR	Peptide
4	E	133	TYR	Mainchain,Peptide
4	E	137	ASP	Mainchain
4	E	139	GLN	Mainchain
4	E	146	ARG	Mainchain
4	E	148	GLN	Peptide
4	E	152	ALA	Mainchain
4	E	154	GLU	Mainchain
4	E	155	VAL	Mainchain
4	E	16	LYS	Mainchain
4	E	160	SER	Peptide
4	E	172	ILE	Mainchain,Peptide
4	E	174	PRO	Mainchain
4	E	18	ILE	Mainchain
4	E	180	ASN	Mainchain,Peptide
4	E	181	GLY	Mainchain,Peptide
4	E	182	GLU	Mainchain
4	E	187	HIS	Mainchain
4	E	189	PRO	Mainchain
4	E	190	ALA	Mainchain
4	E	196	TRP	Mainchain
4	E	201	ASP	Mainchain
4	E	205	PHE	Mainchain
4	E	206	GLN	Mainchain
4	E	217	LYS	Mainchain
4	E	22	LYS	Mainchain
4	E	221	TYR	Mainchain
4	E	226	ILE	Mainchain
4	E	229	CYS	Mainchain
4	E	23	THR	Mainchain
4	E	236	VAL	Mainchain
4	E	237	VAL	Mainchain
4	E	238	LEU	Mainchain

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Mol	Chain	Res	Type	Group
4	E	24	LEU	Mainchain
4	E	245	GLN	Mainchain
4	E	250	LYS	Peptide
4	E	252	THR	Mainchain,Peptide
4	E	26	HIS	Mainchain,Peptide
4	E	260	ALA	Mainchain
4	E	267	LEU	Mainchain
4	E	270	GLN	Mainchain
4	E	271	LYS	Mainchain
4	E	276	SER	Mainchain
4	E	277	LEU	Mainchain
4	E	278	ASN	Mainchain
4	E	279	VAL	Mainchain
4	E	280	PRO	Mainchain
4	E	281	LEU	Mainchain
4	E	287	ILE	Mainchain
4	E	297	VAL	Mainchain
4	E	303	VAL	Mainchain
4	E	305	ASN	Mainchain
4	E	306	VAL	Mainchain
4	E	307	SER	Mainchain
4	E	308	LEU	Mainchain
4	E	310	THR	Mainchain
4	E	39	LEU	Mainchain
4	E	416	VAL	Mainchain
4	E	417	GLU	Mainchain
4	E	425	SER	Mainchain
4	E	428	GLU	Mainchain
4	E	43	ASN	Mainchain
4	E	434	SER	Mainchain
4	E	453	ILE	Mainchain
4	E	455	LEU	Mainchain
4	E	456	LEU	Mainchain
4	E	460	LEU	Mainchain
4	E	463	LEU	Mainchain
4	E	47	GLU	Mainchain
4	E	473	GLN	Mainchain
4	E	476	GLU	Mainchain
4	E	5	ARG	Mainchain
4	E	59	TRP	Mainchain
4	E	61	ASP	Mainchain
4	E	65	SER	Mainchain

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Mol	Chain	Res	Type	Group
4	E	67	ASN	Mainchain,Peptide
4	E	69	SER	Mainchain
4	E	70	GLU	Mainchain
4	E	72	GLU	Mainchain
4	E	73	GLY	Mainchain
4	E	75	ASP	Mainchain
4	E	78	ARG	Mainchain
4	E	79	ILE	Mainchain,Peptide
4	E	81	SER	Mainchain
4	E	82	GLU	Mainchain
4	E	84	LEU	Mainchain
4	E	85	TRP	Mainchain
4	E	92	GLU	Mainchain
4	E	93	ASN	Mainchain
4	E	95	VAL	Mainchain
4	E	96	ASP	Mainchain
4	E	97	GLY	Mainchain
4	E	98	GLN	Mainchain
4	E	99	PHE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2991	0	3001	903	0
1	D	2991	0	3004	903	0
2	B	2972	0	2952	783	0
3	C	2983	0	2983	892	0
4	E	2987	0	2989	900	0
All	All	14924	0	14929	4213	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 141.

All (4213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:TRP:CD2	1:D:86:TRP:O	1.68	1.44
4:E:217:LYS:O	4:E:217:LYS:CE	1.74	1.36
4:E:284:LYS:N	4:E:284:LYS:HE3	1.42	1.29
2:B:130:ILE:HB	2:B:134:TYR:CD2	1.67	1.27
1:D:86:TRP:O	1:D:86:TRP:CG	1.83	1.26
4:E:217:LYS:O	4:E:217:LYS:HE3	1.11	1.25
3:C:67:LEU:CB	3:C:116:GLY:HA2	1.66	1.25
3:C:278:LEU:C	3:C:278:LEU:HD12	1.58	1.24
4:E:26:HIS:CG	4:E:26:HIS:O	1.92	1.20
3:C:148:PHE:HB2	3:C:215:VAL:CG2	1.72	1.20
2:B:160:HIS:CE1	2:B:207:VAL:HG11	1.76	1.19
1:D:152:ASP:CB	1:D:197:PRO:HA	1.72	1.19
2:B:176:ASN:HB2	2:B:191:LYS:HB3	1.25	1.18
2:B:297:LEU:CD1	2:B:445:THR:HG21	1.72	1.18
4:E:56:GLU:HB2	4:E:118:LEU:HD22	1.21	1.18
1:A:250:LEU:CD2	1:A:292:THR:HG22	1.72	1.18
3:C:12:LEU:HB2	3:C:16:LYS:HG2	1.18	1.18
1:D:245:LEU:HD21	4:E:255:ILE:HG13	1.24	1.17
4:E:79:ILE:HG12	4:E:80:PRO:HD2	1.22	1.17
2:B:104:LEU:HD12	2:B:118:TRP:CH2	1.80	1.17
3:C:67:LEU:HB3	3:C:116:GLY:CA	1.72	1.17
1:D:189:TYR:HA	1:D:197:PRO:HD2	1.21	1.17
4:E:183:TRP:CB	4:E:216:ARG:HG2	1.75	1.17
3:C:247:PHE:CE1	3:C:309:VAL:HG22	1.80	1.16
1:D:87:LEU:HD12	1:D:88:PRO:HD2	1.19	1.16
2:B:263:LEU:HD22	2:B:291:VAL:HG22	1.27	1.16
1:D:160:PRO:HD3	1:D:185:LYS:HB3	1.23	1.16
1:A:256:PHE:CZ	2:B:261:VAL:HG23	1.80	1.16
4:E:45:LYS:HD2	4:E:46:GLU:HG2	1.26	1.16
4:E:235:LEU:HD12	4:E:235:LEU:O	1.45	1.16
1:A:137:PHE:CE1	1:A:210:ILE:HD12	1.80	1.16
1:A:175:GLU:HB3	1:A:211:PRO:CG	1.75	1.15
1:D:36:GLN:CG	1:D:55:ARG:HG3	1.76	1.15
2:B:248:LYS:CD	2:B:252:SER:HB3	1.74	1.15
1:D:131:ILE:HG13	1:D:133:THR:H	1.09	1.15
1:A:57:ARG:HA	1:A:119:THR:CG2	1.75	1.15
1:D:136:PRO:HG3	1:D:274:ILE:HD11	1.29	1.15
1:D:35:LEU:HD11	1:D:54:VAL:HG11	1.22	1.15
4:E:240:TYR:CD2	4:E:453:ILE:HD13	1.82	1.15
2:B:269:LYS:HE3	2:B:270:VAL:CG2	1.74	1.15
1:D:72:TYR:CD1	1:D:72:TYR:C	2.09	1.15
4:E:129:ILE:HG22	4:E:133:TYR:CD2	1.82	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:CA	1:A:119:THR:HG22	1.78	1.14
1:D:198:TYR:HD1	1:D:198:TYR:N	1.40	1.14
1:A:380:LYS:HB3	2:B:408:ILE:HD13	1.20	1.14
2:B:248:LYS:HD3	2:B:252:SER:CB	1.76	1.14
3:C:285:VAL:O	3:C:285:VAL:CG2	1.81	1.13
1:D:166:ASP:HB2	1:D:181:TYR:CB	1.77	1.13
4:E:138:TRP:CZ2	4:E:215:GLN:HB2	1.84	1.13
4:E:62:TYR:O	4:E:62:TYR:HD1	1.30	1.13
3:C:242:LEU:HD22	3:C:267:GLN:HB3	1.17	1.12
2:B:28:LYS:HB2	2:B:156:VAL:HA	1.29	1.12
4:E:79:ILE:HG12	4:E:80:PRO:CD	1.78	1.12
1:A:133:THR:HA	1:A:274:ILE:HG22	1.13	1.12
2:B:28:LYS:HG2	2:B:155:GLU:HA	1.27	1.12
1:D:175:GLU:HB3	1:D:211:PRO:HD3	1.14	1.12
2:B:133:MET:HG2	2:B:140:GLN:HG3	1.12	1.12
3:C:445:ASN:HA	3:C:448:LEU:HG	1.23	1.12
1:D:145:LYS:CG	1:D:202:THR:HG23	1.78	1.12
2:B:269:LYS:HE3	2:B:270:VAL:HG22	1.17	1.11
3:C:122:PRO:HB2	3:C:123:PRO:HD2	1.14	1.11
3:C:142:GLN:HG3	3:C:143:ASN:H	1.07	1.11
1:A:160:PRO:HG3	1:A:185:LYS:CB	1.80	1.11
2:B:176:ASN:HD22	2:B:188:ILE:HG21	1.10	1.10
1:A:380:LYS:CB	2:B:408:ILE:HD13	1.79	1.10
1:D:129:GLU:OE1	1:D:129:GLU:HA	1.37	1.10
4:E:44:GLU:HB3	4:E:280:PRO:CD	1.81	1.10
4:E:90:VAL:HG22	4:E:95:VAL:HG11	1.33	1.10
1:D:175:GLU:HB3	1:D:211:PRO:CD	1.79	1.10
4:E:44:GLU:CG	4:E:280:PRO:HB3	1.79	1.10
4:E:236:VAL:HA	4:E:239:VAL:HG23	1.31	1.10
2:B:87:GLN:HB3	2:B:104:LEU:HD11	1.32	1.10
2:B:91:VAL:HA	2:B:96:ASN:ND2	1.66	1.10
1:D:145:LYS:C	1:D:146:LEU:HD12	1.72	1.10
1:A:94:ASN:O	1:A:94:ASN:ND2	1.83	1.10
1:A:130:ILE:HD13	1:A:131:ILE:H	1.07	1.10
1:A:257:LEU:HD13	1:A:285:VAL:HG23	1.31	1.10
3:C:138:PRO:HB3	3:C:290:LYS:HE3	1.27	1.10
1:A:274:ILE:HG12	1:A:277:TYR:HD1	1.15	1.09
1:D:152:ASP:HB3	1:D:197:PRO:HA	1.13	1.09
4:E:44:GLU:HB3	4:E:280:PRO:HD3	1.30	1.09
4:E:44:GLU:CB	4:E:280:PRO:HB3	1.82	1.09
1:D:46:VAL:HA	1:D:272:PRO:CD	1.81	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:THR:HB	2:B:204:TYR:HB2	1.18	1.09
2:B:185:GLN:HB3	2:B:219:PHE:HE2	1.11	1.09
1:A:145:LYS:HG3	1:A:202:THR:HG22	1.22	1.09
1:A:175:GLU:HB3	1:A:211:PRO:HG3	1.21	1.09
3:C:113:ARG:HD2	3:C:117:TYR:HB3	1.18	1.09
1:D:379:VAL:HA	1:D:382:ILE:CG1	1.81	1.09
1:A:236:PRO:HB3	1:A:299:HIS:CE1	1.88	1.09
1:D:145:LYS:HG3	1:D:202:THR:CG2	1.82	1.09
2:B:46:LYS:HE2	2:B:278:PRO:HG3	1.23	1.08
4:E:56:GLU:CB	4:E:118:LEU:HD22	1.83	1.08
1:A:380:LYS:HB3	2:B:408:ILE:CD1	1.81	1.08
1:D:72:TYR:HB2	1:D:112:TYR:HB2	1.16	1.08
1:D:167:LEU:HG	1:D:178:MET:HB2	1.33	1.08
2:B:243:PRO:HB3	2:B:435:ALA:HB1	1.28	1.08
3:C:94:LEU:HB2	3:C:98:ASN:HB2	1.33	1.08
1:D:113:THR:HG22	1:D:114:GLY:HA3	1.13	1.08
1:D:20:ARG:HG2	1:D:20:ARG:HH11	1.10	1.08
1:A:406:ILE:HG23	1:A:409:ILE:HD11	1.30	1.07
2:B:191:LYS:HG3	2:B:191:LYS:O	1.30	1.07
4:E:56:GLU:HA	4:E:118:LEU:HB2	1.31	1.07
3:C:434:LYS:HD3	3:C:435:GLU:HG3	1.30	1.07
4:E:37:THR:HA	4:E:176:ASP:HB3	1.30	1.07
4:E:189:PRO:HD2	4:E:211:PHE:CB	1.83	1.07
1:A:155:LYS:CE	4:E:76:LEU:HD13	1.85	1.07
1:A:72:TYR:HB2	1:A:112:TYR:HB3	1.11	1.07
3:C:50:GLU:HA	3:C:132:ILE:HD13	1.37	1.07
4:E:54:TRP:HB3	4:E:118:LEU:HD11	1.28	1.07
1:A:38:ILE:HD11	1:A:55:ARG:HG3	1.07	1.06
2:B:75:ILE:CD1	2:B:78:LEU:HD13	1.85	1.06
1:D:91:VAL:HG22	1:D:96:ALA:HB2	1.32	1.06
1:A:113:THR:O	1:A:113:THR:HG22	1.53	1.06
1:A:251:LEU:HD22	4:E:260:ALA:CB	1.84	1.06
2:B:308:SER:HB2	2:B:311:THR:HG22	1.09	1.06
1:A:131:ILE:HD11	1:A:140:GLN:CD	1.74	1.06
1:A:160:PRO:HG3	1:A:185:LYS:HB3	1.12	1.06
1:D:46:VAL:HA	1:D:272:PRO:HD3	1.14	1.06
1:D:398:GLU:HA	1:D:401:TYR:CZ	1.90	1.06
2:B:75:ILE:O	2:B:75:ILE:HG13	1.55	1.06
1:A:250:LEU:HD22	1:A:292:THR:HG22	1.31	1.06
2:B:129:THR:HG23	2:B:129:THR:O	1.56	1.06
4:E:91:LEU:HD13	4:E:145:PHE:HB3	1.10	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HD13	1:A:285:VAL:CG2	1.86	1.05
2:B:189:GLU:HG3	2:B:468:PHE:HB3	1.35	1.05
3:C:69:TRP:HZ2	3:C:112:VAL:HG12	1.16	1.05
1:D:169:THR:O	1:D:169:THR:HG22	1.49	1.05
1:A:279:LEU:HA	1:A:282:MET:HB2	1.37	1.05
1:D:238:ASP:HB3	4:E:308:LEU:HD23	1.38	1.05
4:E:44:GLU:HG2	4:E:280:PRO:HB3	1.36	1.05
4:E:47:GLU:HA	4:E:129:ILE:HD11	1.34	1.05
4:E:246:ALA:HB1	4:E:250:LYS:HG3	1.36	1.05
1:A:87:LEU:HD22	1:A:87:LEU:H	1.21	1.05
1:A:250:LEU:HD11	1:A:296:ILE:HG21	1.38	1.05
3:C:69:TRP:CZ2	3:C:112:VAL:HG12	1.91	1.05
3:C:279:PRO:HA	3:C:282:ALA:HB3	1.35	1.05
1:D:166:ASP:HB2	1:D:181:TYR:HB2	1.39	1.05
4:E:183:TRP:HB3	4:E:216:ARG:HG2	1.38	1.05
1:A:113:THR:O	1:A:113:THR:CG2	2.05	1.05
1:D:160:PRO:CD	1:D:185:LYS:HB3	1.87	1.05
4:E:80:PRO:HB2	4:E:83:LEU:HD23	1.37	1.05
2:B:37:LEU:CA	2:B:54:VAL:HG12	1.85	1.04
3:C:31:VAL:O	3:C:31:VAL:HG13	1.54	1.04
3:C:78:SER:C	3:C:114:PRO:HB3	1.78	1.04
1:A:133:THR:HA	1:A:274:ILE:CG2	1.88	1.04
3:C:48:THR:HA	3:C:286:PRO:HD3	1.33	1.04
1:D:189:TYR:HA	1:D:197:PRO:CD	1.87	1.04
1:D:152:ASP:HB3	1:D:197:PRO:CA	1.86	1.04
3:C:316:THR:CG2	3:C:317:PRO:HD2	1.86	1.03
1:D:32:THR:HB	1:D:59:GLN:HB3	1.39	1.03
4:E:211:PHE:C	4:E:212:LEU:HD12	1.78	1.03
2:B:131:LYS:HD3	2:B:132:VAL:H	0.90	1.03
2:B:224:THR:C	2:B:227:PRO:HD2	1.79	1.03
3:C:426:THR:HG22	3:C:426:THR:O	1.54	1.03
1:D:35:LEU:HD12	1:D:36:GLN:H	1.22	1.03
1:A:46:VAL:HG23	1:A:271:VAL:N	1.74	1.03
2:B:48:GLU:HA	2:B:130:ILE:HD11	1.38	1.03
2:B:92:LEU:H	2:B:96:ASN:HB2	1.14	1.03
2:B:134:TYR:CE1	2:B:213:ILE:HG13	1.94	1.03
4:E:44:GLU:HB3	4:E:280:PRO:CB	1.88	1.03
1:A:2:GLU:O	1:A:2:GLU:HG2	1.57	1.03
3:C:288:ILE:CD1	3:C:290:LYS:HE2	1.89	1.03
1:D:379:VAL:HA	1:D:382:ILE:HG13	1.36	1.03
1:A:166:ASP:HB2	1:A:181:TYR:CG	1.94	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:ILE:HD11	2:B:78:LEU:HD13	1.39	1.02
2:B:297:LEU:HD11	2:B:445:THR:HG21	1.34	1.02
2:B:308:SER:CB	2:B:311:THR:HG22	1.88	1.02
3:C:115:ASN:O	3:C:115:ASN:ND2	1.91	1.02
3:C:285:VAL:O	3:C:285:VAL:HG22	1.52	1.02
4:E:189:PRO:CD	4:E:211:PHE:HB2	1.89	1.02
1:A:207:MET:O	1:A:207:MET:HG2	1.56	1.02
2:B:131:LYS:HD3	2:B:132:VAL:N	1.74	1.02
3:C:319:THR:O	3:C:319:THR:HG23	1.56	1.02
1:A:251:LEU:HD22	4:E:260:ALA:HB3	1.40	1.02
1:A:419:ILE:HG23	1:A:420:ILE:H	1.17	1.02
2:B:104:LEU:HA	2:B:118:TRP:CH2	1.94	1.02
1:A:250:LEU:CD1	1:A:296:ILE:HG21	1.88	1.02
1:A:256:PHE:CE1	2:B:261:VAL:HG23	1.93	1.02
2:B:142:CYS:HB3	2:B:211:LEU:HG	1.38	1.02
1:D:36:GLN:HG3	1:D:55:ARG:HG3	1.04	1.02
1:D:46:VAL:CA	1:D:272:PRO:HD3	1.87	1.02
3:C:316:THR:HG22	3:C:317:PRO:HD2	1.36	1.02
1:D:78:ILE:HD12	1:D:78:ILE:O	1.59	1.01
1:D:236:PRO:HB3	1:D:299:HIS:NE2	1.75	1.01
4:E:34:LEU:HD12	4:E:210:PHE:CE2	1.95	1.01
4:E:62:TYR:O	4:E:62:TYR:CD1	2.12	1.01
1:A:77:LYS:HG3	1:A:77:LYS:O	1.56	1.01
1:A:239:SER:HB2	2:B:312:HIS:HB3	1.43	1.01
3:C:296:MET:HA	3:C:296:MET:CE	1.90	1.01
1:D:35:LEU:HD11	1:D:54:VAL:CG1	1.89	1.01
1:D:75:ILE:HG13	1:D:78:ILE:HG23	1.42	1.01
4:E:26:HIS:O	4:E:26:HIS:CD2	2.13	1.01
4:E:223:ILE:HA	4:E:226:ILE:HB	1.40	1.01
1:A:155:LYS:HE3	4:E:76:LEU:CD1	1.89	1.01
2:B:10:VAL:HG13	2:B:11:LEU:HD22	1.40	1.01
3:C:17:TYR:CE2	3:C:19:LYS:HB2	1.96	1.01
3:C:288:ILE:HD11	3:C:290:LYS:HE2	1.02	1.01
2:B:37:LEU:HA	2:B:54:VAL:CG1	1.90	1.01
4:E:91:LEU:CD1	4:E:145:PHE:HB3	1.90	1.01
4:E:189:PRO:HD2	4:E:211:PHE:HB2	1.04	1.01
1:A:189:TYR:HA	1:A:197:PRO:HD2	1.43	1.01
3:C:155:ALA:HB2	3:C:211:ASN:HA	1.40	1.01
1:D:43:VAL:HG22	1:D:50:VAL:HA	1.39	1.01
1:D:136:PRO:HG3	1:D:274:ILE:CD1	1.89	1.01
4:E:184:THR:CG2	4:E:215:GLN:HG2	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:134:PHE:HB3	4:E:282:ILE:HG21	1.39	1.00
1:A:76:LYS:HG2	1:A:77:LYS:H	1.24	1.00
4:E:279:VAL:HB	4:E:280:PRO:HD2	1.43	1.00
1:A:20:ARG:HG2	1:A:20:ARG:HH11	1.26	1.00
1:A:38:ILE:CD1	1:A:55:ARG:HG3	1.90	1.00
3:C:273:LEU:HA	3:C:276:GLN:HG2	1.41	1.00
3:C:113:ARG:HE	3:C:119:THR:HG23	1.25	1.00
1:D:7:LEU:CD2	1:D:70:ALA:HB1	1.92	1.00
1:A:16:ASN:HB2	1:A:19:ILE:HD12	1.43	1.00
1:A:38:ILE:HD11	1:A:55:ARG:CG	1.92	0.99
1:A:46:VAL:HG21	1:A:270:ALA:HA	1.44	0.99
3:C:159:SER:HA	3:C:213:GLN:HG3	1.39	0.99
3:C:60:HIS:HB3	3:C:62:TRP:HZ3	1.27	0.99
2:B:186:TRP:HB3	2:B:215:ARG:CG	1.92	0.99
1:D:160:PRO:HD3	1:D:185:LYS:CB	1.91	0.99
2:B:37:LEU:HA	2:B:54:VAL:HG12	1.00	0.99
4:E:69:SER:O	4:E:69:SER:OG	1.59	0.99
3:C:78:SER:CA	3:C:114:PRO:HB3	1.92	0.99
3:C:278:LEU:C	3:C:278:LEU:CD1	2.28	0.99
1:A:20:ARG:HG3	1:A:22:VAL:HG22	1.44	0.99
2:B:9:SER:HA	2:B:12:PHE:CD1	1.98	0.99
3:C:190:TRP:CD1	3:C:221:ILE:HD12	1.98	0.99
1:D:175:GLU:CB	1:D:211:PRO:HD3	1.93	0.99
4:E:94:ASN:HB3	4:E:125:SER:HB3	1.43	0.99
1:A:274:ILE:HG12	1:A:277:TYR:CD1	1.96	0.98
3:C:180:ASP:OD1	3:C:192:ILE:HG21	1.63	0.98
3:C:50:GLU:CA	3:C:132:ILE:HD13	1.92	0.98
1:A:148:ILE:HG22	1:A:198:TYR:HD2	1.28	0.98
2:B:425:LYS:HA	2:B:428:TRP:CD1	1.97	0.98
1:D:40:LEU:HD13	1:D:52:THR:HB	1.44	0.98
2:B:131:LYS:CD	2:B:132:VAL:H	1.77	0.98
4:E:66:TRP:HE1	4:E:111:ASN:HA	1.27	0.98
4:E:91:LEU:HD13	4:E:145:PHE:CB	1.94	0.98
4:E:94:ASN:HD22	4:E:125:SER:HB2	1.25	0.98
4:E:183:TRP:HB2	4:E:216:ARG:HG2	1.46	0.98
3:C:285:VAL:O	3:C:285:VAL:HG23	1.63	0.98
4:E:94:ASN:ND2	4:E:143:LEU:HD23	1.78	0.98
3:C:247:PHE:HE1	3:C:309:VAL:HG22	1.17	0.98
1:A:135:PHE:O	1:A:135:PHE:CD1	2.17	0.97
2:B:186:TRP:HB3	2:B:215:ARG:HG3	1.44	0.97
2:B:220:TYR:HD2	2:B:223:TYR:HH	1.07	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:66:TRP:NE1	4:E:111:ASN:HA	1.78	0.97
3:C:159:SER:HA	3:C:213:GLN:CG	1.93	0.97
3:C:195:LYS:HE3	3:C:217:PHE:HB3	1.45	0.97
4:E:6:LEU:HD12	4:E:69:SER:HB3	1.45	0.97
4:E:6:LEU:CD1	4:E:69:SER:HB3	1.93	0.97
2:B:132:VAL:HG13	2:B:279:ILE:HA	1.43	0.97
3:C:452:THR:O	3:C:452:THR:HG23	1.60	0.97
2:B:91:VAL:HG11	2:B:149:TYR:CD1	1.99	0.97
1:D:187:TRP:HB2	1:D:199:LEU:HD23	1.44	0.97
4:E:14:TYR:HE2	4:E:16:LYS:HE3	1.30	0.97
4:E:44:GLU:HB3	4:E:280:PRO:CG	1.94	0.97
1:A:130:ILE:HD13	1:A:131:ILE:N	1.78	0.97
2:B:189:GLU:HG3	2:B:468:PHE:CB	1.95	0.97
3:C:115:ASN:O	3:C:115:ASN:CG	2.01	0.97
3:C:145:SER:C	3:C:146:LEU:HD12	1.83	0.97
3:C:242:LEU:HD22	3:C:267:GLN:CB	1.93	0.97
1:D:239:SER:HB2	1:D:242:LYS:HE2	1.44	0.97
4:E:138:TRP:HB2	4:E:213:ILE:HG12	1.46	0.96
1:A:209:ARG:HG3	1:A:210:ILE:H	1.30	0.96
1:A:420:ILE:HG13	1:A:421:GLY:N	1.79	0.96
3:C:138:PRO:HB3	3:C:290:LYS:CE	1.96	0.96
1:D:167:LEU:CG	1:D:178:MET:HB2	1.95	0.96
4:E:284:LYS:N	4:E:284:LYS:CE	2.28	0.96
3:C:288:ILE:HD11	3:C:290:LYS:CE	1.95	0.96
4:E:80:PRO:HB2	4:E:83:LEU:CD2	1.95	0.96
3:C:42:LEU:HD22	3:C:190:TRP:CH2	2.00	0.96
3:C:1:VAL:HA	3:C:4:GLU:HG2	1.48	0.96
3:C:278:LEU:HD12	3:C:278:LEU:O	1.63	0.96
3:C:319:THR:HB	3:C:447:ASN:HB3	1.48	0.96
2:B:142:CYS:HB3	2:B:211:LEU:CG	1.95	0.96
3:C:83:ARG:O	3:C:87:ILE:HG13	1.65	0.96
4:E:129:ILE:HG22	4:E:133:TYR:HD2	1.23	0.96
4:E:184:THR:HG21	4:E:215:GLN:HG2	1.48	0.96
4:E:188:ARG:HG3	4:E:188:ARG:O	1.65	0.96
4:E:146:ARG:NH1	4:E:205:PHE:HB3	1.81	0.95
4:E:197:GLN:HG2	4:E:198:LEU:H	1.29	0.95
4:E:456:LEU:O	4:E:456:LEU:HD22	1.66	0.95
3:C:138:PRO:HG3	3:C:288:ILE:CD1	1.96	0.95
1:A:160:PRO:HG2	1:A:185:LYS:NZ	1.80	0.95
3:C:138:PRO:HG3	3:C:288:ILE:HD11	1.45	0.95
4:E:89:VAL:HG23	4:E:99:PHE:CZ	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:HG2	1:A:185:LYS:CE	1.96	0.95
1:D:170:PHE:HE2	1:D:176:TRP:CD1	1.83	0.95
1:D:187:TRP:CZ2	1:D:189:TYR:HB3	2.02	0.95
1:A:64:ARG:HA	1:A:66:ARG:NH1	1.80	0.95
2:B:176:ASN:ND2	2:B:188:ILE:HG21	1.80	0.95
2:B:185:GLN:HB3	2:B:219:PHE:CE2	2.01	0.95
3:C:247:PHE:HE1	3:C:309:VAL:CG2	1.78	0.95
4:E:44:GLU:HB3	4:E:280:PRO:HB3	1.42	0.95
1:D:26:THR:HG22	1:D:27:HIS:H	1.29	0.95
3:C:249:LEU:HB3	3:C:256:LYS:NZ	1.80	0.95
1:D:152:ASP:CA	1:D:197:PRO:HA	1.95	0.95
3:C:149:THR:HG21	3:C:214:ASP:HB3	1.48	0.95
1:A:416:LEU:O	1:A:419:ILE:HG22	1.65	0.95
1:A:152:ASP:HA	1:A:198:TYR:H	1.30	0.94
4:E:236:VAL:HA	4:E:239:VAL:CG2	1.96	0.94
1:A:406:ILE:CG2	1:A:409:ILE:HD11	1.96	0.94
3:C:42:LEU:HG	3:C:54:THR:HG23	1.49	0.94
3:C:149:THR:CG2	3:C:214:ASP:HB3	1.98	0.94
1:D:217:ASN:HA	1:D:220:ILE:HD11	1.47	0.94
4:E:183:TRP:HB3	4:E:216:ARG:CG	1.97	0.94
1:A:245:LEU:HD22	2:B:250:SER:HA	1.49	0.94
2:B:68:ASP:HB3	2:B:69:PRO:CD	1.97	0.94
2:B:311:THR:HB	2:B:430:TYR:HD2	1.31	0.94
4:E:305:ASN:HA	4:E:308:LEU:HD12	1.49	0.94
1:D:28:PHE:HD2	1:D:157:SER:HB3	1.28	0.94
1:D:78:ILE:CD1	1:D:110:LEU:HB3	1.98	0.94
1:A:152:ASP:HB3	1:A:197:PRO:HA	1.49	0.94
2:B:191:LYS:O	2:B:191:LYS:CG	2.16	0.94
4:E:249:GLN:HE22	4:E:250:LYS:HE3	1.30	0.94
2:B:311:THR:HB	2:B:430:TYR:CD2	2.02	0.94
1:D:49:ILE:HG21	1:D:125:LYS:NZ	1.83	0.94
1:D:187:TRP:HB2	1:D:199:LEU:CD2	1.97	0.94
1:D:203:TYR:N	1:D:203:TYR:HD1	1.66	0.94
4:E:262:THR:HG23	4:E:265:LEU:HD12	1.50	0.94
4:E:313:THR:HB	4:E:440:VAL:HG12	1.47	0.94
3:C:443:VAL:HA	3:C:446:TRP:CD1	2.01	0.94
1:D:77:LYS:HA	1:D:111:ASP:HA	1.48	0.94
4:E:44:GLU:CD	4:E:129:ILE:HB	1.87	0.94
1:A:148:ILE:HD11	1:A:156:VAL:HG13	1.50	0.94
4:E:44:GLU:HA	4:E:129:ILE:CD1	1.98	0.94
4:E:90:VAL:HG13	4:E:95:VAL:HB	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:449:ALA:HA	4:E:452:TRP:CD1	2.02	0.94
1:A:72:TYR:HB2	1:A:112:TYR:CB	1.95	0.93
1:A:102:ILE:O	1:A:102:ILE:HG22	1.67	0.93
2:B:132:VAL:CG1	2:B:279:ILE:HA	1.98	0.93
1:D:282:MET:HG3	1:D:286:ILE:HD11	1.49	0.93
3:C:4:GLU:HG3	3:C:5:GLU:H	1.33	0.93
1:D:166:ASP:HB2	1:D:181:TYR:HB3	1.47	0.93
4:E:436:ASN:HA	4:E:439:TRP:HE1	1.33	0.93
1:D:130:ILE:HG12	1:D:131:ILE:N	1.83	0.93
2:B:226:VAL:HG22	2:B:227:PRO:HD3	1.50	0.93
3:C:309:VAL:O	3:C:313:HIS:HB3	1.68	0.93
4:E:134:PHE:HB3	4:E:282:ILE:CG2	1.97	0.93
3:C:115:ASN:N	3:C:115:ASN:HD22	1.65	0.93
3:C:52:LEU:HD21	3:C:130:CYS:HB2	1.51	0.93
1:A:245:LEU:CD2	2:B:250:SER:HA	1.98	0.93
2:B:279:ILE:CG2	2:B:280:ILE:HD13	1.99	0.93
3:C:122:PRO:HB2	3:C:123:PRO:CD	1.96	0.93
1:D:189:TYR:CA	1:D:197:PRO:HD2	1.98	0.93
1:A:145:LYS:HG3	1:A:202:THR:CG2	1.99	0.92
3:C:434:LYS:HG3	1:D:386:MET:CE	1.98	0.92
2:B:9:SER:HA	2:B:12:PHE:CE1	2.04	0.92
3:C:48:THR:HB	3:C:284:ALA:C	1.89	0.92
1:D:261:VAL:HA	1:D:264:ILE:HD12	1.50	0.92
1:D:302:SER:HB3	1:D:400:LYS:HG2	1.50	0.92
1:A:142:CYS:HB2	1:A:205:PHE:HB2	1.51	0.92
4:E:31:THR:O	4:E:32:LEU:HD23	1.69	0.92
4:E:67:ASN:HD22	4:E:67:ASN:N	1.64	0.92
4:E:284:LYS:HE3	4:E:284:LYS:H	1.30	0.92
3:C:69:TRP:HE3	3:C:73:GLU:HB3	1.33	0.92
3:C:113:ARG:HD2	3:C:117:TYR:CB	2.00	0.92
1:D:217:ASN:HA	1:D:220:ILE:CD1	1.99	0.92
1:D:104:HIS:HB2	1:D:105:MET:SD	2.10	0.92
4:E:282:ILE:HG23	4:E:282:ILE:O	1.69	0.92
1:A:267:THR:HG23	1:A:271:VAL:HG22	1.50	0.92
3:C:56:VAL:HG13	3:C:126:PHE:HE2	1.35	0.92
3:C:247:PHE:CD2	3:C:460:ILE:HG12	2.05	0.92
1:D:56:LEU:N	1:D:56:LEU:HD23	1.85	0.92
4:E:56:GLU:HA	4:E:118:LEU:CB	1.99	0.92
4:E:173:ASP:CG	4:E:185:ILE:HD13	1.90	0.92
1:A:397:GLU:HA	1:A:400:LYS:HD2	1.52	0.92
4:E:45:LYS:HE2	4:E:278:ASN:C	1.90	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD23	1:D:254:THR:N	1.84	0.91
4:E:129:ILE:HG22	4:E:133:TYR:CE2	2.04	0.91
4:E:219:LEU:HB3	4:E:222:ILE:HB	1.50	0.91
1:A:133:THR:CA	1:A:274:ILE:HG22	1.98	0.91
2:B:130:ILE:HB	2:B:134:TYR:CE2	2.06	0.91
2:B:421:PHE:HA	2:B:424:LEU:HB2	1.49	0.91
3:C:253:SER:HB2	1:D:306:HIS:HB3	1.52	0.91
1:D:45:GLU:HB3	1:D:271:VAL:CG2	1.99	0.91
1:A:133:THR:O	1:A:133:THR:HG22	1.70	0.91
1:A:176:TRP:CB	1:A:209:ARG:HD2	2.00	0.91
3:C:42:LEU:HG	3:C:54:THR:CG2	2.01	0.91
1:D:302:SER:HB2	1:D:305:THR:HG23	1.52	0.91
3:C:319:THR:O	3:C:319:THR:CG2	2.15	0.91
4:E:39:LEU:HD23	4:E:183:TRP:HZ2	1.35	0.91
4:E:44:GLU:HG2	4:E:280:PRO:CB	2.01	0.91
1:A:41:ILE:HD11	1:A:51:GLU:HB3	1.53	0.91
1:A:160:PRO:CG	1:A:185:LYS:HB3	2.00	0.91
3:C:7:LEU:HD23	3:C:10:ASP:HB2	1.50	0.91
4:E:36:LEU:CD2	4:E:51:THR:HG21	2.01	0.91
4:E:247:GLY:H	4:E:250:LYS:HZ2	1.16	0.91
1:D:238:ASP:HB3	4:E:308:LEU:CD2	2.01	0.91
3:C:144:CYS:SG	3:C:146:LEU:HD11	2.11	0.91
4:E:172:ILE:HD12	4:E:188:ARG:HB3	1.50	0.91
2:B:160:HIS:NE2	2:B:207:VAL:HG11	1.84	0.91
2:B:287:ILE:HA	2:B:290:LEU:HD12	1.52	0.91
4:E:138:TRP:HB2	4:E:213:ILE:CG1	2.01	0.91
1:D:113:THR:HG22	1:D:114:GLY:CA	2.00	0.90
4:E:32:LEU:O	4:E:33:LYS:HG3	1.70	0.90
1:A:47:ASN:O	1:A:49:ILE:HG13	1.71	0.90
2:B:406:GLU:HA	2:B:409:LYS:HD2	1.52	0.90
1:D:252:SER:HB2	4:E:259:LEU:HD13	1.53	0.90
1:D:405:VAL:O	1:D:409:ILE:HG23	1.71	0.90
1:D:35:LEU:HD23	1:D:164:ARG:NH1	1.87	0.90
4:E:235:LEU:HD12	4:E:235:LEU:C	1.91	0.90
1:A:64:ARG:HA	1:A:66:ARG:HH11	1.36	0.90
4:E:27:VAL:HG12	4:E:154:GLU:HA	1.53	0.90
4:E:76:LEU:HD23	4:E:77:VAL:H	1.35	0.90
1:A:155:LYS:HE3	4:E:76:LEU:HD13	0.93	0.90
1:D:28:PHE:CD2	1:D:157:SER:HB3	2.07	0.90
1:D:78:ILE:O	1:D:78:ILE:CD1	2.19	0.90
3:C:110:VAL:HG13	3:C:120:TRP:HB2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:141:CYS:HB3	4:E:212:LEU:HB2	1.53	0.90
1:A:33:VAL:CG2	1:A:158:ILE:HG12	2.00	0.90
4:E:6:LEU:HD12	4:E:69:SER:CB	2.00	0.90
2:B:133:MET:CG	2:B:140:GLN:HG3	2.02	0.90
2:B:104:LEU:HD12	2:B:118:TRP:CZ3	2.06	0.89
1:D:118:TRP:HE1	1:D:120:PRO:HB3	1.35	0.89
1:D:305:THR:CG2	1:D:400:LYS:HB3	2.01	0.89
4:E:67:ASN:HD22	4:E:67:ASN:H	0.90	0.89
4:E:136:PHE:CZ	4:E:217:LYS:HD2	2.07	0.89
1:A:106:THR:HG22	1:A:107:LYS:H	1.36	0.89
1:A:152:ASP:HA	1:A:198:TYR:N	1.87	0.89
1:D:37:LEU:HD12	1:D:53:ASN:O	1.72	0.89
4:E:31:THR:HB	4:E:58:GLN:HB2	1.54	0.89
1:A:166:ASP:HB3	1:A:178:MET:CE	2.02	0.89
3:C:148:PHE:HB2	3:C:215:VAL:HG22	1.54	0.89
1:D:48:GLN:HB3	1:D:130:ILE:CD1	2.02	0.89
1:D:91:VAL:HG22	1:D:96:ALA:CB	2.01	0.89
3:C:269:VAL:HG13	3:C:270:PHE:CD1	2.07	0.89
1:D:72:TYR:C	1:D:72:TYR:HD1	1.73	0.89
1:D:301:ARG:HH12	1:D:406:ILE:HD11	1.36	0.89
4:E:37:THR:HA	4:E:176:ASP:CB	2.00	0.89
4:E:37:THR:CA	4:E:176:ASP:HB3	2.02	0.89
1:A:235:LEU:HD21	1:A:242:LYS:HE3	1.54	0.89
2:B:247:GLU:C	2:B:249:MET:HG3	1.92	0.89
1:D:29:VAL:HG12	1:D:60:TRP:CD1	2.06	0.89
4:E:44:GLU:CB	4:E:280:PRO:HD3	2.02	0.89
4:E:66:TRP:CD1	4:E:111:ASN:HA	2.08	0.89
4:E:66:TRP:HB2	4:E:71:TYR:H	1.36	0.89
2:B:129:THR:CG2	2:B:142:CYS:HA	2.02	0.89
3:C:80:LEU:HD11	1:D:20:ARG:HH22	1.38	0.89
1:D:137:PHE:HD2	1:D:431:ILE:HG21	1.36	0.89
4:E:279:VAL:CB	4:E:280:PRO:HD2	2.03	0.89
4:E:284:LYS:CE	4:E:284:LYS:H	1.86	0.89
2:B:91:VAL:HG23	2:B:96:ASN:CG	1.92	0.89
1:D:36:GLN:HG3	1:D:55:ARG:CG	1.99	0.89
1:D:305:THR:HG1	1:D:401:TYR:HD2	0.94	0.89
1:D:20:ARG:HH11	1:D:20:ARG:CG	1.85	0.89
1:D:75:ILE:HG13	1:D:78:ILE:CG2	2.03	0.89
1:A:380:LYS:CA	2:B:408:ILE:HD13	2.03	0.88
2:B:263:LEU:HD22	2:B:291:VAL:CG2	2.02	0.88
3:C:453:ILE:HG23	3:C:454:ASP:H	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HD2	1:A:107:LYS:HD2	1.55	0.88
2:B:269:LYS:CE	2:B:270:VAL:HG22	2.02	0.88
4:E:271:LYS:C	4:E:273:PRO:HD2	1.93	0.88
2:B:407:ALA:O	2:B:411:ILE:HG13	1.72	0.88
3:C:65:HIS:CD2	3:C:65:HIS:H	1.91	0.88
4:E:44:GLU:CG	4:E:129:ILE:HB	2.03	0.88
4:E:149:THR:HG23	4:E:150:TYR:H	1.38	0.88
2:B:2:VAL:HG12	2:B:69:PRO:HG3	1.55	0.88
2:B:129:THR:HG22	2:B:142:CYS:HA	1.55	0.88
4:E:172:ILE:HD11	4:E:187:HIS:CA	2.03	0.88
1:A:63:VAL:O	1:A:66:ARG:HD2	1.73	0.88
1:A:141:ASN:HA	1:A:205:PHE:O	1.74	0.88
1:A:175:GLU:CB	1:A:211:PRO:HG3	2.04	0.88
1:D:38:ILE:C	1:D:169:THR:HG21	1.94	0.88
1:D:412:CYS:O	1:D:416:LEU:HD23	1.74	0.88
4:E:244:ALA:HB2	4:E:446:ILE:CG2	2.03	0.88
3:C:434:LYS:CE	3:C:435:GLU:HG2	2.04	0.88
4:E:172:ILE:HD11	4:E:187:HIS:C	1.94	0.88
1:A:251:LEU:CD2	4:E:260:ALA:HB3	2.03	0.88
2:B:175:ILE:HG12	2:B:176:ASN:H	1.38	0.88
2:B:186:TRP:HB3	2:B:215:ARG:CD	2.04	0.88
3:C:45:LEU:HD12	3:C:190:TRP:CE3	2.09	0.88
3:C:279:PRO:HA	3:C:282:ALA:CB	2.03	0.88
3:C:434:LYS:HD3	3:C:435:GLU:CG	2.03	0.88
4:E:66:TRP:CD1	4:E:111:ASN:HB2	2.09	0.88
1:D:203:TYR:N	1:D:203:TYR:CD1	2.34	0.88
4:E:249:GLN:NE2	4:E:250:LYS:HE3	1.88	0.88
1:A:247:ILE:O	1:A:247:ILE:HD13	1.74	0.88
1:D:31:ILE:HG22	1:D:158:ILE:HG23	1.56	0.88
1:D:72:TYR:HB2	1:D:112:TYR:CB	2.04	0.88
4:E:44:GLU:HG3	4:E:129:ILE:CG1	2.05	0.88
4:E:292:VAL:O	4:E:296:ILE:HG23	1.74	0.88
1:A:29:VAL:HG21	1:A:86:TRP:CZ3	2.09	0.87
1:A:148:ILE:CG2	1:A:198:TYR:HD2	1.87	0.87
2:B:45:GLU:OE1	2:B:277:VAL:HB	1.73	0.87
3:C:247:PHE:CE2	3:C:460:ILE:HD11	2.09	0.87
4:E:262:THR:CG2	4:E:265:LEU:HD12	2.03	0.87
1:A:41:ILE:HD11	1:A:51:GLU:CD	1.93	0.87
3:C:113:ARG:CD	3:C:117:TYR:HB3	2.03	0.87
4:E:36:LEU:HD23	4:E:51:THR:HG21	1.56	0.87
4:E:44:GLU:HA	4:E:129:ILE:HD12	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ASP:HB3	2:B:125:ARG:HG3	1.56	0.87
4:E:67:ASN:H	4:E:67:ASN:ND2	1.72	0.87
2:B:28:LYS:CB	2:B:156:VAL:HA	2.03	0.87
1:D:112:TYR:HD1	1:D:113:THR:H	1.14	0.87
1:D:167:LEU:N	1:D:167:LEU:HD12	1.90	0.87
1:A:79:ARG:CD	1:A:107:LYS:HD2	2.03	0.87
4:E:152:ALA:H	4:E:205:PHE:HD1	1.22	0.87
1:A:238:ASP:HB3	2:B:306:HIS:CE1	2.10	0.87
1:D:274:ILE:HB	1:D:276:LYS:HD3	1.56	0.87
1:D:7:LEU:HD22	1:D:70:ALA:HB1	1.57	0.87
4:E:185:ILE:HG12	4:E:214:ILE:CG2	2.05	0.87
4:E:33:LYS:HE3	4:E:160:SER:CB	2.05	0.87
1:A:46:VAL:HG21	1:A:270:ALA:CA	2.05	0.86
1:A:101:ALA:HB3	1:A:123:ILE:O	1.74	0.86
3:C:18:ASN:CB	3:C:21:VAL:HB	2.04	0.86
1:D:48:GLN:OE1	1:D:130:ILE:HD13	1.75	0.86
1:D:60:TRP:CZ2	1:D:86:TRP:CZ3	2.63	0.86
1:D:187:TRP:CZ3	1:D:189:TYR:CD1	2.63	0.86
2:B:56:LEU:CD1	2:B:103:THR:HG23	2.04	0.86
1:A:176:TRP:HB3	1:A:209:ARG:HD2	1.56	0.86
2:B:34:GLY:C	2:B:35:LEU:HD23	1.94	0.86
2:B:232:SER:O	2:B:236:ILE:HG22	1.75	0.86
3:C:296:MET:HA	3:C:296:MET:HE3	1.57	0.86
4:E:267:LEU:O	4:E:270:GLN:HG3	1.75	0.86
2:B:23:GLN:HE21	2:B:23:GLN:N	1.73	0.86
3:C:18:ASN:HB3	3:C:21:VAL:HB	1.56	0.86
3:C:299:VAL:O	3:C:303:VAL:HG23	1.75	0.86
2:B:436:ASP:O	2:B:440:LEU:HD12	1.75	0.86
3:C:16:LYS:HA	3:C:16:LYS:HE3	1.55	0.86
3:C:204:ASP:OD1	3:C:205:LYS:HD3	1.76	0.86
4:E:159:LEU:HD21	4:E:208:ILE:HG23	1.57	0.86
4:E:173:ASP:CB	4:E:185:ILE:HD13	2.06	0.86
3:C:154:ASN:HA	3:C:211:ASN:HB2	1.56	0.86
2:B:31:VAL:HG21	2:B:86:TRP:HZ3	1.40	0.86
3:C:190:TRP:CB	3:C:223:ARG:HB2	2.04	0.86
3:C:249:LEU:HB3	3:C:256:LYS:HZ2	1.36	0.86
1:D:107:LYS:HD3	1:D:107:LYS:N	1.88	0.86
1:D:239:SER:O	1:D:242:LYS:HG2	1.75	0.86
4:E:446:ILE:HG22	4:E:447:ASP:N	1.89	0.86
3:C:122:PRO:CB	3:C:123:PRO:HD2	2.04	0.86
3:C:212:TYR:CD1	3:C:212:TYR:O	2.29	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PHE:C	1:D:135:PHE:CD1	2.48	0.86
1:A:2:GLU:OE2	1:A:74:GLY:HA2	1.74	0.86
1:A:245:LEU:HD11	2:B:250:SER:O	1.76	0.86
1:D:41:ILE:HD12	1:D:51:GLU:O	1.76	0.86
1:D:46:VAL:HB	1:D:271:VAL:HA	1.57	0.86
1:D:72:TYR:CB	1:D:112:TYR:HB2	2.05	0.86
1:D:414:PHE:O	1:D:414:PHE:CD1	2.29	0.86
4:E:250:LYS:HA	4:E:253:LEU:HB3	1.58	0.86
2:B:176:ASN:CB	2:B:191:LYS:HB3	2.03	0.86
2:B:297:LEU:HD12	2:B:445:THR:HG21	1.58	0.85
3:C:8:ILE:HG23	3:C:8:ILE:O	1.74	0.85
4:E:217:LYS:O	4:E:217:LYS:HE2	1.75	0.85
4:E:271:LYS:HZ3	4:E:271:LYS:HB2	1.40	0.85
1:D:419:ILE:HD12	1:D:420:ILE:N	1.91	0.85
4:E:54:TRP:CB	4:E:118:LEU:HD11	2.06	0.85
4:E:62:TYR:HD1	4:E:62:TYR:C	1.78	0.85
3:C:56:VAL:HG13	3:C:126:PHE:CE2	2.11	0.85
3:C:449:VAL:HG12	3:C:452:THR:HB	1.57	0.85
1:D:213:TYR:O	1:D:216:VAL:HG23	1.76	0.85
4:E:109:VAL:HG12	4:E:110:TYR:O	1.76	0.85
1:A:145:LYS:C	1:A:146:LEU:HD12	1.96	0.85
3:C:155:ALA:CB	3:C:211:ASN:HA	2.06	0.85
3:C:282:ALA:HB2	3:C:287:LEU:HD11	1.58	0.85
4:E:236:VAL:CA	4:E:239:VAL:HG23	2.06	0.85
1:A:47:ASN:O	1:A:48:GLN:HG2	1.75	0.85
3:C:30:VAL:HG22	3:C:157:GLU:C	1.96	0.85
3:C:48:THR:HA	3:C:286:PRO:CD	2.06	0.85
3:C:307:GLY:HA2	3:C:310:LEU:HD23	1.58	0.85
2:B:104:LEU:HA	2:B:118:TRP:HH2	1.34	0.85
2:B:243:PRO:HB3	2:B:435:ALA:CB	2.05	0.85
1:A:216:VAL:HG13	1:A:220:ILE:HD11	1.56	0.85
1:A:277:TYR:HA	1:A:280:PHE:CZ	2.12	0.85
1:A:304:SER:HA	1:A:400:LYS:HD3	1.59	0.85
2:B:236:ILE:HB	2:B:446:MET:CE	2.07	0.85
1:A:76:LYS:HG3	1:A:112:TYR:CE2	2.12	0.85
2:B:46:LYS:HG3	2:B:278:PRO:HD2	1.58	0.85
3:C:42:LEU:HA	3:C:54:THR:HG22	1.57	0.85
3:C:154:ASN:HB3	3:C:211:ASN:HB3	1.59	0.85
3:C:194:HIS:CG	3:C:195:LYS:H	1.95	0.85
1:D:379:VAL:HA	1:D:382:ILE:HG12	1.57	0.85
3:C:35:LEU:HD22	3:C:215:VAL:HG11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:PHE:O	3:C:230:ILE:HG12	1.76	0.85
1:D:257:LEU:HD12	1:D:258:LEU:N	1.90	0.85
4:E:45:LYS:NZ	4:E:278:ASN:HA	1.91	0.85
1:D:291:VAL:O	1:D:295:VAL:HG13	1.76	0.85
4:E:268:ILE:HG13	4:E:269:ALA:N	1.90	0.84
4:E:284:LYS:O	4:E:287:ILE:HG23	1.77	0.84
4:E:449:ALA:O	4:E:452:TRP:HB2	1.77	0.84
1:A:148:ILE:HG22	1:A:198:TYR:CD2	2.11	0.84
3:C:220:ILE:HG13	3:C:220:ILE:O	1.77	0.84
1:D:48:GLN:HB3	1:D:130:ILE:HD12	1.59	0.84
2:B:176:ASN:HD22	2:B:188:ILE:CG2	1.89	0.84
3:C:434:LYS:HG3	1:D:386:MET:HE2	1.57	0.84
2:B:7:LEU:O	2:B:11:LEU:HD23	1.77	0.84
1:D:107:LYS:NZ	4:E:149:THR:HA	1.93	0.84
3:C:159:SER:CA	3:C:213:GLN:HG3	2.07	0.84
3:C:179:ILE:HG13	3:C:181:PRO:HD3	1.57	0.84
1:D:20:ARG:HG2	1:D:20:ARG:NH1	1.78	0.84
1:D:49:ILE:HD12	1:D:125:LYS:HE3	1.57	0.84
4:E:28:ILE:HD11	4:E:60:ASN:O	1.77	0.84
1:A:102:ILE:O	1:A:102:ILE:CG2	2.26	0.84
2:B:259:LEU:HD23	2:B:259:LEU:O	1.78	0.84
1:D:132:VAL:C	1:D:274:ILE:HG23	1.97	0.84
3:C:78:SER:HA	3:C:114:PRO:HB3	1.56	0.84
4:E:140:ASN:C	4:E:140:ASN:HD22	1.79	0.84
1:A:77:LYS:O	1:A:77:LYS:CG	2.25	0.84
1:D:203:TYR:HD1	1:D:203:TYR:H	1.20	0.84
2:B:46:LYS:HG3	2:B:278:PRO:CD	2.08	0.84
2:B:306:HIS:C	2:B:306:HIS:ND1	2.32	0.84
1:D:229:THR:O	1:D:232:VAL:HB	1.77	0.84
4:E:142:SER:OG	4:E:209:ILE:HD11	1.78	0.84
1:A:239:SER:CB	2:B:312:HIS:HB3	2.07	0.84
3:C:59:ASP:OD1	3:C:121:LEU:HB2	1.78	0.84
1:D:77:LYS:HG3	1:D:77:LYS:O	1.75	0.84
1:D:415:MET:O	1:D:419:ILE:HG23	1.78	0.84
1:A:35:LEU:HD21	1:A:37:LEU:HD23	1.60	0.83
3:C:296:MET:HA	3:C:296:MET:HE2	1.58	0.83
1:D:253:LEU:HD23	1:D:254:THR:H	1.42	0.83
4:E:28:ILE:HG21	4:E:85:TRP:CZ3	2.13	0.83
4:E:62:TYR:CD1	4:E:62:TYR:C	2.50	0.83
1:A:265:PRO:HA	1:A:268:SER:HB3	1.60	0.83
1:A:419:ILE:HG23	1:A:420:ILE:N	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:PRO:HD3	3:C:22:ARG:HH22	1.41	0.83
2:B:435:ALA:O	2:B:439:PHE:HB3	1.79	0.83
3:C:253:SER:HB2	1:D:306:HIS:CB	2.07	0.83
1:D:65:LEU:HD23	1:D:110:LEU:CD1	2.08	0.83
4:E:182:GLU:O	4:E:218:PRO:HD2	1.77	0.83
3:C:241:PHE:HA	3:C:244:ALA:HB3	1.60	0.83
1:D:7:LEU:HD21	1:D:70:ALA:HB1	1.57	0.83
1:D:245:LEU:HD21	4:E:255:ILE:CG1	2.06	0.83
2:B:104:LEU:HD12	2:B:118:TRP:HH2	1.40	0.83
1:D:228:LEU:O	1:D:232:VAL:HG23	1.78	0.83
1:A:175:GLU:HB3	1:A:211:PRO:CD	2.09	0.83
1:D:92:LEU:HD13	1:D:146:LEU:HG	1.61	0.83
1:D:151:TYR:O	1:D:198:TYR:HB3	1.79	0.83
1:D:414:PHE:O	1:D:414:PHE:HD1	1.61	0.83
4:E:222:ILE:O	4:E:226:ILE:HG13	1.78	0.83
1:A:108:LEU:HD13	1:A:118:TRP:HB2	1.61	0.83
2:B:405:VAL:O	2:B:408:ILE:HG22	1.78	0.83
1:D:64:ARG:HA	1:D:66:ARG:NH1	1.93	0.83
1:D:232:VAL:HG22	1:D:250:LEU:HD11	1.59	0.83
4:E:197:GLN:HG2	4:E:198:LEU:N	1.93	0.83
4:E:229:CYS:HA	4:E:232:ILE:HB	1.58	0.83
1:A:37:LEU:CD2	1:A:54:VAL:HG12	2.08	0.83
3:C:110:VAL:CG1	3:C:120:TRP:HB2	2.08	0.83
4:E:144:VAL:HA	4:E:208:ILE:O	1.79	0.83
4:E:159:LEU:HD12	4:E:191:LYS:C	2.00	0.83
1:A:43:VAL:HG22	1:A:50:VAL:HG13	1.61	0.82
2:B:90:ILE:HG23	2:B:147:LYS:H	1.41	0.82
3:C:138:PRO:CB	3:C:290:LYS:HE3	2.09	0.82
4:E:173:ASP:HB3	4:E:185:ILE:HD13	1.61	0.82
2:B:185:GLN:CB	2:B:217:PRO:HB3	2.09	0.82
2:B:408:ILE:HG23	2:B:409:LYS:N	1.92	0.82
3:C:216:THR:C	3:C:217:PHE:HD1	1.83	0.82
1:D:176:TRP:HB3	1:D:209:ARG:HD2	1.59	0.82
1:A:43:VAL:HG13	1:A:50:VAL:HG22	1.61	0.82
3:C:31:VAL:O	3:C:31:VAL:CG1	2.23	0.82
3:C:319:THR:HB	3:C:447:ASN:CB	2.08	0.82
3:C:426:THR:O	3:C:426:THR:CG2	2.25	0.82
1:D:141:ASN:HA	1:D:205:PHE:O	1.78	0.82
1:D:198:TYR:N	1:D:198:TYR:CD1	2.13	0.82
1:A:107:LYS:C	1:A:108:LEU:HD23	2.00	0.82
2:B:129:THR:HG22	2:B:142:CYS:SG	2.20	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:MET:SD	3:C:92:ILE:HD11	2.20	0.82
3:C:316:THR:HG22	3:C:317:PRO:CD	2.09	0.82
1:D:276:LYS:H	1:D:276:LYS:HD2	1.44	0.82
4:E:89:VAL:CG2	4:E:99:PHE:CE2	2.63	0.82
4:E:265:LEU:O	4:E:268:ILE:HG23	1.79	0.82
1:A:136:PRO:HA	1:A:277:TYR:OH	1.79	0.82
3:C:319:THR:HG22	3:C:320:HIS:N	1.94	0.82
4:E:162:GLU:HA	4:E:190:ALA:H	1.45	0.82
1:A:155:LYS:CG	4:E:78:ARG:HH21	1.93	0.82
2:B:216:LYS:HD2	2:B:216:LYS:O	1.79	0.82
3:C:38:THR:CG2	3:C:57:TRP:CE3	2.63	0.82
1:D:376:ILE:HG22	1:D:380:LYS:NZ	1.94	0.82
4:E:76:LEU:HD23	4:E:77:VAL:N	1.95	0.82
1:A:136:PRO:HD3	1:A:274:ILE:HG23	1.59	0.82
1:A:242:LYS:HB2	1:A:245:LEU:HB2	1.60	0.82
1:A:419:ILE:CG2	1:A:420:ILE:H	1.93	0.82
3:C:438:ALA:HA	3:C:441:GLU:CD	2.00	0.82
1:D:201:ILE:HG22	1:D:203:TYR:CE1	2.14	0.82
1:D:229:THR:HA	1:D:232:VAL:CG2	2.10	0.82
4:E:35:THR:HG23	4:E:175:GLU:OE1	1.78	0.82
2:B:52:THR:HG22	2:B:53:SER:H	1.44	0.82
2:B:65:LEU:HD23	2:B:110:VAL:CG1	2.09	0.82
1:D:60:TRP:CE2	1:D:86:TRP:CH2	2.68	0.82
4:E:151:ASN:HA	4:E:205:PHE:CD1	2.15	0.82
1:A:251:LEU:HD13	4:E:260:ALA:HB2	1.60	0.82
4:E:74:ILE:HG12	4:E:76:LEU:O	1.79	0.81
2:B:185:GLN:CB	2:B:219:PHE:HE2	1.92	0.81
2:B:241:LEU:HG	2:B:248:LYS:HE2	1.62	0.81
3:C:276:GLN:O	3:C:279:PRO:HD2	1.79	0.81
1:D:10:ASN:OD1	1:D:11:LEU:HD23	1.80	0.81
1:A:2:GLU:CD	1:A:74:GLY:HA2	2.00	0.81
2:B:230:LEU:HA	2:B:233:ILE:HG13	1.61	0.81
3:C:94:LEU:CB	3:C:98:ASN:HB2	2.09	0.81
3:C:245:LEU:O	3:C:249:LEU:HD13	1.81	0.81
3:C:463:PRO:HA	3:C:466:VAL:HG23	1.61	0.81
1:D:175:GLU:HB3	1:D:211:PRO:CG	2.09	0.81
1:D:379:VAL:O	1:D:379:VAL:HG12	1.77	0.81
4:E:33:LYS:HG2	4:E:160:SER:HB3	1.61	0.81
1:D:187:TRP:CZ2	1:D:196:THR:HG23	2.16	0.81
4:E:44:GLU:CA	4:E:129:ILE:HD12	2.10	0.81
4:E:267:LEU:HD12	4:E:270:GLN:CD	2.01	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HG22	1:A:107:LYS:N	1.95	0.81
1:D:102:ILE:HD12	4:E:98:GLN:NE2	1.95	0.81
1:D:395:ALA:O	1:D:398:GLU:HG2	1.79	0.81
2:B:2:VAL:CG1	2:B:69:PRO:HG3	2.09	0.81
2:B:31:VAL:HG21	2:B:86:TRP:CZ3	2.15	0.81
2:B:46:LYS:HB2	2:B:276:SER:C	2.01	0.81
2:B:405:VAL:HG12	2:B:409:LYS:NZ	1.95	0.81
1:D:250:LEU:HD22	1:D:292:THR:CB	2.10	0.81
3:C:137:PHE:CD1	3:C:288:ILE:HB	2.15	0.81
3:C:192:ILE:HD12	3:C:219:LEU:HD11	1.63	0.81
3:C:478:PHE:CD1	3:C:478:PHE:C	2.53	0.81
4:E:146:ARG:CZ	4:E:205:PHE:HB3	2.11	0.81
4:E:183:TRP:HB3	4:E:216:ARG:CD	2.10	0.81
4:E:436:ASN:HA	4:E:439:TRP:NE1	1.95	0.81
2:B:306:HIS:ND1	2:B:306:HIS:O	2.14	0.81
3:C:478:PHE:C	3:C:478:PHE:HD1	1.84	0.81
1:D:113:THR:CG2	1:D:114:GLY:HA3	2.06	0.81
1:D:215:VAL:O	1:D:219:ILE:HG23	1.81	0.81
1:A:152:ASP:CB	1:A:197:PRO:HA	2.10	0.81
3:C:106:TYR:O	3:C:106:TYR:HD1	1.63	0.81
1:D:239:SER:CB	1:D:242:LYS:HE2	2.11	0.81
1:D:408:HIS:O	1:D:412:CYS:HB2	1.81	0.81
2:B:1:SER:O	2:B:1:SER:OG	1.98	0.81
4:E:135:PRO:HG2	4:E:137:ASP:O	1.79	0.81
1:A:133:THR:O	1:A:136:PRO:HG2	1.81	0.80
1:A:148:ILE:HG21	1:A:198:TYR:HB2	1.63	0.80
2:B:92:LEU:N	2:B:96:ASN:HB2	1.95	0.80
3:C:30:VAL:HG22	3:C:157:GLU:CA	2.12	0.80
3:C:47:GLU:HG2	3:C:286:PRO:HD2	1.62	0.80
1:D:30:ASP:OD1	1:D:30:ASP:N	2.11	0.80
1:D:106:THR:HG23	1:D:107:LYS:CE	2.11	0.80
1:D:305:THR:HG22	1:D:400:LYS:HB3	1.62	0.80
4:E:94:ASN:CG	4:E:143:LEU:HD23	2.01	0.80
2:B:409:LYS:NZ	3:C:423:ILE:HG23	1.96	0.80
2:B:24:THR:HG22	2:B:25:VAL:H	1.47	0.80
1:D:257:LEU:HD12	1:D:257:LEU:C	2.01	0.80
4:E:122:ILE:H	4:E:122:ILE:HD13	1.46	0.80
4:E:185:ILE:HG12	4:E:214:ILE:HG22	1.61	0.80
1:A:382:ILE:O	1:A:386:MET:HG2	1.81	0.80
3:C:11:LEU:O	3:C:16:LYS:HB2	1.80	0.80
3:C:431:LYS:HZ1	1:D:379:VAL:HG22	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:PHE:CZ	1:D:291:VAL:HG11	2.15	0.80
4:E:39:LEU:HD23	4:E:183:TRP:CZ2	2.15	0.80
2:B:191:LYS:HA	2:B:210:TYR:O	1.81	0.80
3:C:47:GLU:HB3	3:C:285:VAL:HB	1.64	0.80
3:C:180:ASP:HB3	3:C:181:PRO:HD3	1.61	0.80
3:C:190:TRP:HB3	3:C:223:ARG:HB2	1.64	0.80
1:D:135:PHE:C	1:D:135:PHE:HD1	1.84	0.80
1:D:136:PRO:HA	1:D:277:TYR:OH	1.82	0.80
4:E:63:ARG:HB2	4:E:63:ARG:HH11	1.46	0.80
4:E:94:ASN:ND2	4:E:125:SER:HB2	1.96	0.80
2:B:70:ALA:O	2:B:74:GLY:HA3	1.81	0.80
2:B:147:LYS:HG3	2:B:148:SER:N	1.96	0.80
2:B:301:VAL:O	2:B:304:LEU:HB3	1.80	0.80
3:C:137:PHE:HZ	3:C:291:TYR:CD2	1.99	0.80
4:E:463:LEU:HD12	4:E:463:LEU:O	1.81	0.80
2:B:31:VAL:HG12	2:B:158:LEU:HD21	1.64	0.80
3:C:121:LEU:HD12	3:C:121:LEU:O	1.80	0.80
3:C:275:SER:O	3:C:279:PRO:HD3	1.81	0.80
1:A:257:LEU:CD1	1:A:285:VAL:CG2	2.60	0.80
1:A:267:THR:HG23	1:A:271:VAL:CG2	2.11	0.80
2:B:160:HIS:HE1	2:B:207:VAL:HG11	1.41	0.80
1:D:55:ARG:HA	1:D:120:PRO:O	1.82	0.80
1:A:56:LEU:O	1:A:119:THR:HA	1.81	0.80
1:A:141:ASN:HB3	1:A:206:ILE:HG13	1.64	0.80
3:C:472:ILE:HB	3:C:475:MET:SD	2.21	0.80
1:D:60:TRP:CH2	1:D:86:TRP:CZ3	2.69	0.80
1:D:432:GLU:HG2	1:D:435:GLN:NE2	1.95	0.80
2:B:175:ILE:HG12	2:B:176:ASN:N	1.97	0.80
3:C:29:GLU:O	3:C:30:VAL:HG23	1.81	0.80
3:C:142:GLN:HG3	3:C:143:ASN:N	1.92	0.80
3:C:316:THR:CG2	3:C:317:PRO:CD	2.60	0.80
1:A:255:VAL:O	1:A:259:VAL:HG23	1.82	0.79
2:B:243:PRO:CB	2:B:435:ALA:HB1	2.09	0.79
3:C:148:PHE:HB2	3:C:215:VAL:HG21	1.60	0.79
1:D:85:VAL:HG13	1:D:86:TRP:CE3	2.17	0.79
1:D:88:PRO:HG2	1:D:88:PRO:O	1.81	0.79
4:E:100:GLU:HB2	4:E:122:ILE:CD1	2.12	0.79
1:A:155:LYS:HG3	4:E:78:ARG:HH21	1.46	0.79
1:A:207:MET:O	1:A:207:MET:CG	2.30	0.79
2:B:56:LEU:HB2	2:B:120:PRO:HG2	1.62	0.79
2:B:132:VAL:HG13	2:B:279:ILE:CA	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HD12	3:C:116:GLY:C	2.01	0.79
3:C:69:TRP:HB2	3:C:74:TYR:HB2	1.64	0.79
3:C:288:ILE:HG12	3:C:289:GLY:H	1.47	0.79
1:D:187:TRP:HZ2	1:D:196:THR:HA	1.47	0.79
4:E:127:CYS:SG	4:E:128:PRO:HD2	2.22	0.79
4:E:138:TRP:CE2	4:E:215:GLN:HB2	2.16	0.79
4:E:262:THR:CB	4:E:265:LEU:HD12	2.12	0.79
3:C:275:SER:O	3:C:278:LEU:HB3	1.81	0.79
1:D:45:GLU:HB3	1:D:271:VAL:HG23	1.64	0.79
4:E:159:LEU:HB2	4:E:192:LYS:HB2	1.62	0.79
4:E:191:LYS:O	4:E:209:ILE:HG22	1.82	0.79
1:A:94:ASN:HD22	1:A:94:ASN:C	1.83	0.79
1:A:209:ARG:CG	1:A:210:ILE:H	1.95	0.79
3:C:69:TRP:CZ2	3:C:112:VAL:CG1	2.65	0.79
3:C:479:ASN:ND2	3:C:479:ASN:C	2.36	0.79
4:E:138:TRP:HB3	4:E:214:ILE:O	1.82	0.79
2:B:90:ILE:HG23	2:B:147:LYS:N	1.98	0.79
2:B:266:LEU:O	2:B:269:LYS:HG3	1.81	0.79
3:C:42:LEU:HD22	3:C:190:TRP:CZ2	2.18	0.79
3:C:453:ILE:HG23	3:C:454:ASP:N	1.98	0.79
3:C:471:PHE:HD1	3:C:471:PHE:C	1.86	0.79
4:E:45:LYS:HE2	4:E:278:ASN:O	1.82	0.79
4:E:313:THR:O	4:E:313:THR:OG1	2.00	0.79
1:A:56:LEU:HD23	1:A:57:ARG:N	1.98	0.79
3:C:37:LEU:HD12	3:C:217:PHE:CD2	2.17	0.79
3:C:201:ILE:HG13	3:C:211:ASN:O	1.81	0.79
1:D:35:LEU:HD12	1:D:36:GLN:N	1.96	0.79
4:E:433:GLY:O	4:E:436:ASN:HB2	1.82	0.79
1:A:17:LYS:HE3	1:A:84:ASP:HA	1.65	0.79
2:B:40:LEU:HD23	2:B:52:THR:OG1	1.82	0.79
3:C:106:TYR:C	3:C:107:PHE:HD1	1.85	0.79
4:E:140:ASN:HD21	4:E:211:PHE:HA	1.47	0.79
4:E:184:THR:HG23	4:E:215:GLN:HG2	1.63	0.79
1:A:41:ILE:HD11	1:A:51:GLU:CB	2.13	0.79
1:A:304:SER:HB2	1:A:400:LYS:NZ	1.98	0.79
2:B:68:ASP:O	2:B:72:TYR:HB3	1.82	0.79
3:C:7:LEU:HD23	3:C:10:ASP:CB	2.12	0.79
1:D:175:GLU:OE1	1:D:211:PRO:HB3	1.82	0.79
1:A:242:LYS:HB2	1:A:245:LEU:CB	2.12	0.79
3:C:190:TRP:HD1	3:C:221:ILE:HD12	1.48	0.79
1:D:87:LEU:HD12	1:D:88:PRO:CD	2.09	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PHE:HZ	1:D:273:LEU:HD12	1.47	0.79
1:D:232:VAL:CG2	1:D:250:LEU:HD11	2.13	0.79
4:E:33:LYS:HE3	4:E:160:SER:HB2	1.65	0.79
4:E:172:ILE:HD11	4:E:187:HIS:HA	1.65	0.79
1:A:302:SER:HB2	1:A:306:HIS:C	2.02	0.79
2:B:242:PRO:HD3	2:B:248:LYS:HE3	1.64	0.79
3:C:279:PRO:CA	3:C:282:ALA:HB3	2.11	0.79
4:E:162:GLU:O	4:E:189:PRO:HA	1.83	0.79
1:A:420:ILE:HG13	1:A:421:GLY:H	1.46	0.78
2:B:55:PHE:HA	2:B:120:PRO:O	1.83	0.78
2:B:131:LYS:NZ	2:B:132:VAL:HB	1.97	0.78
2:B:197:TRP:CD1	2:B:204:TYR:HB3	2.18	0.78
2:B:112:HIS:CD2	2:B:113:THR:HG23	2.18	0.78
1:D:187:TRP:CZ3	1:D:189:TYR:HD1	2.01	0.78
4:E:89:VAL:HG23	4:E:99:PHE:CE2	2.19	0.78
3:C:3:GLU:OE1	3:C:7:LEU:HD12	1.83	0.78
3:C:273:LEU:HD23	3:C:276:GLN:CG	2.13	0.78
3:C:210:THR:HG22	3:C:211:ASN:H	1.47	0.78
1:D:244:THR:HG23	1:D:245:LEU:N	1.98	0.78
4:E:262:THR:HG23	4:E:265:LEU:CD1	2.14	0.78
1:A:59:GLN:HE22	1:A:117:MET:CG	1.97	0.78
1:A:76:LYS:HG2	1:A:77:LYS:N	1.99	0.78
1:A:189:TYR:HA	1:A:197:PRO:CD	2.13	0.78
1:A:251:LEU:HD22	4:E:260:ALA:HB1	1.66	0.78
2:B:279:ILE:HG22	2:B:280:ILE:HD13	1.66	0.78
1:D:401:TYR:O	1:D:401:TYR:HD1	1.67	0.78
2:B:31:VAL:HG12	2:B:158:LEU:CD2	2.14	0.78
2:B:46:LYS:HE2	2:B:278:PRO:CG	2.10	0.78
2:B:311:THR:CB	2:B:430:TYR:CD2	2.66	0.78
4:E:470:HIS:CE1	4:E:474:VAL:HG23	2.18	0.78
1:A:245:LEU:HD13	2:B:250:SER:HB2	1.65	0.78
3:C:50:GLU:HA	3:C:132:ILE:CD1	2.13	0.78
1:D:60:TRP:CZ2	1:D:86:TRP:CH2	2.71	0.78
4:E:209:ILE:HG12	4:E:211:PHE:HE1	1.49	0.78
4:E:283:GLY:O	4:E:287:ILE:HG22	1.84	0.78
1:A:305:THR:HB	1:A:400:LYS:HB2	1.64	0.78
1:A:422:THR:O	1:A:425:VAL:HG12	1.83	0.78
3:C:38:THR:CG2	3:C:57:TRP:HE3	1.96	0.78
1:D:46:VAL:HB	1:D:271:VAL:CA	2.14	0.78
1:D:101:ALA:C	1:D:102:ILE:HD13	2.04	0.78
1:A:41:ILE:HD11	1:A:51:GLU:OE1	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:CD1	1:A:285:VAL:HG23	2.13	0.78
2:B:442:ILE:O	2:B:446:MET:HG2	1.84	0.78
4:E:237:VAL:CG2	4:E:457:LEU:HD21	2.14	0.78
1:A:35:LEU:HD21	1:A:37:LEU:CD2	2.14	0.78
1:A:151:TYR:O	1:A:198:TYR:HB3	1.84	0.78
1:D:92:LEU:CD2	1:D:92:LEU:H	1.96	0.78
1:D:187:TRP:CH2	1:D:189:TYR:HB3	2.18	0.78
4:E:132:THR:O	4:E:135:PRO:HD3	1.84	0.78
4:E:187:HIS:CE1	4:E:189:PRO:HG3	2.19	0.78
4:E:435:GLU:HB3	4:E:439:TRP:CZ2	2.19	0.78
1:A:135:PHE:HB3	1:A:273:LEU:HA	1.66	0.77
4:E:215:GLN:HG3	4:E:216:ARG:N	1.98	0.77
2:B:81:PRO:HD3	3:C:22:ARG:NH2	1.99	0.77
3:C:12:LEU:HB2	3:C:16:LYS:CG	2.09	0.77
3:C:12:LEU:CB	3:C:16:LYS:HG2	2.08	0.77
3:C:160:MET:H	3:C:213:GLN:HB2	1.49	0.77
3:C:242:LEU:HD21	3:C:263:VAL:HG12	1.65	0.77
1:D:72:TYR:HD1	1:D:72:TYR:O	1.65	0.77
1:D:131:ILE:HG13	1:D:133:THR:N	1.95	0.77
1:D:137:PHE:HD2	1:D:431:ILE:CG2	1.97	0.77
4:E:141:CYS:SG	4:E:143:LEU:HD11	2.25	0.77
4:E:273:PRO:HG2	4:E:274:GLU:H	1.49	0.77
1:D:302:SER:CB	1:D:305:THR:HG23	2.15	0.77
1:A:137:PHE:HB3	1:A:435:GLN:HG3	1.65	0.77
4:E:79:ILE:O	4:E:79:ILE:CG2	2.33	0.77
1:A:2:GLU:O	1:A:7:LEU:HD21	1.83	0.77
1:A:43:VAL:CG1	1:A:50:VAL:HG22	2.15	0.77
1:A:95:ASN:HA	1:A:127:TYR:HB3	1.66	0.77
3:C:143:ASN:OD1	3:C:220:ILE:HB	1.83	0.77
3:C:466:VAL:O	3:C:470:ILE:HG12	1.85	0.77
4:E:233:SER:O	4:E:237:VAL:HG23	1.84	0.77
1:A:41:ILE:CD1	1:A:51:GLU:HB3	2.14	0.77
2:B:241:LEU:HD21	2:B:251:LEU:HD11	1.66	0.77
2:B:449:ILE:HA	2:B:452:PHE:CD2	2.20	0.77
3:C:155:ALA:N	3:C:211:ASN:HA	1.99	0.77
4:E:20:PRO:HG3	4:E:61:ASP:HA	1.66	0.77
4:E:310:THR:HB	4:E:313:THR:HG22	1.67	0.77
2:B:9:SER:HA	2:B:12:PHE:HD1	1.48	0.77
2:B:10:VAL:CG1	2:B:11:LEU:HD22	2.13	0.77
2:B:68:ASP:HB3	2:B:69:PRO:HD3	1.65	0.77
2:B:186:TRP:HB3	2:B:215:ARG:HD2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:HIS:HB3	1:D:7:LEU:HG	1.64	0.77
4:E:279:VAL:HB	4:E:280:PRO:CD	2.15	0.77
2:B:20:ARG:HD3	2:B:20:ARG:H	1.48	0.77
2:B:278:PRO:O	2:B:278:PRO:HG2	1.85	0.77
3:C:195:LYS:HG3	3:C:195:LYS:O	1.83	0.77
3:C:471:PHE:C	3:C:471:PHE:CD1	2.56	0.77
1:A:57:ARG:HD3	1:A:161:GLU:OE1	1.85	0.77
2:B:38:THR:HG22	2:B:55:PHE:HE1	1.50	0.77
3:C:148:PHE:CB	3:C:215:VAL:CG2	2.61	0.77
1:D:58:GLN:NE2	1:D:88:PRO:HG3	2.00	0.77
1:D:153:GLY:HA3	1:D:196:THR:HG22	1.66	0.77
1:A:43:VAL:CG2	1:A:50:VAL:HG22	2.15	0.76
1:A:207:MET:H	1:A:207:MET:HE2	1.48	0.76
3:C:22:ARG:O	3:C:24:VAL:HG23	1.85	0.76
3:C:113:ARG:NE	3:C:119:THR:HG23	1.99	0.76
4:E:152:ALA:HB3	4:E:204:ASP:O	1.84	0.76
4:E:250:LYS:HB3	4:E:253:LEU:HD23	1.67	0.76
2:B:185:GLN:HB3	2:B:217:PRO:HB3	1.66	0.76
1:D:40:LEU:CD1	1:D:52:THR:HB	2.14	0.76
1:D:72:TYR:CD1	1:D:72:TYR:O	2.38	0.76
4:E:14:TYR:CE2	4:E:16:LYS:HE3	2.19	0.76
4:E:262:THR:OG1	4:E:265:LEU:HD12	1.85	0.76
1:A:60:TRP:HE1	1:A:116:ILE:HD12	1.51	0.76
1:A:66:ARG:HD3	1:A:66:ARG:N	2.00	0.76
1:A:380:LYS:HD3	2:B:408:ILE:HB	1.67	0.76
2:B:47:ASN:HB2	2:B:49:GLU:OE1	1.84	0.76
3:C:4:GLU:HG3	3:C:5:GLU:N	2.00	0.76
3:C:453:ILE:CG2	3:C:454:ASP:H	1.97	0.76
4:E:44:GLU:HG3	4:E:129:ILE:CB	2.15	0.76
1:A:90:LEU:CD1	1:A:100:PHE:HE2	1.99	0.76
1:A:174:GLY:HA2	1:A:176:TRP:CZ3	2.21	0.76
2:B:287:ILE:C	2:B:287:ILE:HD12	2.06	0.76
3:C:318:SER:HB2	3:C:447:ASN:HD22	1.49	0.76
4:E:39:LEU:HD12	4:E:49:LEU:HD13	1.66	0.76
1:A:2:GLU:O	1:A:2:GLU:CG	2.34	0.76
2:B:47:ASN:O	2:B:48:GLU:HG2	1.85	0.76
3:C:67:LEU:C	3:C:116:GLY:H	1.89	0.76
3:C:316:THR:HG21	3:C:447:ASN:HB3	1.67	0.76
3:C:137:PHE:CD1	3:C:137:PHE:C	2.59	0.76
1:A:3:HIS:HB2	1:A:7:LEU:CD2	2.16	0.76
1:A:46:VAL:CG2	1:A:270:ALA:CA	2.63	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:HIS:O	1:A:306:HIS:CD2	2.38	0.76
2:B:65:LEU:HD23	2:B:110:VAL:HG11	1.66	0.76
2:B:212:ILE:HG22	2:B:212:ILE:O	1.86	0.76
3:C:84:PRO:HG3	3:C:107:PHE:O	1.86	0.76
3:C:135:LEU:O	3:C:138:PRO:HD2	1.86	0.76
3:C:161:ASP:HA	3:C:199:LYS:HG2	1.68	0.76
1:A:155:LYS:HG3	4:E:78:ARG:HE	1.50	0.76
2:B:56:LEU:HD11	2:B:103:THR:HG23	1.66	0.76
2:B:439:PHE:HA	2:B:442:ILE:HB	1.67	0.76
3:C:36:SER:HB3	3:C:59:ASP:CB	2.16	0.76
1:D:86:TRP:O	1:D:86:TRP:CE2	2.37	0.76
1:D:233:PHE:HZ	1:D:291:VAL:HG11	1.49	0.76
1:A:94:ASN:ND2	1:A:94:ASN:C	2.35	0.76
3:C:58:MET:SD	3:C:92:ILE:CD1	2.74	0.76
1:D:49:ILE:HG22	1:D:49:ILE:O	1.84	0.76
1:D:401:TYR:O	1:D:401:TYR:CD1	2.39	0.76
1:D:412:CYS:HB3	1:D:413:VAL:HG23	1.67	0.76
1:A:139:GLN:HG3	1:A:207:MET:N	2.00	0.76
1:A:291:VAL:O	1:A:295:VAL:HG23	1.86	0.76
3:C:445:ASN:CA	3:C:448:LEU:HG	2.12	0.76
1:D:231:LEU:O	1:D:235:LEU:HG	1.86	0.76
4:E:66:TRP:CD1	4:E:111:ASN:CA	2.69	0.76
4:E:173:ASP:HB3	4:E:185:ILE:HG21	1.67	0.76
4:E:211:PHE:O	4:E:212:LEU:HD12	1.83	0.76
1:A:43:VAL:HG22	1:A:50:VAL:HG22	1.66	0.75
3:C:273:LEU:HD23	3:C:276:GLN:CB	2.16	0.75
1:D:166:ASP:CB	1:D:181:TYR:HB2	2.16	0.75
1:D:271:VAL:O	1:D:271:VAL:CG1	2.34	0.75
4:E:91:LEU:HB2	4:E:95:VAL:H	1.51	0.75
1:A:107:LYS:HE2	2:B:150:THR:HB	1.66	0.75
1:A:107:LYS:CE	2:B:150:THR:HB	2.16	0.75
1:A:209:ARG:C	1:A:210:ILE:HG13	2.05	0.75
1:A:293:VAL:HG22	4:E:238:LEU:HD21	1.66	0.75
2:B:265:LEU:HA	2:B:268:ASP:OD2	1.87	0.75
3:C:316:THR:HG21	3:C:447:ASN:CB	2.16	0.75
1:D:260:ILE:HG22	1:D:264:ILE:HD11	1.66	0.75
1:A:282:MET:O	1:A:286:ILE:HG13	1.85	0.75
2:B:181:THR:CG2	2:B:184:GLY:H	1.99	0.75
2:B:263:LEU:CD2	2:B:291:VAL:HG22	2.13	0.75
1:D:118:TRP:NE1	1:D:120:PRO:HB3	2.02	0.75
1:D:384:GLU:HG2	4:E:422:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:90:VAL:CG2	4:E:95:VAL:HG11	2.14	0.75
1:A:256:PHE:CE1	2:B:261:VAL:CG2	2.70	0.75
1:D:176:TRP:CB	1:D:209:ARG:HD2	2.16	0.75
1:A:406:ILE:HG23	1:A:409:ILE:CD1	2.15	0.75
2:B:112:HIS:NE2	2:B:113:THR:HG23	2.00	0.75
3:C:77:ILE:CD1	3:C:80:LEU:HD13	2.15	0.75
3:C:431:LYS:NZ	1:D:379:VAL:HG22	2.01	0.75
1:D:49:ILE:HG21	1:D:125:LYS:HZ1	1.50	0.75
4:E:101:VAL:CG2	4:E:101:VAL:O	2.35	0.75
3:C:132:ILE:O	3:C:136:TYR:HB2	1.87	0.75
3:C:241:PHE:CD1	3:C:245:LEU:HD22	2.20	0.75
3:C:280:GLU:HG3	3:C:281:THR:N	2.00	0.75
3:C:443:VAL:O	3:C:443:VAL:HG12	1.86	0.75
1:D:11:LEU:O	1:D:15:TYR:HB2	1.86	0.75
1:D:101:ALA:O	1:D:102:ILE:HD13	1.86	0.75
4:E:159:LEU:HD12	4:E:192:LYS:CA	2.16	0.75
1:A:135:PHE:N	1:A:136:PRO:HD2	2.02	0.75
2:B:304:LEU:HD23	2:B:304:LEU:C	2.07	0.75
3:C:33:ILE:O	3:C:160:MET:HA	1.87	0.75
3:C:78:SER:O	3:C:114:PRO:HB3	1.87	0.75
3:C:431:LYS:CE	1:D:379:VAL:HG22	2.16	0.75
1:D:63:VAL:O	1:D:63:VAL:HG22	1.86	0.75
1:D:109:LEU:O	1:D:116:ILE:HG22	1.86	0.75
1:D:167:LEU:N	1:D:167:LEU:CD1	2.48	0.75
1:A:276:LYS:HD2	1:A:276:LYS:H	1.52	0.75
1:D:216:VAL:O	1:D:220:ILE:HG13	1.86	0.75
2:B:223:TYR:O	2:B:226:VAL:HG22	1.86	0.75
3:C:242:LEU:HD22	3:C:267:GLN:CG	2.17	0.75
3:C:248:TYR:C	3:C:250:PRO:HD2	2.08	0.75
3:C:282:ALA:HB2	3:C:287:LEU:CD1	2.16	0.75
1:D:222:CYS:SG	1:D:225:PHE:CZ	2.79	0.75
4:E:44:GLU:CB	4:E:129:ILE:HD12	2.17	0.75
4:E:100:GLU:HB2	4:E:122:ILE:HD11	1.69	0.75
1:A:131:ILE:HD11	1:A:140:GLN:CG	2.16	0.74
1:A:433:LEU:O	1:A:433:LEU:HD12	1.87	0.74
3:C:78:SER:HA	3:C:114:PRO:CB	2.17	0.74
1:D:255:VAL:O	1:D:259:VAL:HG23	1.87	0.74
4:E:55:ILE:HG13	4:E:57:ILE:HG13	1.67	0.74
4:E:66:TRP:CD1	4:E:111:ASN:CB	2.69	0.74
4:E:188:ARG:O	4:E:188:ARG:CG	2.35	0.74
1:A:52:THR:O	1:A:123:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:TRP:HB2	2:B:72:TYR:HB2	1.67	0.74
2:B:131:LYS:HZ2	2:B:132:VAL:HB	1.49	0.74
2:B:289:ILE:HG22	2:B:293:PHE:CZ	2.22	0.74
3:C:48:THR:N	3:C:285:VAL:HA	2.01	0.74
1:D:109:LEU:HD12	1:D:117:MET:HB3	1.69	0.74
4:E:183:TRP:HA	4:E:216:ARG:HA	1.69	0.74
1:A:251:LEU:CD2	4:E:260:ALA:CB	2.63	0.74
1:D:229:THR:HA	1:D:232:VAL:HG23	1.68	0.74
4:E:45:LYS:N	4:E:280:PRO:HA	2.03	0.74
4:E:448:LYS:N	4:E:448:LYS:HD2	1.99	0.74
1:A:137:PHE:CD1	1:A:210:ILE:HD12	2.22	0.74
3:C:30:VAL:CG2	3:C:157:GLU:CA	2.66	0.74
3:C:81:ARG:NH1	3:C:111:LEU:HB2	2.03	0.74
3:C:93:VAL:HG11	3:C:151:LEU:HD13	1.68	0.74
1:A:148:ILE:HD11	1:A:156:VAL:CG1	2.16	0.74
1:A:148:ILE:CG2	1:A:198:TYR:CD2	2.69	0.74
2:B:155:GLU:O	2:B:156:VAL:HG13	1.87	0.74
3:C:138:PRO:CA	3:C:288:ILE:HD12	2.17	0.74
1:D:92:LEU:HD22	1:D:92:LEU:N	2.02	0.74
1:A:379:VAL:HA	1:A:382:ILE:HD11	1.69	0.74
3:C:269:VAL:HG13	3:C:270:PHE:HD1	1.51	0.74
1:D:63:VAL:O	1:D:63:VAL:CG2	2.35	0.74
1:D:227:PHE:O	1:D:230:VAL:HG12	1.87	0.74
1:A:380:LYS:HD3	2:B:408:ILE:CB	2.16	0.74
3:C:25:LYS:HG3	3:C:25:LYS:O	1.87	0.74
3:C:179:ILE:CG2	3:C:181:PRO:HD2	2.17	0.74
1:A:156:VAL:HG22	1:A:157:SER:N	2.02	0.74
1:A:218:VAL:HG13	1:A:219:ILE:N	2.02	0.74
1:A:423:VAL:O	1:A:426:PHE:HB3	1.87	0.74
3:C:316:THR:HG23	3:C:317:PRO:HD2	1.70	0.74
1:D:237:THR:OG1	1:D:406:ILE:HG23	1.88	0.74
4:E:19:LYS:NZ	4:E:154:GLU:HB3	2.03	0.74
2:B:33:VAL:HG21	2:B:158:LEU:HD13	1.69	0.74
3:C:13:ILE:O	3:C:17:TYR:HB3	1.87	0.74
3:C:470:ILE:O	3:C:474:VAL:HG23	1.88	0.74
1:D:64:ARG:HH11	1:D:64:ARG:HG3	1.52	0.74
1:D:132:VAL:O	1:D:274:ILE:HG12	1.87	0.74
1:D:166:ASP:OD2	1:D:181:TYR:HB2	1.88	0.74
4:E:144:VAL:HG12	4:E:209:ILE:HA	1.68	0.74
4:E:35:THR:HG23	4:E:175:GLU:CD	2.08	0.74
4:E:59:TRP:C	4:E:60:ASN:HD22	1.91	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:HB2	1:A:7:LEU:HD21	1.70	0.73
1:A:54:VAL:CG2	1:A:122:ALA:HB3	2.18	0.73
1:A:281:THR:O	1:A:285:VAL:HG12	1.88	0.73
1:A:87:LEU:H	1:A:87:LEU:CD2	1.98	0.73
1:A:236:PRO:HB3	1:A:299:HIS:NE2	2.03	0.73
1:A:250:LEU:HD11	1:A:296:ILE:CG2	2.16	0.73
3:C:434:LYS:HE2	3:C:435:GLU:HG2	1.69	0.73
1:D:398:GLU:HA	1:D:401:TYR:CE1	2.22	0.73
1:D:409:ILE:HA	1:D:412:CYS:HB2	1.71	0.73
4:E:80:PRO:CB	4:E:83:LEU:HD23	2.18	0.73
1:A:41:ILE:CG1	1:A:51:GLU:HB3	2.17	0.73
1:A:139:GLN:NE2	1:A:206:ILE:HG23	2.03	0.73
1:A:259:VAL:HG13	1:A:262:GLU:OE1	1.88	0.73
3:C:138:PRO:HB2	3:C:140:ASP:OD1	1.88	0.73
4:E:44:GLU:HG3	4:E:129:ILE:HB	1.69	0.73
4:E:138:TRP:CE3	4:E:215:GLN:HA	2.22	0.73
4:E:463:LEU:HG	4:E:464:ALA:N	2.03	0.73
1:A:145:LYS:HZ2	1:A:202:THR:HG23	1.54	0.73
2:B:415:LEU:HD13	2:B:415:LEU:C	2.08	0.73
3:C:102:TYR:CE1	3:C:106:TYR:HB3	2.24	0.73
1:D:142:CYS:SG	1:D:144:MET:HG3	2.28	0.73
1:D:301:ARG:HH22	1:D:406:ILE:CD1	2.01	0.73
4:E:14:TYR:HE2	4:E:16:LYS:CE	2.01	0.73
4:E:444:LYS:O	4:E:448:LYS:HG2	1.89	0.73
4:E:416:VAL:HG22	4:E:417:GLU:N	2.04	0.73
1:A:406:ILE:CG2	1:A:409:ILE:CD1	2.67	0.73
1:D:53:ASN:HB2	1:D:123:ILE:HG12	1.70	0.73
1:D:56:LEU:HD21	1:D:122:ALA:HB3	1.70	0.73
2:B:160:HIS:H	2:B:195:LYS:HZ1	1.37	0.73
3:C:196:PRO:HD2	3:C:218:TYR:O	1.87	0.73
1:D:252:SER:HB2	4:E:259:LEU:CD1	2.18	0.73
4:E:262:THR:HG23	4:E:265:LEU:HB2	1.69	0.73
1:A:41:ILE:HG13	1:A:42:ASN:N	2.04	0.73
2:B:48:GLU:HB2	2:B:130:ILE:HG12	1.71	0.73
2:B:251:LEU:C	2:B:251:LEU:HD12	2.08	0.73
3:C:223:ARG:O	3:C:224:LYS:HG3	1.88	0.73
3:C:232:PHE:C	3:C:235:PRO:HD2	2.09	0.73
1:D:65:LEU:HD23	1:D:110:LEU:HD13	1.67	0.73
1:D:86:TRP:O	1:D:86:TRP:CE3	2.38	0.73
4:E:44:GLU:CG	4:E:129:ILE:HD12	2.17	0.73
1:A:148:ILE:HG21	1:A:198:TYR:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:N	2:B:23:GLN:NE2	2.36	0.73
2:B:129:THR:O	2:B:129:THR:CG2	2.25	0.73
1:D:38:ILE:HG22	1:D:38:ILE:O	1.89	0.73
1:D:92:LEU:CB	1:D:95:ASN:HB2	2.19	0.73
4:E:42:LEU:HD22	4:E:183:TRP:CZ2	2.24	0.73
4:E:79:ILE:HG12	4:E:80:PRO:HD3	1.70	0.73
1:A:148:ILE:CG2	1:A:198:TYR:HB2	2.19	0.73
2:B:297:LEU:O	2:B:297:LEU:HD23	1.89	0.73
3:C:155:ALA:HB2	3:C:211:ASN:CA	2.18	0.73
3:C:434:LYS:HG3	1:D:386:MET:HE1	1.69	0.73
1:D:43:VAL:HG22	1:D:50:VAL:CA	2.18	0.73
4:E:267:LEU:HD12	4:E:270:GLN:OE1	1.87	0.73
2:B:27:ASP:C	2:B:28:LYS:HG3	2.08	0.72
2:B:236:ILE:HB	2:B:446:MET:HE3	1.69	0.72
3:C:252:GLU:HG3	1:D:300:HIS:CB	2.19	0.72
1:D:78:ILE:HD12	1:D:110:LEU:HB3	1.70	0.72
1:D:236:PRO:HB3	1:D:299:HIS:HE2	1.53	0.72
4:E:219:LEU:HB3	4:E:222:ILE:CB	2.19	0.72
3:C:65:HIS:CD2	3:C:65:HIS:N	2.54	0.72
3:C:69:TRP:CE3	3:C:73:GLU:HB3	2.21	0.72
1:D:91:VAL:CG2	1:D:96:ALA:CB	2.67	0.72
3:C:51:THR:HA	3:C:128:SER:O	1.89	0.72
3:C:455:ARG:O	3:C:459:PHE:HD1	1.73	0.72
4:E:20:PRO:HB3	4:E:61:ASP:OD1	1.88	0.72
2:B:248:LYS:HD3	2:B:252:SER:HB3	0.82	0.72
1:D:157:SER:HA	1:D:199:LEU:HD12	1.70	0.72
4:E:270:GLN:C	4:E:273:PRO:HD2	2.09	0.72
2:B:109:LEU:HB2	2:B:119:HIS:NE2	2.05	0.72
2:B:218:LEU:HD13	2:B:221:ILE:CG1	2.19	0.72
3:C:278:LEU:CD1	3:C:278:LEU:O	2.35	0.72
1:D:176:TRP:CE3	1:D:209:ARG:NE	2.57	0.72
4:E:27:VAL:HG12	4:E:153:HIS:C	2.10	0.72
4:E:66:TRP:HD1	4:E:111:ASN:HB2	1.53	0.72
4:E:216:ARG:O	4:E:217:LYS:HG3	1.90	0.72
1:A:233:PHE:O	1:A:236:PRO:HG2	1.89	0.72
3:C:46:LYS:HG3	3:C:49:ASP:OD1	1.90	0.72
1:D:136:PRO:CG	1:D:274:ILE:HD11	2.15	0.72
1:D:167:LEU:CD1	1:D:178:MET:HB2	2.19	0.72
1:A:171:MET:HE3	1:A:176:TRP:CZ2	2.23	0.72
1:A:250:LEU:HD22	1:A:292:THR:CG2	2.13	0.72
2:B:181:THR:HG23	2:B:184:GLY:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:469:THR:O	3:C:473:PHE:HB2	1.90	0.72
1:D:15:TYR:CE2	1:D:84:ASP:HB3	2.25	0.72
1:D:169:THR:O	1:D:169:THR:CG2	2.27	0.72
4:E:35:THR:HB	4:E:54:TRP:HE3	1.54	0.72
1:A:179:LYS:HE2	1:A:208:GLN:CD	2.09	0.72
1:A:406:ILE:HA	1:A:409:ILE:HD11	1.70	0.72
3:C:43:ILE:H	3:C:43:ILE:HD12	1.52	0.72
3:C:141:TRP:CZ3	3:C:223:ARG:HB3	2.24	0.72
1:D:201:ILE:O	1:D:203:TYR:HE1	1.73	0.72
1:D:379:VAL:CA	1:D:382:ILE:HG13	2.17	0.72
4:E:469:GLY:O	4:E:473:GLN:HB2	1.90	0.72
1:A:155:LYS:HG3	4:E:78:ARG:NH2	2.05	0.72
2:B:176:ASN:ND2	2:B:188:ILE:HD12	2.05	0.72
3:C:67:LEU:HD21	3:C:112:VAL:HG13	1.71	0.72
1:A:46:VAL:CG2	1:A:270:ALA:C	2.58	0.72
3:C:162:LEU:C	3:C:162:LEU:HD22	2.09	0.72
1:D:398:GLU:HA	1:D:401:TYR:CE2	2.25	0.72
4:E:284:LYS:HE3	4:E:284:LYS:CA	2.19	0.72
2:B:28:LYS:CG	2:B:155:GLU:HA	2.13	0.71
2:B:91:VAL:HA	2:B:96:ASN:HD22	1.52	0.71
2:B:425:LYS:HA	2:B:428:TRP:HD1	1.52	0.71
3:C:7:LEU:HA	3:C:10:ASP:OD2	1.90	0.71
3:C:137:PHE:CD1	3:C:137:PHE:O	2.43	0.71
1:D:191:THR:O	1:D:191:THR:HG22	1.88	0.71
4:E:55:ILE:CG2	4:E:119:PRO:HG2	2.20	0.71
4:E:162:GLU:HA	4:E:190:ALA:N	2.04	0.71
4:E:431:ASP:O	4:E:435:GLU:HG3	1.90	0.71
2:B:142:CYS:O	2:B:210:TYR:HA	1.91	0.71
2:B:277:VAL:H	2:B:278:PRO:HD3	1.55	0.71
1:D:287:SER:HA	1:D:290:ILE:CD1	2.20	0.71
1:A:57:ARG:HA	1:A:119:THR:HG22	0.84	0.71
1:A:237:THR:OG1	1:A:406:ILE:HB	1.91	0.71
1:A:413:VAL:O	1:A:416:LEU:HB3	1.89	0.71
3:C:60:HIS:CD2	3:C:92:ILE:HD13	2.24	0.71
3:C:247:PHE:CE1	3:C:309:VAL:CG2	2.61	0.71
3:C:296:MET:CE	3:C:296:MET:CA	2.68	0.71
1:D:133:THR:HG23	1:D:274:ILE:HD13	1.70	0.71
1:D:141:ASN:HB3	1:D:206:ILE:CD1	2.20	0.71
1:D:152:ASP:HA	1:D:197:PRO:HA	1.71	0.71
4:E:91:LEU:HB3	4:E:94:ASN:H	1.55	0.71
4:E:138:TRP:CZ2	4:E:215:GLN:CB	2.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:NE2	2:B:23:GLN:H	1.88	0.71
2:B:130:ILE:HB	2:B:134:TYR:HD2	1.52	0.71
3:C:272:LEU:O	3:C:276:GLN:HG2	1.90	0.71
1:D:289:ILE:HG22	1:D:290:ILE:N	2.04	0.71
2:B:132:VAL:CG1	2:B:279:ILE:CA	2.68	0.71
2:B:281:ILE:HG22	2:B:285:MET:N	2.05	0.71
3:C:457:SER:O	3:C:461:ILE:HG13	1.91	0.71
1:D:395:ALA:HB1	1:D:399:TRP:CZ2	2.25	0.71
4:E:79:ILE:CG1	4:E:80:PRO:CD	2.63	0.71
4:E:236:VAL:O	4:E:239:VAL:HG23	1.88	0.71
1:A:278:MET:O	1:A:281:THR:HG22	1.90	0.71
3:C:30:VAL:HG21	3:C:158:ILE:N	2.04	0.71
3:C:42:LEU:HD22	3:C:190:TRP:HH2	1.49	0.71
3:C:319:THR:H	3:C:447:ASN:CB	2.03	0.71
1:D:170:PHE:CE2	1:D:176:TRP:CD1	2.75	0.71
4:E:81:SER:O	4:E:86:LEU:HD11	1.91	0.71
4:E:174:PRO:HA	4:E:177:PHE:HB2	1.72	0.71
1:A:56:LEU:HD22	1:A:58:GLN:HG3	1.72	0.71
1:A:250:LEU:CD2	1:A:292:THR:CG2	2.61	0.71
1:A:380:LYS:HB3	2:B:408:ILE:CG1	2.21	0.71
2:B:91:VAL:C	2:B:92:LEU:HD23	2.11	0.71
3:C:58:MET:HE1	3:C:105:ALA:O	1.90	0.71
1:A:46:VAL:HG23	1:A:270:ALA:C	2.10	0.71
1:A:239:SER:HB2	2:B:312:HIS:CB	2.19	0.71
2:B:266:LEU:O	2:B:270:VAL:HG23	1.91	0.71
2:B:438:LEU:HA	2:B:441:TYR:HB3	1.71	0.71
3:C:52:LEU:HD23	3:C:128:SER:OG	1.90	0.71
3:C:90:PRO:HD2	3:C:120:TRP:HZ3	1.55	0.71
3:C:318:SER:HB2	3:C:447:ASN:ND2	2.05	0.71
1:D:7:LEU:O	1:D:11:LEU:HG	1.91	0.71
1:A:52:THR:O	1:A:123:ILE:HA	1.90	0.71
2:B:109:LEU:HB3	2:B:117:SER:HB2	1.71	0.71
3:C:79:ILE:HG23	3:C:111:LEU:HD11	1.70	0.71
1:D:37:LEU:HD11	1:D:52:THR:OG1	1.90	0.71
1:D:391:GLU:HA	1:D:394:ASN:OD1	1.90	0.71
4:E:82:GLU:C	4:E:83:LEU:HD22	2.11	0.71
4:E:214:ILE:C	4:E:214:ILE:HD12	2.10	0.71
4:E:240:TYR:CG	4:E:453:ILE:HD13	2.26	0.71
2:B:141:ASN:ND2	2:B:212:ILE:HG12	2.06	0.70
3:C:36:SER:HB3	3:C:59:ASP:HB3	1.71	0.70
3:C:463:PRO:O	3:C:467:LEU:HD23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:132:THR:C	4:E:135:PRO:HD3	2.11	0.70
2:B:11:LEU:H	2:B:11:LEU:CD2	2.04	0.70
2:B:287:ILE:HA	2:B:290:LEU:CD1	2.21	0.70
3:C:443:VAL:HA	3:C:446:TRP:HD1	1.50	0.70
1:D:160:PRO:CG	1:D:185:LYS:HB3	2.21	0.70
4:E:28:ILE:HG21	4:E:85:TRP:HZ3	1.56	0.70
3:C:60:HIS:HB3	3:C:62:TRP:CZ3	2.18	0.70
3:C:138:PRO:CG	3:C:288:ILE:CD1	2.70	0.70
3:C:452:THR:HA	3:C:455:ARG:HD3	1.72	0.70
1:D:80:LEU:O	1:D:108:LEU:HB3	1.91	0.70
1:D:129:GLU:OE1	1:D:129:GLU:CA	2.25	0.70
1:A:166:ASP:HB3	1:A:178:MET:HE1	1.73	0.70
1:A:167:LEU:HD12	1:A:178:MET:HB2	1.72	0.70
2:B:224:THR:O	2:B:227:PRO:HD2	1.90	0.70
3:C:137:PHE:CZ	3:C:291:TYR:CD2	2.79	0.70
3:C:269:VAL:HG13	3:C:270:PHE:CE1	2.27	0.70
1:D:146:LEU:HD13	1:D:203:TYR:CE1	2.27	0.70
1:A:72:TYR:CD1	1:A:72:TYR:C	2.63	0.70
1:A:245:LEU:HD13	2:B:250:SER:CB	2.21	0.70
2:B:287:ILE:CA	2:B:290:LEU:HD12	2.22	0.70
3:C:38:THR:HG22	3:C:57:TRP:CE3	2.25	0.70
4:E:6:LEU:HD11	4:E:69:SER:HB3	1.73	0.70
2:B:220:TYR:HB3	2:B:223:TYR:CE2	2.26	0.70
2:B:265:LEU:O	2:B:268:ASP:HB2	1.92	0.70
3:C:80:LEU:CD1	1:D:20:ARG:HH22	2.04	0.70
3:C:431:LYS:HE2	1:D:379:VAL:HG13	1.72	0.70
1:D:290:ILE:O	1:D:293:VAL:HB	1.90	0.70
4:E:172:ILE:CD1	4:E:187:HIS:HA	2.22	0.70
1:A:201:ILE:HG21	1:A:203:TYR:HE1	1.55	0.70
2:B:55:PHE:N	2:B:55:PHE:CD1	2.60	0.70
2:B:176:ASN:HB2	2:B:191:LYS:CB	2.14	0.70
3:C:273:LEU:HD23	3:C:276:GLN:HG3	1.73	0.70
1:D:58:GLN:HE21	1:D:88:PRO:HG3	1.55	0.70
1:D:67:TRP:CD1	1:D:71:ASP:CB	2.75	0.70
1:D:178:MET:SD	1:D:207:MET:HB3	2.32	0.70
1:D:296:ILE:HA	1:D:299:HIS:CB	2.21	0.70
4:E:67:ASN:N	4:E:67:ASN:ND2	2.37	0.70
4:E:152:ALA:HA	4:E:155:VAL:O	1.91	0.70
1:A:41:ILE:HD11	1:A:51:GLU:CG	2.22	0.70
3:C:229:VAL:O	3:C:233:ILE:HG12	1.92	0.70
1:A:256:PHE:CZ	2:B:261:VAL:CG2	2.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:HD1	1:A:427:ALA:N	1.90	0.70
3:C:42:LEU:HD13	3:C:190:TRP:HZ2	1.56	0.70
3:C:223:ARG:HG2	3:C:224:LYS:N	2.05	0.70
1:D:76:LYS:HG2	1:D:112:TYR:CE2	2.27	0.70
1:D:145:LYS:HG3	1:D:202:THR:HG23	0.85	0.70
4:E:30:VAL:O	4:E:158:GLN:HG3	1.92	0.70
4:E:138:TRP:CZ3	4:E:215:GLN:HA	2.27	0.70
1:A:131:ILE:HD11	1:A:140:GLN:NE2	2.05	0.70
2:B:226:VAL:O	2:B:230:LEU:HG	1.91	0.70
3:C:33:ILE:HG12	3:C:62:TRP:HB3	1.72	0.70
3:C:153:TYR:HB2	3:C:158:ILE:HG13	1.74	0.70
4:E:22:LYS:HG3	4:E:23:THR:N	2.05	0.70
4:E:52:ASN:HD21	4:E:120:PRO:HB2	1.57	0.70
2:B:56:LEU:HG	2:B:103:THR:HG23	1.74	0.69
3:C:30:VAL:CG2	3:C:157:GLU:C	2.60	0.69
3:C:38:THR:HG21	3:C:57:TRP:CE3	2.27	0.69
3:C:230:ILE:HG13	3:C:231:ASN:N	2.07	0.69
1:D:20:ARG:CG	1:D:20:ARG:NH1	2.49	0.69
1:D:86:TRP:CD2	1:D:86:TRP:C	2.63	0.69
1:D:398:GLU:CA	1:D:401:TYR:CZ	2.72	0.69
3:C:257:MET:HE1	3:C:314:PHE:HA	1.74	0.69
3:C:319:THR:H	3:C:447:ASN:HB3	1.56	0.69
1:A:75:ILE:HG13	1:A:78:ILE:CG2	2.21	0.69
3:C:38:THR:OG1	3:C:178:ILE:HG21	1.92	0.69
3:C:437:ASN:O	3:C:441:GLU:HG3	1.92	0.69
1:D:107:LYS:CE	4:E:149:THR:HA	2.22	0.69
1:A:87:LEU:O	1:A:87:LEU:HD23	1.92	0.69
1:A:175:GLU:OE1	1:A:175:GLU:HA	1.92	0.69
1:A:229:THR:O	1:A:232:VAL:HB	1.93	0.69
1:A:261:VAL:O	1:A:261:VAL:CG1	2.40	0.69
1:D:132:VAL:HB	1:D:274:ILE:HA	1.73	0.69
2:B:56:LEU:CG	2:B:103:THR:HG23	2.22	0.69
2:B:92:LEU:H	2:B:96:ASN:CB	1.98	0.69
2:B:108:VAL:HG13	2:B:118:TRP:HB2	1.74	0.69
2:B:140:GLN:O	2:B:213:ILE:HD13	1.93	0.69
3:C:87:ILE:HG22	3:C:88:TRP:O	1.93	0.69
3:C:195:LYS:CE	3:C:217:PHE:HB3	2.22	0.69
3:C:234:THR:O	3:C:238:LEU:HD13	1.93	0.69
3:C:241:PHE:CD1	3:C:241:PHE:C	2.65	0.69
1:D:26:THR:CG2	1:D:27:HIS:H	2.05	0.69
4:E:129:ILE:CG2	4:E:133:TYR:HD2	2.02	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PHE:HA	1:A:417:ILE:HD12	1.74	0.69
3:C:162:LEU:HG	3:C:217:PHE:HZ	1.57	0.69
1:D:243:MET:H	1:D:243:MET:HE2	1.58	0.69
3:C:25:LYS:HB3	3:C:28:ASN:HD21	1.57	0.69
4:E:252:THR:O	4:E:252:THR:OG1	2.06	0.69
1:A:43:VAL:HG13	1:A:50:VAL:CG2	2.23	0.69
1:A:286:ILE:O	1:A:289:ILE:HB	1.93	0.69
2:B:46:LYS:HA	2:B:278:PRO:HD2	1.73	0.69
2:B:142:CYS:CB	2:B:211:LEU:HD12	2.23	0.69
2:B:186:TRP:CE3	2:B:215:ARG:CZ	2.75	0.69
2:B:269:LYS:HE3	2:B:270:VAL:HG23	1.69	0.69
3:C:247:PHE:HA	3:C:250:PRO:HG3	1.73	0.69
3:C:279:PRO:C	3:C:282:ALA:HB3	2.13	0.69
3:C:435:GLU:O	3:C:438:ALA:HB3	1.92	0.69
1:D:92:LEU:HD13	1:D:146:LEU:CG	2.23	0.69
1:D:238:ASP:CB	4:E:308:LEU:CD2	2.71	0.69
4:E:237:VAL:HG22	4:E:457:LEU:CD2	2.22	0.69
1:A:130:ILE:O	1:A:134:HIS:HB2	1.92	0.69
1:A:271:VAL:HG23	1:A:271:VAL:O	1.92	0.69
3:C:130:CYS:SG	3:C:146:LEU:HD11	2.33	0.69
3:C:279:PRO:O	3:C:282:ALA:HB3	1.92	0.69
2:B:59:ALA:HA	2:B:116:VAL:O	1.93	0.69
2:B:251:LEU:HD12	2:B:251:LEU:O	1.93	0.69
3:C:77:ILE:O	3:C:77:ILE:HG13	1.91	0.69
1:D:107:LYS:HZ1	4:E:149:THR:HA	1.56	0.69
4:E:55:ILE:C	4:E:118:LEU:HD13	2.13	0.69
4:E:228:PRO:O	4:E:231:LEU:HD23	1.92	0.69
1:A:247:ILE:O	1:A:247:ILE:CD1	2.41	0.68
2:B:28:LYS:HB3	2:B:155:GLU:C	2.12	0.68
3:C:201:ILE:HB	3:C:213:GLN:OE1	1.92	0.68
3:C:233:ILE:HD13	3:C:233:ILE:N	2.07	0.68
3:C:252:GLU:HG3	1:D:300:HIS:C	2.14	0.68
1:A:46:VAL:HG23	1:A:271:VAL:H	1.58	0.68
1:A:292:THR:O	1:A:296:ILE:HG12	1.93	0.68
2:B:152:ASP:HB3	2:B:203:SER:HB2	1.75	0.68
1:D:48:GLN:HB3	1:D:130:ILE:HD13	1.73	0.68
1:D:420:ILE:O	1:D:420:ILE:HG13	1.91	0.68
4:E:42:LEU:HD22	4:E:183:TRP:CE2	2.28	0.68
4:E:138:TRP:HH2	4:E:215:GLN:NE2	1.92	0.68
4:E:284:LYS:H	4:E:284:LYS:CD	2.05	0.68
2:B:46:LYS:HB2	2:B:277:VAL:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:LYS:HA	2:B:207:VAL:HG13	1.76	0.68
2:B:440:LEU:O	2:B:443:PHE:HB3	1.94	0.68
3:C:59:ASP:HA	3:C:121:LEU:CB	2.23	0.68
3:C:138:PRO:N	3:C:288:ILE:HD12	2.08	0.68
3:C:461:ILE:O	3:C:464:VAL:HG12	1.93	0.68
1:A:39:GLN:O	1:A:53:ASN:HB2	1.94	0.68
2:B:284:LEU:HD23	2:B:287:ILE:HD11	1.75	0.68
1:D:35:LEU:CD1	1:D:54:VAL:CG1	2.70	0.68
2:B:186:TRP:CB	2:B:215:ARG:HG3	2.21	0.68
2:B:236:ILE:O	2:B:240:TYR:HB2	1.94	0.68
1:D:171:MET:HG2	1:D:174:GLY:H	1.56	0.68
1:D:376:ILE:O	1:D:380:LYS:HG3	1.93	0.68
1:A:251:LEU:HD13	4:E:260:ALA:CB	2.24	0.68
1:A:270:ALA:O	1:A:271:VAL:HG13	1.92	0.68
1:A:292:THR:HA	1:A:296:ILE:HD11	1.73	0.68
3:C:2:ASN:O	3:C:3:GLU:HB3	1.92	0.68
3:C:81:ARG:CZ	3:C:111:LEU:HD13	2.24	0.68
1:D:282:MET:HG3	1:D:286:ILE:CD1	2.23	0.68
1:D:381:TYR:CE1	4:E:419:CYS:SG	2.80	0.68
1:D:390:GLU:O	1:D:393:SER:HB2	1.94	0.68
4:E:45:LYS:CA	4:E:280:PRO:HA	2.23	0.68
4:E:138:TRP:CH2	4:E:215:GLN:NE2	2.62	0.68
4:E:289:VAL:O	4:E:293:SER:HB3	1.94	0.68
2:B:40:LEU:HA	2:B:52:THR:HG23	1.74	0.68
3:C:299:VAL:O	3:C:302:VAL:HG23	1.93	0.68
1:D:130:ILE:O	1:D:134:HIS:HB2	1.94	0.68
1:D:233:PHE:CE2	1:D:295:VAL:HG11	2.29	0.68
1:D:287:SER:HA	1:D:290:ILE:HG12	1.75	0.68
4:E:172:ILE:CD1	4:E:188:ARG:HB3	2.24	0.68
1:A:37:LEU:HA	1:A:53:ASN:O	1.94	0.68
2:B:222:VAL:O	2:B:225:ILE:HB	1.94	0.68
2:B:269:LYS:C	2:B:271:PRO:HD2	2.14	0.68
1:D:60:TRP:CH2	1:D:86:TRP:HZ3	2.12	0.68
1:A:7:LEU:HD22	1:A:70:ALA:O	1.93	0.68
1:A:34:GLY:HA3	1:A:57:ARG:CD	2.24	0.68
2:B:129:THR:HG22	2:B:142:CYS:CA	2.22	0.68
2:B:147:LYS:HG3	2:B:148:SER:H	1.59	0.68
3:C:18:ASN:HB2	3:C:21:VAL:HB	1.76	0.68
3:C:276:GLN:C	3:C:279:PRO:HD2	2.14	0.68
3:C:460:ILE:O	3:C:463:PRO:HG2	1.94	0.68
1:D:271:VAL:O	1:D:271:VAL:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:34:LEU:HD12	4:E:210:PHE:HE2	1.56	0.68
4:E:44:GLU:HA	4:E:129:ILE:HD11	1.75	0.68
4:E:81:SER:HA	4:E:107:VAL:HG23	1.76	0.68
1:A:132:VAL:O	1:A:274:ILE:HG22	1.94	0.68
1:A:384:GLU:HA	1:A:387:LYS:CG	2.24	0.68
2:B:58:LEU:HD11	2:B:118:TRP:HE3	1.59	0.68
2:B:272:GLU:O	2:B:275:LEU:HB2	1.93	0.68
3:C:137:PHE:H	3:C:138:PRO:CD	2.06	0.68
3:C:434:LYS:HE3	1:D:386:MET:HE1	1.76	0.68
1:D:181:TYR:HE1	1:D:203:TYR:HB3	1.59	0.68
4:E:173:ASP:OD1	4:E:173:ASP:O	2.11	0.68
1:A:41:ILE:CD1	1:A:51:GLU:CD	2.62	0.67
1:A:54:VAL:HG23	1:A:122:ALA:HB3	1.74	0.67
1:A:75:ILE:HG13	1:A:78:ILE:HG21	1.75	0.67
2:B:143:THR:HG23	2:B:208:THR:HG23	1.75	0.67
2:B:218:LEU:HD11	2:B:222:VAL:HG22	1.75	0.67
2:B:226:VAL:CG2	2:B:227:PRO:HD3	2.22	0.67
3:C:30:VAL:HG22	3:C:157:GLU:HA	1.75	0.67
3:C:93:VAL:HG11	3:C:151:LEU:HB2	1.74	0.67
1:D:75:ILE:CG1	1:D:78:ILE:CG2	2.72	0.67
1:D:130:ILE:O	1:D:131:ILE:HG12	1.94	0.67
1:D:178:MET:HA	1:D:207:MET:CB	2.24	0.67
4:E:56:GLU:CA	4:E:118:LEU:HB2	2.17	0.67
1:A:7:LEU:HD22	1:A:70:ALA:C	2.14	0.67
1:A:166:ASP:HB2	1:A:181:TYR:CB	2.23	0.67
2:B:198:ARG:HH11	2:B:198:ARG:HG3	1.59	0.67
3:C:19:LYS:O	3:C:19:LYS:HD2	1.93	0.67
3:C:216:THR:O	3:C:217:PHE:HD1	1.78	0.67
3:C:318:SER:CB	3:C:447:ASN:ND2	2.57	0.67
1:D:214:PHE:O	1:D:218:VAL:HG23	1.93	0.67
1:A:34:GLY:HA3	1:A:57:ARG:HD3	1.76	0.67
2:B:10:VAL:CG1	2:B:11:LEU:CD2	2.72	0.67
2:B:223:TYR:O	2:B:223:TYR:CD1	2.47	0.67
2:B:308:SER:HB2	2:B:311:THR:CG2	2.05	0.67
3:C:14:VAL:HG13	3:C:86:LEU:HD23	1.76	0.67
1:D:145:LYS:O	1:D:146:LEU:HD12	1.93	0.67
1:D:283:ILE:HA	1:D:286:ILE:HD12	1.75	0.67
1:D:287:SER:O	1:D:291:VAL:HG23	1.94	0.67
4:E:134:PHE:CB	4:E:282:ILE:CG2	2.72	0.67
1:A:255:VAL:HA	1:A:258:LEU:HD12	1.76	0.67
2:B:55:PHE:N	2:B:55:PHE:HD1	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:CA	1:A:57:ARG:HG2	2.25	0.67
2:B:28:LYS:HG2	2:B:155:GLU:CA	2.16	0.67
2:B:142:CYS:HB3	2:B:211:LEU:CD1	2.23	0.67
1:D:75:ILE:CD1	1:D:78:ILE:CG2	2.72	0.67
4:E:191:LYS:H	4:E:209:ILE:HG23	1.59	0.67
1:A:235:LEU:HB3	1:A:236:PRO:CD	2.25	0.67
1:A:405:VAL:HG23	1:A:405:VAL:O	1.95	0.67
2:B:262:PHE:CZ	3:C:269:VAL:HB	2.29	0.67
3:C:19:LYS:O	3:C:19:LYS:CD	2.43	0.67
3:C:35:LEU:HD22	3:C:215:VAL:HG21	1.77	0.67
3:C:220:ILE:O	3:C:220:ILE:CG1	2.42	0.67
1:D:252:SER:O	1:D:255:VAL:HG12	1.95	0.67
1:D:393:SER:O	1:D:396:ALA:HB3	1.94	0.67
4:E:131:VAL:HA	4:E:281:LEU:O	1.95	0.67
1:A:66:ARG:O	1:A:66:ARG:CD	2.43	0.67
2:B:263:LEU:CD2	2:B:291:VAL:CG2	2.70	0.67
3:C:67:LEU:HB3	3:C:116:GLY:HA2	0.78	0.67
3:C:296:MET:HE3	3:C:296:MET:CA	2.24	0.67
1:A:124:PHE:CD1	1:A:124:PHE:C	2.67	0.67
1:A:224:LEU:HG	1:A:225:PHE:N	2.10	0.67
2:B:37:LEU:HD23	2:B:179:ALA:HB3	1.76	0.67
4:E:149:THR:HG23	4:E:150:TYR:N	2.08	0.67
1:A:37:LEU:HD23	1:A:54:VAL:HG12	1.75	0.67
1:A:41:ILE:HG12	1:A:51:GLU:O	1.94	0.67
1:A:104:HIS:HB2	1:A:105:MET:SD	2.35	0.67
1:A:380:LYS:O	1:A:384:GLU:HB2	1.94	0.67
2:B:139:TRP:HE3	2:B:468:PHE:CE1	2.11	0.67
2:B:223:TYR:O	2:B:223:TYR:HD1	1.77	0.67
3:C:69:TRP:NE1	3:C:114:PRO:HA	2.09	0.67
4:E:195:ASN:HB3	4:E:205:PHE:H	1.60	0.67
2:B:104:LEU:HA	2:B:118:TRP:CZ2	2.29	0.67
3:C:293:MET:O	3:C:297:SER:HB3	1.95	0.67
1:A:257:LEU:CD1	1:A:285:VAL:HG22	2.25	0.66
3:C:137:PHE:CZ	3:C:291:TYR:CE2	2.83	0.66
1:D:95:ASN:HD22	1:D:127:TYR:H	1.42	0.66
1:D:130:ILE:HG12	1:D:131:ILE:H	1.59	0.66
4:E:283:GLY:C	4:E:284:LYS:HE3	2.13	0.66
4:E:437:GLU:O	4:E:441:LEU:HG	1.95	0.66
2:B:216:LYS:HE3	2:B:216:LYS:H	1.59	0.66
3:C:138:PRO:HG3	3:C:290:LYS:HE2	1.77	0.66
3:C:270:PHE:HD1	3:C:270:PHE:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HA	1:A:224:LEU:HB3	1.77	0.66
2:B:92:LEU:HA	2:B:145:VAL:O	1.95	0.66
3:C:273:LEU:HA	3:C:276:GLN:CG	2.20	0.66
1:D:77:LYS:HB2	1:D:111:ASP:OD1	1.95	0.66
1:D:92:LEU:CD2	1:D:92:LEU:N	2.57	0.66
1:D:102:ILE:HD12	4:E:98:GLN:HE22	1.60	0.66
1:D:130:ILE:HG22	1:D:134:HIS:CD2	2.31	0.66
1:D:137:PHE:CD2	1:D:431:ILE:HG21	2.26	0.66
4:E:59:TRP:CZ2	4:E:115:MET:HB3	2.30	0.66
1:A:380:LYS:HD3	2:B:408:ILE:CG2	2.25	0.66
3:C:30:VAL:CG2	3:C:157:GLU:N	2.59	0.66
1:D:250:LEU:HD22	1:D:292:THR:HB	1.75	0.66
1:A:35:LEU:HD23	1:A:35:LEU:C	2.15	0.66
1:A:187:TRP:CH2	1:A:189:TYR:HB3	2.31	0.66
1:A:216:VAL:HG13	1:A:220:ILE:CD1	2.26	0.66
1:A:243:MET:HG2	1:A:244:THR:H	1.59	0.66
1:A:380:LYS:CD	2:B:408:ILE:HB	2.26	0.66
2:B:118:TRP:CD1	2:B:120:PRO:HD3	2.30	0.66
3:C:266:ALA:HB1	3:C:270:PHE:CZ	2.30	0.66
3:C:270:PHE:CD1	3:C:270:PHE:N	2.62	0.66
4:E:55:ILE:HG23	4:E:119:PRO:CD	2.25	0.66
4:E:282:ILE:CG2	4:E:282:ILE:O	2.43	0.66
1:A:52:THR:C	1:A:123:ILE:HG13	2.15	0.66
1:A:107:LYS:O	1:A:108:LEU:HD23	1.96	0.66
1:A:145:LYS:NZ	1:A:202:THR:CG2	2.58	0.66
1:A:175:GLU:HB3	1:A:211:PRO:HD3	1.77	0.66
1:A:376:ILE:HG23	1:A:380:LYS:NZ	2.10	0.66
2:B:285:MET:O	2:B:289:ILE:HG12	1.96	0.66
3:C:35:LEU:HD12	3:C:60:HIS:NE2	2.10	0.66
4:E:134:PHE:HB3	4:E:282:ILE:CB	2.26	0.66
2:B:405:VAL:HG12	2:B:409:LYS:HZ3	1.58	0.66
3:C:60:HIS:NE2	3:C:92:ILE:HG21	2.10	0.66
3:C:259:THR:O	3:C:263:VAL:HG23	1.94	0.66
3:C:316:THR:CG2	3:C:447:ASN:HB3	2.25	0.66
4:E:146:ARG:HD2	4:E:206:GLN:O	1.95	0.66
1:A:227:PHE:HA	1:A:230:VAL:HB	1.78	0.66
1:A:238:ASP:CB	2:B:306:HIS:CE1	2.78	0.66
2:B:40:LEU:HD13	2:B:41:LEU:N	2.10	0.66
2:B:40:LEU:HD22	2:B:51:THR:O	1.96	0.66
2:B:136:PRO:HD3	2:B:280:ILE:CD1	2.26	0.66
2:B:185:GLN:HB2	2:B:217:PRO:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:HG12	1:D:60:TRP:NE1	2.10	0.66
1:D:106:THR:HG23	1:D:107:LYS:HD3	1.78	0.66
1:D:220:ILE:HG21	4:E:294:LEU:CD1	2.26	0.66
1:D:292:THR:HA	1:D:295:VAL:HG22	1.77	0.66
1:D:410:LEU:O	1:D:414:PHE:HB2	1.95	0.66
1:A:171:MET:HG2	1:A:174:GLY:H	1.59	0.66
1:A:235:LEU:HB3	1:A:236:PRO:HD3	1.77	0.66
2:B:4:GLU:OE1	2:B:8:LEU:HG	1.96	0.66
2:B:128:CYS:SG	2:B:144:MET:HG2	2.36	0.66
2:B:236:ILE:HB	2:B:446:MET:HE1	1.76	0.66
3:C:26:HIS:CE1	3:C:66:ARG:HH22	2.13	0.66
3:C:35:LEU:HD21	3:C:37:LEU:CD2	2.26	0.66
3:C:90:PRO:HD2	3:C:120:TRP:CZ3	2.30	0.66
4:E:237:VAL:HG21	4:E:457:LEU:HD21	1.77	0.66
1:A:139:GLN:HB2	1:A:207:MET:C	2.16	0.66
1:A:216:VAL:CG1	1:A:220:ILE:CD1	2.74	0.66
2:B:47:ASN:HB2	2:B:49:GLU:CD	2.16	0.66
2:B:403:GLU:OE1	2:B:403:GLU:HA	1.95	0.66
3:C:434:LYS:CD	3:C:435:GLU:HG3	2.19	0.66
1:D:67:TRP:CD1	1:D:71:ASP:CG	2.69	0.66
1:D:92:LEU:HB2	1:D:95:ASN:HB2	1.78	0.66
1:D:106:THR:CG2	1:D:107:LYS:H	2.09	0.66
1:D:296:ILE:HA	1:D:299:HIS:HB2	1.78	0.66
4:E:303:VAL:HG12	4:E:304:LEU:N	2.10	0.66
1:A:158:ILE:O	1:A:199:LEU:HB2	1.94	0.65
2:B:65:LEU:CD2	2:B:110:VAL:HG11	2.25	0.65
3:C:68:THR:HA	3:C:115:ASN:HA	1.78	0.65
3:C:191:GLU:CG	3:C:222:ARG:HB3	2.26	0.65
1:D:302:SER:CB	1:D:305:THR:CG2	2.75	0.65
4:E:267:LEU:HA	4:E:270:GLN:CG	2.26	0.65
1:A:34:GLY:HA3	1:A:57:ARG:HG2	1.78	0.65
1:A:36:GLN:C	1:A:36:GLN:OE1	2.33	0.65
1:A:107:LYS:HG2	2:B:150:THR:HG21	1.77	0.65
1:A:243:MET:HG2	1:A:244:THR:N	2.11	0.65
2:B:264:LEU:O	2:B:267:ALA:HB3	1.97	0.65
2:B:408:ILE:CG2	2:B:409:LYS:N	2.58	0.65
3:C:67:LEU:CG	3:C:116:GLY:HA2	2.25	0.65
3:C:93:VAL:CG1	3:C:151:LEU:HB2	2.26	0.65
3:C:179:ILE:HG23	3:C:181:PRO:CD	2.26	0.65
3:C:247:PHE:C	3:C:250:PRO:HD3	2.15	0.65
3:C:432:GLN:O	3:C:436:LYS:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD22	1:D:203:TYR:CZ	2.31	0.65
4:E:32:LEU:HD12	4:E:208:ILE:HD11	1.78	0.65
2:B:130:ILE:HD12	2:B:134:TYR:HE2	1.59	0.65
3:C:282:ALA:CB	3:C:287:LEU:CD1	2.74	0.65
1:D:284:PHE:O	1:D:287:SER:HB3	1.96	0.65
4:E:128:PRO:C	4:E:129:ILE:HG23	2.17	0.65
1:A:156:VAL:CG2	1:A:157:SER:N	2.58	0.65
1:A:378:GLY:O	1:A:382:ILE:HG12	1.97	0.65
2:B:132:VAL:O	2:B:279:ILE:HG23	1.96	0.65
3:C:210:THR:HG22	3:C:211:ASN:N	2.11	0.65
3:C:256:LYS:HB2	3:C:259:THR:HG22	1.79	0.65
1:D:106:THR:HG23	1:D:107:LYS:CD	2.27	0.65
4:E:184:THR:HG23	4:E:215:GLN:CG	2.25	0.65
1:A:146:LEU:HD12	1:A:146:LEU:N	2.11	0.65
1:A:155:LYS:HG3	4:E:78:ARG:NE	2.11	0.65
2:B:35:LEU:HD13	2:B:56:LEU:HD22	1.78	0.65
2:B:153:THR:O	2:B:204:TYR:HD2	1.79	0.65
3:C:102:TYR:HD1	3:C:102:TYR:O	1.78	0.65
3:C:107:PHE:O	3:C:107:PHE:CG	2.50	0.65
1:D:36:GLN:HE21	1:D:38:ILE:HG13	1.62	0.65
1:D:76:LYS:HG2	1:D:112:TYR:CD2	2.31	0.65
1:D:149:TRP:CE2	1:D:150:THR:HB	2.31	0.65
1:A:46:VAL:CG2	1:A:270:ALA:HA	2.23	0.65
2:B:46:LYS:CG	2:B:278:PRO:HD2	2.25	0.65
2:B:145:VAL:CG1	2:B:206:ASP:HB2	2.25	0.65
1:D:187:TRP:CH2	1:D:189:TYR:CD1	2.84	0.65
4:E:32:LEU:HD12	4:E:157:LEU:HD13	1.77	0.65
4:E:146:ARG:HD2	4:E:205:PHE:CD2	2.31	0.65
1:A:108:LEU:CD1	1:A:118:TRP:HB2	2.26	0.65
1:A:235:LEU:N	1:A:236:PRO:HD2	2.11	0.65
3:C:252:GLU:OE2	1:D:301:ARG:HA	1.96	0.65
1:D:187:TRP:CE2	1:D:196:THR:HG23	2.32	0.65
4:E:55:ILE:N	4:E:118:LEU:HD13	2.12	0.65
4:E:132:THR:O	4:E:282:ILE:HD12	1.97	0.65
1:A:45:GLU:HB3	1:A:271:VAL:HA	1.77	0.65
1:A:160:PRO:CG	1:A:185:LYS:CE	2.74	0.65
2:B:35:LEU:HD23	2:B:35:LEU:N	2.10	0.65
1:A:156:VAL:CG2	1:A:157:SER:H	2.10	0.65
1:A:166:ASP:CB	1:A:181:TYR:HB3	2.27	0.65
4:E:49:LEU:O	4:E:124:ARG:HD2	1.97	0.65
4:E:103:TYR:C	4:E:104:TYR:CD1	2.70	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:HIS:CB	1:A:7:LEU:HD23	2.26	0.65
1:A:417:ILE:HA	1:A:420:ILE:HG12	1.79	0.65
2:B:15:TYR:O	2:B:15:TYR:CD1	2.50	0.65
2:B:130:ILE:CB	2:B:134:TYR:CE2	2.79	0.65
3:C:48:THR:HB	3:C:285:VAL:N	2.12	0.65
3:C:462:THR:HB	3:C:463:PRO:CD	2.26	0.65
1:D:36:GLN:CB	1:D:55:ARG:HG3	2.26	0.65
4:E:159:LEU:CD2	4:E:208:ILE:HG23	2.27	0.65
1:A:170:PHE:HE1	1:A:176:TRP:NE1	1.95	0.64
2:B:15:TYR:O	2:B:15:TYR:HD1	1.80	0.64
1:D:87:LEU:HD22	1:D:118:TRP:CH2	2.33	0.64
1:D:132:VAL:O	1:D:274:ILE:HG23	1.97	0.64
4:E:178:THR:HG22	4:E:180:ASN:H	1.62	0.64
1:A:29:VAL:HB	1:A:31:ILE:HD12	1.80	0.64
2:B:223:TYR:O	2:B:227:PRO:HD3	1.97	0.64
2:B:409:LYS:HZ3	3:C:423:ILE:HG23	1.60	0.64
3:C:110:VAL:HG13	3:C:120:TRP:CB	2.26	0.64
3:C:135:LEU:C	3:C:138:PRO:HD2	2.17	0.64
1:D:112:TYR:N	1:D:112:TYR:CD1	2.65	0.64
4:E:134:PHE:CB	4:E:282:ILE:HG21	2.21	0.64
4:E:159:LEU:HD12	4:E:192:LYS:HA	1.79	0.64
4:E:213:ILE:HG23	4:E:213:ILE:O	1.98	0.64
1:A:31:ILE:CG1	1:A:60:TRP:HB3	2.27	0.64
2:B:91:VAL:HG23	2:B:96:ASN:CB	2.27	0.64
2:B:287:ILE:HA	2:B:290:LEU:HB2	1.79	0.64
3:C:59:ASP:OD1	3:C:121:LEU:HD13	1.97	0.64
3:C:80:LEU:CD1	1:D:20:ARG:NH2	2.60	0.64
1:D:274:ILE:HG22	1:D:276:LYS:NZ	2.12	0.64
4:E:237:VAL:HG22	4:E:457:LEU:HD21	1.78	0.64
4:E:444:LYS:CE	4:E:444:LYS:HA	2.27	0.64
1:A:48:GLN:HB2	1:A:128:CYS:O	1.96	0.64
1:A:209:ARG:HG3	1:A:210:ILE:N	2.08	0.64
2:B:11:LEU:HD22	2:B:11:LEU:H	1.62	0.64
2:B:218:LEU:HD13	2:B:221:ILE:HG13	1.77	0.64
2:B:277:VAL:H	2:B:278:PRO:CD	2.10	0.64
3:C:42:LEU:CD2	3:C:190:TRP:CH2	2.77	0.64
3:C:242:LEU:CD2	3:C:267:GLN:HG2	2.27	0.64
3:C:315:ARG:H	3:C:315:ARG:CD	2.11	0.64
1:D:129:GLU:C	1:D:130:ILE:HG23	2.17	0.64
1:D:376:ILE:C	1:D:380:LYS:HE2	2.18	0.64
4:E:33:LYS:CG	4:E:160:SER:HB3	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:LEU:CD1	4:E:49:LEU:HD13	2.26	0.64
2:B:133:MET:HG2	2:B:140:GLN:CG	2.08	0.64
2:B:186:TRP:CB	2:B:215:ARG:CG	2.74	0.64
3:C:63:TYR:CE1	3:C:116:GLY:HA3	2.33	0.64
3:C:142:GLN:CG	3:C:143:ASN:H	1.87	0.64
1:D:36:GLN:NE2	1:D:38:ILE:HG13	2.12	0.64
1:D:46:VAL:HB	1:D:270:ALA:C	2.17	0.64
1:A:36:GLN:HA	1:A:164:ARG:NH2	2.12	0.64
1:A:67:TRP:CG	1:A:71:ASP:HB3	2.32	0.64
2:B:307:ARG:O	2:B:307:ARG:HG2	1.97	0.64
1:D:3:HIS:HB3	1:D:7:LEU:CG	2.27	0.64
1:D:37:LEU:CB	1:D:54:VAL:HG13	2.27	0.64
1:D:187:TRP:CZ2	1:D:196:THR:HA	2.30	0.64
4:E:56:GLU:CA	4:E:118:LEU:HD22	2.28	0.64
4:E:240:TYR:HB3	4:E:453:ILE:CD1	2.28	0.64
3:C:319:THR:CG2	3:C:320:HIS:N	2.60	0.64
1:D:135:PHE:HE1	1:D:277:TYR:CE2	2.16	0.64
1:D:141:ASN:HB3	1:D:206:ILE:HG12	1.79	0.64
1:D:233:PHE:CE2	1:D:413:VAL:HG11	2.32	0.64
4:E:38:ASN:O	4:E:51:THR:HA	1.97	0.64
4:E:212:LEU:HD12	4:E:212:LEU:N	2.13	0.64
2:B:153:THR:HG23	2:B:156:VAL:O	1.97	0.64
3:C:247:PHE:C	3:C:250:PRO:CD	2.66	0.64
1:D:233:PHE:HE2	1:D:295:VAL:HG11	1.63	0.64
1:D:244:THR:HG23	1:D:245:LEU:H	1.62	0.64
1:D:254:THR:HG23	1:D:255:VAL:N	2.12	0.64
1:D:302:SER:HB3	1:D:305:THR:CG2	2.28	0.64
2:B:11:LEU:HD22	2:B:11:LEU:N	2.12	0.64
2:B:40:LEU:HD13	2:B:40:LEU:C	2.18	0.64
2:B:283:TYR:HD1	2:B:283:TYR:H	1.46	0.64
3:C:241:PHE:HD1	3:C:245:LEU:HD22	1.63	0.64
3:C:252:GLU:HG3	1:D:300:HIS:HB3	1.78	0.64
1:D:72:TYR:CD1	1:D:73:GLY:N	2.66	0.64
4:E:159:LEU:HD12	4:E:192:LYS:N	2.12	0.64
4:E:184:THR:O	4:E:214:ILE:HB	1.98	0.64
1:A:104:HIS:C	1:A:105:MET:SD	2.77	0.64
1:A:166:ASP:CB	1:A:178:MET:CE	2.75	0.64
3:C:137:PHE:CD1	3:C:288:ILE:CG2	2.81	0.64
3:C:199:LYS:HD2	3:C:200:ASN:N	2.13	0.64
3:C:257:MET:O	3:C:261:ILE:HG12	1.98	0.64
1:D:30:ASP:O	1:D:60:TRP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:MET:SD	1:D:207:MET:CB	2.86	0.64
4:E:32:LEU:CD1	4:E:157:LEU:HD13	2.26	0.64
4:E:94:ASN:HB3	4:E:125:SER:CB	2.22	0.64
1:A:139:GLN:OE1	1:A:179:LYS:HG3	1.98	0.63
2:B:69:PRO:O	2:B:73:GLU:HB2	1.98	0.63
2:B:134:TYR:HE1	2:B:213:ILE:HG13	1.56	0.63
3:C:1:VAL:O	3:C:1:VAL:HG12	1.96	0.63
3:C:17:TYR:HE2	3:C:19:LYS:HB2	1.58	0.63
3:C:475:MET:HG2	3:C:476:GLY:N	2.12	0.63
4:E:2:GLU:HA	4:E:5:ARG:HG3	1.78	0.63
4:E:313:THR:OG1	4:E:441:LEU:HB3	1.98	0.63
1:A:67:TRP:CD1	1:A:71:ASP:CG	2.71	0.63
1:A:90:LEU:HD13	1:A:100:PHE:HE2	1.62	0.63
1:A:166:ASP:HB3	1:A:178:MET:HE2	1.80	0.63
2:B:218:LEU:HA	2:B:221:ILE:HD11	1.80	0.63
3:C:160:MET:H	3:C:213:GLN:CB	2.10	0.63
3:C:248:TYR:C	3:C:250:PRO:CD	2.66	0.63
1:D:135:PHE:CZ	1:D:273:LEU:HB2	2.33	0.63
1:D:236:PRO:HB3	1:D:299:HIS:CE1	2.33	0.63
1:D:247:ILE:HG22	1:D:248:SER:N	2.13	0.63
1:D:384:GLU:OE1	1:D:384:GLU:HA	1.98	0.63
1:A:176:TRP:HB2	1:A:209:ARG:HD2	1.77	0.63
2:B:147:LYS:CG	2:B:148:SER:N	2.61	0.63
2:B:286:PHE:CE1	2:B:287:ILE:HG23	2.32	0.63
4:E:209:ILE:HG12	4:E:211:PHE:CE1	2.32	0.63
1:A:175:GLU:O	1:A:211:PRO:HB3	1.98	0.63
1:A:279:LEU:CA	1:A:282:MET:HB2	2.21	0.63
2:B:429:GLN:HA	2:B:429:GLN:HE21	1.63	0.63
2:B:434:VAL:CG1	2:B:438:LEU:HD12	2.28	0.63
3:C:262:CYS:SG	1:D:251:LEU:HD11	2.39	0.63
3:C:282:ALA:CB	3:C:287:LEU:HD12	2.29	0.63
3:C:295:ILE:O	3:C:299:VAL:HG23	1.99	0.63
1:D:377:GLU:HB2	4:E:415:CYS:SG	2.39	0.63
4:E:89:VAL:O	4:E:90:VAL:HG23	1.98	0.63
4:E:219:LEU:HB3	4:E:222:ILE:CG2	2.28	0.63
4:E:250:LYS:HD2	4:E:253:LEU:HD22	1.78	0.63
1:A:93:TYR:N	1:A:93:TYR:CD1	2.63	0.63
2:B:48:GLU:HA	2:B:130:ILE:CD1	2.22	0.63
3:C:247:PHE:CD2	3:C:460:ILE:CG1	2.81	0.63
3:C:282:ALA:HB1	3:C:287:LEU:HD12	1.80	0.63
1:D:107:LYS:HE3	4:E:149:THR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:382:ILE:O	1:D:386:MET:HG2	1.98	0.63
4:E:44:GLU:HG3	4:E:129:ILE:HG13	1.81	0.63
1:A:97:ASP:HB2	1:A:127:TYR:HB2	1.78	0.63
3:C:65:HIS:H	3:C:65:HIS:HD2	1.44	0.63
3:C:102:TYR:HE1	3:C:106:TYR:HB3	1.64	0.63
1:D:170:PHE:CD2	1:D:178:MET:HG2	2.32	0.63
4:E:88:ASP:O	4:E:147:SER:HA	1.99	0.63
4:E:303:VAL:CG1	4:E:304:LEU:N	2.61	0.63
4:E:305:ASN:HA	4:E:308:LEU:CD1	2.27	0.63
1:A:35:LEU:HD23	1:A:36:GLN:N	2.12	0.63
1:A:157:SER:HB2	1:A:199:LEU:CD1	2.28	0.63
3:C:37:LEU:HD12	3:C:217:PHE:CE2	2.33	0.63
1:D:92:LEU:HB3	1:D:95:ASN:HB2	1.80	0.63
4:E:6:LEU:HD12	4:E:69:SER:OG	1.98	0.63
4:E:31:THR:CB	4:E:58:GLN:HB2	2.28	0.63
4:E:33:LYS:CE	4:E:160:SER:CB	2.77	0.63
4:E:50:THR:HA	4:E:123:TYR:O	1.97	0.63
4:E:276:SER:HB3	4:E:281:LEU:HD13	1.81	0.63
1:A:34:GLY:HA3	1:A:57:ARG:CG	2.29	0.63
1:A:111:ASP:OD1	1:A:111:ASP:N	2.32	0.63
1:A:129:GLU:OE2	1:A:140:GLN:HG3	1.98	0.63
1:A:171:MET:HG2	1:A:174:GLY:N	2.13	0.63
2:B:147:LYS:CG	2:B:148:SER:H	2.12	0.63
2:B:220:TYR:HE2	3:C:279:PRO:HB2	1.63	0.63
3:C:162:LEU:HG	3:C:217:PHE:CZ	2.34	0.63
3:C:242:LEU:HD21	3:C:263:VAL:CG1	2.27	0.63
3:C:306:CYS:O	3:C:309:VAL:HB	1.98	0.63
3:C:429:ILE:HG13	3:C:430:VAL:N	2.13	0.63
4:E:31:THR:HA	4:E:158:GLN:HG3	1.81	0.63
4:E:140:ASN:OD1	4:E:211:PHE:HB3	1.99	0.63
1:A:92:LEU:CB	1:A:95:ASN:HB2	2.29	0.63
2:B:58:LEU:CD1	2:B:118:TRP:HB3	2.28	0.63
1:D:92:LEU:HD21	1:D:124:PHE:CZ	2.34	0.63
4:E:240:TYR:HB3	4:E:453:ILE:HD11	1.81	0.63
4:E:291:PHE:O	4:E:295:VAL:HG23	1.99	0.63
1:A:35:LEU:HD13	1:A:203:TYR:OH	1.99	0.62
1:A:108:LEU:HB3	1:A:117:MET:O	1.99	0.62
1:A:388:SER:HA	1:A:391:GLU:HB3	1.81	0.62
2:B:111:GLN:CD	2:B:115:ALA:HB3	2.19	0.62
2:B:136:PRO:HD3	2:B:280:ILE:HD11	1.80	0.62
2:B:175:ILE:CG1	2:B:176:ASN:H	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:MET:O	3:C:58:MET:HG2	1.99	0.62
1:D:77:LYS:O	1:D:77:LYS:CG	2.45	0.62
4:E:195:ASN:HB3	4:E:205:PHE:N	2.13	0.62
1:A:133:THR:O	1:A:133:THR:CG2	2.47	0.62
3:C:106:TYR:C	3:C:107:PHE:CD1	2.70	0.62
1:D:242:LYS:HD2	1:D:245:LEU:HD13	1.79	0.62
1:D:260:ILE:HA	1:D:263:LEU:HD12	1.80	0.62
1:D:395:ALA:HB1	1:D:399:TRP:CE2	2.34	0.62
4:E:140:ASN:HD21	4:E:211:PHE:CA	2.12	0.62
4:E:187:HIS:ND1	4:E:189:PRO:HG3	2.13	0.62
4:E:200:LYS:O	4:E:200:LYS:HG3	2.00	0.62
1:A:43:VAL:HG22	1:A:50:VAL:CG1	2.29	0.62
1:A:401:TYR:CD1	1:A:401:TYR:O	2.52	0.62
1:A:419:ILE:CG2	1:A:420:ILE:N	2.58	0.62
3:C:257:MET:CE	3:C:314:PHE:CB	2.78	0.62
3:C:291:TYR:N	3:C:291:TYR:HD1	1.96	0.62
1:D:37:LEU:CD1	1:D:54:VAL:HG13	2.28	0.62
1:D:229:THR:HG22	1:D:253:LEU:CD1	2.29	0.62
1:D:305:THR:HG22	1:D:400:LYS:HG2	1.81	0.62
4:E:66:TRP:HB2	4:E:71:TYR:N	2.10	0.62
4:E:189:PRO:HB2	4:E:211:PHE:CD2	2.35	0.62
2:B:201:ASP:OD1	2:B:202:PRO:HD2	1.99	0.62
1:D:7:LEU:HA	1:D:10:ASN:ND2	2.14	0.62
1:D:187:TRP:HB2	1:D:199:LEU:HD21	1.81	0.62
1:D:187:TRP:CB	1:D:199:LEU:HD23	2.23	0.62
1:D:377:GLU:HG3	4:E:415:CYS:HB2	1.80	0.62
4:E:34:LEU:HB2	4:E:210:PHE:HZ	1.65	0.62
4:E:45:LYS:HZ3	4:E:278:ASN:HA	1.62	0.62
4:E:146:ARG:NH1	4:E:205:PHE:CB	2.61	0.62
1:A:133:THR:C	1:A:136:PRO:HG2	2.20	0.62
1:A:265:PRO:CA	1:A:268:SER:HB3	2.28	0.62
2:B:58:LEU:HD11	2:B:118:TRP:HB3	1.82	0.62
2:B:130:ILE:CB	2:B:134:TYR:CD2	2.63	0.62
3:C:16:LYS:HA	3:C:16:LYS:CE	2.30	0.62
3:C:160:MET:H	3:C:213:GLN:CG	2.10	0.62
3:C:199:LYS:NZ	3:C:199:LYS:O	2.33	0.62
3:C:221:ILE:HG13	3:C:222:ARG:N	2.13	0.62
3:C:431:LYS:CE	1:D:379:VAL:CG2	2.77	0.62
1:D:167:LEU:CD1	1:D:167:LEU:H	2.10	0.62
1:D:301:ARG:HH22	1:D:406:ILE:HD13	1.65	0.62
4:E:238:LEU:C	4:E:242:LEU:HD23	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD12	1:A:100:PHE:HE2	1.65	0.62
1:A:207:MET:O	1:A:207:MET:HE3	1.98	0.62
1:A:236:PRO:CB	1:A:299:HIS:CE1	2.77	0.62
1:A:306:HIS:C	1:A:306:HIS:CD2	2.73	0.62
2:B:251:LEU:HD13	3:C:261:ILE:HG21	1.81	0.62
3:C:455:ARG:H	3:C:455:ARG:HD2	1.63	0.62
1:D:177:VAL:O	1:D:207:MET:HB2	2.00	0.62
4:E:1:ASN:O	4:E:69:SER:HB2	1.98	0.62
4:E:76:LEU:CD2	4:E:77:VAL:N	2.63	0.62
1:A:218:VAL:O	1:A:221:PRO:HD2	1.99	0.62
2:B:129:THR:HG22	2:B:142:CYS:CB	2.30	0.62
2:B:430:TYR:O	2:B:430:TYR:HD1	1.82	0.62
3:C:56:VAL:CG2	3:C:124:ALA:HB3	2.29	0.62
3:C:146:LEU:HD12	3:C:146:LEU:N	2.14	0.62
3:C:147:LYS:HE2	3:C:216:THR:HG23	1.82	0.62
1:D:67:TRP:CD1	1:D:71:ASP:HB3	2.34	0.62
1:D:167:LEU:CD1	1:D:178:MET:CB	2.77	0.62
4:E:27:VAL:HG12	4:E:154:GLU:CA	2.27	0.62
4:E:313:THR:HB	4:E:440:VAL:CG1	2.24	0.62
3:C:42:LEU:HA	3:C:54:THR:CG2	2.29	0.62
3:C:67:LEU:HD12	3:C:116:GLY:O	2.00	0.62
3:C:138:PRO:CB	3:C:290:LYS:CE	2.71	0.62
1:D:86:TRP:O	1:D:86:TRP:CD1	2.49	0.62
4:E:66:TRP:CE3	4:E:70:GLU:HB3	2.34	0.62
4:E:244:ALA:HB2	4:E:446:ILE:HG22	1.79	0.62
1:A:79:ARG:HH11	1:A:107:LYS:NZ	1.96	0.62
1:A:110:LEU:HD12	1:A:111:ASP:N	2.14	0.62
3:C:155:ALA:H	3:C:211:ASN:HB3	1.65	0.62
1:D:63:VAL:HG13	1:D:64:ARG:N	2.14	0.62
1:D:249:VAL:O	1:D:253:LEU:HB3	1.99	0.62
4:E:191:LYS:NZ	4:E:211:PHE:CZ	2.66	0.62
1:A:249:VAL:HG13	1:A:253:LEU:HD23	1.81	0.62
2:B:152:ASP:CB	2:B:203:SER:HB2	2.29	0.62
2:B:263:LEU:O	2:B:266:LEU:HB2	2.00	0.62
3:C:273:LEU:O	3:C:276:GLN:HB2	1.99	0.62
3:C:434:LYS:CD	3:C:435:GLU:CG	2.78	0.62
1:D:106:THR:HG22	1:D:107:LYS:H	1.64	0.62
1:D:176:TRP:HB3	1:D:209:ARG:CD	2.30	0.62
1:D:235:LEU:HD23	1:D:235:LEU:N	2.14	0.62
4:E:14:TYR:CE2	4:E:16:LYS:CE	2.81	0.62
3:C:141:TRP:CH2	3:C:223:ARG:HD3	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:TRP:HB2	3:C:223:ARG:HB2	1.81	0.61
3:C:438:ALA:HA	3:C:441:GLU:OE1	1.99	0.61
1:D:46:VAL:O	1:D:272:PRO:HG3	2.00	0.61
1:D:60:TRP:CZ3	1:D:116:ILE:HG13	2.35	0.61
1:D:243:MET:H	1:D:243:MET:CE	2.13	0.61
4:E:14:TYR:OH	4:E:83:LEU:HB3	2.00	0.61
4:E:303:VAL:O	4:E:303:VAL:HG13	2.00	0.61
1:A:38:ILE:H	1:A:38:ILE:HD12	1.65	0.61
1:A:414:PHE:CD1	1:A:417:ILE:HD12	2.35	0.61
2:B:72:TYR:O	2:B:76:LYS:HG2	2.00	0.61
3:C:137:PHE:CE1	3:C:288:ILE:HG22	2.35	0.61
1:A:148:ILE:CG2	1:A:198:TYR:CB	2.76	0.61
1:A:220:ILE:N	1:A:221:PRO:HD2	2.16	0.61
1:A:304:SER:HB2	1:A:400:LYS:HZ2	1.65	0.61
3:C:115:ASN:ND2	3:C:115:ASN:C	2.45	0.61
3:C:225:PRO:HG2	3:C:228:TYR:CD1	2.35	0.61
3:C:429:ILE:O	3:C:433:ILE:HG13	2.00	0.61
4:E:94:ASN:ND2	4:E:143:LEU:CD2	2.60	0.61
1:A:62:ASP:HB3	1:A:65:LEU:CD1	2.30	0.61
1:A:117:MET:SD	1:A:119:THR:HG21	2.40	0.61
3:C:33:ILE:HG22	3:C:160:MET:SD	2.40	0.61
3:C:55:ASN:HA	3:C:124:ALA:O	2.01	0.61
3:C:69:TRP:HB2	3:C:74:TYR:N	2.16	0.61
1:D:209:ARG:CG	1:D:210:ILE:H	2.12	0.61
1:D:263:LEU:O	1:D:267:THR:HG22	2.00	0.61
1:D:286:ILE:O	1:D:290:ILE:HG23	1.99	0.61
4:E:271:LYS:HB2	4:E:271:LYS:NZ	2.14	0.61
3:C:462:THR:HB	3:C:463:PRO:HD3	1.83	0.61
1:D:46:VAL:CB	1:D:271:VAL:HA	2.30	0.61
1:A:178:MET:HA	1:A:207:MET:CB	2.31	0.61
2:B:75:ILE:HD11	2:B:78:LEU:CD1	2.24	0.61
2:B:81:PRO:HA	2:B:107:ASN:HA	1.83	0.61
2:B:141:ASN:HD21	2:B:212:ILE:HG12	1.65	0.61
3:C:66:ARG:HG2	3:C:66:ARG:HH11	1.63	0.61
1:D:49:ILE:CD1	1:D:125:LYS:HE3	2.27	0.61
1:A:216:VAL:CG1	1:A:220:ILE:HD11	2.27	0.61
2:B:27:ASP:C	2:B:28:LYS:CG	2.69	0.61
2:B:38:THR:HG22	2:B:55:PHE:CE1	2.34	0.61
2:B:58:LEU:HD11	2:B:118:TRP:CE3	2.35	0.61
3:C:137:PHE:CD1	3:C:288:ILE:CB	2.83	0.61
1:A:66:ARG:HA	1:A:113:THR:C	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:PHE:CA	2:B:424:LEU:HB2	2.27	0.61
3:C:35:LEU:O	3:C:162:LEU:HD23	2.01	0.61
3:C:49:ASP:O	3:C:50:GLU:HG3	2.01	0.61
3:C:443:VAL:O	3:C:443:VAL:CG1	2.48	0.61
1:D:249:VAL:HA	1:D:252:SER:HB3	1.80	0.61
1:D:409:ILE:HG13	1:D:410:LEU:N	2.16	0.61
4:E:34:LEU:HD23	4:E:55:ILE:HA	1.82	0.61
4:E:52:ASN:HA	4:E:121:ALA:O	2.01	0.61
2:B:145:VAL:HA	2:B:207:VAL:O	1.99	0.61
2:B:189:GLU:HB3	2:B:212:ILE:HG22	1.83	0.61
2:B:304:LEU:O	2:B:307:ARG:HB3	2.00	0.61
3:C:50:GLU:O	3:C:129:SER:HA	2.00	0.61
3:C:291:TYR:N	3:C:291:TYR:CD1	2.68	0.61
4:E:17:ARG:HH11	4:E:18:ILE:HG22	1.66	0.61
4:E:101:VAL:O	4:E:101:VAL:HG22	2.00	0.61
1:A:50:VAL:HG12	1:A:51:GLU:N	2.16	0.61
1:A:131:ILE:HD11	1:A:140:GLN:HG2	1.82	0.61
1:A:394:ASN:O	1:A:398:GLU:HG3	2.00	0.61
2:B:92:LEU:HD22	2:B:146:PHE:CD1	2.35	0.61
2:B:181:THR:O	2:B:181:THR:HG22	2.01	0.61
3:C:80:LEU:O	3:C:112:VAL:HB	2.00	0.61
1:D:49:ILE:HG21	1:D:125:LYS:HZ2	1.63	0.61
1:D:56:LEU:HD23	1:D:56:LEU:H	1.64	0.61
1:D:133:THR:HG22	1:D:136:PRO:HG2	1.83	0.61
1:D:178:MET:HA	1:D:207:MET:HB2	1.83	0.61
4:E:140:ASN:C	4:E:140:ASN:ND2	2.54	0.61
4:E:140:ASN:HD22	4:E:141:CYS:N	1.99	0.61
4:E:242:LEU:HD12	4:E:242:LEU:O	2.00	0.61
3:C:153:TYR:HB2	3:C:158:ILE:HB	1.83	0.60
3:C:179:ILE:HG23	3:C:181:PRO:HD2	1.81	0.60
3:C:228:TYR:CD1	3:C:229:VAL:N	2.69	0.60
3:C:247:PHE:CE2	3:C:460:ILE:CD1	2.82	0.60
3:C:318:SER:HB2	3:C:444:GLY:HA2	1.83	0.60
4:E:105:ALA:HB3	4:E:117:TRP:HE1	1.65	0.60
4:E:183:TRP:HB3	4:E:216:ARG:NE	2.15	0.60
4:E:219:LEU:CB	4:E:222:ILE:HB	2.28	0.60
1:A:46:VAL:HG12	1:A:47:ASN:ND2	2.16	0.60
4:E:35:THR:CG2	4:E:175:GLU:CD	2.70	0.60
4:E:217:LYS:N	4:E:218:PRO:HD2	2.16	0.60
1:A:187:TRP:HD1	1:A:199:LEU:HD23	1.66	0.60
1:A:201:ILE:CG2	1:A:203:TYR:HE1	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:HG21	1:A:397:GLU:O	2.01	0.60
2:B:29:VAL:H	2:B:156:VAL:HG12	1.65	0.60
3:C:20:HIS:O	3:C:20:HIS:CG	2.54	0.60
3:C:249:LEU:N	3:C:250:PRO:CD	2.63	0.60
1:D:242:LYS:CA	1:D:243:MET:HE2	2.32	0.60
4:E:26:HIS:C	4:E:27:VAL:HG13	2.21	0.60
4:E:83:LEU:HD22	4:E:83:LEU:N	2.16	0.60
4:E:246:ALA:CB	4:E:250:LYS:HG3	2.21	0.60
4:E:416:VAL:CG2	4:E:417:GLU:N	2.63	0.60
1:A:20:ARG:HH11	1:A:20:ARG:CG	2.10	0.60
1:A:145:LYS:HZ2	1:A:202:THR:CG2	2.13	0.60
2:B:108:VAL:HG22	2:B:118:TRP:CG	2.36	0.60
2:B:112:HIS:CG	2:B:113:THR:N	2.68	0.60
2:B:261:VAL:O	2:B:265:LEU:HG	2.02	0.60
3:C:263:VAL:O	3:C:267:GLN:HG2	2.01	0.60
1:D:167:LEU:HD11	1:D:178:MET:CB	2.32	0.60
4:E:33:LYS:CE	4:E:160:SER:HB2	2.31	0.60
4:E:108:LEU:O	4:E:115:MET:HA	2.01	0.60
4:E:310:THR:HB	4:E:313:THR:CG2	2.32	0.60
4:E:444:LYS:HA	4:E:444:LYS:HE3	1.81	0.60
1:A:3:HIS:CB	1:A:7:LEU:CD2	2.79	0.60
1:A:136:PRO:CD	1:A:274:ILE:HG23	2.31	0.60
1:A:147:GLY:HA2	1:A:158:ILE:HD13	1.84	0.60
2:B:65:LEU:HD23	2:B:110:VAL:HG13	1.83	0.60
2:B:452:PHE:O	2:B:456:LEU:HD23	2.02	0.60
1:D:242:LYS:HD2	1:D:245:LEU:CD1	2.32	0.60
4:E:100:GLU:HB2	4:E:122:ILE:CG1	2.31	0.60
1:A:171:MET:HE1	1:A:176:TRP:CH2	2.37	0.60
2:B:142:CYS:HB2	2:B:211:LEU:HD12	1.83	0.60
2:B:227:PRO:O	2:B:231:ILE:HG12	2.01	0.60
2:B:267:ALA:O	2:B:271:PRO:HD3	2.02	0.60
3:C:153:TYR:O	3:C:212:TYR:HB3	2.02	0.60
3:C:258:SER:O	3:C:261:ILE:HB	2.01	0.60
4:E:32:LEU:HA	4:E:56:GLU:O	2.02	0.60
4:E:34:LEU:CD2	4:E:55:ILE:HA	2.32	0.60
4:E:90:VAL:HG22	4:E:95:VAL:CG1	2.22	0.60
1:A:90:LEU:O	1:A:91:VAL:HG23	2.02	0.60
1:A:261:VAL:O	1:A:265:PRO:HD3	2.01	0.60
2:B:142:CYS:O	2:B:210:TYR:HD1	1.85	0.60
2:B:152:ASP:HB3	2:B:203:SER:CB	2.30	0.60
2:B:408:ILE:HG23	2:B:409:LYS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:444:ILE:HG23	2:B:445:THR:N	2.16	0.60
3:C:25:LYS:O	3:C:25:LYS:CG	2.46	0.60
1:D:379:VAL:O	1:D:379:VAL:CG1	2.47	0.60
4:E:9:LYS:O	4:E:9:LYS:HD2	2.02	0.60
1:A:135:PHE:N	1:A:136:PRO:CD	2.65	0.60
1:A:209:ARG:CG	1:A:210:ILE:N	2.65	0.60
2:B:9:SER:CA	2:B:12:PHE:CE1	2.80	0.60
2:B:181:THR:CG2	2:B:181:THR:O	2.50	0.60
2:B:189:GLU:HG3	2:B:468:PHE:HB2	1.81	0.60
3:C:36:SER:HB3	3:C:59:ASP:HB2	1.83	0.60
1:D:191:THR:O	1:D:191:THR:CG2	2.50	0.60
1:D:407:ASP:OD1	1:D:408:HIS:HD2	1.85	0.60
1:D:420:ILE:HA	1:D:423:VAL:CG2	2.31	0.60
4:E:138:TRP:HH2	4:E:215:GLN:HE21	1.48	0.60
1:A:29:VAL:HG21	1:A:86:TRP:HZ3	1.64	0.60
1:A:305:THR:HG22	1:A:305:THR:O	2.02	0.60
2:B:19:VAL:HG22	2:B:20:ARG:HD3	1.82	0.60
3:C:33:ILE:HG12	3:C:62:TRP:CB	2.32	0.60
3:C:42:LEU:CD2	3:C:190:TRP:CZ2	2.85	0.60
1:D:135:PHE:CZ	1:D:273:LEU:HD12	2.35	0.60
4:E:34:LEU:HD12	4:E:210:PHE:CZ	2.37	0.60
4:E:95:VAL:O	4:E:95:VAL:HG12	2.01	0.60
4:E:149:THR:CG2	4:E:150:TYR:H	2.14	0.60
3:C:194:HIS:CG	3:C:195:LYS:N	2.64	0.60
1:D:35:LEU:CD2	1:D:164:ARG:NH1	2.64	0.60
4:E:240:TYR:C	4:E:243:PRO:HD2	2.22	0.60
1:A:218:VAL:CG1	1:A:219:ILE:N	2.65	0.59
1:A:413:VAL:O	1:A:417:ILE:HG13	2.02	0.59
2:B:33:VAL:HG22	2:B:158:LEU:HD22	1.83	0.59
3:C:59:ASP:HA	3:C:121:LEU:HB3	1.84	0.59
1:D:232:VAL:HG22	1:D:250:LEU:CD1	2.32	0.59
4:E:66:TRP:CE3	4:E:70:GLU:CG	2.85	0.59
4:E:86:LEU:HD12	4:E:103:TYR:OH	2.02	0.59
4:E:473:GLN:OE1	4:E:473:GLN:O	2.20	0.59
1:A:85:VAL:CG1	1:A:86:TRP:N	2.65	0.59
1:A:171:MET:HE1	1:A:176:TRP:HH2	1.66	0.59
1:A:406:ILE:HA	1:A:409:ILE:CD1	2.32	0.59
2:B:35:LEU:CD2	2:B:56:LEU:HA	2.32	0.59
2:B:160:HIS:H	2:B:195:LYS:NZ	1.99	0.59
3:C:110:VAL:HG12	3:C:111:LEU:N	2.17	0.59
3:C:155:ALA:CA	3:C:211:ASN:HA	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:HD22	1:D:292:THR:OG1	2.01	0.59
1:D:398:GLU:HG3	1:D:399:TRP:CE3	2.37	0.59
4:E:79:ILE:O	4:E:79:ILE:HG23	2.00	0.59
1:A:79:ARG:HD3	1:A:107:LYS:HD2	1.83	0.59
2:B:108:VAL:CG1	2:B:118:TRP:HB2	2.32	0.59
2:B:139:TRP:HE3	2:B:468:PHE:CZ	2.20	0.59
3:C:67:LEU:HD21	3:C:112:VAL:CG1	2.33	0.59
3:C:247:PHE:CG	3:C:460:ILE:HG12	2.37	0.59
3:C:429:ILE:HG13	3:C:430:VAL:H	1.67	0.59
3:C:434:LYS:CE	3:C:435:GLU:CG	2.79	0.59
1:D:38:ILE:O	1:D:39:GLN:HG3	2.02	0.59
1:D:107:LYS:HE3	4:E:149:THR:O	2.02	0.59
1:D:264:ILE:HA	1:D:267:THR:CG2	2.32	0.59
4:E:470:HIS:NE2	4:E:474:VAL:HG23	2.17	0.59
1:A:36:GLN:O	1:A:38:ILE:HD12	2.02	0.59
1:A:117:MET:CG	1:A:119:THR:HG23	2.32	0.59
2:B:186:TRP:CB	2:B:215:ARG:HD2	2.31	0.59
3:C:115:ASN:ND2	3:C:115:ASN:N	2.39	0.59
3:C:239:ILE:HG22	3:C:240:SER:N	2.17	0.59
1:D:231:LEU:HD22	1:D:235:LEU:HD21	1.84	0.59
4:E:27:VAL:CG1	4:E:154:GLU:HA	2.30	0.59
4:E:100:GLU:HB2	4:E:122:ILE:HG12	1.84	0.59
4:E:261:GLN:HE21	4:E:265:LEU:HD11	1.68	0.59
1:A:284:PHE:CD1	1:A:284:PHE:N	2.70	0.59
2:B:240:TYR:O	2:B:240:TYR:HD1	1.84	0.59
2:B:283:TYR:HA	2:B:286:PHE:CZ	2.37	0.59
1:D:29:VAL:CG1	1:D:60:TRP:HE1	2.15	0.59
1:D:160:PRO:HG3	1:D:185:LYS:HB3	1.84	0.59
1:D:166:ASP:CB	1:D:181:TYR:CB	2.68	0.59
1:D:170:PHE:CE2	1:D:176:TRP:NE1	2.71	0.59
1:D:301:ARG:HH12	1:D:406:ILE:CD1	2.13	0.59
4:E:44:GLU:CD	4:E:129:ILE:CB	2.66	0.59
4:E:247:GLY:N	4:E:250:LYS:HZ2	1.92	0.59
2:B:46:LYS:HD2	2:B:275:LEU:O	2.02	0.59
2:B:101:GLU:C	2:B:102:ILE:HG13	2.23	0.59
2:B:111:GLN:HB2	2:B:115:ALA:HB3	1.83	0.59
3:C:206:PHE:C	3:C:206:PHE:CD1	2.75	0.59
1:D:46:VAL:HA	1:D:272:PRO:HD2	1.81	0.59
4:E:28:ILE:HD13	4:E:85:TRP:HZ3	1.68	0.59
4:E:144:VAL:HG12	4:E:209:ILE:CA	2.32	0.59
4:E:158:GLN:O	4:E:159:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:215:GLN:HG3	4:E:216:ARG:H	1.64	0.59
4:E:244:ALA:HB2	4:E:446:ILE:HG21	1.84	0.59
4:E:454:ALA:O	4:E:457:LEU:HB3	2.01	0.59
1:A:59:GLN:NE2	1:A:117:MET:SD	2.75	0.59
1:A:171:MET:CE	1:A:176:TRP:CH2	2.86	0.59
1:A:207:MET:O	1:A:207:MET:CE	2.50	0.59
1:A:305:THR:HB	1:A:400:LYS:CB	2.33	0.59
3:C:48:THR:HG21	3:C:283:LEU:O	2.03	0.59
3:C:154:ASN:CA	3:C:211:ASN:HB2	2.31	0.59
1:D:152:ASP:HA	1:D:198:TYR:N	2.18	0.59
1:D:259:VAL:HA	1:D:262:GLU:CD	2.22	0.59
1:D:305:THR:HG22	1:D:400:LYS:CB	2.33	0.59
4:E:173:ASP:CB	4:E:185:ILE:HG21	2.31	0.59
1:A:265:PRO:HG2	1:A:266:SER:N	2.18	0.59
2:B:9:SER:HA	2:B:12:PHE:HE1	1.61	0.59
3:C:201:ILE:HD12	3:C:213:GLN:OE1	2.03	0.59
1:D:129:GLU:O	1:D:130:ILE:HG23	2.02	0.59
1:D:176:TRP:CE3	1:D:209:ARG:CZ	2.85	0.59
1:D:260:ILE:O	1:D:264:ILE:HG13	2.03	0.59
4:E:161:ALA:O	4:E:190:ALA:HB3	2.02	0.59
1:A:29:VAL:HB	1:A:31:ILE:CD1	2.32	0.59
1:A:66:ARG:HD3	1:A:66:ARG:O	2.03	0.59
1:A:298:THR:HG23	1:A:301:ARG:HD3	1.85	0.59
2:B:409:LYS:NZ	3:C:423:ILE:CG2	2.65	0.59
3:C:111:LEU:HB3	3:C:119:THR:OG1	2.03	0.59
3:C:137:PHE:H	3:C:138:PRO:HD2	1.66	0.59
1:D:28:PHE:HA	1:D:155:LYS:O	2.02	0.59
1:D:201:ILE:O	1:D:203:TYR:CE1	2.56	0.59
4:E:103:TYR:CG	4:E:104:TYR:N	2.67	0.59
1:A:254:THR:O	1:A:258:LEU:HG	2.02	0.59
1:A:261:VAL:O	1:A:261:VAL:HG12	2.03	0.59
3:C:153:TYR:CB	3:C:158:ILE:HG13	2.33	0.59
4:E:242:LEU:HD12	4:E:242:LEU:C	2.23	0.59
1:A:134:HIS:C	1:A:136:PRO:HD2	2.23	0.58
1:A:139:GLN:NE2	1:A:206:ILE:CG2	2.66	0.58
1:A:216:VAL:HG12	1:A:220:ILE:HD12	1.84	0.58
2:B:268:ASP:O	2:B:271:PRO:HD2	2.03	0.58
3:C:199:LYS:HZ2	3:C:199:LYS:C	2.06	0.58
1:D:175:GLU:HB3	1:D:211:PRO:HG3	1.81	0.58
4:E:41:SER:O	4:E:49:LEU:HA	2.03	0.58
4:E:162:GLU:CA	4:E:190:ALA:H	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:CG2	1:A:107:LYS:H	2.13	0.58
2:B:175:ILE:CG1	2:B:176:ASN:N	2.66	0.58
2:B:439:PHE:O	2:B:442:ILE:HG22	2.04	0.58
1:D:220:ILE:N	1:D:221:PRO:HD2	2.18	0.58
4:E:463:LEU:O	4:E:463:LEU:CD1	2.51	0.58
1:A:92:LEU:HB2	1:A:96:ALA:N	2.18	0.58
1:A:165:PRO:C	1:A:181:TYR:HD1	2.07	0.58
1:A:170:PHE:HE1	1:A:176:TRP:CD1	2.22	0.58
2:B:160:HIS:NE2	2:B:207:VAL:CG1	2.64	0.58
2:B:230:LEU:CA	2:B:233:ILE:HG13	2.33	0.58
3:C:30:VAL:CG2	3:C:158:ILE:N	2.66	0.58
3:C:69:TRP:CH2	3:C:112:VAL:CG1	2.85	0.58
3:C:138:PRO:CG	3:C:288:ILE:HD12	2.33	0.58
1:D:65:LEU:HD23	1:D:110:LEU:HD11	1.86	0.58
1:D:226:SER:O	1:D:230:VAL:HB	2.03	0.58
1:D:278:MET:O	1:D:278:MET:HE3	2.04	0.58
1:D:376:ILE:HG22	1:D:380:LYS:HZ1	1.68	0.58
1:D:412:CYS:O	1:D:415:MET:HE2	2.03	0.58
4:E:19:LYS:NZ	4:E:154:GLU:CB	2.66	0.58
4:E:270:GLN:C	4:E:273:PRO:CD	2.71	0.58
1:A:113:THR:O	1:A:113:THR:HG23	2.01	0.58
2:B:48:GLU:HG3	2:B:48:GLU:O	2.04	0.58
2:B:232:SER:HA	2:B:235:ALA:HB3	1.84	0.58
3:C:14:VAL:HG13	3:C:86:LEU:CD2	2.33	0.58
3:C:50:GLU:CB	3:C:132:ILE:HD13	2.33	0.58
3:C:137:PHE:CE1	3:C:288:ILE:CG2	2.86	0.58
1:D:106:THR:HG23	1:D:107:LYS:HE2	1.85	0.58
1:D:242:LYS:O	1:D:245:LEU:HB3	2.04	0.58
1:D:429:ARG:N	1:D:429:ARG:HE	2.01	0.58
4:E:474:VAL:HG12	4:E:475:PRO:HD3	1.85	0.58
1:A:31:ILE:HG13	1:A:60:TRP:HB3	1.85	0.58
1:A:37:LEU:HD22	1:A:54:VAL:HG12	1.83	0.58
1:A:46:VAL:HG21	1:A:270:ALA:N	2.18	0.58
1:A:166:ASP:CB	1:A:178:MET:HE1	2.33	0.58
2:B:304:LEU:HD23	2:B:304:LEU:O	2.04	0.58
2:B:408:ILE:CG2	2:B:409:LYS:H	2.15	0.58
3:C:35:LEU:HD22	3:C:215:VAL:CG1	2.32	0.58
3:C:242:LEU:CD2	3:C:263:VAL:HG12	2.33	0.58
3:C:447:ASN:O	3:C:449:VAL:HG23	2.04	0.58
1:D:256:PHE:CZ	4:E:263:ILE:CG1	2.87	0.58
4:E:45:LYS:CE	4:E:278:ASN:HA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:162:GLU:HG2	4:E:190:ALA:O	2.03	0.58
1:A:15:TYR:OH	1:A:84:ASP:HB3	2.04	0.58
3:C:472:ILE:HA	3:C:475:MET:HB3	1.85	0.58
4:E:131:VAL:HA	4:E:281:LEU:C	2.24	0.58
1:A:9:ALA:O	1:A:13:GLU:HG3	2.03	0.58
1:A:12:LEU:HG	1:A:13:GLU:N	2.18	0.58
1:A:32:THR:HG23	1:A:159:SER:O	2.04	0.58
1:A:58:GLN:NE2	1:A:90:LEU:HD11	2.19	0.58
1:A:155:LYS:HG3	4:E:78:ARG:CZ	2.33	0.58
1:A:178:MET:HA	1:A:207:MET:HB2	1.85	0.58
2:B:35:LEU:CD1	2:B:56:LEU:HD22	2.34	0.58
2:B:130:ILE:O	2:B:134:TYR:HB2	2.04	0.58
2:B:189:GLU:CG	2:B:468:PHE:CB	2.77	0.58
3:C:60:HIS:CD2	3:C:92:ILE:CD1	2.87	0.58
3:C:159:SER:HA	3:C:213:GLN:HG2	1.83	0.58
3:C:179:ILE:HG21	3:C:181:PRO:HD2	1.85	0.58
3:C:180:ASP:CG	3:C:192:ILE:HG21	2.24	0.58
3:C:434:LYS:NZ	3:C:435:GLU:HG2	2.18	0.58
1:D:45:GLU:HB3	1:D:271:VAL:HG22	1.81	0.58
1:D:129:GLU:O	1:D:142:CYS:HB2	2.04	0.58
1:D:409:ILE:CA	1:D:412:CYS:HB2	2.33	0.58
4:E:77:VAL:CG1	4:E:78:ARG:N	2.67	0.58
1:A:66:ARG:HD3	1:A:66:ARG:H	1.69	0.58
1:A:132:VAL:C	1:A:274:ILE:HG22	2.24	0.58
3:C:147:LYS:HE2	3:C:216:THR:CG2	2.33	0.58
1:D:280:PHE:N	1:D:280:PHE:CD1	2.68	0.58
1:D:286:ILE:HG22	1:D:290:ILE:HG23	1.85	0.58
4:E:91:LEU:H	4:E:95:VAL:CG2	2.17	0.58
4:E:172:ILE:HG23	4:E:174:PRO:CD	2.34	0.58
2:B:136:PRO:CD	2:B:280:ILE:HD11	2.33	0.58
2:B:189:GLU:O	2:B:190:HIS:CD2	2.57	0.58
3:C:42:LEU:CD1	3:C:190:TRP:HZ2	2.16	0.58
3:C:141:TRP:CH2	3:C:223:ARG:HB3	2.38	0.58
3:C:215:VAL:HG23	3:C:215:VAL:O	2.04	0.58
1:D:68:ASN:HB2	1:D:69:PRO:CD	2.33	0.58
4:E:226:ILE:O	4:E:230:VAL:HG23	2.04	0.58
1:A:386:MET:HG3	4:E:427:LYS:HD3	1.86	0.58
1:A:389:ASP:O	1:A:392:SER:HB3	2.04	0.58
2:B:247:GLU:HA	2:B:249:MET:CG	2.34	0.58
3:C:60:HIS:NE2	3:C:92:ILE:HD13	2.19	0.58
3:C:141:TRP:HB2	3:C:222:ARG:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ILE:O	1:D:169:THR:HG21	2.04	0.58
1:A:43:VAL:HG22	1:A:50:VAL:CG2	2.34	0.57
1:A:135:PHE:O	1:A:135:PHE:CG	2.57	0.57
1:A:145:LYS:NZ	1:A:202:THR:HG23	2.19	0.57
2:B:278:PRO:CG	2:B:278:PRO:O	2.49	0.57
3:C:3:GLU:OE1	3:C:3:GLU:O	2.22	0.57
3:C:30:VAL:CG1	3:C:31:VAL:N	2.67	0.57
3:C:137:PHE:HD1	3:C:288:ILE:HB	1.68	0.57
3:C:471:PHE:HD1	3:C:471:PHE:O	1.87	0.57
1:D:298:THR:O	1:D:301:ARG:HD3	2.04	0.57
4:E:159:LEU:HD21	4:E:208:ILE:CG2	2.33	0.57
1:A:25:HIS:O	1:A:25:HIS:CG	2.57	0.57
1:A:166:ASP:OD1	1:A:166:ASP:O	2.21	0.57
1:A:190:TYR:HB2	1:A:192:CYS:SG	2.43	0.57
1:A:271:VAL:CG2	1:A:271:VAL:O	2.52	0.57
1:D:296:ILE:HA	1:D:299:HIS:HB3	1.84	0.57
4:E:49:LEU:HD12	4:E:50:THR:N	2.18	0.57
1:A:108:LEU:HD13	1:A:118:TRP:CB	2.32	0.57
1:A:147:GLY:HA2	1:A:158:ILE:HG21	1.87	0.57
2:B:28:LYS:HB2	2:B:156:VAL:CA	2.20	0.57
2:B:92:LEU:N	2:B:92:LEU:HD23	2.19	0.57
3:C:67:LEU:CD1	3:C:116:GLY:CA	2.82	0.57
3:C:153:TYR:HB2	3:C:158:ILE:CG1	2.34	0.57
4:E:34:LEU:HB2	4:E:210:PHE:CZ	2.39	0.57
2:B:31:VAL:CG2	2:B:86:TRP:HZ3	2.15	0.57
2:B:68:ASP:CB	2:B:69:PRO:CD	2.78	0.57
2:B:69:PRO:HG2	2:B:70:ALA:H	1.68	0.57
1:D:1:SER:N	1:D:4:GLU:HB2	2.19	0.57
1:D:29:VAL:CG1	1:D:60:TRP:NE1	2.67	0.57
1:D:189:TYR:HA	1:D:197:PRO:HD3	1.82	0.57
1:D:291:VAL:O	1:D:295:VAL:HG22	2.04	0.57
4:E:54:TRP:C	4:E:118:LEU:HD13	2.25	0.57
4:E:138:TRP:CH2	4:E:215:GLN:CD	2.77	0.57
1:A:166:ASP:HB2	1:A:181:TYR:HB3	1.86	0.57
2:B:288:MET:O	2:B:291:VAL:HG12	2.04	0.57
3:C:30:VAL:HG23	3:C:156:ASN:C	2.25	0.57
3:C:52:LEU:HD22	3:C:52:LEU:N	2.18	0.57
3:C:92:ILE:HA	3:C:149:THR:O	2.04	0.57
3:C:316:THR:HG23	3:C:317:PRO:CD	2.31	0.57
1:D:91:VAL:CG2	1:D:96:ALA:HB1	2.33	0.57
4:E:146:ARG:HB3	4:E:207:GLU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:HB3	1:A:65:LEU:HD12	1.86	0.57
1:A:305:THR:OG1	1:A:400:LYS:HB3	2.05	0.57
3:C:219:LEU:HD11	3:C:221:ILE:HG22	1.86	0.57
1:D:38:ILE:O	1:D:38:ILE:CG2	2.53	0.57
4:E:59:TRP:HH2	4:E:107:VAL:CG1	2.17	0.57
3:C:318:SER:CA	3:C:447:ASN:ND2	2.68	0.57
1:D:48:GLN:CD	1:D:130:ILE:HD13	2.25	0.57
1:D:233:PHE:CZ	1:D:291:VAL:CG1	2.88	0.57
1:D:233:PHE:O	1:D:236:PRO:HG2	2.04	0.57
1:D:287:SER:HA	1:D:290:ILE:CG1	2.34	0.57
4:E:61:ASP:OD2	4:E:84:LEU:HD21	2.05	0.57
1:A:38:ILE:HD12	1:A:38:ILE:N	2.19	0.57
1:A:105:MET:O	1:A:105:MET:HG2	2.03	0.57
1:A:136:PRO:HG3	1:A:274:ILE:CG2	2.34	0.57
1:A:244:THR:O	1:A:247:ILE:HG22	2.03	0.57
3:C:106:TYR:CD1	3:C:107:PHE:CD1	2.93	0.57
3:C:234:THR:N	3:C:235:PRO:HD2	2.20	0.57
3:C:482:PRO:HG2	3:C:483:ALA:N	2.19	0.57
1:D:75:ILE:CG1	1:D:78:ILE:HG23	2.27	0.57
4:E:453:ILE:O	4:E:457:LEU:HB2	2.04	0.57
1:A:134:HIS:N	1:A:136:PRO:HD2	2.20	0.57
1:A:175:GLU:CB	1:A:211:PRO:HD3	2.34	0.57
2:B:33:VAL:HG11	2:B:158:LEU:HD11	1.87	0.57
2:B:252:SER:O	2:B:255:ALA:HB3	2.05	0.57
1:D:102:ILE:O	1:D:102:ILE:HG22	2.05	0.57
1:D:209:ARG:C	1:D:210:ILE:HG13	2.24	0.57
4:E:232:ILE:HG22	4:E:233:SER:N	2.20	0.57
1:A:43:VAL:CB	1:A:50:VAL:HG22	2.34	0.57
2:B:95:ASN:HB3	2:B:127:SER:H	1.69	0.57
3:C:12:LEU:HB3	3:C:15:ASN:HB3	1.87	0.57
4:E:45:LYS:HE2	4:E:278:ASN:CA	2.35	0.57
4:E:138:TRP:CZ2	4:E:215:GLN:CD	2.78	0.57
4:E:144:VAL:HG23	4:E:144:VAL:O	2.05	0.57
4:E:195:ASN:HB2	4:E:205:PHE:O	2.04	0.57
4:E:227:ALA:N	4:E:228:PRO:CD	2.68	0.57
1:A:249:VAL:HG12	1:A:250:LEU:N	2.19	0.56
3:C:199:LYS:HZ3	3:C:200:ASN:HA	1.69	0.56
3:C:249:LEU:N	3:C:250:PRO:HD3	2.20	0.56
1:D:43:VAL:CG2	1:D:50:VAL:HG13	2.34	0.56
1:D:167:LEU:HD11	1:D:178:MET:HB3	1.87	0.56
4:E:44:GLU:OE2	4:E:129:ILE:HB	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:133:TYR:CD1	4:E:139:GLN:CB	2.88	0.56
4:E:235:LEU:C	4:E:235:LEU:CD1	2.62	0.56
1:A:130:ILE:CD1	1:A:130:ILE:H	2.19	0.56
2:B:92:LEU:HD13	2:B:146:PHE:CE1	2.39	0.56
2:B:192:PRO:HD2	2:B:210:TYR:HB2	1.86	0.56
3:C:241:PHE:C	3:C:241:PHE:HD1	2.07	0.56
1:D:32:THR:CB	1:D:59:GLN:HB3	2.23	0.56
1:D:170:PHE:HE2	1:D:176:TRP:NE1	2.03	0.56
4:E:79:ILE:O	4:E:79:ILE:HG22	2.05	0.56
1:A:33:VAL:HG23	1:A:158:ILE:HG12	1.82	0.56
1:A:41:ILE:HG12	1:A:51:GLU:HB3	1.86	0.56
1:A:60:TRP:NE1	1:A:116:ILE:HD12	2.19	0.56
1:A:67:TRP:CD1	1:A:71:ASP:HB3	2.40	0.56
1:A:106:THR:CG2	1:A:107:LYS:N	2.67	0.56
1:A:148:ILE:CD1	1:A:156:VAL:HG13	2.30	0.56
1:A:417:ILE:O	1:A:417:ILE:HG22	2.04	0.56
2:B:185:GLN:HB3	2:B:217:PRO:CB	2.34	0.56
3:C:69:TRP:CH2	3:C:112:VAL:HG11	2.39	0.56
3:C:158:ILE:HG22	3:C:212:TYR:HA	1.86	0.56
3:C:274:THR:HG22	3:C:275:SER:N	2.21	0.56
1:D:56:LEU:N	1:D:56:LEU:CD2	2.58	0.56
1:D:256:PHE:CE2	4:E:263:ILE:HA	2.41	0.56
1:D:427:ALA:O	1:D:431:ILE:HG13	2.06	0.56
4:E:261:GLN:HE22	4:E:296:ILE:HD11	1.71	0.56
1:A:160:PRO:HG3	1:A:185:LYS:HB2	1.81	0.56
3:C:234:THR:HB	3:C:235:PRO:HD3	1.87	0.56
3:C:288:ILE:CD1	3:C:290:LYS:CE	2.69	0.56
3:C:431:LYS:HE2	1:D:379:VAL:CG1	2.36	0.56
1:D:35:LEU:CD1	1:D:36:GLN:H	2.07	0.56
1:D:37:LEU:CA	1:D:54:VAL:HG13	2.36	0.56
1:D:146:LEU:HD12	1:D:146:LEU:N	2.18	0.56
1:D:176:TRP:CE3	1:D:209:ARG:HD2	2.40	0.56
4:E:22:LYS:HG3	4:E:23:THR:HB	1.87	0.56
4:E:80:PRO:HB2	4:E:83:LEU:HD21	1.85	0.56
4:E:273:PRO:HG2	4:E:274:GLU:N	2.19	0.56
1:A:144:MET:HB2	1:A:203:TYR:HB2	1.86	0.56
2:B:75:ILE:O	2:B:75:ILE:CG1	2.40	0.56
2:B:269:LYS:HD2	2:B:270:VAL:N	2.19	0.56
3:C:35:LEU:CD2	3:C:215:VAL:HG11	2.33	0.56
4:E:45:LYS:HA	4:E:280:PRO:HA	1.86	0.56
4:E:246:ALA:HA	4:E:250:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:261:GLN:HG3	4:E:262:THR:N	2.18	0.56
4:E:425:SER:O	4:E:429:GLN:HB3	2.06	0.56
1:A:149:TRP:HH2	4:E:119:PRO:HA	1.71	0.56
1:A:416:LEU:O	1:A:420:ILE:HG23	2.05	0.56
2:B:46:LYS:CG	2:B:278:PRO:CD	2.80	0.56
3:C:35:LEU:HD21	3:C:37:LEU:HD21	1.88	0.56
3:C:69:TRP:HH2	3:C:112:VAL:HG11	1.69	0.56
3:C:257:MET:CE	3:C:314:PHE:HB2	2.35	0.56
1:D:171:MET:SD	1:D:176:TRP:CH2	2.98	0.56
1:D:305:THR:HG21	1:D:400:LYS:HB3	1.86	0.56
4:E:55:ILE:HG23	4:E:119:PRO:HD2	1.87	0.56
4:E:59:TRP:CD2	4:E:115:MET:HB2	2.41	0.56
4:E:61:ASP:OD1	4:E:63:ARG:HB3	2.06	0.56
4:E:173:ASP:HB3	4:E:185:ILE:CD1	2.34	0.56
1:A:4:GLU:HA	1:A:7:LEU:CD1	2.35	0.56
1:A:276:LYS:HD2	1:A:276:LYS:N	2.19	0.56
2:B:268:ASP:C	2:B:271:PRO:HD2	2.26	0.56
2:B:269:LYS:O	2:B:273:THR:HG23	2.06	0.56
3:C:228:TYR:HD1	3:C:229:VAL:H	1.53	0.56
1:D:47:ASN:C	1:D:48:GLN:HG2	2.26	0.56
4:E:93:ASN:CG	4:E:93:ASN:O	2.43	0.56
4:E:287:ILE:HG13	4:E:291:PHE:CE2	2.41	0.56
1:A:56:LEU:HD23	1:A:57:ARG:H	1.71	0.56
1:A:148:ILE:O	1:A:198:TYR:CD2	2.59	0.56
1:A:187:TRP:CZ2	1:A:189:TYR:HB3	2.41	0.56
2:B:197:TRP:CB	2:B:204:TYR:HD1	2.19	0.56
3:C:77:ILE:HD12	3:C:80:LEU:HD13	1.88	0.56
1:D:245:LEU:HD23	1:D:245:LEU:C	2.26	0.56
4:E:45:LYS:N	4:E:280:PRO:CA	2.69	0.56
4:E:138:TRP:O	4:E:213:ILE:HG13	2.06	0.56
1:A:379:VAL:HA	1:A:382:ILE:CD1	2.36	0.56
2:B:9:SER:CA	2:B:12:PHE:HE1	2.17	0.56
2:B:186:TRP:HB2	2:B:215:ARG:HB2	1.88	0.56
3:C:106:TYR:O	3:C:107:PHE:HD1	1.89	0.56
1:D:35:LEU:HD23	1:D:164:ARG:HH11	1.67	0.56
1:D:37:LEU:HB2	1:D:54:VAL:HG13	1.87	0.56
1:D:130:ILE:HG22	1:D:134:HIS:HD2	1.70	0.56
1:D:137:PHE:CD2	1:D:431:ILE:CG2	2.85	0.56
1:D:420:ILE:HA	1:D:423:VAL:HG23	1.88	0.56
4:E:116:TYR:CD1	4:E:116:TYR:C	2.80	0.56
4:E:133:TYR:CG	4:E:139:GLN:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:HIS:HD1	1:A:385:HIS:C	2.10	0.56
2:B:142:CYS:CB	2:B:211:LEU:CD1	2.82	0.56
3:C:29:GLU:O	3:C:156:ASN:HA	2.06	0.56
3:C:319:THR:N	3:C:447:ASN:CB	2.69	0.56
1:D:36:GLN:C	1:D:54:VAL:HG12	2.27	0.56
1:D:88:PRO:O	1:D:88:PRO:CG	2.50	0.56
1:D:261:VAL:O	1:D:261:VAL:CG1	2.53	0.56
4:E:92:GLU:HB3	4:E:144:VAL:HG23	1.87	0.56
4:E:255:ILE:HD11	4:E:304:LEU:HD22	1.87	0.56
4:E:271:LYS:NZ	4:E:271:LYS:CB	2.68	0.56
1:A:17:LYS:HE3	1:A:84:ASP:CA	2.36	0.55
1:A:117:MET:SD	1:A:119:THR:CG2	2.94	0.55
2:B:212:ILE:O	2:B:212:ILE:CG2	2.53	0.55
2:B:240:TYR:O	2:B:244:ASP:HB2	2.06	0.55
2:B:299:VAL:HG12	2:B:299:VAL:O	2.06	0.55
1:D:54:VAL:O	1:D:56:LEU:HD23	2.06	0.55
1:D:57:ARG:CZ	1:D:117:MET:CE	2.84	0.55
1:D:242:LYS:HA	1:D:243:MET:HE2	1.88	0.55
1:D:264:ILE:HB	1:D:265:PRO:HD2	1.87	0.55
4:E:83:LEU:O	4:E:84:LEU:HB2	2.05	0.55
1:A:200:ASP:OD1	1:A:200:ASP:N	2.39	0.55
2:B:82:SER:C	2:B:84:ASP:H	2.09	0.55
3:C:113:ARG:HB2	3:C:117:TYR:O	2.06	0.55
3:C:150:ALA:HB3	3:C:158:ILE:CD1	2.36	0.55
1:D:220:ILE:HG21	4:E:294:LEU:HD11	1.88	0.55
1:D:435:GLN:C	1:D:437:GLY:H	2.09	0.55
4:E:102:ALA:HB2	4:E:121:ALA:HB2	1.88	0.55
4:E:117:TRP:CD1	4:E:119:PRO:HD3	2.42	0.55
4:E:173:ASP:OD1	4:E:173:ASP:C	2.43	0.55
1:A:107:LYS:NZ	2:B:151:TYR:CD1	2.69	0.55
1:A:296:ILE:HD13	1:A:296:ILE:N	2.21	0.55
3:C:193:ILE:HD11	3:C:222:ARG:HB2	1.88	0.55
4:E:79:ILE:CG1	4:E:80:PRO:HD3	2.35	0.55
4:E:133:TYR:C	4:E:135:PRO:HD2	2.27	0.55
1:A:108:LEU:HD22	1:A:118:TRP:HA	1.89	0.55
3:C:42:LEU:CA	3:C:54:THR:HG22	2.32	0.55
3:C:141:TRP:CB	3:C:222:ARG:HA	2.37	0.55
1:D:36:GLN:HB3	1:D:55:ARG:CG	2.36	0.55
1:D:132:VAL:HB	1:D:274:ILE:HG23	1.88	0.55
1:D:144:MET:O	1:D:203:TYR:CD1	2.59	0.55
1:D:280:PHE:HB3	1:D:284:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:59:TRP:N	4:E:59:TRP:CE3	2.75	0.55
4:E:135:PRO:HB2	4:E:137:ASP:OD1	2.07	0.55
1:A:54:VAL:HG22	1:A:122:ALA:HB3	1.89	0.55
1:A:56:LEU:CD2	1:A:57:ARG:N	2.67	0.55
1:A:178:MET:SD	1:A:207:MET:HB3	2.46	0.55
1:A:222:CYS:HA	1:A:225:PHE:HD2	1.71	0.55
2:B:56:LEU:HD11	2:B:103:THR:CG2	2.35	0.55
2:B:185:GLN:O	2:B:217:PRO:HB3	2.06	0.55
2:B:287:ILE:HD12	2:B:288:MET:N	2.21	0.55
2:B:439:PHE:CA	2:B:442:ILE:HB	2.36	0.55
3:C:138:PRO:HA	3:C:288:ILE:HD12	1.89	0.55
3:C:219:LEU:HG	3:C:221:ILE:HG23	1.89	0.55
1:D:295:VAL:O	1:D:299:HIS:HB2	2.06	0.55
4:E:40:ILE:HB	4:E:50:THR:HB	1.88	0.55
4:E:470:HIS:NE2	4:E:474:VAL:CG2	2.69	0.55
1:A:69:PRO:HA	1:A:73:GLY:HA3	1.87	0.55
1:A:214:PHE:CD1	1:A:214:PHE:C	2.79	0.55
2:B:11:LEU:O	2:B:15:TYR:HB3	2.06	0.55
3:C:56:VAL:HG22	3:C:124:ALA:HB3	1.89	0.55
3:C:132:ILE:HG22	3:C:133:ASN:N	2.22	0.55
3:C:138:PRO:CD	3:C:288:ILE:HD12	2.36	0.55
1:D:242:LYS:N	1:D:243:MET:HE2	2.22	0.55
4:E:45:LYS:HB3	4:E:279:VAL:O	2.06	0.55
4:E:66:TRP:CE3	4:E:70:GLU:CB	2.90	0.55
2:B:56:LEU:HB2	2:B:120:PRO:CG	2.32	0.55
2:B:85:VAL:HG12	2:B:86:TRP:N	2.21	0.55
2:B:85:VAL:O	2:B:87:GLN:HG3	2.06	0.55
3:C:425:SER:O	3:C:429:ILE:HG23	2.07	0.55
1:D:176:TRP:CZ3	1:D:209:ARG:CZ	2.90	0.55
1:D:416:LEU:HA	1:D:419:ILE:CG1	2.37	0.55
4:E:143:LEU:O	4:E:210:PHE:HB2	2.06	0.55
4:E:145:PHE:O	4:E:208:ILE:HD12	2.06	0.55
1:A:69:PRO:O	1:A:73:GLY:HA3	2.07	0.55
1:A:124:PHE:C	1:A:124:PHE:HD1	2.08	0.55
1:A:304:SER:CA	1:A:400:LYS:HD3	2.34	0.55
1:A:380:LYS:HB3	2:B:408:ILE:CB	2.37	0.55
1:A:380:LYS:HA	2:B:408:ILE:HD13	1.86	0.55
3:C:38:THR:HG21	3:C:57:TRP:CZ3	2.42	0.55
1:D:28:PHE:HB3	1:D:156:VAL:C	2.27	0.55
1:D:167:LEU:HD21	1:D:178:MET:O	2.07	0.55
1:D:222:CYS:O	1:D:225:PHE:CD1	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:GLU:C	1:D:243:MET:HE2	2.27	0.55
4:E:143:LEU:H	4:E:143:LEU:HD12	1.72	0.55
4:E:200:LYS:O	4:E:200:LYS:CG	2.54	0.55
4:E:246:ALA:HB1	4:E:250:LYS:CG	2.25	0.55
4:E:436:ASN:CA	4:E:439:TRP:NE1	2.70	0.55
2:B:4:GLU:HG2	2:B:70:ALA:HB3	1.89	0.55
3:C:288:ILE:HG12	3:C:289:GLY:N	2.21	0.55
1:D:35:LEU:HB3	1:D:164:ARG:CZ	2.37	0.55
1:D:419:ILE:O	1:D:423:VAL:HG23	2.06	0.55
4:E:103:TYR:C	4:E:104:TYR:HD1	2.07	0.55
4:E:136:PHE:CZ	4:E:217:LYS:CD	2.87	0.55
4:E:138:TRP:HE1	4:E:186:ARG:HD2	1.70	0.55
1:A:108:LEU:HD21	1:A:118:TRP:CD1	2.43	0.55
1:A:223:LEU:HA	1:A:226:SER:OG	2.07	0.55
2:B:112:HIS:CG	2:B:113:THR:H	2.25	0.55
2:B:263:LEU:HA	2:B:266:LEU:HD12	1.88	0.55
1:D:58:GLN:NE2	1:D:88:PRO:CG	2.70	0.55
1:D:76:LYS:HA	1:D:112:TYR:CD2	2.42	0.55
1:D:79:ARG:NH1	4:E:154:GLU:CD	2.60	0.55
4:E:33:LYS:HG2	4:E:160:SER:CB	2.33	0.55
1:A:33:VAL:HG22	1:A:158:ILE:HG12	1.85	0.54
1:A:131:ILE:CD1	1:A:140:GLN:NE2	2.70	0.54
1:A:166:ASP:OD2	1:A:178:MET:HE1	2.07	0.54
2:B:28:LYS:HD3	2:B:156:VAL:N	2.22	0.54
2:B:130:ILE:HD12	2:B:134:TYR:CE2	2.42	0.54
2:B:187:SER:O	2:B:188:ILE:HG12	2.07	0.54
3:C:33:ILE:CG2	3:C:160:MET:SD	2.94	0.54
3:C:305:ASN:O	3:C:309:VAL:HG23	2.08	0.54
3:C:479:ASN:C	3:C:479:ASN:HD22	2.10	0.54
1:D:1:SER:H3	1:D:4:GLU:HB2	1.72	0.54
1:D:51:GLU:HA	1:D:124:PHE:O	2.07	0.54
1:D:85:VAL:HG13	1:D:86:TRP:HE3	1.71	0.54
1:D:419:ILE:O	1:D:422:THR:HG22	2.07	0.54
4:E:143:LEU:HD12	4:E:143:LEU:N	2.22	0.54
4:E:293:SER:O	4:E:296:ILE:HG12	2.08	0.54
1:A:250:LEU:CD1	1:A:296:ILE:CG2	2.77	0.54
2:B:218:LEU:CD1	2:B:221:ILE:CG1	2.84	0.54
3:C:68:THR:HG22	3:C:69:TRP:N	2.20	0.54
3:C:242:LEU:CD2	3:C:267:GLN:CG	2.83	0.54
3:C:252:GLU:CG	1:D:300:HIS:C	2.75	0.54
3:C:278:LEU:N	3:C:279:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:THR:CG2	1:D:245:LEU:N	2.68	0.54
4:E:134:PHE:HB3	4:E:282:ILE:HB	1.88	0.54
4:E:273:PRO:CG	4:E:274:GLU:H	2.18	0.54
1:A:3:HIS:HB3	1:A:7:LEU:HD23	1.89	0.54
1:A:137:PHE:CE1	1:A:210:ILE:CD1	2.73	0.54
2:B:3:MET:O	2:B:7:LEU:HG	2.07	0.54
2:B:46:LYS:HG3	2:B:278:PRO:CG	2.37	0.54
2:B:139:TRP:CE3	2:B:468:PHE:CZ	2.95	0.54
2:B:239:PHE:N	2:B:239:PHE:CD1	2.72	0.54
3:C:160:MET:N	3:C:213:GLN:HB2	2.19	0.54
1:D:188:VAL:O	1:D:197:PRO:HB2	2.07	0.54
4:E:48:ALA:HA	4:E:125:SER:O	2.06	0.54
2:B:40:LEU:CA	2:B:52:THR:HG23	2.36	0.54
2:B:145:VAL:HG12	2:B:206:ASP:HB2	1.88	0.54
2:B:274:SER:O	2:B:278:PRO:HD3	2.08	0.54
1:D:90:LEU:O	1:D:91:VAL:HB	2.06	0.54
1:D:178:MET:HE3	1:D:207:MET:HB3	1.89	0.54
1:D:239:SER:CB	1:D:242:LYS:CE	2.84	0.54
4:E:44:GLU:HG3	4:E:129:ILE:CD1	2.37	0.54
4:E:452:TRP:CE3	4:E:452:TRP:HA	2.43	0.54
1:A:165:PRO:C	1:A:181:TYR:CD1	2.81	0.54
1:A:165:PRO:O	1:A:181:TYR:CE1	2.61	0.54
2:B:135:PHE:N	2:B:136:PRO:CD	2.70	0.54
2:B:441:TYR:O	2:B:444:ILE:HG22	2.06	0.54
2:B:463:PRO:HB2	2:B:464:PRO:HD3	1.89	0.54
3:C:228:TYR:CD1	3:C:229:VAL:HG22	2.43	0.54
3:C:257:MET:HE1	3:C:314:PHE:CB	2.36	0.54
4:E:91:LEU:HD13	4:E:145:PHE:CA	2.37	0.54
4:E:449:ALA:HA	4:E:452:TRP:CG	2.42	0.54
1:A:217:ASN:O	1:A:221:PRO:HD3	2.07	0.54
1:A:380:LYS:HB3	2:B:408:ILE:HB	1.88	0.54
1:A:384:GLU:HA	1:A:387:LYS:HG3	1.87	0.54
1:A:431:ILE:HG22	1:A:431:ILE:O	2.07	0.54
2:B:46:LYS:CB	2:B:278:PRO:HD2	2.38	0.54
2:B:304:LEU:C	2:B:304:LEU:CD2	2.76	0.54
3:C:155:ALA:N	3:C:211:ASN:CA	2.70	0.54
3:C:193:ILE:CD1	3:C:222:ARG:HB2	2.38	0.54
3:C:266:ALA:O	3:C:270:PHE:CD1	2.61	0.54
3:C:429:ILE:CG1	3:C:430:VAL:N	2.71	0.54
1:D:37:LEU:HD13	1:D:54:VAL:HG13	1.89	0.54
1:D:253:LEU:HD23	1:D:254:THR:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:MET:H	1:A:207:MET:CE	2.19	0.54
2:B:289:ILE:HG22	2:B:293:PHE:CE2	2.43	0.54
3:C:102:TYR:O	3:C:102:TYR:CD1	2.61	0.54
3:C:150:ALA:CB	3:C:158:ILE:HD12	2.38	0.54
3:C:319:THR:HB	3:C:447:ASN:C	2.28	0.54
4:E:56:GLU:HB2	4:E:118:LEU:CD2	2.15	0.54
4:E:266:PHE:CD1	4:E:266:PHE:O	2.61	0.54
1:A:58:GLN:HB3	1:A:60:TRP:CZ3	2.42	0.54
1:A:190:TYR:HD1	1:A:197:PRO:HG2	1.73	0.54
1:A:306:HIS:O	1:A:306:HIS:CG	2.60	0.54
2:B:453:SER:HA	2:B:456:LEU:HB2	1.90	0.54
3:C:161:ASP:OD1	3:C:199:LYS:HD3	2.07	0.54
3:C:179:ILE:HG13	3:C:181:PRO:CD	2.34	0.54
3:C:231:ASN:O	3:C:235:PRO:HD3	2.07	0.54
3:C:474:VAL:O	3:C:478:PHE:CD2	2.60	0.54
1:D:78:ILE:HD11	1:D:110:LEU:HD23	1.90	0.54
1:D:289:ILE:O	1:D:292:THR:HG22	2.07	0.54
1:D:305:THR:OG1	1:D:305:THR:O	2.24	0.54
4:E:183:TRP:HB2	4:E:215:GLN:O	2.07	0.54
4:E:225:ILE:C	4:E:228:PRO:HD2	2.28	0.54
1:A:304:SER:HB2	1:A:400:LYS:HZ3	1.73	0.54
1:A:379:VAL:HA	1:A:382:ILE:CG1	2.38	0.54
2:B:9:SER:O	2:B:13:GLU:HG3	2.07	0.54
3:C:155:ALA:H	3:C:211:ASN:CB	2.21	0.54
3:C:264:LEU:HD22	3:C:310:LEU:HD21	1.89	0.54
3:C:438:ALA:O	3:C:442:GLU:HB2	2.08	0.54
1:D:40:LEU:HD22	1:D:52:THR:OG1	2.07	0.54
1:D:49:ILE:CG2	1:D:125:LYS:HE3	2.38	0.54
1:D:223:LEU:HD23	1:D:223:LEU:O	2.08	0.54
4:E:54:TRP:C	4:E:118:LEU:CD1	2.77	0.54
1:A:238:ASP:HB3	2:B:306:HIS:NE2	2.23	0.54
2:B:91:VAL:CG2	2:B:96:ASN:CB	2.86	0.54
3:C:137:PHE:O	3:C:137:PHE:CG	2.61	0.54
3:C:154:ASN:CB	3:C:211:ASN:HB3	2.34	0.54
1:D:38:ILE:CA	1:D:169:THR:HG21	2.38	0.54
1:D:102:ILE:O	1:D:102:ILE:CG2	2.56	0.54
1:D:120:PRO:O	1:D:120:PRO:HG2	2.08	0.54
1:D:305:THR:CG2	1:D:400:LYS:CB	2.82	0.54
1:D:419:ILE:HD12	1:D:419:ILE:C	2.28	0.54
4:E:44:GLU:CG	4:E:129:ILE:CB	2.76	0.54
1:A:133:THR:C	1:A:136:PRO:HD2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ILE:HA	1:A:412:CYS:HB2	1.89	0.53
2:B:75:ILE:CD1	2:B:78:LEU:CD1	2.74	0.53
2:B:152:ASP:OD1	2:B:203:SER:HB2	2.09	0.53
2:B:241:LEU:HB3	2:B:242:PRO:CD	2.37	0.53
3:C:252:GLU:HG3	1:D:300:HIS:O	2.08	0.53
3:C:482:PRO:HG2	3:C:483:ALA:H	1.72	0.53
1:D:135:PHE:CE1	1:D:273:LEU:HB2	2.42	0.53
1:A:45:GLU:OE1	1:A:271:VAL:HB	2.08	0.53
1:A:274:ILE:O	1:A:277:TYR:HB2	2.09	0.53
1:A:382:ILE:O	1:A:386:MET:CE	2.56	0.53
2:B:224:THR:C	2:B:227:PRO:CD	2.66	0.53
3:C:63:TYR:HD1	3:C:64:ASP:N	2.04	0.53
3:C:305:ASN:O	3:C:308:ILE:HG22	2.09	0.53
1:D:49:ILE:CG2	1:D:125:LYS:NZ	2.66	0.53
4:E:112:ASP:N	4:E:112:ASP:OD1	2.41	0.53
4:E:184:THR:HG23	4:E:215:GLN:C	2.28	0.53
1:A:129:GLU:CD	1:A:140:GLN:HG3	2.28	0.53
1:A:131:ILE:CD1	1:A:140:GLN:HG2	2.37	0.53
1:A:160:PRO:CG	1:A:185:LYS:HE2	2.38	0.53
1:A:252:SER:O	1:A:256:PHE:CD1	2.62	0.53
1:A:252:SER:OG	2:B:257:LEU:HD22	2.08	0.53
2:B:28:LYS:CB	2:B:156:VAL:CA	2.84	0.53
3:C:80:LEU:O	3:C:112:VAL:HG23	2.09	0.53
4:E:195:ASN:H	4:E:204:ASP:HB3	1.74	0.53
4:E:248:GLY:C	4:E:250:LYS:H	2.12	0.53
4:E:265:LEU:HD21	4:E:296:ILE:HD11	1.89	0.53
1:A:66:ARG:HA	1:A:113:THR:CA	2.37	0.53
1:A:107:LYS:HE3	2:B:150:THR:HB	1.90	0.53
1:A:135:PHE:CD1	1:A:273:LEU:HB2	2.43	0.53
1:A:171:MET:CE	1:A:176:TRP:CZ2	2.89	0.53
1:A:201:ILE:CG2	1:A:203:TYR:CE1	2.91	0.53
1:A:242:LYS:HB2	1:A:245:LEU:HB3	1.89	0.53
1:A:406:ILE:HG22	1:A:409:ILE:CD1	2.38	0.53
2:B:56:LEU:CD1	2:B:103:THR:CG2	2.83	0.53
2:B:104:LEU:CD1	2:B:118:TRP:CZ3	2.87	0.53
3:C:51:THR:C	3:C:52:LEU:HD13	2.28	0.53
1:D:53:ASN:HD21	1:D:121:PRO:C	2.11	0.53
1:D:112:TYR:HD1	1:D:113:THR:N	1.96	0.53
1:D:256:PHE:CZ	4:E:263:ILE:HG13	2.43	0.53
4:E:436:ASN:CA	4:E:439:TRP:HE1	2.15	0.53
4:E:441:LEU:C	4:E:441:LEU:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:HG2	1:A:20:ARG:NH1	2.01	0.53
1:A:92:LEU:HB3	1:A:95:ASN:ND2	2.23	0.53
1:A:186:HIS:CE1	1:A:187:TRP:O	2.61	0.53
1:D:32:THR:HB	1:D:59:GLN:CB	2.26	0.53
1:D:170:PHE:CE1	1:D:171:MET:O	2.61	0.53
1:D:301:ARG:NH2	1:D:406:ILE:CD1	2.71	0.53
4:E:62:TYR:C	4:E:64:LEU:H	2.12	0.53
4:E:88:ASP:O	4:E:88:ASP:OD1	2.26	0.53
1:A:31:ILE:HG12	1:A:60:TRP:HB3	1.90	0.53
1:A:66:ARG:HA	1:A:113:THR:HA	1.89	0.53
1:A:216:VAL:CG1	1:A:220:ILE:HD12	2.38	0.53
1:A:230:VAL:HG22	1:A:414:PHE:HZ	1.74	0.53
2:B:150:THR:O	2:B:150:THR:HG22	2.08	0.53
2:B:160:HIS:NE2	2:B:209:PHE:HE1	2.07	0.53
3:C:80:LEU:HD12	1:D:20:ARG:NH2	2.23	0.53
3:C:148:PHE:CB	3:C:215:VAL:HG22	2.34	0.53
3:C:192:ILE:HD13	3:C:221:ILE:CG2	2.38	0.53
3:C:215:VAL:HB	3:C:217:PHE:CE1	2.43	0.53
3:C:257:MET:HE1	3:C:314:PHE:CA	2.39	0.53
1:D:404:MET:HG3	1:D:405:VAL:HG23	1.91	0.53
4:E:222:ILE:HG23	4:E:223:ILE:H	1.73	0.53
1:A:260:ILE:O	1:A:264:ILE:HG23	2.08	0.53
2:B:218:LEU:C	2:B:219:PHE:CD1	2.82	0.53
2:B:247:GLU:HA	2:B:249:MET:HG3	1.91	0.53
2:B:420:GLU:O	2:B:424:LEU:HG	2.09	0.53
2:B:439:PHE:O	2:B:439:PHE:CD1	2.62	0.53
3:C:194:HIS:ND1	3:C:195:LYS:N	2.54	0.53
1:D:253:LEU:CD2	1:D:254:THR:N	2.65	0.53
1:D:254:THR:CG2	1:D:255:VAL:N	2.71	0.53
1:D:387:LYS:O	1:D:391:GLU:HG3	2.09	0.53
4:E:20:PRO:HG3	4:E:61:ASP:CB	2.39	0.53
4:E:143:LEU:HD12	4:E:210:PHE:O	2.08	0.53
4:E:447:ASP:O	4:E:450:CYS:HB2	2.08	0.53
4:E:453:ILE:C	4:E:453:ILE:HD12	2.29	0.53
1:A:265:PRO:CD	1:A:266:SER:H	2.21	0.53
1:A:396:ALA:O	1:A:399:TRP:HB2	2.09	0.53
2:B:242:PRO:HB2	2:B:243:PRO:HD3	1.91	0.53
2:B:297:LEU:CD1	2:B:445:THR:CG2	2.67	0.53
2:B:406:GLU:HG2	2:B:409:LYS:HD2	1.91	0.53
1:D:130:ILE:CA	1:D:134:HIS:HB2	2.38	0.53
4:E:27:VAL:HG12	4:E:153:HIS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:418:ALA:HA	4:E:421:PHE:CD2	2.43	0.53
1:A:6:ARG:CB	1:A:6:ARG:HH11	2.22	0.53
2:B:46:LYS:CA	2:B:278:PRO:HD2	2.37	0.53
2:B:133:MET:SD	2:B:140:GLN:HB2	2.49	0.53
3:C:25:LYS:HA	3:C:25:LYS:NZ	2.23	0.53
3:C:155:ALA:N	3:C:211:ASN:CB	2.72	0.53
1:D:35:LEU:CD1	1:D:54:VAL:HG12	2.39	0.53
1:D:289:ILE:CG2	1:D:290:ILE:N	2.72	0.53
4:E:116:TYR:HD1	4:E:117:TRP:N	2.07	0.53
4:E:253:LEU:HG	4:E:254:SER:N	2.23	0.53
4:E:471:LEU:O	4:E:471:LEU:HD12	2.09	0.53
1:A:46:VAL:HG21	1:A:269:SER:O	2.09	0.53
1:A:163:ASP:C	1:A:164:ARG:HG3	2.30	0.53
1:A:221:PRO:O	1:A:225:PHE:HB3	2.09	0.53
1:A:388:SER:O	1:A:391:GLU:HB3	2.09	0.53
2:B:450:GLY:O	2:B:454:ILE:HG13	2.09	0.53
1:D:141:ASN:HB3	1:D:206:ILE:CG1	2.38	0.53
1:D:176:TRP:HE3	1:D:209:ARG:NE	2.06	0.53
1:A:72:TYR:CB	1:A:112:TYR:HB3	2.07	0.52
4:E:2:GLU:CA	4:E:5:ARG:HG3	2.38	0.52
4:E:131:VAL:HG22	4:E:281:LEU:HB3	1.90	0.52
1:A:3:HIS:HB2	1:A:7:LEU:HD23	1.88	0.52
2:B:189:GLU:O	2:B:190:HIS:CG	2.62	0.52
3:C:49:ASP:C	3:C:50:GLU:HG3	2.30	0.52
1:D:305:THR:HG22	1:D:400:LYS:CG	2.40	0.52
4:E:59:TRP:CH2	4:E:115:MET:HB3	2.43	0.52
4:E:116:TYR:C	4:E:116:TYR:HD1	2.13	0.52
1:A:66:ARG:O	1:A:66:ARG:CG	2.57	0.52
1:A:87:LEU:CD2	1:A:87:LEU:N	2.66	0.52
1:A:187:TRP:HD1	1:A:199:LEU:CD2	2.23	0.52
2:B:189:GLU:CG	2:B:468:PHE:HB2	2.38	0.52
2:B:308:SER:CB	2:B:311:THR:CG2	2.76	0.52
3:C:191:GLU:HG2	3:C:222:ARG:C	2.30	0.52
1:D:384:GLU:HG2	4:E:422:ILE:CD1	2.38	0.52
4:E:14:TYR:HE1	4:E:84:LEU:HD12	1.74	0.52
4:E:462:THR:O	4:E:466:PHE:HB3	2.10	0.52
1:A:50:VAL:HG12	1:A:52:THR:HG23	1.89	0.52
1:A:176:TRP:CD2	1:A:209:ARG:NH1	2.77	0.52
1:A:225:PHE:CD1	1:A:225:PHE:C	2.81	0.52
2:B:241:LEU:HD12	2:B:241:LEU:O	2.09	0.52
2:B:279:ILE:HG22	2:B:280:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:MET:HE1	3:C:120:TRP:CZ2	2.44	0.52
3:C:113:ARG:HB3	3:C:114:PRO:HD2	1.92	0.52
1:D:72:TYR:HA	1:D:112:TYR:HB3	1.91	0.52
1:D:76:LYS:HD2	1:D:112:TYR:HE2	1.74	0.52
1:D:135:PHE:CZ	1:D:273:LEU:CB	2.92	0.52
4:E:75:ASP:HA	4:E:111:ASN:HD22	1.75	0.52
4:E:126:THR:O	4:E:126:THR:HG22	2.10	0.52
4:E:262:THR:HG23	4:E:265:LEU:CB	2.38	0.52
4:E:414:SER:HA	4:E:416:VAL:HG13	1.91	0.52
4:E:473:GLN:HA	4:E:476:GLU:HB2	1.91	0.52
1:A:46:VAL:HA	1:A:272:PRO:HD2	1.91	0.52
1:A:64:ARG:CA	1:A:66:ARG:HH11	2.16	0.52
3:C:160:MET:N	3:C:213:GLN:HG3	2.25	0.52
1:D:3:HIS:HB3	1:D:7:LEU:CD2	2.39	0.52
1:D:75:ILE:CD1	1:D:78:ILE:HG22	2.39	0.52
1:D:187:TRP:CD1	1:D:197:PRO:O	2.63	0.52
4:E:103:TYR:CD2	4:E:104:TYR:CD1	2.97	0.52
4:E:303:VAL:O	4:E:306:VAL:HB	2.09	0.52
1:A:77:LYS:HA	1:A:110:LEU:O	2.10	0.52
1:A:196:THR:HG22	1:A:196:THR:O	2.09	0.52
1:A:306:HIS:NE2	1:A:401:TYR:HB2	2.25	0.52
2:B:233:ILE:O	2:B:237:LEU:HB2	2.09	0.52
3:C:42:LEU:CG	3:C:54:THR:CG2	2.82	0.52
3:C:143:ASN:OD1	3:C:220:ILE:CB	2.56	0.52
3:C:222:ARG:NH2	3:C:224:LYS:CA	2.73	0.52
1:D:141:ASN:HB3	1:D:206:ILE:HD11	1.90	0.52
4:E:76:LEU:C	4:E:77:VAL:HG23	2.29	0.52
4:E:279:VAL:CG1	4:E:280:PRO:HD2	2.39	0.52
1:A:7:LEU:CD2	1:A:70:ALA:HA	2.39	0.52
2:B:37:LEU:CB	2:B:54:VAL:HG12	2.38	0.52
2:B:220:TYR:CB	2:B:223:TYR:CE2	2.93	0.52
3:C:233:ILE:N	3:C:233:ILE:CD1	2.73	0.52
3:C:315:ARG:CD	3:C:315:ARG:N	2.72	0.52
3:C:431:LYS:NZ	1:D:382:ILE:HD12	2.25	0.52
3:C:431:LYS:HA	3:C:434:LYS:HB3	1.91	0.52
3:C:436:LYS:O	3:C:439:TYR:HB2	2.10	0.52
1:D:144:MET:HE3	1:D:205:PHE:CE1	2.45	0.52
1:D:223:LEU:HD23	1:D:223:LEU:C	2.29	0.52
1:D:381:TYR:CD1	4:E:419:CYS:SG	3.03	0.52
1:D:398:GLU:CA	1:D:401:TYR:CE1	2.92	0.52
4:E:279:VAL:CB	4:E:280:PRO:CD	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:310:THR:OG1	4:E:313:THR:HG23	2.09	0.52
1:A:40:LEU:HB2	1:A:171:MET:HB2	1.90	0.52
1:A:265:PRO:CG	1:A:266:SER:N	2.72	0.52
1:A:277:TYR:HA	1:A:280:PHE:CE1	2.43	0.52
2:B:10:VAL:O	2:B:13:GLU:HB2	2.09	0.52
3:C:150:ALA:CB	3:C:158:ILE:CD1	2.88	0.52
3:C:216:THR:C	3:C:217:PHE:CD1	2.73	0.52
1:D:383:ALA:HA	1:D:386:MET:HG2	1.92	0.52
4:E:83:LEU:CD2	4:E:83:LEU:N	2.73	0.52
4:E:134:PHE:CB	4:E:282:ILE:HB	2.40	0.52
4:E:174:PRO:HA	4:E:177:PHE:CB	2.38	0.52
4:E:262:THR:HA	4:E:265:LEU:HB2	1.90	0.52
1:A:72:TYR:CD1	1:A:73:GLY:N	2.78	0.52
1:A:186:HIS:CE1	1:A:188:VAL:HG22	2.45	0.52
1:A:250:LEU:HD13	1:A:296:ILE:HG21	1.86	0.52
2:B:82:SER:O	2:B:83:ASP:HB3	2.08	0.52
2:B:109:LEU:HB3	2:B:117:SER:CB	2.40	0.52
2:B:261:VAL:HG12	2:B:262:PHE:HD1	1.74	0.52
3:C:94:LEU:N	3:C:94:LEU:HD23	2.25	0.52
3:C:155:ALA:H	3:C:211:ASN:HA	1.72	0.52
3:C:192:ILE:CD1	3:C:221:ILE:CG2	2.88	0.52
3:C:318:SER:CB	3:C:447:ASN:HD22	2.16	0.52
1:D:176:TRP:CG	1:D:209:ARG:HD2	2.45	0.52
1:D:416:LEU:HA	1:D:419:ILE:HG13	1.92	0.52
4:E:103:TYR:CD2	4:E:104:TYR:HD1	2.27	0.52
1:A:65:LEU:HB2	1:A:114:GLY:HA2	1.92	0.52
1:A:67:TRP:NE1	1:A:71:ASP:CG	2.63	0.52
1:A:90:LEU:HD12	1:A:100:PHE:CE2	2.45	0.52
1:A:92:LEU:HB2	1:A:95:ASN:HB2	1.92	0.52
1:A:135:PHE:CD1	1:A:135:PHE:C	2.82	0.52
1:A:262:GLU:C	1:A:265:PRO:HD2	2.30	0.52
1:A:431:ILE:N	1:A:431:ILE:CD1	2.73	0.52
4:E:261:GLN:HE21	4:E:265:LEU:CD1	2.23	0.52
1:A:3:HIS:C	1:A:7:LEU:HG	2.30	0.51
2:B:108:VAL:HG22	2:B:118:TRP:HB2	1.92	0.51
2:B:248:LYS:HA	2:B:251:LEU:HD23	1.91	0.51
2:B:310:ASN:HD22	2:B:429:GLN:HG2	1.75	0.51
3:C:57:TRP:HA	3:C:122:PRO:O	2.10	0.51
3:C:121:LEU:O	3:C:121:LEU:CD1	2.53	0.51
1:D:253:LEU:CD2	1:D:254:THR:H	2.19	0.51
4:E:237:VAL:HG22	4:E:457:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:CD1	1:A:203:TYR:OH	2.58	0.51
1:A:257:LEU:HD13	1:A:285:VAL:HG22	1.78	0.51
2:B:187:SER:C	2:B:188:ILE:HG12	2.30	0.51
2:B:211:LEU:N	2:B:211:LEU:HD23	2.26	0.51
2:B:258:ALA:HB2	3:C:265:LEU:HD13	1.91	0.51
2:B:281:ILE:H	2:B:281:ILE:HD12	1.74	0.51
3:C:38:THR:CG2	3:C:57:TRP:CZ3	2.93	0.51
3:C:222:ARG:NH2	3:C:223:ARG:C	2.64	0.51
3:C:253:SER:CB	1:D:306:HIS:CB	2.86	0.51
1:D:287:SER:O	1:D:290:ILE:HG12	2.10	0.51
4:E:26:HIS:O	4:E:27:VAL:HG22	2.09	0.51
4:E:34:LEU:HA	4:E:54:TRP:O	2.09	0.51
1:A:50:VAL:CG1	1:A:51:GLU:N	2.74	0.51
1:A:165:PRO:O	1:A:181:TYR:CD1	2.63	0.51
1:A:255:VAL:CG1	1:A:256:PHE:N	2.73	0.51
2:B:48:GLU:CA	2:B:130:ILE:HD11	2.26	0.51
2:B:132:VAL:HG12	2:B:279:ILE:C	2.30	0.51
2:B:238:VAL:CG2	2:B:255:ALA:HB1	2.41	0.51
3:C:106:TYR:CE1	3:C:107:PHE:HE1	2.27	0.51
3:C:191:GLU:HG3	3:C:222:ARG:HB3	1.92	0.51
1:D:63:VAL:HG13	1:D:64:ARG:H	1.76	0.51
4:E:45:LYS:HG2	4:E:278:ASN:C	2.31	0.51
4:E:91:LEU:H	4:E:95:VAL:HG23	1.75	0.51
1:A:107:LYS:HE3	2:B:150:THR:CG2	2.40	0.51
1:A:166:ASP:N	1:A:181:TYR:CD1	2.78	0.51
2:B:91:VAL:HG12	2:B:147:LYS:O	2.11	0.51
2:B:103:THR:OG1	2:B:122:ALA:CB	2.58	0.51
3:C:43:ILE:HD12	3:C:43:ILE:N	2.21	0.51
3:C:50:GLU:HB3	3:C:132:ILE:HD13	1.93	0.51
1:D:46:VAL:HA	1:D:271:VAL:HA	1.93	0.51
1:D:106:THR:CG2	1:D:107:LYS:N	2.74	0.51
1:D:152:ASP:HA	1:D:197:PRO:CA	2.39	0.51
1:D:416:LEU:C	1:D:419:ILE:HG13	2.30	0.51
4:E:123:TYR:N	4:E:123:TYR:CD1	2.76	0.51
1:A:4:GLU:HA	1:A:7:LEU:HD12	1.91	0.51
1:A:187:TRP:CD1	1:A:199:LEU:HD23	2.45	0.51
2:B:271:PRO:O	2:B:275:LEU:HD13	2.10	0.51
3:C:106:TYR:HD1	3:C:106:TYR:C	2.14	0.51
3:C:139:PHE:CD2	3:C:224:LYS:NZ	2.76	0.51
3:C:241:PHE:CA	3:C:244:ALA:HB3	2.38	0.51
3:C:434:LYS:CG	1:D:386:MET:HE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:471:PHE:C	3:C:473:PHE:H	2.13	0.51
1:D:33:VAL:HA	1:D:57:ARG:O	2.10	0.51
1:D:167:LEU:HD21	1:D:178:MET:C	2.31	0.51
1:D:392:SER:O	1:D:395:ALA:HB3	2.11	0.51
4:E:58:GLN:C	4:E:59:TRP:HE3	2.13	0.51
1:A:36:GLN:OE1	1:A:36:GLN:O	2.27	0.51
1:A:175:GLU:HB3	1:A:211:PRO:CB	2.37	0.51
2:B:92:LEU:HD22	2:B:146:PHE:HA	1.93	0.51
3:C:110:VAL:HG13	3:C:120:TRP:CA	2.41	0.51
1:D:36:GLN:NE2	1:D:38:ILE:CG1	2.74	0.51
1:D:38:ILE:HA	1:D:169:THR:HG21	1.92	0.51
1:D:140:GLN:HG3	1:D:141:ASN:N	2.26	0.51
1:D:419:ILE:CD1	1:D:420:ILE:HG23	2.41	0.51
4:E:191:LYS:H	4:E:209:ILE:CG2	2.24	0.51
2:B:94:ASN:HB3	2:B:95:ASN:OD1	2.11	0.51
2:B:108:VAL:HG13	2:B:117:SER:O	2.11	0.51
3:C:190:TRP:HB2	3:C:222:ARG:O	2.11	0.51
1:D:37:LEU:HD13	1:D:54:VAL:HG22	1.91	0.51
1:D:152:ASP:HA	1:D:197:PRO:C	2.31	0.51
1:D:176:TRP:CD2	1:D:209:ARG:HD2	2.45	0.51
1:D:398:GLU:OE2	1:D:399:TRP:CZ3	2.63	0.51
4:E:14:TYR:CE1	4:E:84:LEU:HD12	2.46	0.51
4:E:33:LYS:CE	4:E:160:SER:HB3	2.41	0.51
4:E:38:ASN:O	4:E:51:THR:HG23	2.11	0.51
4:E:240:TYR:HD2	4:E:453:ILE:HD13	1.59	0.51
1:A:77:LYS:HB2	1:A:110:LEU:O	2.11	0.51
1:A:176:TRP:CE3	1:A:209:ARG:NH1	2.79	0.51
2:B:2:VAL:CG1	2:B:69:PRO:CG	2.86	0.51
2:B:91:VAL:CG2	2:B:96:ASN:HB3	2.41	0.51
2:B:438:LEU:O	2:B:442:ILE:CD1	2.58	0.51
3:C:30:VAL:HG13	3:C:31:VAL:N	2.26	0.51
3:C:47:GLU:OE1	3:C:285:VAL:CG2	2.58	0.51
3:C:63:TYR:CD1	3:C:116:GLY:HA3	2.45	0.51
3:C:300:THR:HG22	3:C:300:THR:O	2.10	0.51
1:D:46:VAL:C	1:D:272:PRO:HD3	2.31	0.51
1:D:66:ARG:O	1:D:67:TRP:CE3	2.64	0.51
1:D:220:ILE:HG21	4:E:294:LEU:HD13	1.92	0.51
1:D:407:ASP:OD1	1:D:408:HIS:CD2	2.63	0.51
4:E:123:TYR:N	4:E:123:TYR:HD1	2.09	0.51
4:E:133:TYR:CE1	4:E:139:GLN:N	2.79	0.51
4:E:185:ILE:HG12	4:E:214:ILE:HG21	1.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:269:ALA:O	4:E:273:PRO:HD3	2.11	0.51
1:A:67:TRP:CD1	1:A:71:ASP:OD1	2.64	0.51
1:A:92:LEU:HB3	1:A:95:ASN:HD22	1.76	0.51
1:A:107:LYS:O	1:A:108:LEU:CD2	2.59	0.51
1:A:108:LEU:CD2	1:A:118:TRP:CD1	2.94	0.51
1:A:117:MET:HG3	1:A:119:THR:HG23	1.93	0.51
1:A:229:THR:HA	1:A:232:VAL:HB	1.91	0.51
1:A:280:PHE:HB3	1:A:284:PHE:CE2	2.46	0.51
1:A:381:TYR:O	1:A:385:HIS:HB2	2.11	0.51
1:A:431:ILE:N	1:A:431:ILE:HD12	2.26	0.51
2:B:274:SER:HB2	2:B:278:PRO:HB3	1.93	0.51
3:C:150:ALA:HB3	3:C:158:ILE:HD12	1.93	0.51
3:C:190:TRP:CD1	3:C:221:ILE:CD1	2.84	0.51
3:C:219:LEU:HG	3:C:221:ILE:CG2	2.41	0.51
3:C:257:MET:HE3	3:C:314:PHE:HB3	1.93	0.51
1:D:240:GLY:C	1:D:242:LYS:H	2.14	0.51
4:E:270:GLN:O	4:E:273:PRO:CG	2.59	0.51
4:E:289:VAL:HG12	4:E:290:MET:N	2.25	0.51
1:A:385:HIS:C	1:A:385:HIS:ND1	2.64	0.51
2:B:91:VAL:CG1	2:B:149:TYR:CD1	2.85	0.51
3:C:48:THR:CA	3:C:285:VAL:HA	2.40	0.51
3:C:114:PRO:O	3:C:115:ASN:HB3	2.10	0.51
3:C:271:LEU:HD11	3:C:303:VAL:HG22	1.93	0.51
4:E:71:TYR:HA	4:E:111:ASN:HB2	1.92	0.51
1:A:46:VAL:HB	1:A:270:ALA:C	2.32	0.50
1:A:51:GLU:HA	1:A:124:PHE:O	2.11	0.50
1:A:93:TYR:N	1:A:93:TYR:HD1	2.08	0.50
1:A:262:GLU:C	1:A:265:PRO:CD	2.80	0.50
1:A:305:THR:O	1:A:306:HIS:CB	2.59	0.50
2:B:137:PHE:H	2:B:137:PHE:HD1	1.57	0.50
2:B:144:MET:CE	2:B:211:LEU:HD21	2.41	0.50
2:B:153:THR:HB	2:B:204:TYR:CB	2.13	0.50
3:C:307:GLY:O	3:C:310:LEU:HB2	2.11	0.50
3:C:465:MET:O	3:C:465:MET:HG2	2.09	0.50
1:D:137:PHE:HB2	1:D:431:ILE:CG2	2.41	0.50
1:D:420:ILE:HA	1:D:423:VAL:HB	1.93	0.50
4:E:250:LYS:CA	4:E:253:LEU:HB3	2.35	0.50
4:E:313:THR:O	4:E:314:HIS:CG	2.64	0.50
1:A:239:SER:CB	2:B:312:HIS:CB	2.82	0.50
2:B:137:PHE:CD1	2:B:137:PHE:N	2.75	0.50
2:B:283:TYR:CD1	2:B:283:TYR:N	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:LEU:HB3	2:B:428:TRP:CZ2	2.47	0.50
2:B:424:LEU:O	2:B:427:ASP:HB3	2.11	0.50
3:C:16:LYS:CE	3:C:16:LYS:CA	2.89	0.50
3:C:56:VAL:HG23	3:C:124:ALA:HB3	1.93	0.50
1:D:153:GLY:H	1:D:197:PRO:C	2.14	0.50
1:D:241:GLU:O	1:D:243:MET:CE	2.59	0.50
1:D:377:GLU:N	1:D:380:LYS:HE2	2.26	0.50
1:D:409:ILE:HA	1:D:412:CYS:CB	2.38	0.50
4:E:35:THR:HB	4:E:54:TRP:CE3	2.42	0.50
4:E:55:ILE:O	4:E:118:LEU:HB2	2.09	0.50
4:E:128:PRO:C	4:E:129:ILE:HG12	2.31	0.50
4:E:138:TRP:CH2	4:E:215:GLN:CB	2.95	0.50
4:E:231:LEU:HG	4:E:232:ILE:N	2.19	0.50
4:E:474:VAL:HG12	4:E:475:PRO:CD	2.40	0.50
1:A:139:GLN:CB	1:A:207:MET:C	2.79	0.50
1:A:149:TRP:CH2	4:E:119:PRO:HA	2.46	0.50
1:A:250:LEU:HD23	1:A:292:THR:HG22	1.85	0.50
1:A:426:PHE:CD1	1:A:426:PHE:C	2.83	0.50
2:B:69:PRO:HG2	2:B:70:ALA:N	2.27	0.50
2:B:185:GLN:O	2:B:217:PRO:CB	2.59	0.50
2:B:230:LEU:HA	2:B:233:ILE:CG1	2.38	0.50
3:C:68:THR:HA	3:C:115:ASN:CA	2.42	0.50
3:C:89:ILE:CD1	3:C:107:PHE:HB3	2.42	0.50
3:C:200:ASN:ND2	3:C:201:ILE:H	2.10	0.50
1:D:130:ILE:C	1:D:134:HIS:HB2	2.30	0.50
1:D:175:GLU:OE1	1:D:211:PRO:CB	2.57	0.50
1:D:257:LEU:C	1:D:257:LEU:CD1	2.76	0.50
4:E:70:GLU:OE1	4:E:70:GLU:HA	2.12	0.50
1:A:72:TYR:C	1:A:72:TYR:HD1	2.14	0.50
1:A:110:LEU:HD11	1:A:114:GLY:HA2	1.92	0.50
1:A:130:ILE:HD13	1:A:130:ILE:H	1.76	0.50
1:A:265:PRO:C	1:A:268:SER:HB3	2.31	0.50
2:B:3:MET:O	2:B:6:THR:HB	2.12	0.50
2:B:50:MET:HB3	2:B:126:SER:OG	2.11	0.50
2:B:132:VAL:HG12	2:B:279:ILE:HA	1.88	0.50
2:B:297:LEU:HD11	2:B:445:THR:CG2	2.25	0.50
3:C:37:LEU:HD21	3:C:148:PHE:CD2	2.47	0.50
3:C:201:ILE:HG12	3:C:202:TYR:N	2.25	0.50
3:C:205:LYS:HD3	3:C:205:LYS:H	1.76	0.50
3:C:462:THR:O	3:C:466:VAL:HG23	2.12	0.50
1:D:281:THR:O	1:D:285:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:91:LEU:CB	4:E:95:VAL:H	2.21	0.50
4:E:435:GLU:HB3	4:E:439:TRP:CH2	2.46	0.50
1:A:38:ILE:O	1:A:169:THR:HB	2.12	0.50
1:A:229:THR:O	1:A:233:PHE:CD1	2.64	0.50
2:B:160:HIS:CE1	2:B:207:VAL:CG1	2.71	0.50
1:D:16:ASN:C	1:D:17:LYS:HG3	2.32	0.50
1:D:242:LYS:HB2	1:D:245:LEU:HD12	1.94	0.50
1:A:26:THR:O	1:A:28:PHE:CD1	2.65	0.50
1:A:107:LYS:HE3	2:B:150:THR:CB	2.42	0.50
3:C:68:THR:N	3:C:116:GLY:H	2.10	0.50
3:C:115:ASN:HD22	3:C:115:ASN:H	1.54	0.50
3:C:162:LEU:C	3:C:162:LEU:CD2	2.79	0.50
1:D:257:LEU:HA	1:D:260:ILE:HB	1.93	0.50
1:A:45:GLU:CD	1:A:271:VAL:HB	2.31	0.50
1:A:107:LYS:NZ	2:B:151:TYR:CG	2.80	0.50
1:A:110:LEU:HD13	1:A:114:GLY:O	2.11	0.50
2:B:175:ILE:HG23	2:B:178:ASP:H	1.77	0.50
1:D:137:PHE:HB2	1:D:431:ILE:HG22	1.92	0.50
1:D:242:LYS:HB2	1:D:245:LEU:CB	2.41	0.50
4:E:91:LEU:HA	4:E:145:PHE:HA	1.93	0.50
4:E:146:ARG:HH11	4:E:205:PHE:C	2.15	0.50
1:A:50:VAL:HG12	1:A:52:THR:CG2	2.41	0.50
1:A:250:LEU:HD21	1:A:296:ILE:CD1	2.42	0.50
2:B:242:PRO:HD3	2:B:248:LYS:CE	2.38	0.50
1:D:85:VAL:HG13	1:D:86:TRP:N	2.26	0.50
1:D:85:VAL:CG1	1:D:86:TRP:N	2.73	0.50
1:D:135:PHE:CE1	1:D:277:TYR:CE2	2.98	0.50
4:E:88:ASP:O	4:E:88:ASP:CG	2.50	0.50
1:A:27:HIS:C	1:A:28:PHE:CG	2.83	0.50
1:A:133:THR:C	1:A:136:PRO:CG	2.80	0.50
1:A:397:GLU:HA	1:A:400:LYS:CD	2.35	0.50
2:B:135:PHE:N	2:B:136:PRO:HD2	2.26	0.50
2:B:276:SER:C	2:B:277:VAL:CG1	2.80	0.50
3:C:110:VAL:HG12	3:C:111:LEU:H	1.77	0.50
3:C:241:PHE:CE1	3:C:245:LEU:HD22	2.47	0.50
1:D:61:ILE:HA	1:D:116:ILE:HD11	1.93	0.50
1:D:76:LYS:HA	1:D:112:TYR:HD2	1.77	0.50
1:D:91:VAL:CG2	1:D:96:ALA:HB2	2.19	0.50
1:D:186:HIS:CG	1:D:187:TRP:N	2.79	0.50
1:D:198:TYR:HD1	1:D:198:TYR:H	0.65	0.50
1:D:212:LEU:O	1:D:215:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD23	1:D:254:THR:HB	1.94	0.50
1:D:376:ILE:HG22	1:D:380:LYS:HZ3	1.75	0.50
1:A:24:HIS:CD2	1:A:24:HIS:N	2.78	0.49
1:A:267:THR:O	1:A:271:VAL:HG22	2.12	0.49
3:C:300:THR:O	3:C:300:THR:CG2	2.60	0.49
3:C:308:ILE:CG2	3:C:309:VAL:N	2.75	0.49
3:C:315:ARG:N	3:C:315:ARG:HD3	2.27	0.49
1:D:60:TRP:CE2	1:D:86:TRP:HH2	2.28	0.49
1:D:242:LYS:HB2	1:D:245:LEU:CD1	2.42	0.49
4:E:146:ARG:CD	4:E:205:PHE:CD2	2.95	0.49
2:B:152:ASP:OD1	2:B:203:SER:CB	2.61	0.49
2:B:197:TRP:HB3	2:B:204:TYR:HD1	1.75	0.49
2:B:218:LEU:HD13	2:B:221:ILE:HD11	1.93	0.49
2:B:438:LEU:HD23	2:B:441:TYR:CB	2.42	0.49
3:C:93:VAL:HG21	3:C:151:LEU:HD22	1.95	0.49
3:C:210:THR:CG2	3:C:211:ASN:H	2.19	0.49
3:C:262:CYS:SG	1:D:251:LEU:CD1	3.00	0.49
1:D:46:VAL:HB	1:D:271:VAL:N	2.26	0.49
1:D:53:ASN:HD22	1:D:123:ILE:CG1	2.25	0.49
1:D:241:GLU:O	1:D:243:MET:HE1	2.12	0.49
4:E:44:GLU:CG	4:E:129:ILE:CD1	2.90	0.49
4:E:452:TRP:HA	4:E:452:TRP:HE3	1.76	0.49
4:E:455:LEU:HD12	4:E:455:LEU:O	2.12	0.49
1:A:170:PHE:CE1	1:A:176:TRP:CD1	3.00	0.49
3:C:35:LEU:HD12	3:C:92:ILE:HG21	1.93	0.49
3:C:226:LEU:H	3:C:227:PHE:HD1	1.60	0.49
1:D:236:PRO:HA	1:D:240:GLY:HA2	1.94	0.49
4:E:71:TYR:HA	4:E:111:ASN:CB	2.42	0.49
4:E:133:TYR:CD1	4:E:139:GLN:HB3	2.47	0.49
4:E:310:THR:CB	4:E:313:THR:CG2	2.90	0.49
1:A:92:LEU:HB3	1:A:95:ASN:HB2	1.93	0.49
1:A:166:ASP:CB	1:A:178:MET:HE2	2.40	0.49
1:A:287:SER:HA	1:A:290:ILE:HG13	1.93	0.49
1:A:306:HIS:C	1:A:306:HIS:HD2	2.15	0.49
2:B:52:THR:HG22	2:B:53:SER:N	2.20	0.49
2:B:54:VAL:O	2:B:121:SER:HA	2.11	0.49
2:B:244:ASP:CG	3:C:314:PHE:HE1	2.16	0.49
4:E:74:ILE:C	4:E:76:LEU:H	2.14	0.49
4:E:212:LEU:O	4:E:214:ILE:HG23	2.12	0.49
1:A:130:ILE:CD1	1:A:131:ILE:N	2.65	0.49
1:A:376:ILE:O	1:A:380:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ALA:O	1:A:399:TRP:CG	2.65	0.49
2:B:29:VAL:O	2:B:156:VAL:HG12	2.11	0.49
2:B:32:ARG:HH21	2:B:60:TRP:C	2.16	0.49
2:B:90:ILE:HA	2:B:148:SER:HA	1.94	0.49
2:B:112:HIS:C	2:B:114:GLY:H	2.16	0.49
2:B:446:MET:HA	2:B:449:ILE:HG12	1.95	0.49
3:C:6:ARG:O	3:C:9:ASN:HB3	2.11	0.49
3:C:56:VAL:CG1	3:C:126:PHE:CE2	2.93	0.49
3:C:84:PRO:HB2	3:C:107:PHE:HB2	1.94	0.49
3:C:116:GLY:O	3:C:118:VAL:HG23	2.12	0.49
3:C:180:ASP:HB3	3:C:181:PRO:CD	2.37	0.49
3:C:266:ALA:CB	1:D:251:LEU:HD13	2.42	0.49
3:C:278:LEU:N	3:C:279:PRO:HD2	2.28	0.49
3:C:316:THR:CG2	3:C:447:ASN:CB	2.87	0.49
1:D:246:SER:O	1:D:250:LEU:HD12	2.12	0.49
4:E:66:TRP:HD1	4:E:111:ASN:CB	2.18	0.49
4:E:227:ALA:N	4:E:228:PRO:HD2	2.27	0.49
1:A:2:GLU:CG	1:A:74:GLY:HA2	2.42	0.49
2:B:20:ARG:HG3	2:B:155:GLU:OE1	2.12	0.49
2:B:37:LEU:HD12	2:B:54:VAL:HG11	1.95	0.49
2:B:108:VAL:HG13	2:B:117:SER:C	2.32	0.49
2:B:280:ILE:C	2:B:282:SER:H	2.15	0.49
2:B:409:LYS:HZ1	3:C:423:ILE:CG2	2.25	0.49
2:B:438:LEU:HD22	2:B:441:TYR:CD2	2.47	0.49
3:C:77:ILE:HD11	3:C:80:LEU:HD13	1.94	0.49
3:C:223:ARG:HG2	3:C:224:LYS:H	1.76	0.49
4:E:29:ASP:N	4:E:29:ASP:OD1	2.45	0.49
4:E:88:ASP:CG	4:E:149:THR:HB	2.33	0.49
1:A:235:LEU:CD2	1:A:242:LYS:HE3	2.35	0.49
1:A:431:ILE:O	1:A:431:ILE:CG2	2.60	0.49
2:B:132:VAL:C	2:B:279:ILE:HG23	2.33	0.49
3:C:106:TYR:CD1	3:C:107:PHE:HD1	2.31	0.49
3:C:223:ARG:CG	3:C:224:LYS:N	2.73	0.49
3:C:241:PHE:O	3:C:245:LEU:HB2	2.13	0.49
1:D:211:PRO:HB2	1:D:213:TYR:CD2	2.46	0.49
1:D:212:LEU:O	1:D:216:VAL:HG22	2.12	0.49
1:D:256:PHE:CZ	4:E:263:ILE:HG12	2.47	0.49
4:E:55:ILE:HG23	4:E:119:PRO:HG2	1.95	0.49
4:E:133:TYR:C	4:E:135:PRO:CD	2.80	0.49
4:E:207:GLU:C	4:E:208:ILE:HG13	2.29	0.49
1:A:15:TYR:HE2	1:A:84:ASP:OD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:HD22	1:A:87:LEU:N	2.02	0.49
1:A:174:GLY:HA2	1:A:176:TRP:CE3	2.48	0.49
1:A:290:ILE:O	1:A:293:VAL:HG12	2.13	0.49
2:B:139:TRP:O	2:B:140:GLN:HG2	2.12	0.49
3:C:77:ILE:O	3:C:77:ILE:CG1	2.59	0.49
3:C:106:TYR:C	3:C:106:TYR:CD1	2.86	0.49
3:C:234:THR:N	3:C:235:PRO:CD	2.75	0.49
3:C:464:VAL:HG13	3:C:465:MET:N	2.26	0.49
1:D:201:ILE:CG2	1:D:203:TYR:CE1	2.92	0.49
1:D:233:PHE:CE2	1:D:291:VAL:CG1	2.94	0.49
4:E:146:ARG:NE	4:E:205:PHE:HD2	2.10	0.49
4:E:191:LYS:CE	4:E:211:PHE:CZ	2.95	0.49
4:E:216:ARG:C	4:E:218:PRO:HD2	2.32	0.49
1:A:132:VAL:O	1:A:274:ILE:CA	2.61	0.49
1:A:385:HIS:ND1	1:A:385:HIS:O	2.46	0.49
1:A:393:SER:O	1:A:396:ALA:HB3	2.13	0.49
2:B:10:VAL:HG12	2:B:11:LEU:CD2	2.42	0.49
2:B:97:ASP:OD2	2:B:127:SER:HB2	2.13	0.49
2:B:218:LEU:HD13	2:B:221:ILE:CD1	2.42	0.49
1:D:175:GLU:OE1	1:D:175:GLU:HA	2.12	0.49
1:D:175:GLU:O	1:D:209:ARG:HG3	2.13	0.49
1:A:7:LEU:O	1:A:11:LEU:HG	2.12	0.49
1:A:295:VAL:O	1:A:299:HIS:HB2	2.12	0.49
2:B:54:VAL:C	2:B:55:PHE:HD1	2.16	0.49
2:B:132:VAL:HG12	2:B:279:ILE:CA	2.41	0.49
3:C:1:VAL:O	3:C:1:VAL:CG1	2.59	0.49
3:C:7:LEU:O	3:C:10:ASP:HB2	2.13	0.49
3:C:191:GLU:HG3	3:C:191:GLU:O	2.11	0.49
1:D:301:ARG:NH1	1:D:406:ILE:HD11	2.17	0.49
4:E:269:ALA:O	4:E:273:PRO:HG3	2.13	0.49
1:A:52:THR:O	1:A:123:ILE:CG1	2.60	0.48
1:A:56:LEU:CD2	1:A:56:LEU:C	2.81	0.48
1:A:186:HIS:ND1	1:A:187:TRP:N	2.60	0.48
1:A:265:PRO:O	1:A:268:SER:HB3	2.13	0.48
2:B:247:GLU:CA	2:B:249:MET:HG3	2.43	0.48
2:B:255:ALA:O	2:B:258:ALA:HB3	2.13	0.48
3:C:82:LEU:HG	3:C:86:LEU:HB2	1.94	0.48
3:C:179:ILE:CD1	3:C:195:LYS:HB3	2.42	0.48
3:C:266:ALA:HB2	1:D:251:LEU:HD13	1.95	0.48
3:C:429:ILE:HG13	3:C:430:VAL:HG22	1.95	0.48
3:C:464:VAL:CG1	3:C:465:MET:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:CA	1:D:271:VAL:HA	2.42	0.48
1:D:46:VAL:CG2	1:D:270:ALA:C	2.82	0.48
1:D:49:ILE:HG23	1:D:125:LYS:HE3	1.95	0.48
1:D:174:GLY:C	1:D:176:TRP:N	2.67	0.48
1:D:282:MET:C	1:D:286:ILE:HD12	2.34	0.48
4:E:30:VAL:O	4:E:158:GLN:CG	2.60	0.48
4:E:59:TRP:HH2	4:E:107:VAL:HG12	1.76	0.48
4:E:138:TRP:CH2	4:E:215:GLN:HB2	2.45	0.48
4:E:172:ILE:HG23	4:E:174:PRO:HD2	1.94	0.48
1:A:6:ARG:NH1	1:A:6:ARG:HB2	2.28	0.48
1:A:100:PHE:HB3	1:A:103:VAL:CG2	2.43	0.48
1:A:148:ILE:O	1:A:198:TYR:HD2	1.96	0.48
1:A:285:VAL:O	1:A:288:SER:HB3	2.13	0.48
1:A:295:VAL:HB	1:A:296:ILE:HD13	1.94	0.48
2:B:274:SER:O	2:B:278:PRO:HB3	2.12	0.48
2:B:287:ILE:C	2:B:287:ILE:CD1	2.76	0.48
2:B:299:VAL:O	2:B:299:VAL:CG1	2.60	0.48
3:C:3:GLU:O	3:C:3:GLU:CG	2.60	0.48
3:C:63:TYR:HB2	3:C:117:TYR:CE1	2.48	0.48
3:C:68:THR:CG2	3:C:69:TRP:N	2.75	0.48
3:C:431:LYS:HE2	1:D:382:ILE:HG13	1.95	0.48
3:C:452:THR:CA	3:C:455:ARG:HD3	2.41	0.48
1:D:157:SER:CA	1:D:199:LEU:HD12	2.40	0.48
1:D:233:PHE:CZ	1:D:417:ILE:HD11	2.47	0.48
1:D:237:THR:HG1	1:D:406:ILE:HG23	1.78	0.48
4:E:19:LYS:HZ1	4:E:154:GLU:HB3	1.76	0.48
4:E:217:LYS:N	4:E:218:PRO:CD	2.76	0.48
1:A:242:LYS:HD2	1:A:245:LEU:HD23	1.96	0.48
1:A:306:HIS:O	1:A:306:HIS:HD2	1.90	0.48
2:B:226:VAL:C	2:B:230:LEU:HG	2.33	0.48
2:B:409:LYS:CE	3:C:423:ILE:HG23	2.42	0.48
3:C:38:THR:OG1	3:C:178:ILE:HD13	2.13	0.48
3:C:139:PHE:O	3:C:222:ARG:HG2	2.12	0.48
4:E:138:TRP:HB2	4:E:213:ILE:HG13	1.90	0.48
4:E:161:ALA:HA	4:E:163:GLU:OE2	2.13	0.48
1:A:72:TYR:HD1	1:A:72:TYR:O	1.96	0.48
1:A:179:LYS:HE2	1:A:208:GLN:OE1	2.12	0.48
1:A:235:LEU:HD21	1:A:242:LYS:CE	2.34	0.48
1:A:305:THR:CB	1:A:400:LYS:HB2	2.40	0.48
2:B:220:TYR:CD2	2:B:223:TYR:HE2	2.31	0.48
3:C:67:LEU:CD1	3:C:116:GLY:HA2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:ARG:HA	3:C:112:VAL:HG23	1.94	0.48
1:D:274:ILE:HG22	1:D:276:LYS:HZ3	1.77	0.48
4:E:85:TRP:O	4:E:86:LEU:HD23	2.14	0.48
4:E:288:PHE:O	4:E:292:VAL:HG23	2.14	0.48
1:A:59:GLN:HE22	1:A:117:MET:HG3	1.76	0.48
1:A:156:VAL:HG22	1:A:157:SER:H	1.71	0.48
1:A:167:LEU:CD1	1:A:178:MET:HB2	2.41	0.48
1:A:230:VAL:HG22	1:A:414:PHE:CZ	2.48	0.48
2:B:279:ILE:CG2	2:B:280:ILE:N	2.76	0.48
3:C:319:THR:N	3:C:447:ASN:HB2	2.27	0.48
1:D:21:PRO:HB3	1:D:62:ASP:CG	2.34	0.48
1:D:76:LYS:HD2	1:D:112:TYR:CE2	2.48	0.48
1:D:106:THR:CG2	1:D:107:LYS:HE2	2.43	0.48
1:D:132:VAL:HB	1:D:274:ILE:CG2	2.43	0.48
1:D:225:PHE:HD1	1:D:226:SER:N	2.11	0.48
1:D:276:LYS:HD2	1:D:276:LYS:N	2.20	0.48
1:D:419:ILE:HD12	1:D:420:ILE:HG23	1.96	0.48
4:E:33:LYS:CD	4:E:160:SER:HB3	2.43	0.48
1:A:250:LEU:HD21	1:A:296:ILE:HD12	1.95	0.48
1:A:380:LYS:HD3	2:B:408:ILE:HG21	1.95	0.48
2:B:28:LYS:CB	2:B:155:GLU:C	2.82	0.48
3:C:106:TYR:O	3:C:106:TYR:CD1	2.54	0.48
3:C:281:THR:O	3:C:284:ALA:HB3	2.14	0.48
3:C:445:ASN:HA	3:C:448:LEU:CG	2.16	0.48
1:D:110:LEU:HA	1:D:116:ILE:HG22	1.95	0.48
1:D:166:ASP:OD2	1:D:181:TYR:CB	2.61	0.48
1:D:176:TRP:CE3	1:D:209:ARG:CD	2.96	0.48
4:E:20:PRO:HG3	4:E:61:ASP:CG	2.34	0.48
4:E:223:ILE:HG12	4:E:226:ILE:HD12	1.96	0.48
1:A:3:HIS:O	1:A:7:LEU:HG	2.13	0.48
1:A:218:VAL:CG1	1:A:219:ILE:H	2.26	0.48
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.77	0.48
2:B:92:LEU:HB2	2:B:95:ASN:HB2	1.95	0.48
2:B:223:TYR:CD1	2:B:223:TYR:C	2.86	0.48
2:B:249:MET:HE2	2:B:250:SER:N	2.28	0.48
2:B:431:VAL:O	2:B:432:ALA:HB3	2.13	0.48
3:C:26:HIS:HE1	3:C:66:ARG:HH22	1.58	0.48
3:C:148:PHE:CD1	3:C:148:PHE:N	2.82	0.48
3:C:315:ARG:H	3:C:315:ARG:HD2	1.79	0.48
1:D:64:ARG:HH11	1:D:64:ARG:CG	2.22	0.48
1:D:419:ILE:HD12	1:D:420:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:182:GLU:HA	4:E:218:PRO:HG2	1.96	0.48
1:A:1:SER:HA	1:A:4:GLU:HB2	1.94	0.48
1:A:35:LEU:C	1:A:35:LEU:CD2	2.81	0.48
1:A:120:PRO:HA	1:A:121:PRO:HD3	1.65	0.48
1:A:171:MET:HG2	1:A:173:SER:H	1.79	0.48
1:A:264:ILE:N	1:A:265:PRO:CD	2.77	0.48
2:B:269:LYS:CG	2:B:270:VAL:N	2.77	0.48
2:B:438:LEU:O	2:B:442:ILE:HB	2.14	0.48
3:C:39:LEU:HD12	3:C:39:LEU:N	2.28	0.48
3:C:53:THR:HA	3:C:126:PHE:O	2.13	0.48
3:C:216:THR:O	3:C:217:PHE:CD1	2.64	0.48
3:C:257:MET:HE3	3:C:314:PHE:CB	2.43	0.48
3:C:474:VAL:HA	3:C:477:ASN:OD1	2.14	0.48
1:D:105:MET:HG2	1:D:105:MET:O	2.14	0.48
4:E:272:VAL:O	4:E:272:VAL:HG22	2.13	0.48
4:E:302:ILE:O	4:E:305:ASN:HB3	2.14	0.48
4:E:450:CYS:O	4:E:453:ILE:HG13	2.13	0.48
1:A:160:PRO:HG2	1:A:185:LYS:HE2	1.84	0.48
1:A:255:VAL:HG23	1:A:258:LEU:HD12	1.96	0.48
2:B:9:SER:O	2:B:12:PHE:CD1	2.67	0.48
2:B:284:LEU:O	2:B:287:ILE:HG13	2.14	0.48
2:B:451:THR:HA	2:B:454:ILE:HD12	1.95	0.48
3:C:83:ARG:HD3	3:C:83:ARG:HA	1.73	0.48
3:C:120:TRP:CD1	3:C:122:PRO:HD3	2.48	0.48
3:C:135:LEU:C	3:C:137:PHE:H	2.16	0.48
3:C:434:LYS:CG	3:C:435:GLU:N	2.76	0.48
3:C:437:ASN:O	3:C:441:GLU:CG	2.60	0.48
1:D:292:THR:HA	1:D:295:VAL:CG2	2.44	0.48
1:D:305:THR:OG1	1:D:401:TYR:HD2	1.76	0.48
1:D:429:ARG:NE	1:D:429:ARG:HA	2.29	0.48
1:A:56:LEU:HD12	1:A:90:LEU:HD13	1.95	0.48
1:A:67:TRP:CD1	1:A:71:ASP:CB	2.97	0.48
1:A:75:ILE:O	1:A:78:ILE:HG23	2.14	0.48
1:A:166:ASP:HB3	1:A:181:TYR:HB3	1.95	0.48
1:A:166:ASP:C	1:A:168:SER:H	2.17	0.48
1:A:294:VAL:CG1	1:A:295:VAL:N	2.77	0.48
1:A:380:LYS:CB	2:B:408:ILE:HB	2.43	0.48
2:B:175:ILE:HG23	2:B:178:ASP:N	2.29	0.48
2:B:258:ALA:O	2:B:262:PHE:CD1	2.66	0.48
3:C:212:TYR:CD1	3:C:212:TYR:C	2.87	0.48
3:C:217:PHE:CD1	3:C:217:PHE:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:PHE:CZ	3:C:460:ILE:HD11	2.48	0.48
1:D:376:ILE:O	1:D:380:LYS:HE2	2.14	0.48
4:E:30:VAL:HG22	4:E:59:TRP:HB3	1.96	0.48
4:E:293:SER:O	4:E:297:VAL:HG23	2.14	0.48
1:A:20:ARG:CG	1:A:20:ARG:NH1	2.73	0.47
1:A:132:VAL:O	1:A:274:ILE:CG2	2.61	0.47
1:A:244:THR:HA	1:A:247:ILE:HB	1.95	0.47
3:C:106:TYR:CD1	3:C:107:PHE:CE1	3.02	0.47
3:C:319:THR:CB	3:C:447:ASN:C	2.83	0.47
1:D:289:ILE:O	1:D:293:VAL:HG23	2.14	0.47
4:E:1:ASN:C	4:E:3:GLU:N	2.67	0.47
4:E:9:LYS:HG3	4:E:10:LEU:N	2.28	0.47
4:E:219:LEU:HD13	4:E:222:ILE:HB	1.96	0.47
4:E:310:THR:OG1	4:E:313:THR:CG2	2.62	0.47
1:A:6:ARG:CB	1:A:6:ARG:NH1	2.77	0.47
2:B:21:PRO:HB2	2:B:29:VAL:HG21	1.95	0.47
2:B:220:TYR:CG	2:B:223:TYR:HE2	2.32	0.47
3:C:42:LEU:CD2	3:C:190:TRP:HH2	2.20	0.47
3:C:86:LEU:C	3:C:87:ILE:HG12	2.34	0.47
3:C:147:LYS:HA	3:C:215:VAL:O	2.14	0.47
3:C:149:THR:HG22	3:C:214:ASP:HB3	1.90	0.47
3:C:247:PHE:O	3:C:250:PRO:CD	2.62	0.47
1:D:41:ILE:HG21	4:E:96:ASP:OD2	2.13	0.47
1:D:43:VAL:CG1	1:D:50:VAL:HG22	2.44	0.47
1:D:49:ILE:CG1	1:D:125:LYS:HE3	2.44	0.47
4:E:58:GLN:CA	4:E:59:TRP:HE3	2.27	0.47
4:E:159:LEU:CB	4:E:192:LYS:HB2	2.41	0.47
4:E:177:PHE:CE1	4:E:178:THR:O	2.67	0.47
4:E:264:PHE:N	4:E:264:PHE:CD1	2.82	0.47
4:E:416:VAL:HG22	4:E:417:GLU:H	1.73	0.47
4:E:435:GLU:CB	4:E:439:TRP:CZ2	2.95	0.47
1:A:220:ILE:N	1:A:221:PRO:CD	2.77	0.47
1:A:238:ASP:HB2	2:B:306:HIS:HE2	1.79	0.47
1:A:259:VAL:O	1:A:263:LEU:HG	2.13	0.47
2:B:59:ALA:CB	2:B:116:VAL:O	2.62	0.47
2:B:91:VAL:HG11	2:B:149:TYR:CE1	2.49	0.47
2:B:247:GLU:HA	2:B:249:MET:HG2	1.95	0.47
2:B:261:VAL:HG12	2:B:262:PHE:CD1	2.49	0.47
3:C:122:PRO:CB	3:C:123:PRO:CD	2.73	0.47
3:C:449:VAL:O	3:C:452:THR:HG22	2.14	0.47
1:D:166:ASP:CG	1:D:181:TYR:HB2	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:THR:HG22	1:D:253:LEU:HD11	1.94	0.47
1:D:229:THR:HG21	1:D:288:SER:OG	2.15	0.47
1:A:246:SER:O	1:A:250:LEU:HD12	2.14	0.47
1:A:296:ILE:HA	1:A:299:HIS:HB2	1.95	0.47
2:B:174:MET:HG3	2:B:191:LYS:HE2	1.96	0.47
2:B:197:TRP:HB3	2:B:204:TYR:CD1	2.49	0.47
2:B:242:PRO:CD	2:B:248:LYS:HE3	2.38	0.47
2:B:276:SER:C	2:B:277:VAL:HG13	2.34	0.47
2:B:449:ILE:HA	2:B:452:PHE:HD2	1.75	0.47
3:C:118:VAL:HG12	3:C:119:THR:N	2.29	0.47
3:C:230:ILE:CG1	3:C:231:ASN:N	2.76	0.47
3:C:478:PHE:O	3:C:482:PRO:HD3	2.15	0.47
1:D:49:ILE:CG2	1:D:125:LYS:CE	2.92	0.47
1:D:413:VAL:HA	1:D:416:LEU:HB2	1.95	0.47
4:E:44:GLU:HG3	4:E:129:ILE:HD12	1.92	0.47
4:E:240:TYR:O	4:E:243:PRO:CG	2.62	0.47
1:A:31:ILE:HG23	1:A:60:TRP:HE3	1.79	0.47
1:A:133:THR:N	1:A:274:ILE:HG22	2.30	0.47
1:A:294:VAL:HG13	1:A:295:VAL:N	2.30	0.47
2:B:269:LYS:HG3	2:B:270:VAL:H	1.78	0.47
2:B:415:LEU:C	2:B:415:LEU:CD1	2.78	0.47
3:C:121:LEU:O	3:C:121:LEU:CG	2.63	0.47
3:C:154:ASN:HA	3:C:211:ASN:CB	2.37	0.47
1:D:28:PHE:HB3	1:D:156:VAL:CA	2.44	0.47
1:D:56:LEU:HG	1:D:120:PRO:HG2	1.96	0.47
1:D:233:PHE:CE2	1:D:291:VAL:HG11	2.48	0.47
1:D:282:MET:CE	1:D:286:ILE:HD11	2.44	0.47
1:A:39:GLN:C	1:A:40:LEU:HD23	2.35	0.47
1:A:76:LYS:HG3	1:A:112:TYR:CD2	2.49	0.47
1:A:279:LEU:HD13	1:A:282:MET:CB	2.44	0.47
2:B:176:ASN:HD21	2:B:188:ILE:HD12	1.78	0.47
2:B:286:PHE:CD1	2:B:287:ILE:N	2.82	0.47
3:C:63:TYR:CD1	3:C:64:ASP:N	2.83	0.47
3:C:104:VAL:HA	3:C:106:TYR:CE1	2.50	0.47
1:D:43:VAL:HG21	1:D:50:VAL:HG13	1.95	0.47
1:D:47:ASN:C	1:D:48:GLN:CG	2.83	0.47
4:E:33:LYS:HE3	4:E:160:SER:HB3	1.90	0.47
1:A:46:VAL:CG2	1:A:269:SER:O	2.63	0.47
1:A:58:GLN:HE21	1:A:90:LEU:HD21	1.80	0.47
1:A:69:PRO:HA	1:A:73:GLY:CA	2.45	0.47
1:A:80:LEU:HD23	1:A:110:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:CG	1:A:178:MET:CE	2.83	0.47
1:A:255:VAL:O	1:A:258:LEU:HB2	2.15	0.47
1:A:293:VAL:CG2	4:E:238:LEU:HD21	2.41	0.47
2:B:9:SER:CB	2:B:12:PHE:HE1	2.28	0.47
2:B:35:LEU:HD22	2:B:55:PHE:O	2.14	0.47
2:B:58:LEU:HD21	2:B:118:TRP:CE3	2.50	0.47
2:B:59:ALA:CA	2:B:116:VAL:O	2.62	0.47
2:B:108:VAL:CG2	2:B:118:TRP:HB2	2.45	0.47
2:B:245:ALA:O	2:B:248:LYS:HB3	2.14	0.47
3:C:56:VAL:CG1	3:C:126:PHE:HE2	2.16	0.47
3:C:67:LEU:CD1	3:C:116:GLY:C	2.78	0.47
3:C:81:ARG:NH1	3:C:111:LEU:HD13	2.29	0.47
3:C:221:ILE:HG13	3:C:222:ARG:H	1.78	0.47
3:C:264:LEU:HA	3:C:267:GLN:HG3	1.97	0.47
3:C:306:CYS:O	3:C:310:LEU:HD22	2.15	0.47
3:C:482:PRO:CG	3:C:483:ALA:H	2.28	0.47
1:D:76:LYS:CD	1:D:112:TYR:CE2	2.98	0.47
1:D:157:SER:HB2	1:D:199:LEU:CD1	2.44	0.47
1:D:178:MET:CE	1:D:207:MET:HB3	2.44	0.47
1:D:224:LEU:HD21	4:E:297:VAL:HG11	1.97	0.47
4:E:157:LEU:CD1	4:E:208:ILE:HD11	2.44	0.47
4:E:159:LEU:HD11	4:E:208:ILE:HG23	1.96	0.47
4:E:182:GLU:C	4:E:218:PRO:HD2	2.34	0.47
1:A:6:ARG:HH11	1:A:6:ARG:HB3	1.78	0.47
1:A:175:GLU:C	1:A:211:PRO:HD3	2.35	0.47
1:A:265:PRO:HD2	1:A:266:SER:H	1.79	0.47
1:A:406:ILE:HG22	1:A:409:ILE:HD12	1.96	0.47
2:B:241:LEU:HG	2:B:248:LYS:CE	2.40	0.47
1:D:120:PRO:O	1:D:120:PRO:CG	2.63	0.47
1:D:227:PHE:C	1:D:227:PHE:HD1	2.18	0.47
1:D:431:ILE:HG22	1:D:431:ILE:O	2.15	0.47
4:E:272:VAL:HA	4:E:275:THR:OG1	2.15	0.47
1:A:93:TYR:OH	1:A:198:TYR:CE2	2.58	0.47
1:A:110:LEU:HD12	1:A:111:ASP:H	1.76	0.47
1:A:160:PRO:HG2	1:A:185:LYS:HZ3	1.70	0.47
1:A:251:LEU:CD1	4:E:260:ALA:CB	2.93	0.47
2:B:134:TYR:CD1	2:B:213:ILE:HG13	2.48	0.47
3:C:61:ALA:HB1	3:C:113:ARG:NH2	2.30	0.47
3:C:69:TRP:HB2	3:C:74:TYR:CB	2.39	0.47
3:C:142:GLN:CG	3:C:143:ASN:N	2.66	0.47
3:C:247:PHE:O	3:C:250:PRO:CG	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:ILE:HG23	3:C:290:LYS:N	2.30	0.47
1:D:48:GLN:CB	1:D:130:ILE:HD13	2.41	0.47
1:D:54:VAL:O	1:D:56:LEU:CD2	2.63	0.47
1:D:186:HIS:CE1	1:D:187:TRP:O	2.68	0.47
1:D:232:VAL:CG1	1:D:250:LEU:HD11	2.45	0.47
4:E:30:VAL:HG12	4:E:157:LEU:HD22	1.97	0.47
4:E:104:TYR:CD1	4:E:104:TYR:N	2.83	0.47
4:E:232:ILE:O	4:E:236:VAL:HG22	2.15	0.47
1:A:238:ASP:CB	2:B:306:HIS:HE2	2.28	0.47
1:A:376:ILE:HG22	1:A:377:GLU:N	2.29	0.47
2:B:35:LEU:O	2:B:174:MET:CE	2.63	0.47
2:B:68:ASP:HB3	2:B:69:PRO:HD2	1.92	0.47
2:B:95:ASN:HB3	2:B:126:SER:HB2	1.96	0.47
3:C:230:ILE:HG13	3:C:231:ASN:H	1.76	0.47
1:D:145:LYS:C	1:D:146:LEU:CD1	2.64	0.47
1:D:250:LEU:HA	1:D:253:LEU:HD22	1.96	0.47
1:D:274:ILE:HG13	1:D:277:TYR:CD2	2.50	0.47
1:D:376:ILE:HG22	1:D:380:LYS:CE	2.44	0.47
4:E:9:LYS:HD2	4:E:9:LYS:C	2.35	0.47
4:E:60:ASN:HD22	4:E:60:ASN:N	2.11	0.47
4:E:174:PRO:HD3	4:E:185:ILE:HB	1.95	0.47
1:A:282:MET:O	1:A:285:VAL:HG12	2.15	0.46
2:B:221:ILE:C	2:B:224:THR:HB	2.35	0.46
2:B:233:ILE:HG22	2:B:237:LEU:HD22	1.97	0.46
2:B:444:ILE:CG2	2:B:445:THR:N	2.77	0.46
3:C:63:TYR:HE1	3:C:116:GLY:HA3	1.80	0.46
3:C:89:ILE:HD11	3:C:107:PHE:HB3	1.97	0.46
1:D:76:LYS:CG	1:D:112:TYR:CE2	2.96	0.46
1:D:256:PHE:HZ	4:E:263:ILE:HG13	1.80	0.46
1:D:377:GLU:HB2	4:E:415:CYS:HB2	1.97	0.46
4:E:55:ILE:HG13	4:E:57:ILE:CG1	2.40	0.46
4:E:66:TRP:CD2	4:E:70:GLU:HB3	2.49	0.46
4:E:138:TRP:CH2	4:E:215:GLN:CG	2.98	0.46
4:E:145:PHE:CZ	4:E:208:ILE:HD13	2.50	0.46
4:E:456:LEU:O	4:E:456:LEU:CD2	2.53	0.46
1:A:426:PHE:CD1	1:A:427:ALA:N	2.76	0.46
2:B:34:GLY:O	2:B:35:LEU:HD23	2.12	0.46
2:B:162:LEU:C	2:B:174:MET:N	2.68	0.46
3:C:60:HIS:HE1	3:C:160:MET:CE	2.27	0.46
3:C:281:THR:O	3:C:285:VAL:HG13	2.15	0.46
3:C:316:THR:HB	3:C:320:HIS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ILE:HD12	1:D:78:ILE:HG22	1.95	0.46
1:D:241:GLU:C	1:D:243:MET:CE	2.83	0.46
4:E:19:LYS:HZ3	4:E:154:GLU:CB	2.27	0.46
4:E:222:ILE:O	4:E:225:ILE:HB	2.15	0.46
4:E:302:ILE:O	4:E:306:VAL:HG23	2.15	0.46
1:A:171:MET:CG	1:A:173:SER:H	2.27	0.46
1:A:176:TRP:CE3	1:A:209:ARG:CZ	2.99	0.46
1:A:231:LEU:C	1:A:233:PHE:N	2.69	0.46
1:A:258:LEU:O	1:A:261:VAL:HB	2.15	0.46
2:B:226:VAL:HB	2:B:230:LEU:HD11	1.98	0.46
2:B:233:ILE:O	2:B:236:ILE:HG23	2.14	0.46
1:D:37:LEU:CD1	1:D:54:VAL:HG22	2.45	0.46
1:D:132:VAL:O	1:D:274:ILE:CG1	2.62	0.46
4:E:35:THR:CB	4:E:54:TRP:HE3	2.25	0.46
4:E:182:GLU:HA	4:E:218:PRO:CG	2.45	0.46
1:A:136:PRO:HD3	1:A:274:ILE:CG2	2.38	0.46
1:A:137:PHE:HD1	1:A:137:PHE:HA	1.65	0.46
1:A:137:PHE:CB	1:A:435:GLN:HG3	2.40	0.46
2:B:43:LEU:HD12	2:B:43:LEU:HA	1.78	0.46
2:B:106:VAL:HG12	2:B:118:TRP:NE1	2.31	0.46
1:D:46:VAL:HG21	1:D:270:ALA:C	2.36	0.46
1:D:166:ASP:HB3	1:D:167:LEU:HD12	1.96	0.46
1:D:291:VAL:HG12	1:D:295:VAL:HG11	1.97	0.46
4:E:55:ILE:HG23	4:E:119:PRO:CG	2.45	0.46
4:E:284:LYS:N	4:E:284:LYS:CD	2.72	0.46
1:A:41:ILE:CG2	1:A:123:ILE:HD11	2.46	0.46
1:A:111:ASP:C	1:A:113:THR:N	2.68	0.46
1:A:145:LYS:HZ3	1:A:202:THR:HG21	1.80	0.46
1:A:148:ILE:CG2	1:A:148:ILE:O	2.60	0.46
1:A:255:VAL:HG12	1:A:256:PHE:CD1	2.51	0.46
2:B:132:VAL:HG12	2:B:280:ILE:N	2.31	0.46
2:B:147:LYS:CD	2:B:148:SER:H	2.28	0.46
3:C:242:LEU:HD22	3:C:267:GLN:HG2	1.89	0.46
3:C:316:THR:HB	3:C:319:THR:HG22	1.97	0.46
3:C:471:PHE:CD1	3:C:472:ILE:N	2.84	0.46
4:E:26:HIS:O	4:E:26:HIS:ND1	2.40	0.46
4:E:38:ASN:O	4:E:51:THR:CA	2.63	0.46
4:E:159:LEU:HD23	4:E:159:LEU:HA	1.60	0.46
4:E:239:VAL:O	4:E:243:PRO:HD3	2.16	0.46
4:E:272:VAL:N	4:E:273:PRO:HD2	2.29	0.46
1:A:230:VAL:HG12	1:A:231:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD13	2:B:250:SER:CA	2.46	0.46
2:B:36:THR:O	2:B:55:PHE:CD1	2.69	0.46
2:B:129:THR:N	2:B:142:CYS:SG	2.88	0.46
3:C:249:LEU:N	3:C:249:LEU:CD1	2.79	0.46
1:D:32:THR:O	1:D:58:GLN:HA	2.15	0.46
1:D:132:VAL:CB	1:D:274:ILE:HG23	2.45	0.46
4:E:39:LEU:CD2	4:E:183:TRP:HZ2	2.19	0.46
4:E:44:GLU:CB	4:E:280:PRO:CG	2.82	0.46
4:E:472:ASN:ND2	4:E:472:ASN:O	2.49	0.46
1:A:92:LEU:CD2	1:A:92:LEU:N	2.79	0.46
1:A:129:GLU:CD	1:A:140:GLN:CG	2.84	0.46
1:A:192:CYS:SG	1:A:193:CYS:N	2.89	0.46
1:A:238:ASP:CB	2:B:306:HIS:NE2	2.78	0.46
2:B:101:GLU:OE1	2:B:123:ILE:HG21	2.16	0.46
2:B:218:LEU:CD1	2:B:221:ILE:HD11	2.46	0.46
2:B:248:LYS:HA	2:B:251:LEU:CD2	2.46	0.46
2:B:254:SER:OG	3:C:265:LEU:HD11	2.16	0.46
3:C:267:GLN:HE21	3:C:267:GLN:HB2	1.51	0.46
1:D:26:THR:HG22	1:D:27:HIS:N	2.11	0.46
1:D:44:ASP:OD1	1:D:46:VAL:HG12	2.16	0.46
1:D:57:ARG:CD	1:D:117:MET:SD	3.04	0.46
1:D:243:MET:HE2	1:D:243:MET:N	2.27	0.46
4:E:209:ILE:CG1	4:E:211:PHE:CE1	2.99	0.46
1:A:5:THR:HA	1:A:8:VAL:HG22	1.98	0.46
1:A:79:ARG:HH11	1:A:107:LYS:HZ2	1.62	0.46
1:A:284:PHE:N	1:A:284:PHE:HD1	2.13	0.46
2:B:240:TYR:O	2:B:240:TYR:CD1	2.67	0.46
2:B:281:ILE:HG22	2:B:285:MET:H	1.79	0.46
3:C:10:ASP:O	3:C:16:LYS:HG3	2.15	0.46
3:C:138:PRO:CG	3:C:290:LYS:HE2	2.44	0.46
3:C:212:TYR:O	3:C:212:TYR:HD1	1.94	0.46
1:D:92:LEU:H	1:D:92:LEU:HD22	1.63	0.46
1:A:305:THR:O	1:A:306:HIS:CG	2.69	0.46
2:B:78:LEU:HD23	2:B:80:ILE:HD11	1.97	0.46
2:B:101:GLU:CD	2:B:123:ILE:HG22	2.36	0.46
2:B:298:SER:O	2:B:301:VAL:CG2	2.64	0.46
3:C:110:VAL:CG2	3:C:120:TRP:HB2	2.46	0.46
3:C:482:PRO:CG	3:C:483:ALA:N	2.78	0.46
4:E:45:LYS:CG	4:E:277:LEU:O	2.64	0.46
4:E:215:GLN:CG	4:E:216:ARG:N	2.74	0.46
1:A:54:VAL:HG22	1:A:122:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:CB	1:A:111:ASP:HA	2.45	0.46
1:A:139:GLN:HE21	1:A:206:ILE:HG23	1.80	0.46
1:A:160:PRO:HG2	1:A:185:LYS:HZ1	1.72	0.46
1:A:187:TRP:CD1	1:A:199:LEU:CD2	2.98	0.46
2:B:31:VAL:HG12	2:B:158:LEU:HD23	1.94	0.46
3:C:63:TYR:HD1	3:C:64:ASP:H	1.64	0.46
3:C:288:ILE:CD1	3:C:290:LYS:CD	2.94	0.46
1:D:280:PHE:N	1:D:280:PHE:HD1	2.13	0.46
4:E:116:TYR:CD1	4:E:117:TRP:N	2.84	0.46
4:E:184:THR:CG2	4:E:215:GLN:CG	2.77	0.46
1:A:46:VAL:HB	1:A:270:ALA:O	2.16	0.45
1:A:152:ASP:OD1	1:A:152:ASP:N	2.47	0.45
1:A:166:ASP:CG	1:A:178:MET:HE1	2.37	0.45
1:A:409:ILE:CA	1:A:412:CYS:HB2	2.46	0.45
3:C:154:ASN:CB	3:C:211:ASN:CB	2.94	0.45
3:C:271:LEU:C	3:C:271:LEU:CD2	2.84	0.45
1:D:149:TRP:CG	1:D:150:THR:N	2.85	0.45
1:D:184:TRP:HE3	1:D:185:LYS:O	1.98	0.45
1:D:260:ILE:O	1:D:264:ILE:CD1	2.64	0.45
4:E:146:ARG:CD	4:E:206:GLN:O	2.62	0.45
4:E:304:LEU:C	4:E:306:VAL:H	2.19	0.45
1:A:29:VAL:CG2	1:A:86:TRP:HZ3	2.29	0.45
1:A:160:PRO:CG	1:A:185:LYS:CB	2.73	0.45
1:A:255:VAL:HG12	1:A:256:PHE:N	2.30	0.45
2:B:220:TYR:CG	2:B:223:TYR:CE2	3.04	0.45
3:C:93:VAL:HG11	3:C:151:LEU:CD1	2.41	0.45
3:C:283:LEU:C	3:C:285:VAL:H	2.20	0.45
1:D:46:VAL:HG21	1:D:270:ALA:CA	2.46	0.45
1:D:410:LEU:O	1:D:414:PHE:CB	2.63	0.45
1:D:415:MET:HE2	1:D:415:MET:HB2	1.60	0.45
1:D:435:GLN:C	1:D:437:GLY:N	2.70	0.45
4:E:59:TRP:CZ2	4:E:115:MET:CB	2.99	0.45
1:A:184:TRP:CE3	1:A:185:LYS:O	2.70	0.45
2:B:153:THR:CB	2:B:204:TYR:HB2	2.13	0.45
2:B:175:ILE:HD13	2:B:177:GLN:HB3	1.97	0.45
2:B:251:LEU:HG	2:B:252:SER:N	2.31	0.45
3:C:20:HIS:O	3:C:20:HIS:ND1	2.49	0.45
3:C:153:TYR:HB2	3:C:158:ILE:CB	2.46	0.45
3:C:474:VAL:O	3:C:474:VAL:CG1	2.64	0.45
1:D:130:ILE:C	1:D:131:ILE:HG12	2.36	0.45
1:D:174:GLY:C	1:D:176:TRP:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:138:TRP:CD2	4:E:215:GLN:HA	2.52	0.45
4:E:183:TRP:HB2	4:E:214:ILE:HD13	1.97	0.45
1:A:76:LYS:CG	1:A:77:LYS:N	2.76	0.45
1:A:244:THR:HG23	1:A:245:LEU:N	2.30	0.45
1:A:270:ALA:O	1:A:271:VAL:CG1	2.64	0.45
2:B:111:GLN:NE2	2:B:115:ALA:CB	2.79	0.45
2:B:136:PRO:N	2:B:280:ILE:HD11	2.32	0.45
3:C:63:TYR:O	3:C:65:HIS:CD2	2.69	0.45
3:C:81:ARG:HH12	3:C:111:LEU:HB2	1.79	0.45
3:C:475:MET:HA	3:C:478:PHE:CZ	2.51	0.45
1:D:132:VAL:O	1:D:274:ILE:CG2	2.63	0.45
1:D:229:THR:HA	1:D:232:VAL:HG21	1.95	0.45
1:D:426:PHE:CG	1:D:427:ALA:N	2.84	0.45
4:E:27:VAL:HG12	4:E:154:GLU:N	2.31	0.45
4:E:77:VAL:HG12	4:E:78:ARG:N	2.31	0.45
4:E:173:ASP:H	4:E:188:ARG:HH11	1.64	0.45
1:A:50:VAL:CG1	1:A:52:THR:CG2	2.95	0.45
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.78	0.45
2:B:415:LEU:HD13	2:B:415:LEU:O	2.16	0.45
4:E:38:ASN:ND2	4:E:40:ILE:HG12	2.32	0.45
4:E:258:LEU:O	4:E:258:LEU:HG	2.15	0.45
1:A:245:LEU:CD1	2:B:250:SER:HA	2.47	0.45
1:A:260:ILE:CG2	1:A:261:VAL:N	2.79	0.45
2:B:48:GLU:HB2	2:B:128:CYS:O	2.15	0.45
2:B:53:SER:HA	2:B:122:ALA:O	2.16	0.45
2:B:92:LEU:HD12	2:B:95:ASN:HB2	1.99	0.45
2:B:409:LYS:CE	3:C:423:ILE:HA	2.47	0.45
3:C:30:VAL:HG21	3:C:158:ILE:H	1.79	0.45
3:C:482:PRO:CD	3:C:483:ALA:H	2.30	0.45
1:D:46:VAL:O	1:D:272:PRO:HD3	2.15	0.45
1:D:305:THR:CG2	1:D:400:LYS:HG2	2.47	0.45
4:E:173:ASP:CG	4:E:185:ILE:CD1	2.76	0.45
4:E:283:GLY:O	4:E:286:LEU:HB2	2.15	0.45
1:A:165:PRO:HA	1:A:181:TYR:O	2.17	0.45
1:A:176:TRP:HB3	1:A:209:ARG:CD	2.38	0.45
1:A:256:PHE:CD1	1:A:256:PHE:N	2.85	0.45
1:A:381:TYR:O	1:A:385:HIS:CB	2.65	0.45
2:B:35:LEU:N	2:B:35:LEU:CD2	2.79	0.45
2:B:438:LEU:O	2:B:442:ILE:HD12	2.17	0.45
3:C:25:LYS:HB3	3:C:28:ASN:ND2	2.29	0.45
3:C:58:MET:HE2	3:C:105:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:HIS:HB3	3:C:220:ILE:HG12	1.98	0.45
3:C:222:ARG:HH21	3:C:223:ARG:C	2.20	0.45
1:D:44:ASP:OD2	1:D:46:VAL:HG13	2.17	0.45
1:D:217:ASN:CA	1:D:220:ILE:CD1	2.85	0.45
1:D:302:SER:HB3	1:D:305:THR:HG22	1.98	0.45
4:E:75:ASP:HB3	4:E:110:TYR:CZ	2.52	0.45
4:E:131:VAL:HG12	4:E:131:VAL:O	2.16	0.45
1:A:146:LEU:N	1:A:146:LEU:CD1	2.78	0.45
1:A:171:MET:HG2	1:A:171:MET:O	2.15	0.45
1:A:381:TYR:CD1	1:A:381:TYR:N	2.84	0.45
2:B:91:VAL:HG22	2:B:92:LEU:N	2.31	0.45
2:B:96:ASN:C	2:B:98:GLY:H	2.20	0.45
2:B:220:TYR:CE2	3:C:279:PRO:HB2	2.48	0.45
2:B:284:LEU:HA	2:B:287:ILE:HG13	1.99	0.45
2:B:439:PHE:O	2:B:442:ILE:CG2	2.63	0.45
3:C:290:LYS:HB2	3:C:291:TYR:CD1	2.51	0.45
1:D:242:LYS:CD	1:D:245:LEU:HD13	2.44	0.45
1:D:282:MET:HA	1:D:282:MET:HE3	1.98	0.45
4:E:94:ASN:HD22	4:E:125:SER:CB	2.14	0.45
4:E:135:PRO:CG	4:E:137:ASP:OD1	2.65	0.45
1:A:145:LYS:CG	1:A:202:THR:HG22	2.16	0.45
1:A:171:MET:HE3	1:A:176:TRP:HZ2	1.80	0.45
1:A:410:LEU:HD13	1:A:410:LEU:C	2.38	0.45
2:B:35:LEU:CD1	2:B:56:LEU:HA	2.47	0.45
2:B:91:VAL:HG23	2:B:96:ASN:HB3	1.98	0.45
2:B:281:ILE:HG23	2:B:284:LEU:HB3	1.98	0.45
3:C:16:LYS:HE3	3:C:16:LYS:CA	2.31	0.45
3:C:48:THR:CB	3:C:285:VAL:N	2.78	0.45
3:C:77:ILE:C	3:C:79:ILE:H	2.20	0.45
3:C:469:THR:O	3:C:473:PHE:CB	2.63	0.45
1:D:3:HIS:O	1:D:7:LEU:HG	2.17	0.45
1:D:80:LEU:HD12	1:D:80:LEU:HA	1.75	0.45
1:D:227:PHE:O	1:D:227:PHE:HD1	1.99	0.45
1:D:411:LEU:HD23	1:D:411:LEU:HA	1.74	0.45
4:E:20:PRO:CB	4:E:61:ASP:OD1	2.60	0.45
4:E:45:LYS:CB	4:E:277:LEU:O	2.65	0.45
1:A:174:GLY:CA	1:A:176:TRP:CE3	3.00	0.45
1:A:188:VAL:O	1:A:197:PRO:HB2	2.16	0.45
2:B:220:TYR:CD2	2:B:223:TYR:CE2	3.05	0.45
3:C:137:PHE:N	3:C:138:PRO:CD	2.78	0.45
3:C:316:THR:CG2	3:C:447:ASN:CG	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:HIS:C	1:D:134:HIS:ND1	2.71	0.45
1:D:176:TRP:HB3	1:D:209:ARG:HG3	1.98	0.45
4:E:101:VAL:O	4:E:101:VAL:HG23	2.12	0.45
4:E:273:PRO:CG	4:E:274:GLU:N	2.80	0.45
1:D:160:PRO:HA	1:D:201:ILE:HD11	1.99	0.44
1:D:218:VAL:O	1:D:221:PRO:HG2	2.17	0.44
1:D:257:LEU:HA	1:D:260:ILE:CG1	2.47	0.44
1:D:411:LEU:O	1:D:415:MET:HG3	2.17	0.44
4:E:255:ILE:HG22	4:E:256:SER:N	2.32	0.44
4:E:270:GLN:C	4:E:273:PRO:CG	2.86	0.44
4:E:456:LEU:C	4:E:456:LEU:HD13	2.38	0.44
1:A:93:TYR:CD2	1:A:145:LYS:HB3	2.52	0.44
1:A:267:THR:HA	1:A:270:ALA:HB3	1.99	0.44
1:A:285:VAL:HG13	1:A:286:ILE:HG13	1.99	0.44
1:A:420:ILE:CG1	1:A:421:GLY:N	2.66	0.44
2:B:3:MET:HB3	2:B:6:THR:HB	1.99	0.44
2:B:32:ARG:NH2	2:B:60:TRP:C	2.71	0.44
2:B:101:GLU:OE1	2:B:123:ILE:CG2	2.65	0.44
2:B:159:GLN:HA	2:B:195:LYS:HZ3	1.82	0.44
2:B:218:LEU:C	2:B:219:PHE:CG	2.91	0.44
2:B:239:PHE:HB3	2:B:442:ILE:HG12	1.98	0.44
3:C:64:ASP:O	3:C:116:GLY:HA3	2.17	0.44
3:C:138:PRO:O	3:C:141:TRP:CD1	2.71	0.44
3:C:139:PHE:CE2	3:C:224:LYS:NZ	2.83	0.44
3:C:162:LEU:HB2	3:C:215:VAL:HG12	1.98	0.44
3:C:179:ILE:CG2	3:C:181:PRO:CD	2.87	0.44
3:C:206:PHE:N	3:C:207:PRO:HD2	2.31	0.44
3:C:288:ILE:HG23	3:C:290:LYS:H	1.82	0.44
1:D:37:LEU:HB2	1:D:54:VAL:CG1	2.46	0.44
1:D:57:ARG:CZ	1:D:117:MET:HE3	2.47	0.44
1:D:60:TRP:HZ3	1:D:116:ILE:HG13	1.80	0.44
1:D:228:LEU:HD21	4:E:258:LEU:HD21	2.00	0.44
1:D:238:ASP:CB	4:E:308:LEU:HD22	2.46	0.44
1:D:292:THR:O	1:D:296:ILE:HG12	2.17	0.44
1:A:181:TYR:HB2	1:A:204:HIS:O	2.16	0.44
2:B:46:LYS:HD2	2:B:275:LEU:C	2.38	0.44
2:B:270:VAL:N	2:B:271:PRO:CD	2.81	0.44
1:D:77:LYS:HA	1:D:110:LEU:O	2.18	0.44
1:D:91:VAL:HG21	1:D:96:ALA:HB1	2.00	0.44
1:D:175:GLU:HA	1:D:211:PRO:HB3	1.99	0.44
1:D:187:TRP:CH2	1:D:189:TYR:CG	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:146:ARG:HG3	4:E:147:SER:O	2.18	0.44
4:E:173:ASP:HB3	4:E:185:ILE:CG2	2.41	0.44
4:E:304:LEU:O	4:E:308:LEU:HB2	2.17	0.44
1:A:31:ILE:HA	1:A:59:GLN:O	2.18	0.44
1:A:166:ASP:HB2	1:A:181:TYR:CD1	2.49	0.44
2:B:79:SER:HB2	3:C:153:TYR:HE1	1.82	0.44
2:B:106:VAL:HG12	2:B:118:TRP:HE1	1.83	0.44
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.61	0.44
3:C:80:LEU:O	3:C:112:VAL:CG2	2.65	0.44
1:D:52:THR:O	1:D:123:ILE:HA	2.18	0.44
1:D:76:LYS:HE2	1:D:76:LYS:HB3	1.59	0.44
1:D:145:LYS:CA	1:D:146:LEU:HD12	2.44	0.44
4:E:66:TRP:HD1	4:E:111:ASN:CA	2.24	0.44
4:E:140:ASN:ND2	4:E:212:LEU:H	2.15	0.44
4:E:267:LEU:HD12	4:E:270:GLN:NE2	2.32	0.44
4:E:284:LYS:O	4:E:288:PHE:CE2	2.71	0.44
1:A:227:PHE:CA	1:A:230:VAL:HB	2.46	0.44
1:A:274:ILE:HG12	1:A:277:TYR:CE1	2.50	0.44
1:D:51:GLU:HG3	1:D:125:LYS:HG3	2.00	0.44
1:D:64:ARG:CG	1:D:64:ARG:NH1	2.80	0.44
1:D:116:ILE:O	1:D:116:ILE:HG12	2.17	0.44
1:D:426:PHE:HE1	1:D:430:LEU:HD12	1.83	0.44
4:E:79:ILE:HA	4:E:80:PRO:HD3	1.67	0.44
4:E:91:LEU:HA	4:E:145:PHE:CB	2.47	0.44
4:E:240:TYR:O	4:E:243:PRO:HD2	2.17	0.44
1:A:46:VAL:CG2	1:A:270:ALA:N	2.79	0.44
1:A:152:ASP:HB3	1:A:196:THR:O	2.17	0.44
1:A:178:MET:HE3	1:A:178:MET:HB3	1.87	0.44
1:A:291:VAL:O	1:A:294:VAL:HG12	2.18	0.44
2:B:40:LEU:CB	2:B:52:THR:HG23	2.46	0.44
2:B:146:PHE:O	2:B:147:LYS:HB2	2.17	0.44
3:C:132:ILE:CG2	3:C:133:ASN:N	2.81	0.44
1:D:188:VAL:HG23	1:D:198:TYR:O	2.18	0.44
1:D:229:THR:CG2	1:D:253:LEU:HD12	2.48	0.44
1:D:257:LEU:HD22	1:D:285:VAL:HG22	2.00	0.44
1:A:107:LYS:NZ	2:B:151:TYR:CD2	2.86	0.44
1:A:118:TRP:NE1	1:A:120:PRO:HG3	2.33	0.44
1:A:123:ILE:O	1:A:123:ILE:HG23	2.17	0.44
1:A:129:GLU:O	1:A:142:CYS:SG	2.76	0.44
1:A:262:GLU:O	1:A:265:PRO:HD2	2.17	0.44
2:B:49:GLU:HA	2:B:127:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:GLU:C	2:B:156:VAL:HG22	2.35	0.44
3:C:109:ASN:OD1	3:C:109:ASN:C	2.56	0.44
3:C:110:VAL:CG1	3:C:111:LEU:N	2.81	0.44
3:C:288:ILE:HD13	3:C:288:ILE:HG21	1.57	0.44
1:D:146:LEU:N	1:D:146:LEU:CD1	2.80	0.44
1:D:283:ILE:N	1:D:286:ILE:HD12	2.32	0.44
4:E:45:LYS:HE2	4:E:278:ASN:HA	1.95	0.44
4:E:195:ASN:CB	4:E:205:PHE:H	2.27	0.44
4:E:236:VAL:C	4:E:239:VAL:HG23	2.37	0.44
1:A:145:LYS:NZ	1:A:202:THR:HG21	2.31	0.44
1:A:215:VAL:O	1:A:218:VAL:HG12	2.17	0.44
1:A:237:THR:HB	1:A:406:ILE:HG22	2.00	0.44
1:A:261:VAL:O	1:A:261:VAL:HG13	2.18	0.44
1:A:416:LEU:C	1:A:419:ILE:HG22	2.32	0.44
2:B:10:VAL:HG13	2:B:11:LEU:N	2.33	0.44
2:B:153:THR:O	2:B:204:TYR:CD2	2.65	0.44
2:B:197:TRP:HD1	2:B:204:TYR:HB3	1.79	0.44
2:B:203:SER:O	2:B:205:GLU:HG2	2.17	0.44
2:B:269:LYS:CG	2:B:270:VAL:H	2.31	0.44
3:C:3:GLU:O	3:C:7:LEU:HB2	2.17	0.44
3:C:61:ALA:HB1	3:C:113:ARG:HH22	1.83	0.44
3:C:137:PHE:HD1	3:C:288:ILE:CB	2.28	0.44
3:C:233:ILE:C	3:C:235:PRO:HD2	2.38	0.44
1:D:53:ASN:CB	1:D:123:ILE:HG12	2.46	0.44
1:D:76:LYS:HG2	1:D:112:TYR:HE2	1.79	0.44
1:D:260:ILE:HG22	1:D:264:ILE:CD1	2.43	0.44
4:E:18:ILE:HD13	4:E:18:ILE:HG21	1.84	0.44
4:E:90:VAL:HG22	4:E:99:PHE:HE1	1.82	0.44
4:E:216:ARG:C	4:E:218:PRO:CD	2.86	0.44
4:E:294:LEU:HA	4:E:297:VAL:HG23	2.00	0.44
1:A:121:PRO:HB2	2:B:149:TYR:CZ	2.53	0.44
1:A:382:ILE:O	1:A:386:MET:HE2	2.17	0.44
1:A:397:GLU:O	1:A:400:LYS:HB2	2.18	0.44
2:B:7:LEU:HD11	2:B:69:PRO:HD2	2.00	0.44
2:B:135:PHE:H	2:B:136:PRO:CD	2.30	0.44
2:B:284:LEU:HA	2:B:287:ILE:CG1	2.47	0.44
3:C:41:ASN:HD22	3:C:41:ASN:HA	1.36	0.44
1:D:28:PHE:CZ	1:D:153:GLY:O	2.71	0.44
1:D:53:ASN:HD22	1:D:123:ILE:HG13	1.83	0.44
1:D:167:LEU:H	1:D:167:LEU:HD13	1.82	0.44
1:D:432:GLU:HG2	1:D:435:GLN:HE21	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD13	1:A:203:TYR:CE2	2.52	0.43
1:A:136:PRO:CA	1:A:277:TYR:OH	2.59	0.43
1:A:207:MET:N	1:A:207:MET:SD	2.91	0.43
2:B:35:LEU:CD2	2:B:56:LEU:CA	2.95	0.43
2:B:35:LEU:HD21	2:B:56:LEU:HA	1.99	0.43
2:B:145:VAL:HG13	2:B:208:THR:HA	2.00	0.43
3:C:161:ASP:HA	3:C:199:LYS:CG	2.43	0.43
1:D:166:ASP:OD2	1:D:181:TYR:CG	2.70	0.43
1:D:233:PHE:CZ	1:D:417:ILE:CD1	3.01	0.43
1:D:244:THR:CG2	1:D:245:LEU:H	2.27	0.43
4:E:182:GLU:HG3	4:E:221:TYR:OH	2.17	0.43
4:E:212:LEU:N	4:E:212:LEU:CD1	2.81	0.43
4:E:284:LYS:CE	4:E:284:LYS:CA	2.91	0.43
4:E:313:THR:C	4:E:314:HIS:CG	2.91	0.43
1:A:62:ASP:OD1	1:A:64:ARG:HB2	2.17	0.43
1:A:77:LYS:CA	1:A:110:LEU:O	2.66	0.43
1:A:93:TYR:CZ	1:A:198:TYR:CE2	3.06	0.43
1:A:203:TYR:HB3	1:A:205:PHE:HE1	1.82	0.43
2:B:20:ARG:H	2:B:20:ARG:CD	2.25	0.43
3:C:113:ARG:NE	3:C:119:THR:CG2	2.77	0.43
3:C:228:TYR:CE1	3:C:229:VAL:HG22	2.53	0.43
1:D:78:ILE:O	1:D:78:ILE:HD13	2.13	0.43
1:D:103:VAL:HG13	1:D:118:TRP:CZ2	2.53	0.43
4:E:42:LEU:HD22	4:E:183:TRP:CH2	2.53	0.43
4:E:123:TYR:HD1	4:E:123:TYR:H	1.66	0.43
4:E:129:ILE:HG13	4:E:129:ILE:O	2.18	0.43
4:E:214:ILE:C	4:E:214:ILE:CD1	2.77	0.43
1:A:137:PHE:O	1:A:208:GLN:HB2	2.18	0.43
2:B:248:LYS:HE2	2:B:248:LYS:HB2	1.70	0.43
3:C:68:THR:N	3:C:116:GLY:N	2.67	0.43
3:C:94:LEU:O	3:C:98:ASN:CB	2.66	0.43
3:C:223:ARG:CG	3:C:224:LYS:H	2.31	0.43
1:D:225:PHE:HD1	1:D:225:PHE:C	2.21	0.43
1:D:250:LEU:CD2	1:D:292:THR:HB	2.47	0.43
4:E:56:GLU:CG	4:E:118:LEU:HD22	2.46	0.43
1:A:38:ILE:CD1	1:A:38:ILE:H	2.31	0.43
1:A:79:ARG:HH11	1:A:107:LYS:HZ1	1.63	0.43
1:A:220:ILE:HG22	1:A:220:ILE:O	2.17	0.43
1:A:376:ILE:O	1:A:380:LYS:CE	2.65	0.43
2:B:140:GLN:O	2:B:213:ILE:CD1	2.65	0.43
2:B:202:PRO:HG2	2:B:203:SER:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:LEU:HD23	3:C:52:LEU:HD12	2.00	0.43
3:C:106:TYR:O	3:C:107:PHE:CD1	2.70	0.43
1:D:86:TRP:HE3	1:D:86:TRP:H	1.65	0.43
4:E:20:PRO:HG3	4:E:61:ASP:CA	2.41	0.43
4:E:136:PHE:HZ	4:E:217:LYS:HD2	1.75	0.43
4:E:195:ASN:CB	4:E:205:PHE:O	2.66	0.43
4:E:275:THR:O	4:E:279:VAL:HG23	2.18	0.43
1:A:287:SER:O	1:A:291:VAL:HG23	2.19	0.43
2:B:10:VAL:HG12	2:B:11:LEU:HD23	2.00	0.43
2:B:290:LEU:HD11	2:B:453:SER:CB	2.49	0.43
2:B:411:ILE:HG13	2:B:411:ILE:H	1.69	0.43
2:B:434:VAL:HG12	2:B:438:LEU:HD12	1.98	0.43
3:C:273:LEU:CD2	3:C:276:GLN:CB	2.92	0.43
1:D:57:ARG:CZ	1:D:117:MET:HE1	2.48	0.43
1:D:283:ILE:CA	1:D:286:ILE:HD12	2.46	0.43
1:D:377:GLU:CG	4:E:415:CYS:HB2	2.48	0.43
4:E:30:VAL:HG22	4:E:59:TRP:CB	2.48	0.43
4:E:59:TRP:N	4:E:59:TRP:HE3	2.16	0.43
1:A:72:TYR:CB	1:A:112:TYR:CB	2.83	0.43
1:A:107:LYS:CE	2:B:150:THR:CB	2.94	0.43
1:A:201:ILE:HG22	1:A:203:TYR:CE1	2.54	0.43
2:B:105:HIS:N	2:B:118:TRP:CH2	2.86	0.43
2:B:187:SER:OG	2:B:216:LYS:HE2	2.19	0.43
2:B:431:VAL:CG2	2:B:433:MET:HG2	2.49	0.43
3:C:69:TRP:CD1	3:C:114:PRO:C	2.92	0.43
3:C:141:TRP:HH2	3:C:223:ARG:HD3	1.80	0.43
3:C:149:THR:HA	3:C:160:MET:HE2	2.00	0.43
1:D:36:GLN:O	1:D:54:VAL:HA	2.19	0.43
1:D:68:ASN:HB2	1:D:69:PRO:HD3	1.99	0.43
1:D:92:LEU:HG	1:D:124:PHE:CE1	2.53	0.43
1:D:411:LEU:HD23	1:D:414:PHE:HD2	1.82	0.43
4:E:27:VAL:CG1	4:E:153:HIS:C	2.84	0.43
4:E:139:GLN:O	4:E:213:ILE:HA	2.17	0.43
1:A:167:LEU:HA	1:A:170:PHE:HB2	2.01	0.43
1:A:227:PHE:HD1	1:A:230:VAL:HB	1.83	0.43
1:A:410:LEU:HD13	1:A:414:PHE:HD2	1.84	0.43
2:B:38:THR:CG2	2:B:55:PHE:HE1	2.27	0.43
2:B:238:VAL:HG21	2:B:255:ALA:HB1	1.99	0.43
2:B:274:SER:O	2:B:278:PRO:CD	2.66	0.43
2:B:468:PHE:O	2:B:469:ALA:HB2	2.18	0.43
3:C:40:SER:O	3:C:41:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ILE:HD13	3:C:89:ILE:HG21	1.62	0.43
3:C:232:PHE:O	3:C:235:PRO:HD2	2.18	0.43
3:C:288:ILE:HD13	3:C:290:LYS:CD	2.48	0.43
3:C:429:ILE:C	3:C:429:ILE:HD12	2.38	0.43
1:D:36:GLN:NE2	1:D:36:GLN:HA	2.28	0.43
1:D:40:LEU:HD22	1:D:52:THR:HG1	1.82	0.43
1:D:75:ILE:CD1	4:E:24:LEU:HD12	2.49	0.43
1:D:114:GLY:O	1:D:116:ILE:HD13	2.19	0.43
4:E:35:THR:HG23	4:E:175:GLU:OE2	2.18	0.43
4:E:58:GLN:HA	4:E:59:TRP:CE3	2.54	0.43
4:E:103:TYR:HD2	4:E:104:TYR:CD1	2.37	0.43
4:E:126:THR:O	4:E:126:THR:CG2	2.66	0.43
4:E:213:ILE:O	4:E:213:ILE:CG2	2.66	0.43
4:E:241:PHE:C	4:E:243:PRO:HD2	2.39	0.43
4:E:287:ILE:HG13	4:E:291:PHE:CD2	2.54	0.43
1:A:265:PRO:CD	1:A:266:SER:N	2.81	0.43
2:B:184:GLY:C	2:B:186:TRP:H	2.21	0.43
2:B:259:LEU:HD23	2:B:259:LEU:C	2.38	0.43
3:C:431:LYS:HZ3	1:D:382:ILE:HD12	1.84	0.43
1:D:16:ASN:HD22	1:D:16:ASN:N	2.17	0.43
1:D:45:GLU:CD	1:D:271:VAL:CG2	2.87	0.43
1:D:160:PRO:HD3	1:D:185:LYS:HB2	1.91	0.43
1:D:240:GLY:O	1:D:243:MET:SD	2.77	0.43
1:D:416:LEU:O	1:D:420:ILE:HG23	2.19	0.43
1:A:7:LEU:HD22	1:A:70:ALA:HA	2.01	0.43
1:A:28:PHE:CD1	1:A:154:THR:O	2.72	0.43
1:A:80:LEU:CD2	1:A:110:LEU:HB2	2.48	0.43
1:A:131:ILE:CG1	1:A:140:GLN:HG2	2.48	0.43
1:A:179:LYS:CE	1:A:208:GLN:OE1	2.66	0.43
1:A:237:THR:HB	1:A:406:ILE:CG2	2.49	0.43
2:B:92:LEU:HD22	2:B:146:PHE:CG	2.54	0.43
2:B:101:GLU:CD	2:B:123:ILE:CG2	2.87	0.43
2:B:105:HIS:H	2:B:118:TRP:HH2	1.65	0.43
3:C:251:ALA:C	3:C:253:SER:H	2.21	0.43
3:C:284:ALA:O	3:C:285:VAL:HG12	2.18	0.43
1:D:37:LEU:N	1:D:54:VAL:HG12	2.34	0.43
4:E:5:ARG:H	4:E:5:ARG:HG2	1.44	0.43
4:E:45:LYS:HG2	4:E:279:VAL:C	2.39	0.43
4:E:140:ASN:CG	4:E:211:PHE:HB3	2.39	0.43
4:E:152:ALA:CB	4:E:204:ASP:O	2.63	0.43
4:E:273:PRO:O	4:E:277:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:287:ILE:HG13	4:E:291:PHE:HE2	1.83	0.43
1:A:35:LEU:HD13	1:A:203:TYR:CZ	2.54	0.43
1:A:41:ILE:CD1	1:A:51:GLU:OE1	2.60	0.43
1:A:77:LYS:HD2	1:A:111:ASP:OD2	2.19	0.43
1:A:139:GLN:HB2	1:A:207:MET:O	2.19	0.43
1:A:409:ILE:H	1:A:409:ILE:HG13	1.54	0.43
2:B:38:THR:HG23	2:B:54:VAL:HA	2.00	0.43
2:B:281:ILE:HG22	2:B:285:MET:CA	2.48	0.43
2:B:296:ILE:O	2:B:296:ILE:CG2	2.67	0.43
3:C:247:PHE:HE1	3:C:309:VAL:HG23	1.77	0.43
1:D:15:TYR:HE2	1:D:84:ASP:HB3	1.81	0.43
1:D:189:TYR:N	1:D:197:PRO:HD2	2.33	0.43
1:D:225:PHE:CD1	1:D:225:PHE:C	2.92	0.43
4:E:104:TYR:N	4:E:104:TYR:HD1	2.16	0.43
4:E:151:ASN:HA	4:E:205:PHE:CG	2.54	0.43
4:E:173:ASP:OD2	4:E:185:ILE:HD13	2.18	0.43
4:E:453:ILE:HD12	4:E:454:ALA:N	2.34	0.43
1:A:20:ARG:CG	1:A:20:ARG:O	2.67	0.42
2:B:93:MET:CG	2:B:206:ASP:HB3	2.49	0.42
2:B:226:VAL:CG2	2:B:227:PRO:CD	2.95	0.42
2:B:277:VAL:N	2:B:278:PRO:CD	2.79	0.42
3:C:35:LEU:HD22	3:C:215:VAL:CG2	2.46	0.42
3:C:54:THR:O	3:C:126:PHE:CD2	2.72	0.42
3:C:72:SER:HA	3:C:76:ASP:HB2	1.99	0.42
3:C:125:ILE:O	3:C:125:ILE:HG22	2.19	0.42
3:C:148:PHE:C	3:C:149:THR:HG22	2.38	0.42
3:C:449:VAL:HG12	3:C:452:THR:CB	2.39	0.42
1:D:18:VAL:O	1:D:18:VAL:HG12	2.19	0.42
4:E:44:GLU:CB	4:E:280:PRO:CB	2.58	0.42
4:E:242:LEU:N	4:E:243:PRO:HD2	2.34	0.42
4:E:242:LEU:HA	4:E:245:GLN:OE1	2.19	0.42
4:E:267:LEU:HA	4:E:270:GLN:HG3	2.00	0.42
1:A:67:TRP:HB2	1:A:112:TYR:O	2.19	0.42
1:A:241:GLU:HG2	1:A:241:GLU:O	2.19	0.42
1:A:267:THR:HG23	1:A:271:VAL:HG21	1.99	0.42
2:B:32:ARG:HH21	2:B:60:TRP:CA	2.31	0.42
2:B:198:ARG:HH11	2:B:198:ARG:CG	2.29	0.42
2:B:216:LYS:O	2:B:216:LYS:CD	2.59	0.42
3:C:30:VAL:HG23	3:C:157:GLU:N	2.30	0.42
3:C:296:MET:HE3	3:C:296:MET:N	2.33	0.42
3:C:474:VAL:O	3:C:474:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:TRP:CD2	1:D:86:TRP:HH2	2.37	0.42
1:D:89:ASP:OD1	1:D:89:ASP:O	2.36	0.42
1:D:176:TRP:HB2	1:D:209:ARG:HA	2.02	0.42
4:E:91:LEU:HB3	4:E:94:ASN:N	2.27	0.42
4:E:127:CYS:SG	4:E:128:PRO:CD	3.02	0.42
4:E:140:ASN:OD1	4:E:211:PHE:CG	2.72	0.42
4:E:296:ILE:CG1	4:E:297:VAL:N	2.81	0.42
1:A:85:VAL:HG12	1:A:86:TRP:N	2.34	0.42
1:A:133:THR:C	1:A:136:PRO:CD	2.87	0.42
1:A:199:LEU:C	1:A:200:ASP:OD1	2.57	0.42
1:A:305:THR:CB	1:A:400:LYS:CB	2.97	0.42
2:B:34:GLY:O	2:B:35:LEU:CD2	2.68	0.42
2:B:276:SER:O	2:B:276:SER:OG	2.35	0.42
2:B:287:ILE:N	2:B:290:LEU:HD12	2.34	0.42
3:C:52:LEU:HD22	3:C:52:LEU:H	1.84	0.42
3:C:59:ASP:OD1	3:C:121:LEU:CD1	2.65	0.42
3:C:92:ILE:HG23	3:C:160:MET:HE1	2.00	0.42
1:D:394:ASN:C	1:D:396:ALA:N	2.67	0.42
1:D:398:GLU:HB2	1:D:401:TYR:CE1	2.54	0.42
4:E:159:LEU:CD1	4:E:191:LYS:C	2.79	0.42
4:E:188:ARG:N	4:E:189:PRO:HD3	2.32	0.42
4:E:450:CYS:O	4:E:454:ALA:HB2	2.19	0.42
1:A:160:PRO:HG2	1:A:185:LYS:CD	2.47	0.42
1:A:195:ASP:OD1	1:A:197:PRO:HG3	2.19	0.42
1:A:380:LYS:HB2	1:A:381:TYR:HD1	1.84	0.42
1:A:382:ILE:HG12	1:A:382:ILE:H	1.66	0.42
1:A:410:LEU:O	1:A:414:PHE:HB2	2.19	0.42
2:B:32:ARG:HE	2:B:59:ALA:C	2.22	0.42
3:C:59:ASP:HA	3:C:121:LEU:HB2	1.97	0.42
3:C:271:LEU:C	3:C:271:LEU:HD23	2.40	0.42
1:D:49:ILE:HA	1:D:49:ILE:HD13	1.72	0.42
1:D:170:PHE:CD1	1:D:170:PHE:C	2.93	0.42
1:D:181:TYR:CE1	1:D:203:TYR:HB3	2.46	0.42
1:D:187:TRP:CH2	1:D:189:TYR:CB	2.96	0.42
1:D:245:LEU:C	1:D:245:LEU:CD2	2.88	0.42
1:D:256:PHE:CZ	4:E:263:ILE:HA	2.54	0.42
1:D:295:VAL:HG23	1:D:296:ILE:N	2.34	0.42
4:E:91:LEU:HD13	4:E:145:PHE:N	2.34	0.42
4:E:242:LEU:HG	4:E:243:PRO:HD3	2.01	0.42
4:E:418:ALA:HA	4:E:421:PHE:HD2	1.84	0.42
1:A:7:LEU:HD22	1:A:70:ALA:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ILE:HG12	1:A:140:GLN:HG2	2.01	0.42
2:B:40:LEU:HB2	2:B:52:THR:HG23	2.00	0.42
2:B:463:PRO:HB2	2:B:464:PRO:CD	2.49	0.42
3:C:74:TYR:O	3:C:78:SER:HA	2.18	0.42
3:C:111:LEU:O	3:C:118:VAL:HG13	2.20	0.42
1:D:37:LEU:HA	1:D:54:VAL:HG13	2.00	0.42
1:D:227:PHE:C	1:D:227:PHE:CD1	2.92	0.42
1:D:252:SER:HB2	4:E:259:LEU:CD2	2.49	0.42
2:B:128:CYS:SG	2:B:144:MET:CG	3.06	0.42
2:B:135:PHE:HB2	2:B:279:ILE:HG21	2.01	0.42
2:B:211:LEU:HB3	2:B:213:ILE:HG23	2.00	0.42
3:C:69:TRP:HB2	3:C:74:TYR:H	1.84	0.42
3:C:80:LEU:O	3:C:112:VAL:CB	2.66	0.42
3:C:274:THR:CG2	3:C:275:SER:N	2.82	0.42
1:D:47:ASN:O	1:D:49:ILE:HG12	2.19	0.42
1:D:63:VAL:C	1:D:65:LEU:H	2.22	0.42
1:D:212:LEU:O	1:D:216:VAL:CG2	2.67	0.42
1:D:407:ASP:HA	1:D:410:LEU:HD23	2.01	0.42
4:E:58:GLN:HA	4:E:59:TRP:HE3	1.84	0.42
4:E:128:PRO:HD2	4:E:141:CYS:HA	2.02	0.42
1:A:148:ILE:O	1:A:198:TYR:CE2	2.73	0.42
1:A:235:LEU:HA	2:B:306:HIS:CD2	2.55	0.42
1:A:251:LEU:CG	4:E:260:ALA:CB	2.98	0.42
2:B:160:HIS:HE1	2:B:207:VAL:HG21	1.85	0.42
3:C:154:ASN:CA	3:C:211:ASN:CB	2.95	0.42
3:C:179:ILE:HD11	3:C:195:LYS:HB3	2.02	0.42
3:C:429:ILE:HG13	3:C:430:VAL:CG2	2.50	0.42
3:C:470:ILE:HD13	3:C:470:ILE:HA	1.84	0.42
1:D:60:TRP:O	1:D:116:ILE:HG12	2.20	0.42
1:D:179:LYS:HB2	1:D:206:ILE:HG22	2.01	0.42
1:D:278:MET:HE1	1:D:282:MET:N	2.35	0.42
4:E:66:TRP:CE3	4:E:70:GLU:HG2	2.54	0.42
1:A:12:LEU:HD12	1:A:12:LEU:O	2.20	0.42
1:A:41:ILE:O	1:A:42:ASN:CG	2.57	0.42
1:A:185:LYS:O	1:A:186:HIS:HB2	2.20	0.42
1:A:224:LEU:C	1:A:224:LEU:HD12	2.39	0.42
2:B:46:LYS:HB2	2:B:276:SER:O	2.19	0.42
2:B:186:TRP:CG	2:B:215:ARG:HD2	2.55	0.42
3:C:180:ASP:HB2	3:C:195:LYS:CB	2.50	0.42
3:C:269:VAL:HA	3:C:272:LEU:HD11	2.02	0.42
3:C:431:LYS:HE2	1:D:379:VAL:HG22	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:476:GLY:HA2	3:C:479:ASN:HB3	2.01	0.42
1:D:7:LEU:HD22	1:D:70:ALA:O	2.19	0.42
1:D:36:GLN:HB3	1:D:55:ARG:CB	2.48	0.42
1:D:149:TRP:CZ2	1:D:150:THR:HB	2.55	0.42
1:D:231:LEU:HD23	1:D:231:LEU:HA	1.70	0.42
1:D:398:GLU:CB	1:D:401:TYR:CZ	3.03	0.42
4:E:24:LEU:HA	4:E:24:LEU:HD23	1.48	0.42
4:E:45:LYS:HZ1	4:E:278:ASN:HA	1.82	0.42
4:E:76:LEU:O	4:E:77:VAL:HG23	2.20	0.42
1:A:57:ARG:CG	1:A:57:ARG:O	2.67	0.42
1:A:92:LEU:C	1:A:95:ASN:HD22	2.23	0.42
1:A:130:ILE:CD1	1:A:130:ILE:N	2.81	0.42
1:A:148:ILE:HG21	1:A:198:TYR:HB3	1.99	0.42
1:A:218:VAL:C	1:A:221:PRO:HD2	2.40	0.42
1:A:279:LEU:HD13	1:A:282:MET:HB3	2.01	0.42
1:A:395:ALA:O	1:A:399:TRP:CB	2.68	0.42
2:B:95:ASN:HA	2:B:127:SER:H	1.85	0.42
2:B:139:TRP:O	2:B:140:GLN:CG	2.68	0.42
2:B:456:LEU:N	2:B:456:LEU:CD2	2.82	0.42
3:C:192:ILE:CD1	3:C:221:ILE:HG21	2.49	0.42
1:D:58:GLN:HE22	1:D:87:LEU:HD11	1.85	0.42
1:D:90:LEU:HD23	1:D:90:LEU:HA	1.69	0.42
1:D:429:ARG:N	1:D:429:ARG:NE	2.67	0.42
4:E:26:HIS:CA	4:E:27:VAL:HG13	2.50	0.42
4:E:76:LEU:O	4:E:77:VAL:CG2	2.68	0.42
1:A:46:VAL:HG21	1:A:269:SER:C	2.40	0.42
1:A:157:SER:HB2	1:A:199:LEU:HD11	2.00	0.42
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.79	0.42
1:A:220:ILE:O	1:A:220:ILE:CG2	2.67	0.42
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.94	0.42
1:A:238:ASP:HB3	2:B:306:HIS:HE1	1.74	0.42
3:C:247:PHE:CD2	3:C:460:ILE:CD1	3.02	0.42
3:C:467:LEU:O	3:C:468:GLY:C	2.57	0.42
1:D:19:ILE:H	1:D:19:ILE:HG13	1.66	0.42
1:D:247:ILE:HA	1:D:247:ILE:HD13	1.61	0.42
1:D:429:ARG:NE	1:D:429:ARG:CA	2.83	0.42
4:E:63:ARG:O	4:E:64:LEU:HG	2.20	0.42
4:E:75:ASP:HB3	4:E:110:TYR:OH	2.20	0.42
4:E:94:ASN:ND2	4:E:126:THR:H	2.18	0.42
4:E:172:ILE:CG2	4:E:174:PRO:HD2	2.49	0.42
4:E:267:LEU:CD1	4:E:270:GLN:OE1	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG3	1:A:274:ILE:HG23	2.01	0.41
1:A:159:SER:HB2	1:A:160:PRO:CD	2.50	0.41
1:A:163:ASP:O	1:A:164:ARG:HG3	2.19	0.41
1:A:189:TYR:CA	1:A:197:PRO:HD2	2.32	0.41
1:A:245:LEU:HD21	2:B:250:SER:HA	1.93	0.41
2:B:409:LYS:HE2	3:C:423:ILE:HA	2.02	0.41
1:D:106:THR:HG23	1:D:107:LYS:NZ	2.35	0.41
4:E:59:TRP:CH2	4:E:107:VAL:CG1	3.02	0.41
1:A:232:VAL:O	1:A:236:PRO:HG3	2.20	0.41
2:B:456:LEU:CD2	2:B:456:LEU:H	2.33	0.41
3:C:110:VAL:HG22	3:C:120:TRP:CG	2.55	0.41
3:C:303:VAL:O	3:C:306:CYS:HB2	2.20	0.41
3:C:435:GLU:O	3:C:439:TYR:HD1	2.03	0.41
1:D:95:ASN:ND2	1:D:127:TYR:C	2.74	0.41
1:D:176:TRP:HB3	1:D:209:ARG:CG	2.50	0.41
4:E:44:GLU:CG	4:E:129:ILE:CG1	2.89	0.41
4:E:133:TYR:CG	4:E:139:GLN:CB	3.03	0.41
1:A:103:VAL:HG12	1:A:104:HIS:N	2.35	0.41
1:A:213:TYR:CG	1:A:214:PHE:N	2.88	0.41
2:B:248:LYS:O	2:B:249:MET:C	2.58	0.41
3:C:58:MET:SD	3:C:92:ILE:HD12	2.58	0.41
3:C:431:LYS:NZ	1:D:382:ILE:CD1	2.83	0.41
1:D:63:VAL:CG1	1:D:64:ARG:N	2.81	0.41
1:D:250:LEU:O	1:D:254:THR:HG22	2.20	0.41
1:D:419:ILE:CD1	1:D:420:ILE:CG2	2.98	0.41
4:E:17:ARG:NH1	4:E:18:ILE:HG22	2.33	0.41
4:E:66:TRP:CD1	4:E:66:TRP:N	2.88	0.41
4:E:103:TYR:HD1	4:E:117:TRP:HH2	1.68	0.41
4:E:181:GLY:HA2	4:E:183:TRP:CE3	2.55	0.41
4:E:297:VAL:O	4:E:300:CYS:HB3	2.20	0.41
1:A:157:SER:HB2	1:A:199:LEU:HD12	2.00	0.41
1:A:257:LEU:O	1:A:260:ILE:HG22	2.20	0.41
1:A:384:GLU:OE2	1:A:387:LYS:HG3	2.21	0.41
3:C:149:THR:HB	3:C:214:ASP:HA	2.02	0.41
1:D:45:GLU:CB	1:D:271:VAL:CG2	2.86	0.41
1:D:46:VAL:HG21	1:D:270:ALA:HA	2.02	0.41
1:D:57:ARG:NE	1:D:117:MET:HE3	2.36	0.41
1:D:78:ILE:CD1	1:D:78:ILE:C	2.89	0.41
4:E:44:GLU:CG	4:E:280:PRO:CB	2.65	0.41
4:E:117:TRP:O	4:E:118:LEU:CB	2.68	0.41
1:A:136:PRO:HB3	1:A:138:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASP:N	1:A:181:TYR:HD1	2.17	0.41
1:A:420:ILE:CG1	1:A:421:GLY:H	2.26	0.41
2:B:198:ARG:HG3	2:B:198:ARG:NH1	2.33	0.41
2:B:248:LYS:CD	2:B:252:SER:CB	2.62	0.41
3:C:148:PHE:N	3:C:148:PHE:HD1	2.18	0.41
3:C:191:GLU:CD	3:C:222:ARG:HB3	2.40	0.41
3:C:201:ILE:HA	3:C:213:GLN:HA	2.01	0.41
1:D:79:ARG:HH12	4:E:154:GLU:CD	2.23	0.41
1:D:137:PHE:HE1	1:D:210:ILE:HD12	1.86	0.41
1:D:216:VAL:O	1:D:220:ILE:CG1	2.64	0.41
1:D:291:VAL:HG12	1:D:295:VAL:CG1	2.50	0.41
4:E:2:GLU:HB3	4:E:6:LEU:HG	2.01	0.41
4:E:19:LYS:HZ1	4:E:154:GLU:CB	2.31	0.41
4:E:91:LEU:HB2	4:E:95:VAL:HG23	2.03	0.41
4:E:159:LEU:CD1	4:E:192:LYS:HA	2.47	0.41
4:E:237:VAL:O	4:E:237:VAL:HG12	2.21	0.41
4:E:242:LEU:HG	4:E:243:PRO:CD	2.51	0.41
1:A:92:LEU:HD23	1:A:92:LEU:H	1.86	0.41
1:A:398:GLU:HA	1:A:401:TYR:CE1	2.56	0.41
2:B:138:ASP:OD1	2:B:464:PRO:HB2	2.21	0.41
2:B:186:TRP:HB2	2:B:187:SER:H	1.66	0.41
2:B:258:ALA:CB	3:C:265:LEU:HD13	2.50	0.41
3:C:222:ARG:NH2	3:C:224:LYS:N	2.68	0.41
3:C:446:TRP:HA	3:C:446:TRP:CE3	2.55	0.41
1:D:92:LEU:H	1:D:92:LEU:HD23	1.80	0.41
1:D:107:LYS:HE3	4:E:149:THR:CA	2.47	0.41
1:D:295:VAL:HG13	1:D:295:VAL:H	1.44	0.41
1:D:420:ILE:HA	1:D:423:VAL:CB	2.51	0.41
4:E:55:ILE:HG13	4:E:55:ILE:O	2.20	0.41
4:E:58:GLN:HA	4:E:115:MET:O	2.21	0.41
4:E:88:ASP:OD2	4:E:149:THR:HB	2.20	0.41
4:E:133:TYR:CD1	4:E:139:GLN:N	2.77	0.41
4:E:133:TYR:HA	4:E:135:PRO:HD2	2.03	0.41
1:A:51:GLU:HG3	1:A:125:LYS:HD2	2.02	0.41
1:A:137:PHE:HE1	1:A:210:ILE:HB	1.84	0.41
1:A:293:VAL:O	1:A:297:ASN:HB3	2.20	0.41
1:A:387:LYS:H	1:A:387:LYS:HG2	1.55	0.41
2:B:40:LEU:CD2	2:B:52:THR:OG1	2.63	0.41
2:B:201:ASP:CG	2:B:202:PRO:HD2	2.40	0.41
2:B:437:ARG:HG2	2:B:437:ARG:HH11	1.86	0.41
3:C:130:CYS:SG	3:C:131:PRO:HD2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:PHE:O	3:C:141:TRP:HD1	2.02	0.41
1:D:144:MET:CE	1:D:205:PHE:CE1	3.03	0.41
4:E:45:LYS:HB3	4:E:277:LEU:O	2.21	0.41
4:E:270:GLN:O	4:E:273:PRO:HG2	2.21	0.41
4:E:297:VAL:HB	4:E:298:THR:H	1.57	0.41
1:A:92:LEU:CB	1:A:95:ASN:HD22	2.34	0.41
1:A:133:THR:O	1:A:140:GLN:HB2	2.20	0.41
1:A:245:LEU:CD1	2:B:250:SER:CA	2.98	0.41
1:A:305:THR:O	1:A:306:HIS:HB3	2.20	0.41
2:B:147:LYS:HE2	2:B:148:SER:OG	2.20	0.41
2:B:232:SER:HA	2:B:235:ALA:CB	2.48	0.41
2:B:260:THR:O	2:B:264:LEU:HG	2.20	0.41
2:B:286:PHE:CD1	2:B:287:ILE:HG23	2.54	0.41
2:B:465:ASP:CG	2:B:466:ASN:H	2.23	0.41
3:C:132:ILE:O	3:C:133:ASN:HB2	2.18	0.41
3:C:201:ILE:CG1	3:C:211:ASN:O	2.59	0.41
3:C:471:PHE:C	3:C:473:PHE:N	2.74	0.41
1:D:137:PHE:HE1	1:D:210:ILE:CD1	2.32	0.41
1:D:264:ILE:HA	1:D:267:THR:HG22	2.02	0.41
1:D:423:VAL:HA	1:D:426:PHE:HB3	2.02	0.41
4:E:177:PHE:CD1	4:E:178:THR:O	2.74	0.41
4:E:436:ASN:HA	4:E:439:TRP:CD1	2.54	0.41
1:A:41:ILE:HG21	1:A:123:ILE:HD11	2.01	0.41
1:A:56:LEU:CD1	1:A:90:LEU:HD13	2.51	0.41
1:A:146:LEU:HD22	1:A:203:TYR:CZ	2.55	0.41
1:A:217:ASN:O	1:A:221:PRO:CD	2.68	0.41
1:A:293:VAL:CG1	1:A:294:VAL:N	2.84	0.41
2:B:28:LYS:CD	2:B:156:VAL:N	2.84	0.41
2:B:132:VAL:CG1	2:B:279:ILE:C	2.89	0.41
2:B:185:GLN:CB	2:B:219:PHE:CE2	2.83	0.41
2:B:202:PRO:HG2	2:B:203:SER:H	1.86	0.41
2:B:227:PRO:O	2:B:231:ILE:CG1	2.67	0.41
2:B:242:PRO:HG2	2:B:243:PRO:HD2	2.01	0.41
2:B:424:LEU:HD23	2:B:424:LEU:HA	1.81	0.41
2:B:431:VAL:HG23	2:B:433:MET:H	1.86	0.41
3:C:69:TRP:HB2	3:C:74:TYR:CA	2.51	0.41
3:C:288:ILE:CG1	3:C:289:GLY:H	2.21	0.41
3:C:291:TYR:O	3:C:295:ILE:HG13	2.21	0.41
3:C:316:THR:HG21	3:C:447:ASN:CG	2.41	0.41
3:C:462:THR:N	3:C:463:PRO:HD2	2.35	0.41
1:D:32:THR:HG21	1:D:59:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ILE:O	1:D:39:GLN:CG	2.66	0.41
1:D:109:LEU:O	1:D:116:ILE:HA	2.21	0.41
1:D:135:PHE:N	1:D:136:PRO:CD	2.84	0.41
1:D:192:CYS:SG	1:D:193:CYS:N	2.93	0.41
4:E:32:LEU:HD12	4:E:208:ILE:CD1	2.49	0.41
4:E:47:GLU:HA	4:E:129:ILE:CD1	2.26	0.41
4:E:49:LEU:HD12	4:E:49:LEU:C	2.41	0.41
4:E:103:TYR:CD2	4:E:104:TYR:N	2.89	0.41
4:E:146:ARG:NH1	4:E:205:PHE:C	2.74	0.41
4:E:225:ILE:HD12	4:E:225:ILE:HA	1.38	0.41
4:E:269:ALA:O	4:E:273:PRO:CG	2.69	0.41
4:E:453:ILE:HA	4:E:456:LEU:HB3	2.02	0.41
1:A:39:GLN:O	1:A:40:LEU:HD23	2.21	0.41
1:A:146:LEU:HD22	1:A:203:TYR:OH	2.21	0.41
1:A:245:LEU:HD21	2:B:253:ILE:HB	2.03	0.41
2:B:36:THR:HB	2:B:55:PHE:CD2	2.57	0.41
2:B:68:ASP:CB	2:B:69:PRO:HD2	2.51	0.41
2:B:72:TYR:HD1	2:B:112:HIS:HB2	1.85	0.41
2:B:87:GLN:HB3	2:B:104:LEU:CD1	2.23	0.41
2:B:262:PHE:HA	2:B:265:LEU:HD12	2.03	0.41
3:C:1:VAL:HA	3:C:4:GLU:CG	2.35	0.41
3:C:19:LYS:O	3:C:19:LYS:CE	2.69	0.41
3:C:26:HIS:CE1	3:C:66:ARG:NH2	2.84	0.41
3:C:192:ILE:CD1	3:C:221:ILE:HG22	2.50	0.41
3:C:431:LYS:O	3:C:434:LYS:HB3	2.20	0.41
1:D:220:ILE:HG13	1:D:220:ILE:H	1.72	0.41
1:D:220:ILE:HB	1:D:221:PRO:CD	2.51	0.41
1:D:229:THR:CG2	1:D:253:LEU:CD1	2.96	0.41
4:E:27:VAL:HB	4:E:154:GLU:C	2.41	0.41
4:E:35:THR:CG2	4:E:175:GLU:OE1	2.60	0.41
4:E:150:TYR:O	4:E:205:PHE:CD1	2.74	0.41
4:E:182:GLU:OE1	4:E:182:GLU:CA	2.69	0.41
4:E:264:PHE:N	4:E:264:PHE:HD1	2.19	0.41
2:B:104:LEU:CA	2:B:118:TRP:HH2	2.18	0.40
2:B:286:PHE:HD1	2:B:290:LEU:CD1	2.33	0.40
3:C:26:HIS:ND1	3:C:26:HIS:N	2.66	0.40
3:C:69:TRP:NE1	3:C:114:PRO:CA	2.81	0.40
3:C:78:SER:HA	3:C:114:PRO:HB2	1.99	0.40
1:D:132:VAL:O	1:D:274:ILE:CB	2.69	0.40
1:D:153:GLY:HA3	1:D:196:THR:O	2.21	0.40
1:D:225:PHE:CZ	1:D:285:VAL:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:VAL:HA	1:D:262:GLU:OE1	2.22	0.40
1:D:264:ILE:HG13	1:D:264:ILE:H	1.18	0.40
1:D:274:ILE:HG22	1:D:276:LYS:HZ2	1.83	0.40
1:D:274:ILE:CB	1:D:276:LYS:HD3	2.39	0.40
4:E:13:ASP:OD1	4:E:13:ASP:C	2.60	0.40
4:E:262:THR:CG2	4:E:265:LEU:HB2	2.44	0.40
1:A:58:GLN:HB2	1:A:118:TRP:HB3	2.02	0.40
1:A:166:ASP:CA	1:A:181:TYR:CD1	3.04	0.40
1:A:380:LYS:HB2	1:A:381:TYR:CD1	2.56	0.40
2:B:56:LEU:N	2:B:56:LEU:CD2	2.84	0.40
2:B:417:SER:HB2	2:B:421:PHE:HZ	1.86	0.40
3:C:431:LYS:HZ1	1:D:382:ILE:CD1	2.33	0.40
3:C:446:TRP:HA	3:C:446:TRP:HE3	1.86	0.40
1:D:166:ASP:OD1	1:D:178:MET:CE	2.69	0.40
1:D:188:VAL:CG1	1:D:190:TYR:CE1	3.04	0.40
4:E:10:LEU:HD22	4:E:64:LEU:HD21	2.02	0.40
4:E:66:TRP:NE1	4:E:111:ASN:CA	2.67	0.40
4:E:70:GLU:O	4:E:74:ILE:HD13	2.21	0.40
4:E:187:HIS:ND1	4:E:188:ARG:N	2.66	0.40
4:E:255:ILE:HD13	4:E:255:ILE:HA	1.61	0.40
4:E:255:ILE:O	4:E:256:SER:C	2.57	0.40
1:A:17:LYS:HZ3	1:A:83:ASP:HB3	1.87	0.40
1:A:34:GLY:O	1:A:57:ARG:HG2	2.22	0.40
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.96	0.40
2:B:414:GLN:O	2:B:418:ALA:CB	2.69	0.40
3:C:3:GLU:O	3:C:3:GLU:HG2	2.21	0.40
3:C:50:GLU:HB3	3:C:132:ILE:HB	2.03	0.40
3:C:180:ASP:HB2	3:C:195:LYS:HB3	2.04	0.40
3:C:427:ASN:O	3:C:431:LYS:HG3	2.21	0.40
1:D:36:GLN:NE2	1:D:36:GLN:CA	2.81	0.40
1:D:252:SER:CB	4:E:259:LEU:HD22	2.51	0.40
1:D:274:ILE:HG13	1:D:277:TYR:HD2	1.86	0.40
1:D:301:ARG:NH1	1:D:406:ILE:CD1	2.80	0.40
4:E:59:TRP:CE2	4:E:115:MET:CB	3.04	0.40
4:E:60:ASN:N	4:E:60:ASN:ND2	2.68	0.40
4:E:145:PHE:O	4:E:208:ILE:CD1	2.70	0.40
4:E:202:ASP:C	4:E:203:ILE:HG13	2.41	0.40
4:E:271:LYS:N	4:E:273:PRO:HD2	2.35	0.40
1:A:43:VAL:CG1	1:A:50:VAL:CG2	2.90	0.40
1:A:118:TRP:C	1:A:120:PRO:HD3	2.41	0.40
1:A:218:VAL:HG13	1:A:219:ILE:H	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG12	1:A:256:PHE:HD1	1.86	0.40
2:B:24:THR:HG22	2:B:25:VAL:N	2.25	0.40
2:B:425:LYS:CA	2:B:428:TRP:CD1	2.86	0.40
2:B:429:GLN:HA	2:B:429:GLN:NE2	2.34	0.40
3:C:195:LYS:HD2	3:C:218:TYR:O	2.21	0.40
3:C:211:ASN:HB2	3:C:212:TYR:H	1.67	0.40
1:D:72:TYR:HA	1:D:112:TYR:CB	2.52	0.40
1:D:255:VAL:CG1	1:D:256:PHE:N	2.84	0.40
1:D:267:THR:HG23	1:D:268:SER:H	1.86	0.40
4:E:91:LEU:CG	4:E:145:PHE:HB3	2.50	0.40
4:E:117:TRP:NE1	4:E:119:PRO:HD3	2.35	0.40
4:E:133:TYR:CD2	4:E:139:GLN:HB3	2.56	0.40
2:B:143:THR:CG2	2:B:145:VAL:HG22	2.50	0.40
2:B:160:HIS:NE2	2:B:209:PHE:CE1	2.89	0.40
2:B:218:LEU:CD1	2:B:221:ILE:HG12	2.50	0.40
2:B:269:LYS:CE	2:B:270:VAL:CG2	2.69	0.40
2:B:269:LYS:CD	2:B:270:VAL:N	2.83	0.40
3:C:110:VAL:CG1	3:C:111:LEU:H	2.34	0.40
3:C:210:THR:CG2	3:C:211:ASN:N	2.77	0.40
3:C:219:LEU:CD1	3:C:221:ILE:HG22	2.51	0.40
3:C:241:PHE:CD1	3:C:242:LEU:N	2.89	0.40
3:C:249:LEU:HB3	3:C:256:LYS:HZ1	1.75	0.40
3:C:453:ILE:CG2	3:C:454:ASP:N	2.63	0.40
1:D:280:PHE:O	1:D:284:PHE:CD1	2.75	0.40
1:D:412:CYS:O	1:D:415:MET:CE	2.68	0.40
4:E:44:GLU:OE1	4:E:129:ILE:HD12	2.22	0.40
4:E:59:TRP:CE3	4:E:115:MET:HB2	2.56	0.40
4:E:67:ASN:O	4:E:71:TYR:HD2	2.05	0.40
4:E:133:TYR:CA	4:E:135:PRO:HD2	2.52	0.40
4:E:222:ILE:C	4:E:226:ILE:HG13	2.40	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 PDB entries followed by that with respect to all EM entries.

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	366/461 (79%)	251 (69%)	68 (19%)	47 (13%)	0 5
1	D	366/461 (79%)	265 (72%)	54 (15%)	47 (13%)	0 5
2	B	364/493 (74%)	238 (65%)	85 (23%)	41 (11%)	0 7
3	C	364/522 (70%)	244 (67%)	74 (20%)	46 (13%)	0 5
4	E	365/488 (75%)	239 (66%)	76 (21%)	50 (14%)	0 4
All	All	1825/2425 (75%)	1237 (68%)	357 (20%)	231 (13%)	1 5

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	7	LEU
1	A	48	GLN
1	A	83	ASP
1	A	93	TYR
1	A	97	ASP
1	A	102	ILE
1	A	112	TYR
1	A	131	ILE
1	A	149	TRP
1	A	198	TYR
1	A	215	VAL
1	A	248	SER
1	A	249	VAL
1	A	282	MET
1	A	292	THR
1	A	293	VAL
1	A	303	PRO
1	A	304	SER
1	A	392	SER
1	A	420	ILE
2	B	2	VAL
2	B	27	ASP
2	B	48	GLU
2	B	68	ASP
2	B	81	PRO
2	B	89	ASP
2	B	90	ILE

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Mol	Chain	Res	Type
2	B	93	MET
2	B	94	ASN
2	B	99	SER
2	B	107	ASN
2	B	129	THR
2	B	156	VAL
2	B	185	GLN
2	B	206	ASP
2	B	277	VAL
2	B	280	ILE
2	B	306	HIS
2	B	307	ARG
3	C	2	ASN
3	C	13	ILE
3	C	30	VAL
3	C	71	ALA
3	C	99	ASP
3	C	115	ASN
3	C	131	PRO
3	C	132	ILE
3	C	180	ASP
3	C	212	TYR
3	C	224	LYS
3	C	239	ILE
3	C	253	SER
3	C	288	ILE
3	C	301	GLY
3	C	303	VAL
3	C	310	LEU
3	C	434	LYS
3	C	453	ILE
3	C	475	MET
3	C	484	LYS
1	D	3	HIS
1	D	24	HIS
1	D	27	HIS
1	D	30	ASP
1	D	45	GLU
1	D	64	ARG
1	D	74	GLY
1	D	75	ILE
1	D	93	TYR

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Mol	Chain	Res	Type
1	D	94	ASN
1	D	97	ASP
1	D	102	ILE
1	D	113	THR
1	D	130	ILE
1	D	131	ILE
1	D	136	PRO
1	D	153	GLY
1	D	235	LEU
1	D	239	SER
1	D	241	GLU
1	D	276	LYS
1	D	282	MET
1	D	301	ARG
1	D	436	GLU
4	E	2	GLU
4	E	16	LYS
4	E	27	VAL
4	E	68	THR
4	E	82	GLU
4	E	84	LEU
4	E	95	VAL
4	E	98	GLN
4	E	110	TYR
4	E	128	PRO
4	E	152	ALA
4	E	173	ASP
4	E	217	LYS
4	E	222	ILE
4	E	246	ALA
4	E	249	GLN
4	E	253	LEU
4	E	271	LYS
4	E	298	THR
4	E	429	GLN
4	E	438	ASN
1	A	21	PRO
1	A	28	PHE
1	A	75	ILE
1	A	82	SER
1	A	216	VAL
1	A	239	SER

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Mol	Chain	Res	Type
1	A	426	PHE
2	B	86	TRP
2	B	184	GLY
2	B	198	ARG
2	B	249	MET
2	B	281	ILE
2	B	468	PHE
3	C	87	ILE
3	C	116	GLY
3	C	205	LYS
3	C	471	PHE
1	D	2	GLU
1	D	4	GLU
1	D	280	PHE
1	D	423	VAL
1	D	426	PHE
4	E	47	GLU
4	E	101	VAL
4	E	129	ILE
4	E	161	ALA
4	E	443	GLY
4	E	461	GLY
4	E	464	ALA
1	A	4	GLU
1	A	27	HIS
1	A	76	LYS
1	A	148	ILE
1	A	212	LEU
1	A	436	GLU
2	B	76	LYS
2	B	95	ASN
2	B	137	PHE
3	C	240	SER
3	C	440	ASP
3	C	482	PRO
1	D	28	PHE
1	D	68	ASN
1	D	76	LYS
1	D	84	ASP
1	D	162	SER
1	D	174	GLY
1	D	210	ILE

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Mol	Chain	Res	Type
1	D	252	SER
1	D	399	TRP
1	D	403	ALA
4	E	74	ILE
4	E	92	GLU
4	E	133	TYR
4	E	135	PRO
4	E	200	LYS
4	E	206	GLN
4	E	284	LYS
4	E	309	ARG
4	E	439	TRP
1	A	26	THR
1	A	129	GLU
1	A	135	PHE
1	A	162	SER
1	A	180	ASP
1	A	210	ILE
1	A	214	PHE
2	B	39	SER
2	B	102	ILE
2	B	120	PRO
2	B	139	TRP
2	B	147	LYS
2	B	153	THR
2	B	466	ASN
3	C	72	SER
3	C	76	ASP
3	C	137	PHE
3	C	295	ILE
3	C	458	MET
1	D	148	ILE
1	D	236	PRO
4	E	13	ASP
4	E	63	ARG
4	E	280	PRO
4	E	432	SER
1	A	13	GLU
1	A	17	LYS
1	A	167	LEU
1	A	271	VAL
1	A	419	ILE

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Mol	Chain	Res	Type
2	B	75	ILE
2	B	97	ASP
3	C	5	GLU
3	C	95	GLN
3	C	122	PRO
3	C	134	VAL
3	C	211	ASN
1	D	264	ILE
4	E	184	THR
4	E	203	ILE
4	E	231	LEU
4	E	431	ASP
3	C	77	ILE
3	C	136	TYR
1	D	120	PRO
4	E	120	PRO
4	E	279	VAL
2	B	236	ILE
2	B	295	VAL
3	C	138	PRO
3	C	309	VAL
1	D	114	GLY
4	E	297	VAL
1	D	121	PRO
2	B	135	PHE
2	B	463	PRO
3	C	229	VAL
3	C	302	VAL
3	C	449	VAL
1	D	428	GLY
4	E	257	VAL
4	E	446	ILE
1	A	428	GLY
1	D	135	PHE
3	C	104	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	343/427 (80%)	224 (65%)	119 (35%)	0 1
1	D	343/427 (80%)	222 (65%)	121 (35%)	0 1
2	B	340/449 (76%)	240 (71%)	100 (29%)	0 2
3	C	335/475 (70%)	217 (65%)	118 (35%)	0 1
4	E	337/447 (75%)	219 (65%)	118 (35%)	0 1
All	All	1698/2225 (76%)	1122 (66%)	576 (34%)	1 1

All (576) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	GLU
1	A	3	HIS
1	A	6	ARG
1	A	7	LEU
1	A	12	LEU
1	A	20	ARG
1	A	22	VAL
1	A	24	HIS
1	A	25	HIS
1	A	26	THR
1	A	29	VAL
1	A	30	ASP
1	A	36	GLN
1	A	46	VAL
1	A	56	LEU
1	A	61	ILE
1	A	63	VAL
1	A	66	ARG
1	A	68	ASN
1	A	72	TYR
1	A	77	LYS
1	A	87	LEU
1	A	92	LEU
1	A	94	ASN
1	A	95	ASN
1	A	100	PHE
1	A	103	VAL
1	A	105	MET

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Mol	Chain	Res	Type
1	A	107	LYS
1	A	108	LEU
1	A	110	LEU
1	A	111	ASP
1	A	112	TYR
1	A	116	ILE
1	A	124	PHE
1	A	125	LYS
1	A	126	SER
1	A	130	ILE
1	A	132	VAL
1	A	139	GLN
1	A	141	ASN
1	A	142	CYS
1	A	144	MET
1	A	145	LYS
1	A	149	TRP
1	A	156	VAL
1	A	162	SER
1	A	164	ARG
1	A	167	LEU
1	A	168	SER
1	A	173	SER
1	A	180	ASP
1	A	181	TYR
1	A	185	LYS
1	A	189	TYR
1	A	190	TYR
1	A	191	THR
1	A	193	CYS
1	A	195	ASP
1	A	198	TYR
1	A	200	ASP
1	A	207	MET
1	A	209	ARG
1	A	224	LEU
1	A	225	PHE
1	A	227	PHE
1	A	235	LEU
1	A	243	MET
1	A	246	SER
1	A	247	ILE

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Mol	Chain	Res	Type
1	A	248	SER
1	A	254	THR
1	A	255	VAL
1	A	256	PHE
1	A	257	LEU
1	A	260	ILE
1	A	265	PRO
1	A	266	SER
1	A	267	THR
1	A	268	SER
1	A	273	LEU
1	A	274	ILE
1	A	279	LEU
1	A	280	PHE
1	A	282	MET
1	A	284	PHE
1	A	290	ILE
1	A	292	THR
1	A	293	VAL
1	A	296	ILE
1	A	297	ASN
1	A	304	SER
1	A	306	HIS
1	A	374	SER
1	A	381	TYR
1	A	382	ILE
1	A	387	LYS
1	A	389	ASP
1	A	390	GLU
1	A	391	GLU
1	A	399	TRP
1	A	401	TYR
1	A	402	VAL
1	A	405	VAL
1	A	408	HIS
1	A	409	ILE
1	A	410	LEU
1	A	414	PHE
1	A	415	MET
1	A	419	ILE
1	A	420	ILE
1	A	425	VAL

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Mol	Chain	Res	Type
1	A	426	PHE
1	A	430	LEU
1	A	431	ILE
1	A	433	LEU
1	A	434	SER
1	A	435	GLN
2	B	15	TYR
2	B	16	ASN
2	B	18	LYS
2	B	19	VAL
2	B	20	ARG
2	B	21	PRO
2	B	23	GLN
2	B	25	VAL
2	B	27	ASP
2	B	28	LYS
2	B	29	VAL
2	B	33	VAL
2	B	37	LEU
2	B	41	LEU
2	B	42	ILE
2	B	43	LEU
2	B	53	SER
2	B	55	PHE
2	B	56	LEU
2	B	58	LEU
2	B	64	ARG
2	B	69	PRO
2	B	73	GLU
2	B	79	SER
2	B	81	PRO
2	B	82	SER
2	B	89	ASP
2	B	95	ASN
2	B	97	ASP
2	B	102	ILE
2	B	107	ASN
2	B	117	SER
2	B	119	HIS
2	B	120	PRO
2	B	129	THR
2	B	133	MET

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Mol	Chain	Res	Type
2	B	134	TYR
2	B	135	PHE
2	B	136	PRO
2	B	137	PHE
2	B	138	ASP
2	B	145	VAL
2	B	149	TYR
2	B	156	VAL
2	B	158	LEU
2	B	159	GLN
2	B	180	PHE
2	B	181	THR
2	B	182	GLU
2	B	188	ILE
2	B	189	GLU
2	B	191	LYS
2	B	196	ASN
2	B	200	ASP
2	B	201	ASP
2	B	202	PRO
2	B	213	ILE
2	B	216	LYS
2	B	220	TYR
2	B	221	ILE
2	B	225	ILE
2	B	233	ILE
2	B	236	ILE
2	B	237	LEU
2	B	240	TYR
2	B	241	LEU
2	B	248	LYS
2	B	249	MET
2	B	251	LEU
2	B	253	ILE
2	B	261	VAL
2	B	263	LEU
2	B	269	LYS
2	B	275	LEU
2	B	277	VAL
2	B	280	ILE
2	B	281	ILE
2	B	282	SER

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Mol	Chain	Res	Type
2	B	283	TYR
2	B	284	LEU
2	B	288	MET
2	B	291	VAL
2	B	300	VAL
2	B	304	LEU
2	B	307	ARG
2	B	311	THR
2	B	312	HIS
2	B	411	ILE
2	B	421	PHE
2	B	426	LYS
2	B	429	GLN
2	B	436	ASP
2	B	437	ARG
2	B	439	PHE
2	B	440	LEU
2	B	442	ILE
2	B	447	CYS
2	B	462	VAL
2	B	464	PRO
2	B	468	PHE
3	C	2	ASN
3	C	3	GLU
3	C	5	GLU
3	C	7	LEU
3	C	13	ILE
3	C	15	ASN
3	C	16	LYS
3	C	22	ARG
3	C	25	LYS
3	C	27	ASN
3	C	28	ASN
3	C	41	ASN
3	C	43	ILE
3	C	45	LEU
3	C	46	LYS
3	C	48	THR
3	C	50	GLU
3	C	52	LEU
3	C	54	THR
3	C	55	ASN

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Mol	Chain	Res	Type
3	C	60	HIS
3	C	63	TYR
3	C	65	HIS
3	C	66	ARG
3	C	67	LEU
3	C	69	TRP
3	C	78	SER
3	C	85	GLU
3	C	87	ILE
3	C	91	ASP
3	C	92	ILE
3	C	94	LEU
3	C	96	ASN
3	C	99	ASP
3	C	102	TYR
3	C	104	VAL
3	C	106	TYR
3	C	107	PHE
3	C	114	PRO
3	C	115	ASN
3	C	121	LEU
3	C	130	CYS
3	C	140	ASP
3	C	148	PHE
3	C	149	THR
3	C	158	ILE
3	C	160	MET
3	C	162	LEU
3	C	179	ILE
3	C	180	ASP
3	C	199	LYS
3	C	200	ASN
3	C	201	ILE
3	C	202	TYR
3	C	206	PHE
3	C	211	ASN
3	C	214	ASP
3	C	222	ARG
3	C	225	PRO
3	C	228	TYR
3	C	229	VAL
3	C	233	ILE

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Mol	Chain	Res	Type
3	C	241	PHE
3	C	242	LEU
3	C	245	LEU
3	C	249	LEU
3	C	252	GLU
3	C	256	LYS
3	C	259	THR
3	C	262	CYS
3	C	264	LEU
3	C	267	GLN
3	C	271	LEU
3	C	272	LEU
3	C	274	THR
3	C	276	GLN
3	C	278	LEU
3	C	279	PRO
3	C	280	GLU
3	C	285	VAL
3	C	291	TYR
3	C	293	MET
3	C	296	MET
3	C	297	SER
3	C	299	VAL
3	C	302	VAL
3	C	303	VAL
3	C	310	LEU
3	C	311	ASN
3	C	315	ARG
3	C	318	SER
3	C	319	THR
3	C	421	SER
3	C	423	ILE
3	C	426	THR
3	C	428	TYR
3	C	429	ILE
3	C	430	VAL
3	C	432	GLN
3	C	442	GLU
3	C	446	TRP
3	C	451	GLN
3	C	452	THR
3	C	455	ARG

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Mol	Chain	Res	Type
3	C	456	LEU
3	C	458	MET
3	C	460	ILE
3	C	465	MET
3	C	467	LEU
3	C	471	PHE
3	C	472	ILE
3	C	473	PHE
3	C	475	MET
3	C	478	PHE
3	C	479	ASN
3	C	480	ARG
3	C	482	PRO
3	C	484	LYS
1	D	3	HIS
1	D	8	VAL
1	D	16	ASN
1	D	17	LYS
1	D	20	ARG
1	D	22	VAL
1	D	25	HIS
1	D	26	THR
1	D	30	ASP
1	D	36	GLN
1	D	40	LEU
1	D	41	ILE
1	D	46	VAL
1	D	54	VAL
1	D	55	ARG
1	D	56	LEU
1	D	60	TRP
1	D	61	ILE
1	D	62	ASP
1	D	66	ARG
1	D	72	TYR
1	D	76	LYS
1	D	78	ILE
1	D	79	ARG
1	D	80	LEU
1	D	84	ASP
1	D	86	TRP
1	D	91	VAL

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Mol	Chain	Res	Type
1	D	92	LEU
1	D	94	ASN
1	D	95	ASN
1	D	100	PHE
1	D	102	ILE
1	D	105	MET
1	D	106	THR
1	D	107	LYS
1	D	108	LEU
1	D	112	TYR
1	D	116	ILE
1	D	118	TRP
1	D	120	PRO
1	D	123	ILE
1	D	126	SER
1	D	129	GLU
1	D	130	ILE
1	D	133	THR
1	D	135	PHE
1	D	142	CYS
1	D	143	THR
1	D	145	LYS
1	D	149	TRP
1	D	151	TYR
1	D	152	ASP
1	D	154	THR
1	D	156	VAL
1	D	158	ILE
1	D	160	PRO
1	D	164	ARG
1	D	167	LEU
1	D	170	PHE
1	D	176	TRP
1	D	177	VAL
1	D	180	ASP
1	D	185	LYS
1	D	188	VAL
1	D	193	CYS
1	D	198	TYR
1	D	200	ASP
1	D	202	THR
1	D	203	TYR

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Mol	Chain	Res	Type
1	D	207	MET
1	D	209	ARG
1	D	210	ILE
1	D	216	VAL
1	D	219	ILE
1	D	220	ILE
1	D	221	PRO
1	D	222	CYS
1	D	225	PHE
1	D	226	SER
1	D	227	PHE
1	D	230	VAL
1	D	238	ASP
1	D	243	MET
1	D	244	THR
1	D	245	LEU
1	D	247	ILE
1	D	248	SER
1	D	250	LEU
1	D	252	SER
1	D	253	LEU
1	D	257	LEU
1	D	265	PRO
1	D	267	THR
1	D	271	VAL
1	D	272	PRO
1	D	273	LEU
1	D	274	ILE
1	D	278	MET
1	D	280	PHE
1	D	281	THR
1	D	285	VAL
1	D	295	VAL
1	D	377	GLU
1	D	382	ILE
1	D	387	LYS
1	D	389	ASP
1	D	394	ASN
1	D	399	TRP
1	D	400	LYS
1	D	402	VAL
1	D	406	ILE

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Mol	Chain	Res	Type
1	D	407	ASP
1	D	408	HIS
1	D	409	ILE
1	D	410	LEU
1	D	414	PHE
1	D	418	CYS
1	D	422	THR
1	D	426	PHE
1	D	435	GLN
4	E	5	ARG
4	E	13	ASP
4	E	15	ASP
4	E	17	ARG
4	E	18	ILE
4	E	19	LYS
4	E	25	ASP
4	E	27	VAL
4	E	29	ASP
4	E	31	THR
4	E	44	GLU
4	E	45	LYS
4	E	49	LEU
4	E	52	ASN
4	E	55	ILE
4	E	60	ASN
4	E	62	TYR
4	E	63	ARG
4	E	66	TRP
4	E	67	ASN
4	E	69	SER
4	E	70	GLU
4	E	71	TYR
4	E	74	ILE
4	E	75	ASP
4	E	79	ILE
4	E	80	PRO
4	E	81	SER
4	E	82	GLU
4	E	83	LEU
4	E	84	LEU
4	E	86	LEU
4	E	87	PRO

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Mol	Chain	Res	Type
4	E	89	VAL
4	E	90	VAL
4	E	101	VAL
4	E	104	TYR
4	E	106	ASN
4	E	107	VAL
4	E	110	TYR
4	E	116	TYR
4	E	120	PRO
4	E	122	ILE
4	E	123	TYR
4	E	124	ARG
4	E	125	SER
4	E	127	CYS
4	E	134	PHE
4	E	135	PRO
4	E	140	ASN
4	E	143	LEU
4	E	147	SER
4	E	148	GLN
4	E	151	ASN
4	E	154	GLU
4	E	156	ASN
4	E	158	GLN
4	E	162	GLU
4	E	172	ILE
4	E	176	ASP
4	E	177	PHE
4	E	179	GLU
4	E	182	GLU
4	E	184	THR
4	E	188	ARG
4	E	191	LYS
4	E	194	TYR
4	E	195	ASN
4	E	196	TRP
4	E	201	ASP
4	E	202	ASP
4	E	204	ASP
4	E	210	PHE
4	E	212	LEU
4	E	213	ILE

Continued on next page...

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Mol	Chain	Res	Type
4	E	217	LYS
4	E	220	PHE
4	E	221	TYR
4	E	225	ILE
4	E	231	LEU
4	E	232	ILE
4	E	235	LEU
4	E	238	LEU
4	E	239	VAL
4	E	242	LEU
4	E	252	THR
4	E	254	SER
4	E	255	ILE
4	E	256	SER
4	E	258	LEU
4	E	263	ILE
4	E	268	ILE
4	E	270	GLN
4	E	271	LYS
4	E	275	THR
4	E	276	SER
4	E	279	VAL
4	E	284	LYS
4	E	286	LEU
4	E	287	ILE
4	E	291	PHE
4	E	293	SER
4	E	294	LEU
4	E	296	ILE
4	E	297	VAL
4	E	301	VAL
4	E	303	VAL
4	E	309	ARG
4	E	310	THR
4	E	439	TRP
4	E	444	LYS
4	E	452	TRP
4	E	456	LEU
4	E	465	ILE
4	E	467	LEU
4	E	471	LEU
4	E	472	ASN

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Mol	Chain	Res	Type
4	E	473	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	24	HIS
1	A	27	HIS
1	A	58	GLN
1	A	59	GLN
1	A	95	ASN
1	A	299	HIS
1	A	306	HIS
1	A	435	GLN
2	B	23	GLN
2	B	87	GLN
2	B	95	ASN
2	B	96	ASN
2	B	111	GLN
2	B	141	ASN
2	B	176	ASN
2	B	190	HIS
2	B	303	ASN
2	B	305	HIS
2	B	310	ASN
2	B	312	HIS
2	B	429	GLN
2	B	460	HIS
3	C	9	ASN
3	C	15	ASN
3	C	26	HIS
3	C	28	ASN
3	C	41	ASN
3	C	55	ASN
3	C	65	HIS
3	C	97	ASN
3	C	103	ASN
3	C	115	ASN
3	C	200	ASN
3	C	267	GLN
3	C	447	ASN
3	C	479	ASN

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Mol	Chain	Res	Type
1	D	16	ASN
1	D	25	HIS
1	D	36	GLN
1	D	53	ASN
1	D	58	GLN
1	D	59	GLN
1	D	94	ASN
1	D	95	ASN
1	D	141	ASN
1	D	408	HIS
1	D	435	GLN
4	E	1	ASN
4	E	26	HIS
4	E	52	ASN
4	E	60	ASN
4	E	67	ASN
4	E	93	ASN
4	E	94	ASN
4	E	98	GLN
4	E	111	ASN
4	E	140	ASN
4	E	148	GLN
4	E	156	ASN
4	E	158	GLN
4	E	197	GLN
4	E	206	GLN
4	E	215	GLN
4	E	261	GLN
4	E	472	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	126:THR	C	127:CYS	N	1.19
1	E	309:ARG	C	310:THR	N	1.19
1	B	129:THR	C	130:ILE	N	1.12

6 Map visualisation (i)

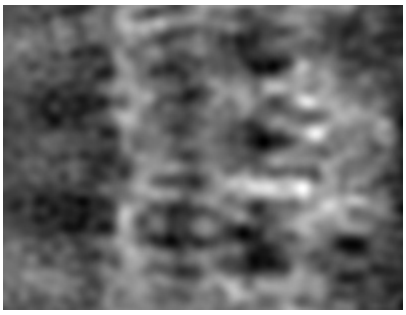
This section contains visualisations of the EMDB entry EMD-2072. These allow visual inspection of the internal detail of the map and identification of artifacts.

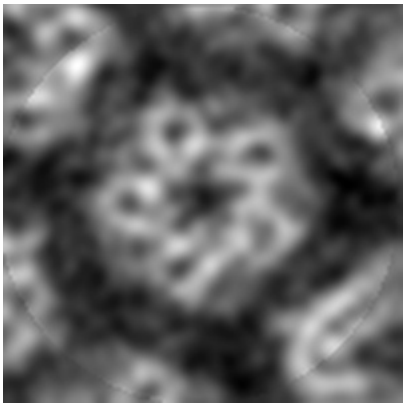
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map

X


Y

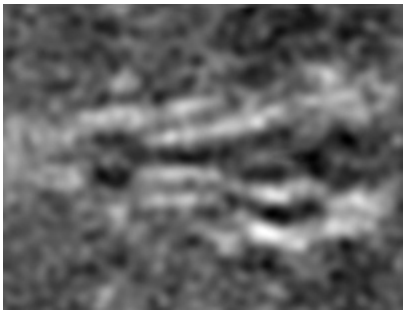

Z

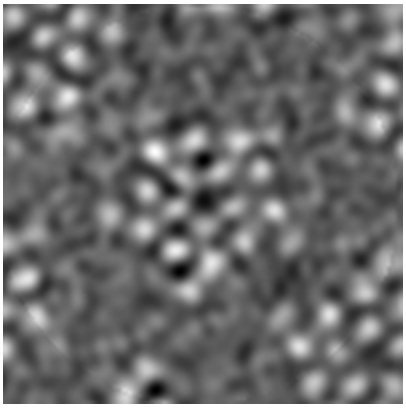
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 64


Y Index: 64

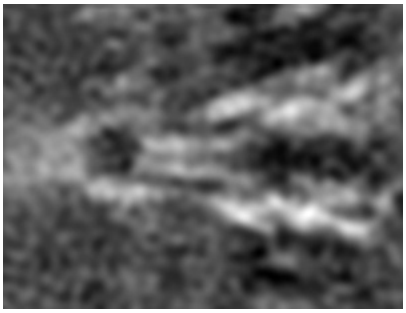

Z Index: 84

The images above show central slices of the map in three orthogonal directions.

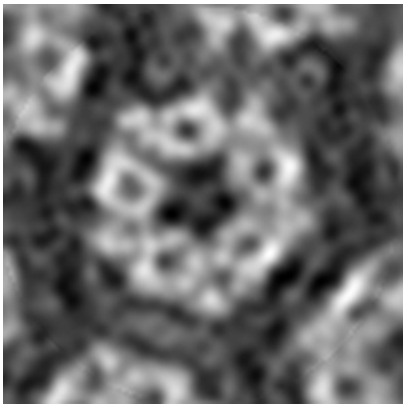
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 63



Y Index: 71

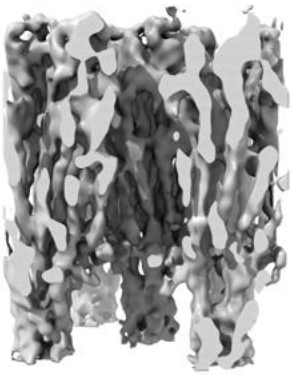


Z Index: 145

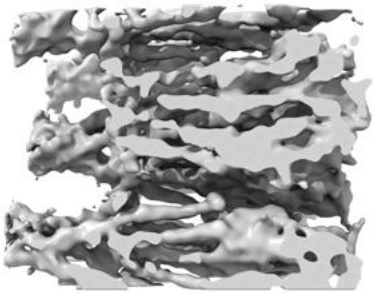
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

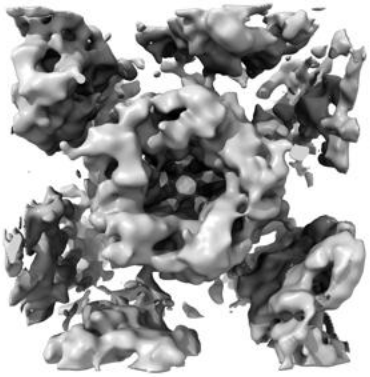
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

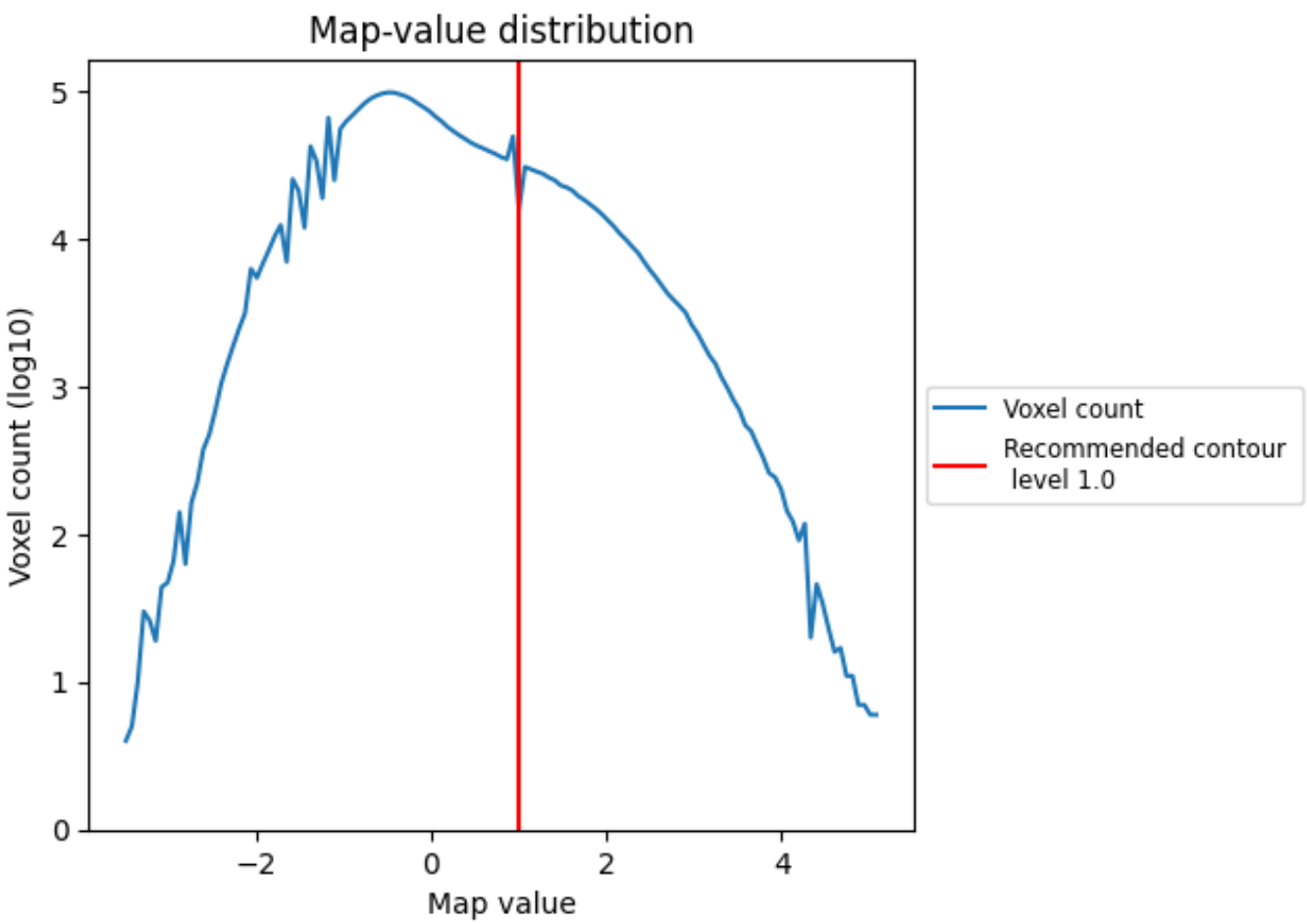
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

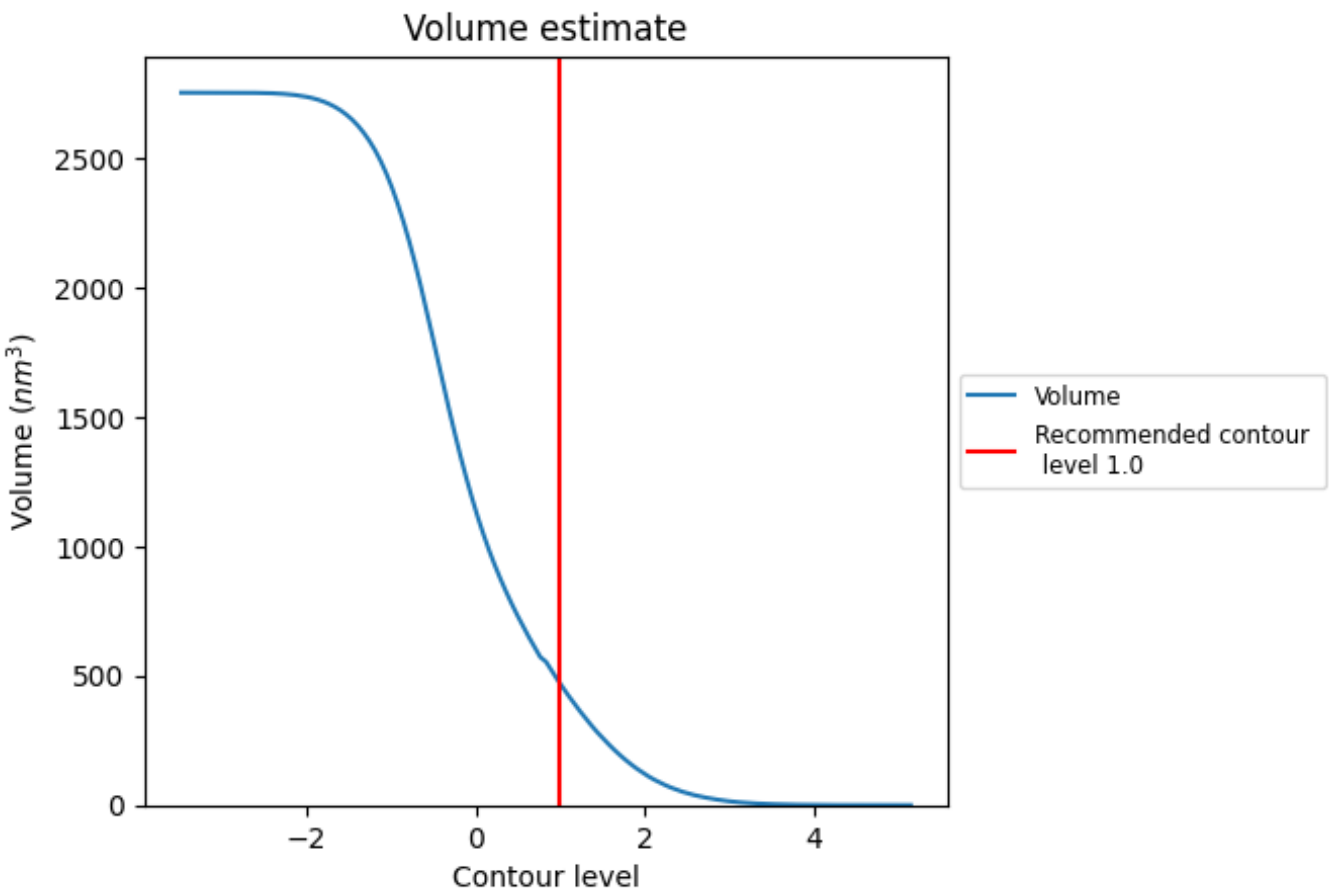
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)



The volume at the recommended contour level is 469 nm^3; this corresponds to an approximate mass of 424 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

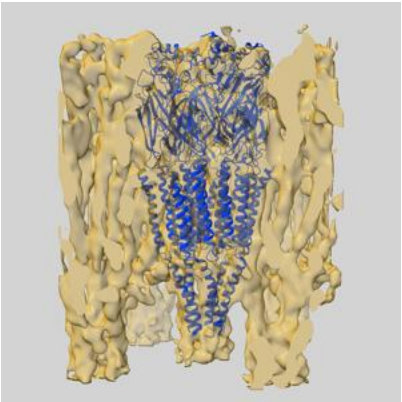
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

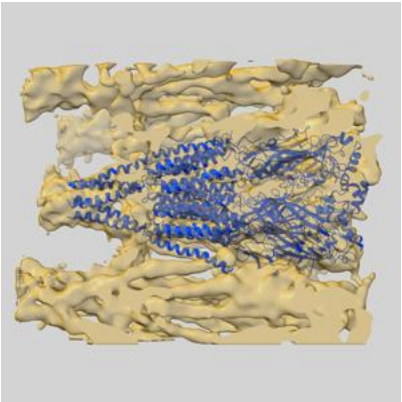
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2072 and PDB model 4AQ9. Per-residue inclusion information can be found in section 3 on page 4.

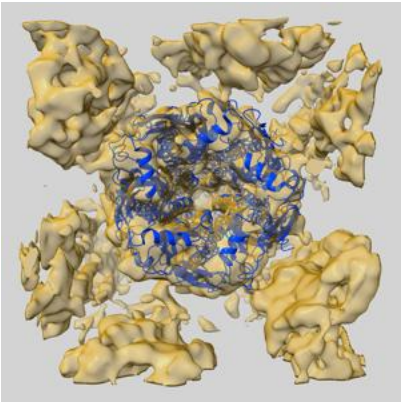
9.1 Map-model overlay (i)



X



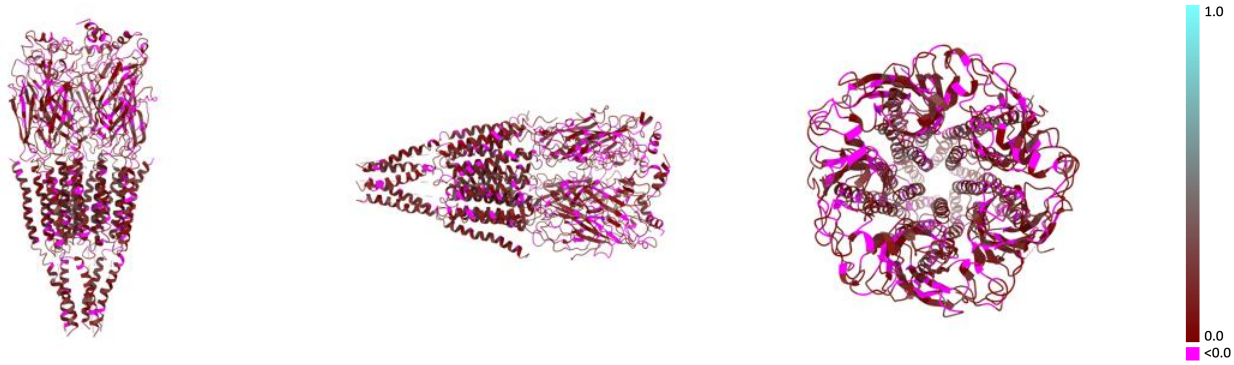
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

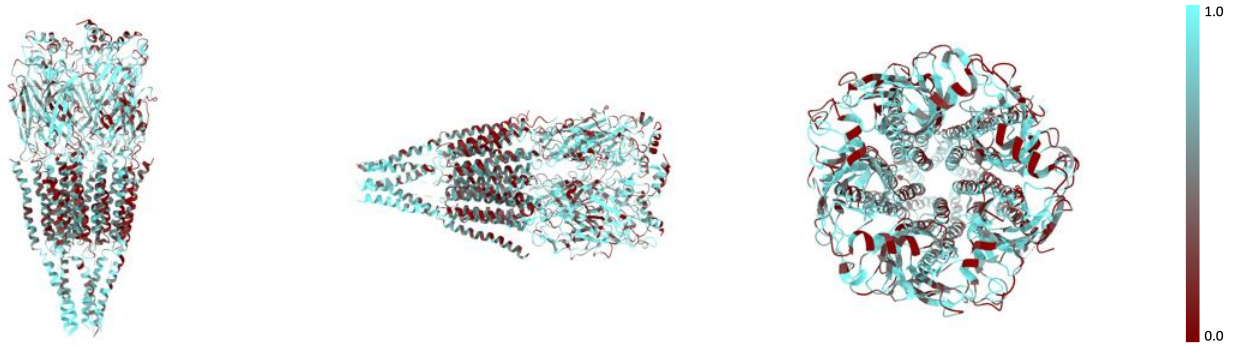
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

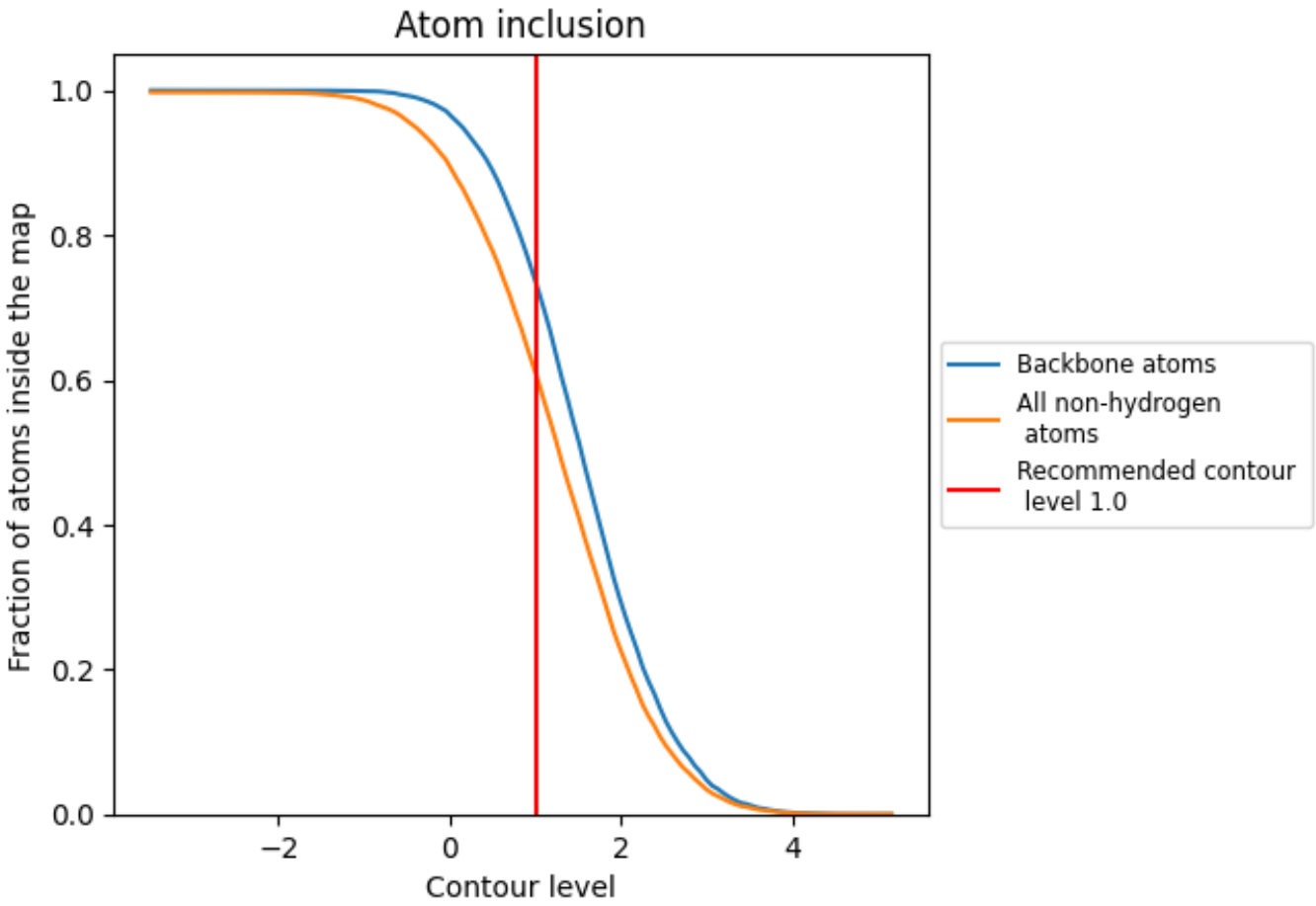
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6095	0.1030
A	0.6077	0.1060
B	0.5775	0.0910
C	0.5742	0.0980
D	0.6268	0.1090
E	0.6612	0.1100