Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 11:07 pm GMT

PDB ID	:	2C6S
Title	:	human adenovirus penton base 2 12 chimera
Authors	:	Zubieta, C.; Blanchoin, L.; Cusack, S.
Deposited on	:	2005-11-11
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

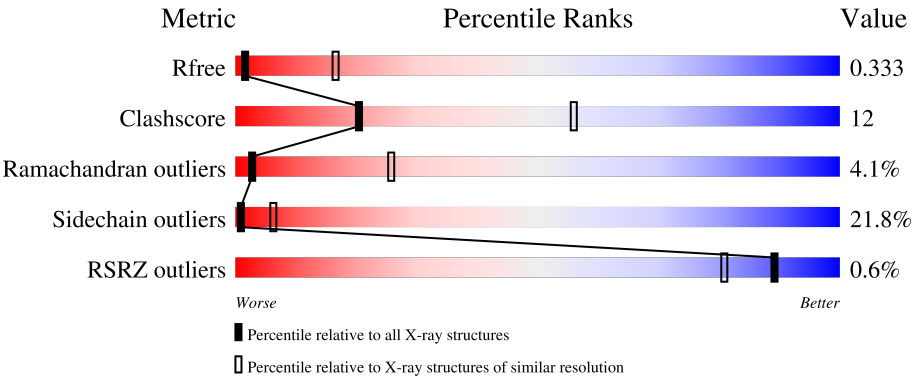
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	523	38% 33% 11% 15%
1	B	523	35% 34% 13% 15%
1	C	523	38% 33% 10% 15%
1	D	523	41% 28% 12% 15%
1	E	523	37% 33% 12% 15%

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Mol	Chain	Length	Quality of chain
1	F	523	38% 32% 12% 15%
1	G	523	38% 31% 13% 15%
1	H	523	38% 31% 13% 15%
1	I	523	37% 34% 11% 15%
1	J	523	37% 33% 12% 15%
1	K	523	33% 33% 15% 15%
1	L	523	34% 34% 13% 15%
1	M	523	38% 33% 12% 15%
1	N	523	36% 34% 11% 15%
1	O	523	37% 33% 12% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 53010 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 ADENOVIRUS 2,12 PENTON BASE CHIMERA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	B	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	C	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	D	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	E	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	F	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	G	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	H	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	I	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	J	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	K	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	L	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	M	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	N	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			
1	O	444	Total	C	N	O	S	0	0	1
			3534	2235	611	676	12			

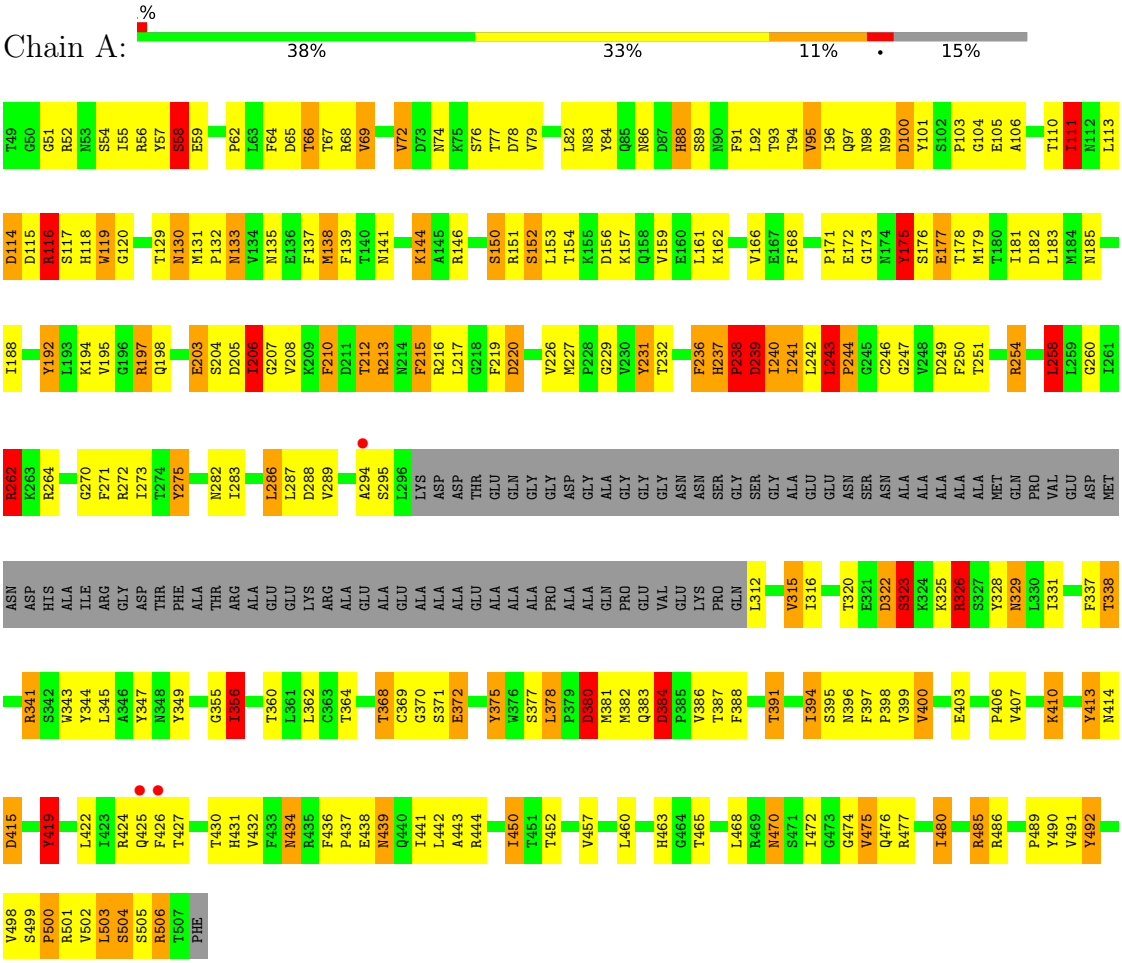
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	LEU	LYS	conflict	UNP P03276
B	312	LEU	LYS	conflict	UNP P03276
C	312	LEU	LYS	conflict	UNP P03276
D	312	LEU	LYS	conflict	UNP P03276
E	312	LEU	LYS	conflict	UNP P03276
F	312	LEU	LYS	conflict	UNP P03276
G	312	LEU	LYS	conflict	UNP P03276
H	312	LEU	LYS	conflict	UNP P03276
I	312	LEU	LYS	conflict	UNP P03276
J	312	LEU	LYS	conflict	UNP P03276
K	312	LEU	LYS	conflict	UNP P03276
L	312	LEU	LYS	conflict	UNP P03276
M	312	LEU	LYS	conflict	UNP P03276
N	312	LEU	LYS	conflict	UNP P03276
O	312	LEU	LYS	conflict	UNP P03276

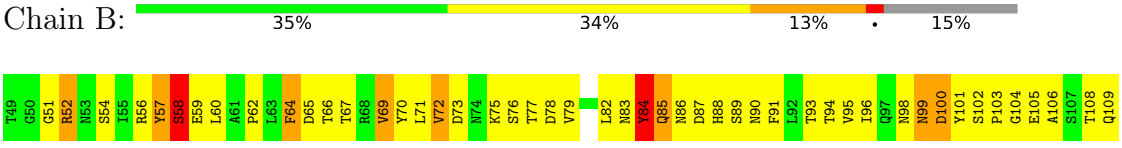
3 Residue-property plots (i)

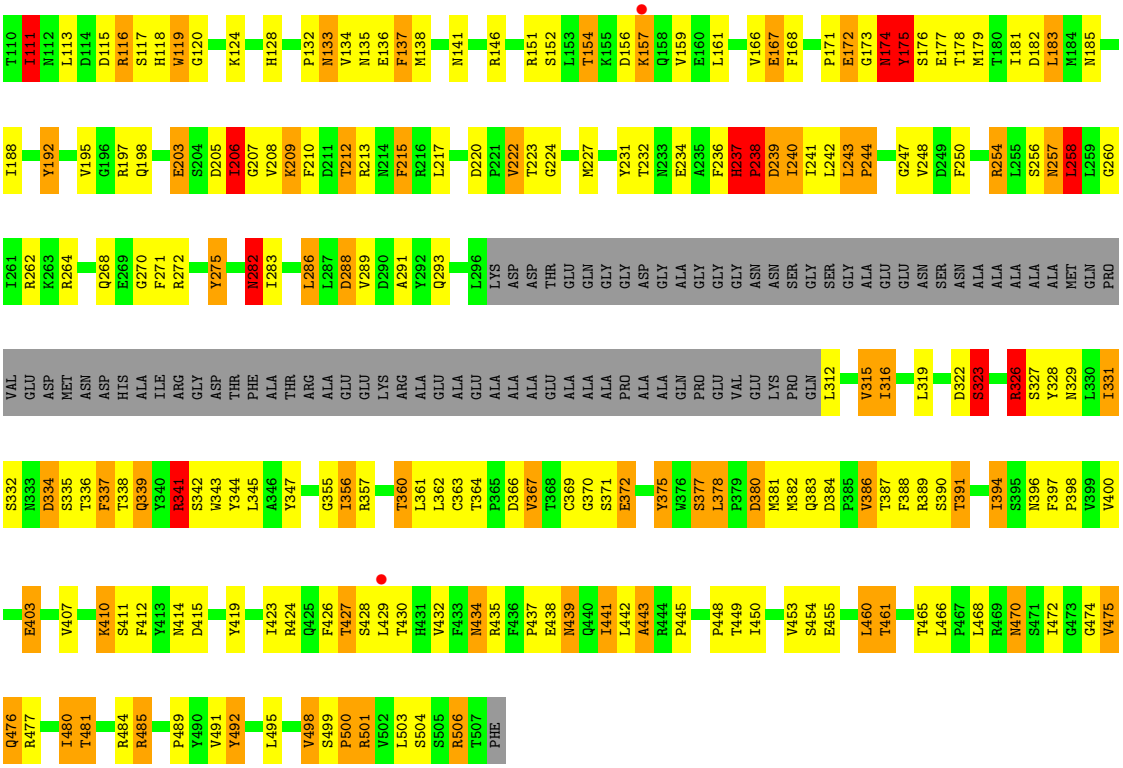
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ADENOVIRUS 2,12 PENTON BASE CHIMERA



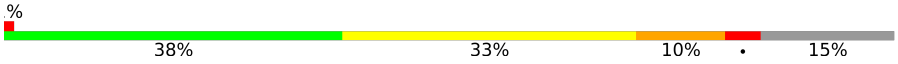
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

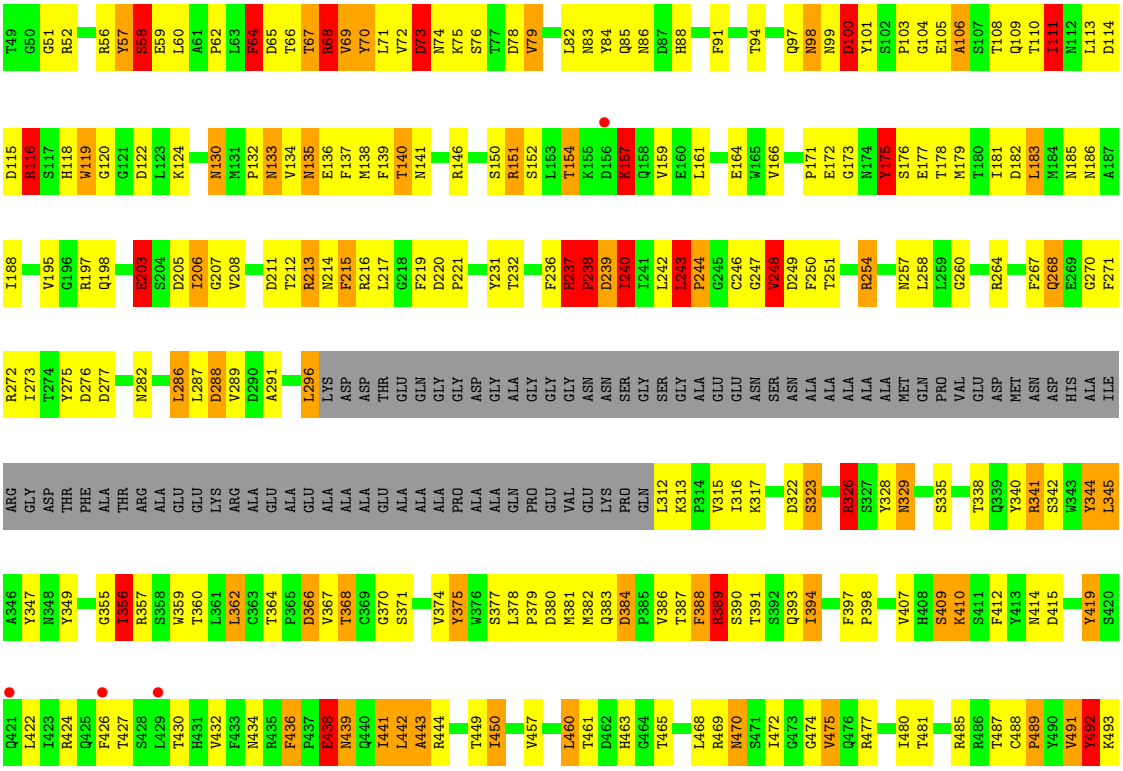


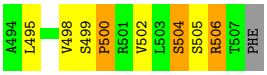


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain C:

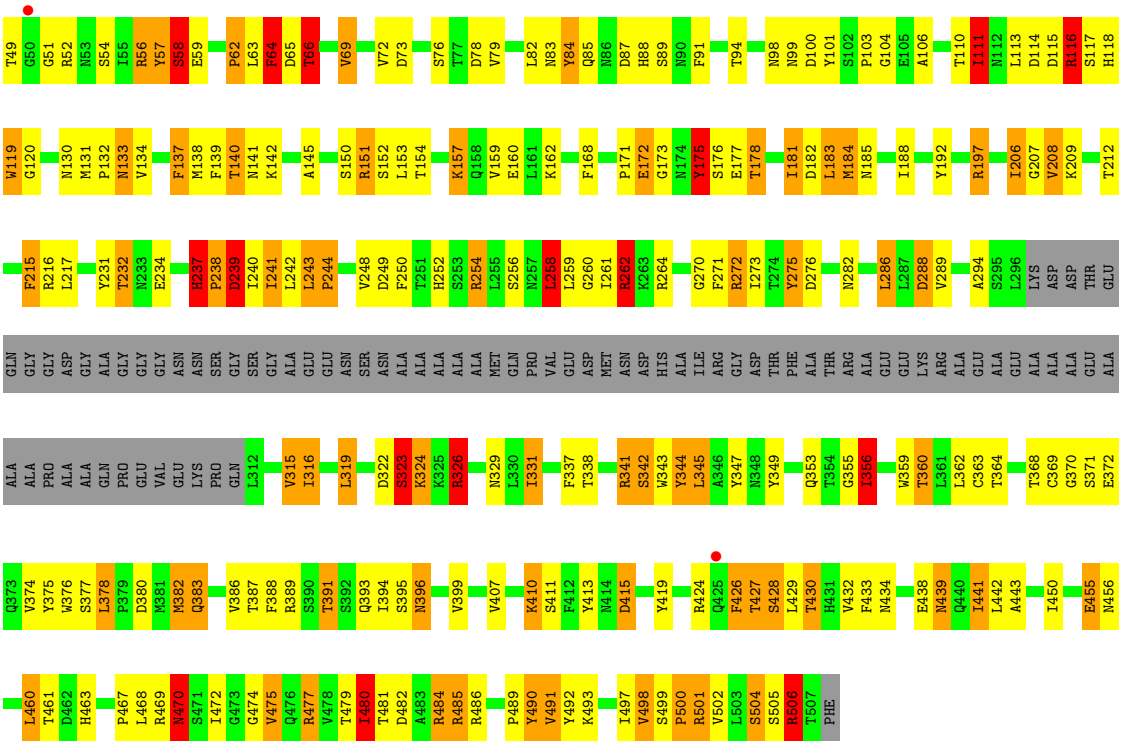






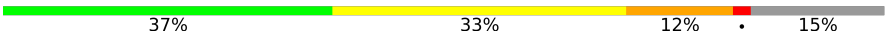
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

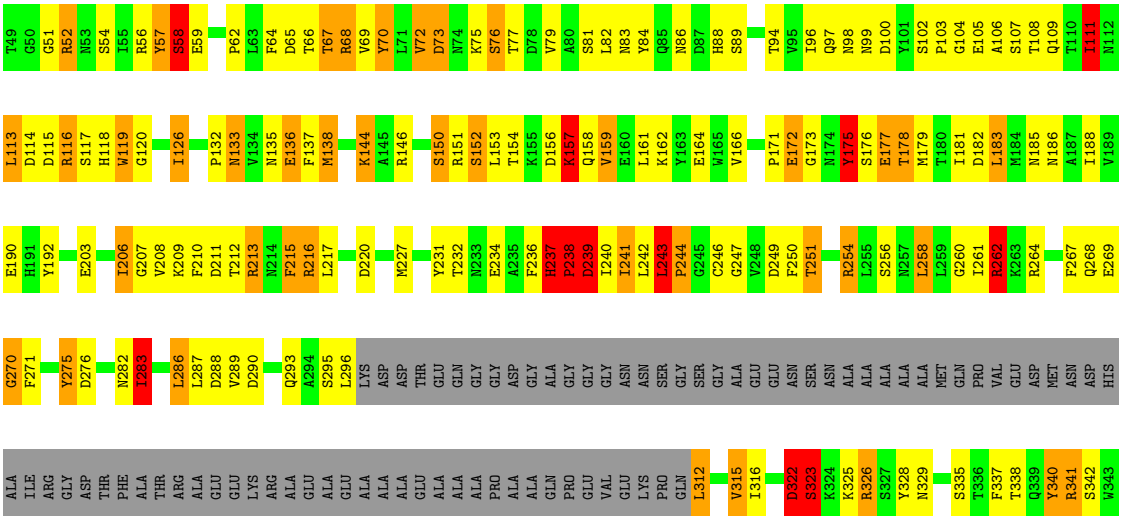
Chain D:



• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain E:





Y344 L345 A346 Y347 Q353 T354 G355 I356 W359 T360 L361 L362 C363 T364 P365 D366 V367 T368 C369 G370 S371 E372 Q373 V374 Y375 W376 S377 L378 M381 M382 Q383 D384 P385 V386 T387 F388 R389 S390 T391 S392 Q393 I394 S395 N396 F397 P398 A402 E403 L404 V407 H408 S409 K410 Y419

S420 Q421 L422 I423 R424 Q425 F426 T427 S428 L429 T430 H431 V432 F433 N434 R435 N439 Q440 I441 L442 A443 P448 T449 I450 T451 T452 L460 T461 L466 R469 N470 S471 I472 G473 G474 V475 Q476 R477 T481 D482 A483 R484 R485 R486 T487 C488 P489 Y490 V491 Y492 L495 V498

S499 P500 R501 V502 L503 S504 S505 R506 T507 PHE

• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain F: 38% 32% 12% • 15%

T49 G50 G51 R52 R56 Y57 S58 E59 P62 L63 F64 D65 T66 T67 R68 V69 Y70 L71 V72 D73 N74 K75 S76 T77 D78 L82 N83 Y84 Q85 N86 D87 H88 S89 N90 F91 L92 T93 T94 V95 I96 Q97 N98 N99 D100 Y101 S102 P103 G104 E105 A106 Q109 T110 I111 N112 L113 D114

D115 R116 S117 H118 W119 G120 P132 N133 V134 N135 E136 F137 M138 F139 T140 N141 V147 S150 R151 S152 L153 T154 K155 D156 K157 Q158 L161 E164 W165 V166 E167 F168 P171 E172 G173 N174 Y175 S176 E177 T178 I181 D182 L183 N186 H191 Y192 L193 K194 V195 G196 R197

Q198 L202 E203 I206 G207 T212 R213 N214 F215 R216 L217 G218 F219 D220 P221 V222 M227 Y231 T232 F236 H237 P238 D239 I240 I241 L242 L243 P244 V248 D249 F250 T251 R254 N257 L258 L259 G260 I261 R262 K263 R264 Q265 G270 F271 Y275 L278 N282

L286 L287 D288 V289 Y292 Q293 A294 S295 L296 LYS ASP ASP THR GLU GLN GLY GLY ASP GLY ALA GLY GLY GLY ASN ASN SER GLY SER GLY ALA GLU GLU ASN SER ASN ALA ALA ALA ALA ALA MET GLN PRO VAL GLU ASP MET ASN ASP HIS ALA ILE ARG GLY ASP THR PHE ALA

THR ARG ALA GLU GLU LYS ARG ALA GLU ALA GLU ALA ALA ALA GLU ALA ALA ALA PRO ALA ALA GLN PRO GLU VAL GLU LYS PRO GLN L312 V315 I316 K317 P318 L319 T320 E321 D322 S323 K324 K325 R326 S327 Y328 N329 L330 I331 S332 N333 D334 S335 T336 F337 T338 Q339 Y340 R341 Y344

L345 A346 Y347 D351 G355 I356 R357 S358 W359 T360 L361 L362 C363 T364 V367 T368 C369 G370 S371 E372 Q373 V374 Y375 W376 S377 L378 M381 M382 Q383 D384 P385 V386 T387 F388 R389 S390 T391 I394 S395 N396 F397 P398 A402 V407 K410 Y413 Y419 S420 Q421 L422

I423 R424 Q425 F426 T427 S428 L429 T430 H431 V432 F433 N434 R435 F436 P437 E438 N439 Q440 I441 L442 A443 R444 T449 I450 T451 T452 V453 S454 L460 T461 D462 H463 G464 T465 L466 P467 L468 R469 N470 S471 I472 G473 G474 V475 Q476 R477 I480 T481 R485 R486 T487 C488 P489 Y490 V491 Y492

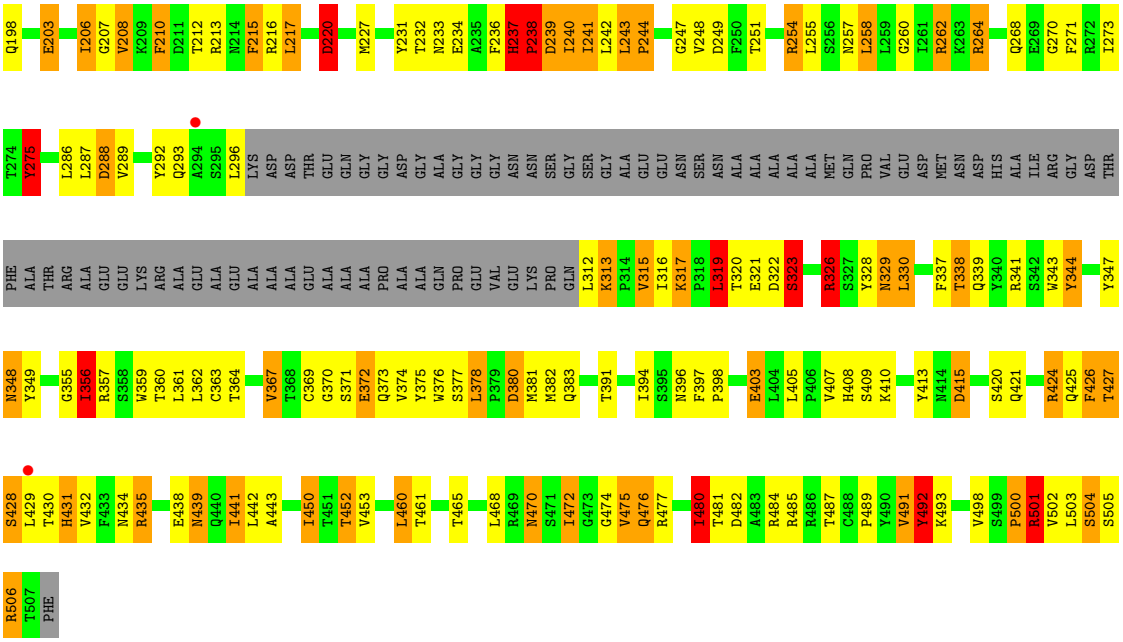
K493 V498 S499 P500 R501 V502 L503 S504 S505 R506 T507 PHE

• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain G: 38% 31% 13% • 15%

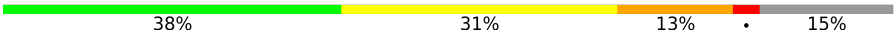
T49 G50 G51 R52 I55 R56 Y57 S58 E59 L60 A61 P62 L63 F64 D65 T66 T67 R68 V69 Y70 L71 V72 D73 N74 K75 S76 T77 D78 V79 L82 N83 Y84 Q85 N86 D87 H88 S89 N90 F91 L92 T93 T94 V95 I96 Q97 N98 N99 D100 Y101 S102 P103 G104 E105 A106 Q109 T110 I111

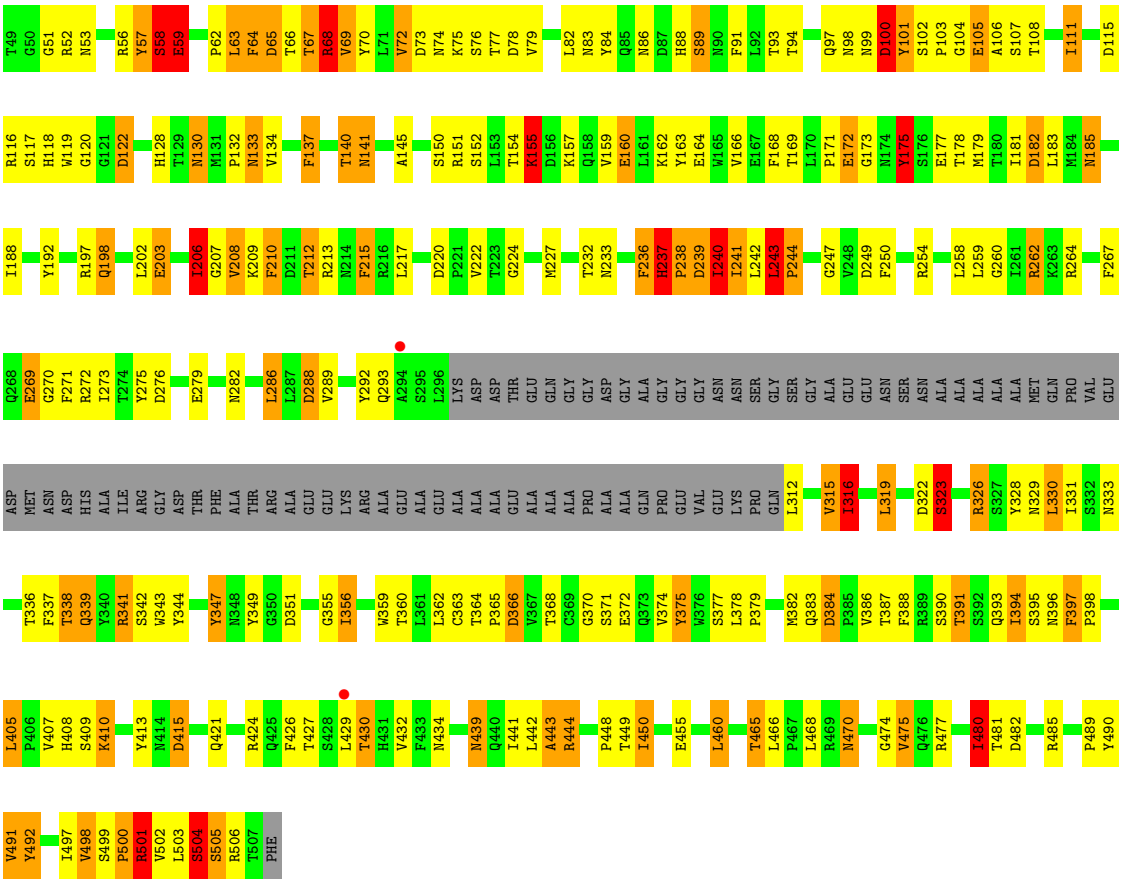
N112 L113 H118 W119 G120 H128 T129 N130 M131 P132 N133 V134 N135 E136 F137 M138 F139 T140 N141 K142 F143 S150 R151 S152 L153 T154 K155 D156 K157 Q158 V159 E160 L161 V166 T169 L170 P171 E172 G173 N174 Y175 S176 E177 I181 D182 L183 M184 N185 I188 Y192 R197



• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

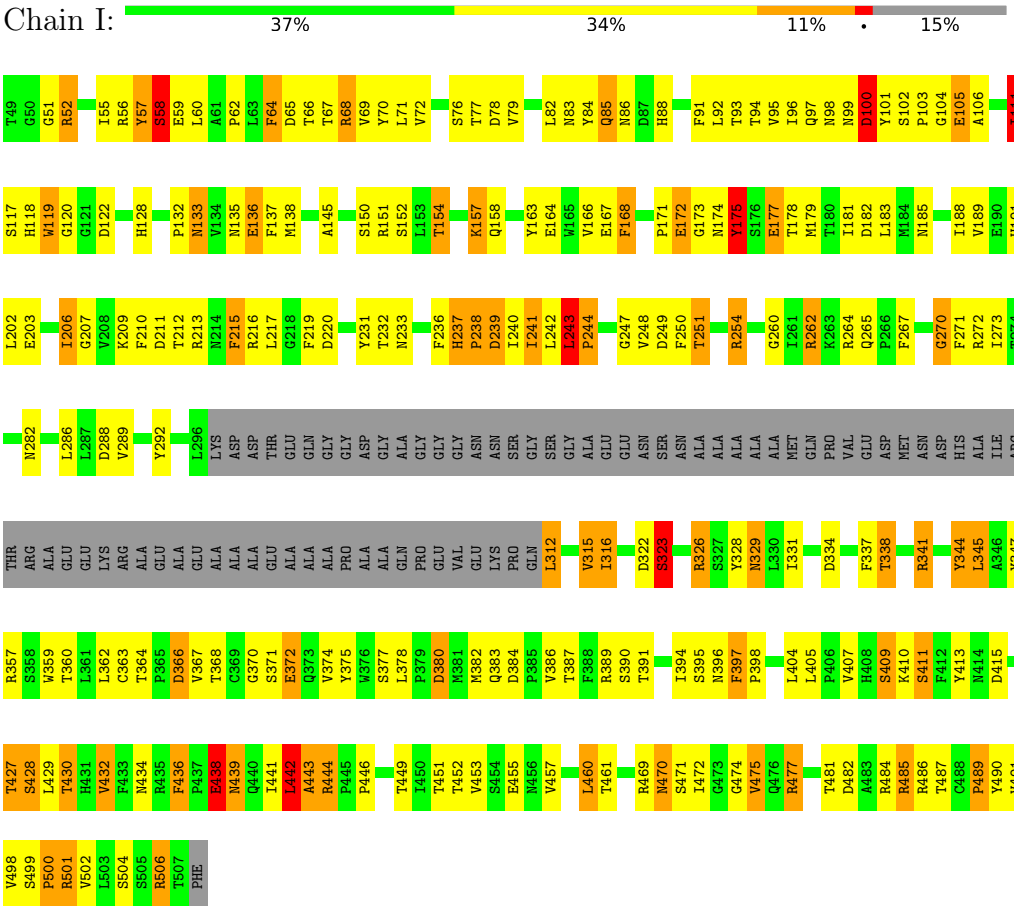
Chain H:





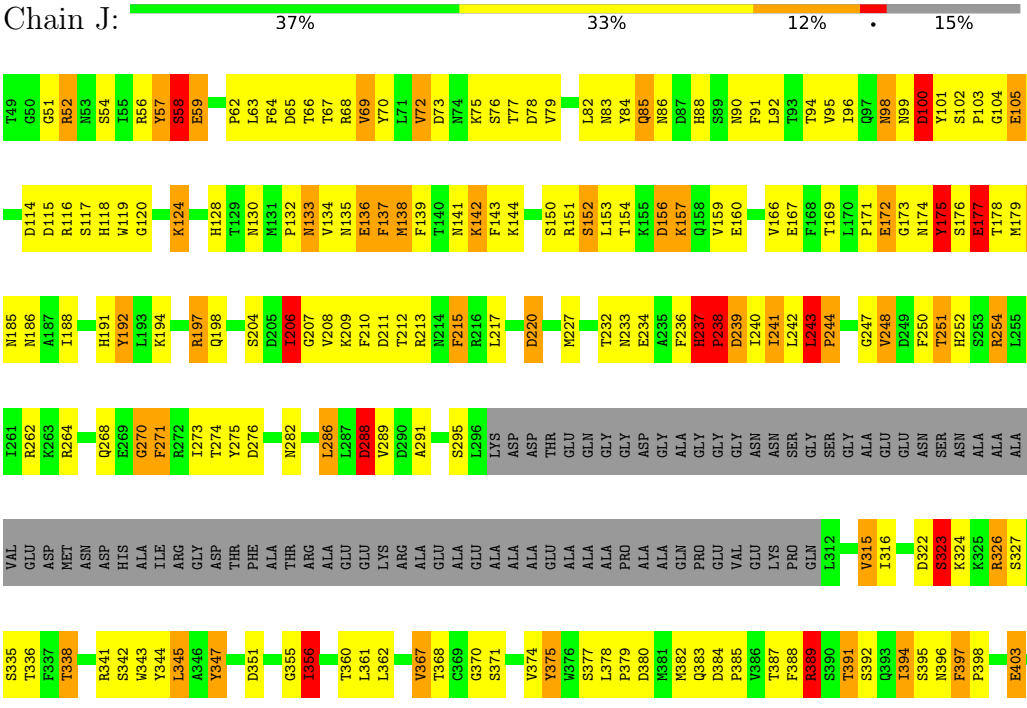
• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

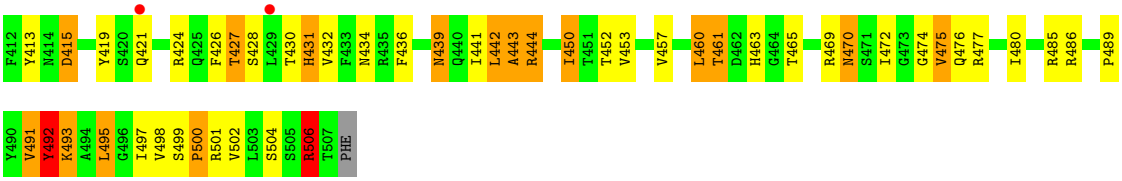
Chain I:



• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

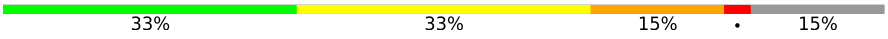
Chain J:

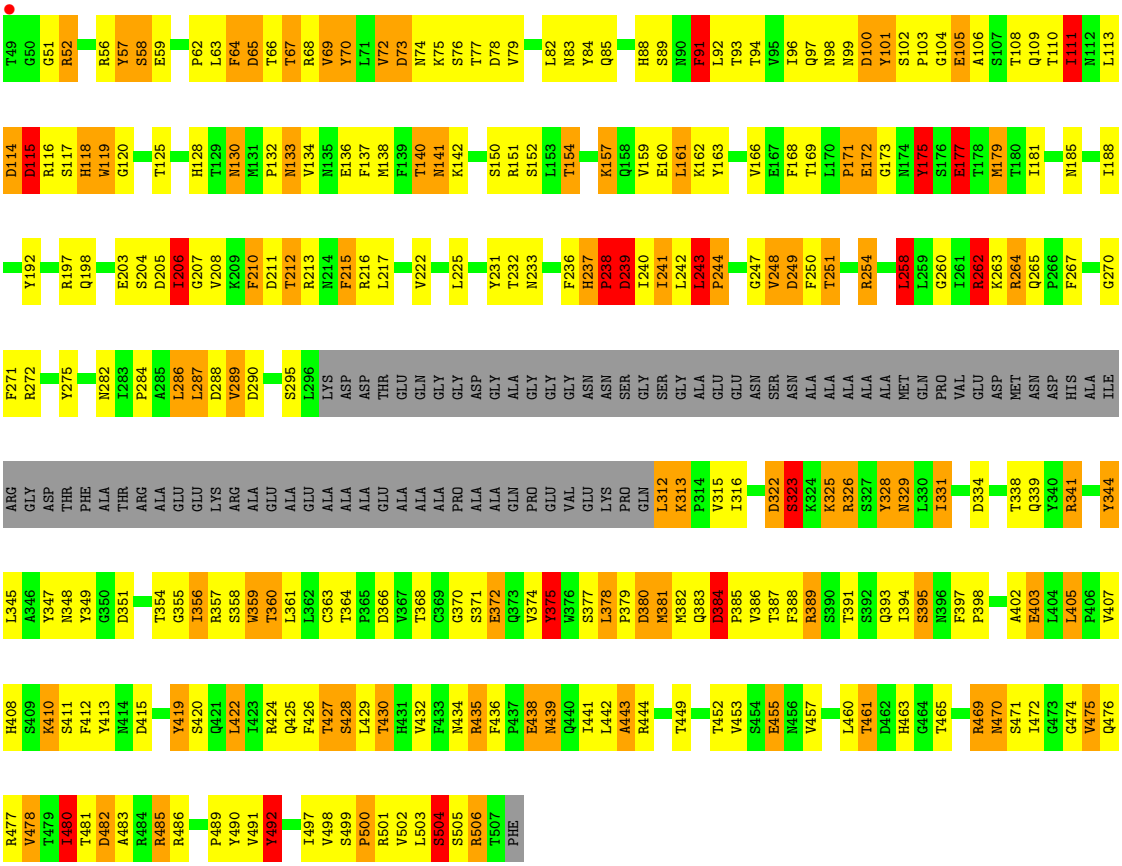




• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

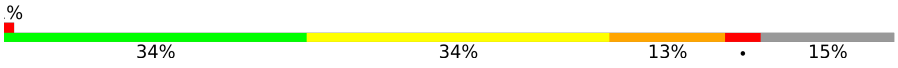
Chain K:

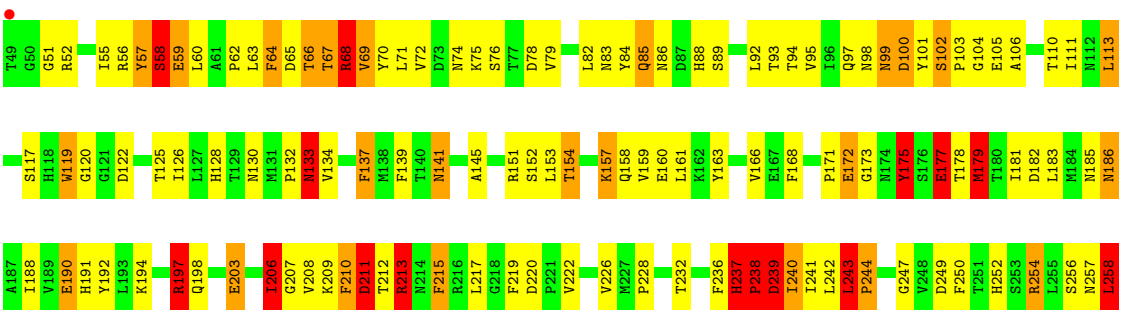


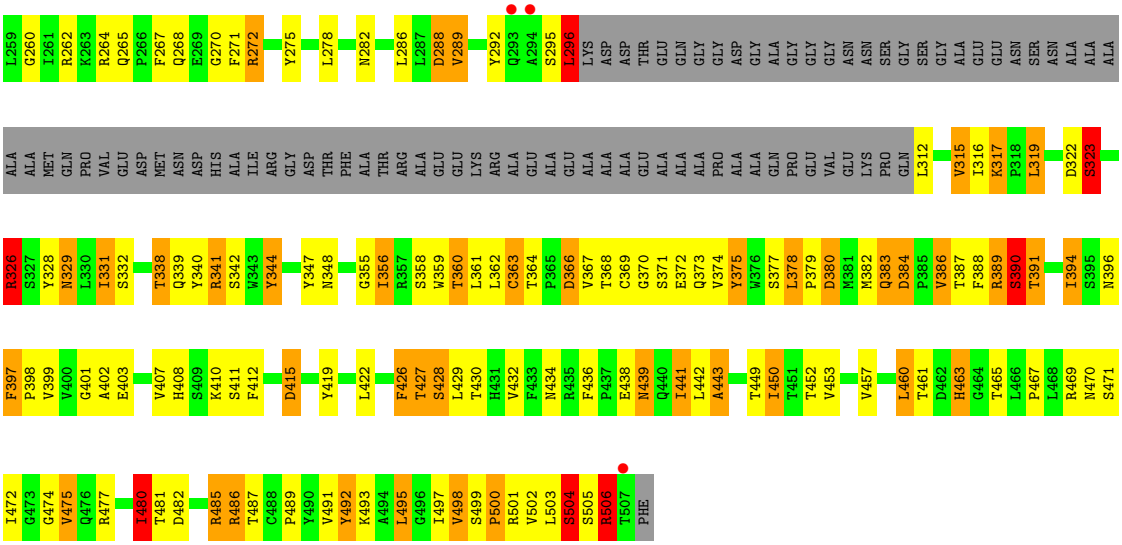


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain L:

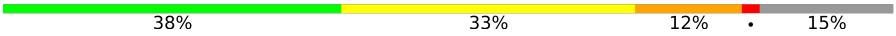


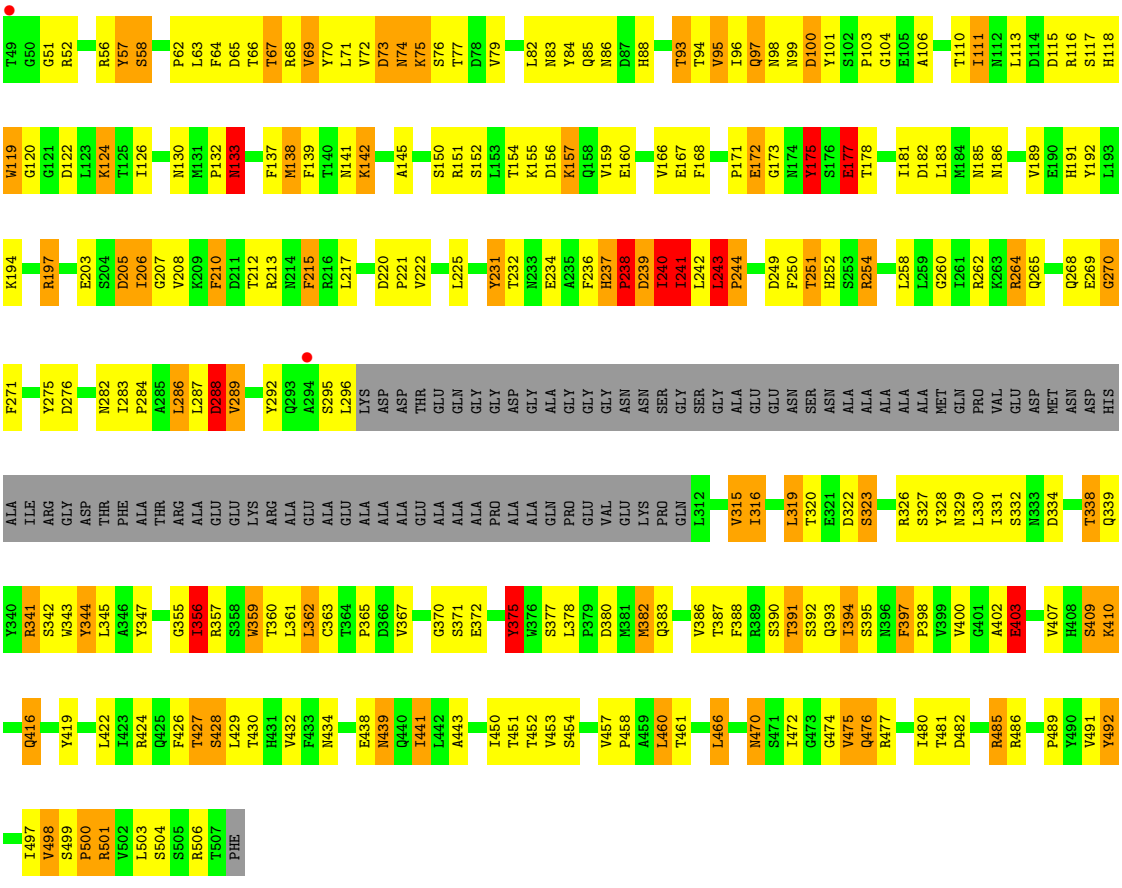




• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

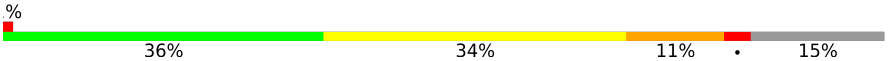
Chain M:

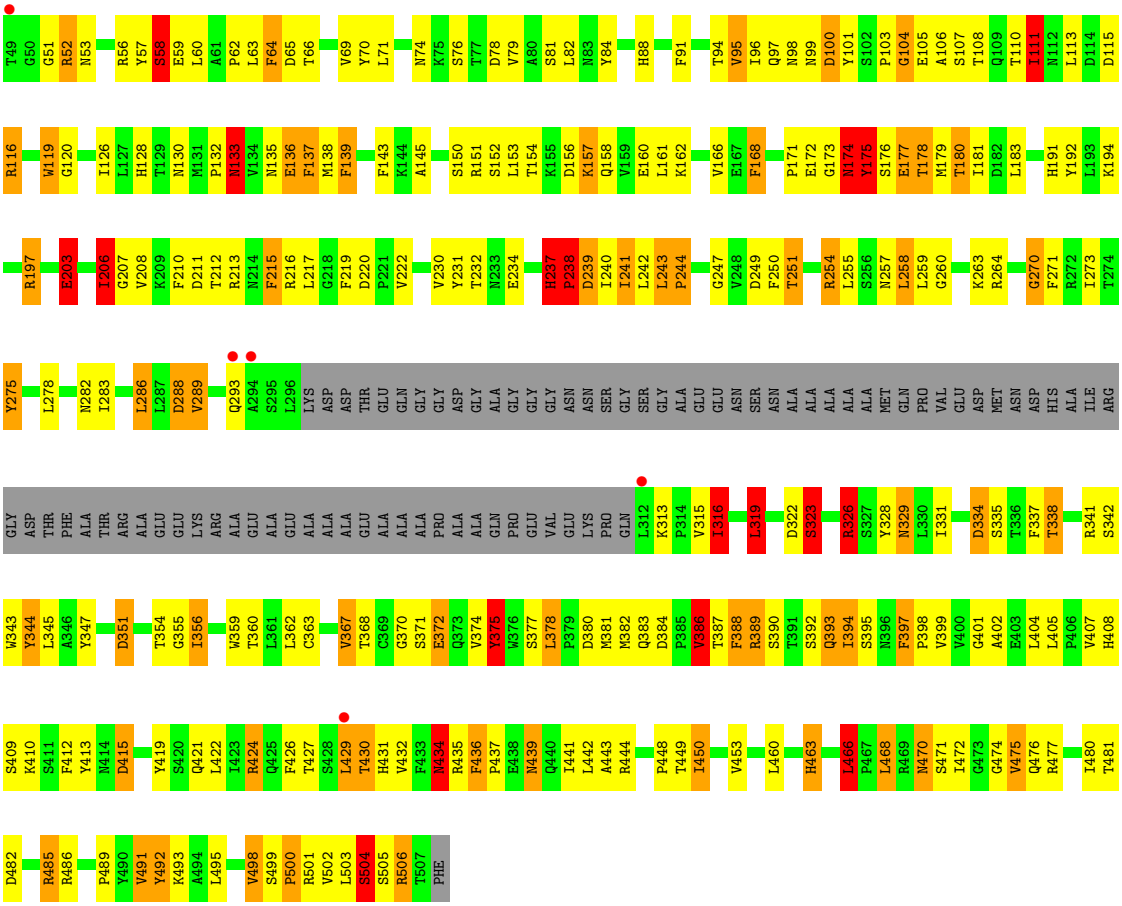




• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

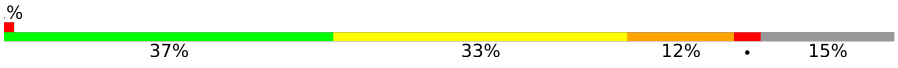
Chain N:

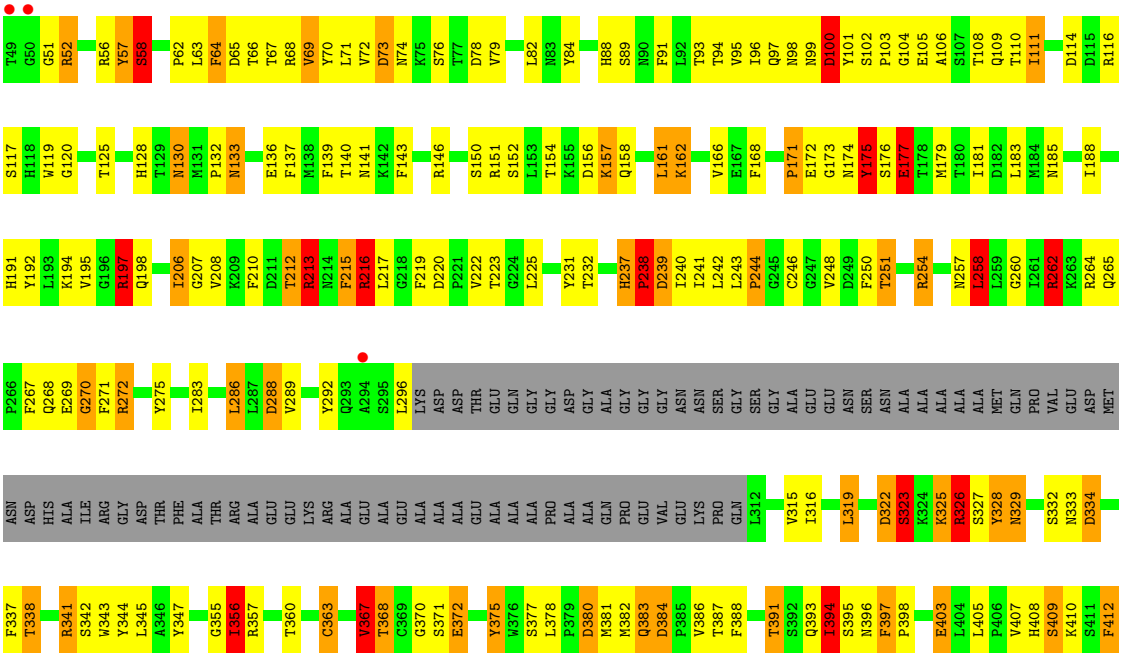


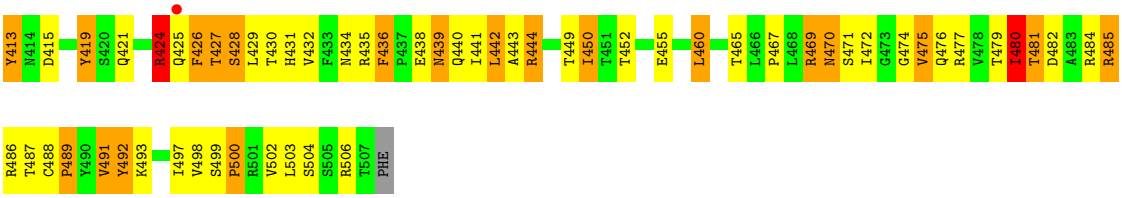


• Molecule 1: ADENOVIRUS 2,12 PENTON BASE CHIMERA

Chain O:






Y413 N414 D415 Y419 S420 Q421 R424 Q425 F426 T427 S428 L429 T430 H431 V432 F433 N434 R435 F436 P437 E438 N439 Q440 I441 L442 A443 R444 T449 I450 T451 T452 E455 L460 T465 L466 P467 L468 R469 N470 S471 I472 G473 G474 V475 Q476 R477 V478 T479 I480 T481 D482 A483 R484 R485

R486 T487 C488 P489 Y490 V491 Y492 K493 I497 V498 S499 P500 R501 V502 L503 S504 S505 R506 T507 PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	266.50Å 292.90Å 307.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.60 15.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.60) 89.3 (15.00-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.275 , 0.340 0.277 , 0.333	Depositor DCC
R_{free} test set	3041 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	131.0	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	53010	wwPDB-VP
Average B, all atoms (Å^2)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	6/3617 (0.2%)	1.06	13/4926 (0.3%)
1	B	1.23	23/3617 (0.6%)	1.17	16/4926 (0.3%)
1	C	1.17	16/3617 (0.4%)	1.11	21/4926 (0.4%)
1	D	1.06	13/3617 (0.4%)	1.11	21/4926 (0.4%)
1	E	1.08	9/3617 (0.2%)	1.09	13/4926 (0.3%)
1	F	1.20	20/3617 (0.6%)	1.13	20/4926 (0.4%)
1	G	1.16	21/3617 (0.6%)	1.11	19/4926 (0.4%)
1	H	1.05	13/3617 (0.4%)	1.09	18/4926 (0.4%)
1	I	0.96	5/3617 (0.1%)	1.07	12/4926 (0.2%)
1	J	1.03	9/3617 (0.2%)	1.06	13/4926 (0.3%)
1	K	1.12	20/3617 (0.6%)	1.11	20/4926 (0.4%)
1	L	1.07	17/3617 (0.5%)	1.09	20/4926 (0.4%)
1	M	1.25	24/3617 (0.7%)	1.12	17/4926 (0.3%)
1	N	1.11	19/3617 (0.5%)	1.11	16/4926 (0.3%)
1	O	1.31	26/3617 (0.7%)	1.17	22/4926 (0.4%)
All	All	1.13	241/54255 (0.4%)	1.11	261/73890 (0.4%)

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	109
1	B	0	105
1	C	0	111
1	D	0	107
1	E	0	103
1	F	0	108
1	G	0	113
1	H	0	114
1	I	0	115
1	J	0	112

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	119
1	L	0	115
1	M	0	105
1	N	0	116
1	O	0	115
All	All	0	1667

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	372	GLU	CD-OE1	28.94	1.57	1.25
1	A	372	GLU	CD-OE2	27.62	1.56	1.25
1	C	157	LYS	CE-NZ	23.22	2.07	1.49
1	C	157	LYS	CD-CE	19.96	2.01	1.51
1	F	194	LYS	CE-NZ	19.88	1.98	1.49
1	B	167	GLU	CD-OE1	19.26	1.46	1.25
1	M	403	GLU	CD-OE2	19.18	1.46	1.25
1	N	372	GLU	CD-OE2	19.09	1.46	1.25
1	F	326	ARG	CZ-NH1	18.69	1.57	1.33
1	G	220	ASP	CG-OD2	18.61	1.68	1.25
1	G	317	LYS	CD-CE	16.65	1.92	1.51
1	M	124	LYS	CD-CE	16.27	1.92	1.51
1	B	167	GLU	CG-CD	16.18	1.76	1.51
1	O	403	GLU	CD-OE1	16.00	1.43	1.25
1	D	324	LYS	CE-NZ	15.53	1.87	1.49
1	E	190	GLU	CD-OE1	15.17	1.42	1.25
1	M	142	LYS	CD-CE	15.12	1.89	1.51
1	O	455	GLU	CD-OE1	14.84	1.42	1.25
1	L	203	GLU	CD-OE2	14.79	1.42	1.25
1	B	146	ARG	CZ-NH1	14.44	1.51	1.33
1	B	424	ARG	CZ-NH1	14.38	1.51	1.33
1	F	194	LYS	CD-CE	14.09	1.86	1.51
1	E	144	LYS	CE-NZ	14.03	1.84	1.49
1	M	142	LYS	CE-NZ	13.60	1.83	1.49
1	O	269	GLU	CD-OE2	13.59	1.40	1.25
1	K	325	LYS	CE-NZ	13.29	1.82	1.49
1	F	203	GLU	CD-OE2	12.83	1.39	1.25
1	A	144	LYS	CE-NZ	12.70	1.80	1.49
1	O	325	LYS	CD-CE	12.69	1.82	1.51
1	L	317	LYS	CD-CE	12.68	1.82	1.51
1	B	424	ARG	CZ-NH2	12.35	1.49	1.33
1	E	216	ARG	CZ-NH1	12.27	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	216	ARG	CZ-NH1	12.00	1.48	1.33
1	M	124	LYS	CE-NZ	11.97	1.78	1.49
1	H	366	ASP	CG-OD2	11.94	1.52	1.25
1	E	157	LYS	CD-CE	11.90	1.80	1.51
1	J	124	LYS	CD-CE	11.63	1.80	1.51
1	O	421	GLN	CD-NE2	11.48	1.61	1.32
1	M	416	GLN	CD-OE1	11.43	1.49	1.24
1	F	100	ASP	CG-OD2	10.87	1.50	1.25
1	K	455	GLU	CD-OE1	10.85	1.37	1.25
1	B	167	GLU	CD-OE2	10.80	1.37	1.25
1	I	366	ASP	CG-OD2	10.78	1.50	1.25
1	K	313	LYS	CG-CD	10.75	1.89	1.52
1	C	130	ASN	CG-OD1	10.72	1.47	1.24
1	H	59	GLU	CD-OE1	10.57	1.37	1.25
1	O	162	LYS	CD-CE	10.54	1.77	1.51
1	H	421	GLN	CD-NE2	10.53	1.59	1.32
1	K	290	ASP	CG-OD2	10.39	1.49	1.25
1	O	424	ARG	CZ-NH1	10.31	1.46	1.33
1	H	269	GLU	CD-OE2	10.27	1.36	1.25
1	M	424	ARG	CZ-NH1	10.25	1.46	1.33
1	J	100	ASP	CG-OD2	10.12	1.48	1.25
1	C	164	GLU	CD-OE2	10.10	1.36	1.25
1	J	142	LYS	CD-CE	10.09	1.76	1.51
1	L	366	ASP	CG-OD2	10.03	1.48	1.25
1	N	326	ARG	CZ-NH2	9.96	1.46	1.33
1	G	421	GLN	CD-NE2	9.72	1.57	1.32
1	O	425	GLN	CG-CD	9.57	1.73	1.51
1	G	313	LYS	CG-CD	9.55	1.84	1.52
1	F	372	GLU	CD-OE1	9.55	1.36	1.25
1	L	411	SER	CB-OG	9.49	1.54	1.42
1	E	366	ASP	CG-OD2	9.44	1.47	1.25
1	G	339	GLN	CD-OE1	9.42	1.44	1.24
1	M	124	LYS	CG-CD	9.31	1.84	1.52
1	N	203	GLU	CD-OE2	9.28	1.35	1.25
1	E	269	GLU	CD-OE2	9.25	1.35	1.25
1	G	100	ASP	CG-OD2	9.19	1.46	1.25
1	N	263	LYS	CD-CE	9.13	1.74	1.51
1	K	101	TYR	CD2-CE2	9.08	1.52	1.39
1	C	157	LYS	CG-CD	9.07	1.83	1.52
1	H	101	TYR	CD2-CE2	8.84	1.52	1.39
1	L	102	SER	CB-OG	8.83	1.53	1.42
1	G	372	GLU	CD-OE1	8.75	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ASN	CG-ND2	8.73	1.54	1.32
1	F	197	ARG	CZ-NH1	8.60	1.44	1.33
1	N	100	ASP	CG-OD2	8.54	1.45	1.25
1	N	421	GLN	CD-OE1	8.54	1.42	1.24
1	F	197	ARG	CZ-NH2	8.54	1.44	1.33
1	K	435	ARG	CZ-NH1	8.48	1.44	1.33
1	C	366	ASP	CG-OD2	8.46	1.44	1.25
1	F	372	GLU	CD-OE2	8.44	1.34	1.25
1	M	416	GLN	CD-NE2	8.43	1.53	1.32
1	B	84	TYR	CD2-CE2	8.42	1.51	1.39
1	N	421	GLN	CD-NE2	8.36	1.53	1.32
1	C	164	GLU	CD-OE1	8.31	1.34	1.25
1	K	263	LYS	CD-CE	8.30	1.72	1.51
1	M	167	GLU	CD-OE1	8.21	1.34	1.25
1	B	84	TYR	CE1-CZ	8.18	1.49	1.38
1	N	372	GLU	CD-OE1	8.13	1.34	1.25
1	K	366	ASP	CG-OD2	8.12	1.44	1.25
1	H	155	LYS	CE-NZ	8.08	1.69	1.49
1	N	326	ARG	CZ-NH1	8.04	1.43	1.33
1	A	146	ARG	CZ-NH1	7.96	1.43	1.33
1	B	341	ARG	CZ-NH1	7.96	1.43	1.33
1	F	174	ASN	CG-OD1	7.95	1.41	1.24
1	D	363	CYS	CB-SG	-7.83	1.69	1.82
1	F	372	GLU	CG-CD	7.78	1.63	1.51
1	F	454	SER	CB-OG	7.77	1.52	1.42
1	C	384	ASP	CG-OD2	7.68	1.43	1.25
1	C	393	GLN	CD-OE1	7.65	1.40	1.24
1	B	137	PHE	CE1-CZ	7.64	1.51	1.37
1	J	124	LYS	CG-CD	7.54	1.78	1.52
1	G	424	ARG	CZ-NH1	7.51	1.42	1.33
1	K	313	LYS	CB-CG	7.47	1.72	1.52
1	M	403	GLU	CG-CD	7.45	1.63	1.51
1	O	326	ARG	CZ-NH1	7.40	1.42	1.33
1	M	339	GLN	CD-OE1	7.39	1.40	1.24
1	B	293	GLN	CD-NE2	7.39	1.51	1.32
1	O	220	ASP	CG-OD2	7.38	1.42	1.25
1	O	431	HIS	CG-CD2	7.33	1.48	1.35
1	O	216	ARG	CD-NE	7.27	1.58	1.46
1	G	425	GLN	CD-NE2	7.26	1.50	1.32
1	K	422	LEU	CG-CD1	7.23	1.78	1.51
1	N	372	GLU	CB-CG	7.18	1.65	1.52
1	M	424	ARG	CD-NE	7.17	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	414	ASN	CG-ND2	7.16	1.50	1.32
1	G	421	GLN	CD-OE1	7.11	1.39	1.24
1	F	203	GLU	CD-OE1	7.07	1.33	1.25
1	K	290	ASP	CG-OD1	7.07	1.41	1.25
1	N	372	GLU	CG-CD	7.01	1.62	1.51
1	B	372	GLU	CD-OE1	7.00	1.33	1.25
1	D	455	GLU	CG-CD	6.99	1.62	1.51
1	O	269	GLU	CD-OE1	6.87	1.33	1.25
1	E	209	LYS	CE-NZ	6.84	1.66	1.49
1	L	359	TRP	CE3-CZ3	6.81	1.50	1.38
1	J	59	GLU	CD-OE1	6.72	1.33	1.25
1	B	339	GLN	CD-NE2	6.61	1.49	1.32
1	K	422	LEU	CG-CD2	6.59	1.76	1.51
1	O	326	ARG	CZ-NH2	6.54	1.41	1.33
1	F	372	GLU	CB-CG	6.53	1.64	1.52
1	O	158	GLN	CD-OE1	6.50	1.38	1.24
1	I	359	TRP	CE3-CZ3	6.50	1.49	1.38
1	M	74	ASN	CG-ND2	6.44	1.49	1.32
1	M	269	GLU	CD-OE1	6.41	1.32	1.25
1	C	130	ASN	CB-CG	6.39	1.65	1.51
1	H	339	GLN	CD-OE1	6.39	1.38	1.24
1	B	424	ARG	NE-CZ	6.38	1.41	1.33
1	L	190	GLU	CD-OE2	6.38	1.32	1.25
1	D	142	LYS	CD-CE	6.38	1.67	1.51
1	J	142	LYS	CE-NZ	6.37	1.65	1.49
1	G	425	GLN	CG-CD	6.32	1.65	1.51
1	K	263	LYS	CE-NZ	6.32	1.64	1.49
1	O	425	GLN	CD-NE2	6.31	1.48	1.32
1	G	317	LYS	CE-NZ	6.28	1.64	1.49
1	J	421	GLN	CD-NE2	6.23	1.48	1.32
1	D	142	LYS	CE-NZ	6.23	1.64	1.49
1	G	372	GLU	CD-OE2	6.17	1.32	1.25
1	N	359	TRP	CE3-CZ3	6.17	1.49	1.38
1	F	339	GLN	CD-NE2	6.16	1.48	1.32
1	M	416	GLN	CB-CG	6.15	1.69	1.52
1	K	359	TRP	CE3-CZ3	6.14	1.48	1.38
1	G	413	TYR	CD2-CE2	6.11	1.48	1.39
1	B	366	ASP	CG-OD2	6.10	1.39	1.25
1	B	167	GLU	CB-CG	6.08	1.63	1.52
1	M	100	ASP	CG-OD1	6.04	1.39	1.25
1	H	59	GLU	CG-CD	6.03	1.60	1.51
1	H	444	ARG	CZ-NH2	6.03	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	197	ARG	CZ-NH1	6.03	1.40	1.33
1	M	403	GLU	CB-CG	6.03	1.63	1.52
1	C	317	LYS	CD-CE	6.02	1.66	1.51
1	O	425	GLN	CB-CG	6.01	1.68	1.52
1	G	425	GLN	CB-CG	6.00	1.68	1.52
1	F	462	ASP	CG-OD2	6.00	1.39	1.25
1	E	359	TRP	CE3-CZ3	5.99	1.48	1.38
1	L	137	PHE	CE1-CZ	5.98	1.48	1.37
1	L	429	LEU	CG-CD2	5.96	1.74	1.51
1	M	160	GLU	CD-OE2	5.96	1.32	1.25
1	O	194	LYS	CD-CE	5.94	1.66	1.51
1	O	413	TYR	CE2-CZ	5.94	1.46	1.38
1	C	203	GLU	CD-OE2	5.93	1.32	1.25
1	J	444	ARG	CZ-NH1	5.88	1.40	1.33
1	B	174	ASN	CG-OD1	5.86	1.36	1.24
1	A	425	GLN	CG-CD	5.85	1.64	1.51
1	M	240	ILE	CB-CG2	-5.80	1.34	1.52
1	F	137	PHE	CD2-CE2	5.79	1.50	1.39
1	F	339	GLN	CG-CD	5.78	1.64	1.51
1	D	455	GLU	CB-CG	5.75	1.63	1.52
1	J	137	PHE	CE1-CZ	5.74	1.48	1.37
1	N	203	GLU	CG-CD	5.66	1.60	1.51
1	L	429	LEU	CG-CD1	5.64	1.72	1.51
1	M	288	ASP	CG-OD2	5.57	1.38	1.25
1	G	84	TYR	CD2-CE2	5.56	1.47	1.39
1	B	240	ILE	CB-CG2	-5.54	1.35	1.52
1	D	324	LYS	CD-CE	5.54	1.65	1.51
1	K	372	GLU	CD-OE1	5.52	1.31	1.25
1	E	421	GLN	CD-NE2	5.51	1.46	1.32
1	O	424	ARG	NE-CZ	5.51	1.40	1.33
1	I	136	GLU	CD-OE1	5.49	1.31	1.25
1	L	190	GLU	CD-OE1	5.49	1.31	1.25
1	D	376	TRP	CB-CG	-5.47	1.40	1.50
1	G	349	TYR	CD2-CE2	5.47	1.47	1.39
1	L	375	TYR	CE2-CZ	5.43	1.45	1.38
1	I	372	GLU	CD-OE1	5.39	1.31	1.25
1	B	414	ASN	CG-OD1	5.38	1.35	1.24
1	N	139	PHE	CE1-CZ	5.37	1.47	1.37
1	M	167	GLU	CD-OE2	5.37	1.31	1.25
1	H	137	PHE	CD2-CE2	5.36	1.50	1.39
1	O	216	ARG	CZ-NH2	5.34	1.40	1.33
1	L	317	LYS	CE-NZ	5.34	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	349	TYR	CE2-CZ	5.32	1.45	1.38
1	N	316	ILE	CA-CB	5.31	1.67	1.54
1	A	438	GLU	CB-CG	5.30	1.62	1.52
1	C	359	TRP	CE3-CZ3	5.29	1.47	1.38
1	B	337	PHE	CE2-CZ	5.26	1.47	1.37
1	G	403	GLU	CG-CD	5.26	1.59	1.51
1	L	100	ASP	CG-OD2	5.25	1.37	1.25
1	D	84	TYR	CD1-CE1	5.25	1.47	1.39
1	F	421	GLN	CD-NE2	5.25	1.46	1.32
1	H	269	GLU	CG-CD	5.24	1.59	1.51
1	D	137	PHE	CD1-CE1	5.23	1.49	1.39
1	M	100	ASP	CG-OD2	5.22	1.37	1.25
1	H	240	ILE	CB-CG2	-5.22	1.36	1.52
1	C	240	ILE	CB-CG2	-5.21	1.36	1.52
1	K	59	GLU	CD-OE1	5.21	1.31	1.25
1	O	363	CYS	CB-SG	-5.19	1.73	1.81
1	K	375	TYR	CE2-CZ	5.18	1.45	1.38
1	L	59	GLU	CD-OE2	5.18	1.31	1.25
1	I	275	TYR	CD2-CE2	5.18	1.47	1.39
1	K	366	ASP	CB-CG	5.17	1.62	1.51
1	A	403	GLU	CG-CD	5.16	1.59	1.51
1	M	359	TRP	CE3-CZ3	5.16	1.47	1.38
1	C	268	GLN	CD-OE1	5.15	1.35	1.24
1	K	455	GLU	CB-CG	5.13	1.61	1.52
1	F	175	TYR	CE2-CZ	5.12	1.45	1.38
1	D	137	PHE	CB-CG	5.11	1.60	1.51
1	G	359	TRP	CE3-CZ3	5.11	1.47	1.38
1	K	115	ASP	CB-CG	5.11	1.62	1.51
1	C	488	CYS	CB-SG	-5.10	1.73	1.81
1	H	359	TRP	CE3-CZ3	5.10	1.47	1.38
1	N	334	ASP	CG-OD2	5.10	1.37	1.25
1	D	64	PHE	CE2-CZ	5.08	1.47	1.37
1	B	484	ARG	CG-CD	5.08	1.64	1.51
1	O	372	GLU	CG-CD	5.08	1.59	1.51
1	N	203	GLU	CB-CG	5.06	1.61	1.52
1	L	190	GLU	CG-CD	5.05	1.59	1.51
1	D	359	TRP	CE3-CZ3	5.04	1.47	1.38
1	N	137	PHE	CE1-CZ	5.04	1.47	1.37
1	L	137	PHE	CE2-CZ	5.04	1.47	1.37
1	G	376	TRP	CB-CG	-5.03	1.41	1.50
1	O	413	TYR	CD2-CE2	5.03	1.46	1.39

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	424	ARG	NE-CZ-NH2	-26.19	107.20	120.30
1	F	197	ARG	NE-CZ-NH2	-17.45	111.58	120.30
1	N	326	ARG	NE-CZ-NH2	-17.36	111.62	120.30
1	O	326	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	O	216	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	O	424	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	G	100	ASP	CB-CG-OD2	-11.65	107.82	118.30
1	B	424	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	G	220	ASP	CB-CG-OD2	-11.19	108.23	118.30
1	F	100	ASP	CB-CG-OD2	-10.53	108.82	118.30
1	M	100	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	F	194	LYS	CD-CE-NZ	-10.20	88.25	111.70
1	G	424	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	N	466	LEU	CB-CG-CD1	-9.63	94.62	111.00
1	C	157	LYS	CG-CD-CE	-9.54	83.26	111.90
1	F	372	GLU	OE1-CD-OE2	-9.38	112.05	123.30
1	B	146	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	C	157	LYS	CD-CE-NZ	-8.93	91.17	111.70
1	N	197	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	E	216	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	B	146	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	I	506	ARG	O-C-N	-8.35	109.35	122.70
1	H	444	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	D	175	TYR	CB-CG-CD1	-8.23	116.06	121.00
1	O	220	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	J	100	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	D	239	ASP	CB-CG-OD1	-7.94	111.16	118.30
1	G	317	LYS	CD-CE-NZ	-7.84	93.66	111.70
1	E	366	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	G	312	LEU	CA-CB-CG	7.56	132.68	115.30
1	H	269	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	E	312	LEU	CA-CB-CG	7.51	132.57	115.30
1	L	312	LEU	CA-CB-CG	7.41	132.35	115.30
1	C	422	LEU	CA-CB-CG	7.41	132.34	115.30
1	L	506	ARG	O-C-N	-7.40	110.86	122.70
1	A	258	LEU	CA-CB-CG	7.31	132.10	115.30
1	B	460	LEU	CB-CG-CD1	7.30	123.41	111.00
1	M	142	LYS	CD-CE-NZ	-7.29	94.93	111.70
1	I	422	LEU	CA-CB-CG	7.26	131.99	115.30
1	G	506	ARG	O-C-N	-7.10	111.33	122.70
1	O	469	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	O	442	LEU	CA-CB-CG	7.00	131.39	115.30
1	K	405	LEU	CA-CB-CG	6.99	131.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	506	ARG	O-C-N	-6.96	111.57	122.70
1	F	429	LEU	CA-CB-CG	6.93	131.25	115.30
1	M	124	LYS	CG-CD-CE	-6.91	91.19	111.90
1	F	442	LEU	CA-CB-CG	6.90	131.17	115.30
1	M	175	TYR	CA-CB-CG	6.89	126.49	113.40
1	C	312	LEU	CA-CB-CG	6.87	131.11	115.30
1	N	372	GLU	OE1-CD-OE2	-6.84	115.09	123.30
1	M	63	LEU	CA-CB-CG	6.84	131.03	115.30
1	K	313	LYS	CB-CG-CD	-6.82	93.88	111.60
1	H	503	LEU	CA-CB-CG	6.81	130.96	115.30
1	L	363	CYS	CA-CB-SG	6.80	126.24	114.00
1	E	258	LEU	CA-CB-CG	6.78	130.90	115.30
1	K	238	PRO	CA-C-N	-6.74	102.38	117.20
1	D	175	TYR	CA-CB-CG	6.73	126.18	113.40
1	M	429	LEU	CA-CB-CG	6.73	130.77	115.30
1	M	403	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	H	238	PRO	CA-C-N	-6.67	102.52	117.20
1	D	183	LEU	CA-CB-CG	6.66	130.63	115.30
1	C	130	ASN	CB-CG-OD1	-6.65	108.29	121.60
1	F	262	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	C	258	LEU	CA-CB-CG	6.65	130.59	115.30
1	M	460	LEU	CB-CG-CD1	6.64	122.30	111.00
1	C	345	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	312	LEU	CA-CB-CG	6.63	130.55	115.30
1	H	78	ASP	CB-CG-OD2	6.62	124.25	118.30
1	I	100	ASP	CB-CG-OD1	6.61	124.25	118.30
1	K	258	LEU	CA-CB-CG	6.58	130.44	115.30
1	G	238	PRO	CA-C-N	-6.58	102.73	117.20
1	I	429	LEU	CA-CB-CG	6.57	130.41	115.30
1	C	243	LEU	CA-CB-CG	6.54	130.34	115.30
1	D	238	PRO	CA-C-N	-6.52	102.85	117.20
1	N	506	ARG	O-C-N	-6.51	112.29	122.70
1	G	175	TYR	CA-CB-CG	6.48	125.71	113.40
1	H	366	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	238	PRO	CA-C-N	-6.47	102.97	117.20
1	B	442	LEU	CA-CB-CG	6.45	130.12	115.30
1	L	238	PRO	CA-C-N	-6.44	103.04	117.20
1	J	361	LEU	CB-CG-CD2	-6.43	100.07	111.00
1	M	238	PRO	CA-C-N	-6.41	103.09	117.20
1	H	312	LEU	CA-CB-CG	6.40	130.02	115.30
1	O	238	PRO	CA-C-N	-6.38	103.16	117.20
1	O	71	LEU	CB-CG-CD1	-6.38	100.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	506	ARG	O-C-N	-6.36	112.53	122.70
1	D	324	LYS	CD-CE-NZ	-6.33	97.13	111.70
1	C	238	PRO	CA-C-N	-6.33	103.28	117.20
1	G	460	LEU	CA-CB-CG	6.31	129.81	115.30
1	F	238	PRO	CA-C-N	-6.31	103.33	117.20
1	N	238	PRO	CA-C-N	-6.29	103.37	117.20
1	O	161	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	238	PRO	CA-C-N	-6.27	103.41	117.20
1	J	243	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	243	LEU	CA-CB-CG	6.22	129.61	115.30
1	G	313	LYS	CB-CG-CD	-6.19	95.50	111.60
1	F	326	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	J	238	PRO	CA-C-N	-6.18	103.61	117.20
1	D	197	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	H	405	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	506	ARG	O-C-N	-6.14	112.88	122.70
1	N	429	LEU	CA-CB-CG	6.12	129.39	115.30
1	O	460	LEU	CB-CG-CD1	6.11	121.39	111.00
1	I	238	PRO	CA-C-N	-6.09	103.80	117.20
1	G	319	LEU	CA-CB-CG	6.07	129.26	115.30
1	E	238	PRO	CA-C-N	-6.07	103.85	117.20
1	L	243	LEU	CA-CB-CG	6.06	129.25	115.30
1	B	460	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	167	GLU	CB-CG-CD	-6.04	97.88	114.20
1	O	375	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	H	330	LEU	CA-CB-CG	6.02	129.14	115.30
1	G	429	LEU	CA-CB-CG	6.00	129.11	115.30
1	H	466	LEU	CB-CG-CD2	-6.00	100.81	111.00
1	F	194	LYS	CG-CD-CE	-5.98	93.95	111.90
1	H	501	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	C	68	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	J	175	TYR	CA-CB-CG	5.95	124.70	113.40
1	J	460	LEU	CA-CB-CG	5.95	128.98	115.30
1	K	312	LEU	CA-CB-CG	5.94	128.97	115.30
1	G	317	LYS	CG-CD-CE	-5.92	94.14	111.90
1	K	375	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	C	175	TYR	CA-CB-CG	5.91	124.63	113.40
1	M	422	LEU	CA-CB-CG	5.90	128.87	115.30
1	L	175	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	D	153	LEU	CA-CB-CG	5.88	128.83	115.30
1	O	325	LYS	CD-CE-NZ	-5.88	98.18	111.70
1	E	243	LEU	CA-CB-CG	5.87	128.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	124	LYS	CG-CD-CE	-5.86	94.31	111.90
1	H	175	TYR	CA-CB-CG	5.84	124.49	113.40
1	M	243	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	153	LEU	CA-CB-CG	5.83	128.70	115.30
1	G	71	LEU	CA-CB-CG	-5.82	101.93	115.30
1	E	262	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	151	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	D	237	HIS	C-N-CD	5.80	140.58	128.40
1	N	63	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	L	429	LEU	CA-CB-CG	5.76	128.54	115.30
1	H	243	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	262	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	M	288	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	A	384	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	K	243	LEU	CA-CB-CG	5.73	128.48	115.30
1	M	375	TYR	CB-CG-CD2	-5.69	117.58	121.00
1	C	492	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	K	435	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	M	205	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	L	460	LEU	CB-CG-CD1	5.65	120.60	111.00
1	I	243	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	135	ASN	N-CA-CB	-5.63	100.46	110.60
1	M	63	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	I	202	LEU	CA-CB-CG	5.63	128.24	115.30
1	F	422	LEU	CA-CB-CG	5.61	128.20	115.30
1	K	161	LEU	CA-CB-CG	5.61	128.19	115.30
1	L	460	LEU	CA-CB-CG	5.60	128.19	115.30
1	G	68	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	L	296	LEU	CA-CB-CG	5.58	128.15	115.30
1	L	495	LEU	CA-CB-CG	-5.57	102.50	115.30
1	E	404	LEU	CA-CB-CG	-5.53	102.57	115.30
1	N	389	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	O	506	ARG	O-C-N	-5.53	113.86	122.70
1	C	64	PHE	CB-CG-CD1	-5.52	116.93	120.80
1	F	197	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	K	469	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	O	197	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	L	386	VAL	CB-CA-C	-5.50	100.95	111.40
1	L	175	TYR	CA-CB-CG	5.49	123.82	113.40
1	B	341	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	389	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	L	258	LEU	CA-CB-CG	5.47	127.88	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	184	MET	CA-CB-CG	5.47	122.60	113.30
1	D	506	ARG	O-C-N	-5.47	113.95	122.70
1	N	386	VAL	CB-CA-C	-5.46	101.03	111.40
1	E	175	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	H	405	LEU	CB-CG-CD1	5.46	120.28	111.00
1	K	175	TYR	CA-CB-CG	5.45	123.75	113.40
1	B	258	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	429	LEU	CA-CB-CG	5.44	127.82	115.30
1	D	258	LEU	CA-CB-CG	5.44	127.81	115.30
1	L	100	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	L	179	MET	CG-SD-CE	5.44	108.90	100.20
1	G	161	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	237	HIS	C-N-CD	5.42	139.78	128.40
1	C	197	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	J	237	HIS	C-N-CD	5.40	139.75	128.40
1	L	237	HIS	C-N-CD	5.40	139.73	128.40
1	D	243	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	322	ASP	CB-CG-OD1	5.38	123.15	118.30
1	H	63	LEU	CA-CB-CG	5.38	127.67	115.30
1	M	296	LEU	CA-CB-CG	5.37	127.66	115.30
1	J	506	ARG	O-C-N	-5.36	114.12	122.70
1	H	429	LEU	CA-CB-CG	5.35	127.61	115.30
1	N	319	LEU	CA-CB-CG	5.35	127.61	115.30
1	N	100	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	F	243	LEU	CA-CB-CG	5.34	127.58	115.30
1	G	217	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	B	222	VAL	CB-CA-C	5.34	121.54	111.40
1	B	175	TYR	CA-CB-CG	5.33	123.53	113.40
1	K	442	LEU	CA-CB-CG	5.33	127.56	115.30
1	J	389	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	380	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	O	213	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	G	102	SER	CB-CA-C	-5.32	99.99	110.10
1	A	287	LEU	CA-CB-CG	5.32	127.54	115.30
1	K	175	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	N	375	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	K	380	ASP	CB-CA-C	5.31	121.02	110.40
1	E	68	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	J	345	LEU	CB-CG-CD2	5.30	120.01	111.00
1	O	258	LEU	CB-CG-CD1	5.29	120.00	111.00
1	K	290	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	N	63	LEU	CA-CB-CG	5.29	127.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	429	LEU	CA-CB-CG	5.29	127.46	115.30
1	F	68	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	429	LEU	CA-CB-CG	5.27	127.42	115.30
1	J	142	LYS	CD-CE-NZ	-5.27	99.57	111.70
1	D	485	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	O	100	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	E	237	HIS	C-N-CD	5.27	139.46	128.40
1	K	389	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	326	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	N	237	HIS	CB-CA-C	5.26	120.92	110.40
1	I	460	LEU	CB-CG-CD1	5.26	119.94	111.00
1	O	405	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	460	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	137	PHE	N-CA-CB	5.22	120.00	110.60
1	H	460	LEU	CB-CG-CD1	5.22	119.87	111.00
1	C	287	LEU	CA-CB-CG	5.21	127.29	115.30
1	A	506	ARG	O-C-N	-5.21	114.36	122.70
1	F	462	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	485	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	K	83	ASN	N-CA-CB	5.17	119.91	110.60
1	F	175	TYR	CA-CB-CG	5.17	123.21	113.40
1	E	157	LYS	CG-CD-CE	-5.16	96.42	111.90
1	I	312	LEU	CB-CA-C	5.16	120.00	110.20
1	J	237	HIS	CB-CA-C	5.15	120.70	110.40
1	A	503	LEU	CA-CB-CG	5.14	127.12	115.30
1	F	337	PHE	CB-CG-CD1	-5.12	117.21	120.80
1	D	345	LEU	CA-CB-CG	5.12	127.08	115.30
1	O	421	GLN	CG-CD-NE2	-5.12	104.41	116.70
1	L	153	LEU	CA-CB-CG	5.12	127.07	115.30
1	H	68	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	K	405	LEU	CB-CG-CD1	5.11	119.69	111.00
1	F	213	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	I	442	LEU	CA-CB-CG	5.10	127.04	115.30
1	K	429	LEU	CA-CB-CG	5.10	127.04	115.30
1	L	442	LEU	CA-CB-CG	5.10	127.03	115.30
1	G	330	LEU	CA-CB-CG	5.09	127.01	115.30
1	N	175	TYR	CA-CB-CG	5.09	123.06	113.40
1	K	366	ASP	CB-CG-OD1	5.08	122.88	118.30
1	I	175	TYR	CA-CB-CG	5.07	123.04	113.40
1	L	68	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	I	92	LEU	CA-CB-CG	5.07	126.95	115.30
1	M	441	ILE	CG1-CB-CG2	-5.06	100.26	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	161	LEU	CA-CB-CG	5.06	126.94	115.30
1	D	482	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	C	237	HIS	C-N-CD	5.03	138.97	128.40
1	O	326	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	460	LEU	CB-CG-CD1	5.03	119.55	111.00
1	C	366	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	237	HIS	CB-CA-C	5.01	120.42	110.40
1	O	63	LEU	CB-CG-CD2	-5.00	102.49	111.00

There are no chirality outliers.

All (1667) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ASP	Sidechain
1	A	101	TYR	Sidechain
1	A	103	PRO	Mainchain
1	A	104	GLY	Mainchain
1	A	106	ALA	Mainchain
1	A	111	ILE	Mainchain
1	A	114	ASP	Sidechain
1	A	116	ARG	Sidechain
1	A	118	HIS	Sidechain
1	A	119	TRP	Mainchain
1	A	132	PRO	Mainchain
1	A	137	PHE	Sidechain,Mainchain
1	A	139	PHE	Sidechain
1	A	151	ARG	Mainchain
1	A	168	PHE	Sidechain
1	A	171	PRO	Mainchain
1	A	173	GLY	Mainchain
1	A	175	TYR	Sidechain
1	A	177	GLU	Mainchain
1	A	178	THR	Mainchain
1	A	181	ILE	Mainchain
1	A	192	TYR	Mainchain
1	A	197	ARG	Mainchain
1	A	203	GLU	Mainchain
1	A	205	ASP	Sidechain
1	A	206	ILE	Mainchain
1	A	210	PHE	Sidechain
1	A	213	ARG	Sidechain
1	A	215	PHE	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	A	219	PHE	Sidechain
1	A	220	ASP	Sidechain
1	A	231	TYR	Sidechain
1	A	236	PHE	Sidechain
1	A	238	PRO	Mainchain
1	A	239	ASP	Sidechain
1	A	249	ASP	Sidechain
1	A	250	PHE	Sidechain
1	A	254	ARG	Mainchain
1	A	258	LEU	Mainchain
1	A	260	GLY	Mainchain
1	A	262	ARG	Sidechain
1	A	264	ARG	Mainchain
1	A	270	GLY	Mainchain
1	A	271	PHE	Sidechain
1	A	272	ARG	Sidechain
1	A	275	TYR	Sidechain
1	A	288	ASP	Mainchain
1	A	289	VAL	Mainchain
1	A	294	ALA	Mainchain
1	A	315	VAL	Mainchain
1	A	322	ASP	Mainchain
1	A	323	SER	Mainchain
1	A	326	ARG	Sidechain
1	A	328	TYR	Sidechain
1	A	329	ASN	Mainchain
1	A	337	PHE	Sidechain
1	A	338	THR	Mainchain
1	A	347	TYR	Sidechain
1	A	349	TYR	Sidechain
1	A	355	GLY	Mainchain
1	A	368	THR	Mainchain
1	A	371	SER	Mainchain
1	A	372	GLU	Mainchain
1	A	375	TYR	Sidechain
1	A	378	LEU	Peptide,Mainchain
1	A	380	ASP	Sidechain
1	A	383	GLN	Mainchain
1	A	384	ASP	Sidechain
1	A	391	THR	Mainchain
1	A	394	ILE	Mainchain
1	A	410	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	413	TYR	Sidechain
1	A	415	ASP	Mainchain
1	A	419	TYR	Sidechain
1	A	424	ARG	Sidechain
1	A	427	THR	Mainchain
1	A	431	HIS	Sidechain
1	A	436	PHE	Sidechain
1	A	439	ASN	Mainchain
1	A	441	ILE	Mainchain
1	A	463	HIS	Sidechain
1	A	485	ARG	Mainchain
1	A	486	ARG	Sidechain
1	A	489	PRO	Mainchain
1	A	492	TYR	Sidechain
1	A	500	PRO	Mainchain
1	A	504	SER	Mainchain
1	A	506	ARG	Sidechain,Mainchain
1	A	52	ARG	Mainchain
1	A	56	ARG	Sidechain,Mainchain
1	A	57	TYR	Sidechain
1	A	58	SER	Mainchain
1	A	62	PRO	Mainchain
1	A	64	PHE	Sidechain,Mainchain
1	A	76	SER	Mainchain
1	A	78	ASP	Sidechain
1	A	79	VAL	Mainchain
1	A	84	TYR	Sidechain,Mainchain
1	A	88	HIS	Sidechain
1	A	91	PHE	Sidechain
1	A	98	ASN	Mainchain
1	A	99	ASN	Mainchain
1	B	100	ASP	Sidechain
1	B	103	PRO	Mainchain
1	B	104	GLY	Mainchain
1	B	106	ALA	Mainchain
1	B	111	ILE	Mainchain
1	B	116	ARG	Sidechain
1	B	118	HIS	Sidechain
1	B	119	TRP	Mainchain
1	B	128	HIS	Sidechain
1	B	132	PRO	Mainchain
1	B	137	PHE	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	B	151	ARG	Mainchain
1	B	168	PHE	Sidechain
1	B	171	PRO	Mainchain
1	B	173	GLY	Mainchain
1	B	174	ASN	Sidechain
1	B	175	TYR	Sidechain
1	B	177	GLU	Mainchain
1	B	178	THR	Mainchain
1	B	181	ILE	Mainchain
1	B	182	ASP	Sidechain
1	B	192	TYR	Mainchain
1	B	205	ASP	Sidechain
1	B	206	ILE	Mainchain
1	B	210	PHE	Sidechain
1	B	215	PHE	Sidechain,Mainchain
1	B	231	TYR	Sidechain
1	B	234	GLU	Mainchain
1	B	236	PHE	Sidechain
1	B	238	PRO	Mainchain
1	B	250	PHE	Mainchain
1	B	254	ARG	Mainchain
1	B	257	ASN	Sidechain
1	B	258	LEU	Mainchain
1	B	260	GLY	Mainchain
1	B	264	ARG	Mainchain
1	B	270	GLY	Mainchain
1	B	271	PHE	Sidechain
1	B	272	ARG	Sidechain
1	B	275	TYR	Sidechain
1	B	282	ASN	Sidechain
1	B	288	ASP	Mainchain
1	B	289	VAL	Mainchain
1	B	315	VAL	Mainchain
1	B	322	ASP	Mainchain
1	B	323	SER	Mainchain
1	B	326	ARG	Sidechain
1	B	328	TYR	Sidechain
1	B	329	ASN	Mainchain
1	B	334	ASP	Sidechain
1	B	338	THR	Mainchain
1	B	347	TYR	Sidechain
1	B	355	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	B	357	ARG	Sidechain
1	B	367	VAL	Mainchain
1	B	371	SER	Mainchain
1	B	372	GLU	Sidechain,Mainchain
1	B	375	TYR	Sidechain
1	B	378	LEU	Peptide,Mainchain
1	B	383	GLN	Mainchain
1	B	388	PHE	Sidechain
1	B	389	ARG	Sidechain
1	B	390	SER	Mainchain
1	B	391	THR	Mainchain
1	B	394	ILE	Mainchain
1	B	403	GLU	Sidechain
1	B	410	LYS	Mainchain
1	B	412	PHE	Mainchain
1	B	427	THR	Mainchain
1	B	435	ARG	Sidechain
1	B	439	ASN	Mainchain
1	B	441	ILE	Mainchain
1	B	443	ALA	Mainchain
1	B	476	GLN	Sidechain
1	B	477	ARG	Mainchain
1	B	480	ILE	Mainchain
1	B	485	ARG	Sidechain,Mainchain
1	B	489	PRO	Mainchain
1	B	492	TYR	Sidechain
1	B	500	PRO	Mainchain
1	B	501	ARG	Sidechain
1	B	504	SER	Mainchain
1	B	506	ARG	Mainchain
1	B	52	ARG	Mainchain
1	B	56	ARG	Mainchain
1	B	57	TYR	Sidechain
1	B	58	SER	Mainchain
1	B	62	PRO	Mainchain
1	B	64	PHE	Sidechain,Mainchain
1	B	70	TYR	Sidechain
1	B	76	SER	Mainchain
1	B	78	ASP	Mainchain
1	B	79	VAL	Mainchain
1	B	84	TYR	Sidechain,Mainchain
1	B	90	ASN	Sidechain

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Mol	Chain	Res	Type	Group
1	B	91	PHE	Sidechain
1	B	98	ASN	Mainchain
1	B	99	ASN	Mainchain
1	C	100	ASP	Sidechain
1	C	101	TYR	Sidechain
1	C	103	PRO	Mainchain
1	C	104	GLY	Mainchain
1	C	106	ALA	Mainchain
1	C	111	ILE	Mainchain
1	C	116	ARG	Sidechain
1	C	118	HIS	Sidechain
1	C	119	TRP	Mainchain
1	C	130	ASN	Sidechain
1	C	132	PRO	Mainchain
1	C	137	PHE	Sidechain,Mainchain
1	C	139	PHE	Sidechain
1	C	151	ARG	Sidechain,Mainchain
1	C	171	PRO	Mainchain
1	C	173	GLY	Mainchain
1	C	175	TYR	Sidechain
1	C	177	GLU	Sidechain,Mainchain
1	C	178	THR	Mainchain
1	C	181	ILE	Mainchain
1	C	203	GLU	Mainchain
1	C	205	ASP	Sidechain
1	C	206	ILE	Mainchain
1	C	213	ARG	Sidechain
1	C	215	PHE	Mainchain
1	C	219	PHE	Sidechain
1	C	231	TYR	Sidechain
1	C	236	PHE	Sidechain,Mainchain
1	C	238	PRO	Mainchain
1	C	248	VAL	Mainchain
1	C	249	ASP	Sidechain
1	C	250	PHE	Mainchain
1	C	254	ARG	Mainchain
1	C	260	GLY	Mainchain
1	C	264	ARG	Mainchain
1	C	267	PHE	Sidechain
1	C	270	GLY	Mainchain
1	C	271	PHE	Sidechain
1	C	275	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	C	277	ASP	Mainchain
1	C	288	ASP	Mainchain
1	C	289	VAL	Mainchain
1	C	315	VAL	Mainchain
1	C	322	ASP	Mainchain
1	C	323	SER	Mainchain
1	C	326	ARG	Sidechain
1	C	328	TYR	Sidechain
1	C	329	ASN	Mainchain
1	C	338	THR	Mainchain
1	C	340	TYR	Sidechain
1	C	344	TYR	Sidechain
1	C	347	TYR	Sidechain
1	C	349	TYR	Sidechain
1	C	355	GLY	Mainchain
1	C	366	ASP	Sidechain
1	C	368	THR	Mainchain
1	C	371	SER	Mainchain
1	C	375	TYR	Sidechain
1	C	378	LEU	Peptide,Mainchain
1	C	383	GLN	Mainchain
1	C	388	PHE	Sidechain
1	C	389	ARG	Sidechain
1	C	390	SER	Mainchain
1	C	391	THR	Mainchain
1	C	394	ILE	Mainchain
1	C	410	LYS	Mainchain
1	C	412	PHE	Mainchain
1	C	419	TYR	Sidechain
1	C	424	ARG	Sidechain
1	C	426	PHE	Sidechain
1	C	427	THR	Mainchain
1	C	438	GLU	Mainchain
1	C	439	ASN	Mainchain
1	C	441	ILE	Mainchain
1	C	443	ALA	Mainchain
1	C	463	HIS	Sidechain
1	C	469	ARG	Sidechain
1	C	477	ARG	Sidechain
1	C	480	ILE	Mainchain
1	C	485	ARG	Mainchain
1	C	489	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	C	491	VAL	Mainchain
1	C	492	TYR	Sidechain
1	C	500	PRO	Mainchain
1	C	504	SER	Mainchain
1	C	506	ARG	Sidechain,Mainchain
1	C	52	ARG	Sidechain,Mainchain
1	C	56	ARG	Mainchain
1	C	57	TYR	Sidechain
1	C	58	SER	Mainchain
1	C	62	PRO	Mainchain
1	C	64	PHE	Sidechain,Mainchain
1	C	68	ARG	Sidechain
1	C	70	TYR	Sidechain
1	C	73	ASP	Mainchain
1	C	76	SER	Mainchain
1	C	78	ASP	Mainchain
1	C	79	VAL	Mainchain
1	C	84	TYR	Sidechain,Mainchain
1	C	91	PHE	Sidechain
1	C	98	ASN	Mainchain
1	C	99	ASN	Mainchain
1	D	100	ASP	Sidechain
1	D	101	TYR	Sidechain
1	D	103	PRO	Mainchain
1	D	104	GLY	Mainchain
1	D	106	ALA	Mainchain
1	D	111	ILE	Mainchain
1	D	113	LEU	Mainchain
1	D	114	ASP	Sidechain
1	D	116	ARG	Sidechain
1	D	118	HIS	Sidechain
1	D	119	TRP	Mainchain
1	D	132	PRO	Mainchain
1	D	137	PHE	Mainchain
1	D	139	PHE	Sidechain
1	D	151	ARG	Mainchain
1	D	171	PRO	Mainchain
1	D	173	GLY	Mainchain
1	D	175	TYR	Sidechain
1	D	177	GLU	Mainchain
1	D	178	THR	Mainchain
1	D	181	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	D	192	TYR	Mainchain
1	D	197	ARG	Sidechain,Mainchain
1	D	206	ILE	Mainchain
1	D	215	PHE	Mainchain
1	D	231	TYR	Sidechain
1	D	238	PRO	Mainchain
1	D	239	ASP	Sidechain
1	D	241	ILE	Mainchain
1	D	250	PHE	Mainchain
1	D	252	HIS	Sidechain
1	D	254	ARG	Sidechain,Mainchain
1	D	258	LEU	Mainchain
1	D	260	GLY	Mainchain
1	D	262	ARG	Sidechain
1	D	264	ARG	Mainchain
1	D	270	GLY	Mainchain
1	D	271	PHE	Sidechain
1	D	272	ARG	Sidechain
1	D	275	TYR	Sidechain
1	D	288	ASP	Mainchain
1	D	289	VAL	Mainchain
1	D	294	ALA	Mainchain
1	D	315	VAL	Mainchain
1	D	322	ASP	Mainchain
1	D	323	SER	Mainchain
1	D	326	ARG	Sidechain
1	D	329	ASN	Mainchain
1	D	337	PHE	Sidechain
1	D	338	THR	Mainchain
1	D	341	ARG	Sidechain
1	D	344	TYR	Sidechain
1	D	347	TYR	Sidechain
1	D	349	TYR	Sidechain
1	D	355	GLY	Mainchain
1	D	371	SER	Mainchain
1	D	372	GLU	Mainchain
1	D	375	TYR	Sidechain
1	D	378	LEU	Peptide,Mainchain
1	D	383	GLN	Mainchain
1	D	388	PHE	Sidechain
1	D	391	THR	Mainchain
1	D	394	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	D	410	LYS	Mainchain
1	D	413	TYR	Sidechain
1	D	424	ARG	Sidechain
1	D	427	THR	Mainchain
1	D	433	PHE	Sidechain
1	D	439	ASN	Mainchain
1	D	441	ILE	Mainchain
1	D	443	ALA	Mainchain
1	D	456	ASN	Sidechain
1	D	463	HIS	Sidechain
1	D	469	ARG	Sidechain
1	D	470	ASN	Sidechain
1	D	477	ARG	Sidechain
1	D	480	ILE	Mainchain
1	D	484	ARG	Sidechain
1	D	485	ARG	Sidechain,Mainchain
1	D	486	ARG	Sidechain
1	D	489	PRO	Mainchain
1	D	490	TYR	Sidechain
1	D	491	VAL	Mainchain
1	D	492	TYR	Sidechain
1	D	500	PRO	Mainchain
1	D	501	ARG	Sidechain
1	D	504	SER	Mainchain
1	D	506	ARG	Mainchain
1	D	52	ARG	Mainchain
1	D	56	ARG	Mainchain
1	D	57	TYR	Sidechain
1	D	58	SER	Mainchain
1	D	62	PRO	Mainchain
1	D	64	PHE	Sidechain,Mainchain
1	D	76	SER	Mainchain
1	D	78	ASP	Mainchain
1	D	79	VAL	Mainchain
1	D	84	TYR	Sidechain,Mainchain
1	D	91	PHE	Sidechain
1	D	98	ASN	Mainchain
1	D	99	ASN	Mainchain
1	E	103	PRO	Mainchain
1	E	104	GLY	Mainchain
1	E	106	ALA	Mainchain
1	E	111	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	E	113	LEU	Mainchain
1	E	116	ARG	Sidechain
1	E	118	HIS	Sidechain
1	E	119	TRP	Mainchain
1	E	132	PRO	Mainchain
1	E	137	PHE	Sidechain,Mainchain
1	E	151	ARG	Sidechain,Mainchain
1	E	153	LEU	Mainchain
1	E	171	PRO	Mainchain
1	E	173	GLY	Mainchain
1	E	175	TYR	Sidechain
1	E	177	GLU	Mainchain
1	E	178	THR	Mainchain
1	E	181	ILE	Mainchain
1	E	192	TYR	Sidechain,Mainchain
1	E	206	ILE	Mainchain
1	E	213	ARG	Sidechain
1	E	215	PHE	Sidechain,Mainchain
1	E	231	TYR	Sidechain
1	E	236	PHE	Sidechain,Mainchain
1	E	238	PRO	Mainchain
1	E	239	ASP	Sidechain
1	E	249	ASP	Sidechain
1	E	254	ARG	Mainchain
1	E	258	LEU	Mainchain
1	E	260	GLY	Mainchain
1	E	262	ARG	Sidechain
1	E	264	ARG	Sidechain,Mainchain
1	E	270	GLY	Mainchain
1	E	275	TYR	Sidechain
1	E	283	ILE	Mainchain
1	E	288	ASP	Mainchain
1	E	289	VAL	Mainchain
1	E	315	VAL	Mainchain
1	E	322	ASP	Mainchain
1	E	323	SER	Mainchain
1	E	329	ASN	Sidechain,Mainchain
1	E	337	PHE	Sidechain
1	E	338	THR	Mainchain
1	E	340	TYR	Sidechain
1	E	344	TYR	Sidechain
1	E	347	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	355	GLY	Mainchain
1	E	366	ASP	Sidechain
1	E	367	VAL	Mainchain
1	E	371	SER	Mainchain
1	E	372	GLU	Mainchain
1	E	375	TYR	Sidechain
1	E	378	LEU	Peptide,Mainchain
1	E	383	GLN	Mainchain
1	E	388	PHE	Sidechain
1	E	390	SER	Mainchain
1	E	391	THR	Mainchain
1	E	394	ILE	Mainchain
1	E	408	HIS	Sidechain
1	E	410	LYS	Mainchain
1	E	419	TYR	Sidechain
1	E	424	ARG	Sidechain
1	E	426	PHE	Sidechain
1	E	435	ARG	Sidechain
1	E	439	ASN	Mainchain
1	E	441	ILE	Mainchain
1	E	469	ARG	Sidechain
1	E	470	ASN	Sidechain
1	E	477	ARG	Mainchain
1	E	482	ASP	Mainchain
1	E	484	ARG	Sidechain
1	E	485	ARG	Mainchain
1	E	486	ARG	Sidechain
1	E	489	PRO	Mainchain
1	E	490	TYR	Sidechain
1	E	491	VAL	Mainchain
1	E	492	TYR	Sidechain
1	E	500	PRO	Mainchain
1	E	501	ARG	Sidechain
1	E	504	SER	Mainchain
1	E	506	ARG	Mainchain
1	E	52	ARG	Mainchain
1	E	56	ARG	Mainchain
1	E	57	TYR	Sidechain
1	E	58	SER	Mainchain
1	E	62	PRO	Mainchain
1	E	64	PHE	Sidechain,Mainchain
1	E	70	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	73	ASP	Mainchain
1	E	76	SER	Mainchain
1	E	79	VAL	Mainchain
1	E	84	TYR	Mainchain
1	E	98	ASN	Mainchain
1	E	99	ASN	Mainchain
1	F	100	ASP	Sidechain
1	F	103	PRO	Mainchain
1	F	104	GLY	Mainchain
1	F	106	ALA	Mainchain
1	F	111	ILE	Mainchain
1	F	115	ASP	Sidechain
1	F	118	HIS	Sidechain
1	F	119	TRP	Mainchain
1	F	132	PRO	Mainchain
1	F	137	PHE	Sidechain,Mainchain
1	F	139	PHE	Sidechain
1	F	151	ARG	Mainchain
1	F	168	PHE	Sidechain
1	F	171	PRO	Mainchain
1	F	173	GLY	Mainchain
1	F	175	TYR	Sidechain
1	F	177	GLU	Mainchain
1	F	178	THR	Mainchain
1	F	181	ILE	Mainchain
1	F	191	HIS	Sidechain
1	F	197	ARG	Mainchain
1	F	206	ILE	Mainchain
1	F	213	ARG	Sidechain
1	F	215	PHE	Mainchain
1	F	219	PHE	Sidechain
1	F	231	TYR	Sidechain
1	F	236	PHE	Sidechain,Mainchain
1	F	238	PRO	Mainchain
1	F	249	ASP	Sidechain
1	F	254	ARG	Mainchain
1	F	258	LEU	Mainchain
1	F	260	GLY	Mainchain
1	F	262	ARG	Sidechain
1	F	264	ARG	Sidechain,Mainchain
1	F	270	GLY	Mainchain
1	F	271	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	F	275	TYR	Sidechain
1	F	288	ASP	Mainchain
1	F	289	VAL	Mainchain
1	F	292	TYR	Sidechain
1	F	315	VAL	Mainchain
1	F	322	ASP	Mainchain
1	F	323	SER	Mainchain
1	F	326	ARG	Sidechain
1	F	328	TYR	Sidechain
1	F	329	ASN	Mainchain
1	F	334	ASP	Sidechain
1	F	337	PHE	Sidechain
1	F	338	THR	Mainchain
1	F	340	TYR	Sidechain
1	F	344	TYR	Sidechain
1	F	347	TYR	Sidechain
1	F	351	ASP	Sidechain
1	F	355	GLY	Mainchain
1	F	371	SER	Mainchain
1	F	372	GLU	Sidechain
1	F	375	TYR	Sidechain
1	F	378	LEU	Peptide,Mainchain
1	F	383	GLN	Mainchain
1	F	390	SER	Mainchain
1	F	391	THR	Mainchain
1	F	394	ILE	Mainchain
1	F	397	PHE	Sidechain
1	F	410	LYS	Mainchain
1	F	413	TYR	Sidechain
1	F	419	TYR	Sidechain
1	F	431	HIS	Sidechain
1	F	434	ASN	Sidechain
1	F	436	PHE	Sidechain
1	F	439	ASN	Mainchain
1	F	441	ILE	Mainchain
1	F	462	ASP	Sidechain
1	F	463	HIS	Sidechain
1	F	477	ARG	Sidechain
1	F	480	ILE	Mainchain
1	F	485	ARG	Sidechain,Mainchain
1	F	486	ARG	Sidechain
1	F	489	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	F	490	TYR	Sidechain
1	F	491	VAL	Mainchain
1	F	492	TYR	Sidechain
1	F	500	PRO	Mainchain
1	F	501	ARG	Sidechain
1	F	504	SER	Mainchain
1	F	506	ARG	Sidechain,Mainchain
1	F	52	ARG	Mainchain
1	F	56	ARG	Mainchain
1	F	57	TYR	Sidechain
1	F	58	SER	Mainchain
1	F	59	GLU	Sidechain
1	F	62	PRO	Mainchain
1	F	64	PHE	Sidechain,Mainchain
1	F	68	ARG	Sidechain
1	F	76	SER	Mainchain
1	F	78	ASP	Mainchain
1	F	84	TYR	Sidechain,Mainchain
1	F	91	PHE	Sidechain
1	F	98	ASN	Mainchain
1	F	99	ASN	Sidechain,Mainchain
1	G	100	ASP	Sidechain
1	G	101	TYR	Sidechain
1	G	103	PRO	Mainchain
1	G	104	GLY	Mainchain
1	G	106	ALA	Mainchain
1	G	111	ILE	Mainchain
1	G	113	LEU	Mainchain
1	G	118	HIS	Sidechain
1	G	119	TRP	Mainchain
1	G	128	HIS	Sidechain
1	G	132	PRO	Mainchain
1	G	135	ASN	Sidechain
1	G	137	PHE	Sidechain,Mainchain
1	G	139	PHE	Sidechain
1	G	143	PHE	Sidechain
1	G	151	ARG	Mainchain
1	G	171	PRO	Mainchain
1	G	172	GLU	Sidechain
1	G	173	GLY	Mainchain
1	G	175	TYR	Sidechain
1	G	177	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	G	181	ILE	Mainchain
1	G	192	TYR	Mainchain
1	G	197	ARG	Mainchain
1	G	203	GLU	Mainchain
1	G	206	ILE	Mainchain
1	G	210	PHE	Sidechain
1	G	215	PHE	Mainchain
1	G	216	ARG	Sidechain
1	G	220	ASP	Sidechain
1	G	231	TYR	Sidechain
1	G	236	PHE	Sidechain
1	G	237	HIS	Sidechain
1	G	238	PRO	Mainchain
1	G	248	VAL	Mainchain
1	G	249	ASP	Sidechain
1	G	254	ARG	Mainchain
1	G	258	LEU	Mainchain
1	G	260	GLY	Mainchain
1	G	262	ARG	Sidechain
1	G	264	ARG	Mainchain
1	G	270	GLY	Mainchain
1	G	271	PHE	Sidechain
1	G	275	TYR	Sidechain
1	G	288	ASP	Mainchain
1	G	289	VAL	Mainchain
1	G	315	VAL	Mainchain
1	G	322	ASP	Mainchain
1	G	323	SER	Mainchain
1	G	326	ARG	Sidechain
1	G	328	TYR	Sidechain
1	G	329	ASN	Sidechain,Mainchain
1	G	337	PHE	Sidechain
1	G	338	THR	Mainchain
1	G	344	TYR	Sidechain
1	G	347	TYR	Sidechain
1	G	355	GLY	Mainchain
1	G	357	ARG	Sidechain
1	G	367	VAL	Mainchain
1	G	371	SER	Mainchain
1	G	372	GLU	Mainchain
1	G	375	TYR	Sidechain
1	G	378	LEU	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	G	380	ASP	Sidechain
1	G	383	GLN	Mainchain
1	G	394	ILE	Mainchain
1	G	408	HIS	Sidechain
1	G	410	LYS	Mainchain
1	G	415	ASP	Mainchain
1	G	420	SER	Mainchain
1	G	424	ARG	Sidechain
1	G	426	PHE	Sidechain
1	G	427	THR	Mainchain
1	G	431	HIS	Sidechain
1	G	435	ARG	Sidechain
1	G	439	ASN	Mainchain
1	G	441	ILE	Mainchain
1	G	443	ALA	Mainchain
1	G	476	GLN	Sidechain
1	G	477	ARG	Sidechain
1	G	480	ILE	Mainchain
1	G	482	ASP	Sidechain
1	G	484	ARG	Sidechain
1	G	485	ARG	Mainchain
1	G	489	PRO	Mainchain
1	G	491	VAL	Mainchain
1	G	492	TYR	Sidechain
1	G	500	PRO	Mainchain
1	G	501	ARG	Sidechain
1	G	504	SER	Mainchain
1	G	506	ARG	Mainchain
1	G	52	ARG	Sidechain,Mainchain
1	G	56	ARG	Mainchain
1	G	57	TYR	Sidechain
1	G	58	SER	Mainchain
1	G	62	PRO	Mainchain
1	G	64	PHE	Sidechain,Mainchain
1	G	68	ARG	Sidechain
1	G	70	TYR	Sidechain
1	G	73	ASP	Sidechain,Mainchain
1	G	76	SER	Mainchain
1	G	78	ASP	Mainchain
1	G	79	VAL	Mainchain
1	G	84	TYR	Mainchain
1	G	91	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	G	98	ASN	Mainchain
1	G	99	ASN	Mainchain
1	H	100	ASP	Sidechain
1	H	101	TYR	Sidechain
1	H	103	PRO	Mainchain
1	H	104	GLY	Mainchain
1	H	106	ALA	Mainchain
1	H	111	ILE	Mainchain
1	H	116	ARG	Sidechain
1	H	118	HIS	Sidechain
1	H	119	TRP	Mainchain
1	H	122	ASP	Sidechain
1	H	132	PRO	Mainchain
1	H	137	PHE	Sidechain,Mainchain
1	H	151	ARG	Mainchain
1	H	160	GLU	Sidechain
1	H	163	TYR	Sidechain
1	H	168	PHE	Sidechain
1	H	171	PRO	Mainchain
1	H	173	GLY	Mainchain
1	H	175	TYR	Sidechain
1	H	177	GLU	Mainchain
1	H	178	THR	Mainchain
1	H	181	ILE	Mainchain
1	H	182	ASP	Sidechain
1	H	185	ASN	Sidechain
1	H	192	TYR	Mainchain
1	H	197	ARG	Mainchain
1	H	203	GLU	Mainchain
1	H	206	ILE	Mainchain
1	H	210	PHE	Sidechain
1	H	215	PHE	Sidechain,Mainchain
1	H	236	PHE	Sidechain
1	H	237	HIS	Sidechain
1	H	238	PRO	Mainchain
1	H	241	ILE	Mainchain
1	H	249	ASP	Sidechain
1	H	250	PHE	Mainchain
1	H	254	ARG	Mainchain
1	H	260	GLY	Mainchain
1	H	264	ARG	Sidechain,Mainchain
1	H	267	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	H	269	GLU	Sidechain
1	H	270	GLY	Mainchain
1	H	271	PHE	Sidechain
1	H	275	TYR	Sidechain
1	H	288	ASP	Mainchain
1	H	289	VAL	Mainchain
1	H	292	TYR	Sidechain
1	H	315	VAL	Mainchain
1	H	322	ASP	Mainchain
1	H	323	SER	Mainchain
1	H	328	TYR	Sidechain
1	H	329	ASN	Mainchain
1	H	337	PHE	Sidechain
1	H	338	THR	Mainchain
1	H	347	TYR	Sidechain
1	H	349	TYR	Sidechain
1	H	355	GLY	Mainchain
1	H	366	ASP	Sidechain
1	H	371	SER	Mainchain
1	H	372	GLU	Mainchain
1	H	375	TYR	Sidechain
1	H	378	LEU	Peptide,Mainchain
1	H	383	GLN	Mainchain
1	H	384	ASP	Sidechain
1	H	390	SER	Mainchain
1	H	391	THR	Mainchain
1	H	394	ILE	Mainchain
1	H	397	PHE	Sidechain
1	H	408	HIS	Sidechain
1	H	410	LYS	Mainchain
1	H	413	TYR	Sidechain
1	H	415	ASP	Mainchain
1	H	424	ARG	Sidechain
1	H	426	PHE	Sidechain
1	H	427	THR	Mainchain
1	H	439	ASN	Mainchain
1	H	441	ILE	Mainchain
1	H	443	ALA	Mainchain
1	H	444	ARG	Sidechain
1	H	477	ARG	Mainchain
1	H	480	ILE	Mainchain
1	H	482	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	H	485	ARG	Sidechain,Mainchain
1	H	489	PRO	Mainchain
1	H	490	TYR	Sidechain
1	H	491	VAL	Mainchain
1	H	492	TYR	Sidechain
1	H	500	PRO	Mainchain
1	H	504	SER	Mainchain
1	H	506	ARG	Sidechain,Mainchain
1	H	52	ARG	Mainchain
1	H	53	ASN	Mainchain
1	H	56	ARG	Mainchain
1	H	57	TYR	Sidechain
1	H	58	SER	Mainchain
1	H	59	GLU	Sidechain
1	H	62	PRO	Mainchain
1	H	64	PHE	Mainchain
1	H	65	ASP	Sidechain
1	H	68	ARG	Sidechain
1	H	70	TYR	Sidechain
1	H	73	ASP	Mainchain
1	H	76	SER	Mainchain
1	H	79	VAL	Mainchain
1	H	84	TYR	Mainchain
1	H	91	PHE	Sidechain
1	H	98	ASN	Mainchain
1	H	99	ASN	Mainchain
1	I	101	TYR	Sidechain
1	I	103	PRO	Mainchain
1	I	104	GLY	Mainchain
1	I	106	ALA	Mainchain
1	I	111	ILE	Mainchain
1	I	113	LEU	Mainchain
1	I	118	HIS	Sidechain
1	I	119	TRP	Mainchain
1	I	122	ASP	Sidechain
1	I	128	HIS	Sidechain
1	I	132	PRO	Mainchain
1	I	135	ASN	Sidechain
1	I	137	PHE	Mainchain
1	I	151	ARG	Sidechain,Mainchain
1	I	163	TYR	Sidechain
1	I	167	GLU	Sidechain

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Mol	Chain	Res	Type	Group
1	I	168	PHE	Sidechain
1	I	171	PRO	Mainchain
1	I	173	GLY	Mainchain
1	I	175	TYR	Sidechain
1	I	177	GLU	Mainchain
1	I	178	THR	Mainchain
1	I	179	MET	Mainchain
1	I	181	ILE	Mainchain
1	I	182	ASP	Sidechain
1	I	191	HIS	Sidechain
1	I	192	TYR	Mainchain
1	I	203	GLU	Mainchain
1	I	206	ILE	Mainchain
1	I	215	PHE	Mainchain
1	I	219	PHE	Sidechain
1	I	220	ASP	Sidechain
1	I	231	TYR	Sidechain
1	I	236	PHE	Sidechain
1	I	238	PRO	Mainchain
1	I	249	ASP	Sidechain
1	I	250	PHE	Sidechain,Mainchain
1	I	254	ARG	Sidechain,Mainchain
1	I	260	GLY	Mainchain
1	I	262	ARG	Sidechain
1	I	264	ARG	Mainchain
1	I	267	PHE	Sidechain
1	I	270	GLY	Mainchain
1	I	271	PHE	Sidechain
1	I	272	ARG	Sidechain
1	I	275	TYR	Sidechain
1	I	288	ASP	Mainchain
1	I	289	VAL	Mainchain
1	I	292	TYR	Sidechain
1	I	312	LEU	Mainchain
1	I	315	VAL	Mainchain
1	I	322	ASP	Mainchain
1	I	323	SER	Mainchain
1	I	326	ARG	Sidechain
1	I	328	TYR	Sidechain
1	I	329	ASN	Mainchain
1	I	337	PHE	Sidechain
1	I	338	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	I	341	ARG	Sidechain
1	I	344	TYR	Sidechain
1	I	347	TYR	Sidechain
1	I	349	TYR	Sidechain
1	I	355	GLY	Mainchain
1	I	357	ARG	Sidechain
1	I	371	SER	Mainchain
1	I	372	GLU	Mainchain
1	I	375	TYR	Sidechain
1	I	378	LEU	Peptide,Mainchain
1	I	383	GLN	Mainchain
1	I	390	SER	Mainchain
1	I	394	ILE	Mainchain
1	I	397	PHE	Sidechain
1	I	413	TYR	Sidechain
1	I	424	ARG	Sidechain
1	I	426	PHE	Sidechain
1	I	427	THR	Mainchain
1	I	432	VAL	Mainchain
1	I	436	PHE	Sidechain
1	I	438	GLU	Mainchain
1	I	439	ASN	Mainchain
1	I	441	ILE	Mainchain
1	I	443	ALA	Mainchain
1	I	444	ARG	Sidechain
1	I	469	ARG	Sidechain
1	I	477	ARG	Mainchain
1	I	485	ARG	Mainchain
1	I	486	ARG	Sidechain
1	I	489	PRO	Mainchain
1	I	490	TYR	Sidechain
1	I	492	TYR	Sidechain
1	I	500	PRO	Mainchain
1	I	501	ARG	Sidechain
1	I	504	SER	Mainchain
1	I	506	ARG	Sidechain,Mainchain
1	I	52	ARG	Sidechain,Mainchain
1	I	56	ARG	Mainchain
1	I	57	TYR	Sidechain
1	I	58	SER	Mainchain
1	I	62	PRO	Mainchain
1	I	64	PHE	Mainchain

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Mol	Chain	Res	Type	Group
1	I	70	TYR	Sidechain
1	I	76	SER	Mainchain
1	I	78	ASP	Mainchain
1	I	79	VAL	Mainchain
1	I	84	TYR	Mainchain
1	I	91	PHE	Sidechain
1	I	98	ASN	Sidechain,Mainchain
1	I	99	ASN	Mainchain
1	J	100	ASP	Sidechain
1	J	101	TYR	Sidechain
1	J	103	PRO	Mainchain
1	J	104	GLY	Mainchain
1	J	106	ALA	Mainchain
1	J	111	ILE	Mainchain
1	J	114	ASP	Sidechain
1	J	118	HIS	Sidechain
1	J	119	TRP	Mainchain
1	J	128	HIS	Sidechain
1	J	132	PRO	Mainchain
1	J	137	PHE	Sidechain,Mainchain
1	J	139	PHE	Sidechain
1	J	143	PHE	Sidechain
1	J	151	ARG	Sidechain,Mainchain
1	J	156	ASP	Sidechain
1	J	171	PRO	Mainchain
1	J	173	GLY	Mainchain
1	J	175	TYR	Sidechain
1	J	177	GLU	Mainchain
1	J	178	THR	Mainchain
1	J	181	ILE	Mainchain
1	J	191	HIS	Sidechain
1	J	192	TYR	Mainchain
1	J	197	ARG	Mainchain
1	J	206	ILE	Mainchain
1	J	213	ARG	Sidechain
1	J	215	PHE	Sidechain,Mainchain
1	J	220	ASP	Sidechain
1	J	233	ASN	Sidechain
1	J	234	GLU	Mainchain
1	J	236	PHE	Sidechain,Mainchain
1	J	238	PRO	Mainchain
1	J	241	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	J	248	VAL	Mainchain
1	J	250	PHE	Mainchain
1	J	252	HIS	Sidechain
1	J	254	ARG	Sidechain,Mainchain
1	J	260	GLY	Mainchain
1	J	264	ARG	Mainchain
1	J	270	GLY	Mainchain
1	J	271	PHE	Sidechain
1	J	275	TYR	Sidechain
1	J	288	ASP	Mainchain
1	J	289	VAL	Mainchain
1	J	295	SER	Mainchain
1	J	315	VAL	Mainchain
1	J	322	ASP	Mainchain
1	J	323	SER	Mainchain
1	J	326	ARG	Sidechain
1	J	329	ASN	Mainchain
1	J	334	ASP	Sidechain
1	J	338	THR	Mainchain
1	J	347	TYR	Sidechain
1	J	355	GLY	Mainchain
1	J	367	VAL	Mainchain
1	J	371	SER	Mainchain
1	J	375	TYR	Sidechain
1	J	378	LEU	Peptide,Mainchain
1	J	383	GLN	Mainchain
1	J	388	PHE	Sidechain
1	J	389	ARG	Sidechain
1	J	391	THR	Mainchain
1	J	394	ILE	Mainchain
1	J	397	PHE	Sidechain
1	J	410	LYS	Mainchain
1	J	413	TYR	Sidechain
1	J	415	ASP	Mainchain
1	J	419	TYR	Sidechain
1	J	424	ARG	Sidechain
1	J	426	PHE	Sidechain
1	J	427	THR	Mainchain
1	J	431	HIS	Sidechain
1	J	436	PHE	Sidechain
1	J	439	ASN	Mainchain
1	J	441	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	J	443	ALA	Mainchain
1	J	463	HIS	Sidechain
1	J	476	GLN	Sidechain
1	J	477	ARG	Sidechain
1	J	485	ARG	Sidechain,Mainchain
1	J	486	ARG	Sidechain
1	J	489	PRO	Mainchain
1	J	491	VAL	Mainchain
1	J	492	TYR	Sidechain
1	J	500	PRO	Mainchain
1	J	504	SER	Mainchain
1	J	506	ARG	Mainchain
1	J	52	ARG	Mainchain
1	J	56	ARG	Sidechain,Mainchain
1	J	57	TYR	Sidechain
1	J	58	SER	Mainchain
1	J	62	PRO	Mainchain
1	J	64	PHE	Sidechain,Mainchain
1	J	70	TYR	Sidechain
1	J	76	SER	Mainchain
1	J	78	ASP	Mainchain
1	J	79	VAL	Mainchain
1	J	84	TYR	Sidechain,Mainchain
1	J	91	PHE	Sidechain
1	J	98	ASN	Mainchain
1	J	99	ASN	Mainchain
1	K	100	ASP	Sidechain
1	K	101	TYR	Sidechain
1	K	103	PRO	Mainchain
1	K	104	GLY	Mainchain
1	K	106	ALA	Mainchain
1	K	111	ILE	Mainchain
1	K	114	ASP	Mainchain
1	K	115	ASP	Sidechain
1	K	118	HIS	Sidechain
1	K	119	TRP	Mainchain
1	K	128	HIS	Sidechain
1	K	132	PRO	Mainchain
1	K	137	PHE	Sidechain,Mainchain
1	K	142	LYS	Mainchain
1	K	151	ARG	Mainchain
1	K	163	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	K	168	PHE	Sidechain
1	K	171	PRO	Mainchain
1	K	173	GLY	Mainchain
1	K	175	TYR	Sidechain
1	K	177	GLU	Mainchain
1	K	181	ILE	Mainchain
1	K	192	TYR	Mainchain
1	K	203	GLU	Mainchain
1	K	205	ASP	Sidechain
1	K	206	ILE	Mainchain
1	K	210	PHE	Sidechain
1	K	215	PHE	Mainchain
1	K	236	PHE	Sidechain
1	K	238	PRO	Mainchain
1	K	239	ASP	Sidechain
1	K	248	VAL	Mainchain
1	K	249	ASP	Sidechain
1	K	250	PHE	Sidechain
1	K	254	ARG	Mainchain
1	K	258	LEU	Mainchain
1	K	260	GLY	Mainchain
1	K	262	ARG	Sidechain
1	K	264	ARG	Sidechain,Mainchain
1	K	267	PHE	Sidechain
1	K	270	GLY	Mainchain
1	K	271	PHE	Sidechain
1	K	272	ARG	Sidechain
1	K	275	TYR	Sidechain
1	K	288	ASP	Mainchain
1	K	289	VAL	Mainchain
1	K	315	VAL	Mainchain
1	K	322	ASP	Mainchain
1	K	323	SER	Mainchain
1	K	328	TYR	Sidechain
1	K	329	ASN	Mainchain
1	K	334	ASP	Sidechain
1	K	338	THR	Mainchain
1	K	344	TYR	Sidechain
1	K	347	TYR	Sidechain
1	K	349	TYR	Sidechain
1	K	355	GLY	Mainchain
1	K	371	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	K	372	GLU	Mainchain
1	K	375	TYR	Sidechain
1	K	378	LEU	Peptide,Mainchain
1	K	383	GLN	Mainchain
1	K	384	ASP	Sidechain
1	K	388	PHE	Sidechain
1	K	391	THR	Mainchain
1	K	394	ILE	Mainchain
1	K	408	HIS	Sidechain
1	K	410	LYS	Mainchain
1	K	412	PHE	Sidechain
1	K	413	TYR	Sidechain
1	K	419	TYR	Sidechain
1	K	420	SER	Mainchain
1	K	424	ARG	Sidechain
1	K	426	PHE	Sidechain
1	K	427	THR	Mainchain
1	K	436	PHE	Sidechain
1	K	439	ASN	Mainchain
1	K	441	ILE	Mainchain
1	K	443	ALA	Mainchain
1	K	444	ARG	Sidechain
1	K	455	GLU	Sidechain
1	K	463	HIS	Sidechain
1	K	469	ARG	Sidechain
1	K	477	ARG	Sidechain,Mainchain
1	K	480	ILE	Mainchain
1	K	485	ARG	Sidechain,Mainchain
1	K	486	ARG	Sidechain
1	K	489	PRO	Mainchain
1	K	490	TYR	Sidechain
1	K	492	TYR	Sidechain
1	K	500	PRO	Mainchain
1	K	501	ARG	Sidechain
1	K	504	SER	Mainchain
1	K	506	ARG	Sidechain
1	K	52	ARG	Mainchain
1	K	56	ARG	Mainchain
1	K	57	TYR	Sidechain
1	K	58	SER	Mainchain
1	K	62	PRO	Mainchain
1	K	64	PHE	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	K	65	ASP	Sidechain
1	K	68	ARG	Sidechain
1	K	70	TYR	Sidechain
1	K	73	ASP	Sidechain,Mainchain
1	K	76	SER	Mainchain
1	K	78	ASP	Sidechain,Mainchain
1	K	79	VAL	Mainchain
1	K	84	TYR	Sidechain,Mainchain
1	K	91	PHE	Sidechain
1	K	98	ASN	Mainchain
1	L	100	ASP	Sidechain
1	L	101	TYR	Sidechain
1	L	103	PRO	Mainchain
1	L	104	GLY	Mainchain
1	L	106	ALA	Mainchain
1	L	111	ILE	Mainchain
1	L	113	LEU	Mainchain
1	L	119	TRP	Mainchain
1	L	122	ASP	Sidechain
1	L	128	HIS	Sidechain
1	L	132	PRO	Mainchain
1	L	133	ASN	Sidechain
1	L	137	PHE	Sidechain,Mainchain
1	L	139	PHE	Sidechain
1	L	151	ARG	Mainchain
1	L	160	GLU	Sidechain
1	L	163	TYR	Sidechain
1	L	171	PRO	Mainchain
1	L	173	GLY	Mainchain
1	L	175	TYR	Sidechain
1	L	177	GLU	Mainchain
1	L	178	THR	Mainchain
1	L	179	MET	Mainchain
1	L	181	ILE	Mainchain
1	L	191	HIS	Sidechain
1	L	192	TYR	Mainchain
1	L	197	ARG	Sidechain,Mainchain
1	L	206	ILE	Mainchain
1	L	210	PHE	Sidechain
1	L	211	ASP	Sidechain
1	L	213	ARG	Sidechain
1	L	215	PHE	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	L	219	PHE	Sidechain
1	L	236	PHE	Sidechain
1	L	238	PRO	Mainchain
1	L	239	ASP	Sidechain
1	L	249	ASP	Sidechain
1	L	250	PHE	Sidechain,Mainchain
1	L	252	HIS	Sidechain
1	L	254	ARG	Sidechain,Mainchain
1	L	258	LEU	Mainchain
1	L	260	GLY	Mainchain
1	L	264	ARG	Mainchain
1	L	267	PHE	Sidechain
1	L	270	GLY	Mainchain
1	L	271	PHE	Sidechain
1	L	272	ARG	Sidechain
1	L	275	TYR	Sidechain
1	L	288	ASP	Mainchain
1	L	289	VAL	Mainchain
1	L	292	TYR	Sidechain
1	L	315	VAL	Mainchain
1	L	322	ASP	Mainchain
1	L	323	SER	Mainchain
1	L	326	ARG	Sidechain
1	L	328	TYR	Sidechain
1	L	329	ASN	Mainchain
1	L	338	THR	Mainchain
1	L	340	TYR	Sidechain
1	L	344	TYR	Sidechain
1	L	347	TYR	Sidechain
1	L	355	GLY	Mainchain
1	L	367	VAL	Mainchain
1	L	371	SER	Mainchain
1	L	372	GLU	Mainchain
1	L	375	TYR	Sidechain
1	L	378	LEU	Peptide,Mainchain
1	L	383	GLN	Mainchain
1	L	384	ASP	Sidechain
1	L	388	PHE	Sidechain
1	L	390	SER	Mainchain
1	L	391	THR	Mainchain
1	L	394	ILE	Mainchain
1	L	397	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	L	408	HIS	Sidechain
1	L	412	PHE	Sidechain,Mainchain
1	L	415	ASP	Mainchain
1	L	426	PHE	Sidechain
1	L	427	THR	Mainchain
1	L	436	PHE	Sidechain
1	L	439	ASN	Mainchain
1	L	441	ILE	Mainchain
1	L	443	ALA	Mainchain
1	L	463	HIS	Sidechain
1	L	477	ARG	Sidechain,Mainchain
1	L	480	ILE	Mainchain
1	L	485	ARG	Mainchain
1	L	486	ARG	Sidechain
1	L	489	PRO	Mainchain
1	L	492	TYR	Sidechain
1	L	500	PRO	Mainchain
1	L	504	SER	Mainchain
1	L	506	ARG	Mainchain
1	L	52	ARG	Mainchain
1	L	56	ARG	Mainchain
1	L	57	TYR	Sidechain
1	L	58	SER	Mainchain
1	L	62	PRO	Mainchain
1	L	64	PHE	Sidechain,Mainchain
1	L	70	TYR	Sidechain
1	L	76	SER	Mainchain
1	L	79	VAL	Mainchain
1	L	84	TYR	Mainchain
1	L	98	ASN	Mainchain
1	L	99	ASN	Sidechain,Mainchain
1	M	100	ASP	Sidechain
1	M	101	TYR	Sidechain
1	M	103	PRO	Mainchain
1	M	104	GLY	Mainchain
1	M	106	ALA	Mainchain
1	M	111	ILE	Mainchain
1	M	118	HIS	Sidechain
1	M	119	TRP	Mainchain
1	M	122	ASP	Sidechain
1	M	130	ASN	Sidechain
1	M	132	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	M	133	ASN	Sidechain
1	M	137	PHE	Sidechain,Mainchain
1	M	139	PHE	Sidechain
1	M	151	ARG	Mainchain
1	M	171	PRO	Mainchain
1	M	173	GLY	Mainchain
1	M	175	TYR	Sidechain
1	M	177	GLU	Mainchain
1	M	178	THR	Mainchain
1	M	181	ILE	Mainchain
1	M	182	ASP	Sidechain
1	M	191	HIS	Sidechain
1	M	192	TYR	Mainchain
1	M	197	ARG	Sidechain,Mainchain
1	M	203	GLU	Mainchain
1	M	205	ASP	Sidechain
1	M	206	ILE	Mainchain
1	M	210	PHE	Sidechain
1	M	215	PHE	Sidechain,Mainchain
1	M	231	TYR	Sidechain
1	M	234	GLU	Sidechain,Mainchain
1	M	236	PHE	Sidechain,Mainchain
1	M	238	PRO	Mainchain
1	M	241	ILE	Mainchain
1	M	249	ASP	Sidechain
1	M	250	PHE	Sidechain
1	M	252	HIS	Sidechain
1	M	254	ARG	Sidechain,Mainchain
1	M	260	GLY	Mainchain
1	M	264	ARG	Sidechain,Mainchain
1	M	270	GLY	Mainchain
1	M	271	PHE	Sidechain
1	M	275	TYR	Sidechain
1	M	288	ASP	Mainchain
1	M	289	VAL	Mainchain
1	M	292	TYR	Sidechain
1	M	315	VAL	Mainchain
1	M	322	ASP	Mainchain
1	M	323	SER	Mainchain
1	M	326	ARG	Sidechain
1	M	328	TYR	Sidechain
1	M	329	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	M	338	THR	Mainchain
1	M	344	TYR	Sidechain
1	M	347	TYR	Sidechain
1	M	355	GLY	Mainchain
1	M	371	SER	Mainchain
1	M	372	GLU	Mainchain
1	M	375	TYR	Sidechain
1	M	378	LEU	Peptide,Mainchain
1	M	383	GLN	Mainchain
1	M	388	PHE	Sidechain
1	M	390	SER	Mainchain
1	M	391	THR	Mainchain
1	M	394	ILE	Mainchain
1	M	397	PHE	Sidechain
1	M	410	LYS	Mainchain
1	M	419	TYR	Sidechain
1	M	427	THR	Mainchain
1	M	439	ASN	Mainchain
1	M	441	ILE	Mainchain
1	M	476	GLN	Sidechain
1	M	477	ARG	Sidechain,Mainchain
1	M	485	ARG	Mainchain
1	M	486	ARG	Sidechain
1	M	489	PRO	Mainchain
1	M	492	TYR	Sidechain
1	M	500	PRO	Mainchain
1	M	501	ARG	Sidechain
1	M	504	SER	Mainchain
1	M	506	ARG	Sidechain
1	M	52	ARG	Mainchain
1	M	56	ARG	Sidechain,Mainchain
1	M	57	TYR	Sidechain
1	M	58	SER	Mainchain
1	M	62	PRO	Mainchain
1	M	64	PHE	Sidechain,Mainchain
1	M	70	TYR	Sidechain
1	M	76	SER	Mainchain
1	M	84	TYR	Sidechain,Mainchain
1	M	98	ASN	Mainchain
1	M	99	ASN	Mainchain
1	N	101	TYR	Sidechain
1	N	103	PRO	Mainchain

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Mol	Chain	Res	Type	Group
1	N	104	GLY	Mainchain
1	N	106	ALA	Mainchain
1	N	111	ILE	Mainchain
1	N	119	TRP	Mainchain
1	N	128	HIS	Sidechain
1	N	132	PRO	Mainchain
1	N	133	ASN	Sidechain
1	N	137	PHE	Sidechain,Mainchain
1	N	139	PHE	Sidechain
1	N	143	PHE	Sidechain
1	N	151	ARG	Mainchain
1	N	153	LEU	Mainchain
1	N	168	PHE	Sidechain
1	N	171	PRO	Mainchain
1	N	173	GLY	Mainchain
1	N	174	ASN	Sidechain
1	N	175	TYR	Sidechain
1	N	177	GLU	Mainchain
1	N	178	THR	Mainchain
1	N	181	ILE	Mainchain
1	N	191	HIS	Sidechain
1	N	192	TYR	Sidechain,Mainchain
1	N	197	ARG	Sidechain
1	N	203	GLU	Mainchain
1	N	206	ILE	Mainchain
1	N	210	PHE	Sidechain
1	N	215	PHE	Sidechain,Mainchain
1	N	219	PHE	Sidechain
1	N	220	ASP	Sidechain
1	N	231	TYR	Sidechain
1	N	234	GLU	Mainchain
1	N	237	HIS	Sidechain
1	N	238	PRO	Mainchain
1	N	249	ASP	Sidechain
1	N	250	PHE	Sidechain
1	N	254	ARG	Mainchain
1	N	258	LEU	Mainchain
1	N	260	GLY	Mainchain
1	N	264	ARG	Sidechain,Mainchain
1	N	270	GLY	Mainchain
1	N	271	PHE	Sidechain
1	N	275	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	N	288	ASP	Mainchain
1	N	289	VAL	Mainchain
1	N	315	VAL	Mainchain
1	N	322	ASP	Mainchain
1	N	323	SER	Mainchain
1	N	326	ARG	Sidechain
1	N	328	TYR	Sidechain
1	N	329	ASN	Mainchain
1	N	334	ASP	Sidechain
1	N	337	PHE	Sidechain
1	N	338	THR	Mainchain
1	N	344	TYR	Sidechain
1	N	347	TYR	Sidechain
1	N	351	ASP	Sidechain
1	N	355	GLY	Mainchain
1	N	371	SER	Mainchain
1	N	372	GLU	Mainchain
1	N	375	TYR	Sidechain
1	N	378	LEU	Peptide,Mainchain
1	N	383	GLN	Mainchain
1	N	384	ASP	Sidechain
1	N	388	PHE	Sidechain
1	N	389	ARG	Sidechain
1	N	390	SER	Mainchain
1	N	394	ILE	Mainchain
1	N	397	PHE	Sidechain
1	N	408	HIS	Sidechain
1	N	413	TYR	Sidechain
1	N	415	ASP	Mainchain
1	N	424	ARG	Sidechain
1	N	426	PHE	Sidechain
1	N	427	THR	Mainchain
1	N	431	HIS	Sidechain
1	N	434	ASN	Sidechain
1	N	435	ARG	Sidechain
1	N	436	PHE	Sidechain
1	N	439	ASN	Mainchain
1	N	441	ILE	Mainchain
1	N	463	HIS	Sidechain
1	N	477	ARG	Sidechain
1	N	482	ASP	Sidechain
1	N	485	ARG	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	N	486	ARG	Sidechain
1	N	489	PRO	Mainchain
1	N	491	VAL	Mainchain
1	N	492	TYR	Sidechain
1	N	500	PRO	Mainchain
1	N	501	ARG	Sidechain
1	N	504	SER	Mainchain
1	N	506	ARG	Sidechain
1	N	52	ARG	Mainchain
1	N	56	ARG	Mainchain
1	N	57	TYR	Sidechain
1	N	58	SER	Mainchain
1	N	62	PRO	Mainchain
1	N	64	PHE	Sidechain,Mainchain
1	N	70	TYR	Sidechain
1	N	76	SER	Mainchain
1	N	78	ASP	Mainchain
1	N	79	VAL	Mainchain
1	N	84	TYR	Sidechain,Mainchain
1	N	91	PHE	Sidechain
1	N	98	ASN	Mainchain
1	N	99	ASN	Mainchain
1	O	100	ASP	Sidechain
1	O	101	TYR	Sidechain
1	O	103	PRO	Mainchain
1	O	104	GLY	Mainchain
1	O	106	ALA	Mainchain
1	O	111	ILE	Mainchain
1	O	119	TRP	Mainchain
1	O	128	HIS	Sidechain
1	O	132	PRO	Mainchain
1	O	137	PHE	Sidechain,Mainchain
1	O	139	PHE	Sidechain
1	O	143	PHE	Sidechain
1	O	151	ARG	Mainchain
1	O	168	PHE	Sidechain
1	O	171	PRO	Mainchain
1	O	173	GLY	Mainchain
1	O	175	TYR	Sidechain
1	O	177	GLU	Mainchain
1	O	181	ILE	Mainchain
1	O	191	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	O	192	TYR	Mainchain
1	O	197	ARG	Mainchain
1	O	206	ILE	Mainchain
1	O	210	PHE	Sidechain
1	O	213	ARG	Sidechain
1	O	215	PHE	Sidechain,Mainchain
1	O	216	ARG	Sidechain
1	O	219	PHE	Sidechain
1	O	231	TYR	Sidechain
1	O	238	PRO	Mainchain
1	O	241	ILE	Mainchain
1	O	250	PHE	Mainchain
1	O	254	ARG	Mainchain
1	O	258	LEU	Mainchain
1	O	260	GLY	Mainchain
1	O	262	ARG	Sidechain
1	O	264	ARG	Mainchain
1	O	267	PHE	Sidechain
1	O	270	GLY	Mainchain
1	O	271	PHE	Sidechain
1	O	272	ARG	Sidechain
1	O	275	TYR	Sidechain
1	O	283	ILE	Mainchain
1	O	288	ASP	Mainchain
1	O	289	VAL	Mainchain
1	O	292	TYR	Sidechain
1	O	315	VAL	Mainchain
1	O	322	ASP	Mainchain
1	O	323	SER	Mainchain
1	O	326	ARG	Sidechain
1	O	328	TYR	Sidechain
1	O	329	ASN	Sidechain,Mainchain
1	O	334	ASP	Sidechain
1	O	337	PHE	Sidechain
1	O	338	THR	Mainchain
1	O	347	TYR	Sidechain
1	O	355	GLY	Mainchain
1	O	357	ARG	Sidechain
1	O	367	VAL	Mainchain
1	O	368	THR	Mainchain
1	O	371	SER	Mainchain
1	O	372	GLU	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	O	375	TYR	Sidechain
1	O	378	LEU	Peptide,Mainchain
1	O	383	GLN	Mainchain
1	O	384	ASP	Sidechain
1	O	388	PHE	Sidechain
1	O	391	THR	Mainchain
1	O	394	ILE	Mainchain
1	O	397	PHE	Sidechain
1	O	408	HIS	Sidechain
1	O	410	LYS	Mainchain
1	O	412	PHE	Sidechain
1	O	413	TYR	Sidechain
1	O	419	TYR	Sidechain
1	O	426	PHE	Sidechain
1	O	427	THR	Mainchain
1	O	436	PHE	Sidechain
1	O	439	ASN	Mainchain
1	O	440	GLN	Sidechain
1	O	441	ILE	Mainchain
1	O	469	ARG	Sidechain
1	O	477	ARG	Sidechain,Mainchain
1	O	480	ILE	Mainchain
1	O	485	ARG	Mainchain
1	O	486	ARG	Sidechain
1	O	489	PRO	Mainchain
1	O	491	VAL	Mainchain
1	O	492	TYR	Sidechain
1	O	500	PRO	Mainchain
1	O	504	SER	Mainchain
1	O	52	ARG	Sidechain,Mainchain
1	O	56	ARG	Mainchain
1	O	57	TYR	Sidechain
1	O	58	SER	Mainchain
1	O	62	PRO	Mainchain
1	O	64	PHE	Sidechain,Mainchain
1	O	70	TYR	Sidechain
1	O	73	ASP	Sidechain,Mainchain
1	O	76	SER	Mainchain
1	O	78	ASP	Mainchain
1	O	79	VAL	Mainchain
1	O	84	TYR	Mainchain
1	O	91	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	O	98	ASN	Mainchain
1	O	99	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3534	0	3463	82	0
1	B	3534	0	3463	107	0
1	C	3534	0	3463	95	0
1	D	3534	0	3463	80	0
1	E	3534	0	3463	100	0
1	F	3534	0	3463	91	0
1	G	3534	0	3463	89	0
1	H	3534	0	3463	82	0
1	I	3534	0	3463	92	0
1	J	3534	0	3463	107	0
1	K	3534	0	3463	107	0
1	L	3534	0	3463	100	0
1	M	3534	0	3463	90	0
1	N	3534	0	3463	94	0
1	O	3534	0	3463	91	0
All	All	53010	0	51945	1296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1296) 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:J:124:LYS:CG	1:J:124:LYS:CD	1.78	1.62
1:K:422:LEU:CG	1:K:422:LEU:CD2	1.76	1.62
1:E:157:LYS:CE	1:E:157:LYS:CD	1.81	1.59
1:O:162:LYS:CE	1:O:162:LYS:CD	1.77	1.59
1:C:157:LYS:CD	1:C:157:LYS:CG	1.83	1.57
1:J:142:LYS:CE	1:J:142:LYS:CD	1.76	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:422:LEU:CG	1:K:422:LEU:CD1	1.78	1.56
1:L:317:LYS:CE	1:L:317:LYS:CD	1.83	1.56
1:J:124:LYS:CD	1:J:124:LYS:CE	1.80	1.55
1:B:167:GLU:CD	1:B:167:GLU:CG	1.76	1.54
1:G:313:LYS:CD	1:G:313:LYS:CG	1.84	1.53
1:H:155:LYS:CE	1:H:155:LYS:NZ	1.69	1.52
1:O:325:LYS:CE	1:O:325:LYS:CD	1.83	1.52
1:M:124:LYS:CD	1:M:124:LYS:CG	1.84	1.51
1:K:313:LYS:CD	1:K:313:LYS:CG	1.89	1.51
1:F:194:LYS:CE	1:F:194:LYS:CD	1.86	1.50
1:M:124:LYS:CD	1:M:124:LYS:CE	1.91	1.47
1:M:142:LYS:CE	1:M:142:LYS:CD	1.89	1.47
1:G:317:LYS:CE	1:G:317:LYS:CD	1.92	1.47
1:M:124:LYS:CE	1:M:124:LYS:NZ	1.79	1.45
1:A:144:LYS:CE	1:A:144:LYS:NZ	1.80	1.43
1:K:325:LYS:CE	1:K:325:LYS:NZ	1.82	1.42
1:E:144:LYS:NZ	1:E:144:LYS:CE	1.84	1.40
1:M:142:LYS:CE	1:M:142:LYS:NZ	1.83	1.39
1:C:157:LYS:CD	1:C:157:LYS:CE	2.01	1.38
1:D:324:LYS:CE	1:D:324:LYS:NZ	1.87	1.37
1:G:220:ASP:CG	1:G:220:ASP:OD2	1.68	1.31
1:F:194:LYS:CE	1:F:194:LYS:NZ	1.98	1.25
1:C:157:LYS:CE	1:C:157:LYS:NZ	2.07	1.17
1:A:133:ASN:HB2	1:A:175:TYR:HB3	1.34	1.10
1:E:133:ASN:HB2	1:E:175:TYR:HB3	1.27	1.07
1:M:133:ASN:HB2	1:M:175:TYR:HB3	1.36	1.06
1:G:133:ASN:HB2	1:G:175:TYR:HB3	1.35	1.06
1:O:133:ASN:HB2	1:O:175:TYR:HB3	1.36	1.06
1:C:133:ASN:HB2	1:C:175:TYR:HB3	1.41	1.00
1:D:133:ASN:HB2	1:D:175:TYR:HB3	1.44	0.99
1:N:133:ASN:HB2	1:N:175:TYR:HB3	1.46	0.98
1:H:133:ASN:HB2	1:H:175:TYR:HB3	1.47	0.97
1:J:176:SER:O	1:J:180:THR:OG1	1.83	0.96
1:B:133:ASN:HB2	1:B:175:TYR:HB3	1.48	0.95
1:F:133:ASN:HB2	1:F:175:TYR:HB3	1.50	0.94
1:K:111:ILE:HB	1:K:472:ILE:HB	1.51	0.90
1:J:430:THR:HB	1:J:432:VAL:HG23	1.56	0.88
1:M:133:ASN:CB	1:M:175:TYR:HB3	2.02	0.87
1:C:69:VAL:HG23	1:C:498:VAL:HB	1.54	0.87
1:O:69:VAL:HG23	1:O:498:VAL:HB	1.56	0.87
1:G:430:THR:HB	1:G:432:VAL:HG23	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:ASN:HB2	1:N:175:TYR:CB	2.06	0.85
1:C:157:LYS:CG	1:C:157:LYS:CE	2.55	0.84
1:E:157:LYS:CE	1:E:157:LYS:CG	2.55	0.84
1:D:66:THR:HB	1:D:500:PRO:O	1.76	0.84
1:B:430:THR:HB	1:B:432:VAL:HG23	1.60	0.83
1:D:58:SER:OG	1:D:59:GLU:N	2.11	0.83
1:M:133:ASN:HB2	1:M:175:TYR:CB	2.08	0.83
1:I:111:ILE:HB	1:I:472:ILE:HB	1.61	0.83
1:E:430:THR:HB	1:E:432:VAL:HG23	1.60	0.82
1:I:430:THR:HB	1:I:432:VAL:HG23	1.59	0.82
1:F:133:ASN:HB2	1:F:175:TYR:CB	2.09	0.82
1:H:282:ASN:H	1:H:341:ARG:HG3	1.44	0.82
1:M:430:THR:HB	1:M:432:VAL:HG23	1.60	0.81
1:O:133:ASN:CB	1:O:175:TYR:HB3	2.11	0.81
1:F:194:LYS:CE	1:F:194:LYS:CG	2.57	0.81
1:B:240:ILE:HG23	1:B:344:TYR:H	1.46	0.81
1:C:100:ASP:HB2	1:D:389:ARG:HH21	1.46	0.81
1:G:313:LYS:CD	1:G:313:LYS:CB	2.59	0.81
1:I:133:ASN:HB2	1:I:175:TYR:HB3	1.63	0.80
1:J:133:ASN:HB2	1:J:175:TYR:HB3	1.63	0.80
1:C:238:PRO:HG2	1:C:362:LEU:HD11	1.64	0.79
1:F:430:THR:HB	1:F:432:VAL:HG23	1.64	0.79
1:A:240:ILE:HG23	1:A:344:TYR:H	1.46	0.78
1:N:203:GLU:HB2	1:N:326:ARG:HH12	1.47	0.78
1:L:430:THR:HB	1:L:432:VAL:HG23	1.64	0.78
1:E:326:ARG:HD2	1:E:439:ASN:HB2	1.64	0.78
1:A:356:ILE:O	1:A:360:THR:HG22	1.84	0.78
1:B:101:TYR:OH	1:L:390:SER:OG	2.02	0.77
1:O:356:ILE:O	1:O:360:THR:HG22	1.84	0.77
1:M:240:ILE:HG23	1:M:344:TYR:H	1.48	0.77
1:J:124:LYS:CG	1:J:124:LYS:CE	2.62	0.77
1:O:240:ILE:HG23	1:O:344:TYR:H	1.48	0.77
1:C:326:ARG:HD2	1:C:439:ASN:HB2	1.66	0.77
1:E:185:ASN:HD21	1:E:210:PHE:H	1.32	0.76
1:F:240:ILE:HG23	1:F:344:TYR:H	1.50	0.76
1:L:240:ILE:HG23	1:L:344:TYR:H	1.49	0.76
1:K:313:LYS:CD	1:K:313:LYS:CB	2.64	0.76
1:L:317:LYS:CE	1:L:317:LYS:CG	2.64	0.76
1:J:58:SER:OG	1:J:59:GLU:N	2.18	0.76
1:J:69:VAL:HG23	1:J:498:VAL:HB	1.67	0.76
1:C:133:ASN:HB2	1:C:175:TYR:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:ASN:CB	1:N:175:TYR:HB3	2.15	0.75
1:F:326:ARG:HD2	1:F:439:ASN:HB2	1.67	0.75
1:O:325:LYS:CE	1:O:325:LYS:CG	2.64	0.75
1:B:133:ASN:HB2	1:B:175:TYR:CB	2.16	0.75
1:C:111:ILE:HB	1:C:472:ILE:HB	1.68	0.75
1:C:430:THR:HB	1:C:432:VAL:HG23	1.68	0.75
1:J:197:ARG:HG3	1:J:198:GLN:HE21	1.52	0.75
1:O:430:THR:HB	1:O:432:VAL:HG23	1.68	0.75
1:G:317:LYS:CE	1:G:317:LYS:CG	2.64	0.74
1:M:237:HIS:HB3	1:M:238:PRO:HD3	1.67	0.74
1:B:167:GLU:CD	1:B:167:GLU:CB	2.56	0.74
1:H:133:ASN:HB2	1:H:175:TYR:CB	2.18	0.74
1:K:100:ASP:HB2	1:L:389:ARG:HH21	1.52	0.74
1:L:133:ASN:HB2	1:L:175:TYR:HB3	1.68	0.74
1:J:142:LYS:CE	1:J:142:LYS:CG	2.66	0.74
1:O:111:ILE:HB	1:O:472:ILE:HB	1.69	0.74
1:L:69:VAL:HG23	1:L:498:VAL:HB	1.71	0.73
1:H:240:ILE:HG23	1:H:344:TYR:H	1.52	0.73
1:H:430:THR:HB	1:H:432:VAL:HG23	1.71	0.73
1:L:141:ASN:H	1:L:141:ASN:HD22	1.34	0.73
1:F:58:SER:OG	1:F:59:GLU:N	2.22	0.73
1:I:453:VAL:HG21	1:J:450:ILE:HG21	1.70	0.73
1:K:430:THR:HB	1:K:432:VAL:HG23	1.71	0.73
1:K:133:ASN:HB2	1:K:175:TYR:HB3	1.69	0.72
1:C:240:ILE:HG23	1:C:344:TYR:H	1.52	0.72
1:D:240:ILE:HG23	1:D:344:TYR:H	1.54	0.72
1:K:172:GLU:HB2	1:L:362:LEU:HD23	1.71	0.72
1:G:69:VAL:HG23	1:G:498:VAL:HB	1.71	0.72
1:N:381:MET:HE1	1:N:498:VAL:HG21	1.72	0.71
1:N:282:ASN:H	1:N:341:ARG:HG3	1.54	0.71
1:C:133:ASN:CB	1:C:175:TYR:HB3	2.20	0.71
1:M:142:LYS:CE	1:M:142:LYS:CG	2.67	0.71
1:O:162:LYS:CE	1:O:162:LYS:CG	2.68	0.71
1:A:58:SER:OG	1:A:59:GLU:N	2.24	0.71
1:J:133:ASN:HB2	1:J:175:TYR:CB	2.20	0.71
1:L:133:ASN:HB2	1:L:175:TYR:CB	2.20	0.71
1:C:489:PRO:O	1:D:262:ARG:NH1	2.24	0.71
1:C:238:PRO:HG2	1:C:362:LEU:CD1	2.21	0.70
1:I:58:SER:OG	1:I:59:GLU:N	2.22	0.70
1:B:84:TYR:CZ	1:C:268:GLN:HG3	2.26	0.70
1:G:133:ASN:CB	1:G:175:TYR:HB3	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ASP:OD1	1:C:73:ASP:N	2.18	0.70
1:H:155:LYS:NZ	1:H:155:LYS:CD	2.53	0.70
1:M:124:LYS:CG	1:M:124:LYS:CE	2.68	0.70
1:C:67:THR:OG1	1:C:68:ARG:N	2.23	0.70
1:M:416:GLN:OE1	1:N:415:ASP:HB3	1.92	0.70
1:O:136:GLU:HA	1:O:141:ASN:HD22	1.57	0.70
1:N:453:VAL:HG21	1:O:450:ILE:HG21	1.72	0.69
1:K:73:ASP:HB3	1:K:91:PHE:CE1	2.28	0.69
1:B:185:ASN:HA	1:B:188:ILE:HD12	1.74	0.69
1:D:430:THR:HB	1:D:432:VAL:HG23	1.73	0.69
1:O:470:ASN:OD1	1:O:470:ASN:N	2.24	0.69
1:I:240:ILE:HG23	1:I:344:TYR:H	1.58	0.69
1:K:422:LEU:CD1	1:K:422:LEU:CB	2.69	0.68
1:O:481:THR:OG1	1:O:485:ARG:HA	1.94	0.68
1:G:133:ASN:HB2	1:G:175:TYR:CB	2.17	0.68
1:N:356:ILE:O	1:N:360:THR:HG22	1.93	0.68
1:F:288:ASP:HA	1:F:319:LEU:HD12	1.76	0.68
1:D:288:ASP:HA	1:D:319:LEU:HD12	1.75	0.68
1:M:69:VAL:HG23	1:M:498:VAL:HB	1.76	0.68
1:L:453:VAL:HG21	1:M:450:ILE:HG21	1.76	0.68
1:N:430:THR:HB	1:N:432:VAL:HG23	1.75	0.68
1:G:57:TYR:OH	1:G:109:GLN:OE1	2.11	0.67
1:J:52:ARG:HB2	1:J:116:ARG:HD2	1.77	0.67
1:J:238:PRO:HG2	1:J:362:LEU:HD11	1.75	0.67
1:N:434:ASN:HD21	1:N:437:PRO:HB3	1.59	0.67
1:I:133:ASN:HB2	1:I:175:TYR:CB	2.24	0.67
1:N:382:MET:HG2	1:N:466:LEU:HD12	1.77	0.67
1:A:66:THR:OG1	1:A:500:PRO:O	2.10	0.66
1:C:113:LEU:HB3	1:C:119:TRP:CD1	2.30	0.66
1:D:185:ASN:HA	1:D:188:ILE:HD12	1.76	0.66
1:E:240:ILE:HG23	1:E:344:TYR:H	1.60	0.66
1:M:427:THR:HG22	1:M:428:SER:HB2	1.78	0.66
1:C:134:VAL:HA	1:C:140:THR:HB	1.78	0.66
1:C:356:ILE:O	1:C:360:THR:HG22	1.95	0.66
1:F:360:THR:OG1	1:F:361:LEU:N	2.28	0.66
1:J:356:ILE:O	1:J:360:THR:HG22	1.96	0.66
1:O:73:ASP:OD1	1:O:73:ASP:N	2.24	0.65
1:E:69:VAL:HG23	1:E:498:VAL:HB	1.78	0.65
1:K:422:LEU:CD2	1:K:422:LEU:HG	2.15	0.65
1:I:133:ASN:CB	1:I:175:TYR:HB3	2.26	0.65
1:J:124:LYS:CD	1:J:124:LYS:CB	2.72	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:325:LYS:CD	1:O:325:LYS:NZ	2.60	0.65
1:E:133:ASN:CB	1:E:175:TYR:HB3	2.15	0.65
1:F:238:PRO:HG2	1:F:362:LEU:CD1	2.25	0.65
1:E:88:HIS:HB2	1:E:491:VAL:O	1.97	0.65
1:E:157:LYS:CD	1:E:157:LYS:NZ	2.60	0.65
1:G:240:ILE:HG23	1:G:344:TYR:H	1.61	0.65
1:H:141:ASN:HD22	1:H:141:ASN:H	1.44	0.65
1:K:470:ASN:OD1	1:K:470:ASN:N	2.29	0.65
1:G:55:ILE:HG12	1:G:113:LEU:HD23	1.78	0.64
1:K:240:ILE:HG23	1:K:344:TYR:H	1.62	0.64
1:C:88:HIS:HB2	1:C:491:VAL:O	1.98	0.64
1:L:72:VAL:H	1:L:93:THR:HG21	1.62	0.64
1:J:136:GLU:HA	1:J:141:ASN:HD22	1.62	0.64
1:K:133:ASN:HB2	1:K:175:TYR:CB	2.27	0.64
1:B:133:ASN:CB	1:B:175:TYR:HB3	2.25	0.64
1:E:67:THR:OG1	1:E:68:ARG:N	2.29	0.64
1:J:142:LYS:CD	1:J:142:LYS:NZ	2.60	0.64
1:J:240:ILE:HG23	1:J:344:TYR:H	1.63	0.64
1:K:249:ASP:OD1	1:K:251:THR:HB	1.98	0.64
1:E:113:LEU:HB3	1:E:119:TRP:CD1	2.32	0.64
1:L:58:SER:OG	1:L:59:GLU:N	2.27	0.64
1:F:213:ARG:O	1:F:240:ILE:HD11	1.98	0.64
1:J:282:ASN:H	1:J:341:ARG:HG3	1.63	0.64
1:M:145:ALA:HB3	1:M:168:PHE:HE1	1.63	0.63
1:O:197:ARG:HG3	1:O:198:GLN:HE21	1.64	0.63
1:A:130:ASN:HB3	1:B:363:CYS:HB3	1.81	0.63
1:B:69:VAL:HG23	1:B:498:VAL:HB	1.81	0.63
1:A:133:ASN:CB	1:A:175:TYR:HB3	2.21	0.63
1:A:343:TRP:HE1	1:A:360:THR:HG21	1.63	0.63
1:A:326:ARG:HH11	1:A:326:ARG:HB3	1.64	0.63
1:D:88:HIS:HB2	1:D:491:VAL:O	2.00	0.62
1:N:58:SER:OG	1:N:59:GLU:N	2.26	0.62
1:A:203:GLU:HB2	1:A:326:ARG:HH12	1.63	0.62
1:I:326:ARG:HD2	1:I:439:ASN:HB2	1.81	0.62
1:F:198:GLN:HA	1:F:198:GLN:HE21	1.65	0.62
1:G:317:LYS:CD	1:G:317:LYS:NZ	2.61	0.62
1:H:331:ILE:HD13	1:H:339:GLN:HG2	1.82	0.62
1:K:363:CYS:HB3	1:O:130:ASN:HB3	1.80	0.62
1:L:401:GLY:HA3	1:L:463:HIS:HD2	1.64	0.62
1:F:69:VAL:HG23	1:F:498:VAL:HB	1.81	0.62
1:I:145:ALA:HB3	1:I:168:PHE:HE1	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:124:LYS:CD	1:M:124:LYS:CB	2.78	0.61
1:K:197:ARG:HG3	1:K:198:GLN:HE21	1.64	0.61
1:A:282:ASN:H	1:A:341:ARG:HG3	1.64	0.61
1:H:465:THR:HG21	1:H:501:ARG:HH11	1.65	0.61
1:I:185:ASN:HD21	1:I:210:PHE:H	1.46	0.61
1:A:430:THR:HB	1:A:432:VAL:HG23	1.83	0.61
1:L:67:THR:OG1	1:L:68:ARG:N	2.32	0.61
1:E:427:THR:HG22	1:E:428:SER:HB2	1.82	0.61
1:C:157:LYS:CD	1:C:157:LYS:CB	2.77	0.61
1:M:231:TYR:OH	1:M:284:PRO:O	2.12	0.61
1:D:254:ARG:HB3	1:D:369:CYS:HB3	1.82	0.61
1:H:326:ARG:HH11	1:H:326:ARG:HB3	1.64	0.61
1:A:238:PRO:HG2	1:A:362:LEU:CD1	2.31	0.61
1:N:238:PRO:HG2	1:N:362:LEU:HD11	1.82	0.61
1:O:150:SER:HB2	1:O:162:LYS:HB2	1.83	0.60
1:F:133:ASN:CB	1:F:175:TYR:HB3	2.28	0.60
1:N:212:THR:HA	1:N:239:ASP:HA	1.83	0.60
1:F:212:THR:HA	1:F:239:ASP:HA	1.83	0.60
1:G:102:SER:HB2	1:G:105:GLU:HB3	1.83	0.60
1:J:403:GLU:OE2	1:J:461:THR:OG1	2.18	0.60
1:N:381:MET:CE	1:N:498:VAL:HG21	2.31	0.60
1:M:342:SER:HB3	1:M:345:LEU:HG	1.84	0.60
1:K:231:TYR:OH	1:K:284:PRO:O	2.14	0.60
1:B:238:PRO:HG2	1:B:362:LEU:CD1	2.31	0.60
1:J:212:THR:HA	1:J:239:ASP:HA	1.84	0.60
1:J:88:HIS:HB2	1:J:491:VAL:O	2.02	0.60
1:E:472:ILE:HG22	1:E:476:GLN:HE21	1.66	0.60
1:C:389:ARG:HH11	1:L:389:ARG:NH1	2.00	0.59
1:A:238:PRO:HG2	1:A:362:LEU:HD11	1.83	0.59
1:I:212:THR:HA	1:I:239:ASP:HA	1.84	0.59
1:M:356:ILE:O	1:M:360:THR:HG22	2.03	0.59
1:O:212:THR:HA	1:O:239:ASP:HA	1.84	0.59
1:G:172:GLU:OE1	1:H:347:TYR:HE2	1.85	0.59
1:C:157:LYS:CE	1:C:157:LYS:HG3	2.32	0.59
1:M:212:THR:HA	1:M:239:ASP:HA	1.84	0.59
1:A:185:ASN:ND2	1:A:210:PHE:O	2.34	0.59
1:E:340:TYR:HD1	1:E:441:ILE:HD13	1.67	0.59
1:F:241:ILE:HD13	1:F:248:VAL:HG21	1.85	0.59
1:K:141:ASN:H	1:K:141:ASN:HD22	1.49	0.59
1:G:57:TYR:CD1	1:H:387:THR:HG22	2.38	0.59
1:L:102:SER:HB3	1:L:105:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:HA	1:E:239:ASP:HA	1.84	0.59
1:G:212:THR:HA	1:G:239:ASP:HA	1.85	0.59
1:M:403:GLU:OE2	1:M:461:THR:OG1	2.20	0.59
1:F:72:VAL:O	1:F:93:THR:OG1	2.20	0.59
1:H:133:ASN:CB	1:H:175:TYR:HB3	2.29	0.59
1:B:88:HIS:HB2	1:B:491:VAL:O	2.03	0.59
1:I:177:GLU:HG2	1:I:452:THR:H	1.67	0.59
1:L:212:THR:HA	1:L:239:ASP:HA	1.85	0.59
1:L:360:THR:OG1	1:L:361:LEU:N	2.35	0.59
1:B:238:PRO:HG2	1:B:362:LEU:HD11	1.84	0.58
1:G:203:GLU:O	1:G:206:ILE:HG12	2.02	0.58
1:N:240:ILE:HG23	1:N:344:TYR:H	1.67	0.58
1:A:144:LYS:NZ	1:A:144:LYS:CD	2.64	0.58
1:D:212:THR:HA	1:D:239:ASP:HA	1.84	0.58
1:D:324:LYS:NZ	1:D:324:LYS:CD	2.64	0.58
1:G:89:SER:HA	1:G:480:ILE:HG12	1.84	0.58
1:M:95:VAL:HG21	1:M:476:GLN:HG2	1.84	0.58
1:N:176:SER:O	1:N:180:THR:HB	2.03	0.58
1:I:88:HIS:HB2	1:I:491:VAL:O	2.04	0.58
1:E:322:ASP:HB2	1:E:328:TYR:HE2	1.69	0.58
1:K:422:LEU:CD2	1:K:422:LEU:CB	2.76	0.58
1:C:212:THR:HA	1:C:239:ASP:HA	1.85	0.58
1:J:73:ASP:OD1	1:J:73:ASP:N	2.33	0.58
1:G:427:THR:HG22	1:G:428:SER:HB2	1.86	0.58
1:M:88:HIS:HB2	1:M:491:VAL:O	2.04	0.58
1:M:282:ASN:H	1:M:341:ARG:HG3	1.66	0.58
1:N:104:GLY:O	1:N:107:SER:OG	2.18	0.58
1:J:57:TYR:OH	1:J:109:GLN:OE1	2.19	0.58
1:K:325:LYS:NZ	1:K:325:LYS:CD	2.66	0.58
1:F:419:TYR:HB3	1:F:422:LEU:HB2	1.86	0.58
1:M:72:VAL:O	1:M:93:THR:OG1	2.21	0.58
1:B:212:THR:HA	1:B:239:ASP:HA	1.85	0.57
1:D:241:ILE:HD12	1:D:273:ILE:HD11	1.85	0.57
1:E:83:ASN:HA	1:E:86:ASN:HD22	1.69	0.57
1:I:427:THR:HG22	1:I:428:SER:HB2	1.86	0.57
1:O:288:ASP:HA	1:O:319:LEU:HD12	1.85	0.57
1:A:212:THR:HA	1:A:239:ASP:HA	1.86	0.57
1:M:240:ILE:HG21	1:M:342:SER:OG	2.04	0.57
1:B:403:GLU:OE2	1:B:461:THR:OG1	2.21	0.57
1:K:212:THR:HA	1:K:239:ASP:HA	1.85	0.57
1:K:359:TRP:HD1	1:K:360:THR:HG22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:326:ARG:CD	1:O:439:ASN:HB2	2.34	0.57
1:I:213:ARG:O	1:I:240:ILE:HD11	2.05	0.57
1:L:240:ILE:HG21	1:L:342:SER:OG	2.03	0.57
1:K:134:VAL:HA	1:K:140:THR:HB	1.86	0.57
1:M:343:TRP:HH2	1:M:362:LEU:HD13	1.68	0.57
1:H:89:SER:HA	1:H:480:ILE:HG12	1.86	0.57
1:A:207:GLY:HA2	1:A:244:PRO:HD2	1.86	0.57
1:D:89:SER:HA	1:D:480:ILE:HG12	1.86	0.57
1:G:138:MET:HB3	1:G:254:ARG:HH12	1.69	0.57
1:J:135:ASN:HA	1:J:172:GLU:HG2	1.87	0.57
1:K:326:ARG:HD2	1:K:439:ASN:HB2	1.87	0.57
1:E:240:ILE:HD13	1:E:342:SER:OG	2.05	0.56
1:F:194:LYS:CD	1:F:194:LYS:NZ	2.68	0.56
1:H:185:ASN:HA	1:H:188:ILE:HD12	1.87	0.56
1:I:185:ASN:HA	1:I:188:ILE:HD12	1.86	0.56
1:F:207:GLY:HA2	1:F:244:PRO:HD2	1.87	0.56
1:K:69:VAL:HG23	1:K:498:VAL:HB	1.88	0.56
1:G:177:GLU:HG2	1:G:452:THR:H	1.69	0.56
1:G:381:MET:HB2	1:G:476:GLN:OE1	2.05	0.56
1:H:172:GLU:CB	1:I:362:LEU:HD23	2.36	0.56
1:H:212:THR:HA	1:H:239:ASP:HA	1.86	0.56
1:L:288:ASP:HA	1:L:319:LEU:HD12	1.88	0.56
1:L:254:ARG:HB3	1:L:369:CYS:HB3	1.85	0.56
1:B:100:ASP:HB2	1:C:389:ARG:HH21	1.69	0.56
1:F:402:ALA:HB3	1:J:497:ILE:HD11	1.87	0.56
1:H:134:VAL:HG13	1:H:140:THR:O	2.06	0.56
1:I:356:ILE:O	1:I:360:THR:HG22	2.05	0.56
1:E:220:ASP:HB2	1:E:227:MET:HG2	1.86	0.56
1:M:57:TYR:CD2	1:N:387:THR:HA	2.41	0.56
1:O:326:ARG:HD3	1:O:439:ASN:HB2	1.87	0.56
1:B:326:ARG:HH11	1:B:326:ARG:HB3	1.71	0.56
1:H:172:GLU:HB2	1:I:362:LEU:HD23	1.88	0.56
1:C:113:LEU:HB3	1:C:119:TRP:NE1	2.21	0.56
1:D:69:VAL:HG23	1:D:498:VAL:HB	1.88	0.56
1:F:434:ASN:HD21	1:F:437:PRO:HB3	1.71	0.56
1:G:381:MET:HG3	1:G:472:ILE:HD13	1.88	0.56
1:H:185:ASN:HD21	1:H:210:PHE:H	1.53	0.56
1:I:96:ILE:HA	1:J:387:THR:HG21	1.88	0.56
1:D:134:VAL:HA	1:D:140:THR:HB	1.88	0.55
1:F:102:SER:HB3	1:F:105:GLU:HB3	1.88	0.55
1:B:241:ILE:HD13	1:B:248:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:HIS:HB2	1:G:491:VAL:O	2.06	0.55
1:O:213:ARG:O	1:O:240:ILE:HD11	2.05	0.55
1:F:133:ASN:HD21	1:F:367:VAL:HG22	1.71	0.55
1:I:241:ILE:HD12	1:I:248:VAL:HG21	1.88	0.55
1:M:177:GLU:HG2	1:M:452:THR:H	1.70	0.55
1:C:58:SER:OG	1:C:59:GLU:N	2.39	0.55
1:K:57:TYR:OH	1:K:109:GLN:OE1	2.23	0.55
1:F:237:HIS:HB2	1:F:238:PRO:HD3	1.87	0.55
1:C:67:THR:HG1	1:C:68:ARG:H	1.55	0.55
1:O:251:THR:OG1	1:O:270:GLY:HA2	2.07	0.55
1:H:240:ILE:HG21	1:H:342:SER:OG	2.07	0.55
1:C:342:SER:HB3	1:C:345:LEU:HG	1.88	0.55
1:E:73:ASP:OD1	1:E:73:ASP:N	2.40	0.55
1:F:88:HIS:HB2	1:F:491:VAL:O	2.07	0.55
1:L:55:ILE:HG12	1:L:113:LEU:HD23	1.89	0.55
1:L:380:ASP:OD2	1:L:380:ASP:N	2.40	0.55
1:A:94:THR:HA	1:A:474:GLY:O	2.07	0.55
1:C:215:PHE:HB2	1:C:345:LEU:HD21	1.88	0.55
1:H:470:ASN:OD1	1:H:470:ASN:N	2.38	0.55
1:N:326:ARG:HH11	1:N:326:ARG:HB3	1.72	0.55
1:K:133:ASN:CB	1:K:175:TYR:HB3	2.37	0.54
1:M:94:THR:HA	1:M:474:GLY:O	2.07	0.54
1:N:401:GLY:HA3	1:N:463:HIS:HD2	1.72	0.54
1:O:67:THR:OG1	1:O:68:ARG:N	2.40	0.54
1:H:130:ASN:HB3	1:I:363:CYS:HB3	1.89	0.54
1:C:214:ASN:HB3	1:C:217:LEU:HD22	1.89	0.54
1:I:197:ARG:HE	1:I:198:GLN:HE22	1.54	0.54
1:J:176:SER:HB2	1:J:179:MET:HB3	1.88	0.54
1:B:57:TYR:OH	1:B:109:GLN:OE1	2.15	0.54
1:E:176:SER:HB3	1:E:179:MET:HB3	1.89	0.54
1:G:326:ARG:HD2	1:G:439:ASN:HB2	1.88	0.54
1:N:240:ILE:HG22	1:N:241:ILE:N	2.22	0.54
1:E:111:ILE:HB	1:E:472:ILE:HB	1.88	0.54
1:L:88:HIS:HB2	1:L:491:VAL:O	2.06	0.54
1:L:282:ASN:H	1:L:341:ARG:HG3	1.71	0.54
1:D:240:ILE:HG22	1:D:241:ILE:N	2.23	0.54
1:K:115:ASP:HA	1:K:470:ASN:HD22	1.73	0.54
1:B:96:ILE:HD12	1:B:474:GLY:HA3	1.90	0.54
1:D:282:ASN:H	1:D:341:ARG:HG3	1.72	0.54
1:I:275:TYR:CE1	1:I:341:ARG:HD3	2.42	0.54
1:L:133:ASN:CB	1:L:175:TYR:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:172:GLU:HB2	1:M:362:LEU:HD23	1.89	0.54
1:N:133:ASN:HD21	1:N:367:VAL:HG22	1.73	0.54
1:A:216:ARG:HG3	1:A:345:LEU:HD13	1.90	0.54
1:G:183:LEU:HD21	1:H:236:PHE:HE2	1.72	0.54
1:H:207:GLY:HA2	1:H:244:PRO:HD2	1.90	0.54
1:A:326:ARG:HD2	1:A:439:ASN:HB2	1.90	0.54
1:D:356:ILE:O	1:D:360:THR:HG22	2.08	0.54
1:J:138:MET:O	1:J:254:ARG:NH1	2.41	0.54
1:K:282:ASN:H	1:K:341:ARG:HG3	1.71	0.54
1:L:57:TYR:CD1	1:M:387:THR:HG22	2.43	0.54
1:F:282:ASN:H	1:F:341:ARG:HG3	1.73	0.54
1:L:94:THR:HA	1:L:474:GLY:O	2.08	0.54
1:A:89:SER:HA	1:A:480:ILE:HG12	1.89	0.53
1:C:94:THR:HA	1:C:474:GLY:O	2.08	0.53
1:G:313:LYS:CG	1:G:313:LYS:CE	2.81	0.53
1:J:124:LYS:CD	1:J:124:LYS:NZ	2.68	0.53
1:N:150:SER:HB2	1:N:162:LYS:HB2	1.90	0.53
1:B:220:ASP:HB2	1:B:227:MET:HG2	1.90	0.53
1:L:326:ARG:HD2	1:L:439:ASN:HB2	1.89	0.53
1:M:225:LEU:HD12	1:M:287:LEU:HD12	1.89	0.53
1:M:343:TRP:CH2	1:M:362:LEU:HD13	2.43	0.53
1:A:434:ASN:HD21	1:A:437:PRO:HB3	1.74	0.53
1:B:111:ILE:HB	1:B:472:ILE:HB	1.90	0.53
1:N:254:ARG:O	1:N:257:ASN:HB2	2.08	0.53
1:O:380:ASP:HB2	1:O:476:GLN:HE22	1.73	0.53
1:K:150:SER:HB2	1:K:162:LYS:HB2	1.91	0.53
1:N:207:GLY:HA2	1:N:244:PRO:HD2	1.91	0.53
1:D:172:GLU:HB2	1:E:362:LEU:HD23	1.91	0.53
1:L:497:ILE:HD11	1:M:402:ALA:HB3	1.89	0.53
1:D:131:MET:HA	1:D:490:TYR:CD2	2.44	0.53
1:I:94:THR:HA	1:I:474:GLY:O	2.09	0.53
1:L:207:GLY:HA2	1:L:244:PRO:HD2	1.91	0.53
1:M:67:THR:HG23	1:M:68:ARG:N	2.24	0.53
1:O:88:HIS:HB2	1:O:491:VAL:O	2.08	0.53
1:O:185:ASN:HA	1:O:188:ILE:HD12	1.91	0.53
1:D:275:TYR:CE1	1:D:341:ARG:HD3	2.44	0.53
1:H:58:SER:OG	1:H:59:GLU:N	2.41	0.53
1:I:136:GLU:HB2	1:I:172:GLU:OE2	2.08	0.53
1:L:481:THR:HB	1:L:485:ARG:HA	1.91	0.53
1:A:69:VAL:HG23	1:A:498:VAL:HB	1.90	0.53
1:D:382:MET:SD	1:D:382:MET:N	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:GLN:HE21	1:H:198:GLN:HA	1.74	0.53
1:D:427:THR:HG22	1:D:428:SER:HB2	1.91	0.52
1:F:238:PRO:HG2	1:F:362:LEU:HD11	1.90	0.52
1:F:389:ARG:NH2	1:J:98:ASN:HD21	2.06	0.52
1:G:69:VAL:CG2	1:G:498:VAL:HB	2.38	0.52
1:L:419:TYR:HB3	1:L:422:LEU:HB2	1.90	0.52
1:H:69:VAL:HG23	1:H:498:VAL:HB	1.91	0.52
1:O:427:THR:HG22	1:O:428:SER:HB2	1.91	0.52
1:A:362:LEU:HD23	1:E:172:GLU:HB2	1.90	0.52
1:G:273:ILE:HG21	1:G:356:ILE:HD11	1.90	0.52
1:H:94:THR:HA	1:H:474:GLY:O	2.09	0.52
1:N:326:ARG:HD3	1:N:439:ASN:HD22	1.75	0.52
1:E:126:ILE:HD12	1:E:495:LEU:HD23	1.92	0.52
1:F:340:TYR:CD1	1:F:441:ILE:HG21	2.45	0.52
1:C:213:ARG:O	1:C:240:ILE:HD11	2.10	0.52
1:J:135:ASN:OD1	1:J:136:GLU:N	2.43	0.52
1:J:238:PRO:HG2	1:J:362:LEU:CD1	2.40	0.52
1:L:113:LEU:HB3	1:L:119:TRP:CD1	2.45	0.52
1:N:95:VAL:HG21	1:N:476:GLN:HG2	1.92	0.52
1:B:377:SER:O	1:B:378:LEU:HD23	2.10	0.52
1:E:244:PRO:HA	1:E:275:TYR:CE1	2.45	0.52
1:K:88:HIS:HB2	1:K:491:VAL:O	2.09	0.52
1:O:102:SER:HB2	1:O:105:GLU:HB3	1.90	0.52
1:A:114:ASP:N	1:A:119:TRP:HE1	2.08	0.52
1:F:498:VAL:HG12	1:F:500:PRO:HD3	1.92	0.52
1:G:465:THR:HG21	1:G:501:ARG:HH11	1.74	0.52
1:H:203:GLU:HB2	1:H:326:ARG:HH12	1.75	0.52
1:M:172:GLU:HB2	1:N:362:LEU:HD23	1.91	0.52
1:B:360:THR:OG1	1:B:361:LEU:N	2.40	0.52
1:C:154:THR:HG22	1:C:157:LYS:HA	1.90	0.52
1:C:207:GLY:HA2	1:C:244:PRO:HD2	1.91	0.52
1:B:209:LYS:NZ	1:B:443:ALA:O	2.41	0.52
1:A:55:ILE:HG12	1:A:113:LEU:HD23	1.91	0.51
1:C:185:ASN:HA	1:C:188:ILE:HD12	1.91	0.51
1:E:381:MET:HE3	1:E:472:ILE:HG21	1.93	0.51
1:F:427:THR:HG22	1:F:428:SER:HB2	1.92	0.51
1:K:331:ILE:HD13	1:K:339:GLN:HG2	1.92	0.51
1:A:213:ARG:O	1:A:240:ILE:HD11	2.10	0.51
1:B:94:THR:HA	1:B:474:GLY:O	2.10	0.51
1:H:88:HIS:HB2	1:H:491:VAL:O	2.10	0.51
1:I:209:LYS:HB3	1:I:242:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ASP:HB2	1:I:242:LEU:HD11	1.92	0.51
1:M:238:PRO:HG2	1:M:362:LEU:CD1	2.40	0.51
1:N:239:ASP:OD1	1:N:259:LEU:HA	2.10	0.51
1:B:197:ARG:HG3	1:B:198:GLN:HE21	1.75	0.51
1:D:326:ARG:HD3	1:D:439:ASN:HB2	1.92	0.51
1:J:411:SER:HB3	1:J:452:THR:HG22	1.92	0.51
1:J:209:LYS:HD2	1:J:442:LEU:HA	1.92	0.51
1:N:238:PRO:HG2	1:N:362:LEU:CD1	2.40	0.51
1:D:326:ARG:HB3	1:D:326:ARG:HH11	1.75	0.51
1:G:57:TYR:HD2	1:G:60:LEU:HB2	1.76	0.51
1:J:240:ILE:HG22	1:J:241:ILE:N	2.26	0.51
1:M:97:GLN:HB2	1:N:388:PHE:CE2	2.46	0.51
1:M:264:ARG:NH1	1:M:357:ARG:O	2.44	0.51
1:N:88:HIS:HB2	1:N:491:VAL:O	2.10	0.51
1:N:145:ALA:HB3	1:N:168:PHE:HE1	1.75	0.51
1:I:69:VAL:CG2	1:I:498:VAL:HB	2.41	0.51
1:I:138:MET:HB3	1:I:254:ARG:HH12	1.74	0.51
1:B:96:ILE:HA	1:C:387:THR:HG21	1.93	0.51
1:C:83:ASN:HA	1:C:86:ASN:HB2	1.93	0.51
1:K:313:LYS:CG	1:K:313:LYS:CE	2.82	0.51
1:B:343:TRP:HH2	1:B:362:LEU:HD13	1.76	0.51
1:F:113:LEU:HB3	1:F:119:TRP:CD1	2.46	0.51
1:K:207:GLY:HA2	1:K:244:PRO:HD2	1.92	0.51
1:K:419:TYR:HB3	1:K:422:LEU:HB2	1.93	0.51
1:E:57:TYR:OH	1:E:109:GLN:OE1	2.19	0.51
1:E:213:ARG:O	1:E:240:ILE:HD11	2.10	0.51
1:E:340:TYR:CD1	1:E:441:ILE:HD13	2.45	0.51
1:F:94:THR:HA	1:F:474:GLY:O	2.11	0.51
1:K:102:SER:HB2	1:K:105:GLU:HB3	1.93	0.51
1:L:331:ILE:HD13	1:L:339:GLN:HG2	1.92	0.51
1:M:142:LYS:CD	1:M:142:LYS:NZ	2.74	0.51
1:N:94:THR:HA	1:N:474:GLY:O	2.11	0.51
1:D:94:THR:HA	1:D:474:GLY:O	2.10	0.50
1:H:72:VAL:H	1:H:93:THR:HG21	1.76	0.50
1:F:83:ASN:HA	1:F:86:ASN:HB2	1.93	0.50
1:G:94:THR:HA	1:G:474:GLY:O	2.11	0.50
1:M:96:ILE:HA	1:N:387:THR:HG21	1.93	0.50
1:O:52:ARG:HB3	1:O:114:ASP:OD2	2.11	0.50
1:J:57:TYR:CG	1:J:58:SER:N	2.78	0.50
1:K:225:LEU:HD12	1:K:287:LEU:HD12	1.93	0.50
1:O:207:GLY:HA2	1:O:244:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PHE:CD2	1:A:398:PRO:HA	2.47	0.50
1:F:236:PHE:HE2	1:J:183:LEU:HD21	1.76	0.50
1:I:240:ILE:HG12	1:I:344:TYR:HB2	1.93	0.50
1:J:470:ASN:HD21	1:J:506:ARG:HH22	1.59	0.50
1:K:481:THR:HB	1:K:485:ARG:HA	1.93	0.50
1:E:378:LEU:HD12	1:E:382:MET:HE2	1.94	0.50
1:M:207:GLY:HA2	1:M:244:PRO:HD2	1.93	0.50
1:N:213:ARG:O	1:N:240:ILE:HD11	2.12	0.50
1:O:136:GLU:HA	1:O:141:ASN:ND2	2.25	0.50
1:C:203:GLU:O	1:C:206:ILE:HG12	2.11	0.50
1:D:73:ASP:OD1	1:D:73:ASP:N	2.43	0.50
1:F:237:HIS:CD2	1:J:174:ASN:HA	2.46	0.50
1:I:470:ASN:N	1:I:470:ASN:OD1	2.44	0.50
1:J:207:GLY:HA2	1:J:244:PRO:HD2	1.94	0.50
1:N:237:HIS:O	1:N:239:ASP:OD2	2.29	0.50
1:O:237:HIS:HB2	1:O:238:PRO:HD3	1.94	0.50
1:A:113:LEU:HB3	1:A:119:TRP:CD1	2.46	0.50
1:F:244:PRO:HG3	1:F:340:TYR:HE2	1.76	0.50
1:J:94:THR:HA	1:J:474:GLY:O	2.12	0.50
1:B:254:ARG:HB3	1:B:369:CYS:HB3	1.94	0.50
1:D:57:TYR:CD1	1:E:387:THR:HG22	2.46	0.50
1:E:94:THR:HA	1:E:474:GLY:O	2.12	0.50
1:J:102:SER:HB3	1:J:105:GLU:HB3	1.93	0.50
1:L:403:GLU:OE2	1:L:461:THR:OG1	2.29	0.50
1:N:211:ASP:HB2	1:N:242:LEU:HD11	1.94	0.50
1:B:135:ASN:HB3	1:B:138:MET:HB2	1.94	0.50
1:B:258:LEU:HD22	1:B:367:VAL:HA	1.93	0.50
1:F:111:ILE:HB	1:F:472:ILE:HB	1.93	0.50
1:F:465:THR:O	1:J:68:ARG:NH2	2.45	0.50
1:G:141:ASN:H	1:G:141:ASN:HD22	1.60	0.50
1:L:57:TYR:CD2	1:M:387:THR:HA	2.47	0.50
1:N:113:LEU:HD22	1:N:119:TRP:CD2	2.47	0.50
1:B:326:ARG:HD3	1:B:439:ASN:HB2	1.94	0.49
1:D:172:GLU:CB	1:E:362:LEU:HD23	2.41	0.49
1:D:343:TRP:HE1	1:D:360:THR:HG21	1.77	0.49
1:E:133:ASN:HD21	1:E:367:VAL:HG22	1.77	0.49
1:L:177:GLU:HG2	1:L:452:THR:H	1.77	0.49
1:M:382:MET:N	1:M:382:MET:SD	2.85	0.49
1:G:492:TYR:CZ	1:H:262:ARG:HG3	2.46	0.49
1:N:133:ASN:HB2	1:N:175:TYR:HB2	1.91	0.49
1:D:154:THR:HG22	1:D:157:LYS:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:SER:OG	1:E:59:GLU:N	2.44	0.49
1:J:133:ASN:CB	1:J:175:TYR:HB3	2.38	0.49
1:B:172:GLU:HB2	1:C:362:LEU:HD23	1.95	0.49
1:E:240:ILE:HD13	1:E:342:SER:HG	1.78	0.49
1:G:57:TYR:CG	1:G:58:SER:N	2.80	0.49
1:G:244:PRO:HA	1:G:275:TYR:CD1	2.47	0.49
1:K:185:ASN:ND2	1:K:210:PHE:O	2.45	0.49
1:O:240:ILE:HD13	1:O:342:SER:OG	2.13	0.49
1:E:114:ASP:N	1:E:119:TRP:HE1	2.10	0.49
1:H:213:ARG:O	1:H:240:ILE:HD11	2.13	0.49
1:I:436:PHE:CD1	1:I:442:LEU:HB3	2.47	0.49
1:J:177:GLU:HG2	1:J:452:THR:H	1.77	0.49
1:K:237:HIS:HD2	1:O:174:ASN:HA	1.78	0.49
1:N:381:MET:HG2	1:N:468:LEU:HD11	1.94	0.49
1:B:102:SER:HB3	1:B:105:GLU:HB3	1.95	0.49
1:G:320:THR:HG23	1:G:321:GLU:HG3	1.94	0.49
1:L:141:ASN:H	1:L:141:ASN:ND2	2.07	0.49
1:D:258:LEU:HD23	1:D:369:CYS:SG	2.52	0.49
1:G:391:THR:HG21	1:G:396:ASN:HB3	1.94	0.49
1:I:57:TYR:CD2	1:J:387:THR:HA	2.47	0.49
1:K:240:ILE:HG22	1:K:241:ILE:N	2.28	0.49
1:A:111:ILE:HB	1:A:472:ILE:HB	1.94	0.49
1:B:154:THR:HG22	1:B:157:LYS:HA	1.95	0.49
1:B:240:ILE:CG2	1:B:344:TYR:H	2.22	0.49
1:M:71:LEU:HA	1:M:93:THR:HG21	1.95	0.49
1:B:242:LEU:HA	1:B:341:ARG:O	2.13	0.49
1:B:465:THR:HG21	1:B:501:ARG:HH11	1.77	0.49
1:E:203:GLU:O	1:E:206:ILE:HG12	2.13	0.49
1:I:197:ARG:HE	1:I:198:GLN:NE2	2.10	0.49
1:L:68:ARG:NH1	1:L:499:SER:OG	2.45	0.49
1:O:154:THR:HG22	1:O:157:LYS:HA	1.95	0.49
1:A:67:THR:HG21	1:B:386:VAL:HG13	1.95	0.48
1:A:419:TYR:HB3	1:A:422:LEU:HB2	1.95	0.48
1:B:58:SER:OG	1:B:59:GLU:N	2.42	0.48
1:F:57:TYR:OH	1:F:109:GLN:OE1	2.29	0.48
1:G:240:ILE:HG22	1:G:241:ILE:N	2.27	0.48
1:L:209:LYS:NZ	1:L:443:ALA:O	2.44	0.48
1:B:71:LEU:HA	1:B:93:THR:HG21	1.95	0.48
1:D:188:ILE:HD13	1:D:208:VAL:O	2.12	0.48
1:K:52:ARG:HG3	1:K:116:ARG:CZ	2.43	0.48
1:N:130:ASN:HB3	1:O:363:CYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HG3	1:A:198:GLN:HE21	1.78	0.48
1:F:278:LEU:HB3	1:F:341:ARG:HG2	1.93	0.48
1:G:185:ASN:ND2	1:G:210:PHE:O	2.46	0.48
1:G:207:GLY:HA2	1:G:244:PRO:HD2	1.94	0.48
1:N:439:ASN:ND2	1:N:442:LEU:HD23	2.27	0.48
1:H:145:ALA:HB1	1:H:208:VAL:HG11	1.96	0.48
1:J:144:LYS:HG2	1:J:167:GLU:HG3	1.95	0.48
1:K:497:ILE:HD11	1:L:402:ALA:HB3	1.94	0.48
1:N:375:TYR:HB3	1:N:399:VAL:HG13	1.93	0.48
1:D:130:ASN:HB3	1:E:363:CYS:HB3	1.94	0.48
1:F:481:THR:HB	1:F:485:ARG:HA	1.94	0.48
1:H:504:SER:HB2	1:H:505:SER:H	1.47	0.48
1:K:113:LEU:HB3	1:K:119:TRP:CD1	2.49	0.48
1:A:387:THR:HG22	1:E:57:TYR:CD1	2.48	0.48
1:B:286:LEU:HD23	1:B:286:LEU:HA	1.68	0.48
1:B:481:THR:HB	1:B:485:ARG:HA	1.95	0.48
1:C:242:LEU:HA	1:C:341:ARG:O	2.14	0.48
1:I:237:HIS:O	1:I:239:ASP:N	2.47	0.48
1:K:427:THR:HG22	1:K:428:SER:HB2	1.95	0.48
1:B:343:TRP:CH2	1:B:362:LEU:HD13	2.49	0.48
1:F:71:LEU:HA	1:F:93:THR:HG21	1.94	0.48
1:F:468:LEU:HD12	1:F:468:LEU:HA	1.61	0.48
1:K:359:TRP:CD1	1:K:360:THR:HG22	2.48	0.48
1:G:188:ILE:HG12	1:G:208:VAL:HG23	1.95	0.48
1:K:72:VAL:H	1:K:93:THR:HG21	1.79	0.48
1:L:213:ARG:O	1:L:240:ILE:HD11	2.14	0.48
1:L:391:THR:HG21	1:L:396:ASN:HB3	1.96	0.48
1:O:133:ASN:HB2	1:O:175:TYR:CB	2.26	0.48
1:B:174:ASN:ND2	1:B:183:LEU:HD23	2.29	0.48
1:I:397:PHE:HA	1:I:398:PRO:HD2	1.69	0.48
1:J:206:ILE:HD13	1:J:206:ILE:HA	1.69	0.48
1:K:94:THR:HA	1:K:474:GLY:O	2.13	0.48
1:M:320:THR:HA	1:M:330:LEU:HD11	1.96	0.48
1:D:343:TRP:CH2	1:D:362:LEU:HD13	2.49	0.48
1:D:391:THR:HG21	1:D:396:ASN:HB3	1.96	0.48
1:G:361:LEU:HD23	1:G:363:CYS:SG	2.54	0.48
1:H:239:ASP:HB2	1:H:259:LEU:HD23	1.96	0.48
1:O:242:LEU:HA	1:O:341:ARG:O	2.13	0.48
1:E:138:MET:O	1:E:254:ARG:HD3	2.14	0.47
1:E:240:ILE:HG22	1:E:241:ILE:N	2.29	0.47
1:H:102:SER:HB2	1:H:105:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:SER:HB3	1:I:105:GLU:HB3	1.95	0.47
1:K:91:PHE:CE2	1:K:478:VAL:HB	2.49	0.47
1:L:85:GLN:HE21	1:L:85:GLN:HB3	1.51	0.47
1:L:317:LYS:CD	1:L:317:LYS:NZ	2.74	0.47
1:M:342:SER:CB	1:M:345:LEU:HG	2.44	0.47
1:O:237:HIS:O	1:O:239:ASP:N	2.47	0.47
1:E:388:PHE:CD2	1:E:398:PRO:HA	2.49	0.47
1:F:237:HIS:O	1:F:239:ASP:N	2.48	0.47
1:G:133:ASN:HB3	1:G:134:VAL:H	1.37	0.47
1:H:237:HIS:O	1:H:239:ASP:N	2.47	0.47
1:I:185:ASN:HD21	1:I:210:PHE:N	2.11	0.47
1:K:453:VAL:HG21	1:L:450:ILE:HG21	1.96	0.47
1:N:154:THR:HG22	1:N:157:LYS:HA	1.96	0.47
1:N:241:ILE:HD12	1:N:273:ILE:HD11	1.96	0.47
1:D:111:ILE:HB	1:D:472:ILE:HB	1.95	0.47
1:H:237:HIS:CE1	1:H:448:PRO:HB3	2.48	0.47
1:B:203:GLU:HB2	1:B:326:ARG:HH12	1.79	0.47
1:K:177:GLU:HG2	1:K:452:THR:H	1.78	0.47
1:L:185:ASN:ND2	1:L:210:PHE:O	2.47	0.47
1:L:211:ASP:HB3	1:L:240:ILE:HD12	1.95	0.47
1:G:71:LEU:HA	1:G:93:THR:HG21	1.97	0.47
1:G:93:THR:HG22	1:G:95:VAL:HG22	1.96	0.47
1:J:67:THR:O	1:J:500:PRO:HD2	2.15	0.47
1:J:154:THR:HG22	1:J:157:LYS:HA	1.96	0.47
1:L:453:VAL:HG11	1:M:450:ILE:HD13	1.96	0.47
1:M:237:HIS:O	1:M:239:ASP:N	2.47	0.47
1:N:111:ILE:HB	1:N:472:ILE:HB	1.95	0.47
1:B:136:GLU:OE1	1:C:357:ARG:NH1	2.47	0.47
1:B:400:VAL:HB	1:B:466:LEU:HD13	1.97	0.47
1:C:282:ASN:H	1:C:341:ARG:HG3	1.80	0.47
1:D:242:LEU:HA	1:D:341:ARG:O	2.15	0.47
1:D:383:GLN:HE21	1:D:467:PRO:HB2	1.79	0.47
1:E:144:LYS:NZ	1:E:144:LYS:CD	2.72	0.47
1:F:450:ILE:HG21	1:J:453:VAL:HG21	1.97	0.47
1:G:67:THR:HG21	1:H:386:VAL:HG13	1.97	0.47
1:N:492:TYR:CZ	1:O:262:ARG:HG3	2.49	0.47
1:A:237:HIS:O	1:A:239:ASP:N	2.47	0.47
1:A:254:ARG:HB3	1:A:369:CYS:HB3	1.95	0.47
1:B:243:LEU:HD13	1:B:247:GLY:HA2	1.96	0.47
1:B:381:MET:HG3	1:B:472:ILE:HD13	1.97	0.47
1:B:391:THR:HG21	1:B:396:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TYR:CD2	1:D:387:THR:HA	2.49	0.47
1:C:238:PRO:CG	1:C:362:LEU:HD11	2.38	0.47
1:D:241:ILE:HD13	1:D:248:VAL:HG21	1.97	0.47
1:F:133:ASN:HB2	1:F:175:TYR:HB2	1.92	0.47
1:F:220:ASP:HB2	1:F:227:MET:HG2	1.97	0.47
1:F:244:PRO:HG3	1:F:340:TYR:CE2	2.50	0.47
1:H:241:ILE:HD12	1:H:273:ILE:HD11	1.95	0.47
1:I:216:ARG:HG3	1:I:345:LEU:HD13	1.96	0.47
1:J:185:ASN:ND2	1:J:210:PHE:O	2.48	0.47
1:K:348:ASN:OD1	1:O:171:PRO:HA	2.14	0.47
1:K:379:PRO:HB3	1:K:398:PRO:HG2	1.97	0.47
1:L:133:ASN:HB2	1:L:175:TYR:HB2	1.93	0.47
1:M:154:THR:HG22	1:M:157:LYS:HA	1.97	0.47
1:M:242:LEU:HA	1:M:341:ARG:O	2.15	0.47
1:N:386:VAL:O	1:N:387:THR:OG1	2.28	0.47
1:C:436:PHE:CD1	1:C:442:LEU:HB3	2.50	0.47
1:D:237:HIS:O	1:D:239:ASP:N	2.48	0.47
1:G:120:GLY:O	1:G:500:PRO:HA	2.15	0.47
1:J:343:TRP:CH2	1:J:362:LEU:HD13	2.50	0.47
1:L:254:ARG:NH2	1:L:368:THR:O	2.48	0.47
1:N:237:HIS:O	1:N:239:ASP:N	2.47	0.47
1:O:424:ARG:HH21	1:O:444:ARG:HB2	1.80	0.47
1:F:242:LEU:HA	1:F:341:ARG:O	2.15	0.47
1:I:251:THR:OG1	1:I:270:GLY:HA2	2.14	0.47
1:J:286:LEU:HA	1:J:286:LEU:HD23	1.67	0.47
1:M:185:ASN:ND2	1:M:210:PHE:O	2.47	0.47
1:B:427:THR:HG22	1:B:428:SER:HB2	1.96	0.47
1:E:237:HIS:O	1:E:239:ASP:N	2.48	0.47
1:H:388:PHE:CD2	1:H:398:PRO:HA	2.50	0.47
1:L:186:ASN:ND2	1:L:190:GLU:HG3	2.30	0.47
1:O:52:ARG:HG3	1:O:116:ARG:HE	1.79	0.47
1:O:439:ASN:O	1:O:443:ALA:HB2	2.15	0.47
1:A:262:ARG:NH1	1:E:489:PRO:O	2.48	0.46
1:J:211:ASP:HB2	1:J:242:LEU:HD11	1.97	0.46
1:K:237:HIS:O	1:K:239:ASP:N	2.49	0.46
1:L:89:SER:HB2	1:L:480:ILE:HB	1.96	0.46
1:M:133:ASN:HB3	1:M:175:TYR:HB3	1.95	0.46
1:C:254:ARG:O	1:C:257:ASN:HB2	2.15	0.46
1:F:391:THR:HG21	1:F:396:ASN:HB3	1.97	0.46
1:H:67:THR:O	1:H:500:PRO:HD2	2.15	0.46
1:J:384:ASP:HA	1:J:385:PRO:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:ASP:OD1	1:M:73:ASP:N	2.46	0.46
1:N:244:PRO:HA	1:N:275:TYR:CE1	2.50	0.46
1:A:391:THR:HG21	1:A:396:ASN:HB3	1.96	0.46
1:B:120:GLY:O	1:B:500:PRO:HA	2.16	0.46
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.70	0.46
1:F:397:PHE:HA	1:F:398:PRO:HD2	1.55	0.46
1:G:343:TRP:CH2	1:G:362:LEU:HD13	2.50	0.46
1:J:237:HIS:O	1:J:239:ASP:N	2.48	0.46
1:K:242:LEU:HA	1:K:341:ARG:O	2.16	0.46
1:N:343:TRP:CH2	1:N:362:LEU:HD13	2.51	0.46
1:O:176:SER:HB2	1:O:179:MET:HB3	1.96	0.46
1:A:150:SER:HB2	1:A:162:LYS:HB2	1.97	0.46
1:B:397:PHE:HA	1:B:398:PRO:HD2	1.62	0.46
1:C:75:LYS:O	1:C:79:VAL:HG23	2.16	0.46
1:E:242:LEU:HA	1:E:341:ARG:O	2.15	0.46
1:H:188:ILE:HD11	1:H:210:PHE:CE1	2.51	0.46
1:I:282:ASN:H	1:I:341:ARG:HG3	1.80	0.46
1:L:237:HIS:O	1:L:239:ASP:N	2.49	0.46
1:O:94:THR:HA	1:O:474:GLY:O	2.14	0.46
1:O:254:ARG:O	1:O:257:ASN:HB2	2.16	0.46
1:A:394:ILE:HA	1:A:397:PHE:CE2	2.50	0.46
1:B:470:ASN:OD1	1:B:470:ASN:N	2.47	0.46
1:E:206:ILE:HD13	1:E:206:ILE:HA	1.80	0.46
1:E:241:ILE:HD11	1:E:261:ILE:HD12	1.98	0.46
1:E:283:ILE:HD11	1:E:441:ILE:HG12	1.96	0.46
1:F:111:ILE:HD13	1:F:111:ILE:HA	1.82	0.46
1:H:288:ASP:HA	1:H:319:LEU:HD12	1.97	0.46
1:K:397:PHE:HA	1:K:398:PRO:HD2	1.67	0.46
1:K:492:TYR:CZ	1:L:262:ARG:HG3	2.50	0.46
1:N:242:LEU:HA	1:N:341:ARG:O	2.14	0.46
1:A:242:LEU:HA	1:A:341:ARG:O	2.15	0.46
1:B:237:HIS:O	1:B:239:ASP:N	2.48	0.46
1:C:237:HIS:O	1:C:239:ASP:N	2.48	0.46
1:G:237:HIS:HB2	1:G:238:PRO:HD3	1.96	0.46
1:J:83:ASN:HA	1:J:86:ASN:HD22	1.80	0.46
1:A:88:HIS:HB2	1:A:491:VAL:O	2.16	0.46
1:G:220:ASP:HB2	1:G:227:MET:HG2	1.97	0.46
1:I:67:THR:OG1	1:I:68:ARG:N	2.47	0.46
1:I:215:PHE:HB2	1:I:345:LEU:HD21	1.97	0.46
1:I:242:LEU:HA	1:I:341:ARG:O	2.15	0.46
1:K:120:GLY:O	1:K:500:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:251:THR:OG1	1:N:270:GLY:HA2	2.15	0.46
1:A:83:ASN:HA	1:A:86:ASN:HB2	1.98	0.46
1:C:120:GLY:O	1:C:500:PRO:HA	2.16	0.46
1:G:242:LEU:HA	1:G:341:ARG:O	2.14	0.46
1:I:455:GLU:OE1	1:J:411:SER:OG	2.34	0.46
1:J:120:GLY:O	1:J:500:PRO:HA	2.16	0.46
1:J:242:LEU:HA	1:J:341:ARG:O	2.16	0.46
1:N:343:TRP:CD1	1:N:356:ILE:HD13	2.50	0.46
1:O:240:ILE:HG21	1:O:342:SER:OG	2.15	0.46
1:A:120:GLY:O	1:A:500:PRO:HA	2.16	0.46
1:C:492:TYR:OH	1:D:262:ARG:HB2	2.16	0.46
1:C:504:SER:HB2	1:C:505:SER:H	1.47	0.46
1:D:207:GLY:HA2	1:D:244:PRO:HD2	1.97	0.46
1:I:100:ASP:HB2	1:J:389:ARG:HH21	1.81	0.46
1:I:380:ASP:N	1:I:380:ASP:OD1	2.48	0.46
1:L:242:LEU:HA	1:L:341:ARG:O	2.16	0.46
1:A:326:ARG:CD	1:A:439:ASN:HB2	2.45	0.46
1:G:185:ASN:HD21	1:G:210:PHE:H	1.64	0.46
1:A:397:PHE:HA	1:A:398:PRO:HD2	1.59	0.45
1:B:240:ILE:HD13	1:B:342:SER:OG	2.15	0.45
1:D:66:THR:CB	1:D:500:PRO:O	2.57	0.45
1:E:238:PRO:HG2	1:E:362:LEU:HD11	1.97	0.45
1:F:120:GLY:O	1:F:500:PRO:HA	2.16	0.45
1:F:216:ARG:HB2	1:F:345:LEU:HD22	1.98	0.45
1:F:286:LEU:HA	1:F:286:LEU:HD23	1.69	0.45
1:H:215:PHE:HE1	1:H:242:LEU:HD21	1.81	0.45
1:I:96:ILE:HD12	1:I:474:GLY:HA3	1.97	0.45
1:I:174:ASN:HA	1:J:237:HIS:HD2	1.81	0.45
1:K:482:ASP:CG	1:K:483:ALA:N	2.69	0.45
1:M:497:ILE:HD11	1:N:402:ALA:HB3	1.98	0.45
1:N:120:GLY:O	1:N:500:PRO:HA	2.16	0.45
1:N:343:TRP:HH2	1:N:362:LEU:HD13	1.80	0.45
1:F:154:THR:HG22	1:F:157:LYS:HA	1.98	0.45
1:F:192:TYR:CZ	1:F:197:ARG:HB3	2.51	0.45
1:G:135:ASN:HA	1:G:172:GLU:HG2	1.97	0.45
1:O:57:TYR:CG	1:O:58:SER:N	2.81	0.45
1:C:83:ASN:HA	1:C:86:ASN:HD22	1.81	0.45
1:C:288:ASP:HB3	1:C:291:ALA:HB3	1.99	0.45
1:D:111:ILE:HD13	1:D:111:ILE:HA	1.84	0.45
1:G:83:ASN:HA	1:G:86:ASN:HD22	1.81	0.45
1:G:215:PHE:O	1:G:217:LEU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:THR:OG1	1:H:68:ARG:N	2.48	0.45
1:I:240:ILE:HG22	1:I:241:ILE:N	2.31	0.45
1:K:492:TYR:CE2	1:L:262:ARG:HG3	2.51	0.45
1:L:226:VAL:HG12	1:L:228:PRO:HD2	1.98	0.45
1:N:113:LEU:HB3	1:N:119:TRP:CD1	2.51	0.45
1:O:239:ASP:N	1:O:239:ASP:OD1	2.43	0.45
1:A:399:VAL:HG12	1:E:70:TYR:OH	2.17	0.45
1:C:135:ASN:HB3	1:C:138:MET:HB2	1.99	0.45
1:C:176:SER:HB2	1:C:179:MET:HB3	1.97	0.45
1:D:119:TRP:HD1	1:D:470:ASN:HD22	1.64	0.45
1:G:188:ILE:HD11	1:G:210:PHE:HE1	1.80	0.45
1:M:208:VAL:HG12	1:M:243:LEU:HD22	1.98	0.45
1:B:453:VAL:HG21	1:C:450:ILE:HG21	1.98	0.45
1:C:397:PHE:HA	1:C:398:PRO:HD2	1.61	0.45
1:F:177:GLU:HG2	1:F:452:THR:H	1.81	0.45
1:F:254:ARG:O	1:F:257:ASN:HB2	2.16	0.45
1:G:220:ASP:OD2	1:G:220:ASP:CB	2.60	0.45
1:H:120:GLY:O	1:H:500:PRO:HA	2.17	0.45
1:H:128:HIS:HE1	1:I:366:ASP:OD2	1.98	0.45
1:K:67:THR:O	1:K:500:PRO:HD2	2.17	0.45
1:M:213:ARG:O	1:M:240:ILE:HD11	2.16	0.45
1:M:238:PRO:HG2	1:M:362:LEU:HD11	1.98	0.45
1:N:504:SER:HB2	1:N:505:SER:H	1.49	0.45
1:A:58:SER:HG	1:A:59:GLU:H	1.60	0.45
1:A:439:ASN:O	1:A:443:ALA:HB2	2.16	0.45
1:B:331:ILE:HD13	1:B:339:GLN:HG2	1.98	0.45
1:F:52:ARG:HG3	1:F:116:ARG:NH2	2.32	0.45
1:F:420:SER:HA	1:F:423:ILE:HD12	1.98	0.45
1:I:192:TYR:CZ	1:I:197:ARG:HB3	2.52	0.45
1:J:133:ASN:HB3	1:J:134:VAL:H	1.43	0.45
1:J:215:PHE:H	1:J:345:LEU:HD21	1.82	0.45
1:J:220:ASP:HB2	1:J:227:MET:HG2	1.99	0.45
1:N:52:ARG:HG3	1:N:116:ARG:NH1	2.32	0.45
1:N:96:ILE:HA	1:O:387:THR:HG21	1.98	0.45
1:D:133:ASN:HB3	1:D:134:VAL:H	1.40	0.45
1:G:343:TRP:HH2	1:G:362:LEU:HD13	1.80	0.45
1:H:220:ASP:HB2	1:H:227:MET:HG2	1.99	0.45
1:J:251:THR:OG1	1:J:270:GLY:HA2	2.17	0.45
1:K:171:PRO:HA	1:L:348:ASN:OD1	2.17	0.45
1:O:323:SER:HB3	1:O:438:GLU:HB2	1.97	0.45
1:O:450:ILE:H	1:O:450:ILE:HG13	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:O	1:A:217:LEU:N	2.50	0.45
1:B:207:GLY:HA2	1:B:244:PRO:HD2	1.99	0.45
1:C:389:ARG:HD2	1:L:389:ARG:CZ	2.47	0.45
1:D:326:ARG:CD	1:D:439:ASN:HB2	2.47	0.45
1:J:391:THR:HG21	1:J:396:ASN:HB3	1.99	0.45
1:K:504:SER:HB2	1:K:505:SER:H	1.47	0.45
1:B:331:ILE:H	1:B:331:ILE:HG12	1.66	0.45
1:D:57:TYR:CG	1:D:58:SER:N	2.85	0.45
1:E:152:SER:OG	1:E:159:VAL:HA	2.16	0.45
1:F:504:SER:HB2	1:F:505:SER:H	1.56	0.45
1:G:183:LEU:HD21	1:H:236:PHE:CE2	2.51	0.45
1:H:388:PHE:HD2	1:H:398:PRO:HA	1.82	0.45
1:I:120:GLY:O	1:I:500:PRO:HA	2.17	0.45
1:J:240:ILE:HD13	1:J:342:SER:OG	2.16	0.45
1:N:135:ASN:OD1	1:N:136:GLU:N	2.50	0.45
1:N:288:ASP:HA	1:N:319:LEU:HD12	1.98	0.45
1:N:419:TYR:HB3	1:N:422:LEU:HB2	1.98	0.45
1:C:414:ASN:HD21	1:D:415:ASP:HB2	1.82	0.45
1:E:286:LEU:HD23	1:E:286:LEU:HA	1.77	0.45
1:F:264:ARG:HD2	1:F:360:THR:O	2.16	0.45
1:G:237:HIS:O	1:G:239:ASP:N	2.50	0.45
1:G:450:ILE:H	1:G:450:ILE:HG13	1.64	0.45
1:I:55:ILE:HG12	1:I:113:LEU:HD23	1.99	0.45
1:I:207:GLY:HA2	1:I:244:PRO:HD2	1.97	0.45
1:K:386:VAL:O	1:K:387:THR:OG1	2.27	0.45
1:L:71:LEU:HA	1:L:71:LEU:HD23	1.81	0.45
1:D:120:GLY:O	1:D:500:PRO:HA	2.18	0.44
1:D:150:SER:HB2	1:D:162:LYS:HB2	1.98	0.44
1:E:326:ARG:CD	1:E:439:ASN:HB2	2.42	0.44
1:F:74:ASN:HB2	1:G:373:GLN:HE22	1.83	0.44
1:G:206:ILE:HD13	1:G:206:ILE:HA	1.93	0.44
1:G:213:ARG:O	1:G:240:ILE:HD11	2.16	0.44
1:K:213:ARG:O	1:K:240:ILE:HD11	2.17	0.44
1:N:481:THR:HB	1:N:485:ARG:HA	1.98	0.44
1:O:343:TRP:HE1	1:O:360:THR:HG21	1.82	0.44
1:A:72:VAL:H	1:A:93:THR:HG21	1.82	0.44
1:D:342:SER:HB3	1:D:345:LEU:HG	1.99	0.44
1:E:72:VAL:HG12	1:E:495:LEU:HD11	1.99	0.44
1:J:192:TYR:CZ	1:J:197:ARG:HB3	2.52	0.44
1:L:215:PHE:O	1:L:217:LEU:N	2.50	0.44
1:L:379:PRO:HD2	1:L:380:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:GLY:O	1:M:500:PRO:HA	2.18	0.44
1:O:322:ASP:OD2	1:O:328:TYR:OH	2.34	0.44
1:A:177:GLU:HG2	1:A:452:THR:H	1.82	0.44
1:C:237:HIS:HB2	1:C:238:PRO:HD3	1.99	0.44
1:H:57:TYR:CD1	1:I:387:THR:HG22	2.52	0.44
1:I:111:ILE:HD13	1:I:111:ILE:HA	1.89	0.44
1:K:70:TYR:HE1	1:L:399:VAL:HB	1.81	0.44
1:M:400:VAL:HB	1:M:466:LEU:HD13	1.98	0.44
1:A:226:VAL:HG21	1:A:231:TYR:CE2	2.53	0.44
1:C:133:ASN:HD21	1:C:367:VAL:HG22	1.82	0.44
1:H:57:TYR:CD2	1:I:387:THR:HA	2.51	0.44
1:I:69:VAL:HG23	1:I:498:VAL:HB	1.99	0.44
1:L:323:SER:HB3	1:L:438:GLU:HB2	1.99	0.44
1:M:356:ILE:HG12	1:M:359:TRP:HB3	1.98	0.44
1:O:120:GLY:O	1:O:500:PRO:HA	2.17	0.44
1:E:215:PHE:HB2	1:E:345:LEU:HD21	1.99	0.44
1:E:251:THR:OG1	1:E:270:GLY:HA2	2.17	0.44
1:G:288:ASP:HA	1:G:319:LEU:HD12	1.99	0.44
1:I:154:THR:HG22	1:I:157:LYS:HA	1.99	0.44
1:I:244:PRO:HA	1:I:275:TYR:CE1	2.52	0.44
1:M:113:LEU:HB3	1:M:119:TRP:CD1	2.52	0.44
1:B:135:ASN:HD22	1:B:138:MET:HG2	1.83	0.44
1:B:208:VAL:HG12	1:B:243:LEU:HD22	1.99	0.44
1:E:495:LEU:HD12	1:E:495:LEU:HA	1.77	0.44
1:G:323:SER:HB3	1:G:438:GLU:HB2	1.99	0.44
1:H:100:ASP:HB2	1:I:389:ARG:HH21	1.83	0.44
1:H:215:PHE:O	1:H:217:LEU:N	2.51	0.44
1:L:120:GLY:O	1:L:500:PRO:HA	2.16	0.44
1:B:380:ASP:OD2	1:B:380:ASP:N	2.51	0.44
1:D:331:ILE:H	1:D:331:ILE:HG12	1.64	0.44
1:E:419:TYR:HB3	1:E:422:LEU:HB2	1.98	0.44
1:F:89:SER:HA	1:F:480:ILE:HG12	2.00	0.44
1:G:441:ILE:HG22	1:G:442:LEU:HD13	2.00	0.44
1:H:206:ILE:HD13	1:H:206:ILE:HA	1.79	0.44
1:I:83:ASN:HA	1:I:86:ASN:HD22	1.82	0.44
1:J:85:GLN:HE21	1:J:85:GLN:HB3	1.69	0.44
1:M:251:THR:OG1	1:M:270:GLY:HA2	2.17	0.44
1:B:174:ASN:HA	1:C:237:HIS:HD2	1.83	0.44
1:C:70:TYR:OH	1:D:399:VAL:HG12	2.18	0.44
1:C:388:PHE:CD2	1:C:398:PRO:HA	2.53	0.44
1:E:120:GLY:O	1:E:500:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:ARG:HB2	1:J:492:TYR:OH	2.17	0.44
1:H:150:SER:HB2	1:H:162:LYS:HB2	1.99	0.44
1:H:397:PHE:HA	1:H:398:PRO:HD2	1.66	0.44
1:N:174:ASN:HA	1:O:237:HIS:CD2	2.53	0.44
1:O:57:TYR:OH	1:O:109:GLN:OE1	2.27	0.44
1:A:203:GLU:O	1:A:206:ILE:HG12	2.18	0.44
1:B:215:PHE:O	1:B:217:LEU:N	2.51	0.44
1:B:283:ILE:HD13	1:B:441:ILE:HD11	2.00	0.44
1:E:377:SER:O	1:E:378:LEU:HD23	2.17	0.44
1:F:439:ASN:O	1:F:443:ALA:HB2	2.18	0.44
1:J:397:PHE:HA	1:J:398:PRO:HD2	1.70	0.44
1:K:498:VAL:HG12	1:K:500:PRO:HD3	2.00	0.44
1:L:55:ILE:HD13	1:L:67:THR:HG22	1.99	0.44
1:L:240:ILE:CG2	1:L:344:TYR:H	2.27	0.44
1:M:286:LEU:HA	1:M:286:LEU:HD23	1.62	0.44
1:M:439:ASN:O	1:M:443:ALA:HB2	2.18	0.44
1:E:177:GLU:HG2	1:E:452:THR:H	1.82	0.43
1:E:207:GLY:HA2	1:E:244:PRO:HD2	1.99	0.43
1:G:155:LYS:HD3	1:G:155:LYS:HA	1.85	0.43
1:G:470:ASN:N	1:G:470:ASN:OD1	2.50	0.43
1:H:242:LEU:HA	1:H:341:ARG:O	2.18	0.43
1:H:455:GLU:OE1	1:I:411:SER:OG	2.29	0.43
1:I:215:PHE:O	1:I:217:LEU:N	2.51	0.43
1:K:215:PHE:O	1:K:217:LEU:N	2.51	0.43
1:K:243:LEU:HD22	1:K:247:GLY:HA2	1.99	0.43
1:M:215:PHE:O	1:M:217:LEU:N	2.51	0.43
1:O:223:THR:HG22	1:O:225:LEU:HD12	1.99	0.43
1:A:96:ILE:HA	1:B:387:THR:HG21	1.98	0.43
1:A:129:THR:OG1	1:A:406:PRO:HG2	2.18	0.43
1:A:206:ILE:HD13	1:A:206:ILE:HA	1.82	0.43
1:B:240:ILE:HG22	1:B:241:ILE:N	2.33	0.43
1:C:379:PRO:HB3	1:C:398:PRO:HG2	1.99	0.43
1:E:113:LEU:HB2	1:E:470:ASN:HA	2.00	0.43
1:E:439:ASN:O	1:E:443:ALA:HB2	2.18	0.43
1:F:381:MET:HG2	1:F:468:LEU:HD11	1.98	0.43
1:G:188:ILE:HD11	1:G:210:PHE:CE1	2.53	0.43
1:H:286:LEU:HD23	1:H:286:LEU:HA	1.65	0.43
1:L:238:PRO:HG2	1:L:362:LEU:CD1	2.48	0.43
1:B:83:ASN:HA	1:B:86:ASN:HB2	2.00	0.43
1:B:381:MET:HB2	1:B:476:GLN:OE1	2.18	0.43
1:E:146:ARG:HD2	1:E:246:CYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:LEU:HD13	1:E:247:GLY:HA2	2.01	0.43
1:H:343:TRP:HH2	1:H:362:LEU:HD13	1.82	0.43
1:I:489:PRO:O	1:J:262:ARG:NH1	2.50	0.43
1:K:138:MET:HB3	1:K:254:ARG:HH12	1.83	0.43
1:L:383:GLN:HB2	1:L:467:PRO:HG2	2.00	0.43
1:F:133:ASN:HB3	1:F:134:VAL:H	1.42	0.43
1:F:251:THR:OG1	1:F:270:GLY:HA2	2.18	0.43
1:F:326:ARG:CD	1:F:439:ASN:HB2	2.45	0.43
1:I:68:ARG:NH2	1:J:465:THR:O	2.51	0.43
1:I:113:LEU:HB3	1:I:119:TRP:CD1	2.52	0.43
1:I:367:VAL:HG12	1:I:409:SER:HB2	2.01	0.43
1:O:215:PHE:O	1:O:217:LEU:N	2.51	0.43
1:D:116:ARG:HE	1:D:116:ARG:HB2	1.65	0.43
1:D:215:PHE:O	1:D:217:LEU:N	2.51	0.43
1:D:244:PRO:HA	1:D:275:TYR:CE1	2.53	0.43
1:F:363:CYS:HB3	1:J:130:ASN:HB3	1.99	0.43
1:G:243:LEU:HD22	1:G:247:GLY:HA2	2.00	0.43
1:H:240:ILE:HG22	1:H:241:ILE:N	2.34	0.43
1:I:52:ARG:HB2	1:I:116:ARG:HD2	2.00	0.43
1:N:439:ASN:O	1:N:443:ALA:HB2	2.17	0.43
1:B:52:ARG:HB2	1:B:116:ARG:HD2	2.01	0.43
1:E:83:ASN:HA	1:E:86:ASN:HB2	2.00	0.43
1:F:57:TYR:CG	1:F:58:SER:N	2.86	0.43
1:F:241:ILE:HG23	1:F:243:LEU:HD21	2.01	0.43
1:J:241:ILE:HD12	1:J:273:ILE:HD11	2.00	0.43
1:K:211:ASP:HB2	1:K:242:LEU:HD11	2.01	0.43
1:K:322:ASP:OD2	1:K:328:TYR:OH	2.26	0.43
1:N:240:ILE:HG21	1:N:342:SER:OG	2.17	0.43
1:O:130:ASN:HD22	1:O:130:ASN:HA	1.57	0.43
1:B:238:PRO:HG2	1:B:362:LEU:HD12	2.00	0.43
1:C:296:LEU:HD11	1:C:313:LYS:HG2	2.00	0.43
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.74	0.43
1:F:171:PRO:HA	1:G:348:ASN:CG	2.39	0.43
1:H:172:GLU:HB3	1:I:362:LEU:HD23	2.01	0.43
1:J:135:ASN:HB3	1:J:138:MET:HB2	2.01	0.43
1:M:453:VAL:HG21	1:N:450:ILE:HG21	1.99	0.43
1:N:282:ASN:N	1:N:341:ARG:HG3	2.28	0.43
1:B:240:ILE:HG12	1:B:344:TYR:HB2	2.00	0.43
1:C:114:ASP:N	1:C:119:TRP:HE1	2.17	0.43
1:C:326:ARG:HB2	1:C:439:ASN:HD22	1.84	0.43
1:E:282:ASN:H	1:E:341:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:PHE:O	1:F:217:LEU:N	2.52	0.43
1:D:56:ARG:HG2	1:D:62:PRO:HG3	2.00	0.43
1:F:236:PHE:CE2	1:J:183:LEU:HD21	2.53	0.43
1:G:130:ASN:HB3	1:H:363:CYS:HB3	2.00	0.43
1:J:450:ILE:H	1:J:450:ILE:HG13	1.68	0.43
1:K:387:THR:HG22	1:O:57:TYR:CD1	2.54	0.43
1:M:237:HIS:HB3	1:M:238:PRO:CD	2.42	0.43
1:M:360:THR:OG1	1:M:361:LEU:N	2.50	0.43
1:N:217:LEU:HD12	1:N:217:LEU:HA	1.71	0.43
1:N:343:TRP:HD1	1:N:356:ILE:HD13	1.83	0.43
1:B:89:SER:HB2	1:B:480:ILE:HB	2.00	0.43
1:C:106:ALA:HA	1:C:109:GLN:HE21	1.83	0.43
1:D:134:VAL:HG13	1:D:141:ASN:HA	2.00	0.43
1:D:145:ALA:HB3	1:D:168:PHE:CE1	2.54	0.43
1:J:238:PRO:CG	1:J:362:LEU:HD11	2.47	0.43
1:J:493:LYS:HD2	1:J:495:LEU:HD13	2.00	0.43
1:K:154:THR:HG22	1:K:157:LYS:HA	2.00	0.43
1:K:331:ILE:H	1:K:331:ILE:HG12	1.63	0.43
1:M:213:ARG:HG3	1:M:215:PHE:CE1	2.54	0.43
1:N:215:PHE:O	1:N:217:LEU:N	2.51	0.43
1:O:436:PHE:CD1	1:O:442:LEU:HB3	2.54	0.43
1:A:413:TYR:HD1	1:A:450:ILE:HG23	1.84	0.42
1:B:439:ASN:O	1:B:443:ALA:HB2	2.19	0.42
1:D:497:ILE:HD11	1:E:402:ALA:HB3	2.01	0.42
1:E:185:ASN:HD21	1:E:210:PHE:N	2.07	0.42
1:G:292:TYR:HE1	1:G:313:LYS:HE2	1.84	0.42
1:H:343:TRP:CH2	1:H:362:LEU:HD13	2.54	0.42
1:I:217:LEU:HA	1:I:217:LEU:HD12	1.64	0.42
1:I:248:VAL:HG23	1:I:273:ILE:HG13	2.00	0.42
1:K:179:MET:HB3	1:K:179:MET:HE2	1.76	0.42
1:K:215:PHE:H	1:K:345:LEU:HD21	1.84	0.42
1:K:402:ALA:HB3	1:O:497:ILE:HD11	2.00	0.42
1:L:75:LYS:HB2	1:L:78:ASP:OD1	2.19	0.42
1:L:206:ILE:HD13	1:L:206:ILE:HA	1.65	0.42
1:M:124:LYS:CG	1:M:124:LYS:HE3	2.49	0.42
1:N:286:LEU:HD23	1:N:286:LEU:HA	1.87	0.42
1:E:391:THR:HG21	1:E:396:ASN:HB3	2.01	0.42
1:E:481:THR:HB	1:E:485:ARG:HA	2.00	0.42
1:H:133:ASN:HB3	1:H:134:VAL:H	1.33	0.42
1:J:215:PHE:O	1:J:217:LEU:N	2.51	0.42
1:J:258:LEU:HD22	1:J:367:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:360:THR:OG1	1:K:361:LEU:N	2.52	0.42
1:K:381:MET:HB2	1:K:476:GLN:OE1	2.19	0.42
1:L:75:LYS:NZ	1:M:485:ARG:HH22	2.18	0.42
1:N:113:LEU:HB2	1:N:470:ASN:HA	2.01	0.42
1:O:381:MET:HE1	1:O:498:VAL:HG21	2.01	0.42
1:A:113:LEU:HB3	1:A:119:TRP:NE1	2.34	0.42
1:B:113:LEU:HB2	1:B:470:ASN:HA	2.01	0.42
1:B:133:ASN:HB3	1:B:134:VAL:H	1.38	0.42
1:F:198:GLN:HE21	1:F:198:GLN:CA	2.29	0.42
1:G:397:PHE:HA	1:G:398:PRO:HD2	1.56	0.42
1:J:124:LYS:CG	1:J:124:LYS:HE3	2.48	0.42
1:L:504:SER:HB2	1:L:505:SER:H	1.54	0.42
1:A:220:ASP:HB2	1:A:227:MET:HG2	2.02	0.42
1:A:378:LEU:HD12	1:A:400:VAL:HG21	2.01	0.42
1:C:215:PHE:O	1:C:217:LEU:N	2.52	0.42
1:E:52:ARG:HB2	1:E:116:ARG:HD2	2.01	0.42
1:E:244:PRO:HG3	1:E:340:TYR:CE2	2.53	0.42
1:F:317:LYS:HA	1:F:318:PRO:HD3	1.90	0.42
1:L:492:TYR:CE2	1:M:262:ARG:HG3	2.54	0.42
1:O:383:GLN:HB2	1:O:467:PRO:HB2	2.02	0.42
1:A:95:VAL:HG23	1:A:474:GLY:HA2	2.01	0.42
1:C:114:ASP:OD1	1:C:116:ARG:HB2	2.19	0.42
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.89	0.42
1:G:254:ARG:HB3	1:G:369:CYS:HB3	2.00	0.42
1:K:403:GLU:OE2	1:K:461:THR:OG1	2.37	0.42
1:L:134:VAL:HG13	1:L:141:ASN:HA	2.01	0.42
1:E:96:ILE:HD12	1:E:474:GLY:HA3	2.01	0.42
1:K:118:HIS:HB2	1:K:504:SER:OG	2.20	0.42
1:N:239:ASP:OD2	1:N:239:ASP:N	2.39	0.42
1:A:243:LEU:HD22	1:A:247:GLY:HA2	2.02	0.42
1:B:57:TYR:CG	1:B:58:SER:N	2.87	0.42
1:B:254:ARG:O	1:B:257:ASN:HB2	2.19	0.42
1:E:238:PRO:HG2	1:E:362:LEU:CD1	2.49	0.42
1:E:397:PHE:HA	1:E:398:PRO:HD2	1.63	0.42
1:G:154:THR:HG22	1:G:158:GLN:H	1.84	0.42
1:H:209:LYS:HB3	1:H:242:LEU:HD12	2.01	0.42
1:H:224:GLY:O	1:H:336:THR:HB	2.19	0.42
1:K:96:ILE:HD12	1:K:474:GLY:HA3	2.02	0.42
1:L:145:ALA:HB3	1:L:168:PHE:HE1	1.85	0.42
1:L:243:LEU:HD22	1:L:247:GLY:HA2	2.00	0.42
1:M:288:ASP:HA	1:M:319:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:397:PHE:HA	1:M:398:PRO:HD2	1.56	0.42
1:A:135:ASN:HB3	1:A:138:MET:HB2	2.01	0.42
1:A:384:ASP:OD1	1:A:384:ASP:N	2.39	0.42
1:B:113:LEU:HB3	1:B:119:TRP:CD1	2.55	0.42
1:D:315:VAL:HG23	1:D:316:ILE:HG23	2.01	0.42
1:J:96:ILE:HD12	1:J:474:GLY:HA3	2.02	0.42
1:K:439:ASN:O	1:K:443:ALA:HB2	2.20	0.42
1:N:206:ILE:HD13	1:N:206:ILE:HA	1.78	0.42
1:N:273:ILE:HD12	1:N:278:LEU:HD11	2.00	0.42
1:A:192:TYR:OH	1:A:203:GLU:HG2	2.20	0.42
1:A:381:MET:HB2	1:A:476:GLN:OE1	2.19	0.42
1:D:215:PHE:HB2	1:D:345:LEU:HD21	2.02	0.42
1:G:504:SER:HB2	1:G:505:SER:H	1.54	0.42
1:I:85:GLN:H	1:I:85:GLN:HG2	1.77	0.42
1:I:213:ARG:HH11	1:I:446:PRO:HD3	1.84	0.42
1:J:136:GLU:HA	1:J:141:ASN:ND2	2.30	0.42
1:K:384:ASP:HA	1:K:385:PRO:HD3	1.85	0.42
1:K:389:ARG:HH21	1:O:100:ASP:HB2	1.84	0.42
1:N:133:ASN:CB	1:N:175:TYR:CB	2.85	0.42
1:O:146:ARG:HD2	1:O:246:CYS:HA	2.01	0.42
1:B:323:SER:HB3	1:B:438:GLU:HB2	2.01	0.42
1:C:179:MET:HG2	1:C:183:LEU:HD22	2.02	0.42
1:C:367:VAL:HG12	1:C:409:SER:HB3	2.01	0.42
1:E:69:VAL:CG2	1:E:498:VAL:HB	2.47	0.42
1:I:411:SER:HB3	1:I:452:THR:HG22	2.01	0.42
1:J:343:TRP:HE1	1:J:360:THR:HG21	1.84	0.42
1:K:96:ILE:HA	1:L:387:THR:HG21	2.02	0.42
1:L:133:ASN:HB3	1:L:134:VAL:H	1.46	0.42
1:M:75:LYS:O	1:M:79:VAL:HG23	2.20	0.42
1:A:114:ASP:OD1	1:A:116:ARG:HB2	2.20	0.41
1:A:236:PHE:HE2	1:E:183:LEU:HD21	1.84	0.41
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.85	0.41
1:A:414:ASN:HD21	1:B:415:ASP:HB2	1.84	0.41
1:B:209:LYS:HZ3	1:B:445:PRO:HG3	1.85	0.41
1:C:273:ILE:HG21	1:C:356:ILE:HD11	2.01	0.41
1:F:315:VAL:HG23	1:F:316:ILE:HG23	2.01	0.41
1:H:439:ASN:O	1:H:443:ALA:HB2	2.20	0.41
1:K:113:LEU:HB2	1:K:470:ASN:HA	2.02	0.41
1:K:206:ILE:HD13	1:K:206:ILE:HA	1.82	0.41
1:A:131:MET:HA	1:A:490:TYR:CD2	2.56	0.41
1:C:113:LEU:HB2	1:C:470:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:ASN:HA	1:H:86:ASN:HB2	2.01	0.41
1:J:241:ILE:HD13	1:J:248:VAL:HG21	2.01	0.41
1:J:273:ILE:HG21	1:J:356:ILE:HD11	2.01	0.41
1:K:130:ASN:HD22	1:K:130:ASN:HA	1.65	0.41
1:K:237:HIS:HB2	1:K:238:PRO:HD3	2.01	0.41
1:L:366:ASP:OD1	1:L:369:CYS:N	2.44	0.41
1:L:401:GLY:HA3	1:L:463:HIS:CD2	2.51	0.41
1:M:367:VAL:HG12	1:M:409:SER:HB2	2.02	0.41
1:O:479:THR:HG22	1:O:481:THR:HG22	2.02	0.41
1:A:275:TYR:HE1	1:A:341:ARG:HB2	1.85	0.41
1:C:146:ARG:HD2	1:C:246:CYS:HA	2.02	0.41
1:C:468:LEU:HA	1:C:468:LEU:HD12	1.40	0.41
1:D:326:ARG:HB2	1:D:439:ASN:HD22	1.83	0.41
1:G:111:ILE:HB	1:G:472:ILE:HB	2.01	0.41
1:H:393:GLN:C	1:H:395:SER:H	2.24	0.41
1:I:481:THR:HB	1:I:485:ARG:HA	2.01	0.41
1:J:217:LEU:HA	1:J:217:LEU:HD12	1.79	0.41
1:L:295:SER:OG	1:L:296:LEU:N	2.53	0.41
1:M:126:ILE:HG21	1:N:404:LEU:HD13	2.03	0.41
1:O:68:ARG:HD3	1:O:68:ARG:HA	1.79	0.41
1:B:85:GLN:HE21	1:B:85:GLN:HB3	1.60	0.41
1:B:224:GLY:O	1:B:336:THR:HB	2.21	0.41
1:B:381:MET:HG2	1:B:468:LEU:HD11	2.01	0.41
1:C:495:LEU:HA	1:C:495:LEU:HD12	1.78	0.41
1:D:178:THR:O	1:D:181:ILE:HG12	2.18	0.41
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.83	0.41
1:D:342:SER:CB	1:D:345:LEU:HG	2.51	0.41
1:F:133:ASN:HD22	1:F:175:TYR:HB2	1.84	0.41
1:G:244:PRO:HA	1:G:275:TYR:CE1	2.56	0.41
1:I:96:ILE:CD1	1:I:474:GLY:HA3	2.50	0.41
1:I:439:ASN:O	1:I:443:ALA:HB2	2.20	0.41
1:J:72:VAL:HG12	1:J:495:LEU:HD11	2.02	0.41
1:J:343:TRP:CD1	1:J:356:ILE:HD13	2.56	0.41
1:L:217:LEU:HD12	1:L:217:LEU:HA	1.96	0.41
1:L:427:THR:HG22	1:L:428:SER:HB2	2.01	0.41
1:N:178:THR:OG1	1:N:448:PRO:HD2	2.20	0.41
1:O:367:VAL:HG12	1:O:409:SER:HB2	2.03	0.41
1:O:394:ILE:H	1:O:394:ILE:HG13	1.67	0.41
1:O:397:PHE:HA	1:O:398:PRO:HD2	1.64	0.41
1:O:480:ILE:H	1:O:480:ILE:HG12	1.63	0.41
1:A:113:LEU:HB2	1:A:470:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:SER:HB2	1:A:505:SER:H	1.57	0.41
1:B:495:LEU:HD12	1:B:495:LEU:HA	1.79	0.41
1:D:426:PHE:HD2	1:D:426:PHE:HA	1.78	0.41
1:E:215:PHE:O	1:E:217:LEU:N	2.53	0.41
1:I:71:LEU:HB2	1:I:496:GLY:HA3	2.02	0.41
1:J:243:LEU:HD22	1:J:247:GLY:HA2	2.02	0.41
1:K:323:SER:HB3	1:K:438:GLU:HB2	2.03	0.41
1:L:197:ARG:HG3	1:L:198:GLN:HE21	1.86	0.41
1:L:203:GLU:HB2	1:L:326:ARG:HH12	1.84	0.41
1:N:439:ASN:HD21	1:N:442:LEU:HD23	1.84	0.41
1:O:286:LEU:HD23	1:O:286:LEU:HA	1.86	0.41
1:D:87:ASP:O	1:E:267:PHE:HE1	2.03	0.41
1:E:135:ASN:OD1	1:E:136:GLU:N	2.54	0.41
1:I:404:LEU:HD12	1:I:404:LEU:HA	1.85	0.41
1:K:262:ARG:HG3	1:O:492:TYR:CZ	2.56	0.41
1:B:176:SER:HB2	1:B:179:MET:HB3	2.02	0.41
1:B:326:ARG:HD2	1:B:438:GLU:HG2	2.02	0.41
1:D:249:ASP:OD2	1:D:272:ARG:HB3	2.20	0.41
1:I:185:ASN:ND2	1:I:210:PHE:O	2.53	0.41
1:K:262:ARG:NH1	1:O:489:PRO:O	2.53	0.41
1:O:381:MET:HB3	1:O:381:MET:HE2	1.94	0.41
1:O:488:CYS:HA	1:O:489:PRO:HD3	1.90	0.41
1:B:244:PRO:HA	1:B:275:TYR:CE1	2.55	0.41
1:B:282:ASN:H	1:B:341:ARG:HG3	1.85	0.41
1:C:439:ASN:O	1:C:443:ALA:HB2	2.20	0.41
1:F:217:LEU:HD12	1:F:217:LEU:HA	1.80	0.41
1:M:138:MET:O	1:M:254:ARG:NH1	2.54	0.41
1:N:215:PHE:H	1:N:345:LEU:HD21	1.85	0.41
1:O:393:GLN:C	1:O:395:SER:H	2.24	0.41
1:B:240:ILE:HG23	1:B:344:TYR:N	2.26	0.41
1:B:288:ASP:HB3	1:B:291:ALA:HB3	2.02	0.41
1:B:342:SER:HG	1:B:345:LEU:HG	1.85	0.41
1:B:434:ASN:ND2	1:B:437:PRO:HG3	2.36	0.41
1:C:98:ASN:HD21	1:D:389:ARG:CZ	2.33	0.41
1:C:133:ASN:ND2	1:C:367:VAL:HG22	2.35	0.41
1:C:188:ILE:HD13	1:C:208:VAL:O	2.21	0.41
1:C:220:ASP:HA	1:C:221:PRO:HD2	1.88	0.41
1:C:243:LEU:HD22	1:C:247:GLY:HA2	2.03	0.41
1:C:248:VAL:HG23	1:C:273:ILE:HG13	2.03	0.41
1:D:261:ILE:HG12	1:D:343:TRP:CH2	2.56	0.41
1:E:254:ARG:HB3	1:E:369:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:VAL:HB	1:G:452:THR:OG1	2.21	0.41
1:G:468:LEU:HD12	1:G:468:LEU:HA	1.45	0.41
1:I:323:SER:HB3	1:I:438:GLU:HB2	2.02	0.41
1:J:288:ASP:HB3	1:J:291:ALA:HB3	2.03	0.41
1:J:343:TRP:HH2	1:J:362:LEU:HD13	1.86	0.41
1:J:439:ASN:O	1:J:443:ALA:HB2	2.20	0.41
1:K:264:ARG:NH1	1:K:357:ARG:O	2.54	0.41
1:K:351:ASP:HB3	1:K:354:THR:HB	2.02	0.41
1:K:393:GLN:C	1:K:395:SER:H	2.24	0.41
1:L:154:THR:HG22	1:L:157:LYS:HA	2.03	0.41
1:M:240:ILE:HG22	1:M:241:ILE:N	2.36	0.41
1:N:243:LEU:HD13	1:N:247:GLY:HA2	2.03	0.41
1:N:397:PHE:HA	1:N:398:PRO:HD2	1.53	0.41
1:N:495:LEU:HD12	1:N:495:LEU:HA	1.68	0.41
1:O:89:SER:OG	1:O:480:ILE:O	2.39	0.41
1:A:226:VAL:HG21	1:A:231:TYR:HE2	1.86	0.41
1:C:470:ASN:OD1	1:C:470:ASN:N	2.54	0.41
1:E:504:SER:HB2	1:E:505:SER:H	1.57	0.41
1:F:136:GLU:HA	1:F:141:ASN:HD22	1.86	0.41
1:H:326:ARG:CD	1:H:439:ASN:HB2	2.51	0.41
1:H:379:PRO:HB3	1:H:398:PRO:HG2	2.03	0.41
1:I:243:LEU:HD22	1:I:247:GLY:HA2	2.02	0.41
1:L:185:ASN:HD21	1:L:210:PHE:H	1.69	0.41
1:M:343:TRP:HE1	1:M:360:THR:HG21	1.86	0.41
1:N:71:LEU:HD23	1:N:71:LEU:HA	1.92	0.41
1:B:87:ASP:HB2	1:B:88:HIS:H	1.77	0.40
1:E:114:ASP:OD1	1:E:116:ARG:HB2	2.20	0.40
1:E:244:PRO:HG3	1:E:340:TYR:HE2	1.86	0.40
1:E:340:TYR:CD1	1:E:441:ILE:HG21	2.56	0.40
1:I:113:LEU:HB2	1:I:470:ASN:HA	2.03	0.40
1:L:397:PHE:HA	1:L:398:PRO:HD2	1.62	0.40
1:N:393:GLN:C	1:N:395:SER:H	2.25	0.40
1:O:412:PHE:O	1:O:450:ILE:HA	2.21	0.40
1:A:133:ASN:H	1:A:175:TYR:HD2	1.69	0.40
1:A:229:GLY:C	1:A:286:LEU:HD22	2.41	0.40
1:B:113:LEU:HA	1:B:113:LEU:HD23	1.80	0.40
1:D:393:GLN:C	1:D:395:SER:H	2.23	0.40
1:E:102:SER:HB3	1:E:105:GLU:HB3	2.03	0.40
1:E:178:THR:OG1	1:E:448:PRO:HD2	2.20	0.40
1:E:250:PHE:HB2	1:E:271:PHE:HD2	1.85	0.40
1:F:387:THR:HG21	1:J:96:ILE:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:LEU:HD22	1:H:247:GLY:HA2	2.02	0.40
1:I:72:VAL:H	1:I:93:THR:HG21	1.85	0.40
1:I:492:TYR:CZ	1:J:262:ARG:HG3	2.56	0.40
1:K:52:ARG:HB3	1:K:114:ASP:OD2	2.21	0.40
1:K:89:SER:HA	1:K:480:ILE:HG12	2.02	0.40
1:K:387:THR:HG21	1:O:96:ILE:HA	2.04	0.40
1:L:83:ASN:HA	1:L:86:ASN:HB2	2.03	0.40
1:L:326:ARG:HB2	1:L:439:ASN:HD22	1.86	0.40
1:M:113:LEU:HB2	1:M:470:ASN:HA	2.03	0.40
1:N:238:PRO:CG	1:N:362:LEU:HD11	2.49	0.40
1:N:412:PHE:O	1:N:450:ILE:HA	2.20	0.40
1:O:177:GLU:HG2	1:O:452:THR:H	1.87	0.40
1:O:391:THR:HG21	1:O:396:ASN:HB3	2.04	0.40
1:B:72:VAL:HG12	1:B:495:LEU:HD11	2.03	0.40
1:B:423:ILE:HD13	1:B:423:ILE:HG21	1.92	0.40
1:C:286:LEU:HA	1:C:286:LEU:HD23	1.78	0.40
1:C:326:ARG:NE	1:C:438:GLU:OE1	2.51	0.40
1:C:450:ILE:H	1:C:450:ILE:HG13	1.74	0.40
1:E:150:SER:HB2	1:E:162:LYS:HB2	2.03	0.40
1:G:254:ARG:O	1:G:257:ASN:HB2	2.21	0.40
1:H:316:ILE:H	1:H:316:ILE:HG13	1.70	0.40
1:H:326:ARG:HD2	1:H:439:ASN:HB2	2.03	0.40
1:H:391:THR:HG21	1:H:396:ASN:HB3	2.03	0.40
1:I:111:ILE:HD12	1:I:111:ILE:HG23	1.76	0.40
1:J:133:ASN:HB2	1:J:175:TYR:HB2	2.00	0.40
1:K:130:ASN:HB3	1:L:363:CYS:HB3	2.03	0.40
1:K:286:LEU:HD23	1:K:286:LEU:HA	1.96	0.40
1:L:278:LEU:HB3	1:L:341:ARG:HG2	2.04	0.40
1:M:220:ASP:HA	1:M:221:PRO:HD2	1.93	0.40
1:N:378:LEU:HD23	1:N:378:LEU:HA	1.83	0.40
1:B:206:ILE:HA	1:B:206:ILE:HD13	1.60	0.40
1:C:113:LEU:HD22	1:C:119:TRP:CD2	2.56	0.40
1:D:504:SER:HB2	1:D:505:SER:H	1.55	0.40
1:F:378:LEU:HA	1:F:378:LEU:HD23	1.73	0.40
1:F:385:PRO:HG2	1:F:388:PHE:CD1	2.57	0.40
1:G:453:VAL:HG11	1:H:450:ILE:HD13	2.03	0.40
1:I:57:TYR:CD1	1:J:387:THR:HG22	2.56	0.40
1:J:347:TYR:CE2	1:J:362:LEU:HB2	2.56	0.40
1:K:73:ASP:OD2	1:K:73:ASP:N	2.45	0.40
1:K:411:SER:HB3	1:K:452:THR:HG22	2.04	0.40
1:L:480:ILE:H	1:L:480:ILE:HG12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:83:ASN:HA	1:M:86:ASN:HB2	2.04	0.40
1:M:111:ILE:HD13	1:M:111:ILE:HA	1.99	0.40
1:M:391:THR:OG1	1:M:392:SER:N	2.51	0.40
1:O:342:SER:HG	1:O:345:LEU:HG	1.86	0.40
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.93	0.40
1:A:241:ILE:HD12	1:A:273:ILE:HD11	2.03	0.40
1:B:192:TYR:CZ	1:B:197:ARG:HB3	2.56	0.40
1:B:213:ARG:O	1:B:240:ILE:HD11	2.21	0.40
1:C:71:LEU:HD11	1:C:381:MET:HE1	2.02	0.40
1:E:364:THR:HA	1:E:365:PRO:HD2	1.87	0.40
1:E:393:GLN:C	1:E:395:SER:H	2.25	0.40
1:F:113:LEU:HB2	1:F:470:ASN:HA	2.04	0.40
1:G:111:ILE:HD13	1:G:111:ILE:HA	1.91	0.40
1:G:215:PHE:C	1:G:217:LEU:H	2.25	0.40
1:I:391:THR:HG21	1:I:396:ASN:HB3	2.03	0.40
1:J:256:SER:HB2	1:J:271:PHE:HE2	1.86	0.40
1:J:427:THR:HG22	1:J:428:SER:HB2	2.03	0.40
1:L:378:LEU:HD23	1:L:378:LEU:HA	1.77	0.40
1:O:326:ARG:HB2	1:O:439:ASN:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	3	26
1	B	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	3	26
1	C	440/523 (84%)	357 (81%)	65 (15%)	18 (4%)	3	26
1	D	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	3	26
1	E	440/523 (84%)	358 (81%)	63 (14%)	19 (4%)	2	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	440/523 (84%)	359 (82%)	62 (14%)	19 (4%)	2	24
1	G	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	3	26
1	H	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	3	26
1	I	440/523 (84%)	360 (82%)	62 (14%)	18 (4%)	3	26
1	J	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	3	26
1	K	440/523 (84%)	356 (81%)	65 (15%)	19 (4%)	2	24
1	L	440/523 (84%)	359 (82%)	63 (14%)	18 (4%)	3	26
1	M	440/523 (84%)	358 (81%)	64 (14%)	18 (4%)	3	26
1	N	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	3	26
1	O	440/523 (84%)	361 (82%)	61 (14%)	18 (4%)	3	26
All	All	6600/7845 (84%)	5382 (82%)	945 (14%)	273 (4%)	3	26

All (273) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	172	GLU
1	A	237	HIS
1	A	286	LEU
1	A	323	SER
1	B	66	THR
1	B	172	GLU
1	B	237	HIS
1	B	286	LEU
1	B	323	SER
1	C	66	THR
1	C	172	GLU
1	C	237	HIS
1	C	286	LEU
1	C	323	SER
1	D	66	THR
1	D	172	GLU
1	D	237	HIS
1	D	286	LEU
1	D	323	SER
1	E	66	THR
1	E	172	GLU
1	E	237	HIS

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Mol	Chain	Res	Type
1	E	286	LEU
1	E	323	SER
1	F	66	THR
1	F	172	GLU
1	F	237	HIS
1	F	286	LEU
1	F	323	SER
1	G	66	THR
1	G	172	GLU
1	G	237	HIS
1	G	286	LEU
1	G	323	SER
1	H	66	THR
1	H	172	GLU
1	H	237	HIS
1	H	286	LEU
1	H	323	SER
1	I	66	THR
1	I	172	GLU
1	I	237	HIS
1	I	286	LEU
1	I	323	SER
1	J	66	THR
1	J	172	GLU
1	J	237	HIS
1	J	286	LEU
1	J	323	SER
1	K	66	THR
1	K	172	GLU
1	K	237	HIS
1	K	286	LEU
1	K	323	SER
1	L	66	THR
1	L	172	GLU
1	L	237	HIS
1	L	286	LEU
1	L	323	SER
1	M	66	THR
1	M	172	GLU
1	M	237	HIS
1	M	286	LEU
1	M	323	SER

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Mol	Chain	Res	Type
1	N	66	THR
1	N	172	GLU
1	N	237	HIS
1	N	286	LEU
1	N	323	SER
1	O	66	THR
1	O	172	GLU
1	O	237	HIS
1	O	286	LEU
1	O	323	SER
1	A	152	SER
1	A	232	THR
1	A	244	PRO
1	A	316	ILE
1	A	434	ASN
1	B	232	THR
1	B	244	PRO
1	B	316	ILE
1	B	356	ILE
1	B	434	ASN
1	C	232	THR
1	C	244	PRO
1	C	316	ILE
1	C	434	ASN
1	D	232	THR
1	D	244	PRO
1	D	316	ILE
1	D	434	ASN
1	E	152	SER
1	E	232	THR
1	E	244	PRO
1	E	295	SER
1	E	316	ILE
1	E	434	ASN
1	F	232	THR
1	F	244	PRO
1	F	316	ILE
1	F	434	ASN
1	G	152	SER
1	G	232	THR
1	G	244	PRO
1	G	316	ILE

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Mol	Chain	Res	Type
1	G	434	ASN
1	H	152	SER
1	H	232	THR
1	H	244	PRO
1	H	316	ILE
1	H	434	ASN
1	I	232	THR
1	I	244	PRO
1	I	316	ILE
1	I	434	ASN
1	J	152	SER
1	J	232	THR
1	J	244	PRO
1	J	316	ILE
1	J	434	ASN
1	K	232	THR
1	K	244	PRO
1	K	316	ILE
1	K	434	ASN
1	L	152	SER
1	L	232	THR
1	L	244	PRO
1	L	316	ILE
1	L	434	ASN
1	M	152	SER
1	M	232	THR
1	M	244	PRO
1	M	316	ILE
1	M	434	ASN
1	N	152	SER
1	N	232	THR
1	N	244	PRO
1	N	316	ILE
1	N	434	ASN
1	O	152	SER
1	O	232	THR
1	O	244	PRO
1	O	316	ILE
1	O	356	ILE
1	O	434	ASN
1	A	133	ASN
1	B	133	ASN

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Mol	Chain	Res	Type
1	B	152	SER
1	C	152	SER
1	C	157	LYS
1	D	152	SER
1	E	133	ASN
1	E	356	ILE
1	F	152	SER
1	F	295	SER
1	F	356	ILE
1	G	133	ASN
1	H	133	ASN
1	I	133	ASN
1	I	152	SER
1	J	133	ASN
1	K	133	ASN
1	K	152	SER
1	L	133	ASN
1	M	133	ASN
1	O	133	ASN
1	A	157	LYS
1	A	356	ILE
1	B	157	LYS
1	C	133	ASN
1	D	133	ASN
1	D	157	LYS
1	D	356	ILE
1	E	157	LYS
1	F	133	ASN
1	F	157	LYS
1	G	157	LYS
1	H	157	LYS
1	H	356	ILE
1	I	157	LYS
1	I	356	ILE
1	J	157	LYS
1	K	157	LYS
1	K	295	SER
1	K	356	ILE
1	L	157	LYS
1	L	356	ILE
1	M	157	LYS
1	N	133	ASN

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Mol	Chain	Res	Type
1	N	157	LYS
1	N	356	ILE
1	O	157	LYS
1	A	65	ASP
1	A	370	GLY
1	B	58	SER
1	B	65	ASP
1	B	370	GLY
1	C	58	SER
1	C	65	ASP
1	C	356	ILE
1	C	370	GLY
1	D	58	SER
1	D	65	ASP
1	D	370	GLY
1	E	58	SER
1	E	65	ASP
1	E	370	GLY
1	F	58	SER
1	F	65	ASP
1	F	370	GLY
1	G	58	SER
1	G	65	ASP
1	G	356	ILE
1	G	370	GLY
1	H	65	ASP
1	H	370	GLY
1	I	58	SER
1	I	65	ASP
1	I	370	GLY
1	J	65	ASP
1	J	356	ILE
1	J	370	GLY
1	K	58	SER
1	K	65	ASP
1	K	370	GLY
1	L	65	ASP
1	L	370	GLY
1	M	58	SER
1	M	65	ASP
1	M	356	ILE
1	M	370	GLY

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Mol	Chain	Res	Type
1	N	58	SER
1	N	65	ASP
1	N	370	GLY
1	O	65	ASP
1	O	370	GLY
1	A	58	SER
1	H	58	SER
1	J	58	SER
1	L	58	SER
1	O	58	SER
1	B	51	GLY
1	C	51	GLY
1	D	51	GLY
1	E	51	GLY
1	F	51	GLY
1	G	51	GLY
1	H	51	GLY
1	I	51	GLY
1	J	51	GLY
1	K	51	GLY
1	L	51	GLY
1	M	51	GLY
1	N	51	GLY
1	O	51	GLY
1	A	51	GLY
1	B	475	VAL
1	J	475	VAL
1	K	475	VAL
1	A	475	VAL
1	C	475	VAL
1	D	475	VAL
1	F	475	VAL
1	G	475	VAL
1	H	475	VAL
1	I	475	VAL
1	L	475	VAL
1	M	475	VAL
1	N	475	VAL
1	O	475	VAL
1	E	475	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	400/451 (89%)	310 (78%)	90 (22%)	1	6
1	B	400/451 (89%)	320 (80%)	80 (20%)	1	8
1	C	400/451 (89%)	317 (79%)	83 (21%)	1	7
1	D	400/451 (89%)	317 (79%)	83 (21%)	1	7
1	E	400/451 (89%)	314 (78%)	86 (22%)	1	6
1	F	400/451 (89%)	322 (80%)	78 (20%)	1	9
1	G	400/451 (89%)	315 (79%)	85 (21%)	1	7
1	H	400/451 (89%)	306 (76%)	94 (24%)	1	5
1	I	400/451 (89%)	321 (80%)	79 (20%)	1	8
1	J	400/451 (89%)	311 (78%)	89 (22%)	1	6
1	K	400/451 (89%)	303 (76%)	97 (24%)	0	4
1	L	400/451 (89%)	297 (74%)	103 (26%)	0	4
1	M	400/451 (89%)	312 (78%)	88 (22%)	1	6
1	N	400/451 (89%)	310 (78%)	90 (22%)	1	6
1	O	400/451 (89%)	319 (80%)	81 (20%)	1	8
All	All	6000/6765 (89%)	4694 (78%)	1306 (22%)	1	6

All (1306) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	68	ARG
1	A	69	VAL
1	A	72	VAL
1	A	74	ASN
1	A	77	THR
1	A	82	LEU
1	A	92	LEU
1	A	95	VAL
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	100	ASP
1	A	105	GLU
1	A	110	THR
1	A	111	ILE
1	A	115	ASP
1	A	116	ARG
1	A	117	SER
1	A	130	ASN
1	A	138	MET
1	A	141	ASN
1	A	150	SER
1	A	152	SER
1	A	154	THR
1	A	156	ASP
1	A	159	VAL
1	A	161	LEU
1	A	166	VAL
1	A	175	TYR
1	A	176	SER
1	A	179	MET
1	A	182	ASP
1	A	183	LEU
1	A	188	ILE
1	A	194	LYS
1	A	195	VAL
1	A	204	SER
1	A	206	ILE
1	A	208	VAL
1	A	212	THR
1	A	239	ASP
1	A	240	ILE
1	A	241	ILE
1	A	243	LEU
1	A	246	CYS
1	A	251	THR
1	A	258	LEU
1	A	262	ARG
1	A	283	ILE
1	A	295	SER
1	A	315	VAL
1	A	320	THR
1	A	323	SER

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Mol	Chain	Res	Type
1	A	325	LYS
1	A	326	ARG
1	A	329	ASN
1	A	331	ILE
1	A	338	THR
1	A	341	ARG
1	A	356	ILE
1	A	364	THR
1	A	368	THR
1	A	375	TYR
1	A	377	SER
1	A	380	ASP
1	A	382	MET
1	A	384	ASP
1	A	386	VAL
1	A	395	SER
1	A	400	VAL
1	A	407	VAL
1	A	410	LYS
1	A	415	ASP
1	A	419	TYR
1	A	426	PHE
1	A	442	LEU
1	A	444	ARG
1	A	450	ILE
1	A	457	VAL
1	A	460	LEU
1	A	465	THR
1	A	468	LEU
1	A	470	ASN
1	A	475	VAL
1	A	477	ARG
1	A	480	ILE
1	A	492	TYR
1	A	499	SER
1	A	501	ARG
1	A	502	VAL
1	A	503	LEU
1	B	54	SER
1	B	60	LEU
1	B	64	PHE
1	B	67	THR

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Mol	Chain	Res	Type
1	B	69	VAL
1	B	72	VAL
1	B	73	ASP
1	B	75	LYS
1	B	77	THR
1	B	82	LEU
1	B	85	GLN
1	B	95	VAL
1	B	99	ASN
1	B	108	THR
1	B	111	ILE
1	B	115	ASP
1	B	117	SER
1	B	124	LYS
1	B	141	ASN
1	B	154	THR
1	B	156	ASP
1	B	159	VAL
1	B	161	LEU
1	B	166	VAL
1	B	175	TYR
1	B	183	LEU
1	B	195	VAL
1	B	203	GLU
1	B	206	ILE
1	B	209	LYS
1	B	212	THR
1	B	222	VAL
1	B	223	THR
1	B	239	ASP
1	B	243	LEU
1	B	256	SER
1	B	258	LEU
1	B	262	ARG
1	B	268	GLN
1	B	312	LEU
1	B	315	VAL
1	B	316	ILE
1	B	319	LEU
1	B	326	ARG
1	B	327	SER
1	B	331	ILE

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Mol	Chain	Res	Type
1	B	332	SER
1	B	334	ASP
1	B	335	SER
1	B	337	PHE
1	B	341	ARG
1	B	356	ILE
1	B	360	THR
1	B	364	THR
1	B	375	TYR
1	B	377	SER
1	B	380	ASP
1	B	382	MET
1	B	384	ASP
1	B	386	VAL
1	B	394	ILE
1	B	407	VAL
1	B	410	LYS
1	B	411	SER
1	B	419	TYR
1	B	426	PHE
1	B	448	PRO
1	B	449	THR
1	B	450	ILE
1	B	454	SER
1	B	455	GLU
1	B	460	LEU
1	B	461	THR
1	B	470	ASN
1	B	475	VAL
1	B	481	THR
1	B	492	TYR
1	B	498	VAL
1	B	499	SER
1	B	503	LEU
1	C	60	LEU
1	C	64	PHE
1	C	67	THR
1	C	69	VAL
1	C	72	VAL
1	C	73	ASP
1	C	74	ASN
1	C	82	LEU

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Mol	Chain	Res	Type
1	C	85	GLN
1	C	97	GLN
1	C	100	ASP
1	C	105	GLU
1	C	108	THR
1	C	110	THR
1	C	111	ILE
1	C	115	ASP
1	C	116	ARG
1	C	122	ASP
1	C	124	LYS
1	C	136	GLU
1	C	140	THR
1	C	141	ASN
1	C	150	SER
1	C	151	ARG
1	C	154	THR
1	C	159	VAL
1	C	161	LEU
1	C	166	VAL
1	C	175	TYR
1	C	182	ASP
1	C	183	LEU
1	C	186	ASN
1	C	195	VAL
1	C	198	GLN
1	C	211	ASP
1	C	216	ARG
1	C	239	ASP
1	C	240	ILE
1	C	243	LEU
1	C	248	VAL
1	C	251	THR
1	C	272	ARG
1	C	276	ASP
1	C	296	LEU
1	C	326	ARG
1	C	329	ASN
1	C	335	SER
1	C	341	ARG
1	C	356	ILE
1	C	362	LEU

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Mol	Chain	Res	Type
1	C	364	THR
1	C	368	THR
1	C	374	VAL
1	C	375	TYR
1	C	377	SER
1	C	380	ASP
1	C	382	MET
1	C	384	ASP
1	C	386	VAL
1	C	394	ILE
1	C	407	VAL
1	C	409	SER
1	C	410	LYS
1	C	415	ASP
1	C	419	TYR
1	C	436	PHE
1	C	438	GLU
1	C	441	ILE
1	C	442	LEU
1	C	444	ARG
1	C	449	THR
1	C	450	ILE
1	C	457	VAL
1	C	460	LEU
1	C	461	THR
1	C	465	THR
1	C	470	ASN
1	C	475	VAL
1	C	481	THR
1	C	487	THR
1	C	493	LYS
1	C	499	SER
1	C	502	VAL
1	D	49	THR
1	D	54	SER
1	D	58	SER
1	D	63	LEU
1	D	64	PHE
1	D	66	THR
1	D	69	VAL
1	D	72	VAL
1	D	82	LEU

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Mol	Chain	Res	Type
1	D	83	ASN
1	D	85	GLN
1	D	110	THR
1	D	111	ILE
1	D	115	ASP
1	D	116	ARG
1	D	117	SER
1	D	138	MET
1	D	140	THR
1	D	159	VAL
1	D	160	GLU
1	D	175	TYR
1	D	176	SER
1	D	182	ASP
1	D	183	LEU
1	D	184	MET
1	D	206	ILE
1	D	208	VAL
1	D	209	LYS
1	D	216	ARG
1	D	232	THR
1	D	234	GLU
1	D	239	ASP
1	D	243	LEU
1	D	256	SER
1	D	258	LEU
1	D	259	LEU
1	D	262	ARG
1	D	276	ASP
1	D	319	LEU
1	D	323	SER
1	D	326	ARG
1	D	331	ILE
1	D	342	SER
1	D	353	GLN
1	D	356	ILE
1	D	360	THR
1	D	364	THR
1	D	368	THR
1	D	374	VAL
1	D	377	SER
1	D	380	ASP

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Mol	Chain	Res	Type
1	D	382	MET
1	D	386	VAL
1	D	396	ASN
1	D	407	VAL
1	D	410	LYS
1	D	411	SER
1	D	415	ASP
1	D	419	TYR
1	D	426	PHE
1	D	428	SER
1	D	430	THR
1	D	438	GLU
1	D	441	ILE
1	D	442	LEU
1	D	450	ILE
1	D	455	GLU
1	D	460	LEU
1	D	461	THR
1	D	468	LEU
1	D	470	ASN
1	D	475	VAL
1	D	477	ARG
1	D	479	THR
1	D	480	ILE
1	D	481	THR
1	D	484	ARG
1	D	493	LYS
1	D	498	VAL
1	D	499	SER
1	D	501	ARG
1	D	502	VAL
1	D	506	ARG
1	E	54	SER
1	E	67	THR
1	E	72	VAL
1	E	75	LYS
1	E	76	SER
1	E	77	THR
1	E	81	SER
1	E	82	LEU
1	E	89	SER
1	E	97	GLN

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Mol	Chain	Res	Type
1	E	100	ASP
1	E	107	SER
1	E	108	THR
1	E	111	ILE
1	E	115	ASP
1	E	117	SER
1	E	126	ILE
1	E	136	GLU
1	E	138	MET
1	E	150	SER
1	E	154	THR
1	E	156	ASP
1	E	158	GLN
1	E	159	VAL
1	E	161	LEU
1	E	164	GLU
1	E	166	VAL
1	E	175	TYR
1	E	182	ASP
1	E	183	LEU
1	E	186	ASN
1	E	188	ILE
1	E	208	VAL
1	E	211	ASP
1	E	216	ARG
1	E	234	GLU
1	E	239	ASP
1	E	241	ILE
1	E	243	LEU
1	E	251	THR
1	E	256	SER
1	E	262	ARG
1	E	268	GLN
1	E	276	ASP
1	E	283	ILE
1	E	287	LEU
1	E	290	ASP
1	E	293	GLN
1	E	296	LEU
1	E	312	LEU
1	E	315	VAL
1	E	322	ASP

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Mol	Chain	Res	Type
1	E	323	SER
1	E	325	LYS
1	E	326	ARG
1	E	335	SER
1	E	341	ARG
1	E	353	GLN
1	E	356	ILE
1	E	360	THR
1	E	367	VAL
1	E	368	THR
1	E	374	VAL
1	E	377	SER
1	E	382	MET
1	E	384	ASP
1	E	385	PRO
1	E	386	VAL
1	E	390	SER
1	E	394	ILE
1	E	395	SER
1	E	407	VAL
1	E	428	SER
1	E	442	LEU
1	E	449	THR
1	E	450	ILE
1	E	460	LEU
1	E	461	THR
1	E	466	LEU
1	E	472	ILE
1	E	475	VAL
1	E	484	ARG
1	E	487	THR
1	E	499	SER
1	E	502	VAL
1	E	503	LEU
1	F	56	ARG
1	F	64	PHE
1	F	69	VAL
1	F	75	LYS
1	F	82	LEU
1	F	89	SER
1	F	93	THR
1	F	95	VAL

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Mol	Chain	Res	Type
1	F	97	GLN
1	F	100	ASP
1	F	110	THR
1	F	111	ILE
1	F	116	ARG
1	F	138	MET
1	F	141	ASN
1	F	147	VAL
1	F	150	SER
1	F	156	ASP
1	F	157	LYS
1	F	158	GLN
1	F	164	GLU
1	F	166	VAL
1	F	183	LEU
1	F	186	ASN
1	F	195	VAL
1	F	198	GLN
1	F	202	LEU
1	F	216	ARG
1	F	222	VAL
1	F	239	ASP
1	F	243	LEU
1	F	251	THR
1	F	258	LEU
1	F	262	ARG
1	F	265	GLN
1	F	293	GLN
1	F	312	LEU
1	F	319	LEU
1	F	320	THR
1	F	321	GLU
1	F	325	LYS
1	F	326	ARG
1	F	331	ILE
1	F	332	SER
1	F	336	THR
1	F	338	THR
1	F	341	ARG
1	F	356	ILE
1	F	358	SER
1	F	360	THR

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Mol	Chain	Res	Type
1	F	362	LEU
1	F	364	THR
1	F	368	THR
1	F	374	VAL
1	F	377	SER
1	F	382	MET
1	F	386	VAL
1	F	395	SER
1	F	407	VAL
1	F	410	LYS
1	F	424	ARG
1	F	428	SER
1	F	438	GLU
1	F	444	ARG
1	F	449	THR
1	F	450	ILE
1	F	451	THR
1	F	454	SER
1	F	460	LEU
1	F	465	THR
1	F	466	LEU
1	F	470	ASN
1	F	475	VAL
1	F	480	ILE
1	F	487	THR
1	F	493	LYS
1	F	499	SER
1	F	502	VAL
1	G	63	LEU
1	G	64	PHE
1	G	69	VAL
1	G	72	VAL
1	G	74	ASN
1	G	75	LYS
1	G	82	LEU
1	G	85	GLN
1	G	92	LEU
1	G	93	THR
1	G	95	VAL
1	G	97	GLN
1	G	105	GLU
1	G	110	THR

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Mol	Chain	Res	Type
1	G	111	ILE
1	G	130	ASN
1	G	135	ASN
1	G	136	GLU
1	G	141	ASN
1	G	150	SER
1	G	154	THR
1	G	159	VAL
1	G	161	LEU
1	G	166	VAL
1	G	169	THR
1	G	175	TYR
1	G	177	GLU
1	G	183	LEU
1	G	198	GLN
1	G	208	VAL
1	G	233	ASN
1	G	234	GLU
1	G	239	ASP
1	G	240	ILE
1	G	241	ILE
1	G	243	LEU
1	G	251	THR
1	G	255	LEU
1	G	258	LEU
1	G	262	ARG
1	G	264	ARG
1	G	268	GLN
1	G	275	TYR
1	G	287	LEU
1	G	293	GLN
1	G	296	LEU
1	G	315	VAL
1	G	319	LEU
1	G	326	ARG
1	G	329	ASN
1	G	330	LEU
1	G	338	THR
1	G	348	ASN
1	G	356	ILE
1	G	360	THR
1	G	364	THR

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Mol	Chain	Res	Type
1	G	374	VAL
1	G	377	SER
1	G	378	LEU
1	G	380	ASP
1	G	382	MET
1	G	403	GLU
1	G	405	LEU
1	G	407	VAL
1	G	409	SER
1	G	415	ASP
1	G	426	PHE
1	G	428	SER
1	G	431	HIS
1	G	435	ARG
1	G	450	ILE
1	G	452	THR
1	G	460	LEU
1	G	461	THR
1	G	470	ASN
1	G	472	ILE
1	G	475	VAL
1	G	480	ILE
1	G	481	THR
1	G	487	THR
1	G	492	TYR
1	G	493	LYS
1	G	501	ARG
1	G	502	VAL
1	G	503	LEU
1	H	63	LEU
1	H	64	PHE
1	H	67	THR
1	H	69	VAL
1	H	72	VAL
1	H	74	ASN
1	H	75	LYS
1	H	77	THR
1	H	82	LEU
1	H	89	SER
1	H	97	GLN
1	H	100	ASP
1	H	105	GLU

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Mol	Chain	Res	Type
1	H	107	SER
1	H	108	THR
1	H	111	ILE
1	H	115	ASP
1	H	117	SER
1	H	122	ASP
1	H	130	ASN
1	H	140	THR
1	H	141	ASN
1	H	154	THR
1	H	155	LYS
1	H	159	VAL
1	H	160	GLU
1	H	164	GLU
1	H	166	VAL
1	H	169	THR
1	H	175	TYR
1	H	179	MET
1	H	182	ASP
1	H	183	LEU
1	H	198	GLN
1	H	202	LEU
1	H	206	ILE
1	H	208	VAL
1	H	212	THR
1	H	222	VAL
1	H	233	ASN
1	H	239	ASP
1	H	240	ILE
1	H	243	LEU
1	H	258	LEU
1	H	262	ARG
1	H	272	ARG
1	H	276	ASP
1	H	279	GLU
1	H	293	GLN
1	H	315	VAL
1	H	316	ILE
1	H	319	LEU
1	H	323	SER
1	H	326	ARG
1	H	330	LEU

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Mol	Chain	Res	Type
1	H	333	ASN
1	H	338	THR
1	H	341	ARG
1	H	351	ASP
1	H	356	ILE
1	H	360	THR
1	H	364	THR
1	H	365	PRO
1	H	368	THR
1	H	374	VAL
1	H	375	TYR
1	H	377	SER
1	H	382	MET
1	H	384	ASP
1	H	394	ILE
1	H	405	LEU
1	H	407	VAL
1	H	409	SER
1	H	410	LYS
1	H	415	ASP
1	H	430	THR
1	H	442	LEU
1	H	449	THR
1	H	450	ILE
1	H	460	LEU
1	H	465	THR
1	H	468	LEU
1	H	470	ASN
1	H	475	VAL
1	H	480	ILE
1	H	481	THR
1	H	492	TYR
1	H	497	ILE
1	H	498	VAL
1	H	499	SER
1	H	501	ARG
1	H	502	VAL
1	H	504	SER
1	H	505	SER
1	I	58	SER
1	I	60	LEU
1	I	64	PHE

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Mol	Chain	Res	Type
1	I	68	ARG
1	I	77	THR
1	I	82	LEU
1	I	85	GLN
1	I	95	VAL
1	I	97	GLN
1	I	100	ASP
1	I	105	GLU
1	I	111	ILE
1	I	115	ASP
1	I	116	ARG
1	I	117	SER
1	I	150	SER
1	I	154	THR
1	I	158	GLN
1	I	164	GLU
1	I	166	VAL
1	I	175	TYR
1	I	183	LEU
1	I	189	VAL
1	I	206	ILE
1	I	233	ASN
1	I	239	ASP
1	I	241	ILE
1	I	243	LEU
1	I	251	THR
1	I	262	ARG
1	I	265	GLN
1	I	276	ASP
1	I	278	LEU
1	I	279	GLU
1	I	315	VAL
1	I	316	ILE
1	I	329	ASN
1	I	331	ILE
1	I	334	ASP
1	I	338	THR
1	I	345	LEU
1	I	356	ILE
1	I	364	THR
1	I	368	THR
1	I	374	VAL

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Mol	Chain	Res	Type
1	I	377	SER
1	I	380	ASP
1	I	382	MET
1	I	384	ASP
1	I	386	VAL
1	I	395	SER
1	I	405	LEU
1	I	407	VAL
1	I	409	SER
1	I	410	LYS
1	I	411	SER
1	I	415	ASP
1	I	428	SER
1	I	430	THR
1	I	438	GLU
1	I	442	LEU
1	I	444	ARG
1	I	449	THR
1	I	451	THR
1	I	457	VAL
1	I	460	LEU
1	I	461	THR
1	I	470	ASN
1	I	471	SER
1	I	475	VAL
1	I	477	ARG
1	I	482	ASP
1	I	484	ARG
1	I	487	THR
1	I	492	TYR
1	I	493	LYS
1	I	499	SER
1	I	501	ARG
1	I	502	VAL
1	J	54	SER
1	J	63	LEU
1	J	69	VAL
1	J	72	VAL
1	J	75	LYS
1	J	77	THR
1	J	82	LEU
1	J	85	GLN

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Mol	Chain	Res	Type
1	J	90	ASN
1	J	92	LEU
1	J	95	VAL
1	J	100	ASP
1	J	105	GLU
1	J	111	ILE
1	J	115	ASP
1	J	117	SER
1	J	136	GLU
1	J	138	MET
1	J	150	SER
1	J	152	SER
1	J	153	LEU
1	J	156	ASP
1	J	159	VAL
1	J	160	GLU
1	J	166	VAL
1	J	169	THR
1	J	175	TYR
1	J	177	GLU
1	J	180	THR
1	J	183	LEU
1	J	186	ASN
1	J	188	ILE
1	J	194	LYS
1	J	204	SER
1	J	206	ILE
1	J	208	VAL
1	J	239	ASP
1	J	243	LEU
1	J	251	THR
1	J	258	LEU
1	J	268	GLN
1	J	274	THR
1	J	276	ASP
1	J	288	ASP
1	J	315	VAL
1	J	323	SER
1	J	324	LYS
1	J	326	ARG
1	J	327	SER
1	J	329	ASN

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Mol	Chain	Res	Type
1	J	330	LEU
1	J	335	SER
1	J	336	THR
1	J	338	THR
1	J	351	ASP
1	J	356	ILE
1	J	368	THR
1	J	374	VAL
1	J	375	TYR
1	J	377	SER
1	J	379	PRO
1	J	380	ASP
1	J	382	MET
1	J	392	SER
1	J	394	ILE
1	J	395	SER
1	J	403	GLU
1	J	407	VAL
1	J	410	LYS
1	J	415	ASP
1	J	431	HIS
1	J	442	LEU
1	J	444	ARG
1	J	450	ILE
1	J	457	VAL
1	J	460	LEU
1	J	461	THR
1	J	469	ARG
1	J	470	ASN
1	J	472	ILE
1	J	475	VAL
1	J	480	ILE
1	J	492	TYR
1	J	493	LYS
1	J	495	LEU
1	J	499	SER
1	J	501	ARG
1	J	502	VAL
1	J	506	ARG
1	K	63	LEU
1	K	64	PHE
1	K	67	THR

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Mol	Chain	Res	Type
1	K	69	VAL
1	K	72	VAL
1	K	74	ASN
1	K	75	LYS
1	K	77	THR
1	K	82	LEU
1	K	85	GLN
1	K	91	PHE
1	K	92	LEU
1	K	97	GLN
1	K	99	ASN
1	K	105	GLU
1	K	108	THR
1	K	110	THR
1	K	111	ILE
1	K	117	SER
1	K	125	THR
1	K	130	ASN
1	K	136	GLU
1	K	140	THR
1	K	141	ASN
1	K	154	THR
1	K	159	VAL
1	K	160	GLU
1	K	161	LEU
1	K	166	VAL
1	K	169	THR
1	K	175	TYR
1	K	177	GLU
1	K	179	MET
1	K	188	ILE
1	K	204	SER
1	K	206	ILE
1	K	208	VAL
1	K	212	THR
1	K	216	ARG
1	K	222	VAL
1	K	233	ASN
1	K	239	ASP
1	K	241	ILE
1	K	243	LEU
1	K	248	VAL

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Mol	Chain	Res	Type
1	K	251	THR
1	K	258	LEU
1	K	262	ARG
1	K	265	GLN
1	K	287	LEU
1	K	289	VAL
1	K	312	LEU
1	K	326	ARG
1	K	329	ASN
1	K	331	ILE
1	K	341	ARG
1	K	356	ILE
1	K	358	SER
1	K	360	THR
1	K	364	THR
1	K	368	THR
1	K	374	VAL
1	K	375	TYR
1	K	377	SER
1	K	378	LEU
1	K	380	ASP
1	K	381	MET
1	K	382	MET
1	K	384	ASP
1	K	395	SER
1	K	403	GLU
1	K	405	LEU
1	K	407	VAL
1	K	410	LYS
1	K	415	ASP
1	K	425	GLN
1	K	428	SER
1	K	430	THR
1	K	435	ARG
1	K	438	GLU
1	K	449	THR
1	K	457	VAL
1	K	460	LEU
1	K	461	THR
1	K	465	THR
1	K	470	ASN
1	K	471	SER

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Mol	Chain	Res	Type
1	K	475	VAL
1	K	478	VAL
1	K	480	ILE
1	K	482	ASP
1	K	492	TYR
1	K	499	SER
1	K	502	VAL
1	K	503	LEU
1	K	504	SER
1	K	506	ARG
1	L	58	SER
1	L	60	LEU
1	L	63	LEU
1	L	64	PHE
1	L	66	THR
1	L	67	THR
1	L	68	ARG
1	L	69	VAL
1	L	74	ASN
1	L	82	LEU
1	L	85	GLN
1	L	92	LEU
1	L	95	VAL
1	L	97	GLN
1	L	99	ASN
1	L	110	THR
1	L	117	SER
1	L	125	THR
1	L	126	ILE
1	L	130	ASN
1	L	141	ASN
1	L	154	THR
1	L	158	GLN
1	L	159	VAL
1	L	161	LEU
1	L	166	VAL
1	L	175	TYR
1	L	177	GLU
1	L	179	MET
1	L	182	ASP
1	L	183	LEU
1	L	186	ASN

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Mol	Chain	Res	Type
1	L	188	ILE
1	L	194	LYS
1	L	197	ARG
1	L	206	ILE
1	L	208	VAL
1	L	211	ASP
1	L	213	ARG
1	L	220	ASP
1	L	222	VAL
1	L	239	ASP
1	L	240	ILE
1	L	241	ILE
1	L	243	LEU
1	L	256	SER
1	L	257	ASN
1	L	258	LEU
1	L	265	GLN
1	L	268	GLN
1	L	272	ARG
1	L	289	VAL
1	L	296	LEU
1	L	315	VAL
1	L	319	LEU
1	L	326	ARG
1	L	329	ASN
1	L	331	ILE
1	L	332	SER
1	L	338	THR
1	L	341	ARG
1	L	356	ILE
1	L	358	SER
1	L	360	THR
1	L	364	THR
1	L	373	GLN
1	L	374	VAL
1	L	377	SER
1	L	380	ASP
1	L	382	MET
1	L	384	ASP
1	L	386	VAL
1	L	389	ARG
1	L	390	SER

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Mol	Chain	Res	Type
1	L	394	ILE
1	L	407	VAL
1	L	410	LYS
1	L	415	ASP
1	L	426	PHE
1	L	428	SER
1	L	441	ILE
1	L	449	THR
1	L	450	ILE
1	L	457	VAL
1	L	460	LEU
1	L	465	THR
1	L	469	ARG
1	L	470	ASN
1	L	471	SER
1	L	472	ILE
1	L	475	VAL
1	L	480	ILE
1	L	482	ASP
1	L	486	ARG
1	L	487	THR
1	L	493	LYS
1	L	495	LEU
1	L	498	VAL
1	L	501	ARG
1	L	502	VAL
1	L	503	LEU
1	L	504	SER
1	L	506	ARG
1	M	67	THR
1	M	69	VAL
1	M	73	ASP
1	M	74	ASN
1	M	75	LYS
1	M	77	THR
1	M	82	LEU
1	M	85	GLN
1	M	93	THR
1	M	95	VAL
1	M	97	GLN
1	M	110	THR
1	M	115	ASP

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Mol	Chain	Res	Type
1	M	116	ARG
1	M	117	SER
1	M	138	MET
1	M	141	ASN
1	M	150	SER
1	M	155	LYS
1	M	156	ASP
1	M	159	VAL
1	M	166	VAL
1	M	175	TYR
1	M	177	GLU
1	M	183	LEU
1	M	186	ASN
1	M	189	VAL
1	M	194	LYS
1	M	197	ARG
1	M	206	ILE
1	M	222	VAL
1	M	239	ASP
1	M	240	ILE
1	M	241	ILE
1	M	243	LEU
1	M	251	THR
1	M	258	LEU
1	M	265	GLN
1	M	268	GLN
1	M	276	ASP
1	M	283	ILE
1	M	289	VAL
1	M	295	SER
1	M	315	VAL
1	M	316	ILE
1	M	319	LEU
1	M	327	SER
1	M	331	ILE
1	M	332	SER
1	M	334	ASP
1	M	338	THR
1	M	341	ARG
1	M	356	ILE
1	M	362	LEU
1	M	363	CYS

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Mol	Chain	Res	Type
1	M	365	PRO
1	M	375	TYR
1	M	377	SER
1	M	380	ASP
1	M	382	MET
1	M	386	VAL
1	M	393	GLN
1	M	394	ILE
1	M	395	SER
1	M	403	GLU
1	M	407	VAL
1	M	409	SER
1	M	410	LYS
1	M	426	PHE
1	M	428	SER
1	M	438	GLU
1	M	451	THR
1	M	454	SER
1	M	457	VAL
1	M	458	PRO
1	M	460	LEU
1	M	466	LEU
1	M	470	ASN
1	M	472	ILE
1	M	475	VAL
1	M	480	ILE
1	M	481	THR
1	M	482	ASP
1	M	492	TYR
1	M	498	VAL
1	M	499	SER
1	M	501	ARG
1	M	503	LEU
1	N	53	ASN
1	N	60	LEU
1	N	64	PHE
1	N	69	VAL
1	N	74	ASN
1	N	81	SER
1	N	82	LEU
1	N	95	VAL
1	N	97	GLN

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Mol	Chain	Res	Type
1	N	100	ASP
1	N	105	GLU
1	N	108	THR
1	N	110	THR
1	N	111	ILE
1	N	115	ASP
1	N	116	ARG
1	N	126	ILE
1	N	136	GLU
1	N	138	MET
1	N	156	ASP
1	N	158	GLN
1	N	160	GLU
1	N	161	LEU
1	N	166	VAL
1	N	174	ASN
1	N	175	TYR
1	N	177	GLU
1	N	179	MET
1	N	180	THR
1	N	183	LEU
1	N	194	LYS
1	N	206	ILE
1	N	208	VAL
1	N	216	ARG
1	N	222	VAL
1	N	230	VAL
1	N	239	ASP
1	N	241	ILE
1	N	243	LEU
1	N	251	THR
1	N	255	LEU
1	N	258	LEU
1	N	283	ILE
1	N	289	VAL
1	N	293	GLN
1	N	313	LYS
1	N	316	ILE
1	N	319	LEU
1	N	323	SER
1	N	326	ARG
1	N	329	ASN

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Mol	Chain	Res	Type
1	N	331	ILE
1	N	335	SER
1	N	338	THR
1	N	351	ASP
1	N	354	THR
1	N	363	CYS
1	N	367	VAL
1	N	368	THR
1	N	374	VAL
1	N	377	SER
1	N	380	ASP
1	N	386	VAL
1	N	392	SER
1	N	393	GLN
1	N	394	ILE
1	N	405	LEU
1	N	407	VAL
1	N	409	SER
1	N	410	LYS
1	N	424	ARG
1	N	429	LEU
1	N	430	THR
1	N	436	PHE
1	N	444	ARG
1	N	449	THR
1	N	450	ILE
1	N	460	LEU
1	N	466	LEU
1	N	468	LEU
1	N	470	ASN
1	N	471	SER
1	N	475	VAL
1	N	480	ILE
1	N	493	LYS
1	N	498	VAL
1	N	499	SER
1	N	502	VAL
1	N	503	LEU
1	N	504	SER
1	O	64	PHE
1	O	69	VAL
1	O	72	VAL

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Mol	Chain	Res	Type
1	O	74	ASN
1	O	82	LEU
1	O	93	THR
1	O	95	VAL
1	O	97	GLN
1	O	100	ASP
1	O	108	THR
1	O	110	THR
1	O	117	SER
1	O	125	THR
1	O	130	ASN
1	O	140	THR
1	O	156	ASP
1	O	161	LEU
1	O	166	VAL
1	O	175	TYR
1	O	177	GLU
1	O	183	LEU
1	O	195	VAL
1	O	206	ILE
1	O	208	VAL
1	O	212	THR
1	O	216	ARG
1	O	222	VAL
1	O	239	ASP
1	O	243	LEU
1	O	248	VAL
1	O	251	THR
1	O	258	LEU
1	O	262	ARG
1	O	265	GLN
1	O	268	GLN
1	O	272	ARG
1	O	296	LEU
1	O	319	LEU
1	O	326	ARG
1	O	327	SER
1	O	329	ASN
1	O	332	SER
1	O	333	ASN
1	O	334	ASP
1	O	338	THR

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Mol	Chain	Res	Type
1	O	341	ARG
1	O	356	ILE
1	O	367	VAL
1	O	368	THR
1	O	377	SER
1	O	380	ASP
1	O	382	MET
1	O	384	ASP
1	O	386	VAL
1	O	394	ILE
1	O	403	GLU
1	O	407	VAL
1	O	409	SER
1	O	415	ASP
1	O	419	TYR
1	O	424	ARG
1	O	426	PHE
1	O	428	SER
1	O	435	ARG
1	O	444	ARG
1	O	449	THR
1	O	450	ILE
1	O	460	LEU
1	O	465	THR
1	O	470	ASN
1	O	471	SER
1	O	475	VAL
1	O	480	ILE
1	O	481	THR
1	O	482	ASP
1	O	484	ARG
1	O	487	THR
1	O	493	LYS
1	O	499	SER
1	O	502	VAL
1	O	503	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	198	GLN
1	A	268	GLN
1	A	414	ASN
1	A	440	GLN
1	B	74	ASN
1	B	85	GLN
1	B	90	ASN
1	B	97	GLN
1	B	99	ASN
1	B	130	ASN
1	B	141	ASN
1	B	198	GLN
1	B	268	GLN
1	B	396	ASN
1	B	431	HIS
1	C	85	GLN
1	C	86	ASN
1	C	130	ASN
1	C	133	ASN
1	C	373	GLN
1	C	396	ASN
1	C	414	ASN
1	D	85	GLN
1	D	86	ASN
1	D	128	HIS
1	D	130	ASN
1	D	268	GLN
1	D	339	GLN
1	D	353	GLN
1	D	383	GLN
1	D	414	ASN
1	D	440	GLN
1	E	86	ASN
1	E	130	ASN
1	E	133	ASN
1	E	141	ASN
1	E	185	ASN
1	E	237	HIS
1	E	268	GLN
1	E	339	GLN
1	E	393	GLN
1	E	396	ASN

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Mol	Chain	Res	Type
1	F	130	ASN
1	F	133	ASN
1	F	141	ASN
1	F	198	GLN
1	F	237	HIS
1	F	434	ASN
1	G	85	GLN
1	G	86	ASN
1	G	97	GLN
1	G	133	ASN
1	G	135	ASN
1	G	141	ASN
1	G	237	HIS
1	G	268	GLN
1	G	373	GLN
1	G	393	GLN
1	G	440	GLN
1	G	463	HIS
1	H	86	ASN
1	H	128	HIS
1	H	133	ASN
1	H	141	ASN
1	H	185	ASN
1	H	198	GLN
1	H	237	HIS
1	H	257	ASN
1	H	440	GLN
1	H	463	HIS
1	I	86	ASN
1	I	141	ASN
1	I	185	ASN
1	I	198	GLN
1	I	257	ASN
1	I	265	GLN
1	I	268	GLN
1	I	339	GLN
1	I	383	GLN
1	J	85	GLN
1	J	86	ASN
1	J	130	ASN
1	J	133	ASN
1	J	141	ASN

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Mol	Chain	Res	Type
1	J	198	GLN
1	J	237	HIS
1	J	257	ASN
1	J	268	GLN
1	K	85	GLN
1	K	99	ASN
1	K	130	ASN
1	K	141	ASN
1	K	191	HIS
1	K	198	GLN
1	K	237	HIS
1	K	265	GLN
1	K	329	ASN
1	K	383	GLN
1	K	396	ASN
1	K	414	ASN
1	K	440	GLN
1	L	85	GLN
1	L	86	ASN
1	L	99	ASN
1	L	141	ASN
1	L	186	ASN
1	L	198	GLN
1	L	268	GLN
1	L	393	GLN
1	L	396	ASN
1	L	463	HIS
1	M	85	GLN
1	M	97	GLN
1	M	268	GLN
1	M	439	ASN
1	M	440	GLN
1	N	74	ASN
1	N	86	ASN
1	N	88	HIS
1	N	133	ASN
1	N	198	GLN
1	N	434	ASN
1	N	439	ASN
1	N	440	GLN
1	O	86	ASN
1	O	97	GLN

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Mol	Chain	Res	Type
1	O	130	ASN
1	O	141	ASN
1	O	198	GLN
1	O	237	HIS
1	O	257	ASN
1	O	268	GLN
1	O	329	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

There are no ligands in this entry.

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	444/523 (84%)	-0.50	3 (0%) 87 78	96, 131, 195, 200	0
1	B	444/523 (84%)	-0.44	2 (0%) 91 83	96, 131, 195, 200	0
1	C	444/523 (84%)	-0.44	4 (0%) 84 73	95, 131, 196, 200	0
1	D	444/523 (84%)	-0.43	2 (0%) 91 83	96, 131, 195, 200	0
1	E	444/523 (84%)	-0.49	0 100 100	96, 131, 195, 200	0
1	F	444/523 (84%)	-0.45	3 (0%) 87 78	94, 131, 196, 200	0
1	G	444/523 (84%)	-0.48	3 (0%) 87 78	94, 132, 195, 200	0
1	H	444/523 (84%)	-0.42	2 (0%) 91 83	95, 131, 195, 200	0
1	I	444/523 (84%)	-0.48	0 100 100	96, 131, 195, 200	0
1	J	444/523 (84%)	-0.44	2 (0%) 91 83	95, 131, 196, 200	0
1	K	444/523 (84%)	-0.46	1 (0%) 95 91	96, 131, 196, 200	0
1	L	444/523 (84%)	-0.46	4 (0%) 84 73	95, 131, 196, 200	0
1	M	444/523 (84%)	-0.45	2 (0%) 91 83	95, 132, 196, 200	0
1	N	444/523 (84%)	-0.46	5 (1%) 80 68	95, 131, 196, 200	0
1	O	444/523 (84%)	-0.45	4 (0%) 84 73	94, 131, 195, 200	0
All	All	6660/7845 (84%)	-0.46	37 (0%) 89 81	94, 131, 196, 200	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	429	LEU	4.1
1	O	425	GLN	3.5
1	D	425	GLN	3.5
1	C	426	PHE	3.4
1	L	294	ALA	3.3
1	K	49	THR	3.2
1	L	49	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	156	ASP	3.1
1	M	294	ALA	3.0
1	B	157	LYS	2.9
1	L	507	THR	2.9
1	N	294	ALA	2.9
1	G	429	LEU	2.8
1	H	294	ALA	2.8
1	N	49	THR	2.7
1	F	49	THR	2.7
1	J	429	LEU	2.7
1	F	425	GLN	2.6
1	D	50	GLY	2.6
1	F	294	ALA	2.6
1	A	426	PHE	2.6
1	J	421	GLN	2.5
1	O	49	THR	2.5
1	C	421	GLN	2.4
1	N	429	LEU	2.4
1	N	293	GLN	2.3
1	G	294	ALA	2.3
1	O	50	GLY	2.2
1	B	429	LEU	2.2
1	A	294	ALA	2.2
1	L	293	GLN	2.2
1	C	429	LEU	2.2
1	O	294	ALA	2.1
1	N	312	LEU	2.1
1	M	49	THR	2.1
1	G	49	THR	2.1
1	A	425	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.