Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 09:42 AM EST

PDB ID	:	2YVX
Title	:	Crystal structure of magnesium transporter MgtE
Authors	:	Hattori, M.; Tanaka, Y.; Fukai, S.; Ishitani, R.; Nureki, O.
Deposited on	:	2007-04-18
Resolution	:	3.50 Å(reported)

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

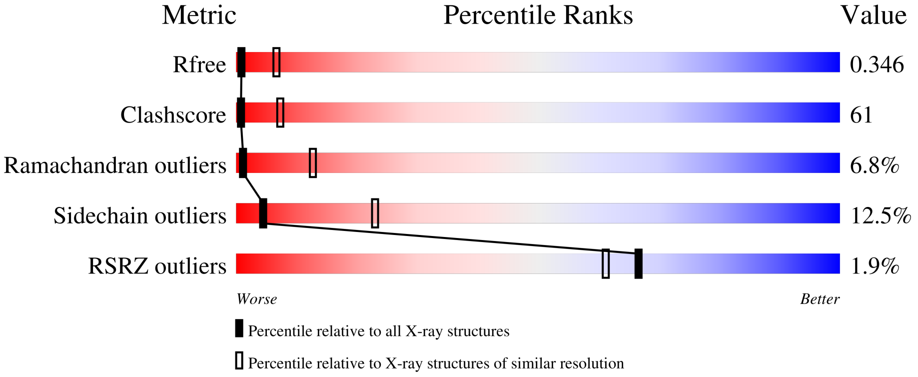
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

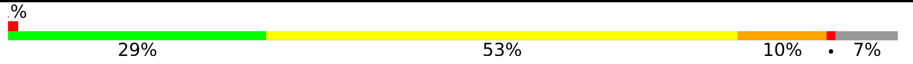
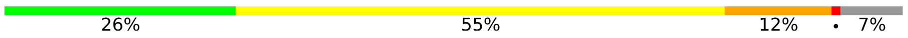
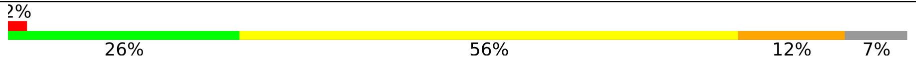
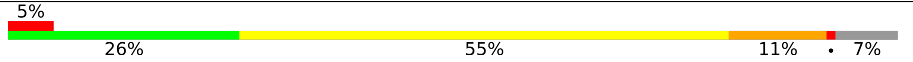
The reported resolution of this entry is 3.50 Å.

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



Metric	**Whole archive (#Entries)**	**Similar resolution (#Entries, resolution range(Å))**
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	**Chain**	**Length**	**Quality of chain**
1	A	473	
1	B	473	
1	C	473	
1	D	473	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	C	453	-	-	-	X

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 13898 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mg2+ transporter MgtE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3470	2238	577	648	7	0	0	0
1	B	442	3470	2238	577	648	7	0	0	0
1	C	442	3470	2238	577	648	7	0	0	0
1	D	442	3470	2238	577	648	7	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q5SMG8
A	-21	GLY	-	expression tag	UNP Q5SMG8
A	-20	SER	-	expression tag	UNP Q5SMG8
A	-19	SER	-	expression tag	UNP Q5SMG8
A	-18	HIS	-	expression tag	UNP Q5SMG8
A	-17	HIS	-	expression tag	UNP Q5SMG8
A	-16	HIS	-	expression tag	UNP Q5SMG8
A	-15	HIS	-	expression tag	UNP Q5SMG8
A	-14	HIS	-	expression tag	UNP Q5SMG8
A	-13	HIS	-	expression tag	UNP Q5SMG8
A	-12	SER	-	expression tag	UNP Q5SMG8
A	-11	SER	-	expression tag	UNP Q5SMG8
A	-10	GLY	-	expression tag	UNP Q5SMG8
A	-9	LEU	-	expression tag	UNP Q5SMG8
A	-8	GLY	-	expression tag	UNP Q5SMG8
A	-7	VAL	-	expression tag	UNP Q5SMG8
A	-6	LEU	-	expression tag	UNP Q5SMG8
A	-5	PRO	-	expression tag	UNP Q5SMG8
A	-4	GLY	-	expression tag	UNP Q5SMG8
A	-3	GLY	-	expression tag	UNP Q5SMG8
A	-2	PRO	-	expression tag	UNP Q5SMG8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	LEU	-	expression tag	UNP Q5SMG8
A	0	HIS	-	expression tag	UNP Q5SMG8
B	-22	MET	-	expression tag	UNP Q5SMG8
B	-21	GLY	-	expression tag	UNP Q5SMG8
B	-20	SER	-	expression tag	UNP Q5SMG8
B	-19	SER	-	expression tag	UNP Q5SMG8
B	-18	HIS	-	expression tag	UNP Q5SMG8
B	-17	HIS	-	expression tag	UNP Q5SMG8
B	-16	HIS	-	expression tag	UNP Q5SMG8
B	-15	HIS	-	expression tag	UNP Q5SMG8
B	-14	HIS	-	expression tag	UNP Q5SMG8
B	-13	HIS	-	expression tag	UNP Q5SMG8
B	-12	SER	-	expression tag	UNP Q5SMG8
B	-11	SER	-	expression tag	UNP Q5SMG8
B	-10	GLY	-	expression tag	UNP Q5SMG8
B	-9	LEU	-	expression tag	UNP Q5SMG8
B	-8	GLY	-	expression tag	UNP Q5SMG8
B	-7	VAL	-	expression tag	UNP Q5SMG8
B	-6	LEU	-	expression tag	UNP Q5SMG8
B	-5	PRO	-	expression tag	UNP Q5SMG8
B	-4	GLY	-	expression tag	UNP Q5SMG8
B	-3	GLY	-	expression tag	UNP Q5SMG8
B	-2	PRO	-	expression tag	UNP Q5SMG8
B	-1	LEU	-	expression tag	UNP Q5SMG8
B	0	HIS	-	expression tag	UNP Q5SMG8
C	-22	MET	-	expression tag	UNP Q5SMG8
C	-21	GLY	-	expression tag	UNP Q5SMG8
C	-20	SER	-	expression tag	UNP Q5SMG8
C	-19	SER	-	expression tag	UNP Q5SMG8
C	-18	HIS	-	expression tag	UNP Q5SMG8
C	-17	HIS	-	expression tag	UNP Q5SMG8
C	-16	HIS	-	expression tag	UNP Q5SMG8
C	-15	HIS	-	expression tag	UNP Q5SMG8
C	-14	HIS	-	expression tag	UNP Q5SMG8
C	-13	HIS	-	expression tag	UNP Q5SMG8
C	-12	SER	-	expression tag	UNP Q5SMG8
C	-11	SER	-	expression tag	UNP Q5SMG8
C	-10	GLY	-	expression tag	UNP Q5SMG8
C	-9	LEU	-	expression tag	UNP Q5SMG8
C	-8	GLY	-	expression tag	UNP Q5SMG8
C	-7	VAL	-	expression tag	UNP Q5SMG8
C	-6	LEU	-	expression tag	UNP Q5SMG8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	PRO	-	expression tag	UNP Q5SMG8
C	-4	GLY	-	expression tag	UNP Q5SMG8
C	-3	GLY	-	expression tag	UNP Q5SMG8
C	-2	PRO	-	expression tag	UNP Q5SMG8
C	-1	LEU	-	expression tag	UNP Q5SMG8
C	0	HIS	-	expression tag	UNP Q5SMG8
D	-22	MET	-	expression tag	UNP Q5SMG8
D	-21	GLY	-	expression tag	UNP Q5SMG8
D	-20	SER	-	expression tag	UNP Q5SMG8
D	-19	SER	-	expression tag	UNP Q5SMG8
D	-18	HIS	-	expression tag	UNP Q5SMG8
D	-17	HIS	-	expression tag	UNP Q5SMG8
D	-16	HIS	-	expression tag	UNP Q5SMG8
D	-15	HIS	-	expression tag	UNP Q5SMG8
D	-14	HIS	-	expression tag	UNP Q5SMG8
D	-13	HIS	-	expression tag	UNP Q5SMG8
D	-12	SER	-	expression tag	UNP Q5SMG8
D	-11	SER	-	expression tag	UNP Q5SMG8
D	-10	GLY	-	expression tag	UNP Q5SMG8
D	-9	LEU	-	expression tag	UNP Q5SMG8
D	-8	GLY	-	expression tag	UNP Q5SMG8
D	-7	VAL	-	expression tag	UNP Q5SMG8
D	-6	LEU	-	expression tag	UNP Q5SMG8
D	-5	PRO	-	expression tag	UNP Q5SMG8
D	-4	GLY	-	expression tag	UNP Q5SMG8
D	-3	GLY	-	expression tag	UNP Q5SMG8
D	-2	PRO	-	expression tag	UNP Q5SMG8
D	-1	LEU	-	expression tag	UNP Q5SMG8
D	0	HIS	-	expression tag	UNP Q5SMG8

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

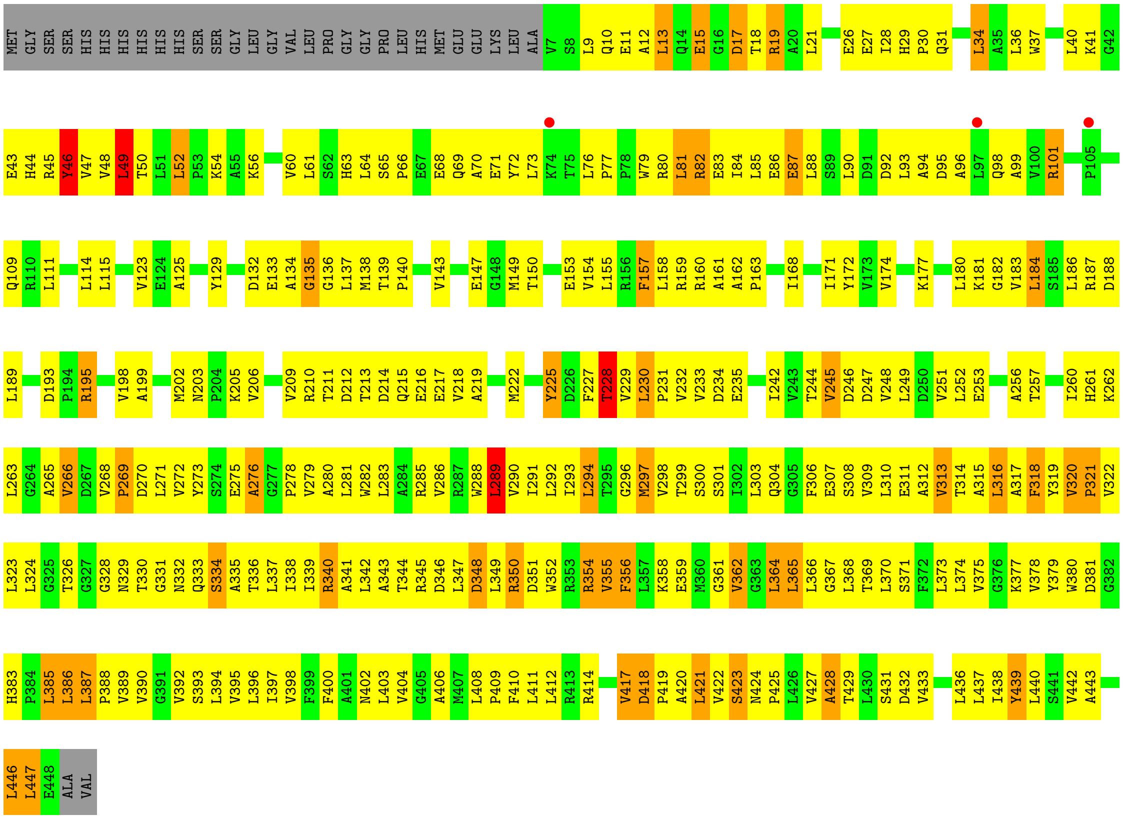
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	5	Total Mg 5 5	0	0
2	C	5	Total Mg 5 5	0	0
2	D	4	Total Mg 4 4	0	0

3 Residue-property plots ⓘ

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

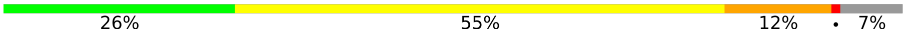
- Molecule 1: Mg2+ transporter MgtE

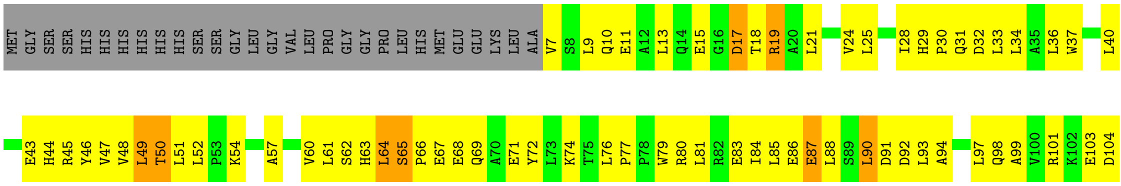
Chain A:

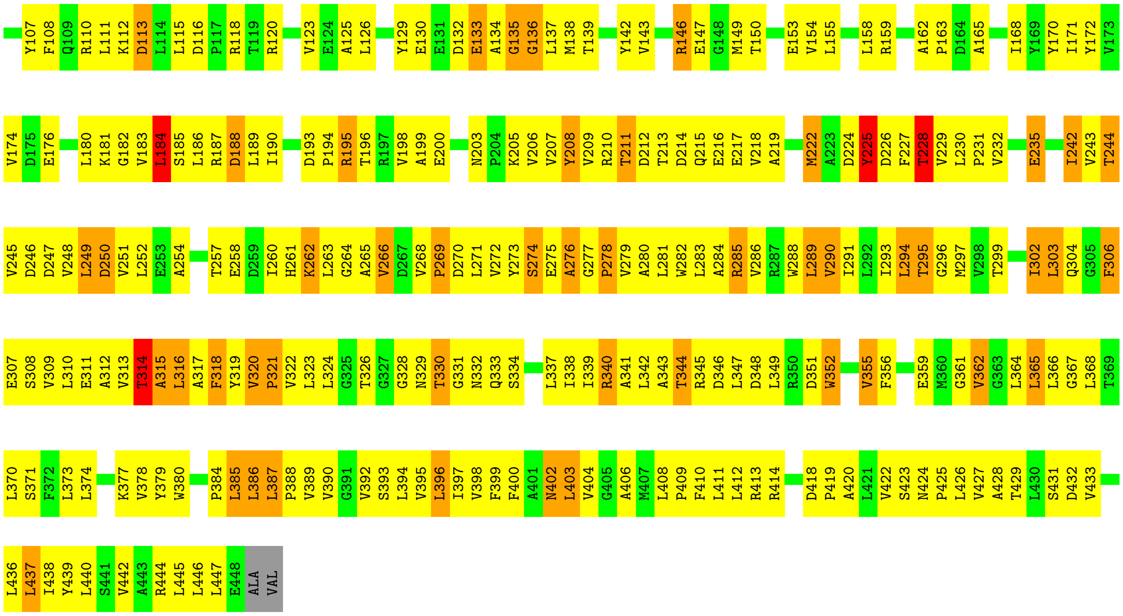


- Molecule 1: Mg2+ transporter MgtE

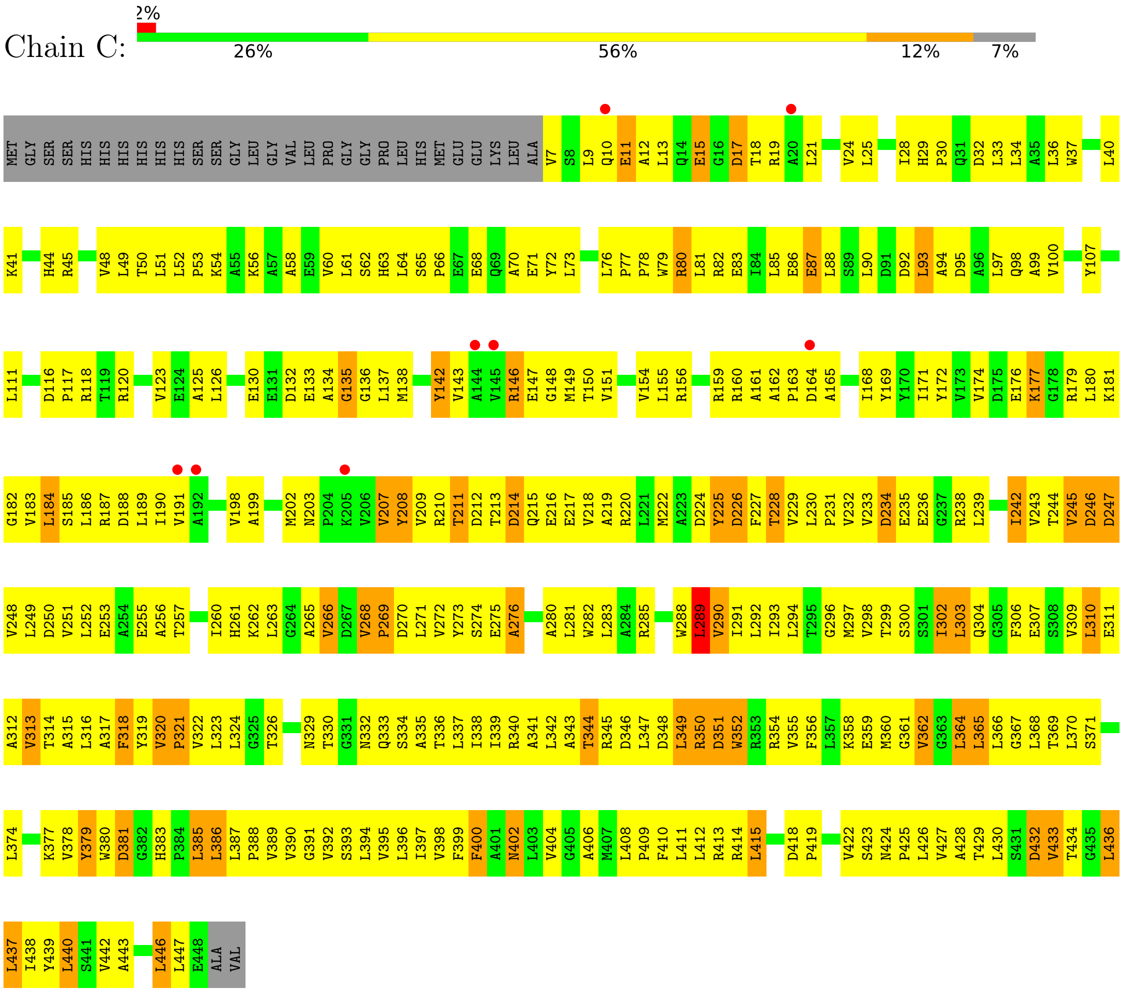
Chain B:





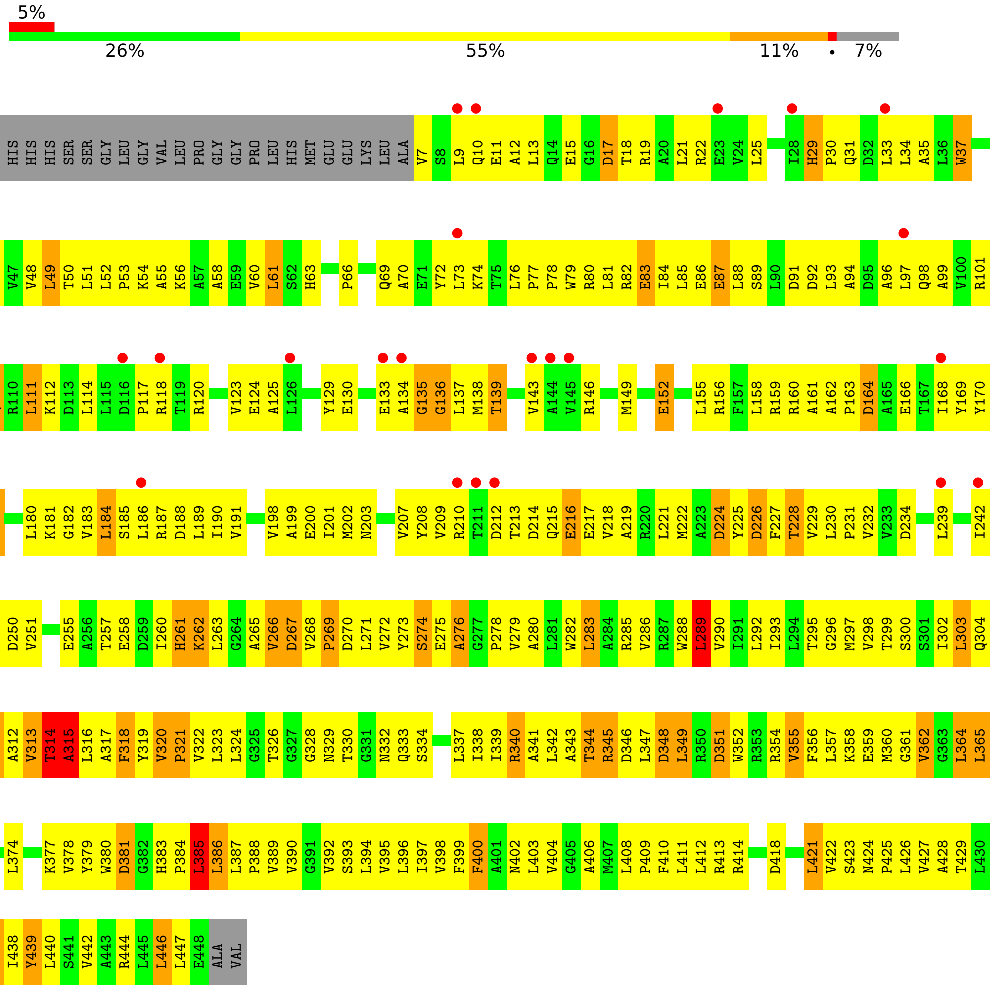


- Molecule 1: Mg2+ transporter MgtE



- Molecule 1: Mg2+ transporter MgtE

Chain D:


5%
26%
55%
11%
•
7%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU GLY VAL LEU PRO GLY GLY PRO LEU HIS MET GLU GLU LYS LEU ALA V7 S8 L9 Q10 E11 A12 L13 Q14 E15 G16 D17 T18 R19 A20 L21 R22 E23 V24 L25 I28 H29 P30 Q31 D32 L33 L34 A35 L36 W37
L40 K41 G42 E43 H44 R45 Y46 V47 V48 L49 T50 L51 L52 P53 K54 A55 K56 A57 A58 E59 V60 L61 S62 H63 P66 Q69 A70 E71 Y72 L73 K74 T75 L76 P77 P78 W79 R80 L81 R82 E83 I84 L85 E86 E87 L88 S89 L90 D91 D92 L93 A94 D95 A96 L97 Q98 A99 V100 R101
K102 E103 D104 Y107 F108 Q109 R110 L111 K112 D113 L114 L115 D116 P117 R118 T119 R120 V123 E124 A125 L126 Y129 E130 E133 A134 G135 G136 L137 M138 T139 V143 A144 V145 R146 M149 E152 L155 R156 F157 L158 R159 R160 A161 A162 P163 D164 A165 E166 T167 I168 Y169 Y170
I171 Y172 V173 V174 D175 E176 K177 L180 K181 G182 V183 L184 S185 L186 R187 D188 L189 I190 V191 V198 A199 E200 I201 M202 N203 V207 Y208 V209 R210 T211 D212 T213 D214 Q215 E216 E217 V218 A219 R220 L221 M222 A223 D224 Y225 D226 F227 T228 V229 L230 P231 V232 V233 D234 L239 I242
V243 T244 V245 D246 D247 V248 L249 D250 V251 E255 A256 T257 E258 D259 I260 H261 K262 L263 G264 A265 V266 D267 V268 P269 D270 L271 V272 Y273 S274 E275 A276 G277 P278 V279 A280 L281 W282 L283 A284 R285 V286 R287 W288 L289 V290 I291 L292 I293 L294 T295 G296 M297 V298 T299 S300 S301 I302 L303 Q304
G305 F306 E307 S308 V309 L310 E311 A312 V313 T314 A315 L316 A317 F318 Y319 V320 P321 V322 L323 L324 G325 T326 G327 G328 N329 T330 G331 N332 Q333 S334 L337 I338 I339 R340 A341 L342 A343 T344 R345 D346 L347 D348 L349 R350 D351 W352 R353 R354 V355 F356 L357 K358 E359 M360 G361 V362 G363 L364 L365
L366 G367 L368 T369 L370 S371 L374 K377 V378 Y379 W380 D381 G382 H383 P384 L385 L386 L387 P388 V389 V390 G391 V392 S393 L394 V395 L396 I397 V398 F399 F400 A401 N402 L403 V404 G405 A406 M407 L408 P409 F410 L411 L412 R413 R414 D418 L421 V422 S423 N424 P425 L426 V427 A428 T429 I430
S431 D432 V433 T434 G435 L436 L437 I438 Y439 L440 S441 V442 A443 R444 L445 L446 L447 E448 ALA VAL

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.31Å 134.90Å 366.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 3.50 49.69 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.69-3.50) 98.3 (49.69-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.294 , 0.341 0.303 , 0.346	Depositor DCC
R_{free} test set	1854 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	97.1	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	13898	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	0/3530	0.76	0/4815
1	B	0.65	0/3530	0.76	2/4815 (0.0%)
1	C	0.56	0/3530	0.70	0/4815
1	D	0.57	3/3530 (0.1%)	0.72	1/4815 (0.0%)
All	All	0.61	3/14120 (0.0%)	0.73	3/19260 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	311	GLU	CB-CG	8.63	1.68	1.52
1	D	315	ALA	CA-CB	-7.63	1.36	1.52
1	D	314	THR	C-O	-6.37	1.11	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	GLU	N-CA-CB	6.01	121.42	110.60
1	B	314	THR	CB-CA-C	-5.83	95.85	111.60
1	B	264	GLY	N-CA-C	-5.27	99.93	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	TYR	Sidechain
1	D	439	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3470	0	3576	445	0
1	B	3470	0	3577	460	0
1	C	3470	0	3577	514	0
1	D	3470	0	3577	524	1
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
All	All	13898	0	14307	1711	1

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 61.

All (1711) 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:C:333:GLN:NE2	1:D:265:ALA:HB3	1.50	1.26
1:A:311:GLU:O	1:A:314:THR:OG1	1.56	1.23
1:C:340:ARG:HH12	1:D:260:ILE:HB	1.08	1.18
1:B:268:VAL:HB	1:B:271:LEU:HD11	1.28	1.15
1:A:378:VAL:HG11	1:A:390:VAL:HG21	1.28	1.15
1:D:314:THR:HG22	1:D:315:ALA:N	1.61	1.15
1:A:378:VAL:HG21	1:A:390:VAL:HG11	1.20	1.14
1:C:378:VAL:HG21	1:C:390:VAL:HG11	1.30	1.13
1:B:285:ARG:HB3	1:B:285:ARG:HH11	1.13	1.11
1:A:296:GLY:O	1:A:299:THR:HG22	1.48	1.10
1:D:316:LEU:HG	1:D:317:ALA:H	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:VAL:HG11	1:B:390:VAL:HG21	1.31	1.10
1:D:378:VAL:HG21	1:D:390:VAL:HG11	1.17	1.09
1:B:378:VAL:HG21	1:B:390:VAL:HG11	1.18	1.09
1:D:359:GLU:HG3	1:D:402:ASN:HD21	1.15	1.08
1:C:378:VAL:HG11	1:C:390:VAL:HG21	1.30	1.07
1:C:266:VAL:HG11	1:D:337:LEU:HD21	1.34	1.07
1:C:336:THR:HG22	1:C:340:ARG:HH21	1.19	1.06
1:D:320:VAL:H	1:D:321:PRO:HD3	1.18	1.06
1:C:183:VAL:HG22	1:C:184:LEU:H	1.19	1.05
1:D:268:VAL:HB	1:D:271:LEU:HD11	1.38	1.05
1:C:333:GLN:HE21	1:D:265:ALA:HB3	0.89	1.05
1:D:183:VAL:HG22	1:D:184:LEU:H	1.22	1.04
1:C:73:LEU:HD22	1:C:111:LEU:HD11	1.39	1.04
1:C:311:GLU:O	1:C:314:THR:OG1	1.76	1.04
1:B:130:GLU:HB2	1:B:133:GLU:HG2	1.40	1.03
1:D:374:LEU:HD22	1:D:394:LEU:HD12	1.39	1.03
1:B:28:ILE:HD12	1:B:33:LEU:HD11	1.37	1.03
1:C:228:THR:HG23	1:C:229:VAL:HG23	1.39	1.03
1:C:90:LEU:HD21	1:C:123:VAL:HG22	1.40	1.02
1:D:309:VAL:O	1:D:313:VAL:HG23	1.60	1.01
1:D:316:LEU:CG	1:D:317:ALA:H	1.71	1.01
1:A:285:ARG:HH12	1:B:402:ASN:HD21	0.99	0.99
1:D:378:VAL:HG11	1:D:390:VAL:HG21	1.45	0.99
1:A:268:VAL:HB	1:A:271:LEU:HD11	1.41	0.98
1:A:336:THR:O	1:A:339:ILE:HG22	1.62	0.98
1:A:322:VAL:HG22	1:B:296:GLY:O	1.63	0.98
1:B:215:GLN:HB3	1:B:251:VAL:HG11	1.46	0.98
1:C:333:GLN:HE21	1:D:265:ALA:CB	1.77	0.97
1:A:392:VAL:O	1:A:396:LEU:HB2	1.63	0.97
1:A:311:GLU:C	1:A:314:THR:OG1	2.01	0.97
1:D:314:THR:O	1:D:316:LEU:N	1.97	0.96
1:A:299:THR:CG2	1:B:322:VAL:HG22	1.95	0.96
1:C:320:VAL:H	1:C:321:PRO:HD3	1.31	0.96
1:A:333:GLN:HE21	1:B:265:ALA:HB3	1.27	0.96
1:C:434:THR:HA	1:C:437:LEU:HD12	1.48	0.95
1:A:337:LEU:HD21	1:B:266:VAL:HG11	1.48	0.95
1:C:88:LEU:HD23	1:C:93:LEU:HD12	1.44	0.95
1:A:354:ARG:HH22	1:B:274:SER:HA	1.32	0.95
1:B:349:LEU:HD11	1:B:414:ARG:HG2	1.48	0.94
1:C:265:ALA:HB3	1:D:333:GLN:HE21	1.33	0.94
1:B:215:GLN:HB3	1:B:251:VAL:CG1	1.96	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:OG1	1:D:321:PRO:HB2	1.67	0.94
1:C:347:LEU:HD11	1:D:273:TYR:HD2	1.29	0.94
1:C:107:TYR:HE2	1:C:111:LEU:HD12	1.34	0.93
1:C:321:PRO:HB2	1:D:299:THR:OG1	1.67	0.93
1:C:333:GLN:NE2	1:D:265:ALA:CB	2.31	0.93
1:C:224:ASP:HB3	1:D:31:GLN:HE21	1.33	0.93
1:A:285:ARG:HH12	1:B:402:ASN:ND2	1.66	0.92
1:A:183:VAL:HG22	1:A:184:LEU:H	1.34	0.92
1:C:265:ALA:HB1	1:C:288:TRP:HB2	1.50	0.92
1:D:54:LYS:HE3	1:D:83:GLU:HG2	1.47	0.92
1:B:334:SER:HB2	1:B:402:ASN:ND2	1.85	0.92
1:C:316:LEU:CG	1:C:317:ALA:H	1.80	0.92
1:A:375:VAL:HG13	1:A:387:LEU:HD11	1.50	0.90
1:C:265:ALA:CB	1:D:333:GLN:HE21	1.83	0.89
1:B:324:LEU:HD21	1:B:436:LEU:HG	1.53	0.89
1:D:228:THR:HG23	1:D:229:VAL:HG23	1.55	0.89
1:B:314:THR:HG22	1:B:315:ALA:N	1.87	0.89
1:C:296:GLY:O	1:D:322:VAL:HG22	1.72	0.89
1:A:257:THR:HA	1:B:340:ARG:HH12	1.37	0.88
1:C:340:ARG:HH12	1:D:260:ILE:CB	1.86	0.88
1:A:195:ARG:HB3	1:A:195:ARG:HH11	1.38	0.88
1:C:268:VAL:HG23	1:C:271:LEU:HD11	1.52	0.88
1:D:209:VAL:HG21	1:D:218:VAL:HG22	1.55	0.88
1:A:299:THR:HG22	1:B:322:VAL:HG22	1.52	0.88
1:C:340:ARG:HH22	1:D:260:ILE:HG22	1.38	0.87
1:C:21:LEU:HD21	1:C:51:LEU:HD13	1.54	0.87
1:A:273:TYR:HD2	1:B:347:LEU:HD11	1.37	0.87
1:B:25:LEU:HB3	1:B:52:LEU:HD23	1.55	0.87
1:B:158:LEU:HD11	1:B:171:ILE:HD11	1.56	0.87
1:C:393:SER:HB3	1:C:442:VAL:HG11	1.54	0.87
1:C:443:ALA:O	1:C:447:LEU:HG	1.75	0.87
1:C:132:ASP:HA	1:C:215:GLN:HE21	1.38	0.86
1:D:133:GLU:HB3	1:D:212:ASP:HA	1.56	0.86
1:B:285:ARG:HB3	1:B:285:ARG:NH1	1.90	0.86
1:C:326:THR:HG23	1:D:293:ILE:HG13	1.58	0.86
1:A:320:VAL:H	1:A:321:PRO:HD2	1.40	0.85
1:C:186:LEU:HD23	1:D:186:LEU:HD23	1.59	0.85
1:B:388:PRO:HG2	1:B:446:LEU:HD11	1.57	0.85
1:B:228:THR:HA	1:B:245:VAL:CG2	2.07	0.85
1:C:322:VAL:HG22	1:D:296:GLY:O	1.77	0.85
1:A:333:GLN:NE2	1:B:265:ALA:HB3	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LEU:HG	1:D:317:ALA:N	1.92	0.85
1:D:314:THR:CG2	1:D:315:ALA:N	2.33	0.84
1:A:338:ILE:HD12	1:A:406:ALA:HA	1.58	0.84
1:A:412:LEU:HD12	1:A:419:PRO:HA	1.56	0.84
1:B:133:GLU:HB3	1:B:212:ASP:HA	1.59	0.84
1:B:228:THR:HA	1:B:245:VAL:HG23	1.59	0.84
1:C:326:THR:CG2	1:D:293:ILE:HG13	2.08	0.83
1:C:336:THR:HG22	1:C:340:ARG:NH2	1.92	0.83
1:C:337:LEU:HD21	1:D:266:VAL:HG11	1.59	0.83
1:D:386:LEU:HD11	1:D:447:LEU:HD21	1.59	0.83
1:C:155:LEU:HD21	1:C:189:LEU:HB3	1.60	0.83
1:D:371:SER:HB2	1:D:395:VAL:CG2	2.09	0.83
1:B:183:VAL:HG22	1:B:184:LEU:H	1.43	0.83
1:D:172:TYR:CE2	1:D:231:PRO:HB3	2.13	0.83
1:B:64:LEU:HD22	1:B:68:GLU:HB3	1.58	0.83
1:D:312:ALA:C	1:D:314:THR:H	1.79	0.83
1:D:320:VAL:N	1:D:321:PRO:HD3	1.92	0.83
1:A:412:LEU:HD11	1:A:422:VAL:HG23	1.60	0.83
1:D:367:GLY:O	1:D:395:VAL:HG22	1.79	0.82
1:B:54:LYS:HE2	1:B:87:GLU:HB2	1.61	0.82
1:C:342:LEU:HB3	1:C:413:ARG:NH1	1.95	0.82
1:D:303:LEU:HD21	1:D:436:LEU:HD13	1.62	0.82
1:A:180:LEU:HD23	1:A:181:LYS:N	1.95	0.82
1:B:171:ILE:HD12	1:B:189:LEU:HD11	1.60	0.82
1:B:273:TYR:HE1	1:B:281:LEU:HD21	1.45	0.82
1:A:425:PRO:HG3	1:B:332:ASN:HD22	1.42	0.81
1:B:34:LEU:HD11	1:B:63:HIS:HB2	1.61	0.81
1:D:320:VAL:N	1:D:321:PRO:CD	2.43	0.81
1:B:371:SER:HB2	1:B:395:VAL:CG2	2.10	0.81
1:A:49:LEU:HB3	1:A:76:LEU:HD11	1.62	0.81
1:B:268:VAL:HB	1:B:271:LEU:CD1	2.09	0.81
1:C:316:LEU:HG	1:C:317:ALA:H	1.43	0.81
1:B:222:MET:CE	1:B:230:LEU:HG	2.11	0.81
1:D:320:VAL:H	1:D:321:PRO:CD	1.92	0.81
1:A:273:TYR:CD2	1:B:347:LEU:HD11	2.15	0.80
1:B:80:ARG:O	1:B:84:ILE:HG13	1.82	0.80
1:C:44:HIS:O	1:C:48:VAL:HG23	1.81	0.80
1:B:320:VAL:H	1:B:321:PRO:HD2	1.47	0.80
1:B:320:VAL:H	1:B:321:PRO:CD	1.95	0.80
1:D:424:ASN:HB2	1:D:425:PRO:HD3	1.63	0.80
1:C:340:ARG:NH1	1:D:260:ILE:HB	1.93	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ALA:C	1:A:314:THR:H	1.84	0.80
1:A:339:ILE:HD11	1:A:420:ALA:HA	1.63	0.80
1:A:52:LEU:HD23	1:A:52:LEU:H	1.48	0.79
1:D:392:VAL:O	1:D:396:LEU:HB2	1.82	0.79
1:B:338:ILE:O	1:B:342:LEU:HD12	1.82	0.79
1:D:374:LEU:CD2	1:D:394:LEU:HD12	2.11	0.79
1:A:132:ASP:HA	1:A:215:GLN:HE21	1.47	0.79
1:C:180:LEU:HD23	1:C:181:LYS:N	1.98	0.79
1:C:316:LEU:HA	1:C:318:PHE:CE1	2.18	0.79
1:C:306:PHE:O	1:C:310:LEU:HB2	1.83	0.79
1:C:371:SER:HA	1:C:394:LEU:HD23	1.65	0.79
1:A:195:ARG:HB3	1:A:195:ARG:NH1	1.96	0.78
1:B:306:PHE:CD2	1:B:440:LEU:HD13	2.18	0.78
1:D:359:GLU:HG3	1:D:402:ASN:ND2	1.97	0.78
1:D:359:GLU:HA	1:D:362:VAL:HG23	1.66	0.78
1:A:281:LEU:HD12	1:A:281:LEU:H	1.48	0.78
1:A:320:VAL:H	1:A:321:PRO:CD	1.96	0.78
1:C:347:LEU:HD11	1:D:273:TYR:CD2	2.15	0.78
1:B:367:GLY:O	1:B:395:VAL:HG22	1.84	0.78
1:C:397:ILE:HG12	1:C:438:ILE:HD12	1.65	0.78
1:D:434:THR:HA	1:D:437:LEU:HD12	1.65	0.78
1:B:388:PRO:CG	1:B:446:LEU:HD11	2.14	0.78
1:B:142:TYR:HB3	1:B:242:ILE:CG2	2.14	0.78
1:B:143:VAL:HG21	1:B:168:ILE:HA	1.63	0.78
1:B:392:VAL:O	1:B:396:LEU:HB2	1.84	0.78
1:C:94:ALA:O	1:C:98:GLN:HG3	1.84	0.78
1:B:361:GLY:O	1:B:365:LEU:HB2	1.84	0.78
1:D:184:LEU:HD21	1:D:189:LEU:HD21	1.66	0.78
1:C:293:ILE:HG13	1:D:326:THR:HG23	1.65	0.78
1:D:207:VAL:HG21	1:D:227:PHE:CE2	2.19	0.77
1:A:371:SER:HA	1:A:394:LEU:HD23	1.66	0.77
1:C:371:SER:HB2	1:C:395:VAL:HG22	1.65	0.77
1:B:323:LEU:HD12	1:B:324:LEU:HD12	1.66	0.77
1:A:215:GLN:HB3	1:A:251:VAL:HG11	1.65	0.77
1:B:400:PHE:O	1:B:404:VAL:HG23	1.85	0.77
1:C:371:SER:HB2	1:C:395:VAL:CG2	2.15	0.77
1:D:265:ALA:HB1	1:D:288:TRP:HB2	1.67	0.77
1:A:340:ARG:NH2	1:A:341:ALA:HB2	2.00	0.77
1:B:320:VAL:N	1:B:321:PRO:HD2	2.00	0.77
1:A:386:LEU:HD11	1:A:447:LEU:HD23	1.65	0.76
1:A:215:GLN:HB3	1:A:251:VAL:CG1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ARG:HG3	1:D:341:ALA:N	1.99	0.76
1:C:229:VAL:HG13	1:C:242:ILE:HD11	1.67	0.76
1:A:371:SER:HB2	1:A:395:VAL:CG2	2.16	0.76
1:B:222:MET:HE3	1:B:230:LEU:HG	1.68	0.76
1:B:142:TYR:HB3	1:B:242:ILE:HG21	1.67	0.76
1:B:399:PHE:O	1:B:403:LEU:HD23	1.86	0.76
1:D:268:VAL:HB	1:D:271:LEU:CD1	2.16	0.76
1:A:320:VAL:N	1:A:321:PRO:HD2	2.01	0.76
1:A:257:THR:HA	1:B:340:ARG:NH1	2.01	0.75
1:B:273:TYR:CE1	1:B:281:LEU:HD21	2.22	0.75
1:C:183:VAL:HG22	1:C:184:LEU:N	1.99	0.75
1:C:316:LEU:CD2	1:C:317:ALA:H	1.98	0.75
1:C:340:ARG:NH2	1:D:260:ILE:HG22	1.99	0.75
1:D:180:LEU:HD23	1:D:181:LYS:N	2.01	0.75
1:B:180:LEU:HD23	1:B:181:LYS:N	2.00	0.75
1:C:172:TYR:CE2	1:C:231:PRO:HB3	2.20	0.75
1:C:392:VAL:O	1:C:396:LEU:HB2	1.86	0.75
1:C:274:SER:CB	1:D:354:ARG:HH22	1.98	0.75
1:C:260:ILE:HD12	1:D:340:ARG:HH12	1.52	0.75
1:C:316:LEU:HD23	1:C:317:ALA:N	2.02	0.75
1:B:303:LEU:HD23	1:B:436:LEU:HD13	1.68	0.74
1:C:111:LEU:O	1:C:111:LEU:HD23	1.85	0.74
1:C:397:ILE:HG12	1:C:438:ILE:CD1	2.16	0.74
1:D:174:VAL:HG12	1:D:180:LEU:HA	1.70	0.74
1:B:172:TYR:CE2	1:B:231:PRO:HB3	2.21	0.74
1:C:335:ALA:O	1:C:339:ILE:HG13	1.87	0.74
1:D:112:LYS:HD2	1:D:124:GLU:OE2	1.88	0.74
1:D:338:ILE:HG21	1:D:410:PHE:CE1	2.22	0.74
1:B:394:LEU:O	1:B:398:VAL:HG23	1.87	0.74
1:C:184:LEU:HD21	1:C:189:LEU:HD21	1.69	0.74
1:D:183:VAL:HG22	1:D:184:LEU:N	2.01	0.74
1:A:268:VAL:HB	1:A:271:LEU:CD1	2.16	0.73
1:C:132:ASP:O	1:C:215:GLN:HG3	1.86	0.73
1:A:442:VAL:O	1:A:442:VAL:HG12	1.86	0.73
1:C:296:GLY:O	1:C:299:THR:HG23	1.89	0.73
1:A:306:PHE:O	1:A:310:LEU:HB2	1.88	0.73
1:B:181:LYS:O	1:B:181:LYS:HG2	1.89	0.73
1:D:180:LEU:HD12	1:D:239:LEU:HD13	1.71	0.73
1:B:265:ALA:HB1	1:B:288:TRP:HB2	1.69	0.73
1:C:143:VAL:HG21	1:C:168:ILE:HA	1.69	0.73
1:D:139:THR:HG21	1:D:166:GLU:OE2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG12	1:B:442:VAL:O	1.89	0.73
1:B:364:LEU:O	1:B:368:LEU:HG	1.87	0.73
1:B:296:GLY:O	1:B:299:THR:HG23	1.89	0.72
1:D:314:THR:HG22	1:D:315:ALA:H	1.51	0.72
1:A:367:GLY:O	1:A:395:VAL:HG22	1.89	0.72
1:C:107:TYR:CE2	1:C:111:LEU:HD12	2.22	0.72
1:C:266:VAL:HG11	1:D:337:LEU:CD2	2.16	0.72
1:C:320:VAL:H	1:C:321:PRO:CD	2.02	0.72
1:C:337:LEU:HD21	1:D:266:VAL:HG21	1.71	0.72
1:C:337:LEU:CG	1:D:266:VAL:HG21	2.19	0.72
1:D:386:LEU:HD21	1:D:447:LEU:HG	1.69	0.72
1:D:146:ARG:NH1	1:D:176:GLU:HA	2.04	0.72
1:B:85:LEU:HB3	1:B:115:LEU:HD11	1.70	0.72
1:A:424:ASN:HB2	1:A:425:PRO:HD3	1.71	0.72
1:B:314:THR:CG2	1:B:315:ALA:N	2.51	0.72
1:C:366:LEU:HD23	1:D:286:VAL:HB	1.70	0.72
1:D:296:GLY:O	1:D:299:THR:HG23	1.88	0.72
1:D:319:TYR:HB2	1:D:439:TYR:OH	1.89	0.72
1:A:260:ILE:HD12	1:B:340:ARG:NH2	2.05	0.72
1:A:378:VAL:CG2	1:A:390:VAL:HG11	2.11	0.71
1:B:374:LEU:O	1:B:378:VAL:HG23	1.89	0.71
1:D:50:THR:HA	1:D:80:ARG:NE	2.04	0.71
1:C:172:TYR:OH	1:C:229:VAL:HG12	1.90	0.71
1:C:329:ASN:OD1	1:D:292:LEU:HD23	1.89	0.71
1:A:340:ARG:NH1	1:B:261:HIS:NE2	2.38	0.71
1:C:320:VAL:N	1:C:321:PRO:HD3	2.05	0.71
1:B:321:PRO:HG2	1:B:322:VAL:H	1.56	0.71
1:C:425:PRO:HG3	1:D:332:ASN:ND2	2.04	0.71
1:B:374:LEU:CD2	1:B:394:LEU:HD22	2.21	0.71
1:C:9:LEU:O	1:C:9:LEU:HD23	1.89	0.71
1:C:133:GLU:HB3	1:C:212:ASP:HA	1.72	0.71
1:C:224:ASP:HB3	1:D:31:GLN:NE2	2.05	0.71
1:D:330:THR:CG2	1:D:402:ASN:HB2	2.21	0.71
1:A:265:ALA:HB3	1:B:333:GLN:HG2	1.73	0.71
1:B:303:LEU:HD23	1:B:436:LEU:CD1	2.21	0.71
1:C:168:ILE:HD11	1:D:187:ARG:HA	1.72	0.71
1:C:364:LEU:O	1:C:368:LEU:HG	1.90	0.71
1:C:320:VAL:N	1:C:321:PRO:CD	2.54	0.71
1:B:72:TYR:O	1:B:76:LEU:HD23	1.90	0.70
1:B:339:ILE:HD11	1:B:422:VAL:HB	1.73	0.70
1:C:394:LEU:O	1:C:398:VAL:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:VAL:N	1:B:321:PRO:CD	2.53	0.70
1:D:400:PHE:O	1:D:404:VAL:HG23	1.90	0.70
1:C:180:LEU:HD23	1:C:181:LYS:H	1.56	0.70
1:A:132:ASP:O	1:A:215:GLN:HG3	1.91	0.70
1:B:132:ASP:HA	1:B:215:GLN:HE21	1.56	0.70
1:C:293:ILE:HD12	1:D:326:THR:OG1	1.90	0.70
1:C:374:LEU:O	1:C:378:VAL:HG23	1.91	0.70
1:C:424:ASN:HB2	1:C:425:PRO:HD3	1.73	0.70
1:A:338:ILE:HG21	1:A:410:PHE:CE1	2.26	0.70
1:C:215:GLN:HB3	1:C:251:VAL:CG1	2.22	0.70
1:C:303:LEU:HD13	1:C:310:LEU:HD11	1.73	0.70
1:D:183:VAL:HG12	1:D:203:ASN:HB2	1.74	0.70
1:A:396:LEU:O	1:A:400:PHE:HD1	1.74	0.70
1:B:424:ASN:HB2	1:B:425:PRO:HD3	1.73	0.70
1:A:324:LEU:CD2	1:A:436:LEU:HG	2.22	0.70
1:C:352:TRP:O	1:C:355:VAL:HG22	1.91	0.70
1:A:412:LEU:HB3	1:A:417:VAL:HG23	1.73	0.70
1:B:307:GLU:HA	1:B:310:LEU:HB3	1.74	0.70
1:C:21:LEU:HD21	1:C:51:LEU:CD1	2.21	0.70
1:C:265:ALA:HB1	1:C:288:TRP:CB	2.22	0.70
1:C:317:ALA:O	1:C:320:VAL:HG23	1.92	0.70
1:D:422:VAL:HA	1:D:426:LEU:HD23	1.74	0.70
1:C:293:ILE:HG13	1:D:326:THR:CG2	2.22	0.69
1:A:326:THR:CG2	1:B:293:ILE:HG13	2.22	0.69
1:C:400:PHE:O	1:C:404:VAL:HG23	1.92	0.69
1:D:364:LEU:CD2	1:D:368:LEU:HD21	2.22	0.69
1:B:80:ARG:HG2	1:B:84:ILE:HD11	1.73	0.69
1:C:15:GLU:HG2	1:C:17:ASP:HB2	1.73	0.69
1:D:442:VAL:O	1:D:442:VAL:HG12	1.92	0.69
1:D:378:VAL:HG21	1:D:390:VAL:CG1	2.09	0.69
1:A:307:GLU:HA	1:A:310:LEU:HB3	1.75	0.69
1:B:107:TYR:CE2	1:B:111:LEU:HD12	2.28	0.69
1:B:277:GLY:O	1:B:278:PRO:C	2.30	0.69
1:C:293:ILE:O	1:C:297:MET:HG3	1.92	0.69
1:D:52:LEU:HD22	1:D:53:PRO:HD2	1.73	0.69
1:A:361:GLY:O	1:A:365:LEU:HB2	1.92	0.69
1:C:25:LEU:HB3	1:C:52:LEU:HD23	1.74	0.69
1:A:338:ILE:HG21	1:A:410:PHE:HE1	1.57	0.69
1:A:133:GLU:HB3	1:A:212:ASP:HA	1.74	0.69
1:A:174:VAL:HG12	1:A:180:LEU:HA	1.74	0.69
1:A:273:TYR:CE1	1:A:281:LEU:HD21	2.28	0.68

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:316:LEU:O	1:A:317:ALA:HB3	1.93	0.68
1:D:279:VAL:O	1:D:283:LEU:HG	1.91	0.68
1:A:279:VAL:HG22	1:D:388:PRO:HG3	1.74	0.68
1:D:318:PHE:H	1:D:318:PHE:HD2	1.37	0.68
1:A:400:PHE:O	1:A:404:VAL:HG23	1.93	0.68
1:C:289:LEU:O	1:C:293:ILE:HG12	1.92	0.68
1:C:338:ILE:HD12	1:C:410:PHE:CE1	2.28	0.68
1:D:52:LEU:CD2	1:D:53:PRO:HD2	2.23	0.68
1:D:215:GLN:HB3	1:D:251:VAL:CG1	2.23	0.68
1:C:365:LEU:HD13	1:D:282:TRP:HB2	1.75	0.68
1:A:138:MET:SD	1:A:232:VAL:HG11	2.33	0.68
1:B:314:THR:O	1:B:316:LEU:N	2.26	0.68
1:B:387:LEU:N	1:B:388:PRO:HD2	2.09	0.68
1:C:61:LEU:HD12	1:C:64:LEU:HD12	1.75	0.68
1:D:143:VAL:HG21	1:D:168:ILE:HA	1.75	0.68
1:A:95:ASP:HA	1:A:98:GLN:OE1	1.94	0.68
1:B:180:LEU:HD22	1:B:206:VAL:HG11	1.76	0.68
1:C:340:ARG:HD3	1:D:257:THR:HG23	1.75	0.68
1:C:387:LEU:N	1:C:388:PRO:HD2	2.08	0.68
1:A:320:VAL:N	1:A:321:PRO:CD	2.57	0.68
1:A:326:THR:HG23	1:B:293:ILE:HG13	1.76	0.68
1:C:366:LEU:HD11	1:D:285:ARG:CD	2.24	0.68
1:A:225:TYR:O	1:A:227:PHE:HD1	1.78	0.67
1:B:387:LEU:N	1:B:388:PRO:CD	2.57	0.67
1:A:187:ARG:NH2	1:B:165:ALA:O	2.26	0.67
1:C:303:LEU:HD23	1:C:436:LEU:HD11	1.75	0.67
1:D:129:TYR:HB3	1:D:135:GLY:HA3	1.76	0.67
1:D:293:ILE:O	1:D:297:MET:HG3	1.95	0.67
1:B:374:LEU:HD22	1:B:394:LEU:HD22	1.77	0.67
1:D:374:LEU:O	1:D:378:VAL:HG23	1.94	0.67
1:C:265:ALA:HB3	1:D:333:GLN:NE2	2.09	0.67
1:C:54:LYS:HE2	1:C:87:GLU:HB2	1.77	0.67
1:C:146:ARG:HG3	1:C:148:GLY:H	1.59	0.67
1:C:174:VAL:HG12	1:C:180:LEU:HA	1.75	0.67
1:C:438:ILE:O	1:C:442:VAL:HB	1.93	0.67
1:D:352:TRP:O	1:D:355:VAL:HG23	1.94	0.67
1:A:133:GLU:HG2	1:A:212:ASP:CA	2.25	0.67
1:A:351:ASP:O	1:A:355:VAL:HG22	1.94	0.67
1:B:186:LEU:O	1:B:190:ILE:HG13	1.95	0.67
1:B:308:SER:O	1:B:311:GLU:HG2	1.95	0.67
1:C:242:ILE:HG12	1:C:243:VAL:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:GLU:HA	1:C:362:VAL:HG23	1.77	0.67
1:C:340:ARG:NE	1:D:261:HIS:CD2	2.63	0.66
1:D:107:TYR:CE2	1:D:111:LEU:HD12	2.30	0.66
1:D:364:LEU:HD23	1:D:368:LEU:HD21	1.77	0.66
1:C:361:GLY:O	1:C:365:LEU:HB2	1.96	0.66
1:C:442:VAL:O	1:C:442:VAL:CG1	2.44	0.66
1:D:215:GLN:HB3	1:D:251:VAL:HG13	1.78	0.66
1:D:280:ALA:HA	1:D:283:LEU:HD12	1.77	0.66
1:B:222:MET:HE2	1:B:229:VAL:N	2.10	0.66
1:C:309:VAL:O	1:C:312:ALA:HB3	1.96	0.66
1:D:130:GLU:HB2	1:D:133:GLU:HG3	1.77	0.66
1:A:427:VAL:C	1:A:429:THR:H	1.99	0.66
1:B:344:THR:HG22	1:B:344:THR:O	1.96	0.66
1:D:138:MET:HB3	1:D:232:VAL:HG21	1.78	0.66
1:D:215:GLN:OE1	1:D:251:VAL:HG13	1.95	0.66
1:A:281:LEU:HD12	1:A:281:LEU:N	2.09	0.65
1:A:324:LEU:HD21	1:A:436:LEU:HG	1.77	0.65
1:B:316:LEU:O	1:B:317:ALA:HB3	1.95	0.65
1:C:338:ILE:HD12	1:C:410:PHE:CZ	2.31	0.65
1:D:155:LEU:O	1:D:159:ARG:HG2	1.96	0.65
1:D:385:LEU:H	1:D:385:LEU:HD12	1.60	0.65
1:C:316:LEU:CG	1:C:317:ALA:N	2.56	0.65
1:A:54:LYS:HG2	1:A:83:GLU:OE1	1.96	0.65
1:A:282:TRP:CD1	1:B:365:LEU:HD22	2.30	0.65
1:A:299:THR:HG23	1:A:300:SER:N	2.12	0.65
1:A:427:VAL:O	1:A:429:THR:N	2.29	0.65
1:D:316:LEU:HA	1:D:318:PHE:CE2	2.32	0.65
1:B:81:LEU:O	1:B:85:LEU:HD13	1.97	0.65
1:C:336:THR:CG2	1:C:340:ARG:HH21	2.04	0.65
1:A:90:LEU:HD13	1:A:140:PRO:CG	2.27	0.65
1:A:387:LEU:N	1:A:388:PRO:CD	2.59	0.65
1:C:319:TYR:HB2	1:C:439:TYR:OH	1.97	0.65
1:D:249:LEU:O	1:D:249:LEU:HD23	1.95	0.65
1:A:94:ALA:O	1:A:98:GLN:HG3	1.96	0.65
1:A:273:TYR:HE1	1:A:281:LEU:HD21	1.62	0.65
1:A:285:ARG:NH1	1:B:402:ASN:HD21	1.84	0.65
1:A:359:GLU:HA	1:A:362:VAL:CG2	2.27	0.65
1:B:279:VAL:O	1:B:283:LEU:HD23	1.97	0.65
1:C:183:VAL:CG2	1:C:184:LEU:H	2.03	0.65
1:D:31:GLN:OE1	1:D:34:LEU:HD12	1.97	0.65
1:A:15:GLU:CD	1:A:15:GLU:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ALA:C	1:D:314:THR:N	2.50	0.65
1:A:338:ILE:O	1:A:342:LEU:HD12	1.97	0.64
1:A:339:ILE:HG23	1:A:340:ARG:N	2.13	0.64
1:C:72:TYR:O	1:C:76:LEU:HD23	1.97	0.64
1:C:220:ARG:HH11	1:C:220:ARG:HG3	1.62	0.64
1:D:22:ARG:NH1	1:D:51:LEU:HG	2.11	0.64
1:B:107:TYR:HE2	1:B:111:LEU:HD12	1.63	0.64
1:B:340:ARG:O	1:B:340:ARG:HD3	1.97	0.64
1:B:162:ALA:N	1:B:163:PRO:HD2	2.12	0.64
1:C:316:LEU:O	1:C:317:ALA:HB3	1.96	0.64
1:C:340:ARG:HH22	1:D:260:ILE:C	2.00	0.64
1:C:344:THR:O	1:C:344:THR:HG22	1.97	0.64
1:D:323:LEU:HD13	1:D:439:TYR:CE1	2.32	0.64
1:D:44:HIS:O	1:D:48:VAL:HG23	1.97	0.64
1:C:215:GLN:HB3	1:C:251:VAL:HG11	1.80	0.64
1:C:248:VAL:HA	1:C:251:VAL:HG23	1.80	0.64
1:D:78:PRO:HA	1:D:81:LEU:HG	1.77	0.64
1:C:190:ILE:O	1:D:159:ARG:HD3	1.98	0.64
1:C:427:VAL:C	1:C:429:THR:H	2.00	0.64
1:D:320:VAL:HG13	1:D:436:LEU:HD21	1.78	0.64
1:C:155:LEU:O	1:C:159:ARG:HG2	1.98	0.64
1:B:174:VAL:HG12	1:B:180:LEU:HA	1.80	0.63
1:C:15:GLU:CD	1:C:15:GLU:H	2.01	0.63
1:D:12:ALA:O	1:D:21:LEU:HD13	1.97	0.63
1:D:309:VAL:O	1:D:313:VAL:CG2	2.44	0.63
1:D:387:LEU:N	1:D:388:PRO:HD2	2.14	0.63
1:A:333:GLN:NE2	1:B:265:ALA:CB	2.62	0.63
1:B:136:GLY:O	1:B:137:LEU:HD23	1.96	0.63
1:D:91:ASP:HB3	1:D:139:THR:HG22	1.80	0.63
1:A:375:VAL:HG13	1:A:387:LEU:CD1	2.24	0.63
1:C:333:GLN:HG2	1:D:265:ALA:H	1.62	0.63
1:D:80:ARG:HD3	1:D:84:ILE:HD11	1.80	0.63
1:C:326:THR:OG1	1:D:293:ILE:HD12	1.98	0.63
1:C:337:LEU:CD2	1:D:266:VAL:HG21	2.27	0.63
1:A:209:VAL:HG21	1:A:218:VAL:HG22	1.78	0.63
1:A:359:GLU:O	1:A:362:VAL:HG23	1.97	0.63
1:A:378:VAL:HG21	1:A:390:VAL:CG1	2.14	0.63
1:D:351:ASP:O	1:D:355:VAL:HG22	1.99	0.63
1:D:386:LEU:CD1	1:D:447:LEU:HD21	2.29	0.63
1:A:29:HIS:ND1	1:A:30:PRO:HD2	2.12	0.63
1:B:77:PRO:HB2	1:B:79:TRP:CD1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:VAL:C	1:D:429:THR:H	2.02	0.63
1:A:312:ALA:C	1:A:314:THR:N	2.50	0.63
1:B:427:VAL:C	1:B:429:THR:H	2.01	0.63
1:C:58:ALA:HB1	1:C:88:LEU:HD13	1.81	0.63
1:C:316:LEU:HD23	1:C:317:ALA:H	1.60	0.63
1:C:370:LEU:HD12	1:C:398:VAL:HG21	1.79	0.63
1:C:387:LEU:N	1:C:388:PRO:CD	2.62	0.63
1:A:337:LEU:HD21	1:B:266:VAL:CG1	2.27	0.62
1:A:447:LEU:O	1:A:447:LEU:HD13	1.99	0.62
1:B:130:GLU:HB2	1:B:133:GLU:CG	2.25	0.62
1:B:340:ARG:HD3	1:B:340:ARG:C	2.20	0.62
1:D:207:VAL:HG21	1:D:227:PHE:HE2	1.60	0.62
1:D:210:ARG:HG3	1:D:210:ARG:HH11	1.64	0.62
1:D:318:PHE:CD2	1:D:318:PHE:N	2.63	0.62
1:C:186:LEU:HB3	1:D:169:TYR:HE2	1.64	0.62
1:C:191:VAL:HG12	1:D:159:ARG:O	1.99	0.62
1:B:427:VAL:O	1:B:429:THR:N	2.31	0.62
1:C:274:SER:HB2	1:D:354:ARG:HH22	1.62	0.62
1:D:22:ARG:HG2	1:D:22:ARG:HH11	1.64	0.62
1:D:342:LEU:HD22	1:D:413:ARG:HD2	1.81	0.62
1:A:133:GLU:HG2	1:A:212:ASP:C	2.19	0.62
1:A:408:LEU:O	1:A:411:LEU:HB3	2.00	0.62
1:D:310:LEU:HA	1:D:313:VAL:CG2	2.29	0.62
1:A:138:MET:HB3	1:A:232:VAL:HG21	1.81	0.62
1:A:367:GLY:HA3	1:A:395:VAL:HG13	1.80	0.62
1:D:107:TYR:HE2	1:D:111:LEU:HD12	1.65	0.62
1:C:37:TRP:HE1	1:C:45:ARG:HH21	1.45	0.62
1:B:49:LEU:HB3	1:B:76:LEU:HD11	1.80	0.62
1:B:277:GLY:O	1:B:279:VAL:N	2.33	0.62
1:D:446:LEU:O	1:D:447:LEU:HG	1.99	0.62
1:A:289:LEU:HD12	1:B:370:LEU:HD21	1.80	0.62
1:A:374:LEU:O	1:A:378:VAL:HG23	1.99	0.62
1:B:277:GLY:O	1:B:280:ALA:N	2.33	0.62
1:D:427:VAL:O	1:D:429:THR:N	2.33	0.62
1:A:332:ASN:ND2	1:A:424:ASN:HB3	2.14	0.62
1:A:339:ILE:CG2	1:A:340:ARG:N	2.62	0.62
1:B:412:LEU:HD12	1:B:422:VAL:HG23	1.81	0.62
1:C:329:ASN:O	1:C:332:ASN:HB2	2.00	0.62
1:D:314:THR:C	1:D:316:LEU:H	2.01	0.62
1:D:386:LEU:HD21	1:D:447:LEU:CG	2.30	0.62
1:B:138:MET:SD	1:B:232:VAL:HG11	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:THR:HB	1:B:200:GLU:OE1	1.99	0.61
1:B:294:LEU:HD23	1:B:295:THR:N	2.15	0.61
1:C:88:LEU:HD23	1:C:93:LEU:CD1	2.27	0.61
1:D:316:LEU:CD1	1:D:317:ALA:H	2.13	0.61
1:B:386:LEU:C	1:B:388:PRO:HD2	2.21	0.61
1:A:77:PRO:HB2	1:A:79:TRP:HD1	1.65	0.61
1:A:257:THR:OG1	1:B:340:ARG:NH1	2.33	0.61
1:A:266:VAL:HG21	1:B:337:LEU:HG	1.82	0.61
1:B:111:LEU:O	1:B:111:LEU:HD23	2.01	0.61
1:D:370:LEU:HD12	1:D:398:VAL:HG21	1.83	0.61
1:D:387:LEU:N	1:D:388:PRO:CD	2.63	0.61
1:A:348:ASP:H	1:A:351:ASP:HB2	1.65	0.61
1:A:402:ASN:OD1	1:B:285:ARG:NH2	2.33	0.61
1:B:193:ASP:O	1:B:196:THR:HG23	2.00	0.61
1:B:309:VAL:O	1:B:312:ALA:HB3	1.99	0.61
1:C:337:LEU:HD11	1:D:266:VAL:CG2	2.29	0.61
1:D:69:GLN:OE1	1:D:96:ALA:HB1	2.01	0.61
1:C:210:ARG:HD2	1:C:212:ASP:OD1	2.01	0.61
1:C:333:GLN:CD	1:D:265:ALA:HB3	2.20	0.61
1:D:209:VAL:HG12	1:D:230:LEU:HD22	1.82	0.61
1:D:338:ILE:HG21	1:D:410:PHE:HE1	1.63	0.61
1:A:272:VAL:HG12	1:A:273:TYR:H	1.66	0.61
1:B:334:SER:HB2	1:B:402:ASN:HD22	1.65	0.61
1:B:352:TRP:O	1:B:355:VAL:HG23	2.00	0.61
1:C:352:TRP:H	1:C:352:TRP:HD1	1.49	0.61
1:C:77:PRO:HB2	1:C:79:TRP:CD1	2.36	0.61
1:C:186:LEU:HD12	1:C:189:LEU:HD12	1.81	0.61
1:D:177:LYS:HA	1:D:177:LYS:HE2	1.81	0.61
1:A:180:LEU:CD2	1:A:206:VAL:HG21	2.30	0.61
1:C:292:LEU:HD23	1:D:329:ASN:OD1	2.01	0.61
1:C:427:VAL:O	1:C:429:THR:N	2.34	0.61
1:D:97:LEU:CD1	1:D:123:VAL:HG11	2.31	0.61
1:D:317:ALA:C	1:D:319:TYR:H	2.03	0.61
1:A:44:HIS:O	1:A:48:VAL:HG23	2.01	0.61
1:A:143:VAL:HG21	1:A:168:ILE:HG22	1.82	0.61
1:B:293:ILE:HG22	1:B:293:ILE:O	1.99	0.61
1:D:397:ILE:HG13	1:D:438:ILE:HG21	1.83	0.61
1:C:249:LEU:O	1:C:249:LEU:HD23	2.01	0.60
1:A:347:LEU:HD11	1:B:273:TYR:CD2	2.37	0.60
1:B:146:ARG:NH2	1:B:176:GLU:HB3	2.16	0.60
1:C:202:MET:HG2	1:C:203:ASN:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LYS:NZ	1:D:120:ARG:HH21	1.98	0.60
1:A:211:THR:HG23	1:A:234:ASP:HA	1.84	0.60
1:B:245:VAL:HA	1:B:248:VAL:HG12	1.83	0.60
1:C:383:HIS:NE2	1:D:304:GLN:NE2	2.49	0.60
1:D:320:VAL:CG1	1:D:436:LEU:HD21	2.30	0.60
1:D:408:LEU:O	1:D:411:LEU:HB3	2.02	0.60
1:C:183:VAL:HG12	1:C:203:ASN:HB2	1.84	0.60
1:C:312:ALA:C	1:C:314:THR:H	2.05	0.60
1:D:364:LEU:HD23	1:D:364:LEU:O	2.02	0.60
1:A:66:PRO:O	1:A:99:ALA:HB1	2.00	0.60
1:A:280:ALA:O	1:A:283:LEU:HG	2.00	0.60
1:A:324:LEU:HG	1:A:432:ASP:OD1	2.00	0.60
1:A:326:THR:HA	1:A:329:ASN:HD22	1.65	0.60
1:B:101:ARG:HD2	1:B:108:PHE:CD2	2.36	0.60
1:B:290:VAL:HG12	1:B:291:ILE:N	2.15	0.60
1:A:293:ILE:O	1:A:293:ILE:HG22	2.02	0.60
1:B:320:VAL:HG13	1:B:324:LEU:HD13	1.84	0.60
1:C:275:GLU:O	1:C:276:ALA:HB2	2.02	0.60
1:C:408:LEU:CD1	1:C:411:LEU:HD23	2.31	0.60
1:A:101:ARG:HH11	1:A:101:ARG:HG3	1.64	0.60
1:A:386:LEU:C	1:A:388:PRO:HD2	2.22	0.60
1:C:365:LEU:HD22	1:D:282:TRP:CD1	2.37	0.60
1:D:89:SER:HB2	1:D:92:ASP:OD2	2.02	0.60
1:A:183:VAL:HG22	1:A:184:LEU:N	2.12	0.60
1:A:282:TRP:NE1	1:B:365:LEU:HD22	2.17	0.60
1:C:260:ILE:HD12	1:D:340:ARG:NH1	2.17	0.60
1:A:31:GLN:HA	1:A:34:LEU:HD12	1.83	0.60
1:B:378:VAL:CG1	1:B:390:VAL:HG21	2.19	0.60
1:A:90:LEU:HD13	1:A:140:PRO:HG3	1.84	0.60
1:B:150:THR:OG1	1:B:153:GLU:HB2	2.01	0.60
1:B:330:THR:HG23	1:B:402:ASN:OD1	2.02	0.60
1:C:340:ARG:CG	1:C:341:ALA:N	2.65	0.60
1:B:330:THR:HG22	1:B:331:GLY:N	2.17	0.59
1:B:446:LEU:HD13	1:B:446:LEU:O	2.02	0.59
1:C:333:GLN:HB2	1:D:285:ARG:NH1	2.16	0.59
1:B:86:GLU:C	1:B:88:LEU:H	2.06	0.59
1:B:265:ALA:HB1	1:B:288:TRP:CB	2.31	0.59
1:C:378:VAL:HG12	1:C:387:LEU:CD1	2.32	0.59
1:D:86:GLU:C	1:D:88:LEU:H	2.05	0.59
1:D:280:ALA:HA	1:D:283:LEU:CD1	2.32	0.59
1:D:307:GLU:HA	1:D:310:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LEU:HD23	1:D:261:HIS:CD2	2.37	0.59
1:C:378:VAL:HG11	1:C:390:VAL:CG2	2.20	0.59
1:D:329:ASN:O	1:D:332:ASN:HB2	2.02	0.59
1:B:34:LEU:HD11	1:B:63:HIS:CB	2.29	0.59
1:D:310:LEU:HA	1:D:313:VAL:HG23	1.84	0.59
1:D:316:LEU:CG	1:D:317:ALA:N	2.45	0.59
1:A:157:PHE:O	1:A:157:PHE:HD1	1.85	0.59
1:C:11:GLU:HG3	1:C:12:ALA:H	1.67	0.59
1:C:378:VAL:HG12	1:C:387:LEU:HD11	1.85	0.59
1:D:364:LEU:O	1:D:368:LEU:HG	2.02	0.59
1:A:86:GLU:C	1:A:88:LEU:H	2.04	0.59
1:A:412:LEU:CD1	1:A:422:VAL:HG23	2.32	0.59
1:B:193:ASP:HB3	1:B:196:THR:HG23	1.85	0.59
1:C:156:ARG:HA	1:C:159:ARG:HG3	1.84	0.59
1:C:412:LEU:HD12	1:C:422:VAL:HG23	1.85	0.59
1:A:328:GLY:HA2	1:A:431:SER:OG	2.03	0.59
1:B:296:GLY:HA2	1:B:299:THR:HG23	1.83	0.59
1:C:185:SER:HB2	1:C:188:ASP:OD2	2.02	0.59
1:C:408:LEU:O	1:C:411:LEU:HB3	2.02	0.59
1:A:133:GLU:HG2	1:A:212:ASP:HA	1.84	0.59
1:C:303:LEU:CD1	1:C:310:LEU:HD11	2.33	0.59
1:B:40:LEU:HB2	1:B:45:ARG:HD2	1.85	0.59
1:B:346:ASP:O	1:B:347:LEU:HB2	2.02	0.59
1:C:397:ILE:HD11	1:C:438:ILE:HB	1.85	0.59
1:A:171:ILE:HD12	1:A:171:ILE:N	2.18	0.58
1:A:290:VAL:HG12	1:A:291:ILE:N	2.17	0.58
1:A:326:THR:OG1	1:B:293:ILE:HG13	2.03	0.58
1:B:183:VAL:HG13	1:B:184:LEU:N	2.16	0.58
1:C:34:LEU:HG	1:C:60:VAL:HG13	1.85	0.58
1:A:339:ILE:CD1	1:A:420:ALA:HA	2.32	0.58
1:B:77:PRO:HB2	1:B:79:TRP:NE1	2.18	0.58
1:D:22:ARG:NH1	1:D:22:ARG:HG2	2.18	0.58
1:A:150:THR:OG1	1:A:153:GLU:HB2	2.03	0.58
1:A:249:LEU:HD23	1:B:249:LEU:HD12	1.85	0.58
1:A:347:LEU:HD11	1:B:273:TYR:HD2	1.68	0.58
1:B:356:PHE:CE2	1:B:403:LEU:HD12	2.38	0.58
1:C:351:ASP:OD1	1:C:354:ARG:HD2	2.03	0.58
1:C:442:VAL:O	1:C:442:VAL:HG12	2.03	0.58
1:A:249:LEU:O	1:A:249:LEU:HD13	2.03	0.58
1:A:339:ILE:HD11	1:A:420:ALA:CA	2.31	0.58
1:B:370:LEU:HD12	1:B:398:VAL:HG21	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:O	1:C:60:VAL:HG23	2.03	0.58
1:C:337:LEU:HD21	1:D:266:VAL:CG1	2.33	0.58
1:C:340:ARG:HH11	1:D:257:THR:HG23	1.67	0.58
1:C:370:LEU:HD11	1:D:289:LEU:HD12	1.85	0.58
1:A:245:VAL:HA	1:A:248:VAL:HG12	1.85	0.58
1:C:257:THR:HA	1:D:340:ARG:NH1	2.18	0.58
1:C:322:VAL:HG13	1:D:296:GLY:C	2.24	0.58
1:D:58:ALA:O	1:D:61:LEU:HG	2.03	0.58
1:D:272:VAL:HG12	1:D:273:TYR:N	2.18	0.58
1:D:317:ALA:C	1:D:319:TYR:N	2.56	0.58
1:B:211:THR:HG21	1:B:235:GLU:OE2	2.03	0.58
1:D:66:PRO:O	1:D:99:ALA:HB1	2.03	0.58
1:C:150:THR:O	1:C:154:VAL:HG23	2.03	0.58
1:D:149:MET:O	1:D:198:VAL:HG23	2.04	0.58
1:D:340:ARG:CZ	1:D:340:ARG:HB2	2.33	0.58
1:A:15:GLU:HG2	1:A:17:ASP:HB2	1.84	0.58
1:A:27:GLU:O	1:B:205:LYS:HE2	2.03	0.58
1:A:386:LEU:CD1	1:A:447:LEU:HD23	2.34	0.58
1:B:319:TYR:HB2	1:B:439:TYR:OH	2.04	0.58
1:B:338:ILE:HG21	1:B:410:PHE:CE1	2.38	0.58
1:B:371:SER:HA	1:B:394:LEU:HD23	1.86	0.58
1:C:90:LEU:HD23	1:C:90:LEU:O	2.02	0.58
1:C:159:ARG:O	1:D:191:VAL:HG12	2.04	0.58
1:D:146:ARG:HH12	1:D:176:GLU:HA	1.69	0.58
1:A:289:LEU:HD23	1:B:333:GLN:NE2	2.18	0.57
1:B:29:HIS:ND1	1:B:30:PRO:HD2	2.18	0.57
1:C:81:LEU:O	1:C:85:LEU:HG	2.04	0.57
1:D:303:LEU:CD2	1:D:436:LEU:HD13	2.32	0.57
1:A:13:LEU:HD23	1:A:13:LEU:O	2.02	0.57
1:B:74:LYS:HA	1:B:107:TYR:OH	2.04	0.57
1:C:66:PRO:O	1:C:99:ALA:HB1	2.04	0.57
1:C:171:ILE:HD12	1:C:171:ILE:N	2.19	0.57
1:C:187:ARG:HA	1:D:168:ILE:HD11	1.87	0.57
1:C:245:VAL:HG11	1:D:245:VAL:HG11	1.86	0.57
1:D:162:ALA:HB3	1:D:163:PRO:HD3	1.87	0.57
1:A:260:ILE:HD12	1:B:340:ARG:HH22	1.69	0.57
1:B:318:PHE:CD2	1:B:318:PHE:N	2.71	0.57
1:C:111:LEU:HD23	1:C:111:LEU:C	2.24	0.57
1:C:425:PRO:HG3	1:D:332:ASN:HD22	1.66	0.57
1:A:275:GLU:O	1:A:276:ALA:HB2	2.04	0.57
1:A:364:LEU:O	1:A:368:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:SER:OG	1:C:406:ALA:HB2	2.05	0.57
1:D:171:ILE:N	1:D:171:ILE:HD12	2.19	0.57
1:D:344:THR:O	1:D:344:THR:HG22	2.03	0.57
1:D:359:GLU:HA	1:D:362:VAL:CG2	2.34	0.57
1:B:222:MET:HG2	1:B:245:VAL:HG22	1.87	0.57
1:C:326:THR:HG23	1:D:293:ILE:CG1	2.33	0.57
1:A:350:ARG:CB	1:A:350:ARG:HH11	2.17	0.57
1:B:306:PHE:O	1:B:310:LEU:HB2	2.04	0.57
1:A:90:LEU:HD23	1:A:90:LEU:C	2.25	0.57
1:B:36:LEU:O	1:B:40:LEU:HG	2.05	0.57
1:B:314:THR:C	1:B:316:LEU:N	2.58	0.57
1:A:80:ARG:O	1:A:84:ILE:HG13	2.05	0.57
1:A:81:LEU:HD12	1:A:111:LEU:CD2	2.35	0.57
1:B:193:ASP:OD2	1:B:195:ARG:HG2	2.04	0.57
1:D:245:VAL:HG13	1:D:246:ASP:N	2.20	0.57
1:C:138:MET:HB3	1:C:232:VAL:HG21	1.87	0.57
1:A:355:VAL:HG21	1:A:410:PHE:CZ	2.40	0.57
1:A:365:LEU:HD22	1:B:282:TRP:CD1	2.40	0.57
1:C:337:LEU:HG	1:D:266:VAL:HG21	1.86	0.57
1:A:245:VAL:HG11	1:B:245:VAL:HG11	1.87	0.56
1:C:296:GLY:HA2	1:C:299:THR:HG23	1.85	0.56
1:C:385:LEU:O	1:C:386:LEU:C	2.43	0.56
1:D:293:ILE:O	1:D:293:ILE:HG22	2.05	0.56
1:B:215:GLN:HB3	1:B:251:VAL:HG13	1.86	0.56
1:C:177:LYS:HE2	1:C:177:LYS:HA	1.86	0.56
1:A:272:VAL:HG12	1:A:273:TYR:N	2.19	0.56
1:A:285:ARG:NH1	1:B:402:ASN:OD1	2.38	0.56
1:B:85:LEU:HD21	1:B:111:LEU:HD21	1.88	0.56
1:B:248:VAL:HA	1:B:251:VAL:HG23	1.88	0.56
1:B:275:GLU:O	1:B:276:ALA:HB2	2.05	0.56
1:B:334:SER:OG	1:B:406:ALA:HB2	2.05	0.56
1:C:116:ASP:OD2	1:C:118:ARG:HB2	2.05	0.56
1:C:245:VAL:CG1	1:D:245:VAL:HG21	2.35	0.56
1:C:293:ILE:CG1	1:D:326:THR:HG23	2.34	0.56
1:D:111:LEU:HD23	1:D:114:LEU:HD12	1.86	0.56
1:D:261:HIS:O	1:D:263:LEU:N	2.38	0.56
1:D:272:VAL:HG12	1:D:273:TYR:H	1.71	0.56
1:A:319:TYR:HB2	1:A:439:TYR:OH	2.05	0.56
1:A:323:LEU:HD13	1:A:439:TYR:CE1	2.40	0.56
1:B:9:LEU:HD23	1:B:9:LEU:C	2.26	0.56
1:C:48:VAL:HA	1:C:51:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:SER:HA	1:C:394:LEU:CD2	2.34	0.56
1:C:11:GLU:HG3	1:C:12:ALA:N	2.20	0.56
1:C:326:THR:OG1	1:D:293:ILE:CD1	2.53	0.56
1:D:97:LEU:HD13	1:D:123:VAL:HG11	1.86	0.56
1:D:265:ALA:HB1	1:D:288:TRP:CB	2.34	0.56
1:A:282:TRP:CE2	1:B:365:LEU:HD22	2.41	0.56
1:A:371:SER:HB2	1:A:395:VAL:HG22	1.85	0.56
1:B:385:LEU:O	1:B:386:LEU:C	2.43	0.56
1:B:408:LEU:O	1:B:411:LEU:HB3	2.06	0.56
1:C:268:VAL:CG2	1:C:271:LEU:HD11	2.29	0.56
1:C:397:ILE:HG13	1:C:438:ILE:HG21	1.87	0.56
1:D:330:THR:HG22	1:D:402:ASN:HB2	1.87	0.56
1:A:36:LEU:O	1:A:40:LEU:HG	2.06	0.56
1:B:97:LEU:HD23	1:B:97:LEU:O	2.05	0.56
1:B:323:LEU:CD1	1:B:324:LEU:HD12	2.36	0.56
1:C:149:MET:O	1:C:198:VAL:HG23	2.06	0.56
1:C:330:THR:OG1	1:D:289:LEU:HD11	2.05	0.56
1:C:446:LEU:O	1:C:447:LEU:HD23	2.06	0.56
1:D:328:GLY:HA2	1:D:431:SER:OG	2.06	0.56
1:B:104:ASP:CG	1:B:107:TYR:HB2	2.26	0.56
1:B:146:ARG:HH22	1:B:176:GLU:HB3	1.70	0.56
1:C:365:LEU:HD22	1:D:282:TRP:CG	2.40	0.56
1:C:422:VAL:HA	1:C:426:LEU:HD23	1.88	0.56
1:D:34:LEU:HG	1:D:60:VAL:HG13	1.88	0.56
1:A:230:LEU:HD23	1:A:231:PRO:HD2	1.88	0.56
1:A:370:LEU:HA	1:A:373:LEU:HD12	1.87	0.56
1:D:306:PHE:O	1:D:310:LEU:HB2	2.06	0.56
1:A:61:LEU:HA	1:A:64:LEU:HD12	1.86	0.55
1:A:257:THR:CB	1:B:340:ARG:NH1	2.69	0.55
1:B:37:TRP:HZ2	1:B:72:TYR:CE2	2.24	0.55
1:C:186:LEU:O	1:C:190:ILE:HG13	2.05	0.55
1:D:217:GLU:O	1:D:221:LEU:HD12	2.06	0.55
1:D:221:LEU:HD12	1:D:221:LEU:H	1.70	0.55
1:A:195:ARG:HH11	1:A:195:ARG:CB	2.15	0.55
1:A:257:THR:CA	1:B:340:ARG:NH1	2.69	0.55
1:A:332:ASN:HD21	1:A:424:ASN:HB3	1.70	0.55
1:B:97:LEU:HD23	1:B:97:LEU:C	2.27	0.55
1:B:348:ASP:OD1	1:B:349:LEU:N	2.32	0.55
1:C:345:ARG:NH2	1:D:35:ALA:HA	2.21	0.55
1:B:116:ASP:OD2	1:B:118:ARG:HD3	2.06	0.55
1:B:155:LEU:O	1:B:159:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ASP:OD1	1:C:349:LEU:N	2.25	0.55
1:D:248:VAL:HA	1:D:251:VAL:HG23	1.87	0.55
1:D:348:ASP:H	1:D:351:ASP:HB2	1.72	0.55
1:A:155:LEU:O	1:A:159:ARG:HG2	2.05	0.55
1:A:329:ASN:OD1	1:B:425:PRO:HB3	2.06	0.55
1:A:388:PRO:HG3	1:A:446:LEU:HD11	1.88	0.55
1:C:356:PHE:O	1:C:360:MET:HG3	2.07	0.55
1:C:366:LEU:HD11	1:D:285:ARG:HD2	1.86	0.55
1:B:180:LEU:CD2	1:B:206:VAL:HG11	2.36	0.55
1:C:86:GLU:C	1:C:88:LEU:H	2.10	0.55
1:C:90:LEU:CD2	1:C:123:VAL:HG22	2.28	0.55
1:A:349:LEU:CD1	1:A:414:ARG:HG2	2.37	0.55
1:A:442:VAL:O	1:A:442:VAL:CG1	2.53	0.55
1:C:37:TRP:NE1	1:C:45:ARG:NH2	2.55	0.55
1:C:220:ARG:HG3	1:C:220:ARG:NH1	2.22	0.55
1:C:303:LEU:CD2	1:C:436:LEU:HD11	2.37	0.55
1:D:25:LEU:HD12	1:D:51:LEU:HB3	1.88	0.55
1:D:394:LEU:HD23	1:D:394:LEU:C	2.26	0.55
1:A:392:VAL:HG12	1:A:396:LEU:HD12	1.88	0.55
1:A:396:LEU:O	1:A:400:PHE:CD1	2.58	0.55
1:B:112:LYS:HD2	1:B:120:ARG:HD3	1.87	0.55
1:A:292:LEU:HD23	1:B:329:ASN:OD1	2.07	0.55
1:A:311:GLU:O	1:A:314:THR:CB	2.53	0.55
1:C:190:ILE:HD11	1:D:186:LEU:HD21	1.88	0.55
1:C:215:GLN:HB3	1:C:251:VAL:HG13	1.89	0.55
1:A:321:PRO:HG2	1:A:322:VAL:H	1.71	0.55
1:C:322:VAL:HG11	1:D:297:MET:HA	1.88	0.55
1:A:265:ALA:HB3	1:B:333:GLN:HE21	1.72	0.55
1:B:320:VAL:O	1:B:324:LEU:HB2	2.06	0.55
1:C:257:THR:HG23	1:D:340:ARG:NH1	2.21	0.55
1:C:282:TRP:CD1	1:D:365:LEU:HB3	2.42	0.55
1:D:378:VAL:CG2	1:D:390:VAL:HG11	2.12	0.55
1:A:31:GLN:HA	1:A:31:GLN:NE2	2.21	0.54
1:A:281:LEU:H	1:A:281:LEU:CD1	2.18	0.54
1:A:326:THR:OG1	1:B:293:ILE:CD1	2.55	0.54
1:A:385:LEU:O	1:A:386:LEU:C	2.46	0.54
1:B:57:ALA:O	1:B:60:VAL:HG12	2.06	0.54
1:B:67:GLU:HG3	1:B:103:GLU:OE1	2.07	0.54
1:B:277:GLY:C	1:B:279:VAL:N	2.59	0.54
1:C:162:ALA:N	1:C:163:PRO:CD	2.70	0.54
1:D:112:LYS:HZ3	1:D:120:ARG:HH21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLY:HA2	1:D:299:THR:HG23	1.89	0.54
1:D:311:GLU:O	1:D:314:THR:OG1	2.18	0.54
1:D:318:PHE:HD2	1:D:318:PHE:N	2.03	0.54
1:D:408:LEU:HD12	1:D:411:LEU:HD23	1.89	0.54
1:C:142:TYR:CD1	1:C:142:TYR:C	2.81	0.54
1:D:77:PRO:HB2	1:D:79:TRP:CD1	2.41	0.54
1:D:261:HIS:C	1:D:263:LEU:H	2.10	0.54
1:B:11:GLU:O	1:B:11:GLU:OE1	2.25	0.54
1:B:330:THR:HG23	1:B:402:ASN:CG	2.28	0.54
1:B:364:LEU:CD1	1:D:392:VAL:HG13	2.38	0.54
1:C:7:VAL:O	1:C:7:VAL:HG12	2.08	0.54
1:C:36:LEU:O	1:C:40:LEU:HG	2.06	0.54
1:D:349:LEU:HD12	1:D:349:LEU:O	2.07	0.54
1:C:340:ARG:HD3	1:D:257:THR:CG2	2.37	0.54
1:C:366:LEU:CD2	1:D:286:VAL:HB	2.35	0.54
1:A:389:VAL:HG12	1:A:443:ALA:HA	1.88	0.54
1:B:66:PRO:O	1:B:99:ALA:HB1	2.07	0.54
1:B:293:ILE:O	1:B:297:MET:HG3	2.07	0.54
1:C:257:THR:HG23	1:D:340:ARG:HD2	1.88	0.54
1:C:350:ARG:HD2	1:C:351:ASP:N	2.23	0.54
1:C:424:ASN:O	1:C:427:VAL:HB	2.06	0.54
1:D:275:GLU:O	1:D:276:ALA:HB2	2.07	0.54
1:D:361:GLY:O	1:D:365:LEU:HB2	2.07	0.54
1:A:87:GLU:HG3	1:A:87:GLU:O	2.07	0.54
1:C:159:ARG:HD3	1:D:190:ILE:O	2.08	0.54
1:C:364:LEU:N	1:C:399:PHE:HD1	2.06	0.54
1:D:377:LYS:C	1:D:379:TYR:H	2.11	0.54
1:A:397:ILE:HG12	1:A:438:ILE:HD12	1.90	0.54
1:B:340:ARG:HG2	1:B:340:ARG:HH11	1.72	0.54
1:C:52:LEU:HD13	1:C:56:LYS:HB3	1.90	0.54
1:C:273:TYR:CE1	1:C:281:LEU:HD21	2.43	0.54
1:C:367:GLY:O	1:C:395:VAL:HG22	2.08	0.54
1:D:138:MET:SD	1:D:232:VAL:HG11	2.48	0.54
1:A:49:LEU:HD21	1:A:61:LEU:HD13	1.89	0.54
1:A:171:ILE:HD12	1:A:171:ILE:H	1.73	0.54
1:A:352:TRP:O	1:A:355:VAL:HG23	2.07	0.54
1:B:85:LEU:N	1:B:85:LEU:HD12	2.23	0.54
1:B:235:GLU:H	1:B:235:GLU:CD	2.11	0.54
1:A:85:LEU:HD22	1:A:93:LEU:CD1	2.38	0.54
1:D:93:LEU:HG	1:D:97:LEU:HD12	1.89	0.54
1:A:261:HIS:O	1:A:263:LEU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:PHE:HE2	1:B:403:LEU:HD12	1.71	0.54
1:C:207:VAL:HG11	1:C:225:TYR:CE2	2.43	0.54
1:D:156:ARG:HA	1:D:159:ARG:HG2	1.89	0.54
1:A:222:MET:CE	1:A:230:LEU:HB2	2.38	0.53
1:A:268:VAL:HG13	1:A:269:PRO:HD2	1.89	0.53
1:B:67:GLU:O	1:B:71:GLU:HB2	2.08	0.53
1:B:323:LEU:HD12	1:B:324:LEU:CD1	2.37	0.53
1:D:360:MET:HA	1:D:399:PHE:CE1	2.43	0.53
1:A:387:LEU:N	1:A:388:PRO:HD2	2.23	0.53
1:D:286:VAL:O	1:D:290:VAL:HG23	2.09	0.53
1:A:12:ALA:O	1:A:21:LEU:HD13	2.09	0.53
1:B:162:ALA:N	1:B:163:PRO:CD	2.71	0.53
1:C:338:ILE:O	1:C:341:ALA:HB3	2.09	0.53
1:A:355:VAL:CG1	1:B:273:TYR:HE2	2.22	0.53
1:B:185:SER:OG	1:B:187:ARG:HG2	2.08	0.53
1:C:202:MET:CG	1:C:203:ASN:N	2.72	0.53
1:A:222:MET:HE1	1:A:230:LEU:HB2	1.89	0.53
1:B:261:HIS:O	1:B:263:LEU:N	2.42	0.53
1:B:171:ILE:HD12	1:B:189:LEU:CD1	2.37	0.53
1:C:272:VAL:HG12	1:C:273:TYR:H	1.72	0.53
1:C:290:VAL:HG12	1:C:291:ILE:N	2.23	0.53
1:C:393:SER:HB3	1:C:442:VAL:CG1	2.32	0.53
1:D:58:ALA:HA	1:D:61:LEU:HD23	1.90	0.53
1:B:40:LEU:HB2	1:B:45:ARG:CD	2.38	0.53
1:D:332:ASN:O	1:D:333:GLN:C	2.46	0.53
1:A:65:SER:HB3	1:A:68:GLU:HG3	1.90	0.53
1:A:157:PHE:O	1:A:157:PHE:CD1	2.60	0.53
1:A:289:LEU:HD23	1:B:333:GLN:CD	2.29	0.53
1:B:314:THR:HG22	1:B:315:ALA:CA	2.39	0.53
1:B:370:LEU:HD12	1:B:398:VAL:HG11	1.90	0.53
1:C:85:LEU:HD11	1:C:111:LEU:HD21	1.90	0.53
1:C:229:VAL:HG13	1:C:242:ILE:CD1	2.37	0.53
1:C:374:LEU:HD22	1:C:394:LEU:HD22	1.90	0.53
1:D:255:GLU:OE1	1:D:255:GLU:HA	2.08	0.53
1:D:288:TRP:O	1:D:290:VAL:N	2.42	0.53
1:B:112:LYS:O	1:B:115:LEU:HB2	2.09	0.53
1:B:193:ASP:HB3	1:B:196:THR:CG2	2.39	0.53
1:B:207:VAL:HG11	1:B:225:TYR:CE2	2.44	0.53
1:D:72:TYR:O	1:D:76:LEU:HD23	2.09	0.53
1:D:185:SER:HB2	1:D:188:ASP:OD2	2.08	0.53
1:D:385:LEU:O	1:D:386:LEU:C	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:111:LEU:HD21	1.90	0.53
1:A:133:GLU:CB	1:A:212:ASP:HA	2.39	0.53
1:B:288:TRP:O	1:B:290:VAL:N	2.41	0.53
1:B:397:ILE:HG12	1:B:438:ILE:HD12	1.90	0.53
1:C:41:LYS:HB2	1:C:44:HIS:ND1	2.24	0.53
1:C:151:VAL:O	1:C:155:LEU:HG	2.08	0.53
1:C:337:LEU:O	1:C:340:ARG:HG2	2.09	0.53
1:A:299:THR:CG2	1:B:322:VAL:CG2	2.81	0.52
1:B:352:TRP:HD1	1:B:352:TRP:H	1.57	0.52
1:B:378:VAL:HB	1:B:387:LEU:HD11	1.91	0.52
1:B:408:LEU:N	1:B:409:PRO:HD2	2.24	0.52
1:C:117:PRO:HA	1:C:120:ARG:HB3	1.92	0.52
1:D:230:LEU:HD23	1:D:231:PRO:N	2.24	0.52
1:A:408:LEU:N	1:A:409:PRO:HD2	2.25	0.52
1:A:423:SER:HB2	1:A:425:PRO:HD2	1.91	0.52
1:B:64:LEU:HD22	1:B:68:GLU:CB	2.36	0.52
1:C:180:LEU:HD12	1:C:239:LEU:HD13	1.92	0.52
1:A:316:LEU:O	1:A:317:ALA:CB	2.56	0.52
1:C:50:THR:HA	1:C:80:ARG:HD2	1.90	0.52
1:C:209:VAL:HG12	1:C:230:LEU:HD22	1.91	0.52
1:C:293:ILE:O	1:C:293:ILE:HG22	2.09	0.52
1:A:370:LEU:HD12	1:A:398:VAL:HG21	1.92	0.52
1:D:364:LEU:HD21	1:D:368:LEU:HD21	1.91	0.52
1:D:397:ILE:O	1:D:398:VAL:C	2.48	0.52
1:A:261:HIS:C	1:A:263:LEU:H	2.12	0.52
1:A:293:ILE:HG13	1:B:326:THR:HG23	1.91	0.52
1:B:9:LEU:C	1:B:11:GLU:H	2.12	0.52
1:B:183:VAL:HG22	1:B:184:LEU:N	2.20	0.52
1:B:359:GLU:OE1	1:B:362:VAL:HB	2.09	0.52
1:C:80:ARG:HG3	1:C:80:ARG:HH11	1.74	0.52
1:C:367:GLY:HA3	1:C:395:VAL:HG13	1.90	0.52
1:A:215:GLN:HB3	1:A:251:VAL:HG13	1.91	0.52
1:A:329:ASN:O	1:A:332:ASN:HB2	2.09	0.52
1:A:397:ILE:O	1:A:398:VAL:C	2.45	0.52
1:B:312:ALA:C	1:B:314:THR:H	2.13	0.52
1:B:314:THR:C	1:B:316:LEU:H	2.12	0.52
1:C:299:THR:HG1	1:D:321:PRO:HB2	1.74	0.52
1:C:323:LEU:HD13	1:C:439:TYR:CE1	2.43	0.52
1:C:332:ASN:ND2	1:D:425:PRO:HG3	2.24	0.52
1:D:129:TYR:CB	1:D:135:GLY:HA3	2.39	0.52
1:D:338:ILE:HD13	1:D:410:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:VAL:HG21	1:D:410:PHE:CZ	2.44	0.52
1:A:216:GLU:O	1:A:219:ALA:HB3	2.09	0.52
1:A:338:ILE:O	1:A:341:ALA:HB3	2.08	0.52
1:A:339:ILE:HD11	1:A:419:PRO:O	2.10	0.52
1:C:117:PRO:HG3	1:C:120:ARG:CZ	2.40	0.52
1:C:318:PHE:HB3	1:D:303:LEU:HB3	1.92	0.52
1:D:33:LEU:HD23	1:D:60:VAL:HG11	1.92	0.52
1:D:370:LEU:CD1	1:D:398:VAL:HG21	2.40	0.52
1:D:442:VAL:O	1:D:442:VAL:CG1	2.57	0.52
1:A:31:GLN:CA	1:A:31:GLN:HE21	2.22	0.52
1:B:19:ARG:NH1	1:B:19:ARG:HB2	2.25	0.52
1:B:185:SER:O	1:B:188:ASP:HB2	2.10	0.52
1:B:346:ASP:OD1	1:B:347:LEU:HG	2.09	0.52
1:B:351:ASP:O	1:B:355:VAL:HG22	2.09	0.52
1:C:280:ALA:O	1:C:283:LEU:HG	2.09	0.52
1:C:11:GLU:CG	1:C:12:ALA:N	2.72	0.52
1:C:182:GLY:HA2	1:C:203:ASN:O	2.10	0.52
1:D:199:ALA:HA	1:D:202:MET:SD	2.50	0.52
1:A:111:LEU:O	1:A:111:LEU:HD13	2.10	0.52
1:A:299:THR:CG2	1:A:300:SER:N	2.73	0.52
1:A:424:ASN:O	1:A:427:VAL:HB	2.10	0.52
1:A:424:ASN:N	1:A:425:PRO:CD	2.73	0.52
1:C:36:LEU:N	1:C:36:LEU:HD12	2.25	0.52
1:A:412:LEU:HD11	1:A:422:VAL:CG2	2.36	0.51
1:C:142:TYR:C	1:C:142:TYR:HD1	2.13	0.51
1:C:245:VAL:HG11	1:D:245:VAL:HG21	1.93	0.51
1:C:288:TRP:O	1:C:290:VAL:N	2.43	0.51
1:C:336:THR:CG2	1:C:340:ARG:NH2	2.67	0.51
1:C:342:LEU:HB3	1:C:413:ARG:HH11	1.72	0.51
1:C:345:ARG:O	1:C:345:ARG:HG2	2.10	0.51
1:D:377:LYS:C	1:D:379:TYR:N	2.63	0.51
1:A:180:LEU:HD22	1:A:206:VAL:HG21	1.92	0.51
1:A:396:LEU:CD2	1:A:400:PHE:HE1	2.23	0.51
1:B:170:TYR:CD1	1:B:229:VAL:HG21	2.45	0.51
1:B:261:HIS:C	1:B:263:LEU:H	2.14	0.51
1:C:234:ASP:OD1	1:C:238:ARG:HG3	2.10	0.51
1:C:346:ASP:O	1:C:347:LEU:HB2	2.10	0.51
1:D:46:TYR:HE1	1:D:76:LEU:HA	1.75	0.51
1:D:50:THR:O	1:D:50:THR:HG22	2.10	0.51
1:B:132:ASP:O	1:B:215:GLN:HG3	2.09	0.51
1:C:326:THR:HA	1:D:293:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ASN:ND2	1:C:424:ASN:HB3	2.25	0.51
1:C:355:VAL:HG23	1:C:356:PHE:N	2.25	0.51
1:C:374:LEU:CD2	1:C:390:VAL:HG12	2.41	0.51
1:D:34:LEU:HD11	1:D:63:HIS:HB2	1.91	0.51
1:D:72:TYR:HB3	1:D:76:LEU:HD23	1.93	0.51
1:C:261:HIS:C	1:C:263:LEU:H	2.13	0.51
1:C:261:HIS:O	1:C:263:LEU:N	2.42	0.51
1:C:345:ARG:HH22	1:D:35:ALA:HA	1.75	0.51
1:D:86:GLU:OE1	1:D:86:GLU:HA	2.11	0.51
1:A:50:THR:HA	1:A:80:ARG:HD2	1.93	0.51
1:A:222:MET:HG3	1:A:227:PHE:HB2	1.93	0.51
1:A:318:PHE:HE1	1:A:383:HIS:NE2	2.08	0.51
1:A:320:VAL:CG1	1:A:436:LEU:HD21	2.40	0.51
1:C:130:GLU:HG3	1:C:133:GLU:OE2	2.09	0.51
1:D:87:GLU:O	1:D:87:GLU:HG3	2.10	0.51
1:A:316:LEU:HA	1:A:318:PHE:CE2	2.46	0.51
1:A:427:VAL:C	1:A:429:THR:N	2.63	0.51
1:B:182:GLY:HA2	1:B:203:ASN:O	2.10	0.51
1:B:424:ASN:CB	1:B:425:PRO:HD3	2.40	0.51
1:D:156:ARG:HA	1:D:159:ARG:CG	2.41	0.51
1:D:268:VAL:CB	1:D:271:LEU:HD11	2.27	0.51
1:A:31:GLN:HA	1:A:31:GLN:HE21	1.76	0.51
1:A:268:VAL:O	1:A:269:PRO:O	2.29	0.51
1:A:293:ILE:HG13	1:B:326:THR:CG2	2.41	0.51
1:A:326:THR:OG1	1:B:293:ILE:HD12	2.11	0.51
1:C:9:LEU:C	1:C:11:GLU:H	2.14	0.51
1:D:356:PHE:O	1:D:360:MET:HG3	2.11	0.51
1:A:180:LEU:O	1:A:181:LYS:HG3	2.10	0.51
1:C:339:ILE:HG23	1:C:419:PRO:HB2	1.93	0.51
1:C:388:PRO:CG	1:C:446:LEU:HD11	2.41	0.51
1:A:111:LEU:HD13	1:A:111:LEU:C	2.30	0.51
1:A:293:ILE:O	1:A:297:MET:HG3	2.11	0.51
1:B:149:MET:O	1:B:198:VAL:HG23	2.11	0.51
1:B:228:THR:HA	1:B:245:VAL:HG21	1.88	0.51
1:B:343:ALA:C	1:B:345:ARG:H	2.14	0.51
1:C:273:TYR:CD2	1:D:347:LEU:HD11	2.45	0.51
1:A:29:HIS:CE1	1:A:30:PRO:HD2	2.46	0.51
1:A:43:GLU:O	1:A:47:VAL:HG23	2.11	0.51
1:A:265:ALA:CB	1:B:333:GLN:HE21	2.23	0.51
1:B:123:VAL:C	1:B:125:ALA:H	2.13	0.51
1:C:88:LEU:CD2	1:C:93:LEU:HD12	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ALA:HB1	1:A:252:LEU:HD21	1.93	0.50
1:A:289:LEU:O	1:A:293:ILE:HG12	2.11	0.50
1:A:315:ALA:O	1:A:318:PHE:CZ	2.64	0.50
1:B:15:GLU:OE1	1:B:17:ASP:HB2	2.11	0.50
1:B:138:MET:HB3	1:B:232:VAL:HG21	1.92	0.50
1:B:442:VAL:O	1:B:442:VAL:CG1	2.58	0.50
1:B:444:ARG:CG	1:B:445:LEU:N	2.74	0.50
1:C:427:VAL:C	1:C:429:THR:N	2.65	0.50
1:D:182:GLY:HA2	1:D:203:ASN:O	2.11	0.50
1:D:386:LEU:HD21	1:D:447:LEU:CD2	2.40	0.50
1:A:265:ALA:HB1	1:A:288:TRP:HB2	1.93	0.50
1:B:54:LYS:CE	1:B:87:GLU:HB2	2.39	0.50
1:C:52:LEU:HD22	1:C:53:PRO:HD2	1.93	0.50
1:C:326:THR:OG1	1:D:293:ILE:HG13	2.11	0.50
1:A:147:GLU:HB2	1:A:199:ALA:HB2	1.93	0.50
1:A:338:ILE:CG2	1:A:410:PHE:CE1	2.93	0.50
1:A:387:LEU:HD12	1:A:387:LEU:O	2.11	0.50
1:B:154:VAL:O	1:B:158:LEU:HG	2.10	0.50
1:B:216:GLU:O	1:B:219:ALA:HB3	2.11	0.50
1:C:216:GLU:O	1:C:219:ALA:HB3	2.11	0.50
1:C:272:VAL:HG12	1:C:273:TYR:N	2.26	0.50
1:C:350:ARG:HD2	1:C:350:ARG:C	2.31	0.50
1:D:70:ALA:HB3	1:D:103:GLU:OE2	2.12	0.50
1:D:180:LEU:HD23	1:D:182:GLY:H	1.77	0.50
1:D:268:VAL:O	1:D:269:PRO:O	2.29	0.50
1:D:320:VAL:O	1:D:320:VAL:HG12	2.10	0.50
1:A:34:LEU:HG	1:A:60:VAL:HG13	1.92	0.50
1:A:48:VAL:C	1:A:50:THR:H	2.15	0.50
1:A:202:MET:CG	1:A:203:ASN:N	2.74	0.50
1:A:332:ASN:O	1:A:333:GLN:C	2.49	0.50
1:A:408:LEU:HD12	1:A:411:LEU:HD23	1.93	0.50
1:A:428:ALA:O	1:A:432:ASP:OD2	2.29	0.50
1:C:318:PHE:O	1:D:300:SER:OG	2.30	0.50
1:C:330:THR:CG2	1:C:402:ASN:HB2	2.42	0.50
1:D:180:LEU:O	1:D:181:LYS:HG3	2.11	0.50
1:A:335:ALA:O	1:A:339:ILE:HB	2.11	0.50
1:B:330:THR:HA	1:B:333:GLN:OE1	2.11	0.50
1:C:34:LEU:HD11	1:C:63:HIS:HB2	1.93	0.50
1:C:245:VAL:CG1	1:C:246:ASP:N	2.73	0.50
1:A:30:PRO:O	1:A:34:LEU:HD12	2.11	0.50
1:A:111:LEU:HD22	1:A:114:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:LEU:HA	1:C:433:VAL:HG23	1.94	0.50
1:D:70:ALA:HA	1:D:73:LEU:HD12	1.93	0.50
1:D:367:GLY:HA3	1:D:395:VAL:HG13	1.94	0.50
1:C:337:LEU:HD11	1:D:266:VAL:HG21	1.93	0.50
1:D:338:ILE:HD12	1:D:406:ALA:HA	1.94	0.50
1:D:386:LEU:C	1:D:388:PRO:HD2	2.32	0.50
1:D:427:VAL:C	1:D:429:THR:N	2.65	0.50
1:B:111:LEU:HD23	1:B:111:LEU:C	2.32	0.50
1:B:316:LEU:O	1:B:317:ALA:CB	2.59	0.50
1:C:228:THR:HG23	1:C:229:VAL:CG2	2.28	0.50
1:C:297:MET:HE3	1:D:374:LEU:HD12	1.93	0.50
1:D:210:ARG:HG3	1:D:210:ARG:NH1	2.25	0.50
1:A:225:TYR:O	1:A:227:PHE:CD1	2.62	0.50
1:A:418:ASP:O	1:A:421:LEU:HD22	2.12	0.50
1:B:94:ALA:O	1:B:98:GLN:HG3	2.12	0.50
1:B:294:LEU:O	1:B:297:MET:HB2	2.12	0.50
1:C:285:ARG:NH1	1:D:333:GLN:HB2	2.27	0.50
1:C:316:LEU:O	1:C:317:ALA:CB	2.60	0.50
1:C:365:LEU:HB3	1:D:282:TRP:CD1	2.47	0.50
1:C:377:LYS:O	1:C:381:ASP:HB2	2.12	0.50
1:A:26:GLU:HA	1:A:26:GLU:OE2	2.12	0.49
1:A:356:PHE:CE2	1:A:403:LEU:HD12	2.47	0.49
1:C:274:SER:HA	1:D:354:ARG:HH12	1.77	0.49
1:C:365:LEU:HD22	1:D:282:TRP:CD2	2.47	0.49
1:D:176:GLU:HG3	1:D:177:LYS:N	2.26	0.49
1:D:397:ILE:CG1	1:D:438:ILE:HG21	2.41	0.49
1:B:24:VAL:HG12	1:B:28:ILE:HD13	1.94	0.49
1:B:225:TYR:O	1:B:227:PHE:HD1	1.95	0.49
1:C:171:ILE:HD12	1:C:171:ILE:H	1.77	0.49
1:C:337:LEU:HD11	1:D:266:VAL:HG22	1.93	0.49
1:C:385:LEU:H	1:C:385:LEU:HD12	1.77	0.49
1:C:397:ILE:O	1:C:398:VAL:C	2.50	0.49
1:D:25:LEU:HB3	1:D:52:LEU:HD23	1.93	0.49
1:D:50:THR:HA	1:D:80:ARG:HE	1.73	0.49
1:D:396:LEU:O	1:D:396:LEU:HD23	2.12	0.49
1:A:320:VAL:HG11	1:A:436:LEU:HD21	1.94	0.49
1:A:371:SER:HA	1:A:394:LEU:CD2	2.38	0.49
1:A:424:ASN:CB	1:A:425:PRO:HD3	2.42	0.49
1:B:21:LEU:HD12	1:B:21:LEU:O	2.12	0.49
1:B:97:LEU:HD21	1:B:108:PHE:CD1	2.47	0.49
1:B:222:MET:HE1	1:B:230:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ALA:CB	1:C:100:VAL:HG22	2.42	0.49
1:C:315:ALA:O	1:C:318:PHE:CZ	2.65	0.49
1:C:332:ASN:O	1:C:333:GLN:C	2.50	0.49
1:D:289:LEU:O	1:D:293:ILE:HG12	2.12	0.49
1:A:388:PRO:CG	1:A:446:LEU:HD11	2.42	0.49
1:B:258:GLU:HG2	1:B:258:GLU:O	2.12	0.49
1:A:93:LEU:O	1:A:94:ALA:C	2.50	0.49
1:A:289:LEU:HD23	1:B:333:GLN:OE1	2.12	0.49
1:B:48:VAL:C	1:B:50:THR:H	2.16	0.49
1:C:169:TYR:CE1	1:D:169:TYR:HB3	2.48	0.49
1:C:343:ALA:C	1:C:345:ARG:H	2.16	0.49
1:D:91:ASP:CB	1:D:139:THR:HG22	2.41	0.49
1:B:280:ALA:O	1:B:283:LEU:HG	2.13	0.49
1:C:24:VAL:HG12	1:C:28:ILE:HD13	1.95	0.49
1:A:48:VAL:O	1:A:52:LEU:HD23	2.13	0.49
1:B:306:PHE:CG	1:B:440:LEU:HD13	2.46	0.49
1:B:332:ASN:O	1:B:333:GLN:C	2.50	0.49
1:B:359:GLU:HA	1:B:362:VAL:HG23	1.94	0.49
1:C:389:VAL:HG12	1:C:443:ALA:HA	1.94	0.49
1:C:425:PRO:CG	1:D:332:ASN:HD22	2.25	0.49
1:A:48:VAL:HG12	1:A:52:LEU:CD2	2.42	0.49
1:B:408:LEU:CD1	1:B:411:LEU:HD23	2.43	0.49
1:D:314:THR:HG22	1:D:315:ALA:CA	2.37	0.49
1:D:378:VAL:HG11	1:D:390:VAL:CG2	2.30	0.49
1:A:69:GLN:OE1	1:A:96:ALA:HB1	2.13	0.49
1:A:72:TYR:HB3	1:A:76:LEU:CD2	2.43	0.49
1:A:359:GLU:HA	1:A:362:VAL:HG23	1.95	0.49
1:A:378:VAL:O	1:A:378:VAL:HG12	2.12	0.49
1:B:272:VAL:HG12	1:B:273:TYR:H	1.78	0.49
1:B:296:GLY:CA	1:B:299:THR:HG23	2.43	0.49
1:C:32:ASP:O	1:C:36:LEU:HD13	2.11	0.49
1:C:313:VAL:HG12	1:C:313:VAL:O	2.13	0.49
1:D:9:LEU:C	1:D:11:GLU:H	2.16	0.49
1:D:408:LEU:CD1	1:D:411:LEU:HD23	2.42	0.49
1:B:397:ILE:O	1:B:398:VAL:C	2.52	0.49
1:C:9:LEU:HD12	1:C:28:ILE:CD1	2.43	0.49
1:C:216:GLU:HG3	1:C:255:GLU:HG3	1.94	0.49
1:A:299:THR:HG23	1:B:322:VAL:HG22	1.87	0.48
1:B:85:LEU:HD12	1:B:85:LEU:H	1.78	0.48
1:C:289:LEU:HD23	1:D:333:GLN:NE2	2.28	0.48
1:C:366:LEU:HD11	1:D:285:ARG:HD3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ASN:ND2	1:D:424:ASN:ND2	2.62	0.48
1:D:22:ARG:HH22	1:D:51:LEU:HA	1.78	0.48
1:D:377:LYS:O	1:D:381:ASP:HB2	2.13	0.48
1:A:29:HIS:CG	1:A:30:PRO:HD2	2.47	0.48
1:A:31:GLN:HA	1:A:34:LEU:CD1	2.43	0.48
1:A:300:SER:HB2	1:B:322:VAL:HG23	1.95	0.48
1:B:371:SER:HB2	1:B:395:VAL:HG23	1.92	0.48
1:C:123:VAL:C	1:C:125:ALA:H	2.16	0.48
1:C:208:TYR:HD1	1:C:208:TYR:H	1.60	0.48
1:C:294:LEU:O	1:C:297:MET:HB2	2.13	0.48
1:C:312:ALA:C	1:C:314:THR:N	2.66	0.48
1:D:34:LEU:CD1	1:D:63:HIS:HB2	2.43	0.48
1:D:282:TRP:O	1:D:286:VAL:HG12	2.14	0.48
1:A:162:ALA:N	1:A:163:PRO:CD	2.77	0.48
1:B:225:TYR:N	1:B:225:TYR:HD1	2.11	0.48
1:D:411:LEU:O	1:D:411:LEU:HD12	2.13	0.48
1:A:358:LYS:HE3	1:B:276:ALA:O	2.13	0.48
1:A:383:HIS:NE2	1:B:304:GLN:NE2	2.58	0.48
1:C:9:LEU:HD23	1:C:9:LEU:C	2.33	0.48
1:A:41:LYS:HB3	1:A:44:HIS:ND1	2.28	0.48
1:A:70:ALA:HA	1:A:73:LEU:HD12	1.94	0.48
1:A:396:LEU:HD23	1:A:400:PHE:CE1	2.48	0.48
1:C:77:PRO:HB2	1:C:79:TRP:HD1	1.76	0.48
1:C:316:LEU:CD2	1:C:317:ALA:N	2.65	0.48
1:C:412:LEU:CD1	1:C:422:VAL:HG23	2.43	0.48
1:D:424:ASN:O	1:D:427:VAL:HB	2.13	0.48
1:A:72:TYR:O	1:A:76:LEU:HD23	2.14	0.48
1:A:160:ARG:O	1:A:161:ALA:HB3	2.14	0.48
1:A:351:ASP:O	1:A:355:VAL:CG2	2.60	0.48
1:B:273:TYR:O	1:B:275:GLU:N	2.47	0.48
1:B:397:ILE:HG12	1:B:438:ILE:CD1	2.44	0.48
1:C:48:VAL:C	1:C:50:THR:H	2.17	0.48
1:C:374:LEU:CD2	1:C:394:LEU:HD22	2.44	0.48
1:A:377:LYS:C	1:A:379:TYR:H	2.15	0.48
1:C:337:LEU:CD1	1:D:266:VAL:HG21	2.44	0.48
1:D:149:MET:C	1:D:198:VAL:HG23	2.34	0.48
1:A:133:GLU:CG	1:A:212:ASP:HA	2.44	0.48
1:A:159:ARG:HH11	1:A:159:ARG:HG3	1.79	0.48
1:A:306:PHE:CG	1:A:440:LEU:HD13	2.49	0.48
1:C:326:THR:OG1	1:D:293:ILE:CG1	2.61	0.48
1:D:48:VAL:C	1:D:50:THR:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LYS:C	1:A:379:TYR:N	2.66	0.48
1:A:397:ILE:HG12	1:A:438:ILE:CD1	2.43	0.48
1:B:317:ALA:O	1:B:320:VAL:HG23	2.14	0.48
1:C:306:PHE:O	1:C:310:LEU:HD12	2.14	0.48
1:C:320:VAL:O	1:C:324:LEU:HB2	2.14	0.48
1:D:74:LYS:HA	1:D:107:TYR:OH	2.14	0.48
1:D:352:TRP:CE2	1:D:414:ARG:NH2	2.82	0.48
1:A:49:LEU:HD11	1:A:61:LEU:HD12	1.96	0.48
1:A:288:TRP:O	1:A:290:VAL:N	2.47	0.48
1:B:208:TYR:CD1	1:B:208:TYR:N	2.82	0.48
1:B:225:TYR:N	1:B:225:TYR:CD1	2.80	0.48
1:C:307:GLU:HA	1:C:310:LEU:HB2	1.95	0.48
1:B:215:GLN:OE1	1:B:251:VAL:HG13	2.14	0.47
1:C:333:GLN:CG	1:D:265:ALA:HB3	2.43	0.47
1:D:219:ALA:HA	1:D:248:VAL:HG21	1.96	0.47
1:B:43:GLU:O	1:B:47:VAL:HG23	2.14	0.47
1:D:323:LEU:HD13	1:D:439:TYR:CD1	2.49	0.47
1:A:90:LEU:HD22	1:A:140:PRO:CD	2.45	0.47
1:A:211:THR:HG23	1:A:233:VAL:O	2.14	0.47
1:A:424:ASN:H	1:A:425:PRO:CD	2.27	0.47
1:C:358:LYS:O	1:D:278:PRO:HG3	2.14	0.47
1:D:22:ARG:NH2	1:D:51:LEU:HD12	2.29	0.47
1:D:25:LEU:CD1	1:D:51:LEU:HB3	2.43	0.47
1:B:24:VAL:O	1:B:28:ILE:HG12	2.13	0.47
1:B:244:THR:CG2	1:B:246:ASP:OD1	2.62	0.47
1:B:338:ILE:HG22	1:B:342:LEU:CD1	2.44	0.47
1:C:117:PRO:HG3	1:C:120:ARG:NH1	2.30	0.47
1:C:333:GLN:HG2	1:D:265:ALA:HB3	1.96	0.47
1:C:388:PRO:HG3	1:C:446:LEU:HD11	1.96	0.47
1:D:262:LYS:HD3	1:D:421:LEU:CD1	2.44	0.47
1:A:292:LEU:CD2	1:B:329:ASN:OD1	2.62	0.47
1:A:340:ARG:HB3	1:A:340:ARG:CZ	2.44	0.47
1:B:446:LEU:O	1:B:446:LEU:CD1	2.61	0.47
1:C:377:LYS:C	1:C:379:TYR:N	2.68	0.47
1:D:91:ASP:HB3	1:D:139:THR:CG2	2.45	0.47
1:D:93:LEU:HD23	1:D:123:VAL:HG21	1.97	0.47
1:D:402:ASN:HD22	1:D:403:LEU:HD22	1.78	0.47
1:A:424:ASN:ND2	1:B:424:ASN:ND2	2.62	0.47
1:C:29:HIS:ND1	1:C:30:PRO:HD2	2.29	0.47
1:C:137:LEU:HD11	1:C:215:GLN:HG2	1.95	0.47
1:C:365:LEU:HD13	1:D:282:TRP:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:MET:HA	1:D:242:ILE:O	2.15	0.47
1:D:402:ASN:ND2	1:D:403:LEU:HD22	2.28	0.47
1:A:129:TYR:HB3	1:A:135:GLY:HA3	1.97	0.47
1:A:309:VAL:O	1:A:312:ALA:HB3	2.14	0.47
1:A:324:LEU:HD11	1:A:432:ASP:HA	1.97	0.47
1:A:339:ILE:CG2	1:A:340:ARG:H	2.27	0.47
1:B:21:LEU:HD11	1:B:25:LEU:HD11	1.97	0.47
1:B:37:TRP:CE2	1:B:45:ARG:HG2	2.50	0.47
1:B:388:PRO:HG3	1:B:446:LEU:HD11	1.92	0.47
1:C:37:TRP:HE1	1:C:45:ARG:NH2	2.11	0.47
1:C:138:MET:HA	1:C:242:ILE:O	2.15	0.47
1:C:213:THR:HG22	1:C:217:GLU:HB3	1.96	0.47
1:C:340:ARG:HH12	1:D:260:ILE:CG2	2.27	0.47
1:C:377:LYS:C	1:C:379:TYR:H	2.18	0.47
1:C:386:LEU:C	1:C:388:PRO:HD2	2.34	0.47
1:C:396:LEU:HD23	1:C:396:LEU:O	2.15	0.47
1:A:31:GLN:NE2	1:A:34:LEU:HD13	2.29	0.47
1:A:326:THR:OG1	1:B:293:ILE:CG1	2.62	0.47
1:D:94:ALA:O	1:D:98:GLN:HG3	2.15	0.47
1:A:172:TYR:OH	1:A:229:VAL:HG12	2.15	0.47
1:A:329:ASN:ND2	1:B:293:ILE:HD11	2.29	0.47
1:B:147:GLU:HB2	1:B:199:ALA:HB2	1.97	0.47
1:B:296:GLY:C	1:B:299:THR:HG23	2.34	0.47
1:C:52:LEU:CD2	1:C:53:PRO:HD2	2.45	0.47
1:C:257:THR:HG23	1:D:340:ARG:CD	2.44	0.47
1:C:268:VAL:HG12	1:C:269:PRO:HD2	1.96	0.47
1:C:360:MET:O	1:C:399:PHE:HE1	1.98	0.47
1:A:135:GLY:C	1:A:137:LEU:H	2.18	0.47
1:A:154:VAL:O	1:A:158:LEU:HG	2.15	0.47
1:A:260:ILE:HG12	1:B:260:ILE:HG12	1.97	0.47
1:D:324:LEU:CG	1:D:432:ASP:HA	2.45	0.47
1:A:230:LEU:CD2	1:A:231:PRO:HD2	2.46	0.46
1:A:340:ARG:NH1	1:A:340:ARG:HB3	2.30	0.46
1:A:343:ALA:C	1:A:345:ARG:H	2.18	0.46
1:B:285:ARG:NH1	1:B:285:ARG:CB	2.70	0.46
1:B:304:GLN:O	1:B:307:GLU:HB3	2.15	0.46
1:C:324:LEU:HG	1:C:432:ASP:HA	1.97	0.46
1:D:37:TRP:CD1	1:D:37:TRP:C	2.88	0.46
1:D:230:LEU:HD23	1:D:231:PRO:CD	2.45	0.46
1:A:71:GLU:HB3	1:A:72:TYR:CD1	2.50	0.46
1:A:82:ARG:HG3	1:A:82:ARG:HH11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG23	1:B:299:THR:OG1	2.16	0.46
1:A:358:LYS:CE	1:B:276:ALA:O	2.64	0.46
1:B:352:TRP:N	1:B:352:TRP:CD1	2.83	0.46
1:C:224:ASP:C	1:C:226:ASP:H	2.19	0.46
1:C:337:LEU:HD21	1:D:266:VAL:CG2	2.41	0.46
1:C:393:SER:CB	1:C:442:VAL:HG11	2.36	0.46
1:D:91:ASP:OD2	1:D:247:ASP:OD2	2.33	0.46
1:D:309:VAL:HG11	1:D:444:ARG:HG3	1.97	0.46
1:B:242:ILE:HG13	1:B:243:VAL:N	2.30	0.46
1:B:306:PHE:N	1:B:306:PHE:CD1	2.84	0.46
1:B:371:SER:HB2	1:B:395:VAL:HG21	1.96	0.46
1:A:245:VAL:CG1	1:A:246:ASP:N	2.78	0.46
1:A:291:ILE:O	1:A:294:LEU:HB3	2.15	0.46
1:A:293:ILE:HD12	1:B:326:THR:OG1	2.15	0.46
1:A:330:THR:OG1	1:B:289:LEU:HD21	2.15	0.46
1:C:21:LEU:CD2	1:C:51:LEU:HD13	2.36	0.46
1:C:72:TYR:HB3	1:C:76:LEU:CD2	2.44	0.46
1:C:351:ASP:O	1:C:355:VAL:HG13	2.15	0.46
1:C:365:LEU:HD22	1:D:282:TRP:CE2	2.51	0.46
1:D:7:VAL:O	1:D:7:VAL:HG12	2.14	0.46
1:D:338:ILE:CG2	1:D:410:PHE:CE1	2.97	0.46
1:A:213:THR:O	1:A:214:ASP:C	2.54	0.46
1:A:313:VAL:O	1:A:313:VAL:HG12	2.16	0.46
1:B:208:TYR:N	1:B:208:TYR:HD1	2.13	0.46
1:B:213:THR:O	1:B:214:ASP:C	2.54	0.46
1:C:183:VAL:HG13	1:C:184:LEU:N	2.30	0.46
1:C:378:VAL:CG2	1:C:390:VAL:HG11	2.22	0.46
1:A:273:TYR:O	1:A:275:GLU:N	2.49	0.46
1:B:37:TRP:CZ2	1:B:45:ARG:HG2	2.51	0.46
1:B:48:VAL:HA	1:B:51:LEU:HD12	1.96	0.46
1:C:266:VAL:CG1	1:D:337:LEU:HD21	2.24	0.46
1:C:340:ARG:NH2	1:D:261:HIS:HA	2.30	0.46
1:D:342:LEU:HD23	1:D:413:ARG:HH11	1.81	0.46
1:D:426:LEU:HD12	1:D:426:LEU:O	2.16	0.46
1:A:213:THR:HG22	1:A:217:GLU:HB3	1.97	0.46
1:C:116:ASP:OD1	1:C:118:ARG:HG3	2.16	0.46
1:C:180:LEU:CD2	1:C:182:GLY:H	2.29	0.46
1:C:289:LEU:HD23	1:D:333:GLN:CD	2.36	0.46
1:A:72:TYR:CD1	1:A:72:TYR:N	2.83	0.46
1:A:183:VAL:O	1:A:184:LEU:HB2	2.14	0.46
1:A:186:LEU:HD12	1:A:189:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:HD12	1:A:406:ALA:CA	2.37	0.46
1:D:40:LEU:HB2	1:D:45:ARG:CD	2.46	0.46
1:D:117:PRO:HA	1:D:120:ARG:HB3	1.98	0.46
1:D:343:ALA:C	1:D:345:ARG:H	2.19	0.46
1:A:9:LEU:C	1:A:11:GLU:H	2.19	0.46
1:A:77:PRO:HB2	1:A:79:TRP:CD1	2.48	0.46
1:A:202:MET:HG2	1:A:203:ASN:N	2.31	0.46
1:B:7:VAL:O	1:B:7:VAL:HG12	2.14	0.46
1:B:389:VAL:HG13	1:B:446:LEU:HD12	1.98	0.46
1:C:268:VAL:O	1:C:269:PRO:O	2.34	0.46
1:C:274:SER:CA	1:D:354:ARG:HH22	2.28	0.46
1:C:340:ARG:HG2	1:C:341:ALA:N	2.30	0.46
1:D:104:ASP:CG	1:D:107:TYR:HB2	2.36	0.46
1:D:261:HIS:C	1:D:263:LEU:N	2.69	0.46
1:A:312:ALA:O	1:A:314:THR:N	2.42	0.46
1:B:268:VAL:O	1:B:269:PRO:O	2.32	0.46
1:C:162:ALA:N	1:C:163:PRO:HD3	2.31	0.46
1:A:329:ASN:HD22	1:B:293:ILE:HD11	1.81	0.45
1:A:333:GLN:HE21	1:B:265:ALA:CB	2.10	0.45
1:B:408:LEU:HD12	1:B:411:LEU:HD23	1.96	0.45
1:C:248:VAL:HG23	1:C:251:VAL:HG21	1.98	0.45
1:A:49:LEU:HD11	1:A:61:LEU:CD1	2.47	0.45
1:B:155:LEU:HD21	1:B:189:LEU:HB3	1.99	0.45
1:B:338:ILE:HG22	1:B:342:LEU:HD11	1.99	0.45
1:B:342:LEU:HB3	1:B:413:ARG:HH11	1.81	0.45
1:B:437:LEU:N	1:B:437:LEU:HD23	2.30	0.45
1:C:30:PRO:O	1:C:33:LEU:HB3	2.16	0.45
1:C:70:ALA:HB1	1:C:100:VAL:HG22	1.98	0.45
1:C:208:TYR:N	1:C:208:TYR:CD1	2.84	0.45
1:C:209:VAL:CG1	1:C:230:LEU:HD22	2.46	0.45
1:D:52:LEU:HD13	1:D:56:LYS:HB3	1.98	0.45
1:D:364:LEU:HD23	1:D:368:LEU:CD2	2.45	0.45
1:A:61:LEU:HD21	1:A:73:LEU:HD21	1.98	0.45
1:B:146:ARG:NH2	1:B:176:GLU:CB	2.79	0.45
1:B:146:ARG:HD2	1:B:174:VAL:O	2.16	0.45
1:B:162:ALA:H	1:B:163:PRO:HD2	1.81	0.45
1:B:364:LEU:HD11	1:D:392:VAL:HG13	1.97	0.45
1:B:379:TYR:HD1	1:B:384:PRO:HB3	1.82	0.45
1:B:424:ASN:O	1:B:427:VAL:HB	2.16	0.45
1:C:95:ASP:HA	1:C:98:GLN:OE1	2.16	0.45
1:C:408:LEU:HB3	1:C:409:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:HIS:ND1	1:D:30:PRO:HD2	2.30	0.45
1:D:149:MET:HB2	1:D:198:VAL:HG21	1.98	0.45
1:B:377:LYS:C	1:B:379:TYR:H	2.18	0.45
1:C:34:LEU:HD21	1:C:60:VAL:O	2.17	0.45
1:C:256:ALA:O	1:C:260:ILE:HG13	2.16	0.45
1:C:300:SER:HB2	1:D:322:VAL:HG23	1.98	0.45
1:D:15:GLU:HG3	1:D:17:ASP:HB2	1.99	0.45
1:D:347:LEU:O	1:D:348:ASP:OD1	2.34	0.45
1:B:28:ILE:CD1	1:B:33:LEU:HD11	2.26	0.45
1:B:93:LEU:O	1:B:94:ALA:C	2.52	0.45
1:B:112:LYS:CD	1:B:120:ARG:HD3	2.47	0.45
1:B:334:SER:HB2	1:B:402:ASN:HD21	1.79	0.45
1:C:146:ARG:HG3	1:C:147:GLU:N	2.32	0.45
1:C:338:ILE:CG2	1:C:410:PHE:CE1	3.00	0.45
1:C:342:LEU:CB	1:C:413:ARG:NH1	2.75	0.45
1:C:352:TRP:O	1:C:355:VAL:CG2	2.63	0.45
1:D:209:VAL:HG12	1:D:230:LEU:CD2	2.44	0.45
1:D:342:LEU:CD2	1:D:413:ARG:HH11	2.30	0.45
1:D:424:ASN:N	1:D:425:PRO:CD	2.78	0.45
1:A:65:SER:HB3	1:A:68:GLU:CG	2.46	0.45
1:A:352:TRP:HA	1:A:355:VAL:HG23	1.97	0.45
1:B:222:MET:HG2	1:B:245:VAL:CG2	2.46	0.45
1:C:186:LEU:HD21	1:D:190:ILE:HD11	1.99	0.45
1:C:207:VAL:CG2	1:C:227:PHE:HE2	2.30	0.45
1:C:340:ARG:HB3	1:C:340:ARG:CZ	2.46	0.45
1:D:22:ARG:CZ	1:D:51:LEU:HG	2.47	0.45
1:D:412:LEU:HD12	1:D:422:VAL:HG23	1.99	0.45
1:A:182:GLY:HA2	1:A:203:ASN:O	2.16	0.45
1:A:260:ILE:HD12	1:B:340:ARG:CZ	2.45	0.45
1:A:296:GLY:O	1:A:299:THR:CG2	2.41	0.45
1:A:364:LEU:O	1:A:364:LEU:HD23	2.17	0.45
1:C:24:VAL:O	1:C:28:ILE:HG12	2.17	0.45
1:C:260:ILE:HG12	1:D:260:ILE:HG12	1.99	0.45
1:C:268:VAL:HB	1:C:271:LEU:HD21	1.99	0.45
1:C:391:GLY:O	1:C:395:VAL:HG23	2.17	0.45
1:A:219:ALA:HA	1:A:248:VAL:HG21	1.98	0.45
1:A:307:GLU:HG3	1:A:308:SER:N	2.31	0.45
1:B:316:LEU:HB3	1:B:317:ALA:H	1.51	0.45
1:B:340:ARG:C	1:B:340:ARG:CD	2.84	0.45
1:B:418:ASP:OD2	1:B:420:ALA:HB3	2.16	0.45
1:C:208:TYR:HD1	1:C:208:TYR:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:OG1	1:C:300:SER:N	2.50	0.45
1:D:61:LEU:C	1:D:61:LEU:HD12	2.38	0.45
1:D:136:GLY:O	1:D:137:LEU:HD23	2.16	0.45
1:D:183:VAL:CG2	1:D:184:LEU:H	2.06	0.45
1:D:317:ALA:O	1:D:319:TYR:N	2.50	0.45
1:A:81:LEU:CD1	1:A:111:LEU:HD21	2.47	0.45
1:A:211:THR:CG2	1:A:234:ASP:HA	2.46	0.45
1:B:65:SER:OG	1:B:68:GLU:HB2	2.17	0.45
1:B:213:THR:CG2	1:B:218:VAL:HG22	2.47	0.45
1:B:224:ASP:C	1:B:226:ASP:H	2.19	0.45
1:B:403:LEU:CD2	1:B:403:LEU:N	2.80	0.45
1:B:427:VAL:C	1:B:429:THR:N	2.65	0.45
1:C:214:ASP:O	1:C:218:VAL:HG23	2.17	0.45
1:C:393:SER:O	1:C:394:LEU:C	2.54	0.45
1:D:296:GLY:C	1:D:299:THR:HG23	2.37	0.45
1:D:324:LEU:HD21	1:D:432:ASP:CA	2.47	0.45
1:A:210:ARG:HH12	1:A:235:GLU:HA	1.81	0.45
1:C:132:ASP:HA	1:C:215:GLN:NE2	2.19	0.45
1:C:208:TYR:CD2	1:C:233:VAL:HG21	2.52	0.45
1:C:257:THR:HA	1:D:340:ARG:HH12	1.80	0.45
1:D:123:VAL:C	1:D:125:ALA:H	2.18	0.45
1:D:273:TYR:O	1:D:275:GLU:N	2.50	0.45
1:D:306:PHE:CG	1:D:440:LEU:HD13	2.52	0.45
1:D:334:SER:OG	1:D:406:ALA:HB2	2.17	0.45
1:D:393:SER:HB3	1:D:442:VAL:HG11	1.99	0.45
1:A:15:GLU:CG	1:A:17:ASP:HB2	2.47	0.44
1:B:225:TYR:HD1	1:B:225:TYR:H	1.64	0.44
1:B:377:LYS:C	1:B:379:TYR:N	2.68	0.44
1:C:242:ILE:CG1	1:C:243:VAL:N	2.79	0.44
1:C:296:GLY:CA	1:C:299:THR:HG23	2.46	0.44
1:C:316:LEU:HG	1:C:317:ALA:N	2.21	0.44
1:C:322:VAL:HG23	1:D:300:SER:HB2	1.98	0.44
1:D:54:LYS:HE3	1:D:83:GLU:CG	2.34	0.44
1:D:180:LEU:CD2	1:D:182:GLY:H	2.30	0.44
1:A:19:ARG:HB3	1:A:19:ARG:CZ	2.47	0.44
1:A:56:LYS:O	1:A:60:VAL:HG23	2.17	0.44
1:A:227:PHE:HB3	1:A:228:THR:H	1.65	0.44
1:C:93:LEU:O	1:C:94:ALA:C	2.56	0.44
1:A:285:ARG:HG2	1:B:333:GLN:NE2	2.32	0.44
1:A:385:LEU:H	1:A:385:LEU:HD12	1.82	0.44
1:A:50:THR:HA	1:A:80:ARG:CD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:HG12	1:B:346:ASP:OD2	2.17	0.44
1:B:288:TRP:C	1:B:290:VAL:N	2.70	0.44
1:B:338:ILE:HD11	1:B:355:VAL:HG11	2.00	0.44
1:C:250:ASP:C	1:C:252:LEU:N	2.71	0.44
1:C:274:SER:HB2	1:D:354:ARG:NH2	2.28	0.44
1:C:296:GLY:C	1:C:299:THR:HG23	2.38	0.44
1:C:334:SER:OG	1:C:406:ALA:N	2.51	0.44
1:D:98:GLN:O	1:D:101:ARG:HB3	2.17	0.44
1:D:268:VAL:HB	1:D:271:LEU:CG	2.46	0.44
1:A:46:TYR:O	1:A:46:TYR:HD1	2.01	0.44
1:A:135:GLY:O	1:A:137:LEU:N	2.51	0.44
1:B:207:VAL:HG11	1:B:225:TYR:CD2	2.53	0.44
1:C:40:LEU:HB2	1:C:45:ARG:HD2	2.00	0.44
1:C:213:THR:O	1:C:214:ASP:C	2.54	0.44
1:C:340:ARG:NH2	1:D:260:ILE:C	2.70	0.44
1:C:367:GLY:C	1:C:395:VAL:HG13	2.37	0.44
1:D:267:ASP:O	1:D:267:ASP:CG	2.55	0.44
1:D:288:TRP:C	1:D:290:VAL:N	2.70	0.44
1:D:386:LEU:HD21	1:D:447:LEU:HD21	2.00	0.44
1:A:285:ARG:HH12	1:B:402:ASN:CG	2.18	0.44
1:B:424:ASN:N	1:B:425:PRO:CD	2.81	0.44
1:C:292:LEU:HD11	1:C:426:LEU:HA	1.98	0.44
1:C:439:TYR:C	1:C:440:LEU:HD23	2.37	0.44
1:D:245:VAL:HA	1:D:248:VAL:HG12	2.00	0.44
1:A:69:GLN:OE1	1:A:96:ALA:CB	2.66	0.44
1:B:280:ALA:HA	1:B:283:LEU:HD21	1.98	0.44
1:B:302:ILE:HD12	1:B:302:ILE:HA	1.90	0.44
1:B:329:ASN:O	1:B:332:ASN:HB2	2.17	0.44
1:D:213:THR:HG22	1:D:217:GLU:HB3	1.99	0.44
1:A:123:VAL:C	1:A:125:ALA:H	2.20	0.44
1:A:266:VAL:HG21	1:B:337:LEU:CD1	2.47	0.44
1:A:366:LEU:CD2	1:B:286:VAL:HB	2.47	0.44
1:C:177:LYS:HB3	1:C:179:ARG:NH1	2.33	0.44
1:C:244:THR:HB	1:C:247:ASP:HB2	2.00	0.44
1:D:199:ALA:HA	1:D:202:MET:HG2	1.99	0.44
1:A:34:LEU:HD21	1:A:63:HIS:HB2	1.99	0.44
1:B:261:HIS:C	1:B:263:LEU:N	2.71	0.44
1:C:73:LEU:HD22	1:C:111:LEU:CD1	2.28	0.44
1:C:149:MET:C	1:C:198:VAL:HG23	2.38	0.44
1:C:209:VAL:HG21	1:C:218:VAL:HG13	1.98	0.44
1:D:81:LEU:O	1:D:85:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:C	1:D:226:ASP:H	2.21	0.44
1:D:228:THR:HA	1:D:245:VAL:HB	2.00	0.44
1:D:332:ASN:ND2	1:D:424:ASN:HB3	2.32	0.44
1:A:133:GLU:HG2	1:A:213:THR:N	2.33	0.43
1:B:62:SER:HA	1:B:69:GLN:NE2	2.32	0.43
1:B:222:MET:HE3	1:B:230:LEU:CG	2.45	0.43
1:C:219:ALA:HA	1:C:248:VAL:HG21	2.00	0.43
1:C:250:ASP:O	1:C:251:VAL:C	2.56	0.43
1:C:338:ILE:HG21	1:C:410:PHE:CE1	2.53	0.43
1:C:410:PHE:O	1:C:414:ARG:HG3	2.18	0.43
1:D:34:LEU:CD2	1:D:60:VAL:HG13	2.48	0.43
1:D:222:MET:HG2	1:D:227:PHE:HB2	1.99	0.43
1:A:40:LEU:HD12	1:A:45:ARG:HG2	1.99	0.43
1:A:340:ARG:NH2	1:A:341:ALA:CB	2.76	0.43
1:B:91:ASP:OD1	1:B:92:ASP:N	2.51	0.43
1:B:110:ARG:O	1:B:113:ASP:HB2	2.18	0.43
1:C:439:TYR:O	1:C:439:TYR:CD2	2.71	0.43
1:D:54:LYS:HG2	1:D:83:GLU:OE2	2.18	0.43
1:D:208:TYR:N	1:D:208:TYR:CD1	2.86	0.43
1:D:374:LEU:HD23	1:D:390:VAL:HG12	2.00	0.43
1:A:285:ARG:NH1	1:B:402:ASN:ND2	2.49	0.43
1:B:208:TYR:HD1	1:B:208:TYR:H	1.65	0.43
1:B:250:ASP:C	1:B:252:LEU:N	2.71	0.43
1:C:77:PRO:HA	1:C:78:PRO:HD2	1.83	0.43
1:C:82:ARG:HH11	1:C:82:ARG:HG3	1.83	0.43
1:C:257:THR:OG1	1:D:340:ARG:CZ	2.67	0.43
1:C:354:ARG:NH1	1:D:274:SER:OG	2.51	0.43
1:C:378:VAL:CG1	1:C:390:VAL:HG21	2.22	0.43
1:D:318:PHE:HE1	1:D:383:HIS:HE2	1.65	0.43
1:D:324:LEU:HD21	1:D:432:ASP:HA	2.00	0.43
1:A:388:PRO:HG2	1:A:389:VAL:N	2.33	0.43
1:B:50:THR:HA	1:B:80:ARG:HD2	1.99	0.43
1:B:80:ARG:O	1:B:83:GLU:HB3	2.18	0.43
1:C:54:LYS:CE	1:C:87:GLU:HB2	2.47	0.43
1:C:176:GLU:HG3	1:C:177:LYS:HD2	2.01	0.43
1:D:217:GLU:O	1:D:221:LEU:CD1	2.66	0.43
1:B:50:THR:O	1:B:51:LEU:HD23	2.18	0.43
1:B:306:PHE:N	1:B:306:PHE:HD1	2.17	0.43
1:D:49:LEU:O	1:D:76:LEU:HD11	2.19	0.43
1:D:111:LEU:CD2	1:D:114:LEU:HD12	2.49	0.43
1:A:157:PHE:CD1	1:A:157:PHE:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:VAL:O	1:A:298:VAL:HG12	2.17	0.43
1:A:396:LEU:CD2	1:A:400:PHE:CE1	3.01	0.43
1:B:268:VAL:HG23	1:B:284:ALA:HB1	2.01	0.43
1:B:302:ILE:HG21	1:B:437:LEU:CD2	2.49	0.43
1:B:379:TYR:CD1	1:B:384:PRO:HB3	2.53	0.43
1:C:261:HIS:C	1:C:263:LEU:N	2.72	0.43
1:D:384:PRO:C	1:D:385:LEU:O	2.56	0.43
1:A:203:ASN:C	1:A:203:ASN:OD1	2.57	0.43
1:A:319:TYR:CB	1:A:439:TYR:OH	2.67	0.43
1:D:134:ALA:O	1:D:135:GLY:C	2.57	0.43
1:D:164:ASP:O	1:D:164:ASP:OD1	2.36	0.43
1:D:393:SER:O	1:D:394:LEU:C	2.55	0.43
1:D:400:PHE:HD2	1:D:400:PHE:HA	1.69	0.43
1:A:72:TYR:HB3	1:A:76:LEU:HD23	2.01	0.43
1:A:268:VAL:HB	1:A:271:LEU:CG	2.49	0.43
1:B:28:ILE:O	1:B:28:ILE:HG13	2.17	0.43
1:C:250:ASP:O	1:C:252:LEU:N	2.52	0.43
1:C:338:ILE:HD12	1:C:410:PHE:HE1	1.78	0.43
1:A:143:VAL:CG2	1:A:168:ILE:HG22	2.48	0.43
1:A:256:ALA:O	1:A:260:ILE:HG13	2.18	0.43
1:B:245:VAL:HA	1:B:248:VAL:CG1	2.47	0.43
1:C:359:GLU:HA	1:C:359:GLU:OE2	2.19	0.43
1:D:447:LEU:HD23	1:D:447:LEU:HA	1.93	0.43
1:A:280:ALA:HA	1:A:283:LEU:HD21	2.01	0.43
1:A:386:LEU:CD2	1:A:446:LEU:HD12	2.49	0.43
1:B:135:GLY:C	1:B:137:LEU:H	2.22	0.43
1:B:315:ALA:O	1:B:318:PHE:CZ	2.72	0.43
1:C:25:LEU:CD1	1:C:51:LEU:HB2	2.48	0.43
1:C:323:LEU:HD13	1:C:439:TYR:HE1	1.84	0.43
1:C:377:LYS:HB2	1:D:297:MET:HE1	2.00	0.43
1:D:216:GLU:O	1:D:219:ALA:HB3	2.19	0.43
1:D:296:GLY:CA	1:D:299:THR:HG23	2.49	0.43
1:D:436:LEU:HD23	1:D:436:LEU:HA	1.87	0.43
1:A:183:VAL:HG13	1:A:184:LEU:N	2.33	0.42
1:A:322:VAL:CG2	1:B:296:GLY:O	2.49	0.42
1:A:338:ILE:HG22	1:A:342:LEU:CD1	2.49	0.42
1:B:258:GLU:O	1:B:262:LYS:HG3	2.19	0.42
1:C:135:GLY:C	1:C:137:LEU:H	2.22	0.42
1:D:215:GLN:HB3	1:D:251:VAL:HG11	1.98	0.42
1:D:316:LEU:HA	1:D:318:PHE:HE2	1.80	0.42
1:A:28:ILE:HG13	1:A:28:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD11	1:A:111:LEU:HD11	2.00	0.42
1:A:86:GLU:C	1:A:88:LEU:N	2.72	0.42
1:A:290:VAL:HG22	1:B:373:LEU:HD13	2.01	0.42
1:B:346:ASP:O	1:B:347:LEU:CB	2.64	0.42
1:C:15:GLU:CG	1:C:17:ASP:HB2	2.43	0.42
1:C:147:GLU:HB2	1:C:199:ALA:HB2	2.01	0.42
1:C:274:SER:HA	1:D:354:ARG:HH22	1.84	0.42
1:C:307:GLU:HA	1:C:310:LEU:CB	2.48	0.42
1:D:268:VAL:HB	1:D:271:LEU:HD21	2.01	0.42
1:D:286:VAL:O	1:D:286:VAL:HG22	2.19	0.42
1:A:340:ARG:HD2	1:B:257:THR:OG1	2.19	0.42
1:A:393:SER:O	1:A:394:LEU:C	2.57	0.42
1:B:84:ILE:HG13	1:B:84:ILE:H	1.67	0.42
1:B:97:LEU:HD21	1:B:108:PHE:CE1	2.55	0.42
1:B:193:ASP:OD2	1:B:193:ASP:C	2.57	0.42
1:C:245:VAL:HG13	1:D:245:VAL:HG21	2.00	0.42
1:C:371:SER:CB	1:C:395:VAL:CG2	2.94	0.42
1:C:397:ILE:HG12	1:C:438:ILE:HD13	1.96	0.42
1:D:227:PHE:HB3	1:D:228:THR:H	1.74	0.42
1:D:424:ASN:H	1:D:425:PRO:CD	2.33	0.42
1:A:134:ALA:O	1:A:135:GLY:C	2.56	0.42
1:A:273:TYR:C	1:A:275:GLU:N	2.72	0.42
1:A:330:THR:HG22	1:A:331:GLY:N	2.32	0.42
1:A:354:ARG:NH2	1:B:274:SER:HA	2.15	0.42
1:B:339:ILE:HG12	1:B:409:PRO:HB3	2.02	0.42
1:C:143:VAL:HG12	1:C:171:ILE:HG23	2.01	0.42
1:C:335:ALA:O	1:C:339:ILE:CG1	2.63	0.42
1:C:366:LEU:HD23	1:D:286:VAL:CB	2.46	0.42
1:D:244:THR:HB	1:D:247:ASP:HB2	2.02	0.42
1:D:314:THR:O	1:D:315:ALA:C	2.45	0.42
1:D:339:ILE:HD11	1:D:422:VAL:HB	2.02	0.42
1:D:346:ASP:O	1:D:347:LEU:CB	2.65	0.42
1:D:360:MET:O	1:D:399:PHE:HE1	2.02	0.42
1:D:408:LEU:HB3	1:D:409:PRO:HD3	2.00	0.42
1:A:266:VAL:CG1	1:B:337:LEU:HD11	2.49	0.42
1:B:244:THR:HG22	1:B:246:ASP:OD1	2.19	0.42
1:B:341:ALA:O	1:B:342:LEU:C	2.57	0.42
1:D:315:ALA:O	1:D:318:PHE:HE2	2.03	0.42
1:A:365:LEU:HD22	1:B:282:TRP:NE1	2.34	0.42
1:B:328:GLY:HA2	1:B:431:SER:OG	2.19	0.42
1:D:50:THR:HA	1:D:80:ARG:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ILE:HD12	1:D:171:ILE:H	1.83	0.42
1:D:329:ASN:N	1:D:329:ASN:HD22	2.17	0.42
1:A:90:LEU:O	1:A:93:LEU:HB3	2.19	0.42
1:A:245:VAL:O	1:A:248:VAL:HG12	2.18	0.42
1:A:337:LEU:O	1:A:340:ARG:NH2	2.52	0.42
1:B:54:LYS:HE2	1:B:87:GLU:CB	2.42	0.42
1:B:135:GLY:O	1:B:137:LEU:N	2.52	0.42
1:C:168:ILE:CD1	1:D:187:ARG:HG3	2.50	0.42
1:C:338:ILE:O	1:C:342:LEU:HG	2.19	0.42
1:C:367:GLY:CA	1:C:395:VAL:HG13	2.49	0.42
1:D:392:VAL:O	1:D:396:LEU:CB	2.63	0.42
1:D:438:ILE:O	1:D:442:VAL:HB	2.20	0.42
1:A:13:LEU:HD23	1:A:13:LEU:C	2.41	0.42
1:A:261:HIS:C	1:A:263:LEU:N	2.73	0.42
1:A:301:SER:O	1:A:304:GLN:HB3	2.18	0.42
1:B:81:LEU:C	1:B:83:GLU:H	2.23	0.42
1:B:273:TYR:C	1:B:275:GLU:N	2.73	0.42
1:B:418:ASP:HA	1:B:419:PRO:HD2	1.84	0.42
1:C:288:TRP:C	1:C:290:VAL:N	2.73	0.42
1:C:342:LEU:O	1:C:413:ARG:NH2	2.53	0.42
1:D:86:GLU:C	1:D:88:LEU:N	2.73	0.42
1:D:183:VAL:O	1:D:184:LEU:HB2	2.19	0.42
1:D:209:VAL:HG21	1:D:218:VAL:CG2	2.40	0.42
1:D:312:ALA:O	1:D:314:THR:N	2.48	0.42
1:A:81:LEU:HD23	1:A:81:LEU:N	2.35	0.42
1:A:135:GLY:HA2	1:A:138:MET:HG2	2.02	0.42
1:A:203:ASN:OD1	1:A:205:LYS:N	2.53	0.42
1:B:250:ASP:O	1:B:251:VAL:C	2.58	0.42
1:C:273:TYR:O	1:C:275:GLU:N	2.53	0.42
1:C:432:ASP:O	1:C:436:LEU:HB2	2.20	0.42
1:D:69:GLN:O	1:D:73:LEU:HG	2.19	0.42
1:D:200:GLU:HG3	1:D:201:ILE:HG23	2.01	0.42
1:D:213:THR:O	1:D:214:ASP:C	2.58	0.42
1:D:295:THR:O	1:D:298:VAL:HG23	2.19	0.42
1:D:388:PRO:HG3	1:D:446:LEU:HD11	2.01	0.42
1:A:266:VAL:CG2	1:B:337:LEU:HD11	2.49	0.42
1:A:346:ASP:O	1:A:347:LEU:CB	2.68	0.42
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.85	0.42
1:B:339:ILE:CG1	1:B:409:PRO:HB3	2.50	0.42
1:C:80:ARG:HG3	1:C:80:ARG:NH1	2.35	0.42
1:C:396:LEU:HD13	1:C:442:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ASN:N	1:C:425:PRO:CD	2.82	0.42
1:A:359:GLU:OE2	1:B:273:TYR:OH	2.38	0.41
1:A:367:GLY:CA	1:A:395:VAL:HG13	2.47	0.41
1:B:321:PRO:HG2	1:B:322:VAL:N	2.30	0.41
1:B:393:SER:O	1:B:394:LEU:C	2.58	0.41
1:D:69:GLN:OE1	1:D:96:ALA:CB	2.67	0.41
1:A:180:LEU:HD23	1:A:182:GLY:H	1.84	0.41
1:A:180:LEU:HD21	1:A:206:VAL:HG21	2.00	0.41
1:A:334:SER:OG	1:A:406:ALA:HB2	2.19	0.41
1:A:436:LEU:O	1:A:439:TYR:N	2.54	0.41
1:B:146:ARG:CD	1:B:174:VAL:O	2.69	0.41
1:B:180:LEU:HD23	1:B:182:GLY:H	1.86	0.41
1:B:250:ASP:O	1:B:252:LEU:N	2.53	0.41
1:B:324:LEU:HB3	1:B:432:ASP:OD1	2.20	0.41
1:B:349:LEU:HD21	1:B:414:ARG:HA	2.01	0.41
1:C:340:ARG:HG2	1:C:341:ALA:H	1.85	0.41
1:C:378:VAL:CG1	1:C:387:LEU:HD11	2.50	0.41
1:C:415:LEU:HD22	1:C:415:LEU:HA	1.81	0.41
1:D:31:GLN:OE1	1:D:31:GLN:HA	2.20	0.41
1:D:111:LEU:HD23	1:D:111:LEU:O	2.19	0.41
1:D:143:VAL:HG11	1:D:158:LEU:HD21	2.03	0.41
1:D:172:TYR:CD2	1:D:180:LEU:HD11	2.55	0.41
1:D:245:VAL:CG1	1:D:246:ASP:N	2.83	0.41
1:D:306:PHE:CD2	1:D:440:LEU:HD13	2.55	0.41
1:D:324:LEU:HD12	1:D:324:LEU:HA	1.84	0.41
1:B:13:LEU:CD2	1:B:44:HIS:HD2	2.33	0.41
1:C:62:SER:OG	1:C:92:ASP:OD1	2.38	0.41
1:C:160:ARG:O	1:C:161:ALA:HB3	2.20	0.41
1:B:183:VAL:O	1:B:184:LEU:HB2	2.20	0.41
1:B:219:ALA:HA	1:B:248:VAL:HG21	2.01	0.41
1:B:316:LEU:HA	1:B:318:PHE:CE2	2.56	0.41
1:C:213:THR:CG2	1:C:218:VAL:HG22	2.50	0.41
1:A:186:LEU:C	1:A:188:ASP:N	2.74	0.41
1:B:317:ALA:C	1:B:319:TYR:H	2.23	0.41
1:C:65:SER:HB3	1:C:68:GLU:HB2	2.02	0.41
1:C:135:GLY:O	1:C:137:LEU:N	2.54	0.41
1:C:222:MET:HG2	1:C:227:PHE:HB2	2.03	0.41
1:C:342:LEU:N	1:C:342:LEU:HD23	2.36	0.41
1:A:318:PHE:O	1:A:321:PRO:HD2	2.20	0.41
1:A:324:LEU:CD1	1:A:432:ASP:HA	2.50	0.41
1:A:371:SER:HB2	1:A:395:VAL:HG21	1.99	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:C:169:TYR:HE1	1:D:170:TYR:CE1	2.38	0.41
1:C:248:VAL:C	1:C:250:ASP:N	2.74	0.41
1:C:322:VAL:CG1	1:D:297:MET:HA	2.49	0.41
1:D:160:ARG:O	1:D:161:ALA:HB3	2.19	0.41
1:D:209:VAL:CG2	1:D:218:VAL:HG22	2.37	0.41
1:D:209:VAL:CG1	1:D:230:LEU:HD22	2.49	0.41
1:D:338:ILE:HD13	1:D:410:PHE:CE1	2.55	0.41
1:A:149:MET:O	1:A:198:VAL:HG23	2.20	0.41
1:A:288:TRP:C	1:A:290:VAL:N	2.74	0.41
1:C:50:THR:HG23	1:C:76:LEU:CD1	2.51	0.41
1:C:293:ILE:CD1	1:D:326:THR:OG1	2.64	0.41
1:C:374:LEU:HD21	1:C:390:VAL:HG12	2.01	0.41
1:D:40:LEU:CD1	1:D:45:ARG:HG3	2.50	0.41
1:D:40:LEU:HD12	1:D:45:ARG:HG3	2.02	0.41
1:D:304:GLN:O	1:D:307:GLU:HB3	2.19	0.41
1:D:386:LEU:O	1:D:389:VAL:HG22	2.20	0.41
1:D:393:SER:O	1:D:397:ILE:HG13	2.21	0.41
1:B:86:GLU:C	1:B:88:LEU:N	2.72	0.41
1:B:281:LEU:O	1:B:285:ARG:HG3	2.20	0.41
1:C:207:VAL:HG21	1:C:227:PHE:HE2	1.84	0.41
1:C:266:VAL:HG23	1:C:266:VAL:O	2.20	0.41
1:D:25:LEU:HD12	1:D:51:LEU:HD23	2.01	0.41
1:D:37:TRP:O	1:D:45:ARG:HD2	2.21	0.41
1:D:55:ALA:N	1:D:87:GLU:HG2	2.35	0.41
1:D:289:LEU:HD22	1:D:289:LEU:HA	1.87	0.41
1:A:19:ARG:NH1	1:A:19:ARG:HB2	2.36	0.41
1:A:285:ARG:CG	1:B:333:GLN:NE2	2.84	0.41
1:A:286:VAL:HB	1:B:366:LEU:CD2	2.50	0.41
1:A:318:PHE:CD2	1:A:318:PHE:N	2.88	0.41
1:A:377:LYS:N	1:A:377:LYS:HD2	2.36	0.41
1:A:418:ASP:HA	1:A:419:PRO:HD2	1.83	0.41
1:B:129:TYR:CD1	1:B:135:GLY:HA3	2.56	0.41
1:B:129:TYR:HD1	1:B:135:GLY:HA3	1.84	0.41
1:B:324:LEU:HD23	1:B:432:ASP:OD1	2.20	0.41
1:B:386:LEU:HD22	1:B:446:LEU:CD1	2.51	0.41
1:B:424:ASN:H	1:B:425:PRO:CD	2.34	0.41
1:B:447:LEU:O	1:B:447:LEU:HG	2.21	0.41
1:C:429:THR:O	1:C:432:ASP:HB2	2.21	0.41
1:D:50:THR:HG21	1:D:77:PRO:HG3	2.02	0.41
1:D:324:LEU:HD22	1:D:436:LEU:HG	2.02	0.41
1:D:384:PRO:O	1:D:385:LEU:O	2.39	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:D:388:PRO:CG	1:D:446:LEU:HD11	2.51	0.41
1:D:438:ILE:C	1:D:440:LEU:H	2.24	0.41
1:B:31:GLN:O	1:B:32:ASP:C	2.60	0.41
1:B:50:THR:HG22	1:B:76:LEU:CD1	2.50	0.41
1:B:64:LEU:HD21	1:B:68:GLU:CD	2.42	0.41
1:C:397:ILE:CG1	1:C:438:ILE:HG21	2.49	0.41
1:D:30:PRO:HB3	1:D:60:VAL:HG23	2.02	0.41
1:A:397:ILE:O	1:A:400:PHE:N	2.54	0.40
1:B:252:LEU:C	1:B:254:ALA:N	2.74	0.40
1:B:389:VAL:HG23	1:B:390:VAL:N	2.35	0.40
1:C:210:ARG:HG2	1:C:211:THR:N	2.36	0.40
1:C:303:LEU:HD12	1:D:318:PHE:HB3	2.03	0.40
1:D:230:LEU:HD23	1:D:231:PRO:HD2	2.03	0.40
1:A:37:TRP:HA	1:A:40:LEU:CD1	2.51	0.40
1:A:294:LEU:O	1:A:297:MET:HB2	2.21	0.40
1:A:317:ALA:C	1:A:319:TYR:H	2.23	0.40
1:A:337:LEU:HD21	1:B:266:VAL:HG21	2.04	0.40
1:C:165:ALA:O	1:D:187:ARG:NH2	2.55	0.40
1:C:172:TYR:CD2	1:C:231:PRO:HB3	2.55	0.40
1:C:302:ILE:C	1:C:304:GLN:N	2.74	0.40
1:C:304:GLN:O	1:C:307:GLU:HB3	2.20	0.40
1:C:418:ASP:HA	1:C:419:PRO:HD2	1.90	0.40
1:D:135:GLY:O	1:D:137:LEU:N	2.54	0.40
1:D:152:GLU:OE1	1:D:152:GLU:O	2.38	0.40
1:D:302:ILE:C	1:D:304:GLN:N	2.75	0.40
1:D:303:LEU:HD22	1:D:303:LEU:HA	1.80	0.40
1:D:357:LEU:O	1:D:358:LYS:C	2.60	0.40
1:A:138:MET:HA	1:A:242:ILE:O	2.21	0.40
1:A:158:LEU:C	1:A:160:ARG:N	2.74	0.40
1:A:265:ALA:CB	1:B:333:GLN:HG2	2.48	0.40
1:A:265:ALA:HB1	1:A:288:TRP:CB	2.52	0.40
1:A:281:LEU:N	1:A:281:LEU:CD1	2.80	0.40
1:A:326:THR:HA	1:A:329:ASN:ND2	2.35	0.40
1:A:364:LEU:CD2	1:A:368:LEU:HD11	2.51	0.40
1:B:90:LEU:HD12	1:B:126:LEU:HD11	2.04	0.40
1:B:134:ALA:O	1:B:135:GLY:C	2.58	0.40
1:B:307:GLU:HG3	1:B:308:SER:N	2.37	0.40
1:B:412:LEU:HD12	1:B:422:VAL:CG2	2.47	0.40
1:B:422:VAL:HA	1:B:426:LEU:HD23	2.03	0.40
1:C:322:VAL:HG13	1:D:297:MET:N	2.36	0.40
1:D:41:LYS:C	1:D:43:GLU:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:GLY:C	1:D:137:LEU:H	2.25	0.40
1:B:291:ILE:O	1:B:294:LEU:HB3	2.21	0.40
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.92	0.40
1:C:326:THR:CB	1:D:293:ILE:HG13	2.51	0.40
1:C:340:ARG:HD2	1:D:261:HIS:NE2	2.36	0.40
1:D:245:VAL:O	1:D:248:VAL:HG12	2.21	0.40
1:A:101:ARG:HG3	1:A:101:ARG:NH1	2.34	0.40
1:A:266:VAL:HG21	1:B:337:LEU:CG	2.49	0.40
1:B:85:LEU:HB3	1:B:115:LEU:CD1	2.48	0.40
1:B:222:MET:HE2	1:B:228:THR:C	2.42	0.40
1:B:252:LEU:O	1:B:254:ALA:N	2.54	0.40
1:B:280:ALA:HA	1:B:283:LEU:CD2	2.52	0.40
1:B:302:ILE:C	1:B:304:GLN:N	2.74	0.40
1:C:80:ARG:HG3	1:C:80:ARG:O	2.21	0.40
1:C:81:LEU:C	1:C:83:GLU:H	2.24	0.40
1:C:134:ALA:O	1:C:135:GLY:C	2.60	0.40
1:D:82:ARG:HH11	1:D:82:ARG:HG3	1.86	0.40
1:D:93:LEU:O	1:D:94:ALA:C	2.60	0.40
1:D:180:LEU:CD1	1:D:239:LEU:HD13	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLN:NE2	1:D:109:GLN:NE2[3_656]	1.97	0.23

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	440/473 (93%)	310 (70%)	100 (23%)	30 (7%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/473 (93%)	312 (71%)	96 (22%)	32 (7%)	1	11
1	C	440/473 (93%)	315 (72%)	98 (22%)	27 (6%)	1	15
1	D	440/473 (93%)	307 (70%)	103 (23%)	30 (7%)	1	13
All	All	1760/1892 (93%)	1244 (71%)	397 (23%)	119 (7%)	1	13

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	LEU
1	A	266	VAL
1	A	269	PRO
1	A	386	LEU
1	A	428	ALA
1	B	266	VAL
1	B	269	PRO
1	B	315	ALA
1	B	386	LEU
1	B	423	SER
1	C	184	LEU
1	C	266	VAL
1	C	269	PRO
1	C	386	LEU
1	D	184	LEU
1	D	266	VAL
1	D	269	PRO
1	D	315	ALA
1	D	386	LEU
1	D	428	ALA
1	A	19	ARG
1	A	136	GLY
1	A	262	LYS
1	A	276	ALA
1	A	289	LEU
1	A	423	SER
1	B	136	GLY
1	B	184	LEU
1	B	262	LYS
1	B	276	ALA
1	B	428	ALA
1	C	19	ARG
1	C	136	GLY

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Mol	Chain	Res	Type
1	C	228	THR
1	C	262	LYS
1	C	276	ALA
1	C	289	LEU
1	C	423	SER
1	C	428	ALA
1	D	19	ARG
1	D	136	GLY
1	D	262	LYS
1	D	276	ALA
1	D	289	LEU
1	D	314	THR
1	D	423	SER
1	A	10	GLN
1	A	225	TYR
1	A	228	THR
1	A	313	VAL
1	A	321	PRO
1	A	433	VAL
1	B	10	GLN
1	B	87	GLU
1	B	225	TYR
1	B	228	THR
1	B	289	LEU
1	B	313	VAL
1	B	321	PRO
1	B	385	LEU
1	C	10	GLN
1	C	18	THR
1	C	225	TYR
1	C	313	VAL
1	C	321	PRO
1	D	10	GLN
1	D	18	THR
1	D	225	TYR
1	D	228	THR
1	D	313	VAL
1	D	321	PRO
1	D	385	LEU
1	A	17	ASP
1	A	18	THR
1	A	46	TYR

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	87	GLU
1	A	385	LEU
1	B	17	ASP
1	B	18	THR
1	B	19	ARG
1	B	49	LEU
1	B	274	SER
1	B	344	THR
1	B	437	LEU
1	C	17	ASP
1	C	87	GLU
1	C	344	THR
1	C	437	LEU
1	D	17	ASP
1	D	49	LEU
1	D	87	GLU
1	A	135	GLY
1	A	334	SER
1	A	344	THR
1	A	437	LEU
1	B	46	TYR
1	B	433	VAL
1	C	13	LEU
1	C	49	LEU
1	C	385	LEU
1	D	13	LEU
1	D	344	THR
1	D	437	LEU
1	A	13	LEU
1	C	433	VAL
1	D	274	SER
1	B	194	PRO
1	C	135	GLY
1	D	433	VAL
1	A	320	VAL
1	B	135	GLY
1	D	135	GLY
1	B	278	PRO
1	B	320	VAL
1	D	320	VAL
1	A	387	LEU

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Mol	Chain	Res	Type
1	C	320	VAL
1	B	387	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/400 (94%)	329 (88%)	47 (12%)	4	23
1	B	376/400 (94%)	330 (88%)	46 (12%)	5	23
1	C	376/400 (94%)	326 (87%)	50 (13%)	4	21
1	D	376/400 (94%)	331 (88%)	45 (12%)	5	24
All	All	1504/1600 (94%)	1316 (88%)	188 (12%)	4	23

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	34	LEU
1	A	46	TYR
1	A	49	LEU
1	A	52	LEU
1	A	81	LEU
1	A	82	ARG
1	A	92	ASP
1	A	101	ARG
1	A	109	GLN
1	A	115	LEU
1	A	139	THR
1	A	157	PHE
1	A	177	LYS
1	A	193	ASP
1	A	195	ARG
1	A	228	THR
1	A	230	LEU
1	A	244	THR

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Mol	Chain	Res	Type
1	A	245	VAL
1	A	247	ASP
1	A	253	GLU
1	A	270	ASP
1	A	278	PRO
1	A	289	LEU
1	A	294	LEU
1	A	297	MET
1	A	303	LEU
1	A	316	LEU
1	A	318	PHE
1	A	340	ARG
1	A	348	ASP
1	A	350	ARG
1	A	354	ARG
1	A	355	VAL
1	A	356	PHE
1	A	362	VAL
1	A	364	LEU
1	A	365	LEU
1	A	369	THR
1	A	380	TRP
1	A	381	ASP
1	A	417	VAL
1	A	418	ASP
1	A	421	LEU
1	A	446	LEU
1	A	447	LEU
1	B	50	THR
1	B	61	LEU
1	B	64	LEU
1	B	65	SER
1	B	90	LEU
1	B	113	ASP
1	B	133	GLU
1	B	139	THR
1	B	146	ARG
1	B	184	LEU
1	B	188	ASP
1	B	195	ARG
1	B	208	TYR
1	B	209	VAL

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Mol	Chain	Res	Type
1	B	211	THR
1	B	217	GLU
1	B	222	MET
1	B	225	TYR
1	B	228	THR
1	B	235	GLU
1	B	242	ILE
1	B	244	THR
1	B	247	ASP
1	B	249	LEU
1	B	250	ASP
1	B	270	ASP
1	B	285	ARG
1	B	290	VAL
1	B	294	LEU
1	B	295	THR
1	B	302	ILE
1	B	303	LEU
1	B	306	PHE
1	B	314	THR
1	B	316	LEU
1	B	318	PHE
1	B	330	THR
1	B	340	ARG
1	B	352	TRP
1	B	355	VAL
1	B	362	VAL
1	B	365	LEU
1	B	380	TRP
1	B	396	LEU
1	B	402	ASN
1	B	403	LEU
1	C	11	GLU
1	C	15	GLU
1	C	71	GLU
1	C	80	ARG
1	C	93	LEU
1	C	97	LEU
1	C	142	TYR
1	C	146	ARG
1	C	164	ASP
1	C	177	LYS

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Mol	Chain	Res	Type
1	C	207	VAL
1	C	208	TYR
1	C	211	THR
1	C	214	ASP
1	C	226	ASP
1	C	234	ASP
1	C	235	GLU
1	C	236	GLU
1	C	242	ILE
1	C	245	VAL
1	C	246	ASP
1	C	247	ASP
1	C	253	GLU
1	C	268	VAL
1	C	270	ASP
1	C	289	LEU
1	C	290	VAL
1	C	298	VAL
1	C	302	ILE
1	C	303	LEU
1	C	310	LEU
1	C	318	PHE
1	C	349	LEU
1	C	350	ARG
1	C	351	ASP
1	C	352	TRP
1	C	362	VAL
1	C	364	LEU
1	C	365	LEU
1	C	369	THR
1	C	379	TYR
1	C	380	TRP
1	C	381	ASP
1	C	400	PHE
1	C	402	ASN
1	C	415	LEU
1	C	432	ASP
1	C	436	LEU
1	C	440	LEU
1	C	446	LEU
1	D	29	HIS
1	D	37	TRP

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Mol	Chain	Res	Type
1	D	43	GLU
1	D	61	LEU
1	D	83	GLU
1	D	109	GLN
1	D	111	LEU
1	D	118	ARG
1	D	139	THR
1	D	152	GLU
1	D	164	ASP
1	D	177	LYS
1	D	216	GLU
1	D	224	ASP
1	D	226	ASP
1	D	234	ASP
1	D	250	ASP
1	D	258	GLU
1	D	261	HIS
1	D	267	ASP
1	D	270	ASP
1	D	283	LEU
1	D	289	LEU
1	D	303	LEU
1	D	310	LEU
1	D	314	THR
1	D	318	PHE
1	D	340	ARG
1	D	345	ARG
1	D	348	ASP
1	D	349	LEU
1	D	351	ASP
1	D	355	VAL
1	D	362	VAL
1	D	364	LEU
1	D	365	LEU
1	D	369	THR
1	D	380	TRP
1	D	381	ASP
1	D	385	LEU
1	D	400	PHE
1	D	418	ASP
1	D	421	LEU
1	D	432	ASP

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Mol	Chain	Res	Type
1	D	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	215	GLN
1	A	424	ASN
1	B	31	GLN
1	B	44	HIS
1	B	332	ASN
1	B	333	GLN
1	B	424	ASN
1	C	10	GLN
1	C	31	GLN
1	C	63	HIS
1	C	215	GLN
1	C	332	ASN
1	C	333	GLN
1	C	424	ASN
1	D	10	GLN
1	D	304	GLN
1	D	332	ASN
1	D	333	GLN
1	D	402	ASN
1	D	424	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB($Å^2$)	Q<0.9
1	A	442/473 (93%)	-0.51	3 (0%)	87	83	41, 99, 150, 167	0
1	B	442/473 (93%)	-0.52	0	100	100	51, 95, 135, 161	0
1	C	442/473 (93%)	-0.32	8 (1%)	68	62	61, 122, 167, 194	0
1	D	442/473 (93%)	-0.12	23 (5%)	27	24	63, 141, 188, 203	0
All	All	1768/1892 (93%)	-0.37	34 (1%)	66	61	41, 108, 174, 203	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	VAL	5.0
1	D	145	VAL	4.6
1	D	134	ALA	4.1
1	D	23	GLU	3.9
1	A	74	LYS	3.8
1	D	144	ALA	3.6
1	C	164	ASP	3.5
1	C	205	LYS	3.4
1	D	118	ARG	3.3
1	D	143	VAL	3.2
1	C	191	VAL	3.1
1	D	10	GLN	3.0
1	D	73	LEU	3.0
1	D	116	ASP	3.0
1	C	20	ALA	2.9
1	C	192	ALA	2.9
1	D	168	ILE	2.7
1	D	211	THR	2.7
1	D	97	LEU	2.5
1	D	212	ASP	2.4
1	C	144	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	2.4
1	D	28	ILE	2.4
1	D	133	GLU	2.3
1	D	33	LEU	2.3
1	D	186	LEU	2.1
1	A	105	PRO	2.1
1	D	172	TYR	2.1
1	D	242	ILE	2.1
1	D	126	LEU	2.1
1	C	10	GLN	2.1
1	D	9	LEU	2.1
1	D	239	LEU	2.0
1	D	210	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled '$Q < 0.9$' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
2	MG	D	452	1/1	0.76	0.28	61,61,61,61	0
2	MG	C	453	1/1	0.77	0.95	60,60,60,60	0
2	MG	D	454	1/1	0.81	0.54	78,78,78,78	0
2	MG	C	455	1/1	0.89	0.31	67,67,67,67	0
2	MG	C	454	1/1	0.90	0.34	53,53,53,53	0
2	MG	D	451	1/1	0.90	0.28	61,61,61,61	0
2	MG	A	451	1/1	0.92	0.29	46,46,46,46	0
2	MG	B	453	1/1	0.93	0.19	40,40,40,40	0
2	MG	B	455	1/1	0.94	0.58	60,60,60,60	0
2	MG	A	452	1/1	0.95	0.26	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MG	C	451	1/1	0.95	0.48	33,33,33,33	0
2	MG	B	451	1/1	0.96	0.55	34,34,34,34	0
2	MG	C	452	1/1	0.96	0.30	38,38,38,38	0
2	MG	D	453	1/1	0.97	0.33	40,40,40,40	0
2	MG	B	452	1/1	0.97	0.23	39,39,39,39	0
2	MG	A	453	1/1	0.98	0.35	40,40,40,40	0
2	MG	B	454	1/1	0.98	0.24	33,33,33,33	0
2	MG	A	454	1/1	0.98	0.54	68,68,68,68	0

6.5 Other polymers

There are no such residues in this entry.