Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 02:54 PM EDT

PDB ID	:	1GLL
Title	:	ESCHERICHIA COLI GLYCEROL KINASE MUTANT WITH BOUND ATP ANALOG SHOWING SUBSTANTIAL DOMAIN MOTION
Authors	:	Bystrom, C.E.; Pettigrew, D.W.; Branchaud, B.P.; Remington, S.J.
Deposited on	:	1998-09-24
Resolution	:	3.00 Å(reported)

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

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

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

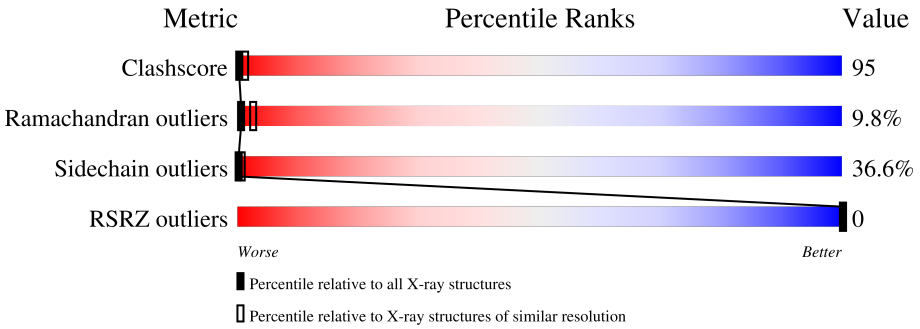
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	O	501	10% 47% 32% 10%
1	Y	501	12% 43% 32% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	O	600	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7896 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 GLYCEROL KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			
1	O	494	Total	C	N	O	S	0	0	0
			3910	2470	683	738	19			

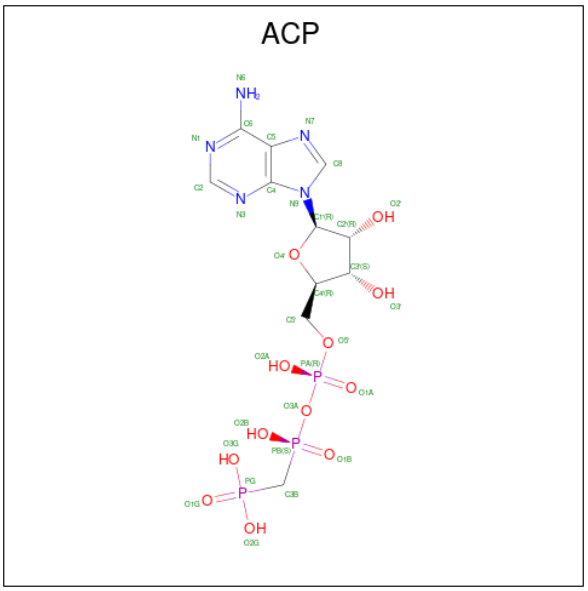
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	TRP	SER	engineered mutation	UNP P0A6F3
O	58	TRP	SER	engineered mutation	UNP P0A6F3

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

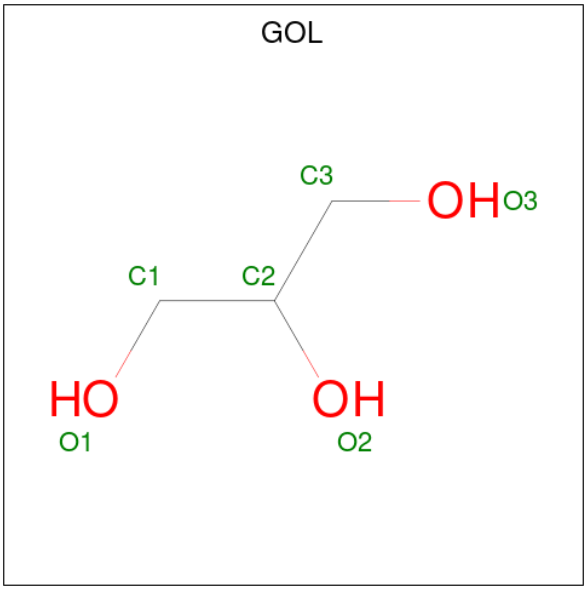
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Y	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	O	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



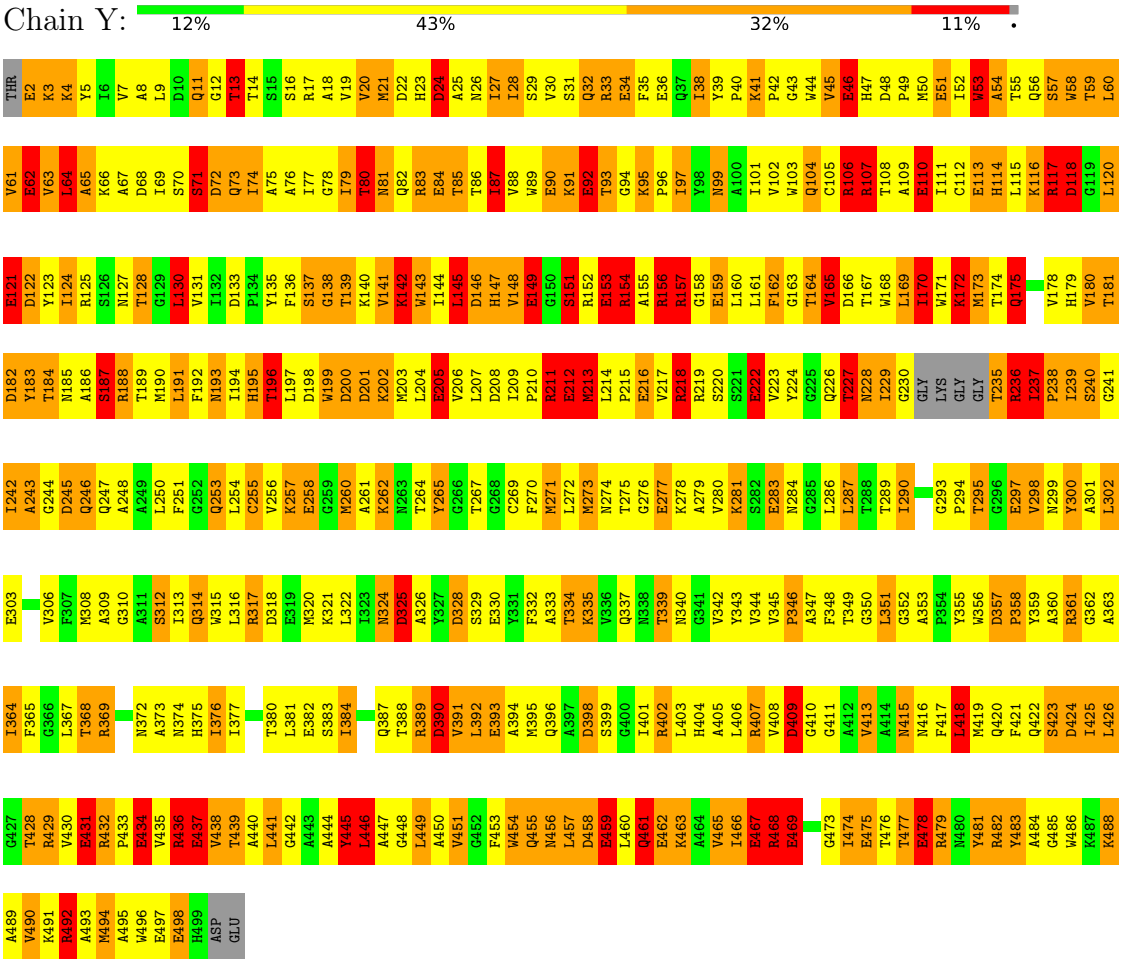
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Y	1	Total	C	O		0	0
			6	3	3			
4	O	1	Total	C	O		0	0
			6	3	3			

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.

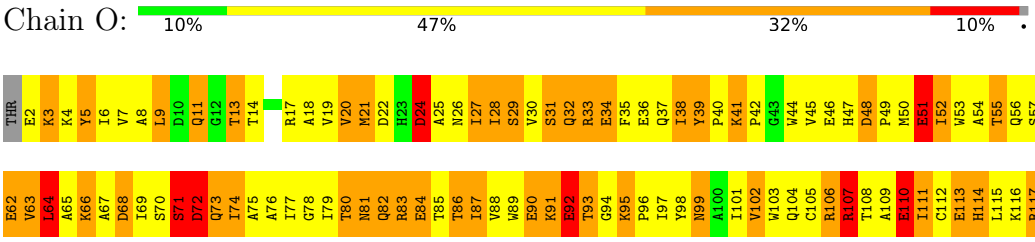
• Molecule 1: GLYCEROL KINASE

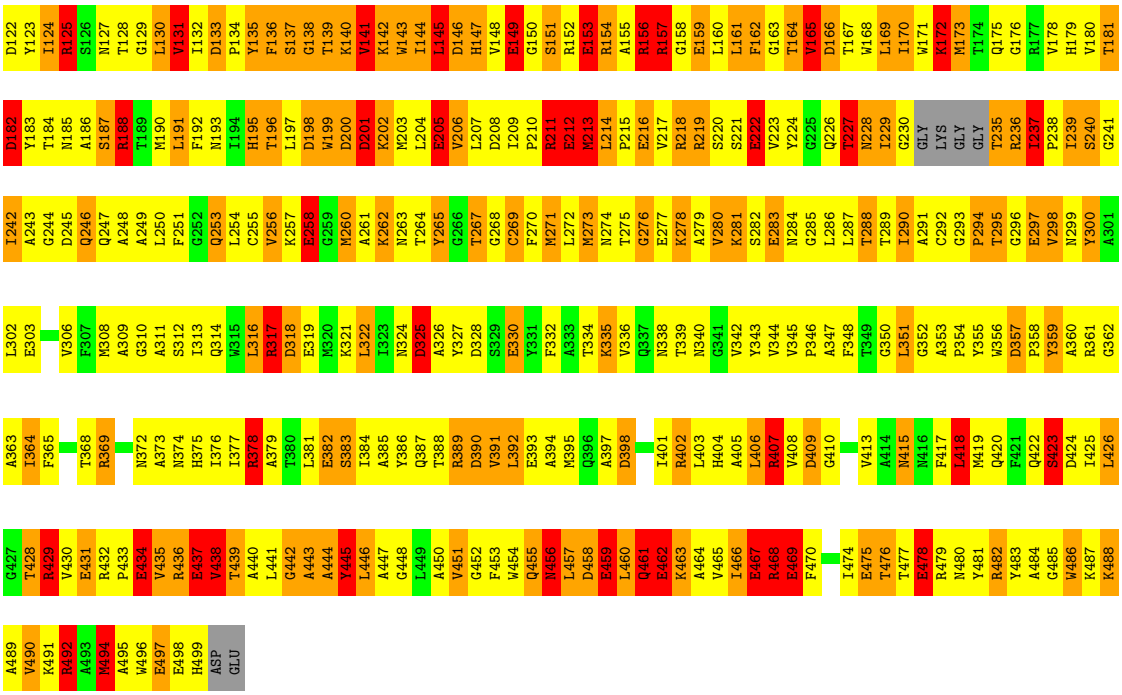
Chain Y:



• Molecule 1: GLYCEROL KINASE

Chain O:




D122 Y123 I124 R125 S126 N127 T128 G129 L130 V131 I132 D133 P134 Y135 F136 S137 G138 T139 K140 V141 K142 W143 I144 L145 D146 H147 V148 E149 G150 S151 R152 E153 R154 A155 R156 R157 G158 E159 L160 L161 F162 G163 T164 V165 D166 T167 W168 L169 I170 W171 K172 M173 T174 Q175 G176 R177 V178 H179 V180 T181
D182 Y183 T184 N185 A186 S187 R188 T189 M190 L191 F192 N193 I194 H195 T196 L197 D198 W199 D200 D201 K202 M203 L204 E205 V206 L207 D208 I209 P210 R211 E212 M213 L214 P215 E216 V217 R218 R219 S220 S221 E222 V223 Y224 G225 Q226 T227 N228 I229 G230 GLY LYS GLY T235 R236 I237 P238 I239 S240 G241
I242 A243 G244 D245 Q246 Q247 A248 A249 L250 F251 G252 Q253 L254 C255 V256 K257 E258 G259 M260 A261 K262 N263 T264 Y265 G266 T267 G268 C269 F270 M271 L272 M273 N274 T275 G276 E277 K278 A279 V280 K281 S282 E283 N284 G285 L286 L287 T288 T289 T290 A291 C292 G293 P294 T295 G296 E297 V298 N299 Y300 A301
L302 E303 V306 F307 M308 A309 G310 A311 S312 I313 Q314 W315 L316 R317 D318 E319 M320 K321 L322 I323 N324 D325 A326 Y327 D328 S329 E330 Y331 F332 A333 T334 K335 V336 Q337 N338 T339 N340 G341 V342 Y343 V344 V345 P346 A347 F348 T349 G350 L351 G352 A353 P354 Y355 W356 D357 P358 Y359 A360 R361 G362
A363 I364 F365 T368 R369 N372 A373 N374 H375 I376 I377 R378 A379 T380 L381 E382 S383 I384 A385 Y386 Q387 T388 R389 D390 V391 L392 E393 A394 M395 Q396 A397 D398 I401 R402 L403 H404 A405 L406 R407 V408 D409 G410 V413 A414 N415 N416 F417 L418 M419 Q420 F421 Q422 S423 D424 I425 L426
G427 T428 R429 V430 E431 R432 P433 E434 V435 R436 E437 V438 T439 A440 L441 G442 A443 A444 Y445 L446 A447 G448 L449 A450 V451 G452 F453 W454 Q455 N456 L457 D458 E459 L460 Q461 E462 K463 A464 V465 I466 E467 R468 E469 F470 I474 E475 T476 T477 E478 R479 N480 Y481 R482 Y483 A484 G485 W486 K487 K488
A489 V490 K491 R492 A493 M494 A495 W496 E497 E498 H499 ASP GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.77Å 201.15Å 114.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 18.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-3.00) 82.7 (18.03-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	93.19 (at 2.97Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.176 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 157.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7896	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 (i)

5.1 Standard geometry (i)

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

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	O	1.27	37/3991 (0.9%)	1.68	72/5412 (1.3%)
1	Y	1.38	35/3991 (0.9%)	1.76	90/5412 (1.7%)
All	All	1.33	72/7982 (0.9%)	1.72	162/10824 (1.5%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	478	GLU	CD-OE2	9.70	1.36	1.25
1	Y	153	GLU	CD-OE1	9.27	1.35	1.25
1	O	258	GLU	CD-OE2	9.23	1.35	1.25
1	Y	34	GLU	CD-OE1	9.09	1.35	1.25
1	Y	478	GLU	CD-OE2	9.08	1.35	1.25
1	Y	84	GLU	CD-OE1	9.01	1.35	1.25
1	Y	110	GLU	CD-OE2	8.68	1.35	1.25
1	O	153	GLU	CD-OE1	8.55	1.35	1.25
1	Y	36	GLU	CD-OE2	8.55	1.35	1.25
1	Y	216	GLU	CD-OE2	8.53	1.35	1.25
1	Y	462	GLU	CD-OE2	8.52	1.35	1.25
1	Y	149	GLU	CD-OE1	8.26	1.34	1.25
1	Y	283	GLU	CD-OE1	8.24	1.34	1.25
1	O	475	GLU	CD-OE2	8.14	1.34	1.25
1	Y	92	GLU	CD-OE1	7.97	1.34	1.25
1	Y	382	GLU	CD-OE2	7.88	1.34	1.25
1	O	462	GLU	CD-OE2	7.83	1.34	1.25
1	Y	475	GLU	CD-OE2	7.73	1.34	1.25
1	O	459	GLU	CD-OE2	7.71	1.34	1.25
1	Y	90	GLU	CD-OE2	7.41	1.33	1.25
1	Y	205	GLU	CD-OE1	7.40	1.33	1.25
1	O	497	GLU	CD-OE1	7.40	1.33	1.25
1	O	36	GLU	CD-OE2	7.39	1.33	1.25
1	O	92	GLU	CD-OE2	7.22	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	34	GLU	CD-OE1	7.21	1.33	1.25
1	Y	2	GLU	CD-OE2	7.18	1.33	1.25
1	O	431	GLU	CD-OE1	7.14	1.33	1.25
1	O	149	GLU	CD-OE2	7.14	1.33	1.25
1	Y	297	GLU	CD-OE2	7.13	1.33	1.25
1	O	469	GLU	CD-OE2	7.11	1.33	1.25
1	O	283	GLU	CD-OE1	7.09	1.33	1.25
1	Y	277	GLU	CD-OE1	7.06	1.33	1.25
1	O	393	GLU	CD-OE1	6.97	1.33	1.25
1	O	159	GLU	CD-OE2	6.95	1.33	1.25
1	Y	498	GLU	CD-OE2	6.90	1.33	1.25
1	O	113	GLU	CD-OE2	6.68	1.33	1.25
1	O	90	GLU	CD-OE2	6.66	1.32	1.25
1	O	121	GLU	CD-OE2	6.63	1.32	1.25
1	Y	431	GLU	CD-OE1	6.61	1.32	1.25
1	O	498	GLU	CD-OE2	6.57	1.32	1.25
1	O	382	GLU	CD-OE2	6.53	1.32	1.25
1	Y	393	GLU	CD-OE1	6.51	1.32	1.25
1	O	319	GLU	CD-OE2	6.51	1.32	1.25
1	O	277	GLU	CD-OE1	6.45	1.32	1.25
1	O	222	GLU	CD-OE2	6.41	1.32	1.25
1	Y	212	GLU	CD-OE2	6.38	1.32	1.25
1	O	62	GLU	CD-OE1	6.37	1.32	1.25
1	Y	51	GLU	CD-OE2	6.30	1.32	1.25
1	O	2	GLU	CD-OE2	6.02	1.32	1.25
1	O	437	GLU	CD-OE1	6.01	1.32	1.25
1	Y	469	GLU	CD-OE2	5.98	1.32	1.25
1	O	110	GLU	CD-OE2	5.97	1.32	1.25
1	O	330	GLU	CD-OE1	5.97	1.32	1.25
1	O	51	GLU	CD-OE1	5.96	1.32	1.25
1	Y	62	GLU	CD-OE1	5.93	1.32	1.25
1	O	84	GLU	CD-OE1	5.85	1.32	1.25
1	O	205	GLU	CD-OE1	5.85	1.32	1.25
1	O	216	GLU	CD-OE2	5.79	1.32	1.25
1	O	212	GLU	CD-OE2	5.75	1.31	1.25
1	Y	159	GLU	CD-OE2	5.69	1.31	1.25
1	Y	437	GLU	CD-OE1	5.67	1.31	1.25
1	Y	459	GLU	CD-OE1	5.62	1.31	1.25
1	Y	434	GLU	CD-OE1	5.58	1.31	1.25
1	Y	113	GLU	CD-OE2	5.53	1.31	1.25
1	O	467	GLU	CD-OE2	5.50	1.31	1.25
1	Y	222	GLU	CD-OE2	5.49	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	297	GLU	CD-OE2	5.38	1.31	1.25
1	Y	467	GLU	CD-OE2	5.27	1.31	1.25
1	Y	46	GLU	CD-OE2	5.27	1.31	1.25
1	Y	121	GLU	CD-OE2	5.26	1.31	1.25
1	Y	258	GLU	CD-OE2	5.19	1.31	1.25
1	O	434	GLU	CD-OE1	5.02	1.31	1.25

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	237	ILE	C-N-CD	-15.74	85.98	120.60
1	Y	83	ARG	C-N-CA	-10.97	94.28	121.70
1	Y	200	ASP	CB-CG-OD2	-10.81	108.57	118.30
1	Y	492	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	O	468	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	O	378	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	O	492	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	O	122	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	Y	328	ASP	CB-CG-OD1	-8.56	110.60	118.30
1	Y	361	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	Y	107	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	Y	424	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	Y	245	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	O	398	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	Y	83	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	O	211	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	O	198	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	Y	334	THR	CA-CB-CG2	-7.87	101.38	112.40
1	Y	80	THR	CA-CB-CG2	-7.82	101.45	112.40
1	O	458	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	Y	117	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	O	198	ASP	CB-CG-OD1	7.71	125.24	118.30
1	Y	107	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	O	107	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	Y	198	ASP	CB-CG-OD1	7.54	125.09	118.30
1	Y	436	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	O	133	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	Y	72	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	Y	409	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	Y	390	ASP	N-CA-CB	7.23	123.62	110.60
1	Y	236	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	O	125	ARG	NE-CZ-NH2	7.21	123.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	378	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	Y	328	ASP	CB-CG-OD2	7.16	124.75	118.30
1	Y	265	TYR	CB-CG-CD2	-7.14	116.72	121.00
1	Y	157	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	Y	357	ASP	CB-CG-OD1	7.01	124.61	118.30
1	O	357	ASP	CB-CG-OD1	6.96	124.56	118.30
1	O	398	ASP	CB-CG-OD2	6.89	124.50	118.30
1	O	146	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	O	318	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	O	118	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	Y	398	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	Y	156	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	O	325	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	Y	64	LEU	N-CA-CB	6.67	123.75	110.40
1	O	317	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	O	188	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	O	182	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	O	458	ASP	CB-CG-OD1	6.61	124.25	118.30
1	Y	80	THR	N-CA-CB	6.58	122.81	110.30
1	O	156	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	O	476	THR	CA-CB-CG2	-6.43	103.40	112.40
1	O	24	ASP	CB-CG-OD2	6.36	124.03	118.30
1	Y	122	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	Y	156	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	Y	325	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	Y	458	ASP	CB-CG-OD1	6.30	123.97	118.30
1	Y	106	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	O	200	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	Y	68	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	O	479	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	Y	83	ARG	O-C-N	-6.18	112.81	122.70
1	Y	24	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	Y	182	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	Y	361	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	Y	227	THR	CA-CB-CG2	-6.04	103.94	112.40
1	Y	62	GLU	N-CA-CB	5.98	121.37	110.60
1	Y	357	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	O	20	VAL	CB-CA-C	-5.95	100.11	111.40
1	Y	20	VAL	CB-CA-C	-5.94	100.11	111.40
1	O	357	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	O	83	ARG	N-CA-C	5.87	126.84	111.00
1	O	68	ASP	CB-CG-OD2	5.85	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	107	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	Y	481	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	Y	200	ASP	CB-CG-OD1	5.83	123.54	118.30
1	Y	255	CYS	CA-CB-SG	-5.82	103.53	114.00
1	Y	104	GLN	N-CA-CB	-5.81	100.15	110.60
1	O	106	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	O	48	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	O	118	ASP	CB-CG-OD1	5.80	123.52	118.30
1	O	407	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	O	342	VAL	CA-CB-CG2	-5.75	102.27	110.90
1	O	83	ARG	C-N-CA	-5.71	107.42	121.70
1	Y	20	VAL	N-CA-CB	5.70	124.04	111.50
1	O	58	TRP	CA-C-N	-5.70	104.66	117.20
1	Y	183	TYR	CA-CB-CG	-5.68	102.61	113.40
1	O	288	THR	CA-CB-CG2	-5.67	104.46	112.40
1	Y	201	ASP	CB-CG-OD1	5.65	123.39	118.30
1	Y	72	ASP	CB-CG-OD1	5.64	123.38	118.30
1	O	200	ASP	CB-CG-OD1	5.64	123.37	118.30
1	Y	445	TYR	CB-CG-CD1	5.61	124.36	121.00
1	O	166	ASP	CB-CG-OD1	5.57	123.32	118.30
1	O	68	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	Y	436	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	Y	481	TYR	CA-CB-CG	-5.56	102.84	113.40
1	O	409	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	O	468	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	Y	114	HIS	CA-CB-CG	-5.51	104.23	113.60
1	O	237	ILE	C-N-CD	-5.50	108.50	120.60
1	O	38	ILE	CB-CA-C	-5.46	100.69	111.60
1	Y	201	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	O	156	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	Y	130	LEU	CA-CB-CG	-5.42	102.84	115.30
1	Y	117	ARG	CB-CA-C	-5.40	99.60	110.40
1	Y	118	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	O	268	GLY	N-CA-C	-5.40	99.60	113.10
1	O	211	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	O	423	SER	N-CA-CB	5.38	118.58	110.50
1	O	265	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	O	201	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	O	494	MET	N-CA-CB	5.35	120.24	110.60
1	O	72	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	Y	380	THR	CA-CB-CG2	-5.33	104.94	112.40
1	Y	492	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	458	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	O	300	TYR	N-CA-CB	5.32	120.17	110.60
1	Y	184	THR	CA-CB-CG2	-5.31	104.96	112.40
1	Y	45	VAL	CA-CB-CG1	-5.31	102.93	110.90
1	Y	211	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	O	267	THR	CA-CB-CG2	-5.29	104.99	112.40
1	Y	409	ASP	CB-CG-OD1	5.29	123.06	118.30
1	Y	413	VAL	CA-CB-CG1	-5.28	102.99	110.90
1	Y	55	THR	N-CA-CB	5.25	120.28	110.30
1	Y	125	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	Y	333	ALA	CB-CA-C	5.24	117.97	110.10
1	Y	24	ASP	CB-CG-OD2	5.23	123.01	118.30
1	Y	390	ASP	CB-CA-C	-5.21	99.97	110.40
1	Y	218	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	O	13	THR	CA-CB-CG2	-5.21	105.11	112.40
1	O	445	TYR	N-CA-CB	5.20	119.95	110.60
1	Y	85	THR	N-CA-CB	-5.20	100.43	110.30
1	O	24	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	Y	13	THR	CA-CB-CG2	-5.18	105.15	112.40
1	O	478	GLU	CG-CD-OE1	5.18	128.65	118.30
1	O	359	TYR	CA-CB-CG	-5.17	103.57	113.40
1	O	429	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	Y	333	ALA	N-CA-CB	-5.13	102.91	110.10
1	O	227	THR	CA-CB-CG2	-5.13	105.22	112.40
1	Y	339	THR	CA-CB-CG2	-5.13	105.22	112.40
1	Y	468	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	Y	243	ALA	N-CA-CB	5.12	117.27	110.10
1	Y	465	VAL	CA-CB-CG1	-5.12	103.23	110.90
1	Y	154	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	Y	84	GLU	O-C-N	5.10	130.85	122.70
1	O	201	ASP	CB-CG-OD1	5.09	122.88	118.30
1	Y	83	ARG	N-CA-C	5.08	124.73	111.00
1	O	72	ASP	CB-CG-OD1	5.08	122.87	118.30
1	O	130	LEU	CA-CB-CG	-5.08	103.62	115.30
1	Y	87	ILE	CB-CA-C	-5.07	101.47	111.60
1	O	39	TYR	CB-CG-CD2	5.07	124.04	121.00
1	Y	390	ASP	CA-CB-CG	5.06	124.53	113.40
1	Y	300	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	Y	117	ARG	N-CA-CB	5.05	119.69	110.60
1	O	492	ARG	CD-NE-CZ	5.05	130.67	123.60
1	Y	398	ASP	CB-CG-OD2	5.05	122.84	118.30
1	O	48	ASP	CB-CG-OD2	5.05	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	193	ASN	N-CA-CB	5.02	119.64	110.60
1	Y	432	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	Y	38	ILE	CB-CA-C	-5.02	101.57	111.60
1	O	438	VAL	CA-CB-CG2	-5.01	103.38	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3910	0	3841	747	0
1	Y	3910	0	3841	743	0
2	O	1	0	0	0	0
2	Y	1	0	0	0	0
3	O	31	0	14	4	0
3	Y	31	0	14	5	0
4	O	6	0	8	7	0
4	Y	6	0	8	2	0
All	All	7896	0	7726	1482	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 95.

All (1482) 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:Y:458:ASP:HA	1:Y:461:GLN:HG3	1.25	1.13
1:O:48:ASP:HB3	1:O:51:GLU:HB3	1.16	1.13
1:O:415:ASN:ND2	1:O:418:LEU:H	1.48	1.11
1:Y:31:SER:HB2	1:Y:63:VAL:HG22	1.28	1.08
1:O:83:ARG:HB2	4:O:600:GOL:H12	1.11	1.08
1:Y:459:GLU:HB2	1:Y:460:LEU:HD12	1.25	1.07
1:Y:84:GLU:HB2	1:Y:103:TRP:HB3	1.36	1.06
1:Y:31:SER:HB3	1:Y:59:THR:HA	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:117:ARG:HH11	1:O:117:ARG:HB2	1.16	1.04
1:O:435:VAL:HG21	1:O:441:LEU:HD11	1.41	1.02
1:O:313:ILE:HD11	1:O:381:LEU:HD23	1.42	1.01
1:O:211:ARG:HG3	1:O:211:ARG:HH11	1.22	1.00
1:O:47:HIS:HB3	1:O:52:ILE:HD11	1.41	0.99
1:O:138:GLY:HA2	1:O:191:LEU:HD21	1.42	0.98
1:O:272:LEU:HD11	1:O:303:GLU:HG3	1.41	0.98
1:Y:246:GLN:HG3	1:Y:262:LYS:HZ1	1.28	0.97
1:Y:460:LEU:HD12	1:Y:460:LEU:H	1.29	0.97
1:O:144:ILE:HD12	1:O:144:ILE:H	1.28	0.96
1:O:460:LEU:HD12	1:O:460:LEU:H	1.31	0.96
1:Y:27:ILE:HD12	1:Y:27:ILE:H	1.31	0.96
1:Y:117:ARG:HH11	1:Y:117:ARG:HB2	1.31	0.96
1:Y:229:ILE:HG21	1:Y:237:ILE:HG12	1.47	0.96
1:Y:226:GLN:HB2	1:Y:236:ARG:HD3	1.50	0.93
1:O:137:SER:O	1:O:138:GLY:C	2.02	0.93
1:Y:152:ARG:HB3	1:Y:156:ARG:HH22	1.34	0.93
1:Y:413:VAL:HG12	1:Y:419:MET:HE3	1.51	0.92
1:O:468:ARG:HG3	1:O:468:ARG:HH11	1.32	0.92
1:O:415:ASN:HD21	1:O:417:PHE:HB3	1.33	0.92
1:Y:117:ARG:HB2	1:Y:117:ARG:NH1	1.84	0.91
1:Y:468:ARG:HD2	1:Y:469:GLU:N	1.85	0.91
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.50	0.91
1:O:415:ASN:HD22	1:O:418:LEU:H	1.01	0.91
1:Y:91:LYS:HB2	1:Y:161:LEU:HD12	1.53	0.91
1:O:27:ILE:H	1:O:27:ILE:HD12	1.35	0.91
1:O:271:MET:HG2	1:O:395:MET:HE2	1.54	0.90
1:O:115:LEU:HD12	1:O:115:LEU:H	1.38	0.89
1:Y:91:LYS:O	1:Y:92:GLU:C	2.05	0.89
1:O:413:VAL:HA	1:O:419:MET:CE	2.03	0.89
1:Y:459:GLU:HB2	1:Y:460:LEU:CD1	2.03	0.88
1:O:463:LYS:HE2	1:O:463:LYS:HA	1.56	0.88
1:O:164:THR:H	1:O:167:THR:HB	1.39	0.87
1:Y:279:ALA:HB2	1:Y:300:TYR:CD2	2.09	0.87
1:Y:196:THR:H	1:Y:197:LEU:HD22	1.39	0.87
1:O:193:ASN:HB3	1:O:196:THR:CG2	2.04	0.87
1:Y:257:LYS:H	1:Y:260:MET:HG3	1.40	0.87
1:O:3:LYS:HG3	1:O:73:GLN:HA	1.57	0.87
1:Y:211:ARG:HG3	1:Y:211:ARG:HH11	1.40	0.87
1:O:203:MET:HA	1:O:206:VAL:HG12	1.57	0.87
1:O:35:PHE:HB2	1:O:51:GLU:HG3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:193:ASN:HB3	1:Y:196:THR:CG2	2.05	0.86
1:Y:31:SER:CB	1:Y:63:VAL:HG22	2.05	0.86
1:O:63:VAL:HA	1:O:66:LYS:HG2	1.55	0.85
1:O:91:LYS:HB2	1:O:161:LEU:HD12	1.57	0.85
1:Y:463:LYS:HA	1:Y:463:LYS:HE2	1.56	0.85
1:Y:468:ARG:HD2	1:Y:469:GLU:H	1.37	0.85
1:O:184:THR:HB	1:O:247:GLN:HG2	1.59	0.85
1:Y:183:TYR:CE1	1:Y:217:VAL:HG12	2.12	0.85
1:O:90:GLU:HB3	1:O:93:THR:HG23	1.58	0.84
1:O:17:ARG:HH22	1:O:437:GLU:HG3	1.40	0.84
1:Y:193:ASN:HB3	1:Y:196:THR:HB	1.58	0.83
1:O:199:TRP:CZ2	1:O:214:LEU:HB3	2.13	0.83
1:Y:84:GLU:HB2	1:Y:103:TRP:CB	2.07	0.83
1:Y:240:SER:HB2	1:Y:450:ALA:CB	2.08	0.83
1:Y:81:ASN:N	1:Y:81:ASN:HD22	1.77	0.83
1:Y:328:ASP:HB3	1:Y:332:PHE:HE2	1.43	0.82
1:O:102:VAL:HG12	1:O:103:TRP:CD1	2.13	0.82
1:O:47:HIS:HB3	1:O:52:ILE:CD1	2.08	0.82
1:O:80:THR:HG21	1:O:245:ASP:HA	1.61	0.82
1:Y:47:HIS:HB3	1:Y:52:ILE:HD11	1.60	0.82
1:Y:458:ASP:HA	1:Y:461:GLN:CG	2.09	0.82
1:O:415:ASN:HD22	1:O:418:LEU:N	1.78	0.82
1:O:459:GLU:HB2	1:O:460:LEU:HD12	1.62	0.82
1:O:114:HIS:HA	1:O:117:ARG:NH1	1.95	0.81
1:Y:433:PRO:HA	1:Y:466:ILE:HA	1.61	0.81
1:O:55:THR:HA	1:O:58:TRP:CD1	2.16	0.81
1:O:91:LYS:O	1:O:92:GLU:C	2.12	0.81
1:O:313:ILE:HD11	1:O:381:LEU:CD2	2.11	0.81
1:O:48:ASP:CB	1:O:51:GLU:HB3	2.08	0.80
1:O:91:LYS:NZ	1:O:91:LYS:HB3	1.94	0.80
1:Y:189:THR:HB	1:Y:191:LEU:HG	1.63	0.80
1:O:193:ASN:HB3	1:O:196:THR:HB	1.62	0.80
1:O:373:ALA:O	1:O:377:ILE:HG13	1.82	0.80
1:Y:195:HIS:N	1:Y:195:HIS:ND1	2.29	0.80
1:Y:251:PHE:CE2	1:Y:446:LEU:HD12	2.17	0.80
1:Y:457:LEU:HA	1:Y:460:LEU:HD13	1.61	0.80
1:O:253:GLN:HE21	1:O:262:LYS:CB	1.96	0.79
1:O:138:GLY:HA2	1:O:191:LEU:CD2	2.12	0.79
1:O:199:TRP:CE2	1:O:214:LEU:HB3	2.18	0.79
1:Y:106:ARG:HD2	1:Y:349:THR:O	1.82	0.79
1:O:48:ASP:HB3	1:O:51:GLU:CB	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:188:ARG:HH21	1:O:289:THR:HG21	1.48	0.79
1:O:272:LEU:CD1	1:O:303:GLU:HG3	2.13	0.78
1:O:463:LYS:HA	1:O:463:LYS:CE	2.13	0.78
1:Y:458:ASP:CA	1:Y:461:GLN:HG3	2.12	0.78
1:Y:3:LYS:HA	1:Y:73:GLN:HA	1.64	0.78
1:Y:413:VAL:HA	1:Y:419:MET:CE	2.13	0.78
1:O:438:VAL:HA	1:O:441:LEU:HD12	1.65	0.78
1:Y:230:GLY:HA2	1:Y:235:THR:CB	2.13	0.78
1:O:40:PRO:HG2	1:O:44:TRP:CB	2.14	0.78
1:Y:415:ASN:HD21	1:Y:417:PHE:HB3	1.47	0.77
1:O:19:VAL:HG12	1:O:21:MET:HE2	1.66	0.77
1:O:146:ASP:HB3	1:O:152:ARG:HH12	1.49	0.77
1:Y:492:ARG:HG2	1:Y:492:ARG:HH11	1.47	0.77
1:O:253:GLN:HE21	1:O:262:LYS:HB2	1.49	0.77
1:Y:413:VAL:HG12	1:Y:419:MET:CE	2.15	0.77
1:O:17:ARG:HH22	1:O:437:GLU:CG	1.98	0.76
1:O:33:ARG:HH21	1:O:58:TRP:HB3	1.50	0.76
1:O:435:VAL:CG2	1:O:441:LEU:HD11	2.14	0.76
1:O:360:ALA:O	1:O:361:ARG:HD3	1.84	0.76
1:Y:286:LEU:C	1:Y:287:LEU:HD23	2.05	0.76
1:O:155:ALA:HB1	1:O:210:PRO:HG2	1.66	0.76
1:Y:127:ASN:HB3	1:Y:193:ASN:ND2	2.00	0.76
1:Y:162:PHE:HB3	1:Y:213:MET:HG3	1.67	0.76
1:Y:373:ALA:O	1:Y:377:ILE:HG13	1.84	0.76
1:O:152:ARG:O	1:O:155:ALA:HB3	1.85	0.76
1:Y:360:ALA:O	1:Y:361:ARG:HD3	1.85	0.76
1:Y:457:LEU:HD22	1:Y:460:LEU:HD13	1.66	0.76
1:O:413:VAL:HA	1:O:419:MET:HE2	1.67	0.76
1:Y:58:TRP:O	1:Y:59:THR:C	2.24	0.76
1:O:173:MET:HB3	1:O:227:THR:HG21	1.67	0.76
1:O:123:TYR:CZ	1:O:202:LYS:HG3	2.20	0.76
1:O:164:THR:H	1:O:167:THR:CB	1.98	0.76
1:Y:141:VAL:O	1:Y:145:LEU:HD22	1.86	0.75
1:Y:267:THR:OG1	3:Y:601:ACP:H3B2	1.86	0.75
1:Y:255:CYS:HB3	1:Y:260:MET:HB2	1.68	0.75
1:Y:269:CYS:HB2	1:Y:306:VAL:HB	1.68	0.75
1:O:31:SER:OG	1:O:62:GLU:HB2	1.85	0.75
1:O:195:HIS:ND1	1:O:195:HIS:N	2.29	0.75
1:Y:152:ARG:O	1:Y:155:ALA:HB3	1.87	0.75
1:O:221:SER:CB	1:O:296:GLY:HA3	2.16	0.75
1:Y:447:ALA:O	1:Y:450:ALA:HB3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:241:GLY:O	1:O:242:ILE:HG13	1.86	0.75
1:Y:193:ASN:HB3	1:Y:196:THR:CB	2.17	0.75
1:O:141:VAL:O	1:O:145:LEU:HD22	1.85	0.75
1:Y:441:LEU:HD22	1:Y:445:TYR:CE1	2.22	0.74
1:O:153:GLU:C	1:O:157:ARG:HD3	2.08	0.74
1:O:156:ARG:HB2	1:O:156:ARG:CZ	2.16	0.74
1:Y:8:ALA:O	1:Y:9:LEU:HD13	1.87	0.74
1:O:184:THR:CG2	1:O:247:GLN:HG2	2.18	0.74
1:O:137:SER:HA	1:O:140:LYS:HD2	1.67	0.74
1:Y:410:GLY:O	1:Y:413:VAL:HG22	1.87	0.74
1:Y:85:THR:HA	1:Y:101:ILE:O	1.87	0.74
1:Y:449:LEU:HD12	1:Y:449:LEU:O	1.87	0.74
1:Y:168:TRP:O	1:Y:172:LYS:HG2	1.88	0.74
1:Y:454:TRP:CD1	1:Y:460:LEU:HD11	2.22	0.74
1:O:276:GLY:HA2	1:O:299:ASN:ND2	2.03	0.74
1:O:332:PHE:O	1:O:335:LYS:HB2	1.87	0.74
1:Y:183:TYR:CD1	1:Y:217:VAL:HG12	2.22	0.74
1:O:3:LYS:HG3	1:O:73:GLN:CA	2.17	0.74
1:Y:120:LEU:HD12	1:Y:120:LEU:H	1.54	0.73
1:O:170:ILE:O	1:O:171:TRP:C	2.25	0.73
1:O:193:ASN:HB3	1:O:196:THR:CB	2.18	0.73
1:O:41:LYS:HG3	1:O:42:PRO:HD2	1.70	0.73
1:O:80:THR:CG2	1:O:245:ASP:HA	2.19	0.73
1:Y:44:TRP:CE2	1:Y:107:ARG:HB2	2.23	0.73
1:O:184:THR:CB	1:O:247:GLN:HG2	2.19	0.73
1:O:221:SER:HB3	1:O:296:GLY:HA3	1.70	0.73
1:O:253:GLN:HG3	1:O:407:ARG:HD2	1.71	0.73
1:O:164:THR:O	1:O:165:VAL:C	2.26	0.72
1:O:226:GLN:CB	1:O:236:ARG:HD3	2.18	0.72
1:Y:415:ASN:ND2	1:Y:418:LEU:H	1.86	0.72
1:O:261:ALA:HB2	1:O:273:MET:HG2	1.71	0.72
1:Y:9:LEU:HD23	1:Y:77:ILE:HG23	1.71	0.72
1:Y:196:THR:N	1:Y:197:LEU:HD22	2.03	0.72
1:O:200:ASP:OD1	1:O:202:LYS:HB2	1.88	0.72
1:O:358:PRO:HG2	1:O:359:TYR:CE2	2.24	0.72
1:O:83:ARG:HB2	4:O:600:GOL:C1	2.06	0.72
1:O:245:ASP:O	1:O:248:ALA:HB3	1.90	0.72
1:O:413:VAL:HA	1:O:419:MET:HE3	1.70	0.72
1:Y:17:ARG:HD3	1:Y:32:GLN:HE21	1.54	0.72
1:O:84:GLU:HB2	1:O:103:TRP:CB	2.20	0.72
1:Y:91:LYS:HG2	1:Y:92:GLU:N	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:256:VAL:HG13	1:O:294:PRO:HG3	1.72	0.71
1:Y:84:GLU:CB	1:Y:103:TRP:HB3	2.19	0.71
1:Y:142:LYS:O	1:Y:143:TRP:C	2.28	0.71
1:Y:279:ALA:HB2	1:Y:300:TYR:CG	2.25	0.71
1:O:254:LEU:HD11	1:O:445:TYR:HE2	1.55	0.71
1:Y:88:VAL:CG2	1:Y:162:PHE:HB2	2.20	0.71
1:Y:262:LYS:HZ3	1:Y:264:THR:HB	1.56	0.71
1:Y:463:LYS:HA	1:Y:463:LYS:CE	2.16	0.71
1:O:253:GLN:CG	1:O:407:ARG:HD2	2.20	0.71
1:Y:137:SER:O	1:Y:138:GLY:C	2.28	0.71
1:O:9:LEU:HD12	1:O:56:GLN:NE2	2.05	0.71
1:O:90:GLU:OE2	1:O:93:THR:HG21	1.91	0.71
1:O:91:LYS:HB2	1:O:161:LEU:CD1	2.21	0.71
1:Y:27:ILE:H	1:Y:27:ILE:CD1	2.03	0.70
1:Y:328:ASP:HB3	1:Y:332:PHE:CE2	2.25	0.70
1:Y:39:TYR:OH	1:O:369:ARG:HD2	1.91	0.70
1:O:203:MET:HA	1:O:206:VAL:CG1	2.20	0.70
1:O:403:LEU:N	1:O:403:LEU:HD12	2.06	0.70
1:Y:31:SER:HB3	1:Y:59:THR:CA	2.20	0.70
1:Y:403:LEU:N	1:Y:403:LEU:HD12	2.05	0.70
1:O:486:TRP:O	1:O:490:VAL:HG23	1.90	0.70
1:Y:348:PHE:CE1	1:Y:362:GLY:HA3	2.27	0.70
1:Y:413:VAL:CG1	1:Y:419:MET:HE3	2.22	0.70
1:Y:467:GLU:HG2	1:Y:468:ARG:N	2.06	0.70
1:Y:422:GLN:O	1:Y:426:LEU:HD22	1.92	0.70
1:Y:230:GLY:HA2	1:Y:235:THR:HB	1.73	0.70
1:Y:413:VAL:HA	1:Y:419:MET:HE2	1.71	0.70
1:O:33:ARG:NH2	1:O:58:TRP:HB3	2.07	0.70
1:O:117:ARG:HH11	1:O:117:ARG:CB	1.98	0.70
1:Y:11:GLN:O	1:Y:81:ASN:HA	1.92	0.70
1:Y:88:VAL:HG22	1:Y:162:PHE:HB2	1.74	0.70
1:O:388:THR:O	1:O:391:VAL:HG13	1.92	0.70
1:Y:154:ARG:HA	1:Y:157:ARG:HG2	1.72	0.69
1:O:40:PRO:HG3	1:O:46:GLU:OE2	1.91	0.69
1:O:74:ILE:HD11	1:O:237:ILE:HG21	1.74	0.69
1:Y:262:LYS:HZ3	1:Y:264:THR:CB	2.05	0.69
1:O:385:ALA:HB1	1:O:422:GLN:NE2	2.06	0.69
1:O:492:ARG:HG2	1:O:492:ARG:HH11	1.56	0.69
1:Y:40:PRO:HG3	1:Y:46:GLU:CD	2.12	0.69
1:O:77:ILE:HB	1:O:238:PRO:O	1.92	0.69
1:O:451:VAL:HG12	1:O:453:PHE:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:154:ARG:O	1:Y:155:ALA:C	2.28	0.69
1:Y:246:GLN:HG3	1:Y:262:LYS:NZ	2.04	0.69
1:Y:143:TRP:O	1:Y:147:HIS:HB2	1.93	0.69
1:Y:26:ASN:O	1:Y:28:ILE:HD13	1.92	0.69
1:Y:246:GLN:HG2	1:Y:270:PHE:CB	2.23	0.69
1:O:117:ARG:HB2	1:O:117:ARG:NH1	2.00	0.69
1:O:322:LEU:N	1:O:322:LEU:HD23	2.07	0.69
1:Y:123:TYR:CZ	1:Y:202:LYS:HG3	2.27	0.69
1:Y:207:LEU:HB3	1:Y:209:ILE:HD12	1.73	0.69
1:O:70:SER:H	1:O:73:GLN:HE21	1.41	0.69
1:Y:35:PHE:HB2	1:Y:51:GLU:HG2	1.75	0.68
1:Y:222:GLU:HG2	1:Y:224:TYR:CE1	2.28	0.68
1:O:439:THR:HG22	1:O:440:ALA:N	2.07	0.68
1:O:444:ALA:O	1:O:445:TYR:C	2.32	0.68
1:Y:115:LEU:HD12	1:Y:115:LEU:H	1.57	0.68
1:Y:257:LYS:C	1:Y:274:ASN:HD22	1.97	0.68
1:Y:317:ARG:O	1:Y:321:LYS:HA	1.93	0.68
1:Y:170:ILE:HG22	1:Y:171:TRP:N	2.07	0.68
1:Y:203:MET:HA	1:Y:206:VAL:HG12	1.75	0.68
1:Y:337:GLN:NE2	1:Y:337:GLN:HA	2.09	0.68
1:O:317:ARG:HG2	1:O:318:ASP:N	2.08	0.68
1:Y:271:MET:HG2	1:Y:395:MET:CE	2.23	0.68
1:O:193:ASN:CB	1:O:196:THR:HB	2.24	0.68
1:Y:124:ILE:HG12	1:Y:203:MET:HE3	1.76	0.68
1:Y:156:ARG:CZ	1:Y:156:ARG:HB2	2.24	0.68
1:O:271:MET:C	1:O:272:LEU:HD12	2.13	0.68
1:Y:151:SER:O	1:Y:152:ARG:C	2.30	0.68
1:Y:169:LEU:O	1:Y:172:LYS:HB2	1.94	0.68
1:O:182:ASP:HB3	1:O:242:ILE:CG2	2.24	0.68
1:Y:124:ILE:HG12	1:Y:203:MET:CE	2.24	0.67
1:O:20:VAL:HG23	1:O:63:VAL:HG11	1.77	0.67
1:O:31:SER:HB2	1:O:63:VAL:CG2	2.25	0.67
1:Y:193:ASN:CB	1:Y:196:THR:HB	2.24	0.67
1:Y:286:LEU:HD11	1:Y:394:ALA:CB	2.25	0.67
1:O:44:TRP:CE2	1:O:107:ARG:HB2	2.30	0.67
1:O:47:HIS:O	1:O:49:PRO:HD3	1.93	0.67
1:O:227:THR:OG1	1:O:239:ILE:HD11	1.94	0.67
1:Y:20:VAL:HG12	1:Y:21:MET:N	2.09	0.67
1:Y:61:VAL:HG12	1:Y:62:GLU:N	2.08	0.67
1:O:226:GLN:HB2	1:O:236:ARG:HD3	1.76	0.67
1:Y:363:ALA:C	1:Y:364:ILE:HD13	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:63:VAL:O	1:O:64:LEU:C	2.32	0.67
1:Y:82:GLN:O	1:Y:165:VAL:HG21	1.94	0.67
1:Y:322:LEU:N	1:Y:322:LEU:HD23	2.09	0.67
1:Y:392:LEU:HD23	1:Y:393:GLU:N	2.10	0.67
1:Y:20:VAL:O	1:Y:28:ILE:N	2.28	0.67
1:O:113:GLU:O	1:O:116:LYS:HB2	1.95	0.67
1:Y:276:GLY:O	1:Y:300:TYR:N	2.29	0.66
1:O:229:ILE:HG21	1:O:237:ILE:HG12	1.78	0.66
1:Y:47:HIS:O	1:Y:99:ASN:HB3	1.96	0.66
1:Y:197:LEU:HD22	1:Y:197:LEU:N	2.10	0.66
1:O:19:VAL:HG12	1:O:21:MET:CE	2.25	0.66
1:O:20:VAL:O	1:O:28:ILE:N	2.29	0.66
1:O:278:LYS:HE3	1:O:280:VAL:HG23	1.77	0.66
1:Y:345:VAL:O	1:Y:362:GLY:HA2	1.96	0.66
1:O:90:GLU:OE1	1:O:95:LYS:HG2	1.94	0.66
1:O:207:LEU:HB3	1:O:209:ILE:CD1	2.26	0.66
1:O:40:PRO:HG2	1:O:44:TRP:HB3	1.77	0.66
1:O:164:THR:O	1:O:167:THR:N	2.29	0.66
1:Y:22:ASP:OD2	1:Y:26:ASN:HB2	1.96	0.66
1:Y:138:GLY:O	1:Y:141:VAL:HG23	1.95	0.66
1:O:3:LYS:HA	1:O:73:GLN:HA	1.77	0.66
1:O:91:LYS:O	1:O:94:GLY:N	2.29	0.66
1:O:181:THR:HG23	1:O:182:ASP:O	1.95	0.66
1:O:197:LEU:N	1:O:197:LEU:HD22	2.10	0.66
1:O:118:ASP:N	1:O:118:ASP:OD1	2.29	0.66
1:O:468:ARG:HG3	1:O:468:ARG:NH1	2.00	0.66
1:Y:153:GLU:O	1:Y:156:ARG:N	2.29	0.66
1:Y:128:THR:HG21	1:Y:190:MET:HA	1.79	0.65
1:Y:166:ASP:OD2	1:Y:242:ILE:HG21	1.95	0.65
1:O:271:MET:HG2	1:O:395:MET:CE	2.26	0.65
1:Y:179:HIS:CD2	1:Y:215:PRO:HA	2.30	0.65
1:Y:205:GLU:O	1:Y:208:ASP:N	2.30	0.65
1:O:26:ASN:O	1:O:28:ILE:HD13	1.97	0.65
1:O:125:ARG:NH1	1:O:282:SER:O	2.29	0.65
1:O:144:ILE:H	1:O:144:ILE:CD1	2.06	0.65
1:O:478:GLU:HA	1:O:478:GLU:OE1	1.96	0.65
1:Y:19:VAL:HG22	1:Y:30:VAL:HG22	1.79	0.65
1:Y:85:THR:HG23	1:Y:102:VAL:HA	1.78	0.65
1:O:84:GLU:CB	1:O:103:TRP:HB3	2.26	0.65
1:O:78:GLY:C	1:O:79:ILE:HG12	2.16	0.65
1:O:183:TYR:CD1	1:O:217:VAL:HG12	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:410:GLY:O	1:O:413:VAL:HG13	1.97	0.65
1:Y:91:LYS:O	1:Y:94:GLY:N	2.30	0.65
1:O:81:ASN:N	1:O:81:ASN:HD22	1.95	0.65
1:O:114:HIS:HA	1:O:117:ARG:CZ	2.26	0.65
1:O:352:GLY:O	1:O:355:TYR:N	2.29	0.65
1:Y:58:TRP:O	1:Y:61:VAL:N	2.30	0.65
1:O:152:ARG:HB3	1:O:156:ARG:HH22	1.61	0.65
1:O:65:ALA:O	1:O:67:ALA:N	2.30	0.65
1:O:205:GLU:O	1:O:208:ASP:N	2.29	0.65
1:O:219:ARG:NH2	1:O:295:THR:OG1	2.29	0.65
1:O:489:ALA:O	1:O:492:ARG:N	2.29	0.65
1:O:84:GLU:N	1:O:84:GLU:OE1	2.29	0.65
1:O:88:VAL:HG22	1:O:162:PHE:HB2	1.78	0.65
1:O:137:SER:O	1:O:140:LYS:N	2.30	0.65
1:O:179:HIS:CD2	1:O:215:PRO:HA	2.32	0.65
1:Y:58:TRP:O	1:Y:60:LEU:N	2.30	0.65
1:Y:212:GLU:O	1:Y:214:LEU:N	2.29	0.65
1:O:40:PRO:HG2	1:O:44:TRP:HB2	1.77	0.65
1:Y:4:LYS:N	1:Y:73:GLN:O	2.30	0.65
1:O:144:ILE:O	1:O:147:HIS:N	2.30	0.65
1:O:420:GLN:NE2	1:O:424:ASP:OD1	2.29	0.65
1:O:451:VAL:CG1	1:O:453:PHE:HB2	2.26	0.65
1:Y:237:ILE:HG22	1:Y:238:PRO:N	2.12	0.64
1:O:220:SER:HB3	1:O:242:ILE:O	1.97	0.64
1:Y:137:SER:OG	1:Y:189:THR:HA	1.97	0.64
1:Y:420:GLN:NE2	1:Y:424:ASP:OD1	2.30	0.64
1:O:146:ASP:HB3	1:O:152:ARG:NH1	2.11	0.64
1:Y:63:VAL:HA	1:Y:66:LYS:HD3	1.78	0.64
1:O:120:LEU:O	1:O:124:ILE:HG13	1.97	0.64
1:O:171:TRP:CE2	1:O:176:GLY:HA2	2.32	0.64
1:Y:205:GLU:HG2	1:Y:206:VAL:N	2.12	0.64
1:Y:314:GLN:O	1:Y:318:ASP:N	2.29	0.64
1:Y:153:GLU:O	1:Y:154:ARG:C	2.32	0.64
1:Y:364:ILE:HD13	1:Y:364:ILE:N	2.13	0.64
1:O:31:SER:HB3	1:O:59:THR:HA	1.79	0.64
1:O:46:GLU:O	1:O:47:HIS:ND1	2.30	0.64
1:O:127:ASN:HD22	1:O:193:ASN:HD21	1.46	0.64
1:O:216:GLU:HG2	1:O:218:ARG:HH11	1.62	0.64
1:O:230:GLY:HA2	1:O:235:THR:CB	2.27	0.64
1:O:33:ARG:HE	1:O:58:TRP:CB	2.11	0.64
1:O:183:TYR:CE1	1:O:217:VAL:HG12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:ILE:HD13	1:O:168:TRP:HB2	1.79	0.64
1:Y:3:LYS:HG3	1:Y:72:ASP:O	1.98	0.64
1:Y:109:ALA:O	1:Y:112:CYS:HB2	1.98	0.64
1:Y:396:GLN:HA	1:Y:399:SER:OG	1.98	0.64
1:Y:130:LEU:HD23	1:Y:130:LEU:N	2.07	0.63
1:Y:157:ARG:HG3	1:Y:159:GLU:OE1	1.98	0.63
1:O:272:LEU:HD11	1:O:303:GLU:CG	2.22	0.63
1:O:143:TRP:O	1:O:147:HIS:HB2	1.98	0.63
1:Y:359:TYR:HB3	1:Y:497:GLU:HB3	1.80	0.63
1:O:353:ALA:HB2	1:O:356:TRP:CZ2	2.34	0.63
1:Y:413:VAL:HA	1:Y:419:MET:HE3	1.81	0.63
1:Y:496:TRP:O	1:O:488:LYS:HE2	1.98	0.63
1:O:286:LEU:HD11	1:O:394:ALA:CB	2.29	0.63
1:O:386:TYR:HB3	1:O:486:TRP:CE2	2.33	0.63
1:Y:9:LEU:HD23	1:Y:77:ILE:CG2	2.29	0.63
1:Y:18:ALA:CB	1:Y:63:VAL:HG21	2.29	0.63
1:Y:153:GLU:C	1:Y:157:ARG:HD3	2.18	0.63
1:Y:229:ILE:CG2	1:Y:237:ILE:HG12	2.23	0.63
1:O:20:VAL:HG12	1:O:21:MET:N	2.14	0.63
1:O:181:THR:HG23	1:O:182:ASP:N	2.13	0.63
1:Y:40:PRO:HG3	1:Y:46:GLU:OE2	1.99	0.63
1:Y:62:GLU:O	1:Y:63:VAL:C	2.32	0.63
1:O:80:THR:HG21	1:O:248:ALA:CB	2.27	0.63
1:O:111:ILE:CD1	1:O:142:LYS:HG2	2.29	0.63
1:Y:29:SER:OG	1:Y:63:VAL:HG12	1.99	0.63
1:Y:182:ASP:HA	1:Y:218:ARG:O	1.99	0.63
1:O:11:GLN:O	1:O:81:ASN:HA	1.98	0.63
1:O:88:VAL:HG13	1:O:161:LEU:O	1.99	0.63
1:O:458:ASP:O	1:O:461:GLN:HB2	1.98	0.63
1:O:267:THR:OG1	3:O:601:ACP:H3B1	1.98	0.62
1:O:459:GLU:HB2	1:O:460:LEU:CD1	2.28	0.62
1:Y:257:LYS:O	1:Y:260:MET:HG2	1.98	0.62
1:Y:140:LYS:O	1:Y:144:ILE:HD12	1.99	0.62
1:Y:14:THR:N	3:Y:601:ACP:O2G	2.30	0.62
1:Y:179:HIS:CE1	1:Y:215:PRO:HB3	2.34	0.62
1:Y:186:ALA:O	1:Y:187:SER:C	2.38	0.62
1:O:67:ALA:HB3	1:O:69:ILE:CD1	2.29	0.62
1:O:179:HIS:O	1:O:216:GLU:N	2.29	0.62
1:Y:478:GLU:HA	1:Y:478:GLU:OE1	1.97	0.62
1:O:166:ASP:OD1	1:O:167:THR:N	2.31	0.62
1:O:208:ASP:O	1:O:209:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:438:VAL:HA	1:O:441:LEU:CD1	2.29	0.62
1:O:447:ALA:O	1:O:450:ALA:HB3	2.00	0.62
1:Y:53:TRP:CH2	1:Y:172:LYS:HB3	2.34	0.62
1:Y:120:LEU:HD12	1:Y:120:LEU:N	2.13	0.62
1:O:91:LYS:HB3	1:O:91:LYS:HZ3	1.65	0.62
1:O:455:GLN:O	1:O:455:GLN:HG3	1.99	0.62
1:Y:211:ARG:HH11	1:Y:211:ARG:CG	2.12	0.62
1:Y:337:GLN:HA	1:Y:337:GLN:HE21	1.64	0.62
1:Y:272:LEU:HG	1:Y:303:GLU:HB2	1.81	0.62
1:Y:87:ILE:HG22	1:Y:88:VAL:H	1.65	0.62
1:O:117:ARG:O	1:O:119:GLY:N	2.30	0.62
1:O:164:THR:O	1:O:166:ASP:N	2.32	0.62
1:O:350:GLY:HA2	1:O:360:ALA:O	2.00	0.62
1:O:483:TYR:O	1:O:487:LYS:HG3	2.00	0.62
1:Y:488:LYS:HD2	1:O:496:TRP:CH2	2.34	0.62
1:O:140:LYS:O	1:O:143:TRP:N	2.33	0.62
1:Y:16:SER:HB3	1:Y:56:GLN:HA	1.82	0.61
1:Y:344:VAL:HG22	1:Y:364:ILE:HD12	1.81	0.61
1:Y:141:VAL:O	1:Y:144:ILE:HB	1.99	0.61
1:Y:310:GLY:O	1:Y:313:ILE:N	2.33	0.61
1:O:105:CYS:SG	1:O:107:ARG:HB3	2.40	0.61
1:O:185:ASN:HD21	1:O:244:GLY:CA	2.12	0.61
1:Y:257:LYS:N	1:Y:260:MET:HG3	2.14	0.61
1:Y:286:LEU:HD11	1:Y:394:ALA:HB1	1.81	0.61
1:O:475:GLU:O	1:O:478:GLU:HB2	2.00	0.61
1:Y:330:GLU:O	1:Y:334:THR:HG23	2.00	0.61
1:O:390:ASP:HA	1:O:483:TYR:OH	2.00	0.61
1:Y:38:ILE:O	1:Y:40:PRO:HD3	2.00	0.61
1:Y:127:ASN:HD22	1:Y:193:ASN:HD21	1.47	0.61
1:Y:287:LEU:HD23	1:Y:287:LEU:N	2.15	0.61
1:O:226:GLN:HB3	1:O:236:ARG:HD3	1.81	0.61
1:Y:81:ASN:N	1:Y:81:ASN:ND2	2.42	0.61
1:Y:114:HIS:O	1:Y:115:LEU:C	2.39	0.61
1:O:279:ALA:HB2	1:O:300:TYR:CD2	2.36	0.61
1:Y:138:GLY:HA2	1:Y:191:LEU:CD2	2.31	0.61
1:O:110:GLU:O	1:O:113:GLU:HB2	2.00	0.61
1:Y:442:GLY:O	1:Y:445:TYR:N	2.33	0.61
1:O:202:LYS:O	1:O:206:VAL:HB	2.00	0.61
1:Y:123:TYR:CD2	1:Y:203:MET:HE2	2.35	0.61
1:Y:142:LYS:O	1:Y:145:LEU:N	2.34	0.61
1:O:91:LYS:CB	1:O:161:LEU:HD12	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:196:THR:HG22	1:O:198:ASP:N	2.16	0.61
1:O:387:GLN:O	1:O:390:ASP:HB2	2.01	0.61
1:Y:152:ARG:CB	1:Y:156:ARG:HH22	2.12	0.60
1:O:63:VAL:CA	1:O:66:LYS:HG2	2.30	0.60
1:O:164:THR:N	1:O:167:THR:HB	2.13	0.60
1:O:213:MET:HG2	1:O:214:LEU:HD12	1.83	0.60
1:Y:123:TYR:OH	1:Y:202:LYS:HG3	2.01	0.60
1:Y:201:ASP:O	1:Y:202:LYS:C	2.38	0.60
1:Y:222:GLU:HG3	1:Y:223:VAL:N	2.15	0.60
1:O:29:SER:OG	1:O:30:VAL:N	2.29	0.60
1:O:216:GLU:HG2	1:O:218:ARG:NH1	2.17	0.60
1:O:262:LYS:HD2	1:O:262:LYS:O	2.01	0.60
1:Y:118:ASP:HB2	1:Y:120:LEU:HD11	1.81	0.60
1:Y:179:HIS:CG	1:Y:215:PRO:HB3	2.37	0.60
1:Y:262:LYS:NZ	1:Y:264:THR:HB	2.15	0.60
1:Y:283:GLU:HA	1:Y:283:GLU:OE1	2.00	0.60
1:Y:387:GLN:O	1:Y:391:VAL:HG12	2.01	0.60
1:O:405:ALA:HB1	1:O:431:GLU:OE2	2.01	0.60
1:Y:477:THR:O	1:Y:478:GLU:C	2.39	0.60
1:O:142:LYS:HE3	1:O:146:ASP:CG	2.22	0.60
1:Y:179:HIS:ND1	1:Y:215:PRO:HB3	2.16	0.60
1:Y:295:THR:N	1:Y:297:GLU:OE1	2.32	0.60
1:O:85:THR:HA	1:O:101:ILE:O	2.01	0.60
1:O:111:ILE:HD13	1:O:142:LYS:HG2	1.82	0.60
1:O:123:TYR:CD2	1:O:203:MET:HE2	2.36	0.60
1:O:211:ARG:HG3	1:O:211:ARG:NH1	1.98	0.60
1:O:227:THR:N	1:O:237:ILE:O	2.33	0.60
1:O:279:ALA:HB2	1:O:300:TYR:CE2	2.37	0.60
1:Y:257:LYS:O	1:Y:258:GLU:C	2.39	0.60
1:O:297:GLU:OE1	1:O:297:GLU:N	2.28	0.60
1:Y:87:ILE:HD12	1:Y:163:GLY:O	2.02	0.60
1:O:90:GLU:N	1:O:95:LYS:O	2.29	0.60
1:O:203:MET:CA	1:O:206:VAL:HG12	2.30	0.60
1:Y:35:PHE:CB	1:Y:51:GLU:HG2	2.32	0.60
1:Y:81:ASN:HD22	1:Y:81:ASN:H	1.47	0.60
1:Y:275:THR:OG1	1:Y:300:TYR:HB2	2.01	0.60
1:Y:388:THR:O	1:Y:391:VAL:HG13	2.01	0.60
1:O:90:GLU:HB3	1:O:93:THR:CG2	2.31	0.60
1:O:278:LYS:CE	1:O:280:VAL:HG23	2.31	0.60
1:Y:255:CYS:CB	1:Y:260:MET:HB2	2.31	0.59
1:O:84:GLU:HG2	1:O:135:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:180:VAL:HG23	1:O:216:GLU:O	2.02	0.59
1:Y:253:GLN:HE21	1:Y:262:LYS:HB2	1.67	0.59
1:O:130:LEU:O	1:O:131:VAL:HG23	2.02	0.59
1:Y:21:MET:CE	1:Y:444:ALA:HB2	2.32	0.59
1:Y:44:TRP:CZ2	1:Y:107:ARG:HB2	2.37	0.59
1:Y:123:TYR:CE2	1:Y:203:MET:HE2	2.37	0.59
1:O:286:LEU:O	1:O:287:LEU:HD23	2.02	0.59
1:O:454:TRP:HD1	1:O:459:GLU:CD	2.06	0.59
1:Y:46:GLU:O	1:Y:47:HIS:ND1	2.32	0.59
1:Y:183:TYR:HE1	1:Y:217:VAL:HG12	1.62	0.59
1:Y:20:VAL:HB	1:Y:28:ILE:HB	1.84	0.59
1:Y:30:VAL:C	1:Y:63:VAL:HG13	2.22	0.59
1:Y:62:GLU:O	1:Y:66:LYS:HG2	2.02	0.59
1:Y:203:MET:O	1:Y:206:VAL:HG12	2.03	0.59
1:Y:261:ALA:HB2	1:Y:273:MET:CG	2.33	0.59
1:Y:423:SER:CB	1:Y:430:VAL:HG23	2.32	0.59
1:O:224:TYR:CZ	1:O:242:ILE:HD12	2.37	0.59
1:O:497:GLU:HA	1:O:497:GLU:OE1	2.01	0.59
1:Y:390:ASP:HA	1:Y:483:TYR:OH	2.02	0.59
1:O:78:GLY:O	1:O:79:ILE:HG12	2.03	0.59
1:O:89:TRP:HB2	1:O:95:LYS:O	2.02	0.59
1:O:254:LEU:CD1	1:O:445:TYR:HE2	2.15	0.59
1:Y:70:SER:H	1:Y:73:GLN:HE21	1.51	0.59
1:Y:144:ILE:HD12	1:Y:144:ILE:H	1.67	0.59
1:O:83:ARG:CB	4:O:600:GOL:H12	2.07	0.59
1:O:246:GLN:NE2	1:O:246:GLN:N	2.50	0.59
1:O:265:TYR:HE1	1:O:408:VAL:CG1	2.16	0.59
1:Y:22:ASP:OD1	1:Y:24:ASP:N	2.35	0.59
1:Y:188:ARG:HH21	1:Y:289:THR:HG21	1.67	0.59
1:Y:242:ILE:HG22	1:Y:243:ALA:H	1.67	0.59
1:Y:415:ASN:O	1:Y:419:MET:HG2	2.03	0.59
1:O:27:ILE:H	1:O:27:ILE:CD1	2.01	0.59
1:O:59:THR:O	1:O:63:VAL:HG23	2.03	0.59
1:O:173:MET:HB3	1:O:227:THR:CG2	2.32	0.59
1:O:205:GLU:HG2	1:O:206:VAL:N	2.17	0.59
1:O:229:ILE:CG2	1:O:237:ILE:HG12	2.33	0.59
1:Y:48:ASP:O	1:Y:52:ILE:HD13	2.03	0.59
1:Y:148:VAL:HG12	1:Y:151:SER:OG	2.03	0.59
1:O:394:ALA:O	1:O:395:MET:C	2.41	0.59
1:O:5:TYR:O	1:O:75:ALA:N	2.29	0.59
1:O:186:ALA:O	1:O:187:SER:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:240:SER:HB2	1:Y:450:ALA:HB3	1.85	0.58
1:Y:432:ARG:HD2	1:Y:436:ARG:NH2	2.17	0.58
1:O:17:ARG:NH2	1:O:437:GLU:HG3	2.15	0.58
1:O:247:GLN:OE1	1:O:247:GLN:N	2.36	0.58
1:Y:317:ARG:HG2	1:Y:318:ASP:N	2.17	0.58
1:O:415:ASN:ND2	1:O:418:LEU:N	2.34	0.58
1:Y:91:LYS:NZ	1:Y:91:LYS:HB3	2.16	0.58
1:Y:280:VAL:HG12	1:Y:281:LYS:N	2.19	0.58
1:O:47:HIS:CB	1:O:52:ILE:HD11	2.25	0.58
1:O:87:ILE:HD13	1:O:168:TRP:CB	2.33	0.58
1:O:415:ASN:O	1:O:419:MET:HG2	2.02	0.58
1:O:438:VAL:O	1:O:441:LEU:HB2	2.02	0.58
1:Y:21:MET:HE3	1:Y:444:ALA:HB2	1.84	0.58
1:Y:48:ASP:C	1:Y:52:ILE:HD13	2.23	0.58
1:O:47:HIS:O	1:O:99:ASN:HB3	2.03	0.58
1:O:345:VAL:O	1:O:362:GLY:HA2	2.03	0.58
1:O:422:GLN:O	1:O:425:ILE:HG22	2.03	0.58
1:Y:372:ASN:O	1:Y:375:HIS:N	2.36	0.58
1:Y:204:LEU:HD22	1:Y:209:ILE:O	2.04	0.58
1:Y:220:SER:O	1:Y:241:GLY:HA2	2.03	0.58
1:Y:458:ASP:O	1:Y:461:GLN:HB2	2.03	0.58
1:O:81:ASN:N	1:O:81:ASN:ND2	2.51	0.58
1:Y:118:ASP:OD1	1:Y:118:ASP:N	2.35	0.58
1:Y:86:THR:HG23	1:Y:162:PHE:HE2	1.68	0.58
1:Y:396:GLN:HA	1:Y:399:SER:HG	1.69	0.58
1:O:50:MET:O	1:O:53:TRP:HB3	2.04	0.58
1:O:237:ILE:N	1:O:237:ILE:HD13	2.19	0.58
1:Y:31:SER:OG	1:Y:63:VAL:N	2.36	0.58
1:Y:70:SER:O	1:Y:73:GLN:HG3	2.04	0.58
1:Y:104:GLN:CG	1:Y:349:THR:HG21	2.33	0.58
1:Y:293:GLY:N	1:Y:297:GLU:O	2.37	0.58
1:Y:432:ARG:O	1:Y:466:ILE:HG12	2.04	0.58
1:Y:445:TYR:O	1:Y:446:LEU:C	2.42	0.58
1:O:115:LEU:H	1:O:115:LEU:CD1	2.14	0.58
1:O:179:HIS:CE1	1:O:215:PRO:HB3	2.39	0.58
1:O:203:MET:O	1:O:207:LEU:N	2.30	0.58
1:Y:193:ASN:HB3	1:Y:196:THR:HG21	1.83	0.57
1:Y:103:TRP:HA	1:Y:140:LYS:HE3	1.86	0.57
1:Y:240:SER:HB2	1:Y:450:ALA:HB1	1.82	0.57
1:O:142:LYS:O	1:O:143:TRP:C	2.41	0.57
1:O:193:ASN:CG	1:O:196:THR:HB	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:314:GLN:O	1:O:318:ASP:N	2.37	0.57
1:Y:128:THR:HB	1:Y:130:LEU:HB2	1.86	0.57
1:Y:144:ILE:O	1:Y:145:LEU:C	2.42	0.57
1:O:463:LYS:HZ3	1:O:465:VAL:HG23	1.69	0.57
1:Y:492:ARG:HH11	1:Y:492:ARG:CG	2.15	0.57
1:O:78:GLY:HA2	1:O:447:ALA:HB2	1.85	0.57
1:O:83:ARG:HE	4:O:600:GOL:C2	2.16	0.57
1:O:184:THR:HG22	1:O:291:ALA:HA	1.85	0.57
1:Y:20:VAL:C	1:Y:21:MET:HG3	2.24	0.57
1:Y:104:GLN:HG3	1:Y:349:THR:HG21	1.87	0.57
1:Y:172:LYS:O	1:Y:175:GLN:N	2.38	0.57
1:O:219:ARG:HG3	1:O:296:GLY:O	2.04	0.57
1:Y:71:SER:HB2	1:Y:235:THR:CG2	2.35	0.57
1:O:182:ASP:CG	1:O:242:ILE:HG22	2.23	0.57
1:O:382:GLU:O	1:O:383:SER:C	2.40	0.57
1:O:423:SER:HB2	1:O:430:VAL:HG23	1.87	0.57
1:Y:154:ARG:HB2	1:Y:159:GLU:HB3	1.86	0.57
1:O:89:TRP:HB2	1:O:95:LYS:C	2.24	0.57
1:O:185:ASN:O	1:O:188:ARG:HB2	2.05	0.57
1:O:445:TYR:O	1:O:448:GLY:N	2.37	0.57
1:Y:88:VAL:HG22	1:Y:162:PHE:HA	1.87	0.57
1:O:230:GLY:HA2	1:O:235:THR:OG1	2.05	0.56
1:O:17:ARG:HG2	1:O:32:GLN:HG2	1.86	0.56
1:Y:53:TRP:CZ2	1:Y:172:LYS:HB3	2.39	0.56
1:Y:110:GLU:O	1:Y:113:GLU:N	2.38	0.56
1:Y:156:ARG:C	1:Y:158:GLY:H	2.09	0.56
1:Y:194:ILE:HG13	1:Y:195:HIS:CE1	2.40	0.56
1:Y:453:PHE:HD2	1:Y:454:TRP:CE3	2.23	0.56
1:O:253:GLN:HE21	1:O:262:LYS:HB3	1.68	0.56
1:O:442:GLY:O	1:O:444:ALA:N	2.38	0.56
1:O:468:ARG:HD2	1:O:469:GLU:N	2.20	0.56
1:Y:137:SER:HA	1:Y:140:LYS:HD2	1.87	0.56
1:Y:192:PHE:CZ	1:Y:197:LEU:HA	2.41	0.56
1:Y:246:GLN:HG2	1:Y:270:PHE:HB2	1.85	0.56
1:Y:496:TRP:CH2	1:O:488:LYS:HD2	2.40	0.56
1:O:85:THR:OG1	1:O:103:TRP:HD1	1.89	0.56
1:O:196:THR:N	1:O:197:LEU:HD22	2.21	0.56
1:Y:110:GLU:O	1:Y:113:GLU:HB2	2.06	0.56
1:Y:181:THR:HG23	1:Y:182:ASP:N	2.21	0.56
1:O:203:MET:O	1:O:206:VAL:HG12	2.05	0.56
1:O:256:VAL:HG13	1:O:294:PRO:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:154:ARG:O	1:O:159:GLU:HB2	2.05	0.56
1:Y:184:THR:HA	1:Y:290:ILE:HG22	1.88	0.56
1:O:83:ARG:HE	4:O:600:GOL:C1	2.19	0.56
1:Y:78:GLY:HA2	1:Y:447:ALA:HB2	1.88	0.56
1:Y:207:LEU:HB3	1:Y:209:ILE:CD1	2.36	0.56
1:Y:357:ASP:O	1:Y:359:TYR:N	2.39	0.56
1:O:83:ARG:HE	4:O:600:GOL:H12	1.70	0.56
1:O:170:ILE:HG22	1:O:171:TRP:N	2.21	0.56
1:O:183:TYR:CB	1:O:290:ILE:HG21	2.36	0.56
1:O:221:SER:HB3	1:O:295:THR:O	2.06	0.56
1:Y:71:SER:HB2	1:Y:235:THR:HG21	1.87	0.56
1:Y:105:CYS:SG	1:Y:107:ARG:HB3	2.46	0.56
1:O:41:LYS:HG3	1:O:42:PRO:CD	2.35	0.56
1:O:130:LEU:HD13	1:O:136:PHE:CD1	2.41	0.56
1:O:251:PHE:CE2	1:O:446:LEU:HD13	2.41	0.56
1:O:442:GLY:O	1:O:443:ALA:C	2.42	0.56
1:O:484:ALA:O	1:O:487:LYS:N	2.36	0.56
1:Y:262:LYS:HD2	1:Y:262:LYS:O	2.06	0.56
1:O:20:VAL:O	1:O:28:ILE:HB	2.05	0.56
1:Y:21:MET:HE3	1:Y:444:ALA:CB	2.37	0.55
1:Y:154:ARG:HG3	1:Y:160:LEU:CD1	2.36	0.55
1:Y:246:GLN:HG2	1:Y:270:PHE:HB3	1.87	0.55
1:Y:441:LEU:HD22	1:Y:445:TYR:HE1	1.67	0.55
1:O:258:GLU:N	1:O:274:ASN:HD22	2.04	0.55
1:Y:340:ASN:HB2	1:Y:375:HIS:CD2	2.42	0.55
1:O:44:TRP:HA	1:O:105:CYS:SG	2.46	0.55
1:O:448:GLY:O	1:O:453:PHE:N	2.35	0.55
1:Y:21:MET:HA	1:Y:26:ASN:O	2.06	0.55
1:Y:53:TRP:HA	1:Y:53:TRP:CE3	2.41	0.55
1:Y:111:ILE:HG22	1:Y:115:LEU:HD13	1.88	0.55
1:Y:498:GLU:OE1	1:Y:498:GLU:HA	2.06	0.55
1:O:6:ILE:O	1:O:20:VAL:HG13	2.06	0.55
1:O:115:LEU:HD12	1:O:115:LEU:N	2.11	0.55
1:O:389:ARG:HA	1:O:426:LEU:HD11	1.88	0.55
1:O:425:ILE:HG22	1:O:426:LEU:HD22	1.88	0.55
1:O:430:VAL:O	1:O:469:GLU:HA	2.06	0.55
1:O:405:ALA:HA	1:O:429:ARG:O	2.07	0.55
1:Y:40:PRO:HG2	1:Y:44:TRP:HB3	1.87	0.55
1:Y:113:GLU:O	1:Y:116:LYS:HB2	2.06	0.55
1:Y:181:THR:O	1:Y:218:ARG:N	2.30	0.55
1:Y:271:MET:C	1:Y:272:LEU:HD12	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:351:LEU:HB2	1:Y:357:ASP:H	1.72	0.55
1:O:97:ILE:O	1:O:98:TYR:HB2	2.07	0.55
1:Y:227:THR:N	1:Y:237:ILE:O	2.28	0.55
1:Y:265:TYR:HE1	1:Y:408:VAL:CG1	2.19	0.55
1:Y:425:ILE:HD12	1:Y:479:ARG:HG2	1.89	0.55
1:O:254:LEU:HD11	1:O:445:TYR:CE2	2.40	0.55
1:Y:286:LEU:HD11	1:Y:395:MET:N	2.22	0.55
1:Y:392:LEU:O	1:Y:395:MET:HB3	2.07	0.55
1:O:137:SER:O	1:O:139:THR:N	2.39	0.55
1:O:286:LEU:HD11	1:O:394:ALA:HB3	1.89	0.55
1:Y:279:ALA:HB2	1:Y:300:TYR:CE2	2.40	0.55
1:Y:445:TYR:O	1:Y:448:GLY:N	2.39	0.55
1:O:430:VAL:O	1:O:470:PHE:N	2.29	0.55
1:Y:91:LYS:HB3	1:Y:91:LYS:HZ3	1.71	0.55
1:Y:164:THR:O	1:Y:165:VAL:C	2.45	0.55
1:Y:404:HIS:O	1:Y:429:ARG:HD2	2.07	0.55
1:O:80:THR:HG22	1:O:245:ASP:N	2.22	0.55
1:Y:18:ALA:HB3	1:Y:63:VAL:HG21	1.87	0.54
1:Y:368:THR:HG23	1:Y:369:ARG:N	2.20	0.54
1:Y:415:ASN:HD22	1:Y:418:LEU:H	1.52	0.54
1:O:275:THR:HG1	1:O:300:TYR:HB2	1.72	0.54
1:O:463:LYS:NZ	1:O:465:VAL:HG23	2.21	0.54
1:Y:85:THR:OG1	1:Y:103:TRP:HD1	1.90	0.54
1:Y:87:ILE:HD13	1:Y:168:TRP:HB2	1.88	0.54
1:Y:189:THR:HB	1:Y:191:LEU:CG	2.35	0.54
1:Y:344:VAL:CG2	1:Y:364:ILE:HG23	2.37	0.54
1:O:170:ILE:HA	1:O:173:MET:HG3	1.89	0.54
1:O:193:ASN:O	1:O:197:LEU:N	2.40	0.54
1:Y:11:GLN:HE22	1:Y:82:GLN:HE21	1.55	0.54
1:Y:63:VAL:HA	1:Y:66:LYS:CD	2.38	0.54
1:Y:228:ASN:HD21	1:Y:235:THR:N	2.05	0.54
1:Y:424:ASP:OD1	1:Y:473:GLY:N	2.29	0.54
1:O:258:GLU:HA	1:O:274:ASN:O	2.07	0.54
1:Y:141:VAL:C	1:Y:145:LEU:HD22	2.27	0.54
1:O:150:GLY:HA3	1:O:154:ARG:HD2	1.89	0.54
1:O:265:TYR:HE1	1:O:408:VAL:HG12	1.72	0.54
1:Y:460:LEU:H	1:Y:460:LEU:CD1	1.98	0.54
1:Y:41:LYS:O	1:Y:44:TRP:HB2	2.08	0.54
1:O:35:PHE:HB2	1:O:51:GLU:CG	2.33	0.54
1:O:162:PHE:HB3	1:O:213:MET:HG3	1.90	0.54
1:Y:53:TRP:HA	1:Y:53:TRP:HE3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:218:ARG:HG3	1:Y:218:ARG:NH1	2.23	0.54
1:O:249:ALA:HB2	1:O:439:THR:OG1	2.07	0.54
1:Y:138:GLY:HA2	1:Y:191:LEU:HD21	1.88	0.54
1:Y:413:VAL:CB	1:Y:419:MET:HE3	2.38	0.54
1:O:101:ILE:HD13	1:O:107:ARG:CZ	2.37	0.54
1:O:240:SER:HB2	1:O:450:ALA:HB3	1.89	0.54
1:Y:38:ILE:O	1:Y:45:VAL:HA	2.08	0.54
1:O:20:VAL:HB	1:O:28:ILE:HB	1.89	0.54
1:O:142:LYS:HE3	1:O:146:ASP:OD2	2.07	0.54
1:Y:29:SER:OG	1:Y:30:VAL:N	2.42	0.54
1:Y:286:LEU:HD21	1:Y:394:ALA:CB	2.37	0.54
1:Y:445:TYR:O	1:Y:447:ALA:N	2.41	0.54
1:O:88:VAL:HA	1:O:161:LEU:O	2.08	0.54
1:O:139:THR:OG1	1:O:140:LYS:N	2.41	0.54
1:Y:203:MET:O	1:Y:207:LEU:HB2	2.08	0.53
1:O:41:LYS:CG	1:O:42:PRO:HD2	2.37	0.53
1:Y:28:ILE:HD13	1:Y:28:ILE:N	2.21	0.53
1:Y:80:THR:HG22	1:Y:243:ALA:O	2.08	0.53
1:Y:86:THR:HG23	1:Y:162:PHE:CE2	2.43	0.53
1:Y:170:ILE:O	1:Y:171:TRP:C	2.45	0.53
1:Y:227:THR:O	1:Y:236:ARG:HA	2.08	0.53
1:Y:332:PHE:O	1:Y:335:LYS:HB2	2.09	0.53
1:Y:416:ASN:O	1:Y:417:PHE:C	2.46	0.53
1:Y:446:LEU:O	1:Y:450:ALA:HB2	2.08	0.53
1:Y:18:ALA:HB3	1:Y:63:VAL:CG2	2.38	0.53
1:Y:325:ASP:O	1:Y:326:ALA:C	2.44	0.53
1:Y:498:GLU:OE2	1:O:488:LYS:HE3	2.08	0.53
1:O:272:LEU:HD12	1:O:272:LEU:N	2.23	0.53
1:O:280:VAL:HG13	1:O:281:LYS:N	2.23	0.53
1:Y:246:GLN:CG	1:Y:270:PHE:HB2	2.38	0.53
1:Y:422:GLN:HE21	1:Y:426:LEU:HD22	1.74	0.53
1:O:193:ASN:HB3	1:O:196:THR:HG21	1.89	0.53
1:Y:137:SER:O	1:Y:140:LYS:N	2.42	0.53
1:Y:17:ARG:HH22	1:Y:437:GLU:HG3	1.72	0.53
1:O:219:ARG:HG2	1:O:221:SER:H	1.74	0.53
1:O:363:ALA:HB3	1:O:365:PHE:CE1	2.43	0.53
1:Y:127:ASN:ND2	1:Y:193:ASN:HD21	2.06	0.53
1:Y:152:ARG:HB3	1:Y:156:ARG:NH2	2.14	0.53
1:Y:201:ASP:HA	1:Y:204:LEU:HB2	1.91	0.53
1:Y:372:ASN:OD1	1:Y:374:ASN:HB2	2.09	0.53
1:Y:405:ALA:HB1	1:Y:431:GLU:OE2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:451:VAL:O	1:Y:451:VAL:HG13	2.07	0.53
1:O:207:LEU:HB3	1:O:209:ILE:HD11	1.89	0.53
1:O:220:SER:HB2	1:O:292:CYS:SG	2.48	0.53
1:O:293:GLY:O	1:O:295:THR:N	2.42	0.53
1:O:401:ILE:HG22	1:O:402:ARG:N	2.23	0.53
1:Y:111:ILE:CG2	1:Y:115:LEU:HD13	2.39	0.53
1:O:63:VAL:HA	1:O:66:LYS:CG	2.33	0.53
1:O:198:ASP:C	1:O:199:TRP:O	2.43	0.53
1:Y:416:ASN:OD1	1:Y:432:ARG:NH1	2.30	0.53
1:Y:441:LEU:O	1:Y:444:ALA:HB3	2.09	0.53
1:O:460:LEU:H	1:O:460:LEU:CD1	1.96	0.53
1:O:434:GLU:OE1	1:O:465:VAL:HB	2.08	0.53
1:O:490:VAL:O	1:O:494:MET:HG2	2.09	0.53
1:Y:67:ALA:HB3	1:Y:69:ILE:CD1	2.38	0.52
1:O:183:TYR:HB3	1:O:290:ILE:HG21	1.91	0.52
1:Y:271:MET:HG2	1:Y:395:MET:HE2	1.90	0.52
1:Y:423:SER:HB2	1:Y:428:THR:O	2.10	0.52
1:O:156:ARG:C	1:O:158:GLY:H	2.13	0.52
1:O:244:GLY:O	1:O:245:ASP:C	2.44	0.52
1:O:253:GLN:NE2	1:O:262:LYS:HB2	2.21	0.52
1:O:263:ASN:HB2	1:O:406:LEU:HD11	1.91	0.52
1:Y:420:GLN:HE21	1:Y:424:ASP:CG	2.12	0.52
1:Y:113:GLU:OE1	1:Y:113:GLU:HA	2.08	0.52
1:O:123:TYR:HD2	1:O:203:MET:CE	2.22	0.52
1:O:140:LYS:O	1:O:141:VAL:C	2.48	0.52
1:O:142:LYS:O	1:O:145:LEU:N	2.43	0.52
1:Y:146:ASP:HB3	1:Y:152:ARG:HH12	1.74	0.52
1:O:422:GLN:O	1:O:426:LEU:HD22	2.10	0.52
1:Y:22:ASP:O	1:Y:25:ALA:N	2.31	0.52
1:Y:295:THR:HG23	1:Y:297:GLU:OE1	2.09	0.52
1:Y:308:MET:HB2	1:Y:346:PRO:HB2	1.91	0.52
1:Y:483:TYR:O	1:Y:486:TRP:HB3	2.09	0.52
1:O:228:ASN:HD21	1:O:235:THR:N	2.07	0.52
1:O:453:PHE:HD2	1:O:454:TRP:CZ3	2.28	0.52
1:Y:50:MET:O	1:Y:53:TRP:HB3	2.09	0.52
1:Y:164:THR:O	1:Y:167:THR:N	2.42	0.52
1:Y:205:GLU:O	1:Y:206:VAL:C	2.43	0.52
1:O:60:LEU:C	1:O:60:LEU:HD12	2.30	0.52
1:O:142:LYS:HG3	1:O:143:TRP:N	2.24	0.52
1:Y:154:ARG:HA	1:Y:157:ARG:CG	2.40	0.52
1:O:9:LEU:HB2	1:O:79:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:ALA:O	1:O:68:ASP:N	2.40	0.52
1:O:154:ARG:HA	1:O:159:GLU:OE1	2.10	0.52
1:Y:78:GLY:C	1:Y:79:ILE:HG12	2.29	0.52
1:Y:151:SER:O	1:Y:153:GLU:N	2.43	0.52
1:O:172:LYS:HD2	1:O:172:LYS:N	2.25	0.52
1:O:415:ASN:HB3	1:O:418:LEU:HB2	1.92	0.52
1:Y:91:LYS:O	1:Y:93:THR:N	2.43	0.52
1:O:67:ALA:HB3	1:O:69:ILE:HD12	1.91	0.52
1:Y:87:ILE:HG22	1:Y:88:VAL:N	2.25	0.51
1:Y:102:VAL:O	1:Y:103:TRP:C	2.47	0.51
1:Y:130:LEU:HD13	1:Y:136:PHE:CD1	2.45	0.51
1:Y:12:GLY:HA3	3:Y:601:ACP:O3G	2.11	0.51
1:Y:144:ILE:HG22	1:Y:145:LEU:N	2.24	0.51
1:Y:272:LEU:HD11	1:Y:303:GLU:HG3	1.92	0.51
1:O:14:THR:N	3:O:601:ACP:O3G	2.43	0.51
1:O:116:LYS:HG2	1:O:132:ILE:HG21	1.92	0.51
1:O:330:GLU:O	1:O:334:THR:HG23	2.09	0.51
1:Y:16:SER:HB3	1:Y:56:GLN:OE1	2.10	0.51
1:O:80:THR:CG2	1:O:248:ALA:HB2	2.41	0.51
1:O:188:ARG:NH2	1:O:289:THR:HG21	2.21	0.51
1:O:298:VAL:HG12	1:O:299:ASN:N	2.25	0.51
1:Y:423:SER:HB2	1:Y:430:VAL:HG23	1.91	0.51
1:O:38:ILE:O	1:O:40:PRO:HD3	2.11	0.51
1:O:261:ALA:HB2	1:O:273:MET:CG	2.39	0.51
1:O:271:MET:O	1:O:272:LEU:HD12	2.11	0.51
1:Y:130:LEU:HD12	1:Y:190:MET:HB2	1.91	0.51
1:Y:235:THR:O	1:Y:237:ILE:HD13	2.11	0.51
1:O:409:ASP:C	1:O:413:VAL:HG11	2.30	0.51
1:O:193:ASN:OD1	1:O:196:THR:HB	2.10	0.51
1:O:455:GLN:O	1:O:456:ASN:HB2	2.09	0.51
1:Y:33:ARG:NE	1:Y:58:TRP:CE3	2.79	0.51
1:Y:172:LYS:O	1:Y:173:MET:C	2.49	0.51
1:O:144:ILE:O	1:O:145:LEU:C	2.49	0.51
1:O:218:ARG:HH11	1:O:218:ARG:CG	2.24	0.51
1:O:278:LYS:O	1:O:278:LYS:HG2	2.09	0.51
1:O:438:VAL:HG12	1:O:439:THR:N	2.24	0.51
1:O:482:ARG:HH11	1:O:482:ARG:CG	2.24	0.51
1:Y:89:TRP:HB2	1:Y:95:LYS:O	2.10	0.51
1:Y:89:TRP:HD1	1:Y:90:GLU:O	1.93	0.51
1:Y:432:ARG:HB3	1:Y:468:ARG:HB3	1.93	0.51
1:O:154:ARG:O	1:O:159:GLU:N	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:89:TRP:HB2	1:Y:95:LYS:C	2.32	0.51
1:Y:115:LEU:HD12	1:Y:115:LEU:N	2.24	0.51
1:Y:179:HIS:CE1	1:Y:215:PRO:HG3	2.46	0.51
1:O:38:ILE:O	1:O:45:VAL:HA	2.10	0.51
1:O:77:ILE:HG22	1:O:239:ILE:HG23	1.93	0.51
1:Y:352:GLY:O	1:Y:353:ALA:C	2.44	0.51
1:Y:422:GLN:NE2	1:Y:426:LEU:HD22	2.25	0.51
1:O:41:LYS:CB	1:O:42:PRO:HD2	2.41	0.51
1:O:56:GLN:O	1:O:59:THR:HB	2.11	0.51
1:Y:124:ILE:CG1	1:Y:203:MET:HE3	2.40	0.50
1:Y:222:GLU:O	1:Y:240:SER:HA	2.11	0.50
1:O:359:TYR:CZ	1:O:499:HIS:CE1	2.99	0.50
1:O:445:TYR:O	1:O:446:LEU:C	2.48	0.50
1:Y:91:LYS:HB2	1:Y:161:LEU:CD1	2.34	0.50
1:Y:108:THR:HG1	1:Y:139:THR:HG1	1.57	0.50
1:Y:237:ILE:HD13	1:Y:237:ILE:N	2.26	0.50
1:Y:456:ASN:O	1:Y:459:GLU:OE2	2.29	0.50
1:Y:491:LYS:O	1:Y:493:ALA:N	2.44	0.50
1:O:114:HIS:CD2	1:O:117:ARG:NH2	2.79	0.50
1:O:137:SER:O	1:O:138:GLY:O	2.29	0.50
1:O:142:LYS:O	1:O:146:ASP:OD1	2.29	0.50
1:O:185:ASN:ND2	1:O:244:GLY:N	2.59	0.50
1:O:283:GLU:HA	1:O:283:GLU:OE1	2.10	0.50
1:O:453:PHE:HD2	1:O:454:TRP:CE3	2.29	0.50
1:Y:242:ILE:HG22	1:Y:243:ALA:N	2.25	0.50
1:O:163:GLY:HA3	1:O:167:THR:HB	1.94	0.50
1:O:182:ASP:OD1	1:O:185:ASN:HB2	2.12	0.50
1:O:428:THR:HG23	1:O:429:ARG:N	2.26	0.50
1:Y:5:TYR:O	1:Y:75:ALA:N	2.33	0.50
1:Y:170:ILE:HA	1:Y:173:MET:HG3	1.93	0.50
1:Y:253:GLN:HE21	1:Y:262:LYS:CB	2.23	0.50
1:Y:267:THR:CB	3:Y:601:ACP:H3B2	2.42	0.50
1:Y:453:PHE:CD2	1:Y:454:TRP:CZ3	2.99	0.50
1:O:184:THR:HA	1:O:290:ILE:HG22	1.94	0.50
1:Y:12:GLY:O	1:Y:35:PHE:HZ	1.95	0.50
1:Y:63:VAL:O	1:Y:64:LEU:O	2.29	0.50
1:Y:211:ARG:HG3	1:Y:211:ARG:NH1	2.15	0.50
1:Y:257:LYS:CA	1:Y:274:ASN:HD22	2.24	0.50
1:O:95:LYS:HG3	1:O:96:PRO:N	2.25	0.50
1:O:103:TRP:CD1	1:O:103:TRP:N	2.80	0.50
1:O:37:GLN:NE2	1:O:47:HIS:CE1	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:44:TRP:CE3	1:O:107:ARG:NH2	2.80	0.50
1:O:101:ILE:HD13	1:O:107:ARG:NE	2.26	0.50
1:O:163:GLY:CA	1:O:167:THR:HB	2.42	0.50
1:O:263:ASN:ND2	1:O:265:TYR:CE1	2.80	0.50
1:Y:3:LYS:HG3	1:Y:73:GLN:CA	2.41	0.50
1:Y:3:LYS:HG3	1:Y:73:GLN:HA	1.93	0.50
1:Y:114:HIS:O	1:Y:117:ARG:N	2.44	0.50
1:Y:444:ALA:O	1:Y:445:TYR:O	2.30	0.50
1:O:153:GLU:O	1:O:157:ARG:HD3	2.12	0.50
1:O:310:GLY:HA3	3:O:601:ACP:O3'	2.10	0.50
1:Y:74:ILE:HD11	1:Y:237:ILE:HG21	1.94	0.50
1:Y:257:LYS:H	1:Y:260:MET:CG	2.19	0.50
1:Y:343:TYR:CD2	1:Y:486:TRP:HA	2.47	0.50
1:O:123:TYR:CE2	1:O:203:MET:HE2	2.47	0.50
1:O:144:ILE:HD12	1:O:144:ILE:N	2.10	0.50
1:O:278:LYS:HD2	1:O:280:VAL:HG23	1.93	0.50
1:O:348:PHE:CD1	1:O:348:PHE:N	2.79	0.50
1:O:386:TYR:HB3	1:O:486:TRP:CD2	2.45	0.50
1:Y:87:ILE:O	1:Y:88:VAL:HG23	2.11	0.50
1:Y:90:GLU:N	1:Y:95:LYS:O	2.36	0.50
1:Y:188:ARG:NH2	1:Y:289:THR:HG21	2.26	0.50
1:O:44:TRP:N	1:O:44:TRP:CD1	2.79	0.50
1:O:148:VAL:HG12	1:O:151:SER:HB3	1.92	0.50
1:O:198:ASP:O	1:O:199:TRP:O	2.30	0.50
1:Y:44:TRP:CD1	1:Y:44:TRP:N	2.78	0.49
1:Y:114:HIS:N	1:Y:114:HIS:CD2	2.78	0.49
1:Y:203:MET:CA	1:Y:206:VAL:HG12	2.42	0.49
1:Y:253:GLN:HG3	1:Y:407:ARG:HD2	1.94	0.49
1:O:11:GLN:NE2	1:O:82:GLN:HG2	2.27	0.49
1:O:138:GLY:O	1:O:141:VAL:HG23	2.12	0.49
1:O:166:ASP:O	1:O:167:THR:C	2.51	0.49
1:O:200:ASP:O	1:O:201:ASP:C	2.50	0.49
1:O:237:ILE:CG2	1:O:238:PRO:HD2	2.42	0.49
1:O:457:LEU:HD22	1:O:460:LEU:HD13	1.93	0.49
1:Y:77:ILE:N	1:Y:238:PRO:O	2.45	0.49
1:Y:88:VAL:HG22	1:Y:162:PHE:CB	2.43	0.49
1:Y:298:VAL:O	1:Y:299:ASN:OD1	2.30	0.49
1:Y:344:VAL:HG22	1:Y:364:ILE:HG23	1.94	0.49
1:O:202:LYS:HA	1:O:205:GLU:OE2	2.12	0.49
1:O:275:THR:OG1	1:O:300:TYR:HB2	2.12	0.49
1:O:326:ALA:O	1:O:327:TYR:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:70:SER:N	1:Y:73:GLN:HE21	2.08	0.49
1:Y:445:TYR:CD2	1:Y:457:LEU:HD11	2.48	0.49
1:O:153:GLU:HA	1:O:156:ARG:NH1	2.27	0.49
1:O:325:ASP:O	1:O:328:ASP:HB2	2.12	0.49
1:O:488:LYS:O	1:O:492:ARG:HD3	2.12	0.49
1:Y:229:ILE:HG23	1:Y:237:ILE:CD1	2.43	0.49
1:Y:271:MET:O	1:Y:272:LEU:HD12	2.12	0.49
1:Y:455:GLN:O	1:Y:456:ASN:OD1	2.30	0.49
1:O:22:ASP:OD2	1:O:26:ASN:HB2	2.11	0.49
1:O:83:ARG:HE	4:O:600:GOL:H2	1.78	0.49
1:Y:173:MET:C	1:Y:175:GLN:H	2.15	0.49
1:Y:454:TRP:HD1	1:Y:459:GLU:CD	2.15	0.49
1:O:155:ALA:CB	1:O:210:PRO:HG2	2.38	0.49
1:O:199:TRP:CG	1:O:214:LEU:HD23	2.47	0.49
1:O:375:HIS:O	1:O:376:ILE:C	2.50	0.49
1:Y:220:SER:O	1:Y:446:LEU:HD23	2.12	0.49
1:Y:256:VAL:CG1	1:Y:294:PRO:HG3	2.42	0.49
1:Y:441:LEU:CD2	1:Y:445:TYR:HE1	2.26	0.49
1:O:420:GLN:HE21	1:O:424:ASP:CG	2.16	0.49
1:Y:31:SER:CB	1:Y:59:THR:HA	2.28	0.49
1:Y:86:THR:HG22	1:Y:87:ILE:N	2.27	0.49
1:Y:205:GLU:C	1:Y:208:ASP:H	2.16	0.49
1:Y:324:ASN:N	1:Y:324:ASN:ND2	2.61	0.49
1:O:7:VAL:HG12	1:O:9:LEU:HD22	1.95	0.49
1:O:21:MET:HB3	1:O:26:ASN:O	2.13	0.49
1:O:54:ALA:O	1:O:55:THR:C	2.49	0.49
1:O:271:MET:CG	1:O:395:MET:HE2	2.37	0.49
1:O:272:LEU:HG	1:O:303:GLU:HB2	1.94	0.49
1:O:422:GLN:NE2	1:O:426:LEU:HD21	2.28	0.49
1:O:91:LYS:O	1:O:92:GLU:O	2.30	0.49
1:O:108:THR:HG21	1:O:140:LYS:HA	1.95	0.49
1:O:264:THR:HA	1:O:409:ASP:O	2.13	0.49
1:Y:7:VAL:O	1:Y:77:ILE:HA	2.13	0.49
1:Y:123:TYR:HD2	1:Y:203:MET:CE	2.26	0.49
1:Y:261:ALA:HB2	1:Y:273:MET:HG3	1.94	0.49
1:O:39:TYR:HA	1:O:44:TRP:O	2.12	0.49
1:O:451:VAL:O	1:O:452:GLY:C	2.46	0.49
1:Y:133:ASP:OD1	1:Y:135:TYR:HB2	2.12	0.49
1:Y:408:VAL:O	1:Y:409:ASP:HB3	2.13	0.49
1:O:48:ASP:O	1:O:51:GLU:N	2.46	0.49
1:Y:69:ILE:HG22	1:Y:70:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:218:ARG:HH11	1:Y:218:ARG:CG	2.25	0.48
1:Y:261:ALA:HB2	1:Y:273:MET:HG2	1.95	0.48
1:O:91:LYS:HG2	1:O:92:GLU:N	2.26	0.48
1:O:196:THR:HG22	1:O:198:ASP:H	1.77	0.48
1:O:219:ARG:HG2	1:O:220:SER:N	2.28	0.48
1:O:451:VAL:O	1:O:451:VAL:HG13	2.11	0.48
1:Y:166:ASP:OD2	1:Y:185:ASN:OD1	2.31	0.48
1:Y:391:VAL:O	1:Y:394:ALA:HB3	2.12	0.48
1:O:141:VAL:C	1:O:145:LEU:HD22	2.34	0.48
1:Y:185:ASN:O	1:Y:188:ARG:HB2	2.13	0.48
1:O:199:TRP:CD2	1:O:214:LEU:HD23	2.48	0.48
1:O:389:ARG:O	1:O:392:LEU:N	2.46	0.48
1:Y:9:LEU:CD2	1:Y:77:ILE:HG23	2.41	0.48
1:Y:146:ASP:OD1	1:Y:146:ASP:N	2.39	0.48
1:Y:348:PHE:CD1	1:Y:348:PHE:N	2.78	0.48
1:O:113:GLU:O	1:O:117:ARG:HD3	2.13	0.48
1:O:481:TYR:O	1:O:484:ALA:HB3	2.13	0.48
1:Y:54:ALA:O	1:Y:57:SER:HB2	2.13	0.48
1:Y:142:LYS:HG3	1:Y:143:TRP:N	2.27	0.48
1:O:93:THR:OG1	1:O:95:LYS:HB3	2.12	0.48
1:O:201:ASP:O	1:O:202:LYS:C	2.52	0.48
1:O:221:SER:HB2	1:O:296:GLY:HA3	1.92	0.48
1:O:387:GLN:O	1:O:388:THR:C	2.51	0.48
1:O:40:PRO:HD2	1:O:44:TRP:O	2.14	0.48
1:O:124:ILE:HG12	1:O:203:MET:CE	2.43	0.48
1:Y:17:ARG:HD3	1:Y:32:GLN:NE2	2.26	0.48
1:Y:17:ARG:HG2	1:Y:32:GLN:HG2	1.95	0.48
1:Y:271:MET:HE1	1:Y:392:LEU:HB2	1.96	0.48
1:O:132:ILE:O	1:O:133:ASP:HB2	2.11	0.48
1:O:150:GLY:HA3	1:O:154:ARG:CD	2.43	0.48
1:O:263:ASN:ND2	1:O:265:TYR:CZ	2.80	0.48
1:Y:22:ASP:O	1:Y:23:HIS:C	2.51	0.48
1:Y:128:THR:C	1:Y:130:LEU:H	2.17	0.48
1:O:61:VAL:O	1:O:62:GLU:C	2.51	0.48
1:Y:222:GLU:HG3	1:Y:223:VAL:H	1.79	0.48
1:O:90:GLU:HB2	1:O:93:THR:OG1	2.14	0.48
1:O:276:GLY:HA2	1:O:299:ASN:HD22	1.77	0.48
1:O:462:GLU:C	1:O:464:ALA:H	2.15	0.48
1:Y:50:MET:O	1:Y:51:GLU:C	2.51	0.48
1:Y:227:THR:O	1:Y:237:ILE:N	2.34	0.48
1:O:278:LYS:HG3	1:O:279:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:20:VAL:HG12	1:Y:21:MET:H	1.77	0.47
1:Y:115:LEU:H	1:Y:115:LEU:CD1	2.26	0.47
1:Y:289:THR:O	1:Y:301:ALA:N	2.43	0.47
1:Y:479:ARG:CG	1:Y:479:ARG:HH11	2.27	0.47
1:O:129:GLY:HA3	1:O:288:THR:HB	1.94	0.47
1:O:140:LYS:O	1:O:144:ILE:HD12	2.14	0.47
1:O:154:ARG:CA	1:O:159:GLU:HB2	2.44	0.47
1:Y:50:MET:O	1:Y:53:TRP:N	2.47	0.47
1:Y:207:LEU:O	1:Y:208:ASP:HB3	2.13	0.47
1:Y:247:GLN:NE2	1:Y:290:ILE:O	2.47	0.47
1:Y:357:ASP:OD2	1:Y:494:MET:HB3	2.14	0.47
1:O:9:LEU:HD13	1:O:9:LEU:HA	1.43	0.47
1:O:118:ASP:HB2	1:O:120:LEU:HD11	1.95	0.47
1:Y:80:THR:HG21	1:Y:248:ALA:HB2	1.95	0.47
1:Y:140:LYS:O	1:Y:143:TRP:HB3	2.13	0.47
1:Y:179:HIS:O	1:Y:216:GLU:N	2.42	0.47
1:Y:193:ASN:CG	1:Y:196:THR:HB	2.33	0.47
1:Y:367:LEU:HD11	1:O:364:ILE:HD13	1.96	0.47
1:Y:468:ARG:HH11	1:Y:468:ARG:HG2	1.78	0.47
1:O:273:MET:HB2	1:O:395:MET:CE	2.44	0.47
1:O:451:VAL:HG12	1:O:453:PHE:CB	2.44	0.47
1:O:458:ASP:HA	1:O:461:GLN:HB2	1.95	0.47
1:Y:350:GLY:HA2	1:Y:360:ALA:O	2.14	0.47
1:O:20:VAL:C	1:O:21:MET:HG3	2.34	0.47
1:O:22:ASP:O	1:O:25:ALA:N	2.43	0.47
1:O:24:ASP:HB3	1:O:26:ASN:HD21	1.80	0.47
1:O:80:THR:HG21	1:O:248:ALA:HB2	1.96	0.47
1:O:247:GLN:O	1:O:250:LEU:HB3	2.15	0.47
1:Y:9:LEU:HD13	1:Y:9:LEU:HA	1.67	0.47
1:Y:329:SER:HB2	1:Y:381:LEU:HD11	1.95	0.47
1:O:31:SER:HB2	1:O:63:VAL:HG23	1.96	0.47
1:O:278:LYS:CD	1:O:280:VAL:HG23	2.44	0.47
1:Y:69:ILE:HD12	1:Y:69:ILE:H	1.80	0.47
1:Y:117:ARG:HB2	1:Y:117:ARG:CZ	2.42	0.47
1:Y:154:ARG:HG3	1:Y:160:LEU:HD11	1.96	0.47
1:Y:310:GLY:O	1:Y:313:ILE:HB	2.15	0.47
1:Y:342:VAL:HA	1:Y:365:PHE:O	2.15	0.47
1:Y:343:TYR:CE2	1:Y:486:TRP:CA	2.98	0.47
1:Y:356:TRP:O	1:Y:358:PRO:HD3	2.15	0.47
1:Y:415:ASN:ND2	1:Y:417:PHE:HB3	2.25	0.47
1:Y:418:LEU:HA	1:Y:418:LEU:HD23	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:438:VAL:HA	1:Y:441:LEU:HD12	1.96	0.47
1:O:24:ASP:O	1:O:25:ALA:HB3	2.15	0.47
1:O:77:ILE:CG2	1:O:79:ILE:HD11	2.44	0.47
1:O:103:TRP:HB2	1:O:135:TYR:CE1	2.50	0.47
1:O:127:ASN:HB3	1:O:193:ASN:ND2	2.30	0.47
1:O:130:LEU:HD12	1:O:190:MET:HB2	1.97	0.47
1:O:257:LYS:O	1:O:258:GLU:O	2.32	0.47
1:O:382:GLU:O	1:O:384:ILE:N	2.48	0.47
1:Y:121:GLU:O	1:Y:122:ASP:C	2.53	0.47
1:Y:169:LEU:O	1:Y:173:MET:HG2	2.14	0.47
1:Y:201:ASP:O	1:Y:204:LEU:N	2.48	0.47
1:Y:428:THR:HG23	1:Y:429:ARG:N	2.30	0.47
1:O:158:GLY:H	1:O:212:GLU:HG2	1.78	0.47
1:O:404:HIS:O	1:O:429:ARG:HD2	2.15	0.47
1:Y:24:ASP:O	1:Y:25:ALA:HB3	2.14	0.47
1:O:95:LYS:HG3	1:O:96:PRO:O	2.14	0.47
1:O:482:ARG:NH1	1:O:482:ARG:HG3	2.30	0.47
1:O:185:ASN:HD21	1:O:244:GLY:HA2	1.79	0.47
1:O:468:ARG:HH11	1:O:468:ARG:CG	2.15	0.47
1:O:494:MET:O	1:O:495:ALA:HB3	2.15	0.47
1:Y:403:LEU:N	1:Y:403:LEU:CD1	2.78	0.46
1:O:148:VAL:CG1	1:O:151:SER:HB3	2.45	0.46
1:O:185:ASN:HD21	1:O:244:GLY:N	2.13	0.46
1:O:351:LEU:HD12	1:O:351:LEU:HA	1.74	0.46
1:Y:180:VAL:CG2	1:Y:181:THR:N	2.78	0.46
1:Y:219:ARG:O	1:Y:224:TYR:OH	2.27	0.46
1:Y:253:GLN:O	1:Y:254:LEU:HB2	2.15	0.46
1:Y:392:LEU:HD23	1:Y:393:GLU:HG2	1.96	0.46
1:O:39:TYR:O	1:O:40:PRO:C	2.53	0.46
1:O:74:ILE:HD12	1:O:76:ALA:N	2.30	0.46
1:Y:152:ARG:C	1:Y:155:ALA:HB3	2.36	0.46
1:O:117:ARG:HD3	1:O:117:ARG:H	1.81	0.46
1:O:439:THR:O	1:O:442:GLY:N	2.48	0.46
1:O:484:ALA:O	1:O:485:GLY:C	2.53	0.46
1:Y:18:ALA:HB1	1:Y:63:VAL:HG21	1.97	0.46
1:Y:343:TYR:CE2	1:Y:486:TRP:HA	2.51	0.46
1:Y:351:LEU:HB3	1:Y:355:TYR:HB2	1.97	0.46
1:O:184:THR:O	1:O:187:SER:HB3	2.16	0.46
1:Y:5:TYR:O	1:Y:74:ILE:HA	2.15	0.46
1:Y:104:GLN:HG2	1:Y:349:THR:HG21	1.97	0.46
1:Y:203:MET:HA	1:Y:206:VAL:CG1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:237:ILE:N	1:Y:237:ILE:CD1	2.78	0.46
1:Y:256:VAL:HG12	1:Y:294:PRO:HG3	1.98	0.46
1:Y:438:VAL:O	1:Y:441:LEU:HB2	2.16	0.46
1:Y:457:LEU:HA	1:Y:460:LEU:CD1	2.39	0.46
1:O:158:GLY:N	1:O:212:GLU:HG2	2.30	0.46
1:O:284:ASN:OD1	1:O:398:ASP:OD1	2.34	0.46
1:Y:170:ILE:CD1	1:Y:170:ILE:N	2.79	0.46
1:Y:422:GLN:NE2	1:Y:426:LEU:CD2	2.78	0.46
1:Y:453:PHE:HD2	1:Y:454:TRP:CZ3	2.34	0.46
1:Y:468:ARG:HH11	1:Y:468:ARG:CG	2.27	0.46
1:O:145:LEU:N	1:O:145:LEU:HD13	2.26	0.46
1:O:224:TYR:CE2	1:O:242:ILE:HD12	2.51	0.46
1:O:245:ASP:OD1	1:O:246:GLN:NE2	2.48	0.46
1:O:435:VAL:CG2	1:O:436:ARG:N	2.79	0.46
1:Y:88:VAL:HG22	1:Y:162:PHE:CA	2.46	0.46
1:Y:114:HIS:O	1:Y:116:LYS:N	2.48	0.46
1:Y:435:VAL:HG21	1:Y:441:LEU:HD11	1.97	0.46
1:O:5:TYR:N	1:O:73:GLN:O	2.44	0.46
1:O:77:ILE:CG2	1:O:239:ILE:HG23	2.45	0.46
1:O:78:GLY:HA3	1:O:443:ALA:O	2.15	0.46
1:O:85:THR:HG23	1:O:102:VAL:HA	1.97	0.46
1:O:154:ARG:HA	1:O:159:GLU:HB2	1.97	0.46
1:O:163:GLY:HA2	1:O:167:THR:HG21	1.98	0.46
1:O:172:LYS:O	1:O:175:GLN:N	2.40	0.46
1:O:269:CYS:HB2	1:O:306:VAL:HB	1.96	0.46
1:O:316:LEU:HA	1:O:316:LEU:HD23	1.26	0.46
1:O:347:ALA:O	1:O:361:ARG:HA	2.16	0.46
1:O:476:THR:O	1:O:477:THR:C	2.51	0.46
1:Y:124:ILE:HG12	1:Y:203:MET:HE1	1.98	0.46
1:Y:181:THR:CG2	1:Y:182:ASP:N	2.79	0.46
1:Y:262:LYS:HD2	1:Y:262:LYS:C	2.36	0.46
1:O:52:ILE:O	1:O:55:THR:OG1	2.34	0.46
1:O:70:SER:O	1:O:73:GLN:HG3	2.16	0.46
1:O:142:LYS:CG	1:O:143:TRP:N	2.79	0.46
1:Y:22:ASP:OD1	1:Y:25:ALA:N	2.49	0.46
1:Y:47:HIS:O	1:Y:49:PRO:HD3	2.16	0.46
1:Y:64:LEU:HB2	1:Y:65:ALA:H	1.54	0.46
1:Y:104:GLN:NE2	1:Y:308:MET:CE	2.79	0.46
1:Y:389:ARG:O	1:Y:390:ASP:C	2.52	0.46
1:O:5:TYR:O	1:O:74:ILE:HA	2.16	0.46
1:O:11:GLN:NE2	1:O:82:GLN:HE21	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:33:ARG:HE	1:O:58:TRP:HB3	1.80	0.46
1:O:113:GLU:OE1	1:O:113:GLU:HA	2.14	0.46
1:O:317:ARG:O	1:O:321:LYS:HA	2.15	0.46
1:Y:50:MET:O	1:Y:52:ILE:N	2.49	0.46
1:Y:120:LEU:O	1:Y:124:ILE:HG13	2.16	0.46
1:Y:244:GLY:O	1:Y:245:ASP:C	2.52	0.46
1:Y:254:LEU:O	1:Y:256:VAL:N	2.48	0.46
1:O:88:VAL:CG2	1:O:162:PHE:HB2	2.46	0.46
1:O:145:LEU:HB3	1:O:152:ARG:CZ	2.46	0.46
1:Y:57:SER:O	1:Y:60:LEU:HD23	2.16	0.45
1:Y:124:ILE:CD1	1:Y:203:MET:HE3	2.46	0.45
1:Y:222:GLU:HG2	1:Y:224:TYR:CD1	2.52	0.45
1:Y:441:LEU:HA	1:Y:441:LEU:HD23	1.67	0.45
1:Y:482:ARG:NH1	1:Y:482:ARG:HG3	2.30	0.45
1:O:161:LEU:CD2	1:O:179:HIS:CE1	2.99	0.45
1:O:179:HIS:CD2	1:O:215:PRO:CA	2.99	0.45
1:O:196:THR:C	1:O:197:LEU:HD22	2.37	0.45
1:O:467:GLU:OE2	1:O:468:ARG:HB2	2.15	0.45
1:Y:101:ILE:HD13	1:Y:107:ARG:NE	2.31	0.45
1:Y:193:ASN:OD1	1:Y:196:THR:HB	2.16	0.45
1:Y:284:ASN:OD1	1:Y:398:ASP:OD1	2.34	0.45
1:Y:394:ALA:O	1:Y:395:MET:C	2.52	0.45
1:O:78:GLY:HA2	1:O:241:GLY:HA3	1.97	0.45
1:O:179:HIS:CG	1:O:215:PRO:HB3	2.52	0.45
1:O:199:TRP:HB3	1:O:204:LEU:HD11	1.98	0.45
1:O:251:PHE:CE2	1:O:446:LEU:CD1	2.98	0.45
1:O:428:THR:CG2	1:O:429:ARG:N	2.79	0.45
1:O:60:LEU:HD12	1:O:60:LEU:O	2.16	0.45
1:O:117:ARG:HD3	1:O:117:ARG:N	2.31	0.45
1:O:191:LEU:HD23	1:O:207:LEU:CD1	2.46	0.45
1:O:230:GLY:HA2	1:O:235:THR:HB	1.98	0.45
1:O:285:GLY:O	1:O:356:TRP:NE1	2.39	0.45
1:O:309:ALA:O	1:O:312:SER:OG	2.30	0.45
1:O:310:GLY:O	1:O:313:ILE:N	2.49	0.45
1:O:401:ILE:CG2	1:O:402:ARG:N	2.79	0.45
1:Y:80:THR:HG21	1:Y:248:ALA:CB	2.47	0.45
1:Y:183:TYR:O	1:Y:184:THR:C	2.55	0.45
1:Y:264:THR:CG2	1:Y:265:TYR:N	2.79	0.45
1:Y:423:SER:HB3	1:Y:430:VAL:HG23	1.98	0.45
1:Y:461:GLN:HE21	1:Y:461:GLN:HB3	1.56	0.45
1:O:145:LEU:HD12	1:O:145:LEU:HA	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:214:LEU:N	1:O:214:LEU:CD1	2.79	0.45
1:O:251:PHE:O	1:O:254:LEU:HD12	2.16	0.45
1:O:298:VAL:O	1:O:299:ASN:OD1	2.35	0.45
1:Y:161:LEU:CD2	1:Y:179:HIS:NE2	2.80	0.45
1:Y:206:VAL:CG1	1:Y:207:LEU:N	2.79	0.45
1:Y:425:ILE:HD12	1:Y:425:ILE:HA	1.53	0.45
1:O:218:ARG:NH1	1:O:218:ARG:CG	2.79	0.45
1:O:438:VAL:CA	1:O:441:LEU:HD12	2.41	0.45
1:Y:53:TRP:CE3	1:Y:53:TRP:CA	3.00	0.45
1:Y:179:HIS:CE1	1:Y:215:PRO:CB	3.00	0.45
1:Y:256:VAL:N	1:Y:260:MET:HG3	2.31	0.45
1:Y:328:ASP:O	1:Y:329:SER:C	2.53	0.45
1:Y:428:THR:CG2	1:Y:429:ARG:N	2.80	0.45
1:O:8:ALA:O	1:O:9:LEU:HD13	2.16	0.45
1:O:13:THR:HB	3:O:601:ACP:O3G	2.16	0.45
1:O:86:THR:CG2	1:O:162:PHE:CE2	2.99	0.45
1:O:153:GLU:O	1:O:156:ARG:N	2.49	0.45
1:O:183:TYR:CD2	1:O:298:VAL:CG2	2.99	0.45
1:O:419:MET:O	1:O:420:GLN:C	2.52	0.45
1:Y:3:LYS:HA	1:Y:73:GLN:CA	2.40	0.45
1:Y:212:GLU:C	1:Y:214:LEU:H	2.19	0.45
1:Y:466:ILE:HD13	1:Y:466:ILE:O	2.17	0.45
1:O:33:ARG:NE	1:O:58:TRP:HB3	2.32	0.45
1:O:105:CYS:SG	1:O:107:ARG:NH1	2.89	0.45
1:O:184:THR:OG1	1:O:243:ALA:HA	2.17	0.45
1:O:406:LEU:CD2	1:O:407:ARG:N	2.79	0.45
1:Y:130:LEU:HB3	1:Y:131:VAL:H	1.41	0.45
1:Y:435:VAL:CG2	1:Y:436:ARG:N	2.79	0.45
1:O:71:SER:OG	1:O:230:GLY:O	2.30	0.45
1:O:180:VAL:CG2	1:O:181:THR:N	2.80	0.45
1:O:182:ASP:OD1	1:O:242:ILE:HG22	2.17	0.45
1:O:257:LYS:CA	1:O:274:ASN:HD22	2.30	0.45
1:O:352:GLY:O	1:O:353:ALA:C	2.51	0.45
1:Y:230:GLY:CA	1:Y:235:THR:HB	2.44	0.45
1:Y:426:LEU:HD12	1:Y:426:LEU:HA	1.71	0.45
1:O:33:ARG:CZ	1:O:58:TRP:HB3	2.47	0.45
1:O:290:ILE:CG2	1:O:291:ALA:N	2.80	0.45
1:Y:79:ILE:HD11	1:Y:239:ILE:HG23	1.98	0.45
1:Y:142:LYS:O	1:Y:145:LEU:HB2	2.17	0.45
1:Y:312:SER:O	1:Y:315:TRP:HB3	2.17	0.45
1:O:11:GLN:HE22	1:O:82:GLN:HG2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:265:TYR:CE1	1:O:408:VAL:CG1	2.99	0.45
1:O:467:GLU:O	1:O:467:GLU:HG2	2.09	0.45
1:Y:102:VAL:O	1:Y:104:GLN:N	2.50	0.44
1:Y:149:GLU:OE1	1:Y:149:GLU:HA	2.17	0.44
1:Y:182:ASP:CG	1:Y:242:ILE:HB	2.37	0.44
1:Y:271:MET:HG2	1:Y:271:MET:O	2.13	0.44
1:Y:309:ALA:O	1:Y:312:SER:OG	2.32	0.44
1:Y:478:GLU:O	1:Y:481:TYR:N	2.50	0.44
1:Y:488:LYS:O	1:Y:492:ARG:HD3	2.17	0.44
1:O:237:ILE:N	1:O:237:ILE:CD1	2.80	0.44
1:O:422:GLN:NE2	1:O:426:LEU:CD2	2.79	0.44
1:O:463:LYS:NZ	1:O:465:VAL:CG2	2.80	0.44
1:Y:59:THR:O	1:Y:60:LEU:C	2.56	0.44
1:Y:111:ILE:O	1:Y:112:CYS:C	2.50	0.44
1:Y:214:LEU:N	1:Y:214:LEU:CD1	2.79	0.44
1:Y:495:ALA:O	1:O:492:ARG:NH2	2.50	0.44
1:O:3:LYS:HG3	1:O:72:ASP:O	2.17	0.44
1:O:65:ALA:C	1:O:67:ALA:H	2.21	0.44
1:O:146:ASP:OD1	1:O:146:ASP:N	2.38	0.44
1:O:389:ARG:O	1:O:390:ASP:C	2.56	0.44
1:Y:70:SER:H	1:Y:73:GLN:HG3	1.82	0.44
1:Y:142:LYS:O	1:Y:146:ASP:OD1	2.35	0.44
1:Y:148:VAL:CG1	1:Y:149:GLU:N	2.80	0.44
1:Y:222:GLU:CG	1:Y:223:VAL:N	2.80	0.44
1:O:37:GLN:HB3	1:O:39:TYR:CZ	2.52	0.44
1:O:37:GLN:HE22	1:O:47:HIS:CE1	2.34	0.44
1:O:53:TRP:O	1:O:54:ALA:C	2.56	0.44
1:O:80:THR:C	1:O:81:ASN:HD22	2.20	0.44
1:O:186:ALA:HB2	1:O:217:VAL:HG13	2.00	0.44
1:O:357:ASP:OD1	1:O:358:PRO:HD2	2.17	0.44
1:Y:3:LYS:HG3	1:Y:72:ASP:C	2.37	0.44
1:Y:31:SER:HB2	1:Y:63:VAL:CG2	2.20	0.44
1:Y:56:GLN:HG3	1:Y:56:GLN:O	2.18	0.44
1:Y:130:LEU:HD13	1:Y:136:PHE:CE1	2.52	0.44
1:O:41:LYS:CG	1:O:42:PRO:N	2.81	0.44
1:O:83:ARG:NH1	1:O:246:GLN:HB2	2.33	0.44
1:Y:228:ASN:HD22	1:Y:230:GLY:N	2.16	0.44
1:O:302:LEU:HD23	1:O:302:LEU:HA	1.62	0.44
1:O:415:ASN:ND2	1:O:417:PHE:HB3	2.15	0.44
1:Y:41:LYS:HB2	1:Y:42:PRO:HD2	2.00	0.44
1:Y:43:GLY:C	1:Y:44:TRP:HD1	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:154:ARG:CA	1:Y:159:GLU:HB2	2.47	0.44
1:Y:255:CYS:HA	1:Y:260:MET:CB	2.47	0.44
1:Y:265:TYR:N	1:Y:409:ASP:O	2.51	0.44
1:Y:434:GLU:HB2	1:Y:465:VAL:O	2.17	0.44
1:O:298:VAL:CG1	1:O:299:ASN:N	2.81	0.44
1:Y:200:ASP:OD1	1:Y:202:LYS:HB2	2.18	0.44
1:Y:253:GLN:CG	1:Y:407:ARG:HD2	2.47	0.44
1:Y:257:LYS:CA	1:Y:274:ASN:ND2	2.81	0.44
1:Y:272:LEU:N	1:Y:272:LEU:CD1	2.80	0.44
1:O:21:MET:HA	1:O:26:ASN:O	2.18	0.44
1:O:130:LEU:HD13	1:O:136:PHE:CG	2.52	0.44
1:O:439:THR:CG2	1:O:440:ALA:N	2.79	0.44
1:Y:74:ILE:HD12	1:Y:75:ALA:N	2.32	0.44
1:Y:97:ILE:H	1:Y:97:ILE:HG13	1.66	0.44
1:Y:218:ARG:NH1	1:Y:218:ARG:CG	2.79	0.44
1:Y:279:ALA:CB	1:Y:300:TYR:CG	2.99	0.44
1:O:183:TYR:O	1:O:187:SER:N	2.37	0.44
1:Y:111:ILE:O	1:Y:115:LEU:HD13	2.18	0.44
1:Y:172:LYS:HA	1:Y:172:LYS:HD2	1.48	0.44
1:O:5:TYR:CE2	1:O:28:ILE:HG13	2.53	0.44
1:O:148:VAL:CG1	1:O:149:GLU:N	2.80	0.44
1:O:185:ASN:ND2	1:O:244:GLY:CA	2.79	0.44
1:O:354:PRO:HD2	1:O:355:TYR:CE2	2.53	0.44
1:O:442:GLY:O	1:O:445:TYR:N	2.51	0.44
1:O:474:ILE:HD12	1:O:474:ILE:HA	1.79	0.44
1:Y:74:ILE:HD12	1:Y:74:ILE:C	2.38	0.43
1:Y:270:PHE:CZ	4:Y:600:GOL:H11	2.53	0.43
1:Y:348:PHE:N	1:Y:348:PHE:HD1	2.14	0.43
1:Y:445:TYR:HD2	1:Y:457:LEU:HD11	1.81	0.43
1:O:74:ILE:HD12	1:O:74:ILE:C	2.38	0.43
1:O:169:LEU:HD13	1:O:169:LEU:HA	1.39	0.43
1:O:453:PHE:CD2	1:O:454:TRP:CZ3	3.05	0.43
1:O:482:ARG:CG	1:O:482:ARG:NH1	2.79	0.43
1:Y:16:SER:CB	1:Y:56:GLN:HA	2.48	0.43
1:Y:64:LEU:O	1:Y:65:ALA:C	2.56	0.43
1:Y:88:VAL:HA	1:Y:161:LEU:O	2.17	0.43
1:Y:476:THR:O	1:Y:477:THR:C	2.56	0.43
1:O:192:PHE:CZ	1:O:197:LEU:HA	2.53	0.43
1:O:246:GLN:H	1:O:246:GLN:HE21	1.65	0.43
1:O:257:LYS:O	1:O:258:GLU:C	2.56	0.43
1:O:394:ALA:O	1:O:397:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:91:LYS:NZ	1:Y:91:LYS:CB	2.79	0.43
1:Y:161:LEU:HD22	1:Y:179:HIS:CE1	2.52	0.43
1:Y:286:LEU:O	1:Y:287:LEU:HD23	2.17	0.43
1:O:84:GLU:HG2	1:O:135:TYR:O	2.19	0.43
1:O:109:ALA:HA	1:O:134:PRO:HG3	2.01	0.43
1:O:114:HIS:O	1:O:117:ARG:N	2.51	0.43
1:O:123:TYR:OH	1:O:200:ASP:OD2	2.31	0.43
1:Y:110:GLU:O	1:Y:111:ILE:C	2.55	0.43
1:Y:436:ARG:C	1:Y:438:VAL:H	2.20	0.43
1:Y:482:ARG:HH11	1:Y:482:ARG:CG	2.30	0.43
1:Y:484:ALA:O	1:Y:485:GLY:C	2.54	0.43
1:O:28:ILE:N	1:O:28:ILE:HD13	2.32	0.43
1:O:141:VAL:O	1:O:142:LYS:C	2.57	0.43
1:O:219:ARG:HD3	1:O:221:SER:O	2.18	0.43
1:Y:41:LYS:CB	1:Y:42:PRO:HD2	2.48	0.43
1:Y:83:ARG:HE	1:Y:83:ARG:HB2	1.64	0.43
1:Y:199:TRP:CE2	1:Y:214:LEU:HD23	2.53	0.43
1:Y:302:LEU:HD23	1:Y:302:LEU:HA	1.33	0.43
1:Y:468:ARG:CG	1:Y:468:ARG:NH1	2.80	0.43
1:Y:489:ALA:O	1:Y:490:VAL:C	2.57	0.43
1:O:363:ALA:HB3	1:O:365:PHE:HE1	1.81	0.43
1:O:385:ALA:CB	1:O:422:GLN:NE2	2.79	0.43
1:O:443:ALA:O	1:O:444:ALA:O	2.35	0.43
1:Y:8:ALA:C	1:Y:9:LEU:HD22	2.39	0.43
1:Y:151:SER:O	1:Y:155:ALA:N	2.46	0.43
1:Y:439:THR:O	1:Y:440:ALA:C	2.56	0.43
1:O:33:ARG:NE	1:O:58:TRP:CB	2.80	0.43
1:O:84:GLU:OE1	1:O:103:TRP:HB3	2.19	0.43
1:O:182:ASP:HB3	1:O:242:ILE:HG21	1.99	0.43
1:Y:13:THR:N	3:Y:601:ACP:O2G	2.52	0.43
1:Y:343:TYR:HE2	1:Y:486:TRP:HB2	1.83	0.43
1:O:204:LEU:HD23	1:O:204:LEU:HA	1.48	0.43
1:O:251:PHE:CD1	1:O:256:VAL:HG21	2.54	0.43
1:Y:74:ILE:HD12	1:Y:76:ALA:N	2.33	0.43
1:Y:475:GLU:O	1:Y:478:GLU:HB2	2.19	0.43
1:O:171:TRP:NE1	1:O:176:GLY:HA2	2.33	0.43
1:O:409:ASP:CA	1:O:413:VAL:HG11	2.49	0.43
1:O:457:LEU:HD22	1:O:457:LEU:HA	1.39	0.43
1:O:460:LEU:O	1:O:462:GLU:N	2.52	0.43
1:Y:179:HIS:CD2	1:Y:215:PRO:CA	2.99	0.43
1:Y:286:LEU:HD21	1:Y:394:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:293:GLY:O	1:Y:295:THR:N	2.52	0.43
1:Y:433:PRO:O	1:Y:436:ARG:NH1	2.52	0.43
1:O:257:LYS:C	1:O:274:ASN:HD22	2.21	0.43
1:O:460:LEU:C	1:O:462:GLU:H	2.22	0.43
1:Y:35:PHE:HB2	1:Y:51:GLU:CG	2.47	0.43
1:Y:38:ILE:HG22	1:Y:40:PRO:HD3	2.01	0.43
1:Y:40:PRO:HD2	1:Y:44:TRP:C	2.38	0.43
1:Y:154:ARG:HA	1:Y:159:GLU:HB2	2.01	0.43
1:Y:179:HIS:CE1	1:Y:215:PRO:CG	3.02	0.43
1:Y:193:ASN:O	1:Y:197:LEU:N	2.52	0.43
1:Y:199:TRP:HZ2	1:Y:215:PRO:O	2.01	0.43
1:Y:251:PHE:C	1:Y:254:LEU:H	2.21	0.43
1:Y:482:ARG:O	1:Y:483:TYR:C	2.53	0.43
1:Y:45:VAL:O	1:Y:102:VAL:HG23	2.19	0.42
1:Y:153:GLU:H	1:Y:153:GLU:HG2	1.68	0.42
1:Y:203:MET:C	1:Y:206:VAL:HG12	2.40	0.42
1:Y:251:PHE:CD2	1:Y:446:LEU:HD12	2.54	0.42
1:Y:325:ASP:O	1:Y:328:ASP:N	2.51	0.42
1:Y:467:GLU:OE2	1:Y:468:ARG:HB2	2.18	0.42
1:Y:478:GLU:O	1:Y:481:TYR:HB3	2.19	0.42
1:O:144:ILE:O	1:O:147:HIS:HB2	2.19	0.42
1:O:228:ASN:HB2	1:O:236:ARG:CZ	2.49	0.42
1:O:276:GLY:O	1:O:300:TYR:N	2.52	0.42
1:O:477:THR:O	1:O:478:GLU:C	2.57	0.42
1:Y:130:LEU:CD1	1:Y:136:PHE:CD1	3.01	0.42
1:Y:174:THR:O	1:Y:175:GLN:C	2.55	0.42
1:Y:401:ILE:HG22	1:Y:402:ARG:N	2.34	0.42
1:O:86:THR:HG23	1:O:162:PHE:CE2	2.54	0.42
1:O:124:ILE:HG12	1:O:203:MET:HE1	2.00	0.42
1:O:154:ARG:H	1:O:154:ARG:HG2	1.34	0.42
1:O:415:ASN:ND2	1:O:418:LEU:HB2	2.33	0.42
1:Y:91:LYS:HZ2	1:Y:161:LEU:CD1	2.33	0.42
1:Y:229:ILE:HG23	1:Y:237:ILE:HD13	2.01	0.42
1:Y:421:PHE:O	1:Y:422:GLN:C	2.57	0.42
1:O:183:TYR:CD2	1:O:298:VAL:HG22	2.55	0.42
1:O:251:PHE:CE1	1:O:256:VAL:HG21	2.55	0.42
1:Y:372:ASN:OD1	1:Y:374:ASN:N	2.52	0.42
1:Y:415:ASN:HD22	1:Y:415:ASN:C	2.23	0.42
1:Y:479:ARG:HH11	1:Y:479:ARG:HG3	1.83	0.42
1:O:7:VAL:HG12	1:O:9:LEU:CD2	2.49	0.42
1:O:152:ARG:C	1:O:155:ALA:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:262:LYS:HA	1:O:407:ARG:O	2.19	0.42
1:O:487:LYS:O	1:O:491:LYS:HG3	2.20	0.42
1:Y:79:ILE:HD11	1:Y:239:ILE:CG2	2.49	0.42
1:Y:204:LEU:O	1:Y:209:ILE:N	2.39	0.42
1:Y:242:ILE:O	1:Y:243:ALA:HB2	2.19	0.42
1:O:286:LEU:HD11	1:O:395:MET:N	2.35	0.42
1:Y:28:ILE:HD12	1:Y:28:ILE:HA	1.79	0.42
1:Y:273:MET:HB2	1:Y:395:MET:CE	2.50	0.42
1:O:102:VAL:H	1:O:102:VAL:HG23	1.50	0.42
1:O:265:TYR:CE1	1:O:408:VAL:HG11	2.55	0.42
1:O:308:MET:HB2	1:O:346:PRO:HB2	2.00	0.42
1:Y:154:ARG:O	1:Y:155:ALA:O	2.38	0.42
1:Y:169:LEU:HA	1:Y:169:LEU:HD12	1.57	0.42
1:Y:280:VAL:HG12	1:Y:281:LYS:H	1.83	0.42
1:Y:368:THR:CG2	1:Y:369:ARG:N	2.82	0.42
1:O:40:PRO:HD2	1:O:44:TRP:C	2.40	0.42
1:O:70:SER:O	1:O:72:ASP:N	2.53	0.42
1:O:84:GLU:HG2	1:O:135:TYR:CE1	2.55	0.42
1:O:120:LEU:O	1:O:121:GLU:C	2.57	0.42
1:O:246:GLN:NE2	1:O:246:GLN:H	2.16	0.42
1:O:486:TRP:CD1	1:O:487:LYS:HG2	2.54	0.42
1:Y:67:ALA:CB	1:Y:69:ILE:CD1	2.98	0.42
1:Y:214:LEU:N	1:Y:214:LEU:HD12	2.33	0.42
1:Y:347:ALA:O	1:Y:362:GLY:N	2.52	0.42
1:O:87:ILE:HD11	1:O:165:VAL:N	2.34	0.42
1:O:101:ILE:HD13	1:O:107:ARG:CD	2.50	0.42
1:O:432:ARG:HA	1:O:433:PRO:HD2	1.84	0.42
1:O:445:TYR:O	1:O:447:ALA:N	2.53	0.42
1:O:457:LEU:HA	1:O:460:LEU:HD13	2.00	0.42
1:O:466:ILE:HD13	1:O:466:ILE:C	2.39	0.42
1:Y:81:ASN:ND2	1:Y:81:ASN:H	2.12	0.42
1:Y:95:LYS:HA	1:Y:96:PRO:HD3	1.92	0.42
1:Y:155:ALA:HB1	1:Y:210:PRO:HG2	2.01	0.42
1:O:13:THR:O	1:O:13:THR:HG22	2.19	0.42
1:O:50:MET:O	1:O:53:TRP:N	2.53	0.42
1:O:117:ARG:C	1:O:119:GLY:H	2.18	0.42
1:O:193:ASN:HB3	1:O:196:THR:HG22	1.95	0.42
1:O:338:ASN:OD1	1:O:340:ASN:N	2.43	0.42
1:Y:70:SER:O	1:Y:71:SER:C	2.59	0.42
1:Y:309:ALA:HA	1:Y:384:ILE:HD13	2.02	0.42
1:Y:320:MET:O	1:Y:321:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:109:ALA:O	1:O:112:CYS:HB2	2.20	0.42
1:O:114:HIS:CD2	1:O:117:ARG:HH22	2.38	0.42
1:O:422:GLN:HG3	1:O:426:LEU:HD23	2.00	0.42
1:Y:20:VAL:CG1	1:Y:21:MET:N	2.80	0.41
1:Y:154:ARG:H	1:Y:154:ARG:HG2	1.41	0.41
1:Y:355:TYR:O	1:Y:356:TRP:HB2	2.20	0.41
1:Y:364:ILE:N	1:Y:364:ILE:CD1	2.83	0.41
1:O:246:GLN:NE2	1:O:246:GLN:CA	2.80	0.41
1:O:378:ARG:O	1:O:379:ALA:C	2.57	0.41
1:Y:453:PHE:CE2	1:Y:454:TRP:CZ3	3.08	0.41
1:Y:482:ARG:NH1	1:Y:482:ARG:CG	2.80	0.41
1:O:3:LYS:HD2	1:O:72:ASP:O	2.20	0.41
1:O:154:ARG:HA	1:O:157:ARG:HG2	2.02	0.41
1:O:272:LEU:CD1	1:O:272:LEU:N	2.82	0.41
1:O:374:ASN:O	1:O:375:HIS:C	2.58	0.41
1:O:487:LYS:O	1:O:488:LYS:C	2.58	0.41
1:Y:3:LYS:HZ2	1:Y:75:ALA:HA	1.85	0.41
1:Y:128:THR:HB	1:Y:130:LEU:H	1.85	0.41
1:Y:180:VAL:HA	1:Y:216:GLU:O	2.20	0.41
1:Y:237:ILE:CG2	1:Y:238:PRO:N	2.80	0.41
1:O:82:GLN:OE1	1:O:102:VAL:HG13	2.21	0.41
1:O:207:LEU:HB3	1:O:209:ILE:HD12	1.99	0.41
1:Y:328:ASP:O	1:Y:332:PHE:HD2	2.03	0.41
1:Y:492:ARG:CG	1:Y:492:ARG:NH1	2.80	0.41
1:O:124:ILE:CD1	1:O:203:MET:CE	2.98	0.41
1:O:311:ALA:O	1:O:312:SER:C	2.59	0.41
1:O:406:LEU:HD22	1:O:407:ARG:N	2.35	0.41
1:Y:286:LEU:CD1	1:Y:394:ALA:HB1	2.47	0.41
1:Y:348:PHE:CD1	1:Y:362:GLY:HA3	2.55	0.41
1:O:86:THR:C	1:O:87:ILE:HG13	2.40	0.41
1:O:199:TRP:HZ2	1:O:215:PRO:O	2.02	0.41
1:O:245:ASP:OD1	1:O:246:GLN:N	2.54	0.41
1:O:251:PHE:CE2	1:O:446:LEU:HB2	2.55	0.41
1:O:489:ALA:O	1:O:490:VAL:C	2.59	0.41
1:Y:144:ILE:O	1:Y:147:HIS:N	2.53	0.41
1:Y:272:LEU:CD1	1:Y:303:GLU:HG3	2.50	0.41
1:Y:376:ILE:HD12	1:Y:376:ILE:HA	1.69	0.41
1:Y:449:LEU:HD13	1:Y:449:LEU:HA	1.55	0.41
1:O:44:TRP:CE3	1:O:107:ARG:CZ	3.04	0.41
1:O:183:TYR:HA	1:O:186:ALA:HB3	2.03	0.41
1:O:286:LEU:HD11	1:O:394:ALA:HB1	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:372:ASN:OD1	1:O:374:ASN:N	2.54	0.41
1:O:389:ARG:HB2	1:O:426:LEU:HD13	2.03	0.41
1:Y:250:LEU:CD1	1:Y:255:CYS:HB2	2.51	0.41
1:Y:251:PHE:O	1:Y:254:LEU:HD12	2.20	0.41
1:Y:466:ILE:HD13	1:Y:466:ILE:C	2.41	0.41
1:Y:488:LYS:HD3	1:O:496:TRP:CZ3	2.56	0.41
1:O:111:ILE:O	1:O:112:CYS:C	2.58	0.41
1:O:123:TYR:CE2	1:O:202:LYS:CB	3.04	0.41
1:O:343:TYR:CE1	1:O:486:TRP:HB2	2.55	0.41
1:O:410:GLY:O	1:O:413:VAL:HG22	2.20	0.41
1:Y:77:ILE:O	1:Y:239:ILE:HA	2.21	0.41
1:Y:142:LYS:HE3	1:Y:146:ASP:OD2	2.21	0.41
1:Y:256:VAL:CG1	1:Y:294:PRO:CG	2.99	0.41
1:O:296:GLY:N	1:O:297:GLU:OE1	2.53	0.41
1:O:347:ALA:O	1:O:348:PHE:C	2.58	0.41
1:Y:8:ALA:HB2	1:Y:21:MET:HE1	2.03	0.41
1:Y:83:ARG:N	4:Y:600:GOL:O2	2.53	0.41
1:Y:127:ASN:CB	1:Y:193:ASN:ND2	2.79	0.41
1:Y:154:ARG:HG3	1:Y:160:LEU:HD12	2.02	0.41
1:Y:154:ARG:CB	1:Y:159:GLU:CB	2.99	0.41
1:Y:183:TYR:CD1	1:Y:183:TYR:N	2.79	0.41
1:Y:183:TYR:CD1	1:Y:217:VAL:CG1	3.00	0.41
1:Y:188:ARG:HH21	1:Y:289:THR:CG2	2.33	0.41
1:Y:375:HIS:O	1:Y:376:ILE:C	2.57	0.41
1:Y:391:VAL:HG22	1:Y:392:LEU:N	2.35	0.41
1:Y:401:ILE:CG2	1:Y:402:ARG:N	2.84	0.41
1:Y:434:GLU:N	1:Y:465:VAL:O	2.54	0.41
1:Y:474:ILE:HA	1:Y:474:ILE:HD12	1.73	0.41
1:O:20:VAL:HG23	1:O:63:VAL:CG1	2.50	0.41
1:O:98:TYR:CD1	1:O:99:ASN:N	2.89	0.41
1:O:133:ASP:OD1	1:O:135:TYR:N	2.43	0.41
1:O:151:SER:HA	1:O:160:LEU:CD1	2.51	0.41
1:O:213:MET:HG2	1:O:214:LEU:CD1	2.49	0.41
1:O:255:CYS:SG	1:O:260:MET:HB3	2.61	0.41
1:O:270:PHE:CD1	1:O:270:PHE:N	2.89	0.41
1:O:394:ALA:O	1:O:398:ASP:N	2.41	0.41
1:Y:123:TYR:CD2	1:Y:203:MET:CE	3.00	0.41
1:Y:142:LYS:O	1:Y:144:ILE:N	2.54	0.41
1:Y:152:ARG:CB	1:Y:156:ARG:NH2	2.80	0.41
1:O:9:LEU:CD1	1:O:18:ALA:CB	2.99	0.41
1:O:168:TRP:O	1:O:172:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:254:LEU:O	1:O:256:VAL:N	2.54	0.41
1:O:348:PHE:CE1	1:O:362:GLY:HA3	2.56	0.41
1:O:372:ASN:O	1:O:373:ALA:C	2.59	0.41
1:O:405:ALA:HB1	1:O:431:GLU:CD	2.42	0.41
1:Y:91:LYS:HZ2	1:Y:161:LEU:HD11	1.86	0.40
1:Y:334:THR:HG23	1:Y:334:THR:H	1.49	0.40
1:Y:413:VAL:CA	1:Y:419:MET:HE3	2.49	0.40
1:O:257:LYS:H	1:O:260:MET:HG3	1.86	0.40
1:Y:166:ASP:O	1:Y:167:THR:C	2.58	0.40
1:Y:277:GLU:O	1:Y:300:TYR:HE2	2.04	0.40
1:O:222:GLU:HG3	1:O:223:VAL:N	2.36	0.40
1:O:344:VAL:O	1:O:346:PRO:HD3	2.20	0.40
1:Y:48:ASP:O	1:Y:52:ILE:N	2.41	0.40
1:Y:54:ALA:O	1:Y:57:SER:N	2.49	0.40
1:Y:124:ILE:CD1	1:Y:203:MET:CE	3.00	0.40
1:Y:295:THR:HG23	1:Y:297:GLU:CD	2.42	0.40
1:Y:316:LEU:HA	1:Y:316:LEU:HD23	1.27	0.40
1:Y:351:LEU:HD22	1:Y:360:ALA:CB	2.52	0.40
1:Y:439:THR:O	1:Y:442:GLY:N	2.55	0.40
1:O:38:ILE:HG22	1:O:40:PRO:N	2.36	0.40
1:O:115:LEU:O	1:O:120:LEU:HD12	2.22	0.40
1:Y:381:LEU:HD23	1:Y:381:LEU:HA	1.85	0.40
1:Y:422:GLN:NE2	1:Y:422:GLN:HA	2.37	0.40
1:Y:453:PHE:CD2	1:Y:454:TRP:CE3	3.07	0.40
1:O:41:LYS:CB	1:O:42:PRO:CD	2.99	0.40
1:O:181:THR:HG22	1:O:217:VAL:HG13	2.02	0.40
1:O:480:ASN:O	1:O:481:TYR:C	2.58	0.40
1:Y:71:SER:OG	1:Y:230:GLY:O	2.29	0.40
1:Y:121:GLU:O	1:Y:124:ILE:N	2.55	0.40
1:Y:162:PHE:O	1:Y:215:PRO:HD3	2.21	0.40
1:Y:251:PHE:O	1:Y:254:LEU:HA	2.22	0.40
1:Y:324:ASN:ND2	1:Y:324:ASN:H	2.19	0.40
1:Y:432:ARG:HG2	1:Y:436:ARG:NH1	2.37	0.40
1:O:44:TRP:CD2	1:O:107:ARG:HB2	2.56	0.40
1:O:228:ASN:HB2	1:O:236:ARG:NH2	2.37	0.40
1:O:336:VAL:HG11	1:O:375:HIS:CD2	2.56	0.40
1:O:347:ALA:HB2	1:O:351:LEU:HD13	2.03	0.40
1:O:389:ARG:HB2	1:O:426:LEU:CD1	2.50	0.40
1:O:422:GLN:HG3	1:O:426:LEU:CD2	2.51	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	O	490/501 (98%)	341 (70%)	102 (21%)	47 (10%)	0	3
1	Y	490/501 (98%)	354 (72%)	87 (18%)	49 (10%)	0	2
All	All	980/1002 (98%)	695 (71%)	189 (19%)	96 (10%)	0	2

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	58	TRP
1	Y	59	THR
1	Y	64	LEU
1	Y	151	SER
1	Y	165	VAL
1	Y	212	GLU
1	Y	213	MET
1	Y	445	TYR
1	Y	446	LEU
1	Y	456	ASN
1	O	66	LYS
1	O	165	VAL
1	O	187	SER
1	O	199	TRP
1	O	258	GLU
1	O	443	ALA
1	O	445	TYR
1	O	446	LEU
1	Y	53	TRP
1	Y	65	ALA
1	Y	92	GLU
1	Y	172	LYS
1	Y	187	SER
1	Y	188	ARG
1	Y	196	THR

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Mol	Chain	Res	Type
1	Y	202	LYS
1	Y	358	PRO
1	Y	439	THR
1	Y	461	GLN
1	Y	477	THR
1	O	64	LEU
1	O	71	SER
1	O	99	ASN
1	O	118	ASP
1	O	119	GLY
1	O	138	GLY
1	O	141	VAL
1	O	172	LYS
1	O	188	ARG
1	O	276	GLY
1	O	294	PRO
1	O	444	ALA
1	O	456	ASN
1	Y	54	ALA
1	Y	61	VAL
1	Y	121	GLU
1	Y	130	LEU
1	Y	138	GLY
1	Y	143	TRP
1	Y	153	GLU
1	Y	199	TRP
1	Y	441	LEU
1	Y	459	GLU
1	Y	478	GLU
1	Y	492	ARG
1	O	143	TRP
1	O	201	ASP
1	O	212	GLU
1	O	213	MET
1	O	390	ASP
1	O	442	GLY
1	O	461	GLN
1	Y	71	SER
1	Y	99	ASN
1	Y	147	HIS
1	Y	175	GLN
1	Y	418	LEU

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Mol	Chain	Res	Type
1	O	55	THR
1	O	140	LYS
1	O	151	SER
1	O	202	LYS
1	Y	110	GLU
1	Y	142	LYS
1	Y	145	LEU
1	Y	298	VAL
1	O	63	VAL
1	O	92	GLU
1	O	111	ILE
1	O	121	GLU
1	O	145	LEU
1	O	242	ILE
1	O	298	VAL
1	O	418	LEU
1	O	459	GLU
1	O	110	GLU
1	O	114	HIS
1	O	131	VAL
1	O	157	ARG
1	Y	27	ILE
1	Y	238	PRO
1	Y	346	PRO
1	Y	411	GLY
1	O	490	VAL
1	Y	170	ILE
1	Y	490	VAL
1	O	144	ILE

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	O	408/412 (99%)	258 (63%)	150 (37%)	0 0
1	Y	408/412 (99%)	259 (64%)	149 (36%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	816/824 (99%)	517 (63%)	299 (37%)	0 1

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	2	GLU
1	Y	3	LYS
1	Y	4	LYS
1	Y	11	GLN
1	Y	13	THR
1	Y	21	MET
1	Y	24	ASP
1	Y	28	ILE
1	Y	32	GLN
1	Y	33	ARG
1	Y	34	GLU
1	Y	41	LYS
1	Y	46	GLU
1	Y	53	TRP
1	Y	57	SER
1	Y	60	LEU
1	Y	62	GLU
1	Y	63	VAL
1	Y	64	LEU
1	Y	71	SER
1	Y	73	GLN
1	Y	74	ILE
1	Y	79	ILE
1	Y	80	THR
1	Y	81	ASN
1	Y	87	ILE
1	Y	91	LYS
1	Y	92	GLU
1	Y	93	THR
1	Y	95	LYS
1	Y	97	ILE
1	Y	106	ARG
1	Y	107	ARG
1	Y	116	LYS
1	Y	117	ARG
1	Y	118	ASP
1	Y	120	LEU

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Mol	Chain	Res	Type
1	Y	124	ILE
1	Y	128	THR
1	Y	130	LEU
1	Y	137	SER
1	Y	139	THR
1	Y	141	VAL
1	Y	142	LYS
1	Y	145	LEU
1	Y	146	ASP
1	Y	148	VAL
1	Y	149	GLU
1	Y	151	SER
1	Y	154	ARG
1	Y	156	ARG
1	Y	157	ARG
1	Y	162	PHE
1	Y	164	THR
1	Y	165	VAL
1	Y	169	LEU
1	Y	170	ILE
1	Y	172	LYS
1	Y	173	MET
1	Y	175	GLN
1	Y	178	VAL
1	Y	180	VAL
1	Y	181	THR
1	Y	187	SER
1	Y	191	LEU
1	Y	195	HIS
1	Y	196	THR
1	Y	205	GLU
1	Y	211	ARG
1	Y	213	MET
1	Y	218	ARG
1	Y	222	GLU
1	Y	227	THR
1	Y	228	ASN
1	Y	229	ILE
1	Y	235	THR
1	Y	236	ARG
1	Y	237	ILE
1	Y	239	ILE

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Mol	Chain	Res	Type
1	Y	240	SER
1	Y	242	ILE
1	Y	246	GLN
1	Y	253	GLN
1	Y	257	LYS
1	Y	260	MET
1	Y	262	LYS
1	Y	271	MET
1	Y	273	MET
1	Y	278	LYS
1	Y	281	LYS
1	Y	287	LEU
1	Y	290	ILE
1	Y	295	THR
1	Y	302	LEU
1	Y	312	SER
1	Y	314	GLN
1	Y	317	ARG
1	Y	324	ASN
1	Y	325	ASP
1	Y	335	LYS
1	Y	339	THR
1	Y	351	LEU
1	Y	364	ILE
1	Y	368	THR
1	Y	369	ARG
1	Y	376	ILE
1	Y	383	SER
1	Y	384	ILE
1	Y	389	ARG
1	Y	390	ASP
1	Y	391	VAL
1	Y	392	LEU
1	Y	402	ARG
1	Y	406	LEU
1	Y	407	ARG
1	Y	409	ASP
1	Y	415	ASN
1	Y	418	LEU
1	Y	423	SER
1	Y	425	ILE
1	Y	426	LEU

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Mol	Chain	Res	Type
1	Y	428	THR
1	Y	429	ARG
1	Y	431	GLU
1	Y	434	GLU
1	Y	436	ARG
1	Y	437	GLU
1	Y	438	VAL
1	Y	445	TYR
1	Y	446	LEU
1	Y	449	LEU
1	Y	451	VAL
1	Y	454	TRP
1	Y	455	GLN
1	Y	457	LEU
1	Y	461	GLN
1	Y	462	GLU
1	Y	463	LYS
1	Y	466	ILE
1	Y	467	GLU
1	Y	468	ARG
1	Y	469	GLU
1	Y	474	ILE
1	Y	479	ARG
1	Y	482	ARG
1	Y	483	TYR
1	Y	488	LYS
1	Y	492	ARG
1	Y	494	MET
1	O	3	LYS
1	O	4	LYS
1	O	5	TYR
1	O	9	LEU
1	O	11	GLN
1	O	21	MET
1	O	24	ASP
1	O	27	ILE
1	O	28	ILE
1	O	29	SER
1	O	31	SER
1	O	32	GLN
1	O	33	ARG
1	O	34	GLU

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Mol	Chain	Res	Type
1	O	41	LYS
1	O	51	GLU
1	O	52	ILE
1	O	57	SER
1	O	60	LEU
1	O	64	LEU
1	O	71	SER
1	O	72	ASP
1	O	73	GLN
1	O	74	ILE
1	O	80	THR
1	O	81	ASN
1	O	82	GLN
1	O	86	THR
1	O	87	ILE
1	O	91	LYS
1	O	92	GLU
1	O	93	THR
1	O	95	LYS
1	O	102	VAL
1	O	104	GLN
1	O	106	ARG
1	O	107	ARG
1	O	117	ARG
1	O	118	ASP
1	O	124	ILE
1	O	125	ARG
1	O	128	THR
1	O	131	VAL
1	O	135	TYR
1	O	136	PHE
1	O	137	SER
1	O	139	THR
1	O	141	VAL
1	O	142	LYS
1	O	145	LEU
1	O	147	HIS
1	O	149	GLU
1	O	153	GLU
1	O	154	ARG
1	O	156	ARG
1	O	157	ARG

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Mol	Chain	Res	Type
1	O	161	LEU
1	O	162	PHE
1	O	164	THR
1	O	165	VAL
1	O	169	LEU
1	O	170	ILE
1	O	172	LYS
1	O	173	MET
1	O	178	VAL
1	O	181	THR
1	O	182	ASP
1	O	188	ARG
1	O	191	LEU
1	O	195	HIS
1	O	196	THR
1	O	201	ASP
1	O	205	GLU
1	O	206	VAL
1	O	211	ARG
1	O	213	MET
1	O	214	LEU
1	O	218	ARG
1	O	219	ARG
1	O	222	GLU
1	O	227	THR
1	O	228	ASN
1	O	229	ILE
1	O	235	THR
1	O	236	ARG
1	O	237	ILE
1	O	239	ILE
1	O	240	SER
1	O	246	GLN
1	O	253	GLN
1	O	256	VAL
1	O	260	MET
1	O	262	LYS
1	O	269	CYS
1	O	271	MET
1	O	273	MET
1	O	278	LYS
1	O	280	VAL

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Mol	Chain	Res	Type
1	O	281	LYS
1	O	290	ILE
1	O	295	THR
1	O	316	LEU
1	O	317	ARG
1	O	322	LEU
1	O	324	ASN
1	O	325	ASP
1	O	335	LYS
1	O	339	THR
1	O	351	LEU
1	O	364	ILE
1	O	368	THR
1	O	369	ARG
1	O	378	ARG
1	O	383	SER
1	O	389	ARG
1	O	391	VAL
1	O	392	LEU
1	O	402	ARG
1	O	406	LEU
1	O	407	ARG
1	O	415	ASN
1	O	418	LEU
1	O	423	SER
1	O	426	LEU
1	O	428	THR
1	O	429	ARG
1	O	434	GLU
1	O	435	VAL
1	O	436	ARG
1	O	437	GLU
1	O	438	VAL
1	O	439	THR
1	O	451	VAL
1	O	455	GLN
1	O	456	ASN
1	O	457	LEU
1	O	460	LEU
1	O	461	GLN
1	O	462	GLU
1	O	463	LYS

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Mol	Chain	Res	Type
1	O	466	ILE
1	O	467	GLU
1	O	468	ARG
1	O	469	GLU
1	O	478	GLU
1	O	482	ARG
1	O	486	TRP
1	O	488	LYS
1	O	492	ARG
1	O	494	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	11	GLN
1	Y	23	HIS
1	Y	26	ASN
1	Y	32	GLN
1	Y	73	GLN
1	Y	81	ASN
1	Y	104	GLN
1	Y	114	HIS
1	Y	127	ASN
1	Y	147	HIS
1	Y	185	ASN
1	Y	228	ASN
1	Y	253	GLN
1	Y	274	ASN
1	Y	284	ASN
1	Y	299	ASN
1	Y	324	ASN
1	Y	337	GLN
1	Y	396	GLN
1	Y	415	ASN
1	Y	420	GLN
1	Y	422	GLN
1	Y	456	ASN
1	Y	461	GLN
1	O	11	GLN
1	O	23	HIS
1	O	26	ASN
1	O	37	GLN

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Mol	Chain	Res	Type
1	O	73	GLN
1	O	81	ASN
1	O	114	HIS
1	O	127	ASN
1	O	147	HIS
1	O	179	HIS
1	O	185	ASN
1	O	228	ASN
1	O	246	GLN
1	O	253	GLN
1	O	274	ASN
1	O	284	ASN
1	O	299	ASN
1	O	337	GLN
1	O	387	GLN
1	O	415	ASN
1	O	420	GLN
1	O	499	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	O	600	-	5,5,5	0.61	0	5,5,5	0.34	0
3	ACP	Y	601	2	27,33,33	2.36	5 (18%)	32,52,52	1.84	4 (12%)
3	ACP	O	601	2	27,33,33	2.90	6 (22%)	32,52,52	2.59	4 (12%)
4	GOL	Y	600	-	5,5,5	0.48	0	5,5,5	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	O	600	-	-	2/4/4/4	-
3	ACP	Y	601	2	-	4/15/38/38	0/3/3/3
3	ACP	O	601	2	-	0/15/38/38	0/3/3/3
4	GOL	Y	600	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	601	ACP	PG-O2G	9.45	1.76	1.54
3	O	601	ACP	PG-O3G	7.72	1.72	1.54
3	Y	601	ACP	PG-O3G	7.50	1.72	1.54
3	O	601	ACP	PG-O1G	6.28	1.63	1.50
3	Y	601	ACP	PG-O2G	5.53	1.67	1.54
3	Y	601	ACP	PB-O3A	5.17	1.64	1.58
3	Y	601	ACP	PG-O1G	4.50	1.59	1.50
3	O	601	ACP	PB-O3A	3.96	1.62	1.58
3	O	601	ACP	PB-O1B	2.38	1.57	1.51
3	O	601	ACP	C4-N3	-2.24	1.32	1.35
3	Y	601	ACP	C4-N3	-2.04	1.32	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	601	ACP	C1'-N9-C4	12.90	149.31	126.64
3	Y	601	ACP	C1'-N9-C4	7.24	139.36	126.64
3	Y	601	ACP	PA-O3A-PB	-3.59	121.17	132.56
3	O	601	ACP	C5-C6-N6	3.40	125.53	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	601	ACP	O1G-PG-C3B	-3.36	104.00	111.24
3	O	601	ACP	PA-O3A-PB	-3.25	122.25	132.56
3	Y	601	ACP	C5-C6-N6	2.82	124.64	120.35
3	O	601	ACP	O1G-PG-C3B	-2.52	105.80	111.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	601	ACP	C5'-O5'-PA-O1A
3	Y	601	ACP	C5'-O5'-PA-O3A
4	Y	600	GOL	C1-C2-C3-O3
4	Y	600	GOL	O2-C2-C3-O3
4	O	600	GOL	C1-C2-C3-O3
4	O	600	GOL	O2-C2-C3-O3
3	Y	601	ACP	C4'-C5'-O5'-PA
3	Y	601	ACP	PG-C3B-PB-O1B

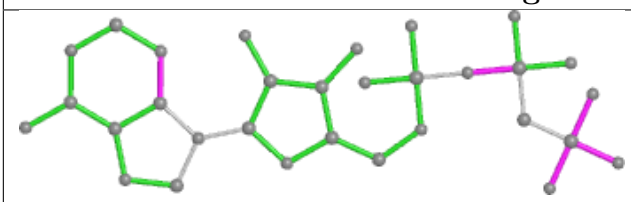
There are no ring outliers.

4 monomers are involved in 18 short contacts:

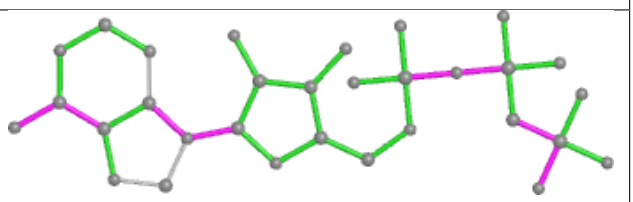
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	600	GOL	7	0
3	Y	601	ACP	5	0
3	O	601	ACP	4	0
4	Y	600	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

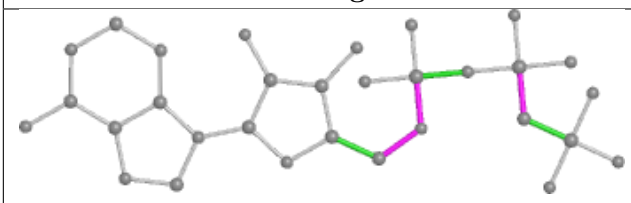
Ligand ACP Y 601



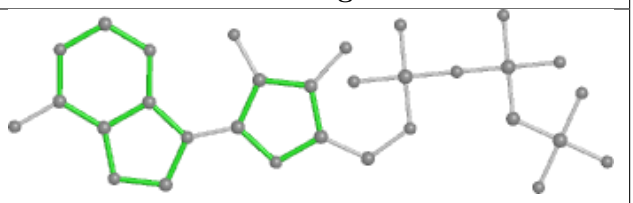
Bond lengths



Bond angles

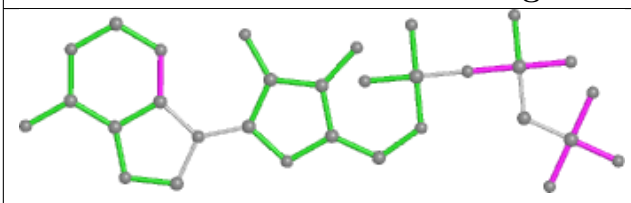


Torsions

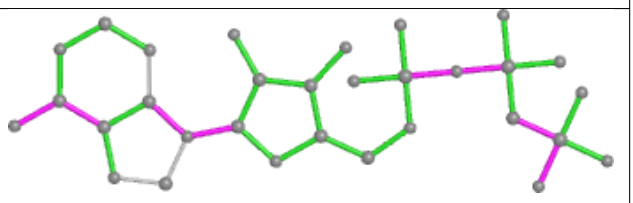


Rings

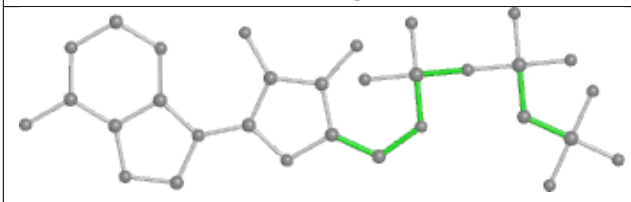
Ligand ACP O 601



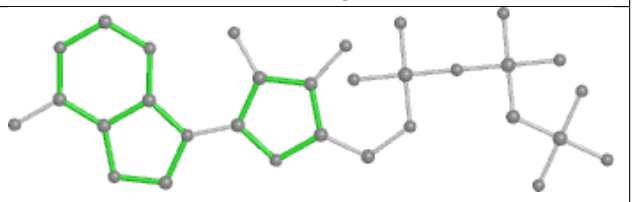
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	O	494/501 (98%)	-0.79	0	100	100	13, 61, 94, 100	0
1	Y	494/501 (98%)	-0.98	0	100	100	7, 48, 81, 98	0
All	All	988/1002 (98%)	-0.88	0	100	100	7, 54, 88, 100	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

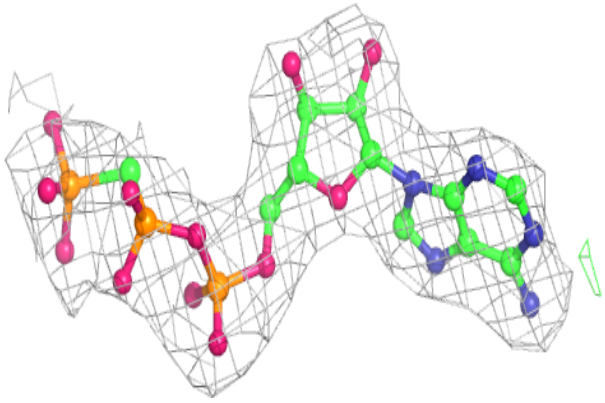
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

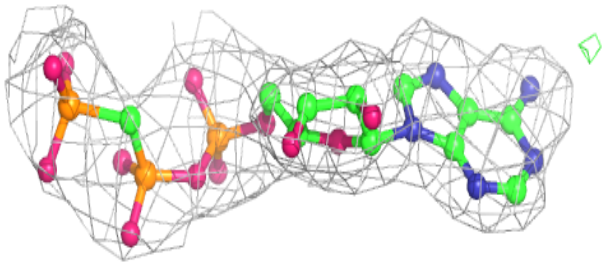
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	O	602	1/1	0.90	0.56	65,65,65,65	0
3	ACP	O	601	31/31	0.96	0.13	60,60,60,60	0
4	GOL	Y	600	6/6	0.96	0.13	32,32,32,32	0
3	ACP	Y	601	31/31	0.97	0.11	47,47,47,47	0
4	GOL	O	600	6/6	0.98	0.09	29,29,29,29	0
2	MG	Y	602	1/1	0.99	0.20	40,40,40,40	0

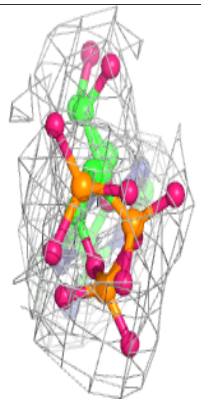
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ACP O 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

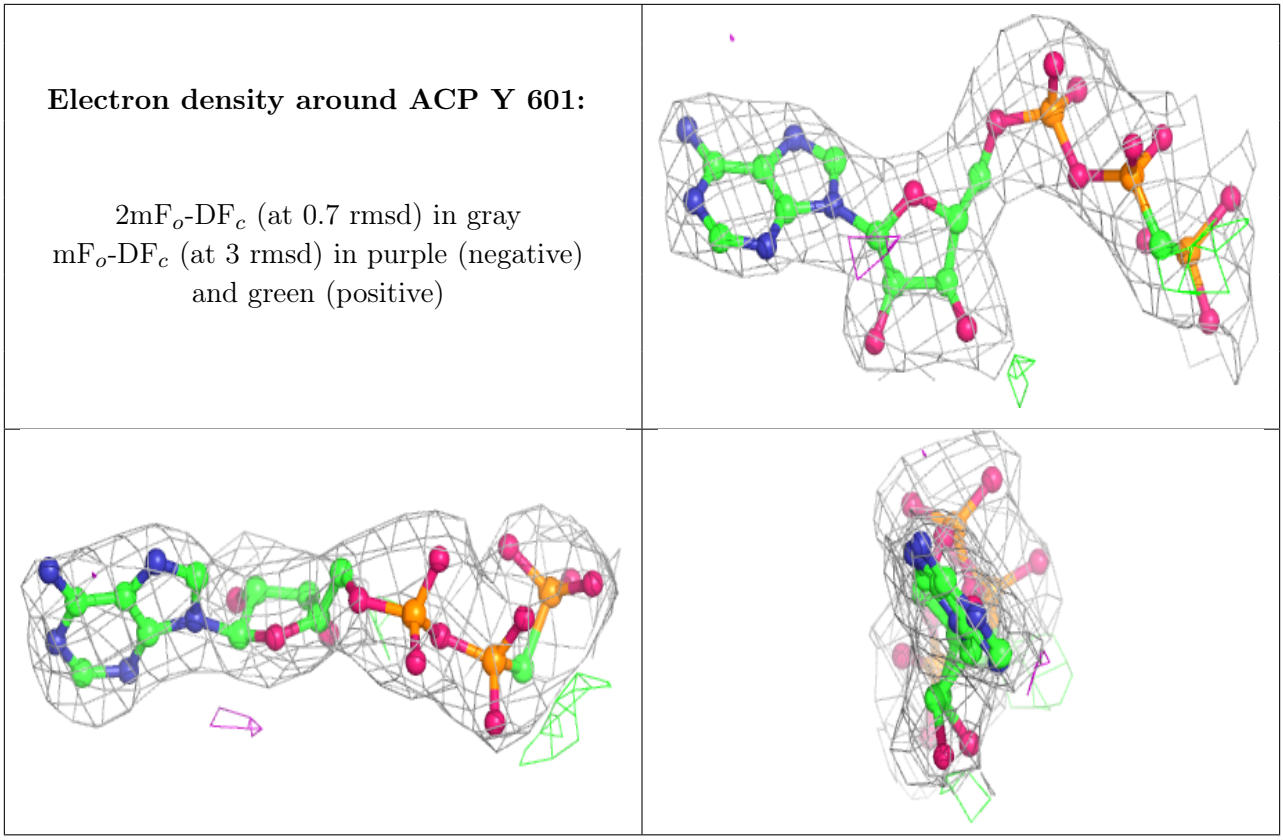






Electron density around ACP Y 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.