Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:42 PM GMT

PDB ID	:	1C2O
Title	:	ELECTROPHORUS ELECTRICUS ACETYLCHOLINESTERASE
Authors	:	Bourne, Y.; Marchot, P.
Deposited on	:	1999-07-26
Resolution	:	4.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

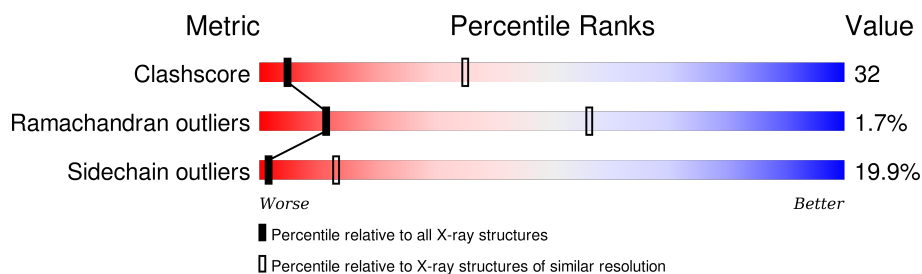|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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

Metric	Percentile Ranks	Value
Clashscore		32
Ramachandran outliers		1.7%
Sidechain outliers		19.9%

Worse　　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	539	41% 46% 12% •
1	B	539	40% 46% 13% •
1	C	539	42% 45% 12% •
1	D	539	42% 45% 12% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16688 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.

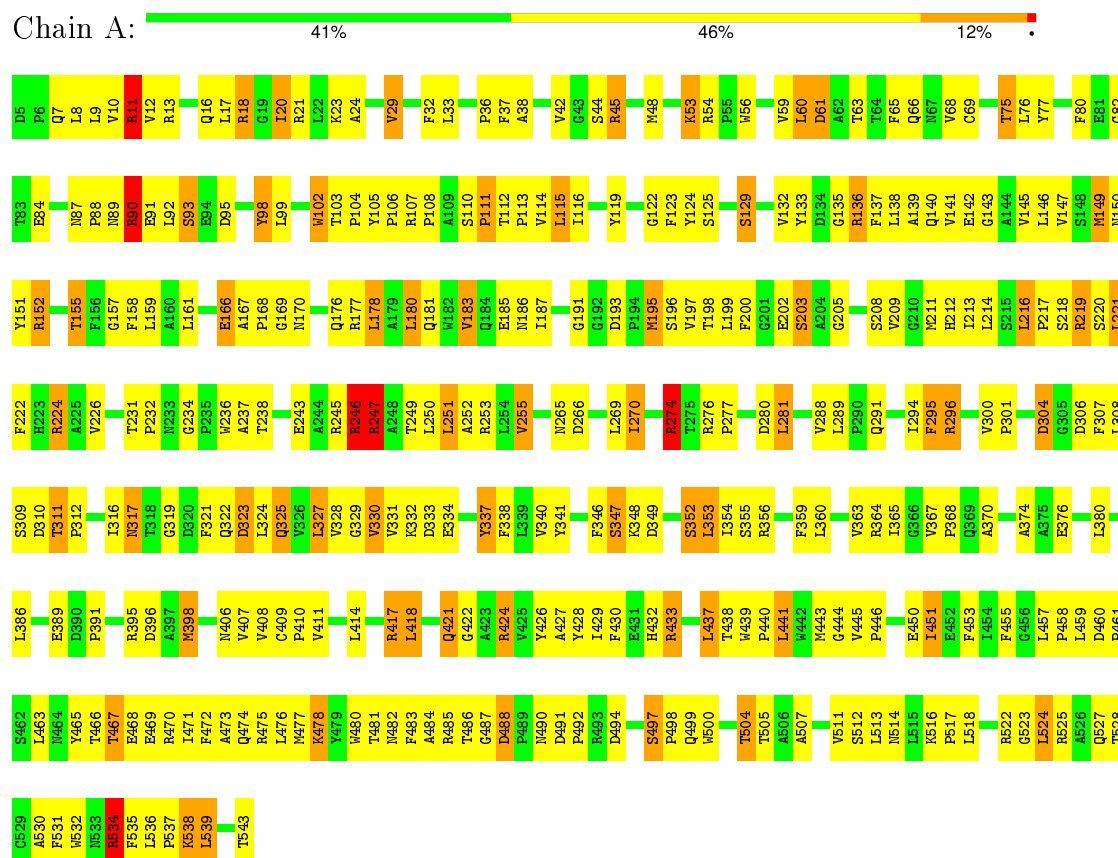- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

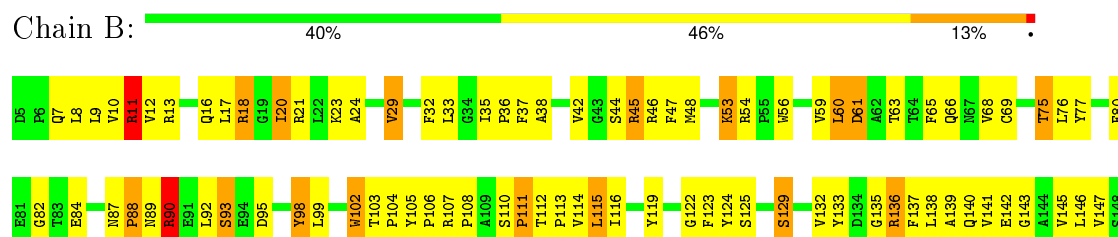| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	B	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	C	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			
1	D	539	Total	C	N	O	S	0	0	0
			4172	2681	723	754	14			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
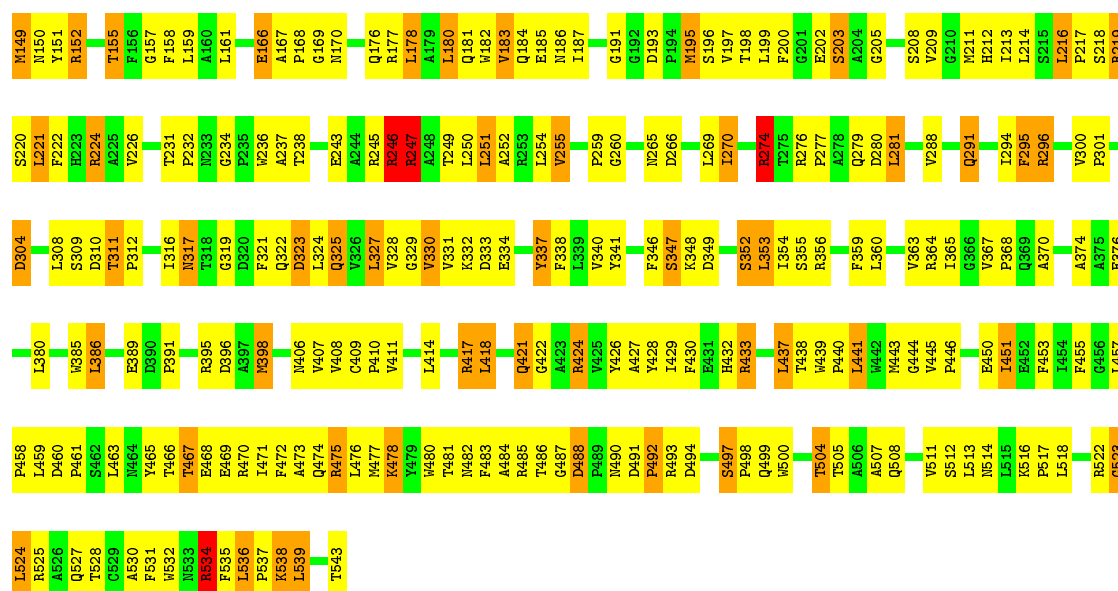
Note EDS was not executed.
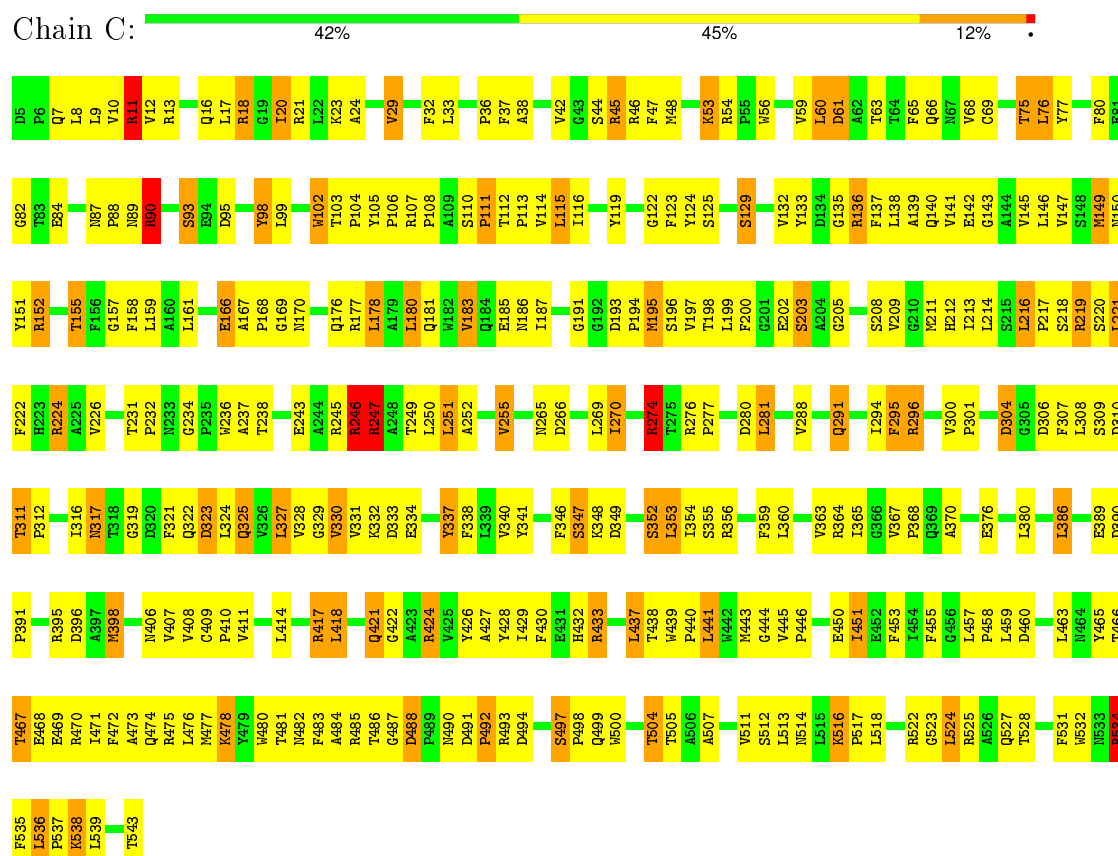
- Molecule 1: ACETYLCHOLINESTERASE
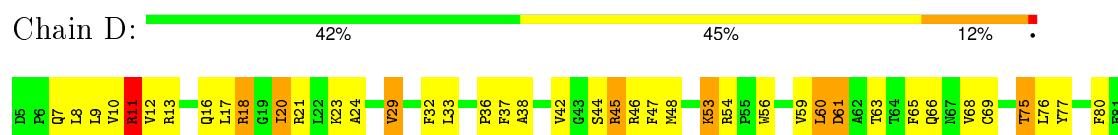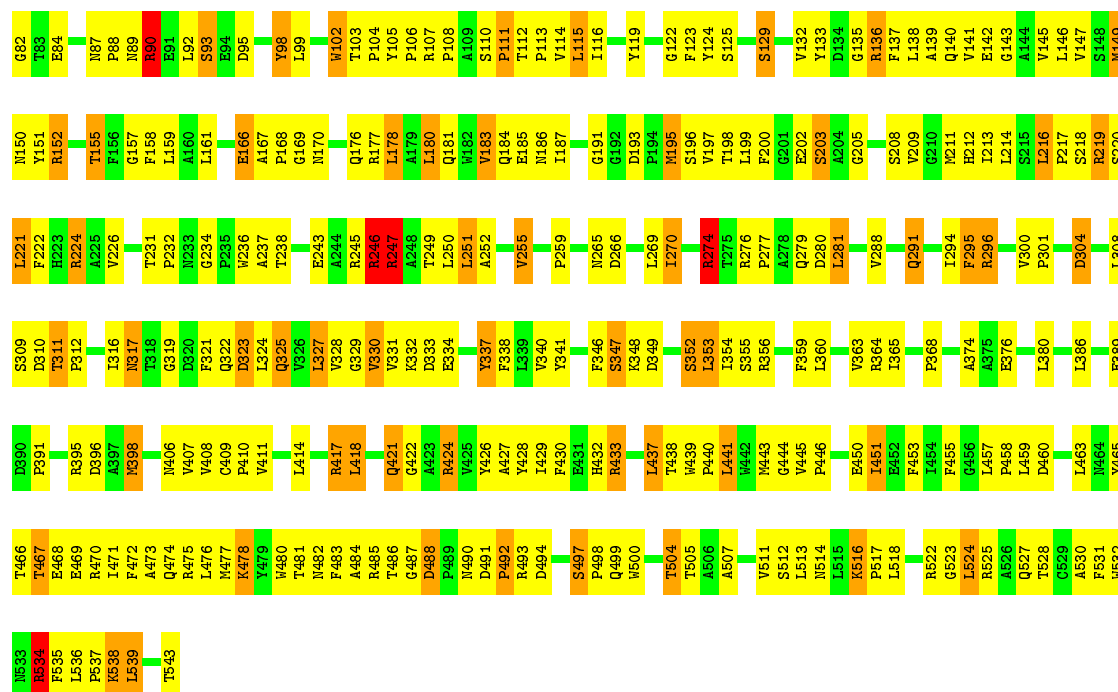
Chain A:

- Molecule 1: ACETYLCHOLINESTERASE

Chain B:

M149 N150 Y151 R152 T155 F156 G157 F158 L159 A160 L161 E166 A167 P168 G169 N170 Q176 R177 L178 A179 L180 Q181 W182 V183 Q184 E185 N186 I187 G191 G192 D193 P194 M195 S196 V197 T198 L199 F200 G201 E202 S203 A204 G205 S208 V209 G210 M211 H212 I213 L214 S215 L216 P217 S218 R219

S220 L221 F222 H223 R224 A225 V226 T231 P232 N233 G234 P235 W236 A237 T238 E243 A244 R245 R246 R247 A248 T249 L250 L251 R253 L254 V255 P259 G260 N265 D266 L269 I270 R274 T275 R276 P277 A278 Q279 D280 L281 V288 Q291 I294 F295 R296 V300 P301

D304 L308 S309 D310 T311 P312 I316 N317 T318 G319 D320 F321 Q322 D323 L324 Q325 V326 L327 V328 G329 V330 V331 K332 D333 E334 Y337 F338 L339 V340 Y341 F346 S347 K348 D349 S352 L353 I354 S355 R356 F359 L360 V363 R364 I365 G366 V367 P368 Q369 A370 A374 A375 E376

L380 W385 L386 E389 D390 P391 R395 D396 A397 M398 N406 V407 V408 C409 P410 V411 L414 R417 L418 Q421 G422 A423 R424 V425 Y426 A427 Y428 I429 F430 E431 H432 R433 L437 T438 W439 P440 L441 W442 M443 G444 V445 P446 E450 I451 E452 F453 I454 F455 G456 L457

P458 L459 D460 P461 S462 L463 M464 Y465 T466 T467 E468 E469 R470 I471 F472 A473 Q474 R475 L476 M477 K478 Y479 W480 T481 N482 F483 A484 R485 T486 G487 D488 P489 N490 D491 P492 R493 D494 S497 P498 Q499 W500 T504 T505 A506 A507 Q508 V511 S512 L513 N514 L515 K516 P517 L518 R522 G523

L524 R525 A526 Q527 T528 C529 A530 F531 W532 N533 R534 F535 L536 P537 K538 L539 T543

● Molecule 1: ACETYLCHOLINESTERASE

Chain C:

42%　　　45%　　　12%　·

D5 P6 Q7 L8 L9 V10 R11 V12 R13 Q16 L17 R18 G19 I20 R21 L22 K23 A24 V29 F32 L33 P36 F37 A38 V42 G43 S44 R45 R46 F47 M48 K53 R54 P55 W56 V59 L60 D61 A62 T63 T64 Q66 M67 V68 C69 T75 L76 Y77 F80 E81

G82 T83 E84 N87 P88 N89 R90 S93 E94 D95 Y98 L99 W102 T103 P104 Y105 P106 R107 P108 A109 S110 P111 T112 P113 V114 L115 I116 Y119 G122 F123 Y124 S125 S129 V132 Y133 D134 G135 R136 F137 L138 A139 Q140 E142 G143 A144 V145 L146 V147 S148 M149 N150

Y151 R152 T155 F156 G157 F158 L159 A160 L161 E166 A167 P168 G169 N170 Q176 R177 L178 A179 L180 Q181 W182 V183 Q184 E185 N186 I187 G191 G192 D193 P194 M195 S196 V197 T198 L199 F200 G201 E202 S203 A204 G205 S208 V209 G210 M211 H212 I213 L214 S215 L216 P217 S218 R219 S220 L221

F222 H223 R224 A225 V226 T231 P232 N233 G234 P235 W236 A237 T238 E243 A244 R245 R246 R247 A248 T249 L250 L251 A252 V255 N265 D266 L269 I270 R274 T275 R276 P277 D280 L281 V288 Q291 I294 F295 R296 V300 P301 D304 G305 D306 F307 L308 S309 D310

T311 P312 I316 N317 T318 G319 D320 Q322 D323 Q325 V326 L327 V328 G329 V330 V331 K332 D333 E334 Y337 F338 L339 V340 Y341 F346 S347 K348 D349 S352 L353 I354 S355 R356 F359 L360 V363 R364 I365 G366 V367 P368 Q369 A370 E376 L380 L386 E389 D390

P391 R395 D396 A397 M398 N406 V407 V408 C409 P410 V411 L414 R417 L418 Q421 G422 A423 R424 V425 Y426 A427 Y428 I429 F430 E431 H432 R433 L437 T438 W439 P440 L441 W442 M443 G444 V445 P446 E450 I451 E452 F453 I454 F455 G456 L457 P458 L459 D460 L463 M464 Y465 T466

T467 E468 E469 R470 I471 F472 A473 Q474 R475 L476 M477 K478 Y479 W480 T481 N482 F483 A484 R485 T486 G487 D488 P489 N490 D491 P492 R493 D494 S497 P498 Q499 W500 T504 T505 A506 A507 V511 S512 L513 N514 L515 K516 P517 L518 R522 G523 L524 R525 A526 Q527 T528 F531 W532 N533 R534

F535 L536 P537 K538 L539 T543

● Molecule 1: ACETYLCHOLINESTERASE

Chain D:

42%　　　45%　　　12%　·

D5 P6 Q7 L8 L9 V10 R11 V12 R13 Q16 L17 R18 G19 I20 R21 L22 K23 A24 V29 F32 L33 P36 F37 A38 V42 G43 S44 R45 R46 F47 M48 K53 R54 P55 W56 V59 L60 D61 A62 T63 T64 F65 Q66 M67 V68 C69 T75 L76 Y77 F80 E81

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.16Å 129.75Å 195.42Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	12.00 – 4.20	Depositor
% Data completeness (in resolution range)	66.0 (12.00-4.20)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.375 , 0.385	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16688	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.66	0/4298	1.42	32/5879 (0.5%)
1	B	0.65	0/4298	1.42	33/5879 (0.6%)
1	C	0.66	0/4298	1.42	33/5879 (0.6%)
1	D	0.66	0/4298	1.42	32/5879 (0.5%)
All	All	0.66	0/17192	1.42	130/23516 (0.6%)

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	247	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	D	247	ARG	NE-CZ-NH2	-13.24	113.68	120.30
1	A	247	ARG	NE-CZ-NH2	-13.17	113.72	120.30
1	C	247	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	C	274	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	B	274	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	D	274	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	A	274	ARG	NE-CZ-NH2	-12.03	114.29	120.30
1	D	247	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	B	247	ARG	NE-CZ-NH1	11.09	125.85	120.30
1	A	247	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	C	247	ARG	NE-CZ-NH1	10.97	125.79	120.30
1	C	246	ARG	NE-CZ-NH2	-10.43	115.08	120.30
1	B	246	ARG	NE-CZ-NH2	-10.42	115.09	120.30
1	D	246	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	246	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	A	247	ARG	CD-NE-CZ	9.18	136.44	123.60
1	C	247	ARG	CD-NE-CZ	9.18	136.44	123.60
1	B	247	ARG	CD-NE-CZ	9.11	136.35	123.60
1	D	247	ARG	CD-NE-CZ	9.08	136.31	123.60
1	B	534	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	D	534	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	C	534	ARG	NE-CZ-NH2	-8.74	115.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	11	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	534	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	11	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	11	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	11	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	534	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	A	534	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	488	ASP	CB-CG-OD1	8.16	125.64	118.30
1	D	534	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	B	488	ASP	CB-CG-OD1	8.08	125.57	118.30
1	B	534	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	D	488	ASP	CB-CG-OD1	7.93	125.44	118.30
1	C	543	THR	CA-C-O	7.91	136.71	120.10
1	A	543	THR	CA-C-O	7.89	136.67	120.10
1	B	543	THR	CA-C-O	7.88	136.66	120.10
1	A	488	ASP	CB-CG-OD1	7.86	125.37	118.30
1	D	543	THR	CA-C-O	7.86	136.60	120.10
1	C	274	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	274	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	274	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	274	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	B	245	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	224	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	D	224	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	C	245	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	245	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	224	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	224	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	D	245	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	265	ASN	N-CA-CB	6.64	122.56	110.60
1	D	265	ASN	N-CA-CB	6.64	122.56	110.60
1	A	265	ASN	N-CA-CB	6.60	122.48	110.60
1	C	265	ASN	N-CA-CB	6.60	122.48	110.60
1	B	475	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	11	ARG	CD-NE-CZ	6.40	132.56	123.60
1	C	475	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	11	ARG	CD-NE-CZ	6.35	132.49	123.60
1	A	475	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	C	11	ARG	CD-NE-CZ	6.30	132.41	123.60
1	D	11	ARG	CD-NE-CZ	6.29	132.40	123.60
1	D	475	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	488	ASP	CB-CG-OD2	-6.22	112.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	488	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	C	152	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	D	488	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	424	ARG	CD-NE-CZ	6.05	132.08	123.60
1	A	296	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	A	424	ARG	CD-NE-CZ	6.03	132.04	123.60
1	D	424	ARG	CD-NE-CZ	6.03	132.04	123.60
1	A	152	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	504	THR	CA-CB-CG2	-6.03	103.96	112.40
1	B	504	THR	CA-CB-CG2	-6.02	103.97	112.40
1	D	504	THR	CA-CB-CG2	-6.01	103.98	112.40
1	A	488	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	296	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	C	424	ARG	CD-NE-CZ	5.98	131.97	123.60
1	B	152	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	424	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	504	THR	CA-CB-CG2	-5.94	104.08	112.40
1	C	424	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	424	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	152	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	C	98	TYR	CB-CG-CD2	5.90	124.54	121.00
1	D	98	TYR	CB-CG-CD2	5.79	124.47	121.00
1	A	98	TYR	CB-CG-CD2	5.77	124.46	121.00
1	B	296	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	238	THR	N-CA-CB	5.74	121.20	110.30
1	D	296	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	B	238	THR	N-CA-CB	5.73	121.19	110.30
1	C	238	THR	N-CA-CB	5.72	121.17	110.30
1	D	238	THR	N-CA-CB	5.72	121.17	110.30
1	B	424	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	102	TRP	CA-CB-CG	5.69	124.51	113.70
1	C	90	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	102	TRP	CA-CB-CG	5.67	124.47	113.70
1	A	102	TRP	CA-CB-CG	5.66	124.45	113.70
1	D	102	TRP	CA-CB-CG	5.65	124.44	113.70
1	B	98	TYR	CB-CG-CD2	5.64	124.38	121.00
1	C	13	ARG	CD-NE-CZ	5.55	131.38	123.60
1	A	13	ARG	CD-NE-CZ	5.51	131.32	123.60
1	B	13	ARG	CD-NE-CZ	5.48	131.27	123.60
1	D	90	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	13	ARG	CD-NE-CZ	5.45	131.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	TRP	N-CA-CB	5.41	120.33	110.60
1	C	102	TRP	N-CA-CB	5.40	120.32	110.60
1	B	102	TRP	N-CA-CB	5.38	120.28	110.60
1	A	90	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	102	TRP	N-CA-CB	5.37	120.27	110.60
1	C	219	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	13	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	219	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	B	90	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	219	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	D	13	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	246	ARG	NH1-CZ-NH2	5.21	125.14	119.40
1	D	219	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	D	337	TYR	CA-CB-CG	5.13	123.16	113.40
1	A	246	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	C	337	TYR	CA-CB-CG	5.10	123.09	113.40
1	B	246	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	B	337	TYR	CA-CB-CG	5.09	123.08	113.40
1	D	246	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	A	337	TYR	CA-CB-CG	5.07	123.03	113.40
1	B	245	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	13	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	245	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4172	0	4052	257	7
1	B	4172	0	4052	272	0
1	C	4172	0	4052	270	10
1	D	4172	0	4052	256	0
All	All	16688	0	16208	1039	17

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 32.

All (1039) 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:A:306:ASP:OD1	1:B:259:PRO:HB2	1.47	1.11
1:A:306:ASP:OD1	1:B:259:PRO:CB	1.98	1.10
1:A:116:ILE:HD11	1:A:183:VAL:HG11	1.43	1.00
1:D:116:ILE:HD11	1:D:183:VAL:HG11	1.43	0.99
1:C:116:ILE:HD11	1:C:183:VAL:HG11	1.43	0.98
1:B:116:ILE:HD11	1:B:183:VAL:HG11	1.43	0.97
1:B:429:ILE:HD11	1:B:524:LEU:HD21	1.46	0.97
1:A:429:ILE:HD11	1:A:524:LEU:HD21	1.47	0.96
1:C:429:ILE:HD11	1:C:524:LEU:HD21	1.46	0.96
1:D:429:ILE:HD11	1:D:524:LEU:HD21	1.47	0.95
1:B:497:SER:CB	1:B:498:PRO:HD3	2.06	0.86
1:C:497:SER:CB	1:C:498:PRO:HD3	2.06	0.86
1:D:497:SER:CB	1:D:498:PRO:HD3	2.06	0.85
1:A:497:SER:CB	1:A:498:PRO:HD3	2.06	0.84
1:A:44:SER:HA	1:A:274:ARG:HD2	1.60	0.83
1:D:44:SER:HA	1:D:274:ARG:HD2	1.60	0.83
1:A:11:ARG:HB2	1:A:11:ARG:HH11	1.44	0.82
1:C:11:ARG:HH11	1:C:11:ARG:HB2	1.44	0.82
1:C:36:PRO:HB2	1:C:53:LYS:HG2	1.62	0.82
1:A:36:PRO:HB2	1:A:53:LYS:HG2	1.62	0.82
1:B:507:ALA:HA	1:B:522:ARG:HH21	1.45	0.81
1:B:11:ARG:HB2	1:B:11:ARG:HH11	1.44	0.81
1:D:507:ALA:HA	1:D:522:ARG:HH21	1.46	0.81
1:C:44:SER:HA	1:C:274:ARG:HD2	1.60	0.81
1:B:36:PRO:HB2	1:B:53:LYS:HG2	1.62	0.81
1:B:44:SER:HA	1:B:274:ARG:HD2	1.60	0.81
1:D:11:ARG:HB2	1:D:11:ARG:HH11	1.44	0.81
1:C:507:ALA:HA	1:C:522:ARG:HH21	1.46	0.80
1:D:36:PRO:HB2	1:D:53:LYS:HG2	1.62	0.80
1:A:507:ALA:HA	1:A:522:ARG:HH21	1.46	0.79
1:C:319:GLY:O	1:C:421:GLN:HG2	1.83	0.79
1:C:24:ALA:HB3	1:C:140:GLN:HG3	1.63	0.79
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.63	0.79
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.63	0.79
1:B:319:GLY:O	1:B:421:GLN:HG2	1.83	0.79
1:D:319:GLY:O	1:D:421:GLN:HG2	1.82	0.79
1:A:112:THR:HG23	1:A:113:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:HB3	1:D:140:GLN:HG3	1.63	0.78
1:C:112:THR:HG23	1:C:113:PRO:HD2	1.65	0.78
1:B:112:THR:HG23	1:B:113:PRO:HD2	1.65	0.78
1:A:319:GLY:O	1:A:421:GLN:HG2	1.83	0.78
1:D:112:THR:HG23	1:D:113:PRO:HD2	1.65	0.77
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.68	0.76
1:C:511:VAL:HB	1:C:518:LEU:HD22	1.68	0.76
1:D:511:VAL:HB	1:D:518:LEU:HD22	1.68	0.76
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.68	0.75
1:A:294:ILE:HG12	1:A:365:ILE:HG22	1.68	0.75
1:C:294:ILE:HG12	1:C:365:ILE:HG22	1.68	0.75
1:B:294:ILE:HG12	1:B:365:ILE:HG22	1.68	0.75
1:A:306:ASP:OD1	1:B:259:PRO:HB3	1.85	0.74
1:A:36:PRO:HB2	1:A:53:LYS:CG	2.18	0.74
1:D:36:PRO:HB2	1:D:53:LYS:CG	2.17	0.74
1:C:36:PRO:HB2	1:C:53:LYS:CG	2.18	0.73
1:B:36:PRO:HB2	1:B:53:LYS:CG	2.18	0.73
1:D:226:VAL:HG11	1:D:480:TRP:HE1	1.54	0.73
1:B:226:VAL:HG11	1:B:480:TRP:HE1	1.54	0.73
1:D:294:ILE:HG12	1:D:365:ILE:HG22	1.69	0.73
1:A:36:PRO:HA	1:A:98:TYR:HD1	1.54	0.72
1:A:37:PHE:HD1	1:A:178:LEU:HD13	1.55	0.72
1:D:37:PHE:HD1	1:D:178:LEU:HD13	1.55	0.72
1:B:36:PRO:HA	1:B:98:TYR:HD1	1.54	0.71
1:A:243:GLU:OE2	1:A:246:ARG:HD3	1.90	0.71
1:B:243:GLU:OE2	1:B:246:ARG:HD3	1.90	0.71
1:C:306:ASP:OD1	1:D:259:PRO:HB2	1.90	0.71
1:C:36:PRO:HA	1:C:98:TYR:HD1	1.54	0.71
1:D:36:PRO:HA	1:D:98:TYR:HD1	1.54	0.71
1:C:68:VAL:HG11	1:C:88:PRO:HB3	1.73	0.71
1:D:243:GLU:OE2	1:D:246:ARG:HD3	1.90	0.71
1:A:226:VAL:HG11	1:A:480:TRP:HE1	1.54	0.71
1:C:226:VAL:HG11	1:C:480:TRP:HE1	1.54	0.71
1:A:329:GLY:HA3	1:A:428:TYR:CE1	2.26	0.71
1:C:329:GLY:HA3	1:C:428:TYR:CE1	2.26	0.71
1:D:329:GLY:HA3	1:D:428:TYR:CE1	2.26	0.71
1:A:68:VAL:HG11	1:A:88:PRO:HB3	1.72	0.71
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.72	0.70
1:B:329:GLY:HA3	1:B:428:TYR:CE1	2.26	0.70
1:B:37:PHE:HD1	1:B:178:LEU:HD13	1.55	0.70
1:C:243:GLU:OE2	1:C:246:ARG:HD3	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:460:ASP:HB3	1:D:463:LEU:HD12	1.73	0.70
1:C:21:ARG:HH21	1:C:23:LYS:NZ	1.89	0.70
1:A:167:ALA:HB3	1:A:270:ILE:HD12	1.73	0.70
1:C:460:ASP:HB3	1:C:463:LEU:HD12	1.74	0.70
1:A:460:ASP:HB3	1:A:463:LEU:HD12	1.74	0.70
1:C:167:ALA:HB3	1:C:270:ILE:HD12	1.73	0.70
1:D:167:ALA:HB3	1:D:270:ILE:HD12	1.74	0.70
1:D:68:VAL:HG11	1:D:88:PRO:HB3	1.73	0.70
1:C:37:PHE:HD1	1:C:178:LEU:HD13	1.55	0.70
1:B:21:ARG:HH21	1:B:23:LYS:NZ	1.89	0.69
1:D:488:ASP:OD1	1:D:490:ASN:HB2	1.92	0.69
1:B:103:THR:HG23	1:B:104:PRO:HD2	1.75	0.69
1:B:167:ALA:HB3	1:B:270:ILE:HD12	1.73	0.69
1:A:488:ASP:OD1	1:A:490:ASN:HB2	1.92	0.69
1:B:488:ASP:OD1	1:B:490:ASN:HB2	1.92	0.69
1:A:21:ARG:HH21	1:A:23:LYS:NZ	1.89	0.69
1:C:488:ASP:OD1	1:C:490:ASN:HB2	1.93	0.69
1:D:21:ARG:HH21	1:D:23:LYS:NZ	1.89	0.69
1:D:103:THR:HG23	1:D:104:PRO:HD2	1.75	0.69
1:C:306:ASP:OD1	1:D:259:PRO:CB	2.41	0.69
1:D:18:ARG:HB2	1:D:18:ARG:HH21	1.58	0.69
1:B:56:TRP:NE1	1:B:60:LEU:HB2	2.08	0.69
1:C:458:PRO:HA	1:C:465:TYR:CD2	2.28	0.69
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.28	0.68
1:C:103:THR:HG23	1:C:104:PRO:HD2	1.75	0.68
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.28	0.68
1:C:56:TRP:NE1	1:C:60:LEU:HB2	2.08	0.68
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.73	0.68
1:A:18:ARG:HH21	1:A:18:ARG:HB2	1.58	0.68
1:C:18:ARG:HB2	1:C:18:ARG:HH21	1.58	0.68
1:A:56:TRP:NE1	1:A:60:LEU:HB2	2.08	0.68
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.28	0.68
1:A:103:THR:HG23	1:A:104:PRO:HD2	1.75	0.68
1:D:365:ILE:O	1:D:368:PRO:HD3	1.94	0.68
1:B:18:ARG:HB2	1:B:18:ARG:HH21	1.58	0.67
1:B:365:ILE:O	1:B:368:PRO:HD3	1.95	0.67
1:C:66:GLN:HB3	1:C:98:TYR:HD2	1.60	0.67
1:A:66:GLN:HB3	1:A:98:TYR:HD2	1.60	0.67
1:D:142:GLU:CB	1:D:481:THR:HG21	2.25	0.67
1:D:56:TRP:NE1	1:D:60:LEU:HB2	2.08	0.67
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:N	1:A:398:MET:HE1	2.10	0.66
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.31	0.66
1:A:407:VAL:O	1:A:411:VAL:HG23	1.96	0.66
1:B:142:GLU:CB	1:B:481:THR:HG21	2.25	0.66
1:A:142:GLU:CB	1:A:481:THR:HG21	2.25	0.66
1:D:66:GLN:HG3	1:D:98:TYR:CD2	2.31	0.66
1:A:440:PRO:HD2	1:A:443:MET:SD	2.36	0.66
1:B:331:VAL:HG12	1:B:430:PHE:HB3	1.77	0.66
1:C:142:GLU:CB	1:C:481:THR:HG21	2.25	0.66
1:A:365:ILE:O	1:A:368:PRO:HD3	1.94	0.66
1:D:407:VAL:O	1:D:411:VAL:HG23	1.96	0.66
1:C:89:ASN:O	1:C:90:ARG:HD3	1.96	0.66
1:B:407:VAL:O	1:B:411:VAL:HG23	1.96	0.66
1:B:440:PRO:HD2	1:B:443:MET:SD	2.36	0.66
1:D:528:THR:O	1:D:531:PHE:HB3	1.96	0.66
1:C:365:ILE:O	1:C:368:PRO:HD3	1.94	0.66
1:D:89:ASN:O	1:D:90:ARG:HD3	1.96	0.66
1:D:331:VAL:HG12	1:D:430:PHE:HB3	1.77	0.66
1:C:300:VAL:HB	1:C:301:PRO:HD2	1.79	0.65
1:A:528:THR:O	1:A:531:PHE:HB3	1.96	0.65
1:C:331:VAL:HG12	1:C:430:PHE:HB3	1.77	0.65
1:C:66:GLN:HG3	1:C:98:TYR:CD2	2.31	0.65
1:D:66:GLN:HB3	1:D:98:TYR:HD2	1.60	0.65
1:B:428:TYR:HB2	1:B:513:LEU:HD23	1.77	0.65
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.77	0.65
1:C:440:PRO:HD2	1:C:443:MET:SD	2.36	0.65
1:C:528:THR:O	1:C:531:PHE:HB3	1.96	0.65
1:A:478:LYS:HZ3	1:A:478:LYS:HB3	1.61	0.65
1:D:440:PRO:HD2	1:D:443:MET:SD	2.36	0.65
1:C:470:ARG:O	1:C:474:GLN:HG3	1.97	0.65
1:B:497:SER:CB	1:B:498:PRO:CD	2.75	0.65
1:B:470:ARG:O	1:B:474:GLN:HG3	1.96	0.65
1:A:428:TYR:HB2	1:A:513:LEU:HD23	1.78	0.65
1:A:89:ASN:O	1:A:90:ARG:HD3	1.96	0.65
1:A:497:SER:CB	1:A:498:PRO:CD	2.75	0.65
1:B:528:THR:O	1:B:531:PHE:HB3	1.96	0.65
1:A:470:ARG:O	1:A:474:GLN:HG3	1.96	0.65
1:D:428:TYR:HB2	1:D:513:LEU:HD23	1.78	0.65
1:B:478:LYS:HB3	1:B:478:LYS:HZ3	1.61	0.65
1:B:534:ARG:HG3	1:B:534:ARG:HH11	1.62	0.65
1:B:66:GLN:HB3	1:B:98:TYR:HD2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:O	1:D:474:GLN:HG3	1.96	0.64
1:B:89:ASN:O	1:B:90:ARG:HD3	1.96	0.64
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.79	0.64
1:C:53:LYS:HD2	1:C:54:ARG:O	1.98	0.64
1:C:407:VAL:O	1:C:411:VAL:HG23	1.96	0.64
1:B:300:VAL:HB	1:B:301:PRO:HD2	1.78	0.64
1:D:497:SER:CB	1:D:498:PRO:CD	2.75	0.64
1:A:36:PRO:HA	1:A:98:TYR:CD1	2.32	0.64
1:C:497:SER:CB	1:C:498:PRO:CD	2.75	0.64
1:C:428:TYR:HB2	1:C:513:LEU:HD23	1.77	0.64
1:D:300:VAL:HB	1:D:301:PRO:HD2	1.79	0.64
1:B:53:LYS:HD2	1:B:54:ARG:O	1.98	0.63
1:C:36:PRO:HA	1:C:98:TYR:CD1	2.32	0.63
1:B:116:ILE:HD12	1:B:197:VAL:HG13	1.80	0.63
1:D:36:PRO:HA	1:D:98:TYR:CD1	2.33	0.63
1:D:53:LYS:HD2	1:D:54:ARG:O	1.97	0.63
1:A:534:ARG:HG3	1:A:534:ARG:HH11	1.62	0.63
1:D:534:ARG:HH11	1:D:534:ARG:HG3	1.62	0.63
1:A:53:LYS:HD2	1:A:54:ARG:O	1.98	0.63
1:D:473:ALA:O	1:D:477:MET:HG3	1.99	0.63
1:C:322:GLN:O	1:C:323:ASP:HB3	1.99	0.63
1:A:473:ALA:O	1:A:477:MET:HG3	1.99	0.63
1:D:426:TYR:HB3	1:D:500:TRP:NE1	2.14	0.63
1:A:331:VAL:HB	1:A:445:VAL:HG12	1.81	0.63
1:B:322:GLN:O	1:B:323:ASP:HB3	1.99	0.63
1:C:331:VAL:HB	1:C:445:VAL:HG12	1.81	0.63
1:C:116:ILE:HD12	1:C:197:VAL:HG13	1.80	0.62
1:C:132:VAL:HG23	1:C:133:TYR:CD1	2.35	0.62
1:A:116:ILE:HD12	1:A:197:VAL:HG13	1.80	0.62
1:C:426:TYR:HB3	1:C:500:TRP:NE1	2.14	0.62
1:B:132:VAL:HG23	1:B:133:TYR:CD1	2.34	0.62
1:D:363:VAL:N	1:D:398:MET:HE1	2.15	0.62
1:C:534:ARG:HH11	1:C:534:ARG:HG3	1.63	0.62
1:B:426:TYR:HB3	1:B:500:TRP:NE1	2.14	0.62
1:A:132:VAL:HG23	1:A:133:TYR:CD1	2.35	0.62
1:C:478:LYS:HZ3	1:C:478:LYS:HB3	1.65	0.62
1:B:36:PRO:HA	1:B:98:TYR:CD1	2.33	0.62
1:A:426:TYR:HB3	1:A:500:TRP:NE1	2.14	0.62
1:D:466:THR:OG1	1:D:469:GLU:HG3	2.00	0.62
1:A:322:GLN:O	1:A:323:ASP:HB3	1.99	0.62
1:D:331:VAL:HB	1:D:445:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ALA:O	1:B:477:MET:HG3	1.99	0.62
1:C:138:LEU:HG	1:C:477:MET:HE3	1.82	0.62
1:C:473:ALA:O	1:C:477:MET:HG3	1.99	0.62
1:D:311:THR:HG22	1:D:312:PRO:HD2	1.83	0.61
1:D:132:VAL:HG23	1:D:133:TYR:CD1	2.35	0.61
1:B:331:VAL:HB	1:B:445:VAL:HG12	1.81	0.61
1:A:138:LEU:HG	1:A:477:MET:HE3	1.81	0.61
1:B:311:THR:HG22	1:B:312:PRO:HD2	1.82	0.61
1:A:311:THR:HG22	1:A:312:PRO:HD2	1.83	0.61
1:D:116:ILE:HD12	1:D:197:VAL:HG13	1.80	0.61
1:C:251:LEU:HD21	1:C:281:LEU:HD12	1.83	0.61
1:D:112:THR:CG2	1:D:113:PRO:HD2	2.31	0.61
1:D:395:ARG:HD2	1:D:396:ASP:OD1	2.01	0.61
1:D:149:MET:HE2	1:D:176:GLN:HA	1.82	0.61
1:B:395:ARG:HD2	1:B:396:ASP:OD1	2.01	0.61
1:D:138:LEU:HG	1:D:477:MET:HE3	1.83	0.61
1:A:340:VAL:HG23	1:A:341:TYR:CD1	2.36	0.61
1:C:466:THR:OG1	1:C:469:GLU:HG3	2.00	0.61
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.01	0.61
1:D:322:GLN:O	1:D:323:ASP:HB3	1.99	0.61
1:C:395:ARG:HD2	1:C:396:ASP:OD1	2.01	0.61
1:C:122:GLY:O	1:C:123:PHE:HB2	2.01	0.60
1:A:466:THR:OG1	1:A:469:GLU:HG3	2.00	0.60
1:D:340:VAL:HG23	1:D:341:TYR:CD1	2.36	0.60
1:A:114:VAL:HG12	1:A:145:VAL:HB	1.84	0.60
1:C:114:VAL:HG12	1:C:145:VAL:HB	1.84	0.60
1:B:340:VAL:HG23	1:B:341:TYR:CD1	2.36	0.60
1:D:251:LEU:HD21	1:D:281:LEU:HD12	1.83	0.60
1:A:114:VAL:HG23	1:A:197:VAL:HA	1.84	0.60
1:C:114:VAL:HG23	1:C:197:VAL:HA	1.84	0.60
1:C:80:PHE:CE2	1:C:82:GLY:HA3	2.37	0.60
1:B:466:THR:OG1	1:B:469:GLU:HG3	2.00	0.60
1:D:122:GLY:O	1:D:123:PHE:HB2	2.01	0.60
1:B:138:LEU:HG	1:B:477:MET:HE3	1.82	0.60
1:B:149:MET:HE2	1:B:176:GLN:HA	1.83	0.60
1:C:311:THR:HG22	1:C:312:PRO:HD2	1.83	0.60
1:C:340:VAL:HG23	1:C:341:TYR:CD1	2.36	0.60
1:A:80:PHE:CE2	1:A:82:GLY:HA3	2.37	0.60
1:B:112:THR:CG2	1:B:113:PRO:HD2	2.31	0.60
1:B:80:PHE:CE2	1:B:82:GLY:HA3	2.37	0.60
1:B:122:GLY:O	1:B:123:PHE:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:VAL:HG12	1:D:145:VAL:HB	1.84	0.59
1:C:17:LEU:HD23	1:C:60:LEU:HB3	1.84	0.59
1:A:149:MET:HE2	1:A:176:GLN:HA	1.83	0.59
1:D:327:LEU:HD23	1:D:328:VAL:N	2.17	0.59
1:B:251:LEU:HD21	1:B:281:LEU:HD12	1.83	0.59
1:B:114:VAL:HG23	1:B:197:VAL:HA	1.84	0.59
1:C:66:GLN:CB	1:C:98:TYR:HD2	2.16	0.59
1:A:66:GLN:CB	1:A:98:TYR:HD2	2.16	0.59
1:D:80:PHE:CE2	1:D:82:GLY:HA3	2.37	0.59
1:B:327:LEU:HD23	1:B:328:VAL:N	2.18	0.59
1:D:17:LEU:HD23	1:D:60:LEU:HB3	1.84	0.59
1:B:66:GLN:CB	1:B:98:TYR:HD2	2.16	0.59
1:A:251:LEU:HD21	1:A:281:LEU:HD12	1.83	0.59
1:C:112:THR:CG2	1:C:113:PRO:HD2	2.31	0.59
1:C:327:LEU:HD23	1:C:328:VAL:N	2.18	0.59
1:D:114:VAL:HG23	1:D:197:VAL:HA	1.84	0.59
1:D:66:GLN:CB	1:D:98:TYR:HD2	2.16	0.59
1:C:18:ARG:NH2	1:C:59:VAL:HG11	2.18	0.59
1:A:122:GLY:O	1:A:123:PHE:HB2	2.01	0.59
1:B:114:VAL:HG12	1:B:145:VAL:HB	1.84	0.59
1:A:329:GLY:HA3	1:A:428:TYR:CD1	2.38	0.59
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.38	0.59
1:B:18:ARG:NH2	1:B:59:VAL:HG11	2.18	0.59
1:C:329:GLY:HA3	1:C:428:TYR:CD1	2.38	0.58
1:A:444:GLY:O	1:A:446:PRO:HD3	2.03	0.58
1:C:224:ARG:HG2	1:C:325:GLN:HB2	1.85	0.58
1:B:329:GLY:HA3	1:B:428:TYR:CD1	2.38	0.58
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.38	0.58
1:A:123:PHE:HB2	1:A:300:VAL:HG12	1.85	0.58
1:C:337:TYR:O	1:C:340:VAL:HG22	2.03	0.58
1:B:21:ARG:HH21	1:B:23:LYS:HZ2	1.50	0.58
1:D:444:GLY:O	1:D:446:PRO:HD3	2.04	0.58
1:D:42:VAL:O	1:D:45:ARG:HB2	2.03	0.58
1:B:17:LEU:HD23	1:B:60:LEU:HB3	1.84	0.58
1:D:123:PHE:HB2	1:D:300:VAL:HG12	1.85	0.58
1:C:329:GLY:HA3	1:C:428:TYR:CZ	2.38	0.58
1:C:42:VAL:O	1:C:45:ARG:HB2	2.03	0.58
1:B:231:THR:HB	1:B:232:PRO:HD2	1.86	0.58
1:A:42:VAL:O	1:A:45:ARG:HB2	2.03	0.58
1:B:386:LEU:HD11	1:C:522:ARG:HB2	1.85	0.58
1:A:112:THR:CG2	1:A:113:PRO:HD2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:HD23	1:A:328:VAL:N	2.18	0.58
1:D:18:ARG:NH2	1:D:59:VAL:HG11	2.18	0.58
1:D:453:PHE:HB3	1:D:476:LEU:HD13	1.86	0.58
1:A:18:ARG:NH2	1:A:59:VAL:HG11	2.18	0.58
1:B:337:TYR:O	1:B:340:VAL:HG22	2.03	0.58
1:C:231:THR:HB	1:C:232:PRO:HD2	1.86	0.58
1:C:444:GLY:O	1:C:446:PRO:HD3	2.03	0.58
1:B:167:ALA:CB	1:B:270:ILE:HD12	2.34	0.58
1:B:444:GLY:O	1:B:446:PRO:HD3	2.03	0.58
1:C:317:ASN:HA	1:C:417:ARG:HH11	1.69	0.58
1:A:337:TYR:O	1:A:340:VAL:HG22	2.03	0.57
1:A:472:PHE:CE1	1:A:476:LEU:HD11	2.40	0.57
1:D:329:GLY:HA3	1:D:428:TYR:CZ	2.38	0.57
1:B:330:VAL:HG23	1:B:411:VAL:HG21	1.87	0.57
1:C:437:LEU:CD1	1:C:439:TRP:H	2.18	0.57
1:D:329:GLY:HA3	1:D:428:TYR:CD1	2.38	0.57
1:D:330:VAL:HG23	1:D:411:VAL:HG21	1.87	0.57
1:D:337:TYR:O	1:D:340:VAL:HG22	2.03	0.57
1:B:317:ASN:HA	1:B:417:ARG:HH11	1.69	0.57
1:A:138:LEU:HD11	1:A:455:PHE:HA	1.86	0.57
1:D:224:ARG:HG2	1:D:325:GLN:HB2	1.86	0.57
1:B:426:TYR:HD2	1:B:500:TRP:CD1	2.23	0.57
1:D:167:ALA:CB	1:D:270:ILE:HD12	2.34	0.57
1:B:123:PHE:HB2	1:B:300:VAL:HG12	1.86	0.57
1:C:149:MET:HE2	1:C:176:GLN:HA	1.86	0.57
1:A:453:PHE:HB3	1:A:476:LEU:HD13	1.86	0.57
1:A:17:LEU:HD23	1:A:60:LEU:HB3	1.84	0.57
1:A:437:LEU:CD1	1:A:439:TRP:H	2.18	0.57
1:B:42:VAL:O	1:B:45:ARG:HB2	2.03	0.57
1:A:167:ALA:CB	1:A:270:ILE:HD12	2.34	0.57
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.85	0.57
1:D:426:TYR:HD2	1:D:500:TRP:CD1	2.23	0.57
1:C:330:VAL:HG23	1:C:411:VAL:HG21	1.87	0.57
1:C:453:PHE:HB3	1:C:476:LEU:HD13	1.86	0.57
1:B:437:LEU:CD1	1:B:439:TRP:H	2.18	0.57
1:B:138:LEU:HD11	1:B:455:PHE:HA	1.86	0.57
1:B:317:ASN:HB2	1:B:417:ARG:NH1	2.20	0.57
1:D:138:LEU:HD11	1:D:455:PHE:HA	1.87	0.56
1:C:317:ASN:HB2	1:C:417:ARG:NH1	2.20	0.56
1:D:472:PHE:CE1	1:D:476:LEU:HD11	2.40	0.56
1:C:123:PHE:HB2	1:C:300:VAL:HG12	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.86	0.56
1:D:231:THR:HB	1:D:232:PRO:HD2	1.86	0.56
1:A:231:THR:HB	1:A:232:PRO:HD2	1.86	0.56
1:B:472:PHE:CE1	1:B:476:LEU:HD11	2.40	0.56
1:B:103:THR:CG2	1:B:104:PRO:HD2	2.36	0.56
1:C:103:THR:CG2	1:C:104:PRO:HD2	2.36	0.56
1:D:437:LEU:CD1	1:D:439:TRP:H	2.18	0.56
1:C:450:GLU:HG2	1:C:451:ILE:N	2.20	0.56
1:D:450:GLU:HG2	1:D:451:ILE:N	2.20	0.56
1:A:317:ASN:HA	1:A:417:ARG:HH11	1.69	0.56
1:B:181:GLN:O	1:B:185:GLU:HG2	2.05	0.56
1:A:426:TYR:HD2	1:A:500:TRP:CD1	2.23	0.56
1:D:317:ASN:HA	1:D:417:ARG:HH11	1.70	0.56
1:D:328:VAL:CG1	1:D:411:VAL:HG13	2.36	0.56
1:C:167:ALA:CB	1:C:270:ILE:HD12	2.34	0.56
1:D:317:ASN:HB2	1:D:417:ARG:NH1	2.20	0.56
1:C:181:GLN:O	1:C:185:GLU:HG2	2.05	0.56
1:C:426:TYR:HD2	1:C:500:TRP:CD1	2.23	0.56
1:A:330:VAL:HG23	1:A:411:VAL:HG21	1.87	0.56
1:B:453:PHE:HB3	1:B:476:LEU:HD13	1.86	0.56
1:C:472:PHE:CE1	1:C:476:LEU:HD11	2.40	0.56
1:C:138:LEU:HD11	1:C:455:PHE:HA	1.86	0.56
1:A:317:ASN:HB2	1:A:417:ARG:NH1	2.20	0.56
1:A:450:GLU:HG2	1:A:451:ILE:N	2.20	0.56
1:A:181:GLN:O	1:A:185:GLU:HG2	2.05	0.56
1:D:103:THR:CG2	1:D:104:PRO:HD2	2.36	0.56
1:A:328:VAL:CG1	1:A:411:VAL:HG13	2.36	0.55
1:C:328:VAL:CG1	1:C:411:VAL:HG13	2.36	0.55
1:D:181:GLN:O	1:D:185:GLU:HG2	2.05	0.55
1:A:266:ASP:O	1:A:270:ILE:HG12	2.06	0.55
1:A:103:THR:CG2	1:A:104:PRO:HD2	2.36	0.55
1:A:180:LEU:O	1:A:183:VAL:HG12	2.06	0.55
1:B:328:VAL:CG1	1:B:411:VAL:HG13	2.36	0.55
1:C:266:ASP:O	1:C:270:ILE:HG12	2.06	0.55
1:B:266:ASP:O	1:B:270:ILE:HG12	2.06	0.55
1:C:18:ARG:HH22	1:C:59:VAL:HG11	1.71	0.55
1:D:266:ASP:O	1:D:270:ILE:HG12	2.06	0.55
1:B:450:GLU:HG2	1:B:451:ILE:N	2.21	0.55
1:A:66:GLN:CB	1:A:98:TYR:CD2	2.90	0.55
1:A:66:GLN:CG	1:A:98:TYR:CD2	2.90	0.55
1:A:20:ILE:HG22	1:A:63:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:O	1:D:183:VAL:HG12	2.06	0.55
1:C:114:VAL:HG11	1:C:187:ILE:HG12	1.89	0.55
1:C:180:LEU:O	1:C:183:VAL:HG12	2.06	0.55
1:D:66:GLN:CB	1:D:98:TYR:CD2	2.90	0.55
1:C:20:ILE:HG22	1:C:63:THR:HA	1.89	0.55
1:B:180:LEU:O	1:B:183:VAL:HG12	2.06	0.55
1:C:66:GLN:CB	1:C:98:TYR:CD2	2.90	0.55
1:D:250:LEU:HG	1:D:288:VAL:HG12	1.89	0.55
1:D:21:ARG:HH21	1:D:23:LYS:HZ2	1.54	0.55
1:D:20:ILE:HG22	1:D:63:THR:HA	1.89	0.55
1:B:330:VAL:CG2	1:B:411:VAL:HG21	2.38	0.54
1:A:114:VAL:HG11	1:A:187:ILE:HG12	1.89	0.54
1:B:20:ILE:HG22	1:B:63:THR:HA	1.89	0.54
1:A:18:ARG:HH22	1:A:59:VAL:HG11	1.71	0.54
1:D:114:VAL:HG11	1:D:187:ILE:HG12	1.88	0.54
1:B:66:GLN:CB	1:B:98:TYR:CD2	2.90	0.54
1:B:250:LEU:HG	1:B:288:VAL:HG12	1.89	0.54
1:B:18:ARG:HH22	1:B:59:VAL:HG11	1.71	0.54
1:D:478:LYS:NZ	1:D:478:LYS:HB3	2.23	0.54
1:C:66:GLN:CG	1:C:98:TYR:CD2	2.90	0.54
1:D:330:VAL:CG2	1:D:411:VAL:HG21	2.38	0.54
1:A:322:GLN:HA	1:A:422:GLY:HA3	1.90	0.54
1:A:535:PHE:O	1:A:538:LYS:HG2	2.07	0.54
1:A:330:VAL:CG2	1:A:411:VAL:HG21	2.38	0.54
1:C:322:GLN:HA	1:C:422:GLY:HA3	1.90	0.54
1:D:535:PHE:O	1:D:538:LYS:HG2	2.07	0.54
1:C:363:VAL:N	1:C:398:MET:HE1	2.23	0.54
1:A:21:ARG:HH21	1:A:23:LYS:HZ2	1.55	0.54
1:A:99:LEU:C	1:A:99:LEU:HD12	2.28	0.54
1:C:250:LEU:HG	1:C:288:VAL:HG12	1.89	0.54
1:B:535:PHE:O	1:B:538:LYS:HG2	2.07	0.54
1:B:66:GLN:CG	1:B:98:TYR:CD2	2.90	0.54
1:B:478:LYS:NZ	1:B:478:LYS:HB3	2.23	0.54
1:B:107:ARG:NH1	1:B:107:ARG:HG3	2.23	0.54
1:D:124:TYR:CD1	1:D:125:SER:HB3	2.42	0.54
1:B:124:TYR:CD1	1:B:125:SER:HB3	2.42	0.54
1:A:124:TYR:CD1	1:A:125:SER:HB3	2.42	0.54
1:B:114:VAL:HG11	1:B:187:ILE:HG12	1.89	0.54
1:A:66:GLN:HB3	1:A:98:TYR:CD2	2.43	0.54
1:A:200:PHE:HB2	1:A:226:VAL:HB	1.90	0.54
1:D:18:ARG:HH22	1:D:59:VAL:HG11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:GLN:HA	1:D:422:GLY:HA3	1.90	0.54
1:C:535:PHE:O	1:C:538:LYS:HG2	2.07	0.54
1:B:99:LEU:HD12	1:B:99:LEU:C	2.28	0.53
1:C:99:LEU:C	1:C:99:LEU:HD12	2.28	0.53
1:A:250:LEU:HG	1:A:288:VAL:HG12	1.89	0.53
1:A:107:ARG:HG3	1:A:107:ARG:NH1	2.23	0.53
1:D:116:ILE:HD13	1:D:180:LEU:HD12	1.90	0.53
1:D:66:GLN:CG	1:D:98:TYR:CD2	2.90	0.53
1:C:142:GLU:HB3	1:C:481:THR:HG21	1.90	0.53
1:B:66:GLN:HB3	1:B:98:TYR:CD2	2.43	0.53
1:C:330:VAL:CG2	1:C:411:VAL:HG21	2.38	0.53
1:A:142:GLU:HB3	1:A:481:THR:HG21	1.90	0.53
1:C:124:TYR:CD1	1:C:125:SER:HB3	2.42	0.53
1:D:205:GLY:O	1:D:208:SER:HB2	2.09	0.53
1:A:205:GLY:O	1:A:208:SER:HB2	2.09	0.53
1:B:328:VAL:O	1:B:427:ALA:HA	2.09	0.53
1:D:107:ARG:HG3	1:D:107:ARG:NH1	2.23	0.53
1:C:107:ARG:NH1	1:C:107:ARG:HG3	2.23	0.53
1:A:116:ILE:HD13	1:A:180:LEU:HD12	1.90	0.53
1:C:116:ILE:HD13	1:C:180:LEU:HD12	1.90	0.53
1:B:116:ILE:HD13	1:B:180:LEU:HD12	1.90	0.53
1:D:142:GLU:HB3	1:D:481:THR:HG21	1.90	0.53
1:A:328:VAL:O	1:A:427:ALA:HA	2.09	0.53
1:D:328:VAL:O	1:D:427:ALA:HA	2.09	0.53
1:D:99:LEU:HD12	1:D:99:LEU:C	2.28	0.53
1:B:508:GLN:OE1	1:C:386:LEU:HD23	2.08	0.53
1:B:328:VAL:HG12	1:B:329:GLY:N	2.24	0.53
1:C:200:PHE:HB2	1:C:226:VAL:HB	1.90	0.53
1:C:478:LYS:NZ	1:C:478:LYS:HB3	2.23	0.53
1:D:124:TYR:CE1	1:D:125:SER:HB3	2.44	0.53
1:B:205:GLY:O	1:B:208:SER:HB2	2.09	0.53
1:A:328:VAL:HG12	1:A:329:GLY:N	2.24	0.52
1:A:478:LYS:NZ	1:A:478:LYS:HB3	2.23	0.52
1:B:322:GLN:HA	1:B:422:GLY:HA3	1.90	0.52
1:B:124:TYR:CE1	1:B:125:SER:HB3	2.44	0.52
1:A:124:TYR:CE1	1:A:125:SER:HB3	2.44	0.52
1:C:306:ASP:OD1	1:D:259:PRO:HB3	2.08	0.52
1:C:205:GLY:O	1:C:208:SER:HB2	2.09	0.52
1:D:66:GLN:HB3	1:D:98:TYR:CD2	2.43	0.52
1:B:142:GLU:HB3	1:B:481:THR:HG21	1.90	0.52
1:C:325:GLN:HB3	1:C:483:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ARG:HB2	1:C:386:LEU:HD11	1.90	0.52
1:C:328:VAL:O	1:C:427:ALA:HA	2.09	0.52
1:D:200:PHE:HB2	1:D:226:VAL:HB	1.90	0.52
1:C:18:ARG:HB2	1:C:18:ARG:NH2	2.24	0.52
1:B:325:GLN:HB3	1:B:483:PHE:CE1	2.45	0.52
1:A:317:ASN:HA	1:A:417:ARG:HD2	1.92	0.52
1:B:18:ARG:HB2	1:B:18:ARG:NH2	2.24	0.52
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.90	0.52
1:D:328:VAL:HG12	1:D:329:GLY:N	2.24	0.52
1:C:328:VAL:HG12	1:C:329:GLY:N	2.24	0.52
1:C:124:TYR:CE1	1:C:125:SER:HB3	2.44	0.52
1:C:197:VAL:HG11	1:C:221:LEU:O	2.10	0.52
1:D:325:GLN:HB3	1:D:483:PHE:CE1	2.45	0.52
1:A:325:GLN:HB3	1:A:483:PHE:CE1	2.45	0.52
1:C:317:ASN:HA	1:C:417:ARG:HD2	1.92	0.51
1:B:363:VAL:HG23	1:B:398:MET:HE1	1.92	0.51
1:A:18:ARG:NH2	1:A:18:ARG:HB2	2.24	0.51
1:D:107:ARG:HH11	1:D:107:ARG:HG3	1.76	0.51
1:B:197:VAL:HG11	1:B:221:LEU:O	2.10	0.51
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.76	0.51
1:D:197:VAL:HG11	1:D:221:LEU:O	2.10	0.51
1:D:89:ASN:OD1	1:D:129:SER:HB2	2.11	0.51
1:D:213:ILE:HG23	1:D:219:ARG:NH1	2.26	0.51
1:D:155:THR:HG22	1:D:159:LEU:HD12	1.93	0.51
1:D:354:ILE:CD1	1:D:359:PHE:HB2	2.41	0.51
1:A:532:TRP:O	1:A:537:PRO:HD3	2.11	0.51
1:A:213:ILE:HG23	1:A:219:ARG:NH1	2.26	0.51
1:C:213:ILE:HG23	1:C:219:ARG:NH1	2.26	0.51
1:A:110:SER:OG	1:A:111:PRO:HD2	2.11	0.51
1:C:110:SER:OG	1:C:111:PRO:HD2	2.11	0.51
1:C:29:VAL:HG12	1:C:103:THR:O	2.11	0.51
1:A:29:VAL:HG12	1:A:103:THR:O	2.11	0.51
1:D:532:TRP:O	1:D:537:PRO:HD3	2.11	0.51
1:A:226:VAL:HG11	1:A:480:TRP:NE1	2.25	0.51
1:C:532:TRP:O	1:C:537:PRO:HD3	2.11	0.51
1:B:110:SER:OG	1:B:111:PRO:HD2	2.11	0.51
1:B:432:HIS:HB3	1:B:472:PHE:HE2	1.76	0.51
1:D:110:SER:OG	1:D:111:PRO:HD2	2.11	0.51
1:B:532:TRP:O	1:B:537:PRO:HD3	2.11	0.51
1:C:353:LEU:HB3	1:C:391:PRO:HB2	1.93	0.51
1:C:354:ILE:CD1	1:C:359:PHE:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:HG23	1:B:219:ARG:NH1	2.26	0.51
1:B:89:ASN:OD1	1:B:129:SER:HB2	2.11	0.50
1:B:45:ARG:O	1:B:48:MET:HB2	2.11	0.50
1:C:107:ARG:HH11	1:C:107:ARG:HG3	1.76	0.50
1:B:155:THR:HG22	1:B:159:LEU:HD12	1.93	0.50
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.93	0.50
1:C:89:ASN:OD1	1:C:129:SER:HB2	2.11	0.50
1:C:409:CYS:N	1:C:410:PRO:CD	2.75	0.50
1:A:89:ASN:OD1	1:A:129:SER:HB2	2.11	0.50
1:B:317:ASN:HA	1:B:417:ARG:HD2	1.92	0.50
1:A:197:VAL:HG11	1:A:221:LEU:O	2.10	0.50
1:B:226:VAL:HG11	1:B:480:TRP:NE1	2.25	0.50
1:A:409:CYS:N	1:A:410:PRO:CD	2.75	0.50
1:A:68:VAL:HG12	1:A:69:CYS:O	2.12	0.50
1:B:68:VAL:HG12	1:B:69:CYS:O	2.12	0.50
1:B:409:CYS:N	1:B:410:PRO:CD	2.75	0.50
1:B:56:TRP:CE2	1:B:60:LEU:HD23	2.47	0.50
1:C:60:LEU:HD12	1:C:61:ASP:N	2.27	0.50
1:B:99:LEU:HA	1:B:149:MET:HA	1.94	0.50
1:B:354:ILE:CD1	1:B:359:PHE:HB2	2.41	0.50
1:C:346:PHE:HA	1:C:352:SER:HB3	1.93	0.50
1:D:346:PHE:HA	1:D:352:SER:HB3	1.93	0.50
1:C:226:VAL:HG11	1:C:480:TRP:NE1	2.25	0.50
1:D:18:ARG:HB2	1:D:18:ARG:NH2	2.24	0.50
1:C:45:ARG:O	1:C:48:MET:HB2	2.11	0.50
1:A:45:ARG:O	1:A:48:MET:HB2	2.11	0.50
1:C:99:LEU:HA	1:C:149:MET:HA	1.94	0.50
1:D:317:ASN:HA	1:D:417:ARG:HD2	1.92	0.50
1:D:409:CYS:N	1:D:410:PRO:CD	2.75	0.50
1:D:29:VAL:HG12	1:D:103:THR:O	2.11	0.50
1:A:60:LEU:HD12	1:A:61:ASP:N	2.27	0.50
1:D:56:TRP:CE2	1:D:60:LEU:HD23	2.47	0.50
1:D:45:ARG:O	1:D:48:MET:HB2	2.11	0.50
1:D:478:LYS:O	1:D:482:ASN:HB2	2.12	0.50
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.76	0.50
1:A:354:ILE:CD1	1:A:359:PHE:HB2	2.41	0.50
1:C:21:ARG:HH21	1:C:23:LYS:HZ2	1.58	0.50
1:D:68:VAL:HG12	1:D:69:CYS:O	2.12	0.50
1:B:60:LEU:HD12	1:B:61:ASP:N	2.27	0.50
1:A:478:LYS:O	1:A:482:ASN:HB2	2.12	0.50
1:B:119:TYR:CE1	1:B:151:TYR:CE1	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:HIS:HB3	1:D:472:PHE:HE2	1.77	0.50
1:B:29:VAL:HG12	1:B:103:THR:O	2.11	0.50
1:D:213:ILE:HG23	1:D:219:ARG:HH12	1.77	0.50
1:A:155:THR:HG22	1:A:159:LEU:HD12	1.93	0.50
1:C:68:VAL:HG12	1:C:69:CYS:O	2.12	0.49
1:C:213:ILE:HG23	1:C:219:ARG:HH12	1.77	0.49
1:A:348:LYS:O	1:A:440:PRO:HG3	2.13	0.49
1:A:432:HIS:HB3	1:A:472:PHE:HE2	1.76	0.49
1:D:476:LEU:CD2	1:D:513:LEU:HD12	2.42	0.49
1:C:478:LYS:O	1:C:482:ASN:HB2	2.12	0.49
1:D:354:ILE:HD11	1:D:359:PHE:HB2	1.94	0.49
1:C:476:LEU:CD2	1:C:513:LEU:HD12	2.42	0.49
1:C:56:TRP:CE2	1:C:60:LEU:HD23	2.47	0.49
1:B:478:LYS:O	1:B:482:ASN:HB2	2.12	0.49
1:B:363:VAL:N	1:B:398:MET:HE1	2.28	0.49
1:A:476:LEU:CD2	1:A:513:LEU:HD12	2.43	0.49
1:A:56:TRP:CE2	1:A:60:LEU:HD23	2.47	0.49
1:D:348:LYS:O	1:D:440:PRO:HG3	2.13	0.49
1:A:99:LEU:HA	1:A:149:MET:HA	1.94	0.49
1:A:249:THR:OG1	1:A:250:LEU:N	2.46	0.49
1:B:213:ILE:HG23	1:B:219:ARG:HH12	1.77	0.49
1:A:119:TYR:CE1	1:A:151:TYR:CE1	3.00	0.49
1:C:155:THR:HG22	1:C:159:LEU:HD12	1.93	0.49
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.93	0.49
1:B:8:LEU:N	1:B:8:LEU:HD23	2.28	0.49
1:C:119:TYR:CE1	1:C:151:TYR:CE1	3.00	0.49
1:D:119:TYR:CE1	1:D:151:TYR:CE1	3.00	0.49
1:A:346:PHE:HA	1:A:352:SER:HB3	1.93	0.49
1:C:252:ALA:CB	1:C:269:LEU:HD21	2.43	0.49
1:A:321:PHE:CD2	1:A:418:LEU:HD12	2.48	0.49
1:A:213:ILE:HG23	1:A:219:ARG:HH12	1.77	0.49
1:D:36:PRO:HB2	1:D:53:LYS:HG3	1.94	0.49
1:B:348:LYS:O	1:B:440:PRO:HG3	2.13	0.49
1:A:354:ILE:HD11	1:A:359:PHE:HB2	1.95	0.49
1:C:66:GLN:HB3	1:C:98:TYR:CD2	2.43	0.49
1:C:432:HIS:HB3	1:C:472:PHE:HE2	1.77	0.49
1:A:478:LYS:HE2	1:A:482:ASN:ND2	2.28	0.49
1:C:321:PHE:CD2	1:C:418:LEU:HD12	2.48	0.49
1:D:84:GLU:O	1:D:87:ASN:HB2	2.13	0.49
1:A:36:PRO:HB2	1:A:53:LYS:HG3	1.95	0.48
1:C:478:LYS:HE2	1:C:482:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:TRP:CZ3	1:D:237:ALA:HB2	2.48	0.48
1:C:354:ILE:HD11	1:C:359:PHE:HB2	1.94	0.48
1:B:236:TRP:CZ3	1:B:237:ALA:HB2	2.48	0.48
1:C:84:GLU:O	1:C:87:ASN:HB2	2.13	0.48
1:B:252:ALA:CB	1:B:269:LEU:HD21	2.43	0.48
1:B:346:PHE:HA	1:B:352:SER:HB3	1.93	0.48
1:B:249:THR:OG1	1:B:250:LEU:N	2.46	0.48
1:D:99:LEU:HA	1:D:149:MET:HA	1.94	0.48
1:B:321:PHE:CD2	1:B:418:LEU:HD12	2.48	0.48
1:D:353:LEU:HB3	1:D:391:PRO:HB2	1.93	0.48
1:B:478:LYS:HE2	1:B:482:ASN:ND2	2.28	0.48
1:D:478:LYS:HE2	1:D:482:ASN:ND2	2.28	0.48
1:A:84:GLU:O	1:A:87:ASN:HB2	2.13	0.48
1:D:249:THR:OG1	1:D:250:LEU:N	2.46	0.48
1:B:476:LEU:CD2	1:B:513:LEU:HD12	2.43	0.48
1:C:75:THR:O	1:C:77:TYR:N	2.47	0.48
1:C:138:LEU:HG	1:C:477:MET:CE	2.44	0.48
1:C:363:VAL:HG23	1:C:398:MET:HE1	1.94	0.48
1:A:7:GLN:HG3	1:A:105:TYR:CE1	2.49	0.48
1:A:139:ALA:O	1:A:143:GLY:HA2	2.14	0.48
1:A:445:VAL:HG12	1:A:445:VAL:O	2.14	0.48
1:A:138:LEU:HG	1:A:477:MET:CE	2.44	0.48
1:D:93:SER:OG	1:D:95:ASP:N	2.45	0.48
1:D:321:PHE:CD2	1:D:418:LEU:HD12	2.48	0.48
1:B:277:PRO:HG2	1:B:280:ASP:OD1	2.13	0.48
1:D:197:VAL:HB	1:D:222:PHE:HA	1.96	0.48
1:A:8:LEU:HD23	1:A:8:LEU:N	2.28	0.48
1:D:60:LEU:HD12	1:D:61:ASP:N	2.27	0.48
1:A:75:THR:O	1:A:77:TYR:N	2.47	0.48
1:B:445:VAL:O	1:B:445:VAL:HG12	2.14	0.48
1:C:348:LYS:O	1:C:440:PRO:HG3	2.13	0.48
1:D:139:ALA:O	1:D:143:GLY:HA2	2.13	0.48
1:D:226:VAL:HG11	1:D:480:TRP:NE1	2.25	0.48
1:D:75:THR:O	1:D:77:TYR:N	2.47	0.48
1:C:198:THR:OG1	1:C:224:ARG:HB2	2.14	0.48
1:C:249:THR:OG1	1:C:250:LEU:N	2.46	0.48
1:B:139:ALA:O	1:B:143:GLY:HA2	2.13	0.48
1:A:252:ALA:CB	1:A:269:LEU:HD21	2.43	0.48
1:B:523:GLY:HA3	1:C:386:LEU:CD2	2.44	0.48
1:D:8:LEU:N	1:D:8:LEU:HD23	2.28	0.48
1:B:75:THR:O	1:B:77:TYR:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:THR:OG1	1:B:224:ARG:HB2	2.14	0.48
1:D:7:GLN:HG3	1:D:105:TYR:CE1	2.49	0.48
1:B:7:GLN:HG3	1:B:105:TYR:CE1	2.49	0.48
1:C:277:PRO:HG2	1:C:280:ASP:OD1	2.13	0.48
1:C:139:ALA:O	1:C:143:GLY:HA2	2.13	0.48
1:D:252:ALA:CB	1:D:269:LEU:HD21	2.43	0.48
1:A:197:VAL:HB	1:A:222:PHE:HA	1.96	0.48
1:C:8:LEU:HD23	1:C:8:LEU:N	2.28	0.48
1:D:198:THR:OG1	1:D:224:ARG:HB2	2.14	0.48
1:C:236:TRP:CZ3	1:C:237:ALA:HB2	2.48	0.48
1:A:277:PRO:HG2	1:A:280:ASP:OD1	2.13	0.48
1:B:84:GLU:O	1:B:87:ASN:HB2	2.13	0.48
1:C:247:ARG:HB3	1:C:288:VAL:CG2	2.44	0.47
1:A:247:ARG:HB3	1:A:288:VAL:CG2	2.44	0.47
1:D:158:PHE:O	1:D:159:LEU:C	2.52	0.47
1:A:486:THR:OG1	1:A:487:GLY:N	2.47	0.47
1:A:93:SER:OG	1:A:95:ASP:N	2.46	0.47
1:B:328:VAL:HG11	1:B:411:VAL:HG13	1.96	0.47
1:B:354:ILE:HD11	1:B:359:PHE:HB2	1.95	0.47
1:B:476:LEU:HD21	1:B:513:LEU:HD12	1.96	0.47
1:C:7:GLN:HG3	1:C:105:TYR:CE1	2.49	0.47
1:D:486:THR:OG1	1:D:487:GLY:N	2.47	0.47
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.70	0.47
1:C:486:THR:OG1	1:C:487:GLY:N	2.47	0.47
1:D:328:VAL:HG11	1:D:411:VAL:HG13	1.96	0.47
1:C:445:VAL:O	1:C:445:VAL:HG12	2.14	0.47
1:B:138:LEU:HG	1:B:477:MET:CE	2.43	0.47
1:D:277:PRO:HG2	1:D:280:ASP:OD1	2.13	0.47
1:B:36:PRO:HB2	1:B:53:LYS:HG3	1.94	0.47
1:C:476:LEU:HD21	1:C:513:LEU:HD12	1.96	0.47
1:A:451:ILE:H	1:A:451:ILE:HG12	1.55	0.47
1:B:197:VAL:HB	1:B:222:PHE:HA	1.96	0.47
1:A:236:TRP:CZ3	1:A:237:ALA:HB2	2.48	0.47
1:D:476:LEU:HD21	1:D:513:LEU:HD12	1.96	0.47
1:C:457:LEU:N	1:C:458:PRO:CD	2.78	0.47
1:B:457:LEU:N	1:B:458:PRO:CD	2.78	0.47
1:C:158:PHE:O	1:C:159:LEU:C	2.52	0.47
1:A:457:LEU:N	1:A:458:PRO:CD	2.78	0.47
1:A:77:TYR:CD2	1:A:348:LYS:HD3	2.50	0.47
1:C:77:TYR:CD2	1:C:348:LYS:HD3	2.50	0.47
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:VAL:HG13	1:D:276:ARG:HD2	1.97	0.47
1:D:457:LEU:N	1:D:458:PRO:CD	2.78	0.47
1:B:77:TYR:CD2	1:B:348:LYS:HD3	2.50	0.47
1:C:45:ARG:HG3	1:C:45:ARG:NH1	2.29	0.47
1:B:45:ARG:NH1	1:B:45:ARG:HG3	2.29	0.47
1:B:486:THR:OG1	1:B:487:GLY:N	2.47	0.47
1:D:247:ARG:HB3	1:D:288:VAL:CG2	2.44	0.46
1:A:328:VAL:HG11	1:A:411:VAL:HG13	1.96	0.46
1:D:45:ARG:HG3	1:D:45:ARG:NH1	2.29	0.46
1:D:478:LYS:HZ3	1:D:478:LYS:HB3	1.80	0.46
1:C:115:LEU:HD11	1:C:484:ALA:HB2	1.97	0.46
1:C:433:ARG:NH2	1:C:441:LEU:HA	2.31	0.46
1:D:77:TYR:CD2	1:D:348:LYS:HD3	2.50	0.46
1:A:152:ARG:O	1:A:157:GLY:HA3	2.15	0.46
1:B:247:ARG:HB3	1:B:288:VAL:CG2	2.44	0.46
1:C:328:VAL:HG11	1:C:411:VAL:HG13	1.96	0.46
1:D:68:VAL:HG21	1:D:88:PRO:HB3	1.97	0.46
1:D:445:VAL:HG12	1:D:445:VAL:O	2.14	0.46
1:D:433:ARG:NH2	1:D:441:LEU:HA	2.31	0.46
1:D:138:LEU:HG	1:D:477:MET:CE	2.44	0.46
1:A:198:THR:OG1	1:A:224:ARG:HB2	2.14	0.46
1:B:116:ILE:CD1	1:B:183:VAL:HG11	2.32	0.46
1:B:115:LEU:HD11	1:B:484:ALA:HB2	1.97	0.46
1:A:45:ARG:HG3	1:A:45:ARG:NH1	2.29	0.46
1:C:152:ARG:O	1:C:157:GLY:HA3	2.15	0.46
1:A:180:LEU:HD11	1:A:199:LEU:CD2	2.46	0.46
1:A:68:VAL:HG21	1:A:88:PRO:HB3	1.97	0.46
1:D:316:ILE:HG21	1:D:414:LEU:CD1	2.46	0.46
1:A:347:SER:OG	1:A:349:ASP:N	2.46	0.46
1:A:10:VAL:HG23	1:A:32:PHE:CE2	2.51	0.46
1:B:152:ARG:O	1:B:157:GLY:HA3	2.15	0.46
1:D:152:ARG:O	1:D:157:GLY:HA3	2.15	0.46
1:A:106:PRO:O	1:A:107:ARG:C	2.54	0.46
1:D:106:PRO:O	1:D:107:ARG:C	2.54	0.46
1:C:211:MET:HG2	1:C:308:LEU:HD21	1.97	0.46
1:C:317:ASN:HA	1:C:417:ARG:NH1	2.31	0.46
1:A:317:ASN:HA	1:A:417:ARG:NH1	2.31	0.46
1:A:158:PHE:O	1:A:159:LEU:C	2.52	0.46
1:B:10:VAL:HG23	1:B:32:PHE:CE2	2.51	0.46
1:A:476:LEU:HD21	1:A:513:LEU:HD12	1.96	0.46
1:A:115:LEU:HD11	1:A:484:ALA:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:TYR:HE2	1:B:150:ASN:HA	1.81	0.46
1:D:119:TYR:HE2	1:D:150:ASN:HA	1.81	0.46
1:C:255:VAL:HG13	1:C:276:ARG:HD2	1.97	0.46
1:B:180:LEU:HD11	1:B:199:LEU:CD2	2.45	0.46
1:C:66:GLN:OE1	1:C:98:TYR:CE2	2.69	0.46
1:A:66:GLN:OE1	1:A:98:TYR:CE2	2.69	0.46
1:C:161:LEU:HD13	1:C:270:ILE:CD1	2.46	0.46
1:D:68:VAL:HG23	1:D:90:ARG:HB2	1.98	0.46
1:A:433:ARG:NH2	1:A:441:LEU:HA	2.31	0.46
1:C:316:ILE:HG21	1:C:414:LEU:CD1	2.46	0.46
1:D:211:MET:HG2	1:D:308:LEU:HD21	1.97	0.46
1:C:106:PRO:O	1:C:107:ARG:C	2.54	0.46
1:D:180:LEU:HD11	1:D:199:LEU:CD2	2.46	0.45
1:C:197:VAL:HB	1:C:222:PHE:HA	1.96	0.45
1:D:161:LEU:HD13	1:D:270:ILE:CD1	2.46	0.45
1:B:158:PHE:O	1:B:159:LEU:C	2.52	0.45
1:B:136:ARG:HG2	1:B:137:PHE:N	2.31	0.45
1:C:68:VAL:HG21	1:C:88:PRO:HB3	1.97	0.45
1:C:334:GLU:HG3	1:C:407:VAL:HB	1.98	0.45
1:B:68:VAL:HG21	1:B:88:PRO:HB3	1.97	0.45
1:B:407:VAL:C	1:B:410:PRO:HD2	2.37	0.45
1:B:161:LEU:HD13	1:B:270:ILE:CD1	2.47	0.45
1:B:433:ARG:NH2	1:B:441:LEU:HA	2.31	0.45
1:C:149:MET:HE1	1:C:176:GLN:HB3	1.98	0.45
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.97	0.45
1:C:10:VAL:HG23	1:C:32:PHE:CE2	2.51	0.45
1:B:169:GLY:O	1:B:170:ASN:HB2	2.16	0.45
1:A:334:GLU:HG3	1:A:407:VAL:HB	1.98	0.45
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.98	0.45
1:D:115:LEU:HD11	1:D:484:ALA:HB2	1.96	0.45
1:A:316:ILE:HG21	1:A:414:LEU:CD1	2.46	0.45
1:B:106:PRO:O	1:B:107:ARG:C	2.54	0.45
1:A:255:VAL:HG13	1:A:276:ARG:HD2	1.98	0.45
1:C:136:ARG:HG2	1:C:137:PHE:N	2.32	0.45
1:B:347:SER:OG	1:B:349:ASP:N	2.46	0.45
1:D:10:VAL:HG23	1:D:32:PHE:CE2	2.51	0.45
1:D:407:VAL:C	1:D:410:PRO:HD2	2.37	0.45
1:B:66:GLN:OE1	1:B:98:TYR:CE2	2.69	0.45
1:D:38:ALA:HA	1:D:53:LYS:N	2.31	0.45
1:D:66:GLN:OE1	1:D:98:TYR:CE2	2.69	0.45
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:HB3	1:A:59:VAL:HG22	1.99	0.45
1:B:317:ASN:HA	1:B:417:ARG:NH1	2.31	0.45
1:C:38:ALA:HA	1:C:53:LYS:N	2.32	0.45
1:B:38:ALA:HA	1:B:53:LYS:N	2.31	0.45
1:A:294:ILE:HG12	1:A:365:ILE:CG2	2.43	0.45
1:D:334:GLU:HG3	1:D:407:VAL:HB	1.98	0.45
1:C:105:TYR:HA	1:C:106:PRO:HA	1.75	0.45
1:A:119:TYR:HE2	1:A:150:ASN:HA	1.81	0.45
1:C:36:PRO:HB2	1:C:53:LYS:HG3	1.94	0.45
1:A:407:VAL:C	1:A:410:PRO:HD2	2.37	0.45
1:D:491:ASP:HA	1:D:492:PRO:HD2	1.77	0.45
1:B:316:ILE:HG21	1:B:414:LEU:CD1	2.46	0.45
1:B:146:LEU:HD23	1:B:147:VAL:N	2.32	0.45
1:C:407:VAL:C	1:C:410:PRO:HD2	2.37	0.45
1:B:16:GLN:HB3	1:B:59:VAL:HG22	1.99	0.45
1:A:169:GLY:O	1:A:170:ASN:HB2	2.17	0.45
1:D:169:GLY:O	1:D:170:ASN:HB2	2.16	0.45
1:C:68:VAL:HG23	1:C:90:ARG:HB2	1.98	0.45
1:C:16:GLN:HB3	1:C:59:VAL:HG22	1.99	0.45
1:D:347:SER:OG	1:D:349:ASP:N	2.46	0.45
1:D:141:VAL:HG21	1:D:459:LEU:HD22	1.99	0.45
1:C:116:ILE:CD1	1:C:183:VAL:HG11	2.32	0.44
1:B:523:GLY:CA	1:C:386:LEU:HD21	2.46	0.44
1:C:421:GLN:HB2	1:C:421:GLN:HE21	1.49	0.44
1:C:119:TYR:HE2	1:C:150:ASN:HA	1.81	0.44
1:A:161:LEU:HD13	1:A:270:ILE:CD1	2.47	0.44
1:A:45:ARG:HH11	1:A:45:ARG:HG3	1.83	0.44
1:B:255:VAL:HG13	1:B:276:ARG:HD2	1.98	0.44
1:B:291:GLN:HE21	1:B:291:GLN:HB2	1.61	0.44
1:A:141:VAL:HG21	1:A:459:LEU:HD22	1.99	0.44
1:A:146:LEU:HD23	1:A:147:VAL:N	2.32	0.44
1:A:421:GLN:HB2	1:A:421:GLN:HE21	1.49	0.44
1:B:294:ILE:HG12	1:B:365:ILE:CG2	2.43	0.44
1:D:294:ILE:HG12	1:D:365:ILE:CG2	2.43	0.44
1:A:166:GLU:HG3	1:A:270:ILE:HG13	2.00	0.44
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.82	0.44
1:B:437:LEU:HD12	1:B:439:TRP:H	1.82	0.44
1:D:291:GLN:HB2	1:D:291:GLN:HE21	1.61	0.44
1:B:243:GLU:OE1	1:B:247:ARG:NH2	2.48	0.44
1:D:146:LEU:HD23	1:D:147:VAL:N	2.32	0.44
1:A:38:ALA:HA	1:A:53:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:GLY:CA	1:C:386:LEU:CD2	2.96	0.44
1:C:481:THR:O	1:C:484:ALA:HB3	2.18	0.44
1:D:363:VAL:HG23	1:D:398:MET:HE1	2.00	0.44
1:D:317:ASN:HA	1:D:417:ARG:NH1	2.31	0.44
1:D:136:ARG:HG2	1:D:137:PHE:N	2.31	0.44
1:A:216:LEU:CB	1:A:217:PRO:HD3	2.48	0.44
1:C:408:VAL:O	1:C:411:VAL:HB	2.18	0.44
1:D:492:PRO:HB2	1:D:493:ARG:H	1.44	0.44
1:A:20:ILE:HG13	1:A:21:ARG:N	2.33	0.44
1:A:103:THR:HG23	1:A:108:PRO:HD3	2.00	0.44
1:D:481:THR:O	1:D:484:ALA:HB3	2.18	0.44
1:A:439:TRP:HB3	1:A:440:PRO:HD2	2.00	0.44
1:C:45:ARG:HH11	1:C:45:ARG:HG3	1.82	0.44
1:C:180:LEU:HD11	1:C:199:LEU:CD2	2.46	0.44
1:C:426:TYR:HB3	1:C:500:TRP:HE1	1.83	0.44
1:A:37:PHE:CD1	1:A:178:LEU:HD13	2.45	0.44
1:B:408:VAL:O	1:B:411:VAL:HB	2.18	0.44
1:C:20:ILE:HG13	1:C:21:ARG:N	2.33	0.44
1:C:103:THR:HG23	1:C:108:PRO:HD3	2.00	0.44
1:A:433:ARG:NH2	1:A:440:PRO:O	2.51	0.44
1:C:316:ILE:HG13	1:C:317:ASN:N	2.33	0.44
1:C:169:GLY:O	1:C:170:ASN:HB2	2.17	0.44
1:A:481:THR:O	1:A:484:ALA:HB3	2.18	0.44
1:B:433:ARG:NH2	1:B:440:PRO:O	2.51	0.44
1:C:439:TRP:HB3	1:C:440:PRO:HD2	2.00	0.44
1:D:439:TRP:HB3	1:D:440:PRO:HD2	2.00	0.44
1:C:467:THR:HG23	1:C:470:ARG:NH1	2.33	0.44
1:B:208:SER:O	1:B:209:VAL:C	2.57	0.44
1:C:146:LEU:HD23	1:C:147:VAL:N	2.32	0.44
1:B:523:GLY:N	1:C:386:LEU:HD21	2.33	0.43
1:D:408:VAL:O	1:D:411:VAL:HB	2.18	0.43
1:B:56:TRP:CD1	1:B:60:LEU:HB2	2.53	0.43
1:D:457:LEU:N	1:D:458:PRO:HD3	2.33	0.43
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.82	0.43
1:D:316:ILE:HG13	1:D:317:ASN:N	2.33	0.43
1:C:327:LEU:HD23	1:C:328:VAL:H	1.83	0.43
1:C:407:VAL:O	1:C:410:PRO:HD2	2.18	0.43
1:D:458:PRO:HB3	1:D:465:TYR:CG	2.53	0.43
1:B:481:THR:O	1:B:484:ALA:HB3	2.18	0.43
1:A:437:LEU:HD12	1:A:439:TRP:H	1.82	0.43
1:B:439:TRP:HB3	1:B:440:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:LEU:HD12	1:C:439:TRP:H	1.82	0.43
1:D:437:LEU:HD12	1:D:439:TRP:H	1.83	0.43
1:B:334:GLU:HG3	1:B:407:VAL:HB	1.99	0.43
1:B:20:ILE:HG13	1:B:21:ARG:N	2.32	0.43
1:D:20:ILE:HG13	1:D:21:ARG:N	2.33	0.43
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.83	0.43
1:C:208:SER:O	1:C:209:VAL:C	2.57	0.43
1:B:216:LEU:CB	1:B:217:PRO:HD3	2.48	0.43
1:D:426:TYR:HB3	1:D:500:TRP:HE1	1.83	0.43
1:B:426:TYR:HB3	1:B:500:TRP:HE1	1.83	0.43
1:D:327:LEU:HD23	1:D:328:VAL:H	1.83	0.43
1:B:407:VAL:O	1:B:410:PRO:HD2	2.18	0.43
1:A:457:LEU:N	1:A:458:PRO:HD3	2.33	0.43
1:B:458:PRO:HB3	1:B:465:TYR:CG	2.54	0.43
1:D:16:GLN:HB3	1:D:59:VAL:HG22	1.99	0.43
1:B:457:LEU:N	1:B:458:PRO:HD3	2.33	0.43
1:A:208:SER:O	1:A:211:MET:N	2.52	0.43
1:D:7:GLN:CB	1:D:105:TYR:HE1	2.31	0.43
1:A:408:VAL:O	1:A:411:VAL:HB	2.18	0.43
1:A:458:PRO:HB3	1:A:465:TYR:CG	2.54	0.43
1:D:534:ARG:HH11	1:D:534:ARG:CG	2.30	0.43
1:C:347:SER:OG	1:C:349:ASP:N	2.46	0.43
1:C:166:GLU:HG3	1:C:270:ILE:HG13	2.00	0.43
1:B:460:ASP:HA	1:B:461:PRO:HD3	1.82	0.43
1:D:433:ARG:NH2	1:D:440:PRO:O	2.51	0.43
1:D:208:SER:O	1:D:211:MET:N	2.52	0.43
1:C:7:GLN:CB	1:C:105:TYR:HE1	2.31	0.43
1:B:93:SER:OG	1:B:95:ASP:N	2.46	0.43
1:D:202:GLU:O	1:D:203:SER:C	2.57	0.43
1:C:216:LEU:CB	1:C:217:PRO:HD3	2.48	0.43
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.84	0.43
1:B:33:LEU:CD1	1:B:33:LEU:N	2.82	0.43
1:C:468:GLU:HA	1:C:471:ILE:HD12	2.01	0.43
1:C:457:LEU:N	1:C:458:PRO:HD3	2.33	0.43
1:C:433:ARG:NH2	1:C:440:PRO:O	2.51	0.43
1:B:467:THR:HG23	1:B:470:ARG:NH1	2.33	0.43
1:C:534:ARG:CG	1:C:534:ARG:HH11	2.30	0.43
1:B:316:ILE:HG13	1:B:317:ASN:N	2.33	0.43
1:A:7:GLN:CB	1:A:105:TYR:HE1	2.31	0.43
1:C:146:LEU:C	1:C:146:LEU:HD23	2.39	0.43
1:D:216:LEU:CB	1:D:217:PRO:HD3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:O	1:A:203:SER:C	2.57	0.43
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.84	0.43
1:A:136:ARG:HG2	1:A:137:PHE:N	2.31	0.43
1:D:166:GLU:HG3	1:D:270:ILE:HG13	2.00	0.43
1:B:166:GLU:HG3	1:B:270:ILE:HG13	2.00	0.43
1:D:103:THR:HG23	1:D:108:PRO:HD3	2.00	0.43
1:C:458:PRO:HB3	1:C:465:TYR:CG	2.54	0.43
1:D:146:LEU:HD23	1:D:146:LEU:C	2.39	0.43
1:B:468:GLU:HA	1:B:471:ILE:HD12	2.01	0.43
1:B:295:PHE:CE2	1:B:338:PHE:CZ	3.07	0.43
1:B:492:PRO:HB2	1:B:493:ARG:H	1.44	0.43
1:A:522:ARG:HH11	1:A:522:ARG:HD3	1.70	0.43
1:C:306:ASP:O	1:C:307:PHE:C	2.57	0.43
1:D:467:THR:HG23	1:D:470:ARG:NH1	2.33	0.43
1:C:208:SER:O	1:C:211:MET:N	2.52	0.43
1:A:146:LEU:HD23	1:A:146:LEU:C	2.39	0.43
1:B:141:VAL:HG21	1:B:459:LEU:HD22	1.99	0.43
1:C:141:VAL:HG21	1:C:459:LEU:HD22	1.99	0.43
1:B:212:HIS:HD2	1:B:218:SER:OG	2.02	0.43
1:A:306:ASP:HB2	1:B:260:GLY:H	1.84	0.42
1:D:407:VAL:O	1:D:410:PRO:HD2	2.18	0.42
1:C:491:ASP:HA	1:C:492:PRO:HD2	1.77	0.42
1:A:108:PRO:HG2	1:A:191:GLY:HA3	2.01	0.42
1:B:146:LEU:HD23	1:B:146:LEU:C	2.39	0.42
1:C:295:PHE:CE2	1:C:338:PHE:CZ	3.07	0.42
1:A:407:VAL:O	1:A:410:PRO:HD2	2.18	0.42
1:B:472:PHE:CZ	1:B:476:LEU:HD11	2.55	0.42
1:B:534:ARG:CG	1:B:534:ARG:HH11	2.30	0.42
1:A:212:HIS:HD2	1:A:218:SER:OG	2.02	0.42
1:A:33:LEU:CD1	1:A:33:LEU:N	2.82	0.42
1:C:500:TRP:HB2	1:C:518:LEU:HD11	2.02	0.42
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.54	0.42
1:B:108:PRO:HG2	1:B:191:GLY:HA3	2.02	0.42
1:A:142:GLU:HB2	1:A:481:THR:HG21	2.01	0.42
1:A:295:PHE:CE2	1:A:338:PHE:CZ	3.07	0.42
1:B:193:ASP:OD1	1:B:195:MET:HB2	2.20	0.42
1:B:475:ARG:HH11	1:B:475:ARG:HD3	1.66	0.42
1:A:56:TRP:CD1	1:A:60:LEU:HB2	2.53	0.42
1:A:316:ILE:HG13	1:A:317:ASN:N	2.33	0.42
1:B:7:GLN:CB	1:B:105:TYR:HE1	2.31	0.42
1:A:468:GLU:HA	1:A:471:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LEU:HA	1:B:536:LEU:HD23	1.89	0.42
1:A:500:TRP:HB2	1:A:518:LEU:HD11	2.02	0.42
1:A:467:THR:HG23	1:A:470:ARG:NH1	2.33	0.42
1:C:310:ASP:OD1	1:C:311:THR:N	2.53	0.42
1:D:208:SER:O	1:D:209:VAL:C	2.57	0.42
1:B:338:PHE:N	1:B:338:PHE:CD1	2.88	0.42
1:C:212:HIS:HD2	1:C:218:SER:OG	2.02	0.42
1:B:12:VAL:HG13	1:B:186:ASN:OD1	2.20	0.42
1:D:295:PHE:CE2	1:D:338:PHE:CZ	3.07	0.42
1:B:103:THR:HG23	1:B:108:PRO:HD3	2.00	0.42
1:C:322:GLN:O	1:C:323:ASP:CB	2.68	0.42
1:A:12:VAL:HG13	1:A:186:ASN:OD1	2.20	0.42
1:D:37:PHE:CD1	1:D:178:LEU:HD13	2.45	0.42
1:C:472:PHE:CZ	1:C:476:LEU:HD11	2.55	0.42
1:C:37:PHE:CD1	1:C:178:LEU:HD13	2.45	0.42
1:D:56:TRP:CD1	1:D:60:LEU:HB2	2.53	0.42
1:B:208:SER:O	1:B:211:MET:N	2.52	0.42
1:A:135:GLY:CA	1:A:146:LEU:HD13	2.50	0.42
1:C:33:LEU:CD1	1:C:33:LEU:N	2.82	0.42
1:B:202:GLU:O	1:B:203:SER:C	2.57	0.42
1:B:21:ARG:NH2	1:B:23:LYS:HZ2	2.17	0.42
1:A:132:VAL:HG23	1:A:133:TYR:CE1	2.55	0.42
1:D:212:HIS:HD2	1:D:218:SER:OG	2.02	0.42
1:D:12:VAL:HG13	1:D:186:ASN:OD1	2.20	0.42
1:A:310:ASP:OD1	1:A:311:THR:N	2.53	0.42
1:A:338:PHE:CD1	1:A:338:PHE:N	2.88	0.42
1:D:33:LEU:CD1	1:D:33:LEU:N	2.82	0.42
1:B:508:GLN:OE1	1:C:386:LEU:CD2	2.67	0.42
1:C:517:PRO:O	1:C:518:LEU:C	2.59	0.42
1:B:517:PRO:O	1:B:518:LEU:C	2.58	0.42
1:D:243:GLU:OE1	1:D:247:ARG:NH2	2.48	0.42
1:B:37:PHE:CD1	1:B:178:LEU:HD13	2.45	0.42
1:D:8:LEU:HD11	1:D:21:ARG:HB2	2.02	0.42
1:C:142:GLU:HB2	1:C:481:THR:HG21	2.01	0.42
1:C:75:THR:HB	1:C:76:LEU:H	1.75	0.42
1:B:170:ASN:ND2	1:B:304:ASP:OD2	2.52	0.42
1:C:294:ILE:HG12	1:C:365:ILE:CG2	2.42	0.41
1:A:327:LEU:HD23	1:A:328:VAL:H	1.83	0.41
1:C:132:VAL:HG23	1:C:133:TYR:CE1	2.55	0.41
1:D:105:TYR:HA	1:D:106:PRO:HA	1.76	0.41
1:D:338:PHE:CD1	1:D:338:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLN:O	1:B:530:ALA:N	2.53	0.41
1:D:193:ASP:OD1	1:D:195:MET:HB2	2.20	0.41
1:D:472:PHE:CZ	1:D:476:LEU:HD11	2.55	0.41
1:D:108:PRO:HG2	1:D:191:GLY:HA3	2.02	0.41
1:C:108:PRO:HG2	1:C:191:GLY:HA3	2.02	0.41
1:C:56:TRP:CD1	1:C:60:LEU:HB2	2.53	0.41
1:B:310:ASP:OD1	1:B:311:THR:N	2.53	0.41
1:B:340:VAL:CG2	1:B:341:TYR:CD1	3.03	0.41
1:B:149:MET:HE1	1:B:176:GLN:HB3	2.02	0.41
1:C:170:ASN:ND2	1:C:304:ASP:OD2	2.53	0.41
1:A:527:GLN:O	1:A:530:ALA:N	2.53	0.41
1:C:93:SER:OG	1:C:95:ASP:N	2.46	0.41
1:A:193:ASP:OD1	1:A:195:MET:HB2	2.20	0.41
1:D:135:GLY:CA	1:D:146:LEU:HD13	2.50	0.41
1:C:135:GLY:CA	1:C:146:LEU:HD13	2.50	0.41
1:C:177:ARG:CZ	1:C:217:PRO:HB2	2.51	0.41
1:C:193:ASP:OD1	1:C:195:MET:HB2	2.20	0.41
1:B:374:ALA:HA	1:B:539:LEU:HD13	2.02	0.41
1:D:374:ALA:HA	1:D:539:LEU:HD13	2.02	0.41
1:B:327:LEU:HD23	1:B:328:VAL:H	1.84	0.41
1:A:306:ASP:O	1:A:307:PHE:C	2.57	0.41
1:A:406:ASN:O	1:A:410:PRO:HG2	2.21	0.41
1:B:8:LEU:HD11	1:B:21:ARG:HB2	2.02	0.41
1:D:170:ASN:ND2	1:D:304:ASP:OD2	2.53	0.41
1:A:367:VAL:HG12	1:A:370:ALA:HB2	2.03	0.41
1:C:12:VAL:HG13	1:C:186:ASN:OD1	2.20	0.41
1:C:367:VAL:HG12	1:C:370:ALA:HB2	2.03	0.41
1:C:291:GLN:HB2	1:C:291:GLN:HE21	1.61	0.41
1:A:253:ARG:HD2	1:A:253:ARG:HH11	1.72	0.41
1:D:322:GLN:O	1:D:323:ASP:CB	2.68	0.41
1:C:390:ASP:HA	1:C:391:PRO:HD2	1.92	0.41
1:B:367:VAL:HG12	1:B:370:ALA:HB2	2.02	0.41
1:B:35:ILE:HA	1:B:36:PRO:HD2	1.98	0.41
1:D:517:PRO:O	1:D:518:LEU:C	2.59	0.41
1:C:406:ASN:O	1:C:410:PRO:HG2	2.21	0.41
1:D:300:VAL:HB	1:D:301:PRO:CD	2.49	0.41
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.50	0.41
1:C:492:PRO:HB2	1:C:493:ARG:H	1.44	0.41
1:C:60:LEU:HD12	1:C:61:ASP:O	2.21	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.91	0.41
1:C:202:GLU:O	1:C:203:SER:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:HD11	1:D:199:LEU:HD21	2.03	0.41
1:A:517:PRO:O	1:A:518:LEU:C	2.59	0.41
1:D:500:TRP:HB2	1:D:518:LEU:HD11	2.02	0.41
1:B:500:TRP:HB2	1:B:518:LEU:HD11	2.01	0.41
1:D:406:ASN:O	1:D:410:PRO:HG2	2.21	0.41
1:B:406:ASN:O	1:B:410:PRO:HG2	2.21	0.41
1:A:60:LEU:HD12	1:A:61:ASP:O	2.21	0.41
1:C:80:PHE:CE1	1:C:348:LYS:NZ	2.85	0.41
1:B:132:VAL:HG23	1:B:133:TYR:CE1	2.55	0.41
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.91	0.41
1:D:177:ARG:CZ	1:D:217:PRO:HB2	2.51	0.41
1:C:46:ARG:HD3	1:C:47:PHE:CZ	2.56	0.41
1:D:527:GLN:O	1:D:530:ALA:N	2.53	0.41
1:C:536:LEU:HA	1:C:536:LEU:HD23	1.89	0.41
1:A:518:LEU:HD23	1:A:518:LEU:HA	1.81	0.41
1:D:132:VAL:HG23	1:D:133:TYR:CE1	2.55	0.41
1:B:135:GLY:CA	1:B:146:LEU:HD13	2.50	0.41
1:B:46:ARG:HD3	1:B:47:PHE:CZ	2.56	0.41
1:C:8:LEU:HD11	1:C:21:ARG:HB2	2.02	0.40
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.50	0.40
1:C:212:HIS:CD2	1:C:218:SER:OG	2.74	0.40
1:D:279:GLN:O	1:D:279:GLN:HG3	2.21	0.40
1:D:468:GLU:HA	1:D:471:ILE:HD12	2.01	0.40
1:D:46:ARG:HD3	1:D:47:PHE:CZ	2.56	0.40
1:D:490:ASN:O	1:D:491:ASP:C	2.60	0.40
1:A:490:ASN:O	1:A:491:ASP:C	2.60	0.40
1:A:208:SER:O	1:A:209:VAL:C	2.56	0.40
1:A:202:GLU:OE1	1:A:203:SER:N	2.55	0.40
1:B:202:GLU:OE1	1:B:203:SER:N	2.55	0.40
1:C:193:ASP:HA	1:C:194:PRO:HD2	1.92	0.40
1:C:202:GLU:OE1	1:C:203:SER:N	2.54	0.40
1:A:374:ALA:HA	1:A:539:LEU:HD13	2.02	0.40
1:D:60:LEU:HD12	1:D:61:ASP:O	2.21	0.40
1:A:363:VAL:HG23	1:A:398:MET:HE1	2.04	0.40
1:A:478:LYS:HD2	1:A:478:LYS:HA	1.93	0.40
1:A:300:VAL:HB	1:A:301:PRO:CD	2.49	0.40
1:D:340:VAL:CG2	1:D:341:TYR:CD1	3.03	0.40
1:C:317:ASN:CB	1:C:417:ARG:NH1	2.83	0.40
1:A:317:ASN:CB	1:A:417:ARG:NH1	2.84	0.40
1:B:279:GLN:O	1:B:279:GLN:HG3	2.21	0.40
1:B:182:TRP:O	1:B:183:VAL:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD11	1:A:21:ARG:HB2	2.02	0.40
1:C:490:ASN:O	1:C:491:ASP:C	2.60	0.40
1:B:60:LEU:HD12	1:B:61:ASP:O	2.21	0.40
1:D:310:ASP:OD1	1:D:311:THR:N	2.53	0.40
1:B:317:ASN:CB	1:B:417:ARG:NH1	2.84	0.40
1:C:451:ILE:H	1:C:451:ILE:HG12	1.55	0.40
1:C:418:LEU:HA	1:C:418:LEU:HD12	1.91	0.40
1:B:385:TRP:HD1	1:C:527:GLN:HG3	1.87	0.40
1:D:184:GLN:HA	1:D:184:GLN:OE1	2.22	0.40
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.84	0.40
1:B:490:ASN:O	1:B:491:ASP:C	2.60	0.40
1:A:534:ARG:HH11	1:A:534:ARG:CG	2.30	0.40
1:A:170:ASN:ND2	1:A:304:ASP:OD2	2.52	0.40
1:D:212:HIS:CD2	1:D:218:SER:OG	2.75	0.40
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.86	0.40
1:C:516:LYS:HA	1:C:516:LYS:HE3	2.04	0.40
1:B:184:GLN:HA	1:B:184:GLN:OE1	2.22	0.40
1:D:516:LYS:HE3	1:D:516:LYS:HA	2.04	0.40

All (17) 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:C:21:ARG:NH2	1:C:105:TYR:CE2[2_655]	0.66	1.54
1:A:88:PRO:O	1:A:91:GLU:CG[2_554]	1.08	1.12
1:C:21:ARG:NH2	1:C:105:TYR:CZ[2_655]	1.12	1.08
1:A:88:PRO:O	1:A:91:GLU:CD[2_554]	1.17	1.03
1:C:23:LYS:NZ	1:C:105:TYR:OH[2_655]	1.21	0.99
1:A:88:PRO:O	1:A:91:GLU:OE1[2_554]	1.53	0.67
1:C:21:ARG:NH1	1:C:21:ARG:NH1[2_655]	1.61	0.59
1:C:21:ARG:CZ	1:C:105:TYR:CE2[2_655]	1.72	0.48
1:C:21:ARG:CD	1:C:21:ARG:NH1[2_655]	1.78	0.42
1:A:87:ASN:O	1:A:91:GLU:OE1[2_554]	1.82	0.38
1:A:88:PRO:C	1:A:91:GLU:OE1[2_554]	1.85	0.35
1:C:21:ARG:NH2	1:C:105:TYR:CD2[2_655]	1.93	0.27
1:C:23:LYS:CE	1:C:105:TYR:OH[2_655]	1.94	0.26
1:C:21:ARG:NH2	1:C:105:TYR:OH[2_655]	1.95	0.25
1:A:87:ASN:C	1:A:91:GLU:OE1[2_554]	2.02	0.18
1:C:21:ARG:CZ	1:C:21:ARG:NH1[2_655]	2.15	0.05
1:A:88:PRO:C	1:A:91:GLU:CG[2_554]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	537/539 (100%)	470 (88%)	58 (11%)	9 (2%)	11	56
1	B	537/539 (100%)	471 (88%)	57 (11%)	9 (2%)	11	56
1	C	537/539 (100%)	470 (88%)	58 (11%)	9 (2%)	11	56
1	D	537/539 (100%)	469 (87%)	59 (11%)	9 (2%)	11	56
All	All	2148/2156 (100%)	1880 (88%)	232 (11%)	36 (2%)	11	56

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	323	ASP
1	A	492	PRO
1	A	494	ASP
1	A	497	SER
1	B	76	LEU
1	B	323	ASP
1	B	492	PRO
1	B	494	ASP
1	B	497	SER
1	C	76	LEU
1	C	323	ASP
1	C	492	PRO
1	C	494	ASP
1	C	497	SER
1	D	76	LEU
1	D	323	ASP
1	D	492	PRO
1	D	494	ASP
1	D	497	SER
1	A	111	PRO
1	B	111	PRO

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Mol	Chain	Res	Type
1	B	203	SER
1	C	111	PRO
1	D	111	PRO
1	A	203	SER
1	C	203	SER
1	D	203	SER
1	A	234	GLY
1	B	234	GLY
1	C	234	GLY
1	D	234	GLY
1	B	523	GLY
1	A	523	GLY
1	C	523	GLY
1	D	523	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/440 (99%)	348 (80%)	86 (20%)	1	13
1	B	434/440 (99%)	347 (80%)	87 (20%)	1	13
1	C	434/440 (99%)	348 (80%)	86 (20%)	1	13
1	D	434/440 (99%)	348 (80%)	86 (20%)	1	13
All	All	1736/1760 (99%)	1391 (80%)	345 (20%)	1	13

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	ARG
1	A	18	ARG
1	A	20	ILE
1	A	29	VAL
1	A	45	ARG
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	60	LEU
1	A	61	ASP
1	A	65	PHE
1	A	75	THR
1	A	90	ARG
1	A	93	SER
1	A	102	TRP
1	A	115	LEU
1	A	129	SER
1	A	136	ARG
1	A	149	MET
1	A	155	THR
1	A	166	GLU
1	A	168	PRO
1	A	178	LEU
1	A	180	LEU
1	A	183	VAL
1	A	195	MET
1	A	196	SER
1	A	214	LEU
1	A	216	LEU
1	A	220	SER
1	A	221	LEU
1	A	246	ARG
1	A	247	ARG
1	A	251	LEU
1	A	255	VAL
1	A	270	ILE
1	A	274	ARG
1	A	281	LEU
1	A	291	GLN
1	A	295	PHE
1	A	296	ARG
1	A	304	ASP
1	A	309	SER
1	A	311	THR
1	A	317	ASN
1	A	324	LEU
1	A	325	GLN
1	A	327	LEU
1	A	330	VAL
1	A	332	LYS

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Mol	Chain	Res	Type
1	A	333	ASP
1	A	347	SER
1	A	352	SER
1	A	353	LEU
1	A	355	SER
1	A	356	ARG
1	A	360	LEU
1	A	364	ARG
1	A	376	GLU
1	A	380	LEU
1	A	386	LEU
1	A	389	GLU
1	A	398	MET
1	A	417	ARG
1	A	418	LEU
1	A	421	GLN
1	A	424	ARG
1	A	433	ARG
1	A	437	LEU
1	A	438	THR
1	A	441	LEU
1	A	451	ILE
1	A	467	THR
1	A	478	LYS
1	A	485	ARG
1	A	499	GLN
1	A	504	THR
1	A	505	THR
1	A	512	SER
1	A	514	ASN
1	A	516	LYS
1	A	524	LEU
1	A	525	ARG
1	A	534	ARG
1	A	536	LEU
1	A	538	LYS
1	A	539	LEU
1	B	9	LEU
1	B	11	ARG
1	B	18	ARG
1	B	20	ILE
1	B	29	VAL

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Mol	Chain	Res	Type
1	B	45	ARG
1	B	53	LYS
1	B	60	LEU
1	B	61	ASP
1	B	65	PHE
1	B	75	THR
1	B	88	PRO
1	B	90	ARG
1	B	93	SER
1	B	102	TRP
1	B	115	LEU
1	B	129	SER
1	B	136	ARG
1	B	149	MET
1	B	155	THR
1	B	166	GLU
1	B	168	PRO
1	B	178	LEU
1	B	180	LEU
1	B	183	VAL
1	B	195	MET
1	B	196	SER
1	B	214	LEU
1	B	216	LEU
1	B	220	SER
1	B	221	LEU
1	B	246	ARG
1	B	247	ARG
1	B	251	LEU
1	B	255	VAL
1	B	270	ILE
1	B	274	ARG
1	B	281	LEU
1	B	291	GLN
1	B	295	PHE
1	B	296	ARG
1	B	304	ASP
1	B	309	SER
1	B	311	THR
1	B	317	ASN
1	B	324	LEU
1	B	325	GLN

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Mol	Chain	Res	Type
1	B	327	LEU
1	B	330	VAL
1	B	332	LYS
1	B	333	ASP
1	B	347	SER
1	B	352	SER
1	B	353	LEU
1	B	355	SER
1	B	356	ARG
1	B	360	LEU
1	B	364	ARG
1	B	376	GLU
1	B	380	LEU
1	B	386	LEU
1	B	389	GLU
1	B	398	MET
1	B	417	ARG
1	B	418	LEU
1	B	421	GLN
1	B	424	ARG
1	B	433	ARG
1	B	437	LEU
1	B	438	THR
1	B	441	LEU
1	B	451	ILE
1	B	467	THR
1	B	478	LYS
1	B	485	ARG
1	B	499	GLN
1	B	504	THR
1	B	505	THR
1	B	512	SER
1	B	514	ASN
1	B	516	LYS
1	B	524	LEU
1	B	525	ARG
1	B	534	ARG
1	B	536	LEU
1	B	538	LYS
1	B	539	LEU
1	C	9	LEU
1	C	11	ARG

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Mol	Chain	Res	Type
1	C	18	ARG
1	C	20	ILE
1	C	29	VAL
1	C	45	ARG
1	C	53	LYS
1	C	60	LEU
1	C	61	ASP
1	C	65	PHE
1	C	75	THR
1	C	90	ARG
1	C	93	SER
1	C	102	TRP
1	C	115	LEU
1	C	129	SER
1	C	136	ARG
1	C	149	MET
1	C	155	THR
1	C	166	GLU
1	C	168	PRO
1	C	178	LEU
1	C	180	LEU
1	C	183	VAL
1	C	195	MET
1	C	196	SER
1	C	214	LEU
1	C	216	LEU
1	C	220	SER
1	C	221	LEU
1	C	246	ARG
1	C	247	ARG
1	C	251	LEU
1	C	255	VAL
1	C	270	ILE
1	C	274	ARG
1	C	281	LEU
1	C	291	GLN
1	C	295	PHE
1	C	296	ARG
1	C	304	ASP
1	C	309	SER
1	C	311	THR
1	C	317	ASN

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Mol	Chain	Res	Type
1	C	324	LEU
1	C	325	GLN
1	C	327	LEU
1	C	330	VAL
1	C	332	LYS
1	C	333	ASP
1	C	347	SER
1	C	352	SER
1	C	353	LEU
1	C	355	SER
1	C	356	ARG
1	C	360	LEU
1	C	364	ARG
1	C	376	GLU
1	C	380	LEU
1	C	386	LEU
1	C	389	GLU
1	C	398	MET
1	C	417	ARG
1	C	418	LEU
1	C	421	GLN
1	C	424	ARG
1	C	433	ARG
1	C	437	LEU
1	C	438	THR
1	C	441	LEU
1	C	451	ILE
1	C	467	THR
1	C	478	LYS
1	C	485	ARG
1	C	499	GLN
1	C	504	THR
1	C	505	THR
1	C	512	SER
1	C	514	ASN
1	C	516	LYS
1	C	524	LEU
1	C	525	ARG
1	C	534	ARG
1	C	536	LEU
1	C	538	LYS
1	C	539	LEU

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Mol	Chain	Res	Type
1	D	9	LEU
1	D	11	ARG
1	D	18	ARG
1	D	20	ILE
1	D	29	VAL
1	D	45	ARG
1	D	53	LYS
1	D	60	LEU
1	D	61	ASP
1	D	65	PHE
1	D	75	THR
1	D	90	ARG
1	D	93	SER
1	D	102	TRP
1	D	115	LEU
1	D	129	SER
1	D	136	ARG
1	D	149	MET
1	D	155	THR
1	D	166	GLU
1	D	168	PRO
1	D	178	LEU
1	D	180	LEU
1	D	183	VAL
1	D	195	MET
1	D	196	SER
1	D	214	LEU
1	D	216	LEU
1	D	220	SER
1	D	221	LEU
1	D	246	ARG
1	D	247	ARG
1	D	251	LEU
1	D	255	VAL
1	D	270	ILE
1	D	274	ARG
1	D	281	LEU
1	D	291	GLN
1	D	295	PHE
1	D	296	ARG
1	D	304	ASP
1	D	309	SER

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Mol	Chain	Res	Type
1	D	311	THR
1	D	317	ASN
1	D	324	LEU
1	D	325	GLN
1	D	327	LEU
1	D	330	VAL
1	D	332	LYS
1	D	333	ASP
1	D	347	SER
1	D	352	SER
1	D	353	LEU
1	D	355	SER
1	D	356	ARG
1	D	360	LEU
1	D	364	ARG
1	D	376	GLU
1	D	380	LEU
1	D	386	LEU
1	D	389	GLU
1	D	398	MET
1	D	417	ARG
1	D	418	LEU
1	D	421	GLN
1	D	424	ARG
1	D	433	ARG
1	D	437	LEU
1	D	438	THR
1	D	441	LEU
1	D	451	ILE
1	D	467	THR
1	D	478	LYS
1	D	485	ARG
1	D	499	GLN
1	D	504	THR
1	D	505	THR
1	D	512	SER
1	D	514	ASN
1	D	516	LYS
1	D	524	LEU
1	D	525	ARG
1	D	534	ARG
1	D	536	LEU

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Mol	Chain	Res	Type
1	D	538	LYS
1	D	539	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	66	GLN
1	A	212	HIS
1	A	291	GLN
1	A	317	ASN
1	A	421	GLN
1	A	464	ASN
1	A	482	ASN
1	A	499	GLN
1	B	16	GLN
1	B	66	GLN
1	B	212	HIS
1	B	291	GLN
1	B	317	ASN
1	B	421	GLN
1	B	464	ASN
1	B	482	ASN
1	B	499	GLN
1	C	16	GLN
1	C	66	GLN
1	C	212	HIS
1	C	291	GLN
1	C	317	ASN
1	C	421	GLN
1	C	464	ASN
1	C	482	ASN
1	C	499	GLN
1	D	16	GLN
1	D	66	GLN
1	D	212	HIS
1	D	291	GLN
1	D	317	ASN
1	D	421	GLN
1	D	464	ASN
1	D	482	ASN
1	D	499	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.