Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:16 PM GMT

PDB ID	:	1JKI
Title	:	myo-Inositol-1-phosphate Synthase Complexed with an Inhibitor, 2-deoxy-glucitol-6-phosphate
Authors	:	Stein, A.J.; Geiger, J.H.
Deposited on	:	2001-07-12
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

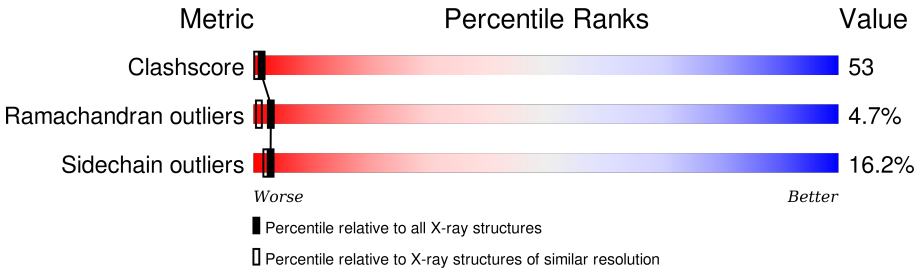
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	34% 43% 17% 5%
1	B	533	28% 41% 23% 7%

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
3	DG6	A	630	X	-	X	-
3	DG6	B	640	X	-	X	-

2 Entry composition (i)

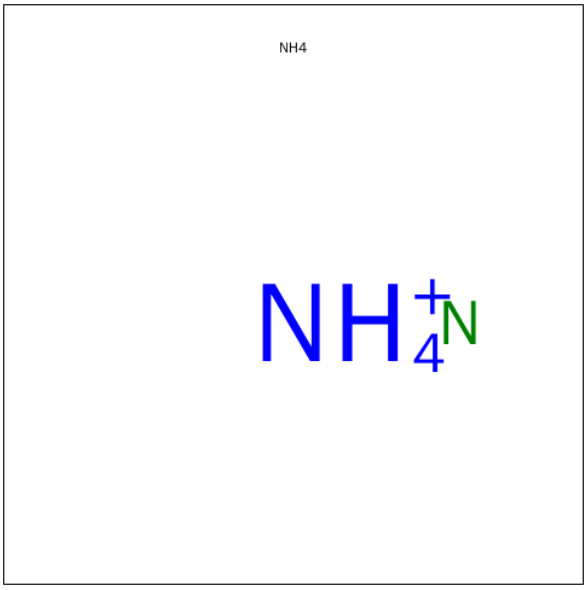
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 myo-inositol-1-phosphate synthase.

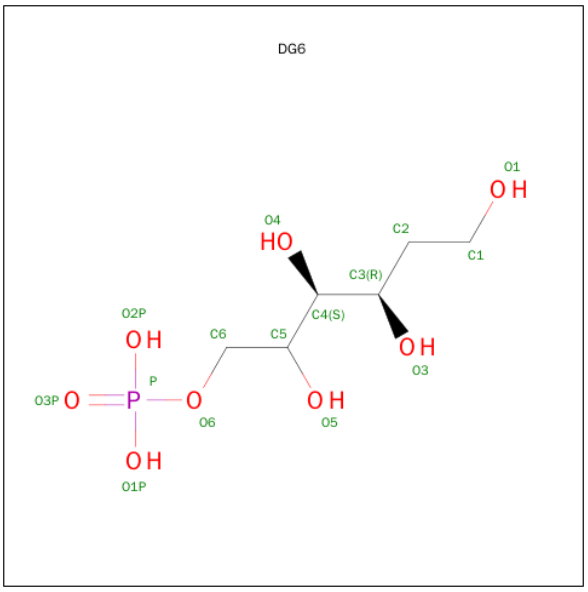
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	524	Total	C	N	O	S	0	0	0
			4130	2626	694	794	16			

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



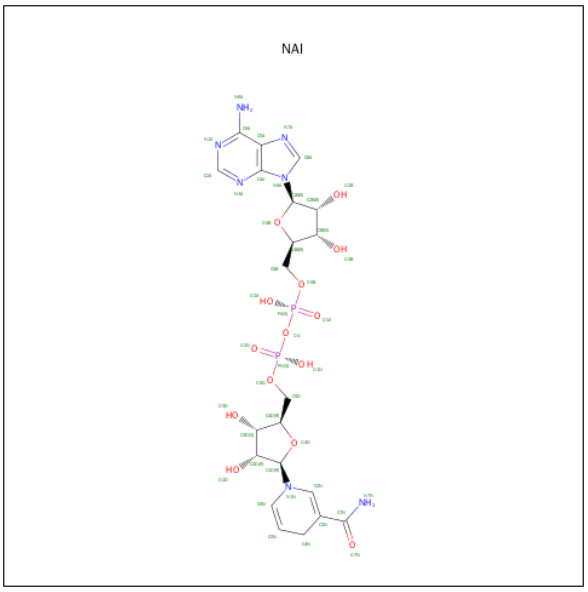
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (three-letter code: DG6) (formula: $C_6H_{15}O_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	315	Total	O	0	0
			315	315		

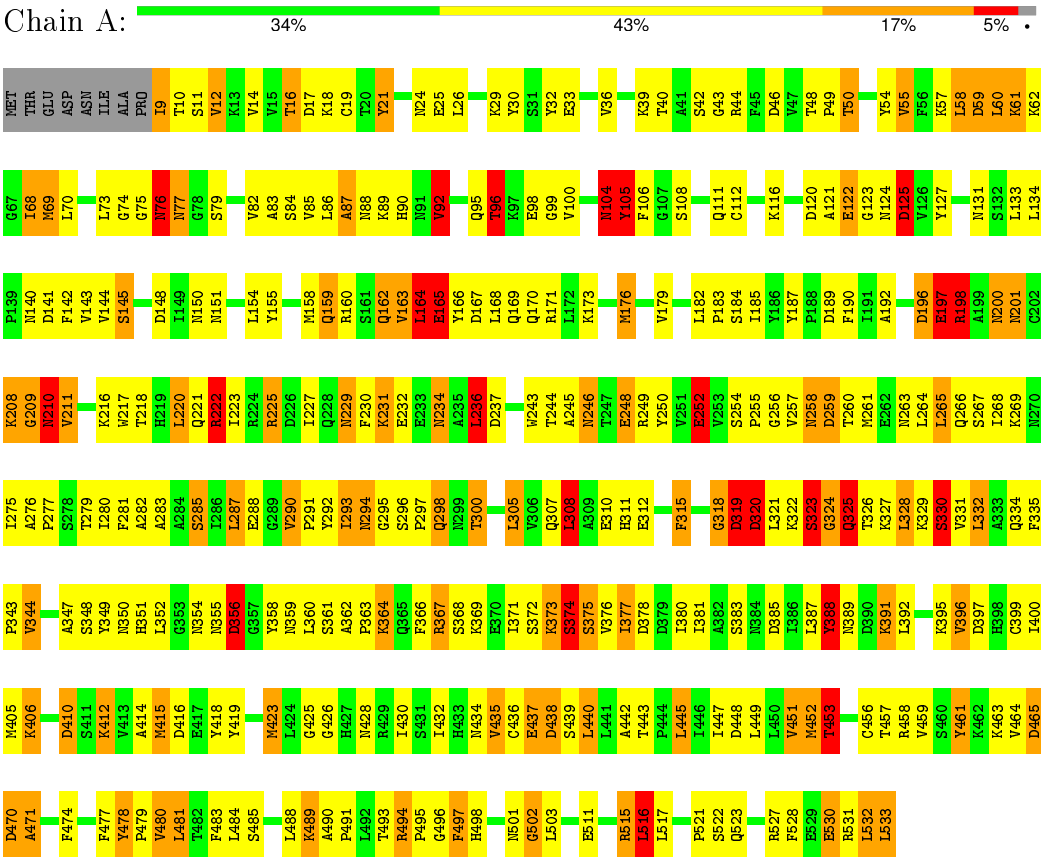
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

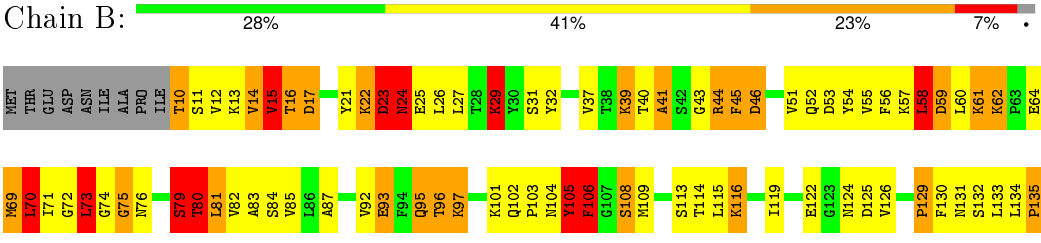
- Molecule 1: myo-inositol-1-phosphate synthase

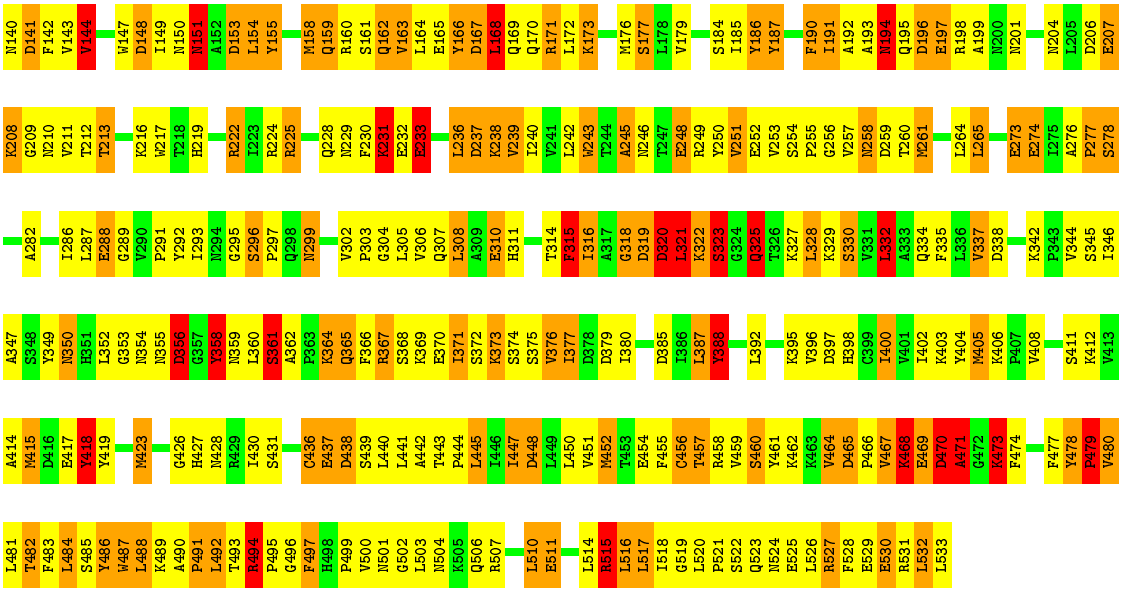
Chain A:



- Molecule 1: myo-inositol-1-phosphate synthase

Chain B:




N140 D141 F142 V143 V144 W147 D148 I149 N150 N151 A152 D153 L154 Y155 M158 Q159 R160 S161 Q162 V163 L164 E165 Y166 D167 L168 Q169 Q170 R171 L172 K173 M176 S177 L178 V179 S184 I185 Y186 Y187 F190 I191 A192 A193 N194 Q195 D196 E197 R198 A199 N200 N201 N204 L205 D206 E207
K208 G209 N210 V211 T212 T213 K216 W217 T218 H219 R222 I223 R224 R225 Q228 N229 F230 K231 E232 E233 L236 D237 K238 V239 I240 V241 L242 W243 T244 A245 N246 T247 E248 R249 Y250 V251 E252 V253 S254 P255 G256 V257 N258 D259 T260 M261 L264 L265 E273 E274 I275 A276 P277 S278
A282 I286 L287 E288 G289 V290 P291 Y292 I293 N294 G295 S296 P297 Q298 N299 V302 P303 G304 L305 V306 Q307 L308 A309 E310 H311 T314 F315 I316 A317 G318 D319 D320 L321 K322 S323 G324 Q325 T326 K327 L328 K329 S330 V331 L332 A333 Q334 F335 L336 V337 D338 K342 P343 V344 S345 I346
A347 S348 Y349 N350 H351 L352 G353 N354 N355 D356 G357 K358 N359 L360 S361 A362 P363 K364 Q365 F366 R367 S368 K369 E370 I371 S372 K373 S374 S375 V376 I377 D378 D379 I380 D385 I386 I387 Y388 I392 K395 V396 D397 H398 C399 I400 V401 I402 K403 Y404 M405 K406 P407 V408 S411 K412 V413
A414 M415 D416 E417 V418 Y419 M423 G426 H427 N428 R429 I430 S431 C436 E437 D438 S439 L440 L441 A442 T443 P444 L445 I446 I447 D448 L449 L450 V451 M452 T453 E454 F455 C456 T457 R458 V459 S460 Y461 K462 K463 V464 D465 P466 V467 K468 E469 D470 A471 G472 K473 F474 F477 Y478 P479 V480
L481 T482 F483 L484 S485 Y486 W487 L488 K489 A490 P491 L492 T493 R494 P495 G496 F497 H498 P499 V500 N501 G502 L503 N504 K505 Q506 R507 L510 E511 L514 R515 L516 L517 I518 G519 L520 P521 S522 Q523 N524 E525 L526 R527 F528 E529 E530 R531 L532 L533

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.73Å 98.31Å 121.86Å 90.00° 126.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.6 (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, NAI, DG6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.87	91/4219 (2.2%)	1.52	58/5719 (1.0%)
1	B	1.95	97/4211 (2.3%)	1.69	81/5708 (1.4%)
All	All	1.91	188/8430 (2.2%)	1.61	139/11427 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	7
All	All	0	12

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	MET	CB-CG	9.86	1.82	1.51
1	A	165	GLU	CB-CG	9.64	1.70	1.52
1	A	32	TYR	CE1-CZ	8.97	1.50	1.38
1	A	356	ASP	CB-CG	8.89	1.70	1.51
1	A	388	TYR	CE1-CZ	8.76	1.50	1.38
1	A	54	TYR	CG-CD2	-8.69	1.27	1.39
1	B	356	ASP	CB-CG	8.58	1.69	1.51
1	A	77	ASN	CB-CG	8.48	1.70	1.51
1	B	437	GLU	CB-CG	-8.37	1.36	1.52
1	A	459	VAL	CA-CB	8.27	1.72	1.54
1	A	136	MET	CG-SD	8.05	2.02	1.81
1	B	75	GLY	CA-C	-8.05	1.39	1.51
1	A	315	PHE	CB-CG	-8.04	1.37	1.51
1	B	84	SER	CB-OG	7.97	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ILE	CA-CB	-7.91	1.36	1.54
1	A	456	CYS	CB-SG	7.76	1.95	1.82
1	B	144	VAL	CB-CG1	-7.74	1.36	1.52
1	B	166	TYR	CB-CG	7.66	1.63	1.51
1	B	155	TYR	CE1-CZ	7.53	1.48	1.38
1	A	145	SER	N-CA	-7.47	1.31	1.46
1	B	344	VAL	CB-CG1	7.26	1.68	1.52
1	B	113	SER	CB-OG	-7.25	1.32	1.42
1	B	451	VAL	CA-CB	-7.11	1.39	1.54
1	B	105	TYR	CD1-CE1	7.07	1.50	1.39
1	B	456	CYS	CB-SG	7.07	1.94	1.82
1	A	163	VAL	CB-CG2	-7.03	1.38	1.52
1	B	155	TYR	CG-CD2	7.01	1.48	1.39
1	B	158	MET	SD-CE	7.00	2.17	1.77
1	B	69	MET	CG-SD	-6.97	1.63	1.81
1	B	238	LYS	CD-CE	6.93	1.68	1.51
1	B	15	VAL	CB-CG2	-6.93	1.38	1.52
1	A	84	SER	CA-CB	6.92	1.63	1.52
1	B	231	LYS	CD-CE	6.85	1.68	1.51
1	B	81	LEU	N-CA	6.85	1.60	1.46
1	B	423	MET	SD-CE	-6.81	1.39	1.77
1	A	85	VAL	CB-CG2	6.80	1.67	1.52
1	A	79	SER	CA-CB	6.77	1.63	1.52
1	A	229	ASN	N-CA	6.72	1.59	1.46
1	B	293	ILE	CA-CB	-6.63	1.39	1.54
1	A	143	VAL	CA-CB	6.57	1.68	1.54
1	A	197	GLU	CG-CD	6.57	1.61	1.51
1	B	80	THR	CA-CB	6.55	1.70	1.53
1	B	515	ARG	CG-CD	6.55	1.68	1.51
1	A	158	MET	CG-SD	-6.54	1.64	1.81
1	A	104	ASN	CB-CG	6.53	1.66	1.51
1	B	105	TYR	CE1-CZ	-6.53	1.30	1.38
1	A	87	ALA	CA-CB	6.51	1.66	1.52
1	B	85	VAL	CB-CG2	6.50	1.66	1.52
1	A	197	GLU	CD-OE1	6.49	1.32	1.25
1	B	464	VAL	CB-CG2	-6.49	1.39	1.52
1	A	274	GLU	CG-CD	6.48	1.61	1.51
1	A	108	SER	CA-CB	6.45	1.62	1.52
1	B	138	SER	CA-CB	-6.45	1.43	1.52
1	B	239	VAL	CB-CG2	6.44	1.66	1.52
1	B	116	LYS	CE-NZ	6.43	1.65	1.49
1	A	69	MET	SD-CE	6.43	2.13	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	TYR	CD1-CE1	-6.43	1.29	1.39
1	A	292	TYR	CG-CD1	6.41	1.47	1.39
1	B	530	GLU	CG-CD	6.36	1.61	1.51
1	A	83	ALA	CA-CB	6.36	1.65	1.52
1	B	105	TYR	CE2-CZ	6.35	1.46	1.38
1	A	54	TYR	CB-CG	-6.35	1.42	1.51
1	B	228	GLN	N-CA	6.31	1.58	1.46
1	B	135	PRO	CG-CD	6.31	1.71	1.50
1	B	415	MET	CG-SD	6.31	1.97	1.81
1	A	511	GLU	CD-OE2	6.31	1.32	1.25
1	A	68	ILE	CB-CG2	6.30	1.72	1.52
1	A	437	GLU	CG-CD	6.30	1.61	1.51
1	A	105	TYR	CD2-CE2	6.28	1.48	1.39
1	A	227	ILE	CA-CB	6.26	1.69	1.54
1	A	75	GLY	CA-C	-6.25	1.41	1.51
1	B	460	SER	CA-CB	6.24	1.62	1.52
1	A	105	TYR	CB-CG	6.22	1.60	1.51
1	A	144	VAL	CB-CG1	6.22	1.66	1.52
1	B	418	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	347	ALA	CA-CB	6.19	1.65	1.52
1	A	248	GLU	CG-CD	6.16	1.61	1.51
1	B	358	TYR	CE1-CZ	6.15	1.46	1.38
1	B	14	VAL	CA-CB	6.14	1.67	1.54
1	B	39	LYS	CE-NZ	6.13	1.64	1.49
1	A	64	GLU	CG-CD	6.11	1.61	1.51
1	B	245	ALA	N-CA	-6.11	1.34	1.46
1	A	293	ILE	C-O	6.09	1.34	1.23
1	B	525	GLU	CD-OE2	6.07	1.32	1.25
1	A	30	TYR	CG-CD2	-6.07	1.31	1.39
1	A	166	TYR	CD2-CE2	6.05	1.48	1.39
1	A	453	THR	CB-CG2	-6.04	1.32	1.52
1	B	358	TYR	CG-CD1	6.03	1.47	1.39
1	A	244	THR	CA-CB	-6.02	1.37	1.53
1	B	83	ALA	CA-CB	6.02	1.65	1.52
1	A	137	VAL	CB-CG1	-6.01	1.40	1.52
1	A	69	MET	CB-CG	5.99	1.70	1.51
1	A	418	TYR	CD2-CE2	5.97	1.48	1.39
1	A	232	GLU	CG-CD	5.95	1.60	1.51
1	B	106	PHE	CB-CG	-5.93	1.41	1.51
1	B	141	ASP	CA-C	-5.91	1.37	1.52
1	A	12	VAL	CA-CB	5.88	1.67	1.54
1	A	448	ASP	CB-CG	-5.86	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ALA	C-O	-5.84	1.12	1.23
1	A	29	LYS	CD-CE	5.82	1.65	1.51
1	A	451	VAL	N-CA	-5.82	1.34	1.46
1	B	108	SER	CA-CB	5.81	1.61	1.52
1	A	344	VAL	CA-CB	5.77	1.66	1.54
1	B	217	TRP	CB-CG	5.75	1.60	1.50
1	B	527	ARG	CG-CD	5.75	1.66	1.51
1	B	79	SER	CA-CB	5.74	1.61	1.52
1	B	151	ASN	CA-C	-5.71	1.38	1.52
1	B	141	ASP	CG-OD2	5.70	1.38	1.25
1	A	414	ALA	CA-CB	5.70	1.64	1.52
1	B	136	MET	SD-CE	-5.70	1.46	1.77
1	B	315	PHE	CB-CG	-5.69	1.41	1.51
1	A	55	VAL	CB-CG1	5.68	1.64	1.52
1	B	310	GLU	CG-CD	5.67	1.60	1.51
1	B	436	CYS	CB-SG	-5.67	1.72	1.81
1	B	288	GLU	CG-CD	5.67	1.60	1.51
1	B	166	TYR	C-O	-5.66	1.12	1.23
1	A	290	VAL	CB-CG2	-5.65	1.41	1.52
1	A	288	GLU	CD-OE2	5.63	1.31	1.25
1	B	405	MET	CG-SD	5.59	1.95	1.81
1	A	252	GLU	CG-CD	5.58	1.60	1.51
1	B	230	PHE	CG-CD1	-5.58	1.30	1.38
1	A	415	MET	SD-CE	5.55	2.08	1.77
1	B	419	TYR	CD1-CE1	5.54	1.47	1.39
1	A	111	GLN	CA-C	-5.54	1.38	1.52
1	B	69	MET	SD-CE	5.52	2.08	1.77
1	B	246	ASN	CG-ND2	5.50	1.46	1.32
1	B	507	ARG	CZ-NH2	5.50	1.40	1.33
1	A	159	GLN	CG-CD	5.46	1.63	1.51
1	B	148	ASP	CB-CG	5.45	1.63	1.51
1	A	105	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	231	LYS	CD-CE	5.45	1.64	1.51
1	B	337	VAL	CA-CB	-5.44	1.43	1.54
1	A	423	MET	SD-CE	-5.44	1.47	1.77
1	B	159	GLN	CG-CD	5.43	1.63	1.51
1	A	252	GLU	CB-CG	5.43	1.62	1.52
1	B	243	TRP	CG-CD1	5.38	1.44	1.36
1	B	232	GLU	CD-OE2	5.38	1.31	1.25
1	B	93	GLU	CG-CD	-5.38	1.43	1.51
1	B	160	ARG	N-CA	-5.37	1.35	1.46
1	A	425	GLY	C-O	-5.35	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	GLU	CG-CD	5.35	1.59	1.51
1	B	288	GLU	CD-OE2	5.34	1.31	1.25
1	A	234	ASN	CG-OD1	-5.34	1.12	1.24
1	A	405	MET	CG-SD	5.33	1.95	1.81
1	A	530	GLU	CG-CD	5.32	1.59	1.51
1	B	45	PHE	CE1-CZ	5.30	1.47	1.37
1	B	511	GLU	CB-CG	-5.29	1.42	1.52
1	A	112	CYS	CB-SG	5.28	1.91	1.82
1	B	194	ASN	CB-CG	5.27	1.63	1.51
1	B	161	SER	CB-OG	5.26	1.49	1.42
1	A	330	SER	CB-OG	5.25	1.49	1.42
1	B	274	GLU	CG-CD	5.25	1.59	1.51
1	A	76	ASN	CB-CG	5.24	1.63	1.51
1	B	388	TYR	CE1-CZ	5.24	1.45	1.38
1	B	72	GLY	C-O	5.24	1.32	1.23
1	A	293	ILE	CA-CB	-5.22	1.42	1.54
1	A	366	PHE	CE1-CZ	5.22	1.47	1.37
1	A	168	LEU	CA-C	-5.21	1.39	1.52
1	B	96	THR	CA-CB	5.21	1.66	1.53
1	B	126	VAL	CB-CG2	5.20	1.63	1.52
1	A	127	TYR	CB-CG	-5.20	1.43	1.51
1	B	442	ALA	N-CA	-5.19	1.35	1.46
1	B	158	MET	CG-SD	-5.18	1.67	1.81
1	A	325	GLN	CG-CD	5.17	1.62	1.51
1	A	19	CYS	CB-SG	5.16	1.91	1.82
1	B	464	VAL	CA-CB	-5.15	1.44	1.54
1	A	435	VAL	CB-CG2	5.15	1.63	1.52
1	A	158	MET	CB-CG	-5.14	1.34	1.51
1	B	143	VAL	CA-CB	5.14	1.65	1.54
1	B	29	LYS	CE-NZ	5.12	1.61	1.49
1	A	54	TYR	CE1-CZ	-5.12	1.31	1.38
1	B	248	GLU	CD-OE2	5.12	1.31	1.25
1	A	61	LYS	CE-NZ	5.12	1.61	1.49
1	B	515	ARG	CZ-NH2	5.11	1.39	1.33
1	A	438	ASP	N-CA	-5.09	1.36	1.46
1	B	478	TYR	CA-C	5.09	1.66	1.52
1	A	95	GLN	CG-CD	-5.09	1.39	1.51
1	A	111	GLN	CG-CD	5.09	1.62	1.51
1	A	471	ALA	CA-CB	5.08	1.63	1.52
1	B	487	TRP	CG-CD1	5.08	1.43	1.36
1	A	69	MET	CG-SD	-5.07	1.68	1.81
1	B	377	ILE	CA-CB	5.06	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	PHE	CE2-CZ	5.06	1.47	1.37
1	A	451	VAL	CA-CB	-5.04	1.44	1.54
1	B	155	TYR	CD2-CE2	5.03	1.46	1.39
1	A	376	VAL	CA-CB	-5.03	1.44	1.54
1	A	325	GLN	CB-CG	5.02	1.66	1.52
1	B	358	TYR	CE2-CZ	5.00	1.45	1.38

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	222	ARG	NE-CZ-NH2	-21.35	109.62	120.30
1	B	222	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	B	321	LEU	CB-CG-CD2	-13.96	87.26	111.00
1	A	423	MET	CG-SD-CE	13.56	121.90	100.20
1	B	153	ASP	CB-CG-OD2	11.97	129.07	118.30
1	B	438	ASP	CB-CG-OD2	-11.48	107.97	118.30
1	A	171	ARG	NE-CZ-NH2	11.17	125.89	120.30
1	B	507	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	B	338	ASP	CB-CG-OD1	-10.04	109.27	118.30
1	A	236	LEU	CA-CB-CG	10.01	138.32	115.30
1	B	224	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	B	321	LEU	CB-CG-CD1	9.61	127.34	111.00
1	A	494	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	198	ARG	N-CA-C	-9.18	86.22	111.00
1	B	338	ASP	CB-CG-OD2	8.78	126.20	118.30
1	B	167	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	171	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	B	526	LEU	C-N-CA	-8.62	100.15	121.70
1	B	59	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	B	158	MET	CA-CB-CG	8.52	127.79	113.30
1	B	44	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	261	MET	CG-SD-CE	8.15	113.25	100.20
1	A	356	ASP	N-CA-CB	-8.13	95.97	110.60
1	B	59	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	158	MET	CG-SD-CE	-8.09	87.26	100.20
1	B	502	GLY	N-CA-C	-8.02	93.05	113.10
1	B	320	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	B	321	LEU	CA-CB-CG	8.00	133.70	115.30
1	A	209	GLY	N-CA-C	-7.95	93.22	113.10
1	A	318	GLY	C-N-CA	7.95	141.58	121.70
1	A	125	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	B	430	ILE	CG1-CB-CG2	-7.73	94.40	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	158	MET	CG-SD-CE	-7.70	87.88	100.20
1	B	448	ASP	CB-CG-OD1	7.67	125.21	118.30
1	B	81	LEU	CA-CB-CG	-7.62	97.76	115.30
1	A	356	ASP	CB-CG-OD1	7.53	125.07	118.30
1	B	323	SER	N-CA-C	-7.52	90.69	111.00
1	B	73	LEU	CB-CG-CD2	7.47	123.70	111.00
1	B	136	MET	CG-SD-CE	-7.46	88.26	100.20
1	B	318	GLY	N-CA-C	7.08	130.81	113.10
1	B	167	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	171	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	516	LEU	CA-CB-CG	6.99	131.37	115.30
1	B	473	LYS	N-CA-C	6.99	129.87	111.00
1	B	516	LEU	CA-CB-CG	6.94	131.27	115.30
1	B	471	ALA	N-CA-C	-6.87	92.44	111.00
1	A	59	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	A	237	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	164	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	470	ASP	N-CA-C	6.71	129.12	111.00
1	B	445	LEU	CB-CG-CD1	-6.69	99.62	111.00
1	B	315	PHE	CB-CA-C	-6.60	97.20	110.40
1	B	323	SER	N-CA-CB	-6.60	100.60	110.50
1	A	92	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	B	459	VAL	CB-CA-C	-6.54	98.97	111.40
1	B	438	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	58	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	17	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	B	325	GLN	N-CA-C	-6.45	93.59	111.00
1	A	141	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	410	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	158	MET	CA-CB-CG	6.38	124.16	113.30
1	A	320	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	356	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	96	THR	OG1-CB-CG2	6.28	124.45	110.00
1	A	448	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	167	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	210	ASN	N-CA-C	6.23	127.83	111.00
1	B	97	LYS	CD-CE-NZ	-6.21	97.41	111.70
1	B	208	LYS	N-CA-C	-6.19	94.29	111.00
1	B	158	MET	N-CA-CB	6.17	121.70	110.60
1	B	46	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	225	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	332	LEU	CA-CB-CG	-6.14	101.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	GLY	N-CA-C	-6.11	97.81	113.10
1	A	60	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	163	VAL	CG1-CB-CG2	6.04	120.57	110.90
1	B	176	MET	CG-SD-CE	6.02	109.83	100.20
1	A	515	ARG	CG-CD-NE	-6.02	99.16	111.80
1	A	143	VAL	N-CA-C	-6.01	94.77	111.00
1	B	222	ARG	CG-CD-NE	-6.00	99.19	111.80
1	B	526	LEU	O-C-N	-6.00	113.09	122.70
1	B	318	GLY	C-N-CA	6.00	136.70	121.70
1	B	448	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	452	MET	CG-SD-CE	5.98	109.77	100.20
1	B	168	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	70	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	153	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	173	LYS	CD-CE-NZ	-5.89	98.16	111.70
1	A	96	THR	N-CA-CB	-5.88	99.13	110.30
1	B	527	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	465	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	379	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	379	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	62	LYS	CD-CE-NZ	5.84	125.12	111.70
1	B	222	ARG	CD-NE-CZ	5.78	131.70	123.60
1	A	318	GLY	CA-C-N	-5.78	104.48	117.20
1	A	59	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	305	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	251	VAL	N-CA-C	-5.70	95.61	111.00
1	B	308	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	46	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	196	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	308	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	323	SER	N-CA-C	5.56	126.01	111.00
1	A	419	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	A	136	MET	CG-SD-CE	-5.55	91.32	100.20
1	B	44	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	435	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	A	452	MET	CB-CG-SD	5.37	128.51	112.40
1	A	17	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	396	VAL	N-CA-C	-5.35	96.55	111.00
1	B	356	ASP	N-CA-CB	-5.33	101.00	110.60
1	A	410	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	B	356	ASP	OD1-CG-OD2	-5.30	113.23	123.30
1	B	133	LEU	CA-CB-CG	5.30	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	B	73	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	137	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	344	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	A	220	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	437	GLU	C-N-CA	-5.18	108.74	121.70
1	A	138	SER	CA-CB-OG	-5.16	97.27	111.20
1	A	182	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	430	ILE	C-N-CA	-5.16	108.81	121.70
1	A	145	SER	CB-CA-C	5.13	119.84	110.10
1	B	24	ASN	N-CA-C	-5.13	97.16	111.00
1	A	222	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	395	LYS	CD-CE-NZ	5.11	123.45	111.70
1	B	494	ARG	N-CA-C	-5.09	97.25	111.00
1	B	296	SER	CB-CA-C	-5.09	100.44	110.10
1	B	23	ASP	C-N-CA	5.08	134.41	121.70
1	B	418	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	187	TYR	N-CA-C	-5.06	97.33	111.00
1	A	452	MET	CG-SD-CE	-5.06	92.11	100.20
1	B	445	LEU	CB-CG-CD2	5.06	119.59	111.00
1	A	439	SER	CA-CB-OG	-5.04	97.58	111.20
1	B	172	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	434	ASN	C-N-CA	-5.03	109.11	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	388	TYR	Sidechain
1	A	461	TYR	Sidechain
1	A	478	TYR	Sidechain
1	B	105	TYR	Sidechain
1	B	186	TYR	Sidechain
1	B	358	TYR	Sidechain
1	B	388	TYR	Sidechain
1	B	418	TYR	Sidechain
1	B	486	TYR	Sidechain
1	B	56	PHE	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4147	420	1
1	B	4130	0	4136	505	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
3	A	15	0	12	10	0
3	B	15	0	12	17	0
4	A	44	0	22	8	0
4	B	44	0	24	3	0
5	A	303	0	0	55	0
5	B	315	0	0	63	0
All	All	9006	0	8353	891	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (891) 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:B:69:MET:CB	1:B:69:MET:CG	1.82	1.54
1:A:136:MET:SD	1:A:136:MET:CG	2.02	1.46
1:B:69:MET:CE	1:B:69:MET:SD	2.08	1.40
1:A:415:MET:CE	1:A:415:MET:SD	2.09	1.40
1:A:69:MET:SD	1:A:69:MET:CE	2.13	1.36
1:A:449:LEU:HD22	5:A:791:HOH:O	1.16	1.32
1:B:158:MET:CE	1:B:158:MET:SD	2.17	1.31
1:B:11:SER:HB3	5:B:760:HOH:O	1.40	1.19
1:B:321:LEU:HD22	5:B:979:HOH:O	1.44	1.18
1:A:318:GLY:HA2	1:A:488:LEU:CD1	1.74	1.16
1:B:76:ASN:O	1:B:80:THR:HG23	1.47	1.14
1:B:347:ALA:HB2	5:B:989:HOH:O	1.49	1.13
1:B:417:GLU:OE2	1:B:431:SER:HB3	1.49	1.11
1:A:77:ASN:OD1	5:A:784:HOH:O	1.69	1.10
1:A:363:PRO:HG2	1:A:364:LYS:HE2	1.34	1.09
1:B:369:LYS:HD2	3:B:640:DG6:HC3	1.35	1.06
1:B:323:SER:HB2	5:B:995:HOH:O	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:HD2	1:B:374:SER:N	1.70	1.06
1:A:327:LYS:HE3	5:A:940:HOH:O	1.56	1.06
1:B:469:GLU:HG2	1:B:470:ASP:H	1.15	1.05
1:B:373:LYS:HD2	1:B:374:SER:H	1.20	1.04
4:A:650:NAI:N7N	4:A:650:NAI:O1N	1.89	1.04
1:B:76:ASN:O	1:B:80:THR:CG2	2.05	1.04
1:B:23:ASP:OD1	1:B:24:ASN:N	1.91	1.03
1:B:315:PHE:CD1	1:B:481:LEU:HD11	1.94	1.03
1:B:95:GLN:HE21	1:B:95:GLN:HA	1.26	1.00
1:A:318:GLY:HA2	1:A:488:LEU:HD13	1.37	1.00
1:A:363:PRO:CG	1:A:364:LYS:HE2	1.92	0.99
1:A:412:LYS:HE2	3:A:630:DG6:O4	1.61	0.98
1:B:469:GLU:HG2	1:B:470:ASP:N	1.76	0.98
4:B:660:NAI:O1N	4:B:660:NAI:N7N	1.96	0.98
1:B:437:GLU:HG3	5:B:746:HOH:O	1.63	0.97
1:B:473:LYS:HE2	1:B:474:PHE:N	1.78	0.97
1:A:318:GLY:CA	1:A:488:LEU:HD13	1.94	0.97
1:A:122:GLU:O	1:A:124:ASN:N	1.96	0.97
1:B:356:ASP:HB3	3:B:640:DG6:O1P	1.64	0.97
1:A:61:LYS:HG3	1:A:61:LYS:O	1.61	0.97
1:B:515:ARG:NH1	1:B:521:PRO:O	1.98	0.96
1:B:365:GLN:HG3	5:B:990:HOH:O	1.66	0.96
1:A:151:ASN:H	1:A:200:ASN:HD21	1.14	0.95
1:B:238:LYS:HE3	5:B:978:HOH:O	1.67	0.94
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.30	0.94
1:A:356:ASP:HB3	3:A:630:DG6:O3P	1.67	0.93
1:B:289:GLY:HA2	1:B:314:THR:HG21	1.51	0.93
5:A:800:HOH:O	1:B:168:LEU:HG	1.67	0.93
1:B:473:LYS:HE2	1:B:474:PHE:H	1.33	0.93
1:B:489:LYS:HZ3	3:B:640:DG6:HC12	1.34	0.92
1:A:300:THR:HG21	5:A:704:HOH:O	1.67	0.92
1:A:435:VAL:HG23	5:A:956:HOH:O	1.66	0.92
1:B:163:VAL:HG22	1:B:164:LEU:HD22	1.52	0.92
1:B:330:SER:OG	1:B:376:VAL:HG21	1.70	0.92
1:A:297:PRO:HD3	1:A:320:ASP:OD2	1.70	0.91
1:B:342:LYS:HE2	5:B:880:HOH:O	1.69	0.91
1:A:64:GLU:O	1:A:65:LYS:HD3	1.70	0.91
1:B:11:SER:CB	5:B:760:HOH:O	2.08	0.91
1:B:286:ILE:HG21	1:B:308:LEU:HD12	1.48	0.91
1:A:58:LEU:HD13	1:A:60:LEU:HD23	1.54	0.90
1:B:369:LYS:HD2	3:B:640:DG6:C3	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:HD1	1:B:481:LEU:HD11	1.34	0.90
1:A:449:LEU:O	1:A:453:THR:HG23	1.71	0.90
1:A:225:ARG:HE	1:A:229:ASN:HD21	1.16	0.90
1:B:23:ASP:CG	1:B:24:ASN:H	1.75	0.90
1:B:61:LYS:NZ	5:B:937:HOH:O	2.02	0.90
1:A:40:THR:O	1:A:43:GLY:N	2.03	0.89
1:B:286:ILE:HG21	1:B:308:LEU:CD1	2.01	0.89
1:B:168:LEU:HD13	1:B:168:LEU:C	1.93	0.89
1:A:449:LEU:O	1:A:453:THR:CG2	2.22	0.88
1:B:116:LYS:HE3	1:B:125:ASP:OD1	1.72	0.88
1:A:363:PRO:CD	1:A:364:LYS:HE2	2.03	0.88
1:A:260:THR:HG23	1:A:263:ASN:H	1.39	0.87
1:B:95:GLN:NE2	1:B:95:GLN:HA	1.89	0.87
1:B:95:GLN:CA	1:B:95:GLN:HE21	1.86	0.87
1:B:115:LEU:HD22	1:B:511:GLU:HG3	1.57	0.86
1:A:449:LEU:CD2	5:A:791:HOH:O	1.91	0.85
1:A:372:SER:HB2	1:A:489:LYS:HE3	1.56	0.85
1:B:237:ASP:HB2	5:B:774:HOH:O	1.76	0.85
1:B:369:LYS:NZ	3:B:640:DG6:HC62	1.91	0.85
1:A:406:LYS:O	1:A:406:LYS:HD2	1.76	0.85
1:B:286:ILE:CG2	1:B:308:LEU:CD1	2.54	0.85
1:B:427:HIS:HE1	5:B:906:HOH:O	1.59	0.85
1:B:297:PRO:HB2	1:B:368:SER:HB3	1.60	0.83
1:B:494:ARG:HG3	5:B:842:HOH:O	1.76	0.83
1:B:198:ARG:HG3	5:B:966:HOH:O	1.79	0.83
1:A:327:LYS:HG2	1:A:503:LEU:HD13	1.61	0.83
5:A:800:HOH:O	1:B:168:LEU:CG	2.26	0.82
1:B:365:GLN:CG	5:B:990:HOH:O	2.23	0.82
1:A:356:ASP:N	1:A:356:ASP:OD2	2.10	0.82
1:B:297:PRO:HD3	1:B:320:ASP:OD1	1.78	0.82
1:A:96:THR:HG23	1:A:98:GLU:H	1.43	0.82
1:A:348:SER:OG	1:A:416:ASP:OD2	1.98	0.82
1:A:89:LYS:NZ	5:A:827:HOH:O	2.11	0.81
1:A:40:THR:HB	1:A:44:ARG:HB3	1.62	0.81
1:A:360:LEU:HD11	3:A:630:DG6:HC61	1.61	0.81
1:B:464:VAL:HG12	1:B:465:ASP:N	1.95	0.81
1:A:364:LYS:HE3	1:A:364:LYS:H	1.46	0.81
1:B:191:ILE:N	1:B:191:ILE:HD13	1.96	0.80
1:A:234:ASN:OD1	5:A:714:HOH:O	2.00	0.80
1:A:136:MET:CG	1:A:136:MET:CE	2.58	0.80
1:B:315:PHE:HD1	1:B:481:LEU:CD1	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LYS:O	1:B:61:LYS:HD2	1.81	0.80
1:A:412:LYS:CE	3:A:630:DG6:O4	2.30	0.80
1:B:23:ASP:OD1	1:B:24:ASN:HB2	1.82	0.80
1:A:257:VAL:HG22	1:A:258:ASN:ND2	1.96	0.79
1:A:533:LEU:HB2	1:B:494:ARG:HH12	1.47	0.79
1:B:251:VAL:H	1:B:299:ASN:HD21	1.29	0.79
1:A:445:LEU:HB2	5:A:754:HOH:O	1.82	0.79
1:B:297:PRO:HD3	1:B:320:ASP:CG	2.03	0.79
1:B:303:PRO:HG2	1:B:304:GLY:H	1.45	0.79
1:A:318:GLY:CA	1:A:488:LEU:CD1	2.55	0.79
1:B:489:LYS:NZ	3:B:640:DG6:HC12	1.97	0.79
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.64	0.79
1:A:436:CYS:HB3	1:B:428:ASN:HD22	1.46	0.79
1:B:115:LEU:CD2	1:B:511:GLU:HG3	2.13	0.79
1:B:464:VAL:CG1	1:B:465:ASP:N	2.45	0.79
1:A:334:GLN:HE22	1:A:380:ILE:HG12	1.48	0.79
1:B:365:GLN:CD	5:B:990:HOH:O	2.21	0.79
1:B:286:ILE:CG2	1:B:308:LEU:HD12	2.11	0.78
1:A:294:ASN:C	1:A:294:ASN:ND2	2.36	0.78
1:B:258:ASN:H	1:B:258:ASN:HD22	1.32	0.78
1:A:294:ASN:C	1:A:294:ASN:HD22	1.84	0.78
1:B:206:ASP:O	1:B:208:LYS:N	2.17	0.78
1:A:258:ASN:H	1:A:258:ASN:HD22	1.29	0.77
1:B:456:CYS:HG	1:B:477:PHE:HE1	1.32	0.77
1:B:69:MET:SD	1:B:69:MET:CB	2.73	0.77
1:A:90:HIS:CE1	5:A:865:HOH:O	2.36	0.77
1:A:150:ASN:ND2	1:A:160:ARG:HH12	1.83	0.77
1:A:329:LYS:NZ	5:A:964:HOH:O	2.17	0.77
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.20	0.77
1:A:104:ASN:HD21	1:B:423:MET:HA	1.49	0.77
1:B:191:ILE:H	1:B:191:ILE:HD13	1.49	0.76
1:B:116:LYS:HE3	1:B:125:ASP:CG	2.06	0.76
1:A:231:LYS:HD3	5:A:873:HOH:O	1.86	0.76
1:B:454:GLU:O	1:B:457:THR:HG22	1.86	0.76
1:A:249:ARG:O	1:A:249:ARG:HG3	1.86	0.76
1:A:363:PRO:HD2	1:A:364:LYS:HE2	1.65	0.76
1:A:9:ILE:N	1:A:9:ILE:HD12	2.01	0.75
1:B:59:ASP:OD1	1:B:61:LYS:HE3	1.85	0.75
1:B:480:VAL:HG12	1:B:482:THR:HG22	1.66	0.75
1:B:261:MET:CE	1:B:308:LEU:HA	2.15	0.75
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLY:HA2	1:B:314:THR:CG2	2.17	0.75
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.17	0.75
1:A:318:GLY:HA2	1:A:488:LEU:CD2	2.17	0.74
1:B:315:PHE:CE1	1:B:481:LEU:HD11	2.21	0.74
1:A:437:GLU:HG3	5:A:685:HOH:O	1.88	0.74
1:B:480:VAL:CG2	1:B:492:LEU:HD12	2.18	0.74
1:B:23:ASP:CG	1:B:24:ASN:N	2.36	0.74
1:A:24:ASN:OD1	5:A:724:HOH:O	2.06	0.74
1:B:159:GLN:O	5:B:691:HOH:O	2.06	0.74
1:B:347:ALA:HB1	1:B:349:TYR:CE2	2.23	0.74
1:B:315:PHE:CD1	1:B:481:LEU:CD1	2.70	0.74
1:B:131:ASN:HA	1:B:136:MET:HE2	1.70	0.74
1:B:480:VAL:HG21	1:B:492:LEU:HD12	1.68	0.73
1:B:373:LYS:HZ1	1:B:376:VAL:HG12	1.53	0.73
1:B:372:SER:OG	1:B:489:LYS:HE3	1.89	0.73
1:B:254:SER:H	1:B:258:ASN:HD21	1.36	0.73
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.89	0.73
1:B:323:SER:CB	5:B:995:HOH:O	2.20	0.73
1:A:122:GLU:CD	1:A:122:GLU:H	1.92	0.73
1:B:109:MET:N	1:B:448:ASP:OD1	2.20	0.73
1:B:327:LYS:HG2	1:B:503:LEU:HD13	1.71	0.73
1:A:363:PRO:HG2	1:A:364:LYS:CE	2.15	0.72
1:B:256:GLY:N	1:B:259:ASP:OD1	2.20	0.72
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.71	0.72
1:B:405:MET:O	1:B:408:VAL:HG22	1.89	0.72
1:B:65:LYS:NZ	1:B:141:ASP:OD2	2.21	0.72
1:A:493:THR:HG23	1:B:530:GLU:OE1	1.90	0.72
1:A:344:VAL:HG23	5:A:728:HOH:O	1.88	0.72
1:B:373:LYS:NZ	1:B:376:VAL:HG12	2.05	0.72
1:A:322:LYS:NZ	1:A:503:LEU:HD12	2.04	0.72
1:B:187:TYR:OH	1:B:219:HIS:HD2	1.73	0.72
1:B:299:ASN:H	1:B:299:ASN:HD22	1.37	0.72
1:B:158:MET:CE	1:B:158:MET:CG	2.67	0.72
1:B:297:PRO:HG3	1:B:369:LYS:HE2	1.73	0.71
1:B:62:LYS:O	5:B:772:HOH:O	2.08	0.71
1:B:109:MET:HE3	1:B:487:TRP:CZ2	2.25	0.71
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.72	0.71
1:A:192:ALA:HB3	1:A:359:ASN:HD22	1.55	0.71
1:A:217:TRP:O	1:A:221:GLN:HG2	1.90	0.71
1:A:381:ILE:HD11	1:A:396:VAL:HG23	1.73	0.71
1:A:354:ASN:OD1	1:A:356:ASP:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ALA:HB1	1:B:364:LYS:NZ	2.06	0.71
1:A:451:VAL:HG12	1:A:451:VAL:O	1.89	0.71
1:B:315:PHE:H	1:B:315:PHE:HD2	1.37	0.71
1:B:75:GLY:O	1:B:79:SER:HB3	1.91	0.71
1:B:367:ARG:O	1:B:370:GLU:HB2	1.91	0.71
1:A:503:LEU:HD22	1:B:335:PHE:HE2	1.54	0.70
1:B:365:GLN:NE2	5:B:990:HOH:O	2.22	0.70
1:B:464:VAL:CG1	1:B:465:ASP:H	2.03	0.70
1:B:396:VAL:O	1:B:398:HIS:HD2	1.74	0.70
1:B:356:ASP:CB	3:B:640:DG6:O3P	2.40	0.70
1:B:303:PRO:CG	1:B:304:GLY:H	2.05	0.70
1:B:12:VAL:O	5:B:911:HOH:O	2.09	0.70
1:A:327:LYS:CE	5:A:940:HOH:O	2.26	0.70
1:A:90:HIS:HE1	5:A:865:HOH:O	1.70	0.70
1:B:371:ILE:HD13	1:B:374:SER:HB3	1.75	0.69
1:A:255:PRO:HA	1:A:259:ASP:OD1	1.93	0.69
1:B:527:ARG:H	1:B:531:ARG:HD2	1.57	0.69
1:B:369:LYS:HZ1	3:B:640:DG6:HC62	1.54	0.69
1:B:273:GLU:HB3	5:B:876:HOH:O	1.91	0.69
1:A:203:ILE:HD12	1:A:222:ARG:HG3	1.74	0.69
1:A:341:ILE:O	1:A:343:PRO:HD2	1.92	0.69
1:A:372:SER:CB	1:A:489:LYS:HE3	2.23	0.69
1:B:456:CYS:SG	1:B:477:PHE:HE1	2.16	0.69
1:B:356:ASP:HB3	3:B:640:DG6:P	2.32	0.69
1:B:131:ASN:HA	1:B:136:MET:CE	2.22	0.69
1:B:373:LYS:O	1:B:374:SER:HB3	1.92	0.69
1:B:168:LEU:HD13	1:B:168:LEU:O	1.91	0.69
1:A:294:ASN:HD22	1:A:295:GLY:N	1.90	0.69
1:A:377:ILE:O	1:A:381:ILE:HG13	1.93	0.69
1:B:362:ALA:HB3	1:B:365:GLN:OE1	1.91	0.69
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.28	0.69
1:A:294:ASN:ND2	1:A:296:SER:H	1.91	0.69
1:B:325:GLN:NE2	1:B:350:ASN:OD1	2.27	0.68
1:A:372:SER:CB	1:A:489:LYS:CE	2.71	0.68
1:A:249:ARG:NH2	5:A:702:HOH:O	2.26	0.68
1:A:331:VAL:O	5:A:907:HOH:O	2.12	0.68
1:A:297:PRO:HG3	1:A:369:LYS:HD2	1.75	0.68
1:A:122:GLU:C	1:A:124:ASN:H	1.97	0.68
1:B:469:GLU:CG	1:B:470:ASP:H	1.89	0.68
1:B:315:PHE:CE1	1:B:481:LEU:HD21	2.29	0.68
1:A:497:PHE:CE2	1:B:530:GLU:HB2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HD23	1:A:516:LEU:C	2.15	0.68
1:B:318:GLY:HA2	1:B:488:LEU:CD2	2.24	0.68
1:B:25:GLU:OE1	1:B:57:LYS:HD2	1.93	0.67
1:A:328:LEU:HD21	1:B:332:LEU:HD11	1.74	0.67
1:A:120:ASP:OD1	1:A:124:ASN:HB2	1.94	0.67
1:B:258:ASN:N	1:B:258:ASN:HD22	1.89	0.67
1:A:412:LYS:O	5:A:956:HOH:O	2.12	0.67
1:B:373:LYS:CD	1:B:374:SER:H	2.01	0.67
1:A:531:ARG:O	1:A:532:LEU:HD12	1.95	0.67
1:B:95:GLN:HB2	1:B:167:ASP:OD1	1.95	0.67
1:B:134:LEU:HD21	1:B:518:ILE:CG2	2.25	0.67
1:B:467:VAL:HG23	5:B:899:HOH:O	1.94	0.67
1:B:366:PHE:CE1	1:B:402:ILE:HG22	2.30	0.67
1:B:354:ASN:OD1	1:B:356:ASP:HB2	1.95	0.67
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.77	0.66
1:B:69:MET:CE	1:B:69:MET:CG	2.74	0.66
1:B:249:ARG:O	1:B:249:ARG:HG3	1.95	0.66
1:B:248:GLU:OE2	1:B:278:SER:HB2	1.95	0.66
1:A:131:ASN:OD1	5:A:900:HOH:O	2.14	0.66
1:A:321:LEU:HD22	1:A:445:LEU:CD2	2.26	0.66
1:A:9:ILE:CD1	1:A:9:ILE:N	2.59	0.66
5:A:800:HOH:O	1:B:168:LEU:CD1	2.43	0.65
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.25	0.65
1:B:142:PHE:O	5:B:685:HOH:O	2.13	0.65
1:B:356:ASP:HB2	3:B:640:DG6:O3P	1.96	0.65
1:B:23:ASP:OD1	1:B:24:ASN:CB	2.44	0.65
1:B:32:TYR:O	5:B:845:HOH:O	2.14	0.65
1:B:297:PRO:HD3	1:B:320:ASP:CB	2.27	0.65
1:A:326:THR:HG21	1:A:489:LYS:HG3	1.79	0.65
1:B:131:ASN:HB2	1:B:136:MET:CE	2.26	0.65
1:A:272:HIS:HD2	1:A:274:GLU:HB2	1.61	0.65
1:A:291:PRO:HG2	5:A:838:HOH:O	1.95	0.65
1:A:375:SER:OG	5:A:965:HOH:O	2.14	0.65
1:A:225:ARG:NE	1:A:229:ASN:HD21	1.89	0.65
1:B:480:VAL:CG1	1:B:482:THR:HG22	2.26	0.65
1:A:416:ASP:OD1	5:A:703:HOH:O	2.14	0.65
1:A:315:PHE:CZ	1:A:481:LEU:HD21	2.32	0.65
1:B:261:MET:HE2	1:B:308:LEU:HA	1.78	0.65
1:A:325:GLN:NE2	3:A:630:DG6:O1	2.30	0.64
1:B:438:ASP:OD2	1:B:438:ASP:N	2.24	0.64
1:B:480:VAL:HG12	1:B:480:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:511:GLU:CG	2.27	0.64
1:B:58:LEU:HD13	1:B:60:LEU:HD23	1.79	0.64
1:A:364:LYS:HE3	1:A:364:LYS:N	2.13	0.64
1:A:154:LEU:HB3	1:A:176:MET:HE2	1.80	0.64
1:B:361:SER:OG	5:B:921:HOH:O	2.15	0.64
1:B:355:ASN:O	1:B:359:ASN:N	2.26	0.64
1:A:120:ASP:OD1	1:A:122:GLU:O	2.15	0.64
1:A:315:PHE:CE1	1:A:481:LEU:HD11	2.33	0.64
1:B:76:ASN:O	1:B:80:THR:HG22	1.96	0.64
1:A:372:SER:HB3	1:A:489:LYS:HE2	1.78	0.64
1:B:364:LYS:H	1:B:364:LYS:HE3	1.63	0.64
1:B:131:ASN:HB2	1:B:136:MET:HE1	1.78	0.64
1:A:389:ASN:OD1	1:A:391:LYS:N	2.30	0.63
1:B:153:ASP:OD2	1:B:155:TYR:HB3	1.96	0.63
1:B:61:LYS:CG	5:B:958:HOH:O	2.46	0.63
1:A:87:ALA:HA	1:A:92:VAL:HG13	1.80	0.63
1:A:503:LEU:HD22	1:B:335:PHE:CE2	2.32	0.63
1:B:295:GLY:HA2	5:B:728:HOH:O	1.98	0.63
1:A:209:GLY:O	1:A:210:ASN:HB2	1.98	0.63
1:A:364:LYS:N	1:A:364:LYS:CE	2.61	0.63
1:A:463:LYS:NZ	1:A:463:LYS:HB2	2.11	0.63
1:A:322:LYS:HG3	1:A:489:LYS:HA	1.80	0.63
1:B:286:ILE:CG2	1:B:308:LEU:HD13	2.28	0.63
1:B:417:GLU:OE2	1:B:431:SER:CB	2.39	0.62
1:B:261:MET:O	1:B:265:LEU:HD22	1.99	0.62
1:B:297:PRO:CD	1:B:320:ASP:OD1	2.47	0.62
1:B:396:VAL:O	1:B:398:HIS:CD2	2.52	0.62
1:A:451:VAL:O	1:A:451:VAL:CG1	2.47	0.62
1:A:478:TYR:CE1	1:A:480:VAL:HB	2.33	0.62
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.34	0.62
1:B:15:VAL:HG23	1:B:15:VAL:O	1.97	0.62
1:A:68:ILE:HD13	1:A:142:PHE:CD1	2.34	0.62
1:A:134:LEU:HB3	1:A:135:PRO:HD2	1.81	0.62
1:A:225:ARG:HH21	1:A:225:ARG:CG	2.12	0.62
1:B:494:ARG:N	5:B:981:HOH:O	2.26	0.62
1:A:203:ILE:HD12	1:A:222:ARG:CG	2.30	0.62
1:A:322:LYS:HZ2	1:A:503:LEU:HD12	1.64	0.62
1:B:116:LYS:HD3	1:B:523:GLN:NE2	2.14	0.62
1:B:190:PHE:HE2	1:B:251:VAL:HG12	1.64	0.62
1:A:498:HIS:CE1	5:A:861:HOH:O	2.52	0.62
1:A:162:GLN:NE2	5:A:774:HOH:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:H	1:A:359:ASN:HD21	1.48	0.62
1:B:516:LEU:O	1:B:519:GLY:N	2.29	0.62
1:B:372:SER:HA	1:B:490:ALA:HB2	1.80	0.62
1:B:503:LEU:HA	1:B:506:GLN:NE2	2.15	0.62
1:B:467:VAL:O	1:B:467:VAL:HG12	2.00	0.62
1:A:291:PRO:CD	5:A:838:HOH:O	2.48	0.62
1:A:463:LYS:CB	1:A:463:LYS:NZ	2.62	0.62
3:A:630:DG6:O1P	4:A:650:NAI:H2D	1.99	0.62
1:B:489:LYS:NZ	3:B:640:DG6:C1	2.61	0.62
1:A:530:GLU:HG3	1:B:497:PHE:CD1	2.34	0.61
1:A:258:ASN:HD22	1:A:258:ASN:N	1.90	0.61
1:A:531:ARG:O	1:A:532:LEU:CD1	2.48	0.61
1:B:116:LYS:CE	1:B:125:ASP:OD1	2.47	0.61
1:B:299:ASN:HD22	1:B:299:ASN:N	1.98	0.61
1:A:287:LEU:HD13	1:A:308:LEU:HD11	1.80	0.61
1:A:318:GLY:HA2	1:A:488:LEU:CG	2.31	0.61
1:A:493:THR:HG22	1:A:494:ARG:N	2.15	0.61
1:A:485:SER:OG	1:A:491:PRO:HB3	2.01	0.61
1:A:406:LYS:HD2	1:A:406:LYS:C	2.17	0.61
1:B:40:THR:O	1:B:41:ALA:CB	2.49	0.61
1:A:297:PRO:CD	1:A:320:ASP:OD2	2.46	0.61
1:B:297:PRO:CG	1:B:369:LYS:HE2	2.31	0.61
1:A:283:ALA:O	1:A:287:LEU:HB2	2.00	0.61
1:A:250:TYR:HD1	1:A:368:SER:HG	1.48	0.61
1:B:342:LYS:HB2	1:B:387:LEU:HG	1.82	0.61
1:B:310:GLU:HG2	1:B:479:PRO:HG2	1.81	0.61
1:A:217:TRP:HB2	1:A:269:LYS:HA	1.83	0.61
1:B:321:LEU:HB2	5:B:979:HOH:O	1.98	0.60
1:B:377:ILE:HG21	1:B:398:HIS:CD2	2.36	0.60
1:B:364:LYS:HB2	1:B:365:GLN:HE22	1.66	0.60
1:A:399:CYS:O	1:A:400:ILE:HD12	2.01	0.60
1:B:385:ASP:HA	1:B:388:TYR:O	2.01	0.60
1:B:261:MET:HE3	1:B:308:LEU:HA	1.81	0.60
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.82	0.60
1:A:442:ALA:HB2	4:A:650:NAI:H42N	1.83	0.60
1:A:334:GLN:NE2	1:A:380:ILE:HG12	2.15	0.60
1:A:478:TYR:HE1	1:A:480:VAL:HB	1.66	0.60
1:A:426:GLY:HA3	1:B:440:LEU:CD1	2.32	0.60
1:B:109:MET:HE3	1:B:487:TRP:HZ2	1.67	0.60
1:A:308:LEU:CD2	1:A:312:GLU:HG2	2.31	0.60
1:B:352:LEU:CD2	1:B:402:ILE:HD11	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:CD	1:A:364:LYS:N	2.64	0.60
1:B:484:LEU:N	1:B:484:LEU:CD2	2.65	0.60
1:A:122:GLU:CD	1:A:122:GLU:N	2.55	0.60
1:A:68:ILE:HD13	1:A:142:PHE:CG	2.36	0.60
1:B:252:GLU:O	1:B:274:GLU:OE2	2.19	0.60
1:A:234:ASN:HB2	1:A:236:LEU:HD22	1.83	0.60
1:B:147:TRP:HB3	1:B:184:SER:HB2	1.83	0.60
1:B:95:GLN:CA	1:B:95:GLN:NE2	2.56	0.60
1:B:59:ASP:OD2	1:B:61:LYS:HG3	2.00	0.60
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.31	0.60
1:A:285:SER:HB3	1:A:290:VAL:HG23	1.83	0.60
1:B:372:SER:CA	1:B:490:ALA:HB2	2.32	0.60
1:B:291:PRO:HB3	1:B:315:PHE:HB2	1.84	0.60
1:B:315:PHE:N	1:B:315:PHE:HD2	1.99	0.60
1:B:259:ASP:HA	1:B:303:PRO:HG2	1.84	0.60
1:B:61:LYS:HG2	5:B:958:HOH:O	2.01	0.60
1:A:323:SER:HB2	1:A:326:THR:HB	1.83	0.59
1:B:264:LEU:CD2	1:B:305:LEU:HD13	2.32	0.59
1:B:367:ARG:HA	1:B:370:GLU:HG3	1.84	0.59
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.37	0.59
1:B:154:LEU:HD22	1:B:179:VAL:CG1	2.32	0.59
1:A:318:GLY:HA2	1:A:488:LEU:HD11	1.74	0.59
1:A:330:SER:O	1:A:331:VAL:C	2.40	0.59
1:A:296:SER:CB	1:A:298:GLN:HE22	2.15	0.59
1:A:364:LYS:H	1:A:364:LYS:CE	2.15	0.59
1:A:259:ASP:OD2	1:A:263:ASN:OD1	2.21	0.59
1:B:129:PRO:HB2	1:B:132:SER:HB3	1.85	0.59
1:B:150:ASN:O	5:B:681:HOH:O	2.16	0.59
1:B:196:ASP:O	1:B:198:ARG:N	2.35	0.59
1:A:92:VAL:HG22	1:A:92:VAL:O	2.02	0.59
1:B:473:LYS:HA	1:B:473:LYS:CE	2.33	0.59
1:B:251:VAL:HG13	5:B:940:HOH:O	2.02	0.59
1:A:493:THR:HG21	1:A:497:PHE:HB2	1.83	0.59
1:B:15:VAL:CG2	1:B:15:VAL:O	2.51	0.59
1:B:347:ALA:HB1	1:B:349:TYR:HE2	1.67	0.59
1:B:352:LEU:HD21	1:B:402:ILE:HD11	1.85	0.59
1:A:368:SER:HA	1:A:371:ILE:CG2	2.32	0.59
1:A:399:CYS:C	1:A:400:ILE:HD12	2.23	0.59
1:B:131:ASN:CB	1:B:136:MET:HE1	2.32	0.59
1:A:438:ASP:OD1	2:A:670:NH4:N	2.36	0.59
1:B:151:ASN:HD22	1:B:151:ASN:C	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HD3	1:B:54:TYR:O	2.02	0.58
1:B:204:ASN:ND2	1:B:212:THR:O	2.32	0.58
1:A:331:VAL:C	5:A:907:HOH:O	2.41	0.58
1:B:345:SER:HA	1:B:397:ASP:O	2.04	0.58
1:B:503:LEU:O	1:B:506:GLN:HB2	2.04	0.58
1:B:23:ASP:OD1	1:B:24:ASN:CA	2.52	0.58
1:B:167:ASP:O	1:B:171:ARG:HG3	2.04	0.58
1:A:372:SER:HB3	1:A:489:LYS:CE	2.33	0.58
1:B:261:MET:HE3	1:B:308:LEU:CA	2.34	0.58
1:B:464:VAL:HG13	1:B:465:ASP:H	1.66	0.58
1:B:523:GLN:HB2	5:B:902:HOH:O	2.02	0.58
1:A:165:GLU:OE1	5:A:695:HOH:O	2.17	0.58
1:A:322:LYS:HE2	5:A:906:HOH:O	2.03	0.58
1:A:322:LYS:HD2	1:A:327:LYS:HG3	1.86	0.58
1:B:469:GLU:CG	1:B:470:ASP:N	2.51	0.58
1:A:480:VAL:O	1:A:480:VAL:HG12	2.02	0.58
1:A:50:THR:CG2	5:A:692:HOH:O	2.51	0.58
1:B:492:LEU:HD13	1:B:493:THR:H	1.69	0.57
1:B:40:THR:HG1	1:B:44:ARG:H	1.50	0.57
1:A:36:VAL:HA	1:B:119:ILE:O	2.04	0.57
1:A:252:GLU:O	1:A:274:GLU:OE1	2.22	0.57
1:A:142:PHE:O	5:A:679:HOH:O	2.17	0.57
1:A:321:LEU:CD2	1:A:445:LEU:HD22	2.34	0.57
1:B:307:GLN:O	1:B:310:GLU:HB2	2.03	0.57
1:A:298:GLN:H	1:A:298:GLN:NE2	2.03	0.57
1:B:494:ARG:O	1:B:497:PHE:HB2	2.04	0.57
1:B:365:GLN:NE2	1:B:365:GLN:N	2.52	0.57
1:A:197:GLU:OE1	1:A:197:GLU:C	2.42	0.57
1:A:355:ASN:HB3	1:A:356:ASP:OD2	2.05	0.57
1:B:297:PRO:HB2	1:B:368:SER:CB	2.34	0.57
1:A:352:LEU:N	1:A:352:LEU:HD23	2.19	0.57
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.69	0.57
1:A:368:SER:HA	1:A:371:ILE:HG22	1.87	0.57
1:B:503:LEU:HA	1:B:506:GLN:HE21	1.69	0.57
1:A:469:GLU:O	1:A:470:ASP:CB	2.52	0.57
1:A:356:ASP:CB	3:A:630:DG6:O3P	2.48	0.56
1:B:315:PHE:N	1:B:315:PHE:CD2	2.67	0.56
1:A:294:ASN:HD21	1:A:296:SER:H	1.52	0.56
1:A:246:ASN:ND2	4:A:650:NAI:H8A	2.19	0.56
1:B:109:MET:CE	1:B:487:TRP:CZ2	2.88	0.56
1:A:12:VAL:HG12	1:A:133:LEU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HE3	1:A:125:ASP:CG	2.25	0.56
1:A:321:LEU:HD22	1:A:445:LEU:HD22	1.88	0.56
1:B:87:ALA:HA	1:B:92:VAL:HG13	1.88	0.56
1:A:449:LEU:O	1:A:453:THR:HG22	2.03	0.56
1:B:198:ARG:NH2	5:B:969:HOH:O	2.38	0.56
1:A:498:HIS:HE1	5:A:861:HOH:O	1.89	0.56
1:B:316:ILE:O	1:B:316:ILE:HD12	2.05	0.56
1:A:291:PRO:HD2	5:A:838:HOH:O	2.05	0.56
1:B:130:PHE:HE2	1:B:452:MET:CE	2.19	0.56
1:B:303:PRO:CG	1:B:304:GLY:N	2.69	0.56
1:A:522:SER:OG	1:B:524:ASN:HB3	2.05	0.56
1:B:14:VAL:HG22	1:B:16:THR:HG22	1.88	0.56
1:B:31:SER:N	5:B:699:HOH:O	1.96	0.56
1:A:318:GLY:HA2	1:A:488:LEU:HD22	1.87	0.56
1:A:363:PRO:HB2	1:A:367:ARG:NH2	2.20	0.56
1:B:356:ASP:OD2	1:B:356:ASP:N	2.22	0.56
1:B:168:LEU:C	1:B:168:LEU:CD1	2.71	0.56
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.06	0.56
1:A:58:LEU:HD13	1:A:60:LEU:CD2	2.33	0.55
1:A:515:ARG:NH1	1:A:521:PRO:O	2.36	0.55
1:A:116:LYS:HE3	1:A:125:ASP:OD1	2.06	0.55
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.41	0.55
1:B:358:TYR:HB2	1:B:404:TYR:CE2	2.41	0.55
1:B:374:SER:O	1:B:376:VAL:N	2.40	0.55
1:A:332:LEU:HD21	1:B:328:LEU:HD21	1.88	0.55
1:A:453:THR:O	1:A:457:THR:HG23	2.06	0.55
1:B:286:ILE:HG22	1:B:308:LEU:CD1	2.33	0.55
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.07	0.55
1:A:310:GLU:OE1	1:A:478:TYR:OH	2.17	0.55
1:B:231:LYS:HG2	1:B:236:LEU:O	2.07	0.55
1:B:486:TYR:CE1	1:B:503:LEU:HG	2.40	0.55
1:B:74:GLY:N	1:B:148:ASP:OD1	2.40	0.55
1:B:321:LEU:HD13	1:B:445:LEU:HD22	1.88	0.55
1:A:371:ILE:O	1:A:374:SER:HB3	2.07	0.55
1:B:468:LYS:O	1:B:468:LYS:HG3	2.06	0.55
1:B:131:ASN:CB	1:B:136:MET:CE	2.84	0.55
1:A:372:SER:CB	1:A:489:LYS:HE2	2.37	0.55
1:A:92:VAL:O	1:A:92:VAL:CG2	2.55	0.55
1:B:366:PHE:HE1	1:B:402:ILE:HG22	1.70	0.55
1:A:151:ASN:H	1:A:200:ASN:ND2	1.95	0.55
1:A:331:VAL:HG12	5:A:907:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:N	1:B:106:PHE:CD1	2.74	0.55
1:A:104:ASN:ND2	1:A:106:PHE:H	2.05	0.54
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.88	0.54
1:A:61:LYS:NZ	5:A:970:HOH:O	2.35	0.54
1:A:96:THR:HG22	1:A:99:GLY:N	2.22	0.54
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.20	0.54
1:B:61:LYS:HG3	5:B:958:HOH:O	2.07	0.54
1:A:170:GLN:NE2	5:A:723:HOH:O	2.41	0.54
1:A:261:MET:HE3	1:A:311:HIS:HB3	1.89	0.54
1:A:14:VAL:O	1:A:16:THR:HG22	2.08	0.54
1:A:364:LYS:N	1:A:364:LYS:HD3	2.23	0.54
1:B:489:LYS:HZ3	3:B:640:DG6:C1	2.12	0.54
1:B:356:ASP:CB	3:B:640:DG6:P	2.96	0.54
1:A:493:THR:CG2	1:A:497:PHE:HB2	2.37	0.54
1:B:22:LYS:O	1:B:23:ASP:C	2.44	0.54
1:B:303:PRO:HG2	1:B:304:GLY:N	2.18	0.54
1:A:246:ASN:HD22	4:A:650:NAI:H51A	1.70	0.54
1:A:246:ASN:ND2	4:A:650:NAI:H51A	2.23	0.54
1:A:96:THR:CG2	1:A:98:GLU:H	2.18	0.54
1:A:12:VAL:CG1	1:A:133:LEU:HA	2.37	0.54
1:A:327:LYS:HG2	1:A:503:LEU:CD1	2.36	0.54
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.72	0.54
1:A:325:GLN:NE2	1:A:350:ASN:OD1	2.40	0.54
1:A:344:VAL:HG21	5:A:851:HOH:O	2.07	0.54
1:B:106:PHE:N	1:B:106:PHE:HD1	2.04	0.54
1:A:527:ARG:HH11	1:A:527:ARG:HG2	1.73	0.54
1:B:134:LEU:HD11	1:B:517:LEU:HB3	1.90	0.54
1:A:423:MET:CE	1:B:443:THR:HB	2.38	0.54
1:A:350:ASN:N	1:A:401:VAL:O	2.42	0.54
1:A:527:ARG:HG2	1:A:527:ARG:NH1	2.23	0.54
1:A:44:ARG:NH2	1:B:13:LYS:HG2	2.23	0.53
1:A:218:THR:HG23	5:A:836:HOH:O	2.08	0.53
1:B:212:THR:OG1	1:B:213:THR:N	2.41	0.53
1:A:298:GLN:HG2	1:A:300:THR:HG22	1.90	0.53
1:A:163:VAL:HG12	1:A:164:LEU:HD13	1.90	0.53
1:A:246:ASN:HD22	1:A:246:ASN:N	2.07	0.53
1:A:96:THR:HG23	1:A:98:GLU:N	2.20	0.53
1:B:299:ASN:H	1:B:299:ASN:ND2	2.06	0.53
1:A:463:LYS:HZ2	1:A:463:LYS:HB2	1.71	0.53
1:A:104:ASN:HD22	1:A:104:ASN:C	2.11	0.53
1:A:363:PRO:HD2	1:A:364:LYS:CE	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ASN:N	1:B:258:ASN:ND2	2.56	0.53
1:A:218:THR:CG2	5:A:836:HOH:O	2.57	0.53
1:B:259:ASP:HA	1:B:303:PRO:CG	2.39	0.53
1:A:61:LYS:CG	1:A:61:LYS:O	2.45	0.52
1:A:258:ASN:ND2	1:A:258:ASN:N	2.53	0.52
1:A:82:VAL:HG21	1:A:154:LEU:CD2	2.38	0.52
1:B:355:ASN:N	1:B:356:ASP:OD2	2.43	0.52
1:A:362:ALA:CB	5:A:879:HOH:O	2.56	0.52
1:B:243:TRP:CE2	1:B:245:ALA:HB3	2.44	0.52
1:B:350:ASN:HD22	1:B:350:ASN:C	2.13	0.52
1:B:315:PHE:CD1	1:B:481:LEU:CG	2.92	0.52
1:A:377:ILE:HD11	5:A:917:HOH:O	2.09	0.52
1:B:105:TYR:CZ	1:B:139:PRO:HG2	2.44	0.52
1:A:463:LYS:CB	1:A:463:LYS:HZ3	2.22	0.52
1:B:259:ASP:OD2	1:B:260:THR:N	2.42	0.52
1:B:130:PHE:CE2	1:B:452:MET:HE3	2.44	0.52
1:B:318:GLY:HA2	1:B:488:LEU:HD21	1.91	0.52
1:B:204:ASN:O	1:B:211:VAL:HA	2.09	0.52
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.24	0.52
1:A:322:LYS:HZ2	1:A:503:LEU:CD1	2.23	0.52
1:B:484:LEU:HD22	1:B:484:LEU:N	2.24	0.52
1:B:473:LYS:HE3	1:B:473:LYS:HA	1.92	0.52
1:A:120:ASP:O	1:A:121:ALA:C	2.47	0.52
1:B:327:LYS:HD2	5:B:993:HOH:O	2.09	0.52
1:A:200:ASN:HD22	1:A:200:ASN:C	2.12	0.52
1:B:288:GLU:OE2	5:B:977:HOH:O	2.19	0.52
1:B:14:VAL:HG11	1:B:518:ILE:O	2.10	0.52
1:B:327:LYS:NZ	5:B:993:HOH:O	2.42	0.51
1:B:194:ASN:HD22	1:B:195:GLN:N	2.07	0.51
1:A:328:LEU:HD13	1:A:432:ILE:HD11	1.92	0.51
1:A:503:LEU:CD2	1:B:335:PHE:CE2	2.94	0.51
1:A:104:ASN:ND2	1:B:423:MET:HA	2.22	0.51
1:A:385:ASP:HA	1:A:388:TYR:O	2.11	0.51
1:A:105:TYR:OH	1:A:140:ASN:ND2	2.43	0.51
1:B:318:GLY:CA	1:B:488:LEU:HD23	2.40	0.51
1:B:62:LYS:N	5:B:847:HOH:O	2.09	0.51
1:A:328:LEU:O	1:A:332:LEU:HB2	2.11	0.51
1:A:25:GLU:OE2	1:A:57:LYS:HD2	2.11	0.51
1:A:296:SER:HB3	1:A:298:GLN:HE22	1.75	0.51
5:A:793:HOH:O	1:B:533:LEU:HD13	2.10	0.51
1:B:261:MET:HE3	1:B:308:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PHE:O	1:B:457:THR:N	2.44	0.51
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.93	0.51
1:A:373:LYS:O	1:A:373:LYS:HG2	2.11	0.51
1:B:500:VAL:HG12	1:B:501:ASN:O	2.11	0.51
1:A:151:ASN:N	1:A:200:ASN:HD21	1.97	0.51
1:B:286:ILE:HG21	1:B:308:LEU:HD13	1.83	0.51
1:A:287:LEU:CD1	1:A:308:LEU:HD21	2.40	0.51
1:A:209:GLY:O	1:A:210:ASN:CB	2.58	0.51
1:A:33:GLU:OE2	5:A:810:HOH:O	2.20	0.51
1:A:59:ASP:OD1	1:A:61:LYS:HG2	2.12	0.50
1:A:296:SER:HB2	1:A:298:GLN:HE22	1.77	0.50
1:B:481:LEU:O	1:B:484:LEU:HD23	2.11	0.50
1:A:207:GLU:O	1:A:208:LYS:HB2	2.11	0.50
1:B:528:PHE:CG	1:B:532:LEU:HD22	2.46	0.50
1:B:350:ASN:HB3	1:B:414:ALA:HA	1.93	0.50
1:B:21:TYR:CE2	1:B:26:LEU:HD13	2.46	0.50
1:B:52:GLN:OE1	1:B:53:ASP:N	2.43	0.50
1:A:74:GLY:N	1:A:148:ASP:OD1	2.44	0.50
1:B:25:GLU:HG3	1:B:57:LYS:HG3	1.94	0.50
1:A:440:LEU:HD23	1:B:426:GLY:HA3	1.92	0.50
1:A:461:TYR:OH	1:B:533:LEU:HB2	2.11	0.50
1:B:51:VAL:HG12	1:B:52:GLN:N	2.26	0.50
1:A:184:SER:OG	1:A:185:ILE:N	2.44	0.50
1:B:286:ILE:O	1:B:288:GLU:N	2.45	0.50
1:A:491:PRO:HD3	1:A:501:ASN:HD21	1.77	0.50
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.93	0.50
1:B:485:SER:OG	1:B:491:PRO:HB3	2.12	0.50
1:B:322:LYS:NZ	5:B:926:HOH:O	2.44	0.50
1:B:302:VAL:HB	1:B:303:PRO:CD	2.40	0.50
1:B:14:VAL:CG1	1:B:518:ILE:O	2.59	0.50
1:A:468:LYS:O	1:A:470:ASP:N	2.44	0.50
1:B:81:LEU:HA	1:B:443:THR:HG23	1.94	0.50
1:B:130:PHE:HZ	1:B:510:LEU:HD12	1.77	0.50
1:B:376:VAL:CG1	1:B:377:ILE:N	2.74	0.50
1:A:327:LYS:HD3	1:B:335:PHE:CE2	2.47	0.50
1:A:497:PHE:CD1	1:A:497:PHE:N	2.80	0.50
1:B:14:VAL:O	1:B:16:THR:HG22	2.12	0.50
1:A:225:ARG:CG	1:A:225:ARG:NH2	2.73	0.50
1:B:187:TYR:OH	1:B:219:HIS:CD2	2.60	0.50
1:A:192:ALA:CB	1:A:359:ASN:HD22	2.22	0.50
1:A:516:LEU:CD2	1:A:516:LEU:C	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LEU:HD13	1:A:445:LEU:HD22	1.93	0.49
1:A:493:THR:HG22	1:A:494:ARG:H	1.77	0.49
1:B:318:GLY:CA	1:B:488:LEU:CD2	2.89	0.49
1:B:184:SER:OG	1:B:185:ILE:N	2.44	0.49
1:B:402:ILE:HG23	1:B:402:ILE:O	2.12	0.49
1:A:120:ASP:OD1	1:A:124:ASN:O	2.30	0.49
1:B:494:ARG:HB3	5:B:981:HOH:O	2.12	0.49
1:B:40:THR:O	1:B:41:ALA:HB3	2.12	0.49
1:A:368:SER:CA	1:A:371:ILE:HG22	2.43	0.49
1:A:367:ARG:O	1:A:371:ILE:HG22	2.12	0.49
1:B:360:LEU:HD11	3:B:640:DG6:HC61	1.94	0.49
1:A:443:THR:CG2	1:B:423:MET:HE1	2.42	0.49
1:A:272:HIS:CD2	1:A:274:GLU:HB2	2.45	0.49
1:B:154:LEU:HD22	1:B:179:VAL:HG11	1.94	0.49
1:B:66:LEU:HD21	1:B:240:ILE:HD12	1.95	0.49
1:A:465:ASP:OD1	1:A:467:VAL:N	2.41	0.49
1:A:362:ALA:HA	5:A:879:HOH:O	2.11	0.49
1:B:352:LEU:HA	1:B:411:SER:O	2.11	0.49
1:A:423:MET:HE1	1:B:443:THR:CG2	2.43	0.49
1:A:497:PHE:CD2	1:B:530:GLU:HB2	2.48	0.49
1:A:349:TYR:HD1	1:A:401:VAL:HB	1.78	0.49
1:A:225:ARG:HH21	1:A:225:ARG:HG2	1.78	0.49
1:A:533:LEU:CB	1:B:494:ARG:HH12	2.22	0.49
1:B:499:PRO:HD2	5:B:886:HOH:O	2.13	0.49
1:B:350:ASN:O	1:B:402:ILE:HA	2.13	0.49
1:B:108:SER:OG	1:B:448:ASP:OD2	2.27	0.49
1:B:173:LYS:NZ	5:B:968:HOH:O	2.26	0.49
3:A:630:DG6:O1P	4:A:650:NAI:H3D	2.12	0.48
1:A:321:LEU:CD1	1:A:445:LEU:HD22	2.42	0.48
1:B:261:MET:H	1:B:307:GLN:NE2	2.11	0.48
1:B:130:PHE:CD2	1:B:130:PHE:O	2.66	0.48
1:A:43:GLY:O	1:B:10:THR:HA	2.14	0.48
1:A:68:ILE:CD1	1:A:142:PHE:CD2	2.96	0.48
1:B:130:PHE:CE2	1:B:452:MET:CE	2.96	0.48
1:A:494:ARG:HG3	1:A:497:PHE:CD1	2.48	0.48
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.95	0.48
1:B:370:GLU:OE2	1:B:400:ILE:HG22	2.13	0.48
1:B:155:TYR:OH	1:B:170:GLN:NE2	2.44	0.48
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.95	0.48
1:B:527:ARG:HD3	5:B:855:HOH:O	2.14	0.48
1:B:31:SER:CB	5:B:699:HOH:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:ILE:O	1:A:371:ILE:HD12	2.14	0.48
1:A:155:TYR:CE1	1:A:173:LYS:HG3	2.49	0.48
1:B:520:LEU:HD12	1:B:520:LEU:HA	1.80	0.48
1:B:243:TRP:CZ2	1:B:245:ALA:HB3	2.49	0.48
1:A:471:ALA:N	5:A:963:HOH:O	2.47	0.48
1:A:383:SER:O	1:B:114:THR:OG1	2.22	0.48
1:B:460:SER:OG	5:B:914:HOH:O	2.20	0.48
1:B:447:ILE:O	1:B:450:LEU:N	2.44	0.48
1:B:369:LYS:HZ1	4:B:660:NAI:H2D	1.78	0.48
1:A:121:ALA:HB3	1:A:122:GLU:CD	2.34	0.48
1:B:364:LYS:HB2	1:B:365:GLN:NE2	2.29	0.48
1:A:351:HIS:HA	1:A:403:LYS:O	2.14	0.48
1:A:192:ALA:CB	1:A:359:ASN:ND2	2.77	0.47
1:B:158:MET:CE	1:B:158:MET:HG3	2.45	0.47
1:B:194:ASN:ND2	1:B:195:GLN:HG2	2.30	0.47
1:A:155:TYR:CD1	1:A:173:LYS:HG3	2.48	0.47
1:B:242:LEU:C	1:B:242:LEU:HD23	2.35	0.47
1:B:122:GLU:HB2	1:B:124:ASN:ND2	2.28	0.47
1:B:229:ASN:ND2	1:B:233:GLU:OE2	2.42	0.47
1:B:319:ASP:N	1:B:319:ASP:OD1	2.47	0.47
1:B:369:LYS:HZ2	3:B:640:DG6:HC62	1.75	0.47
1:A:298:GLN:H	1:A:298:GLN:HE21	1.61	0.47
1:B:489:LYS:C	1:B:491:PRO:HD3	2.34	0.47
1:B:258:ASN:H	1:B:258:ASN:ND2	2.07	0.47
1:A:423:MET:HA	1:B:104:ASN:OD1	2.15	0.47
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.97	0.47
1:B:97:LYS:HG3	5:B:722:HOH:O	2.13	0.47
1:A:249:ARG:CG	1:A:249:ARG:O	2.62	0.47
1:A:68:ILE:CD1	1:A:142:PHE:CG	2.98	0.47
1:A:491:PRO:CD	1:A:501:ASN:HD21	2.28	0.47
1:A:196:ASP:O	1:A:197:GLU:CB	2.63	0.47
1:A:196:ASP:O	1:A:197:GLU:HB3	2.15	0.47
1:A:352:LEU:H	1:A:352:LEU:HD23	1.80	0.47
1:B:353:GLY:CA	1:B:406:LYS:HA	2.44	0.47
1:B:37:VAL:HA	1:B:46:ASP:O	2.15	0.47
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.73	0.47
1:A:360:LEU:CD1	3:A:630:DG6:HC61	2.39	0.47
1:A:250:TYR:HD1	1:A:368:SER:OG	1.98	0.46
1:A:40:THR:N	1:A:44:ARG:O	2.28	0.46
1:A:531:ARG:HD3	1:B:483:PHE:CE2	2.50	0.46
1:A:10:THR:HA	1:B:43:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:N	1:B:191:ILE:CD1	2.75	0.46
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.50	0.46
1:B:327:LYS:HG2	1:B:503:LEU:CD1	2.42	0.46
1:B:486:TYR:CD1	1:B:503:LEU:HG	2.50	0.46
1:A:159:GLN:HA	1:A:169:GLN:HE22	1.80	0.46
1:B:131:ASN:CA	1:B:136:MET:CE	2.92	0.46
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.83	0.46
1:A:185:ILE:CG2	1:A:187:TYR:CE2	2.99	0.46
1:A:374:SER:O	1:A:374:SER:OG	2.34	0.46
1:A:327:LYS:HD3	1:B:335:PHE:CZ	2.50	0.46
1:B:206:ASP:OD1	1:B:210:ASN:HB2	2.15	0.46
1:B:149:ILE:HD12	1:B:199:ALA:HB2	1.98	0.46
1:B:103:PRO:HA	5:B:933:HOH:O	2.14	0.46
1:A:136:MET:SD	1:A:136:MET:CB	2.96	0.46
1:B:408:VAL:O	1:B:411:SER:HB2	2.16	0.46
1:A:82:VAL:HG21	1:A:154:LEU:HD21	1.97	0.46
1:B:354:ASN:CG	1:B:356:ASP:CG	2.74	0.46
1:B:468:LYS:O	1:B:469:GLU:O	2.33	0.46
1:A:254:SER:H	1:A:258:ASN:HD21	1.63	0.46
1:B:231:LYS:HG3	1:B:239:VAL:HG21	1.98	0.46
1:B:353:GLY:N	1:B:408:VAL:HG23	2.31	0.46
1:B:297:PRO:HG3	1:B:369:LYS:CE	2.44	0.46
1:B:486:TYR:CG	1:B:486:TYR:O	2.69	0.46
1:B:80:THR:HB	1:B:164:LEU:HD21	1.97	0.46
1:B:470:ASP:O	1:B:471:ALA:HB2	2.15	0.46
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.51	0.46
1:A:76:ASN:HD22	1:A:76:ASN:N	2.13	0.46
1:A:358:TYR:CD1	1:A:404:TYR:CE2	3.04	0.46
1:B:362:ALA:HB1	1:B:364:LYS:HZ1	1.78	0.46
1:A:96:THR:HA	1:A:165:GLU:OE2	2.16	0.46
1:B:466:PRO:HB2	5:B:899:HOH:O	2.16	0.46
1:A:257:VAL:O	1:A:267:SER:OG	2.31	0.46
1:B:332:LEU:HD23	1:B:332:LEU:N	2.30	0.46
1:B:93:GLU:HB3	1:B:102:GLN:OE1	2.16	0.46
1:B:403:LYS:HB3	5:B:895:HOH:O	2.15	0.46
1:B:369:LYS:HD2	3:B:640:DG6:O3	2.14	0.45
1:B:166:TYR:CE2	1:B:170:GLN:HG3	2.51	0.45
1:A:310:GLU:HA	1:A:479:PRO:HG2	1.97	0.45
1:B:452:MET:HG3	1:B:487:TRP:CH2	2.51	0.45
1:B:332:LEU:HA	1:B:332:LEU:HD22	1.21	0.45
1:A:135:PRO:HG2	1:A:458:ARG:HH12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:O	1:B:177:SER:OG	2.34	0.45
1:A:358:TYR:HD1	1:A:404:TYR:CE2	2.33	0.45
1:B:353:GLY:HA3	1:B:406:LYS:HA	1.97	0.45
1:B:473:LYS:CA	1:B:473:LYS:CE	2.94	0.45
1:A:200:ASN:ND2	1:A:200:ASN:C	2.70	0.45
1:A:265:LEU:O	1:A:269:LYS:HG3	2.16	0.45
1:B:55:VAL:O	1:B:462:LYS:N	2.45	0.45
1:A:503:LEU:CD2	1:B:335:PHE:HE2	2.26	0.45
1:B:167:ASP:CG	1:B:167:ASP:O	2.55	0.45
1:A:530:GLU:CG	1:B:497:PHE:CD1	3.00	0.45
1:B:198:ARG:NE	5:B:969:HOH:O	2.50	0.45
1:B:332:LEU:CD2	1:B:332:LEU:N	2.70	0.45
1:A:268:ILE:HG12	1:A:275:ILE:HG21	1.98	0.45
1:B:186:TYR:CE1	1:B:191:ILE:HD11	2.49	0.45
1:B:334:GLN:NE2	1:B:380:ILE:HG12	2.32	0.45
1:B:67:GLY:O	1:B:240:ILE:N	2.45	0.45
1:A:319:ASP:HB2	1:A:490:ALA:O	2.16	0.45
1:A:412:LYS:C	5:A:956:HOH:O	2.53	0.45
1:A:250:TYR:CE1	1:A:371:ILE:HG21	2.52	0.45
1:A:443:THR:O	1:A:447:ILE:HG13	2.17	0.45
1:B:58:LEU:HA	1:B:458:ARG:O	2.17	0.45
1:A:243:TRP:CD1	1:A:243:TRP:C	2.90	0.45
1:A:145:SER:HB3	1:A:230:PHE:CE1	2.52	0.45
1:A:428:ASN:ND2	1:B:436:CYS:HB3	2.13	0.45
1:A:264:LEU:O	1:A:266:GLN:N	2.50	0.45
1:A:320:ASP:O	1:A:488:LEU:HA	2.18	0.44
1:B:439:SER:OG	4:B:660:NAI:O7N	2.28	0.44
1:B:373:LYS:NZ	1:B:376:VAL:CG1	2.76	0.44
1:B:481:LEU:HB3	1:B:484:LEU:HD23	1.99	0.44
1:B:187:TYR:HD1	1:B:277:PRO:HD3	1.82	0.44
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.52	0.44
1:A:389:ASN:C	1:A:389:ASN:OD1	2.55	0.44
1:B:22:LYS:HE3	1:B:27:LEU:HD12	1.99	0.44
1:B:443:THR:HB	1:B:444:PRO:HD3	2.00	0.44
1:B:198:ARG:CZ	5:B:969:HOH:O	2.66	0.44
1:B:372:SER:CA	5:B:801:HOH:O	2.65	0.44
1:A:322:LYS:NZ	1:A:503:LEU:CD1	2.75	0.44
1:B:64:GLU:HG2	5:B:772:HOH:O	2.17	0.44
1:B:134:LEU:HD21	1:B:518:ILE:HG22	1.99	0.44
1:A:272:HIS:CD2	1:A:274:GLU:H	2.35	0.44
1:A:308:LEU:CD2	1:A:312:GLU:CG	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD23	1:B:73:LEU:HD23	1.99	0.44
1:A:18:LYS:NZ	5:A:713:HOH:O	2.50	0.44
1:A:321:LEU:CD2	1:A:445:LEU:CD2	2.93	0.44
1:B:455:PHE:O	1:B:456:CYS:C	2.56	0.44
1:A:261:MET:H	1:A:307:GLN:NE2	2.15	0.44
1:B:52:GLN:HA	1:B:52:GLN:OE1	2.16	0.44
1:A:207:GLU:CA	1:A:207:GLU:OE1	2.62	0.44
1:A:57:LYS:HE3	1:A:474:PHE:CD1	2.53	0.44
1:B:492:LEU:HD13	1:B:493:THR:N	2.33	0.43
1:A:256:GLY:N	1:A:259:ASP:OD1	2.51	0.43
1:B:478:TYR:CE2	1:B:494:ARG:HB2	2.53	0.43
1:B:187:TYR:CD1	1:B:277:PRO:HD3	2.53	0.43
1:A:285:SER:HB3	1:A:290:VAL:CG2	2.45	0.43
1:A:469:GLU:O	1:A:470:ASP:HB3	2.17	0.43
1:A:136:MET:HG2	1:A:136:MET:CE	2.46	0.43
1:B:438:ASP:OD1	2:B:680:NH4:N	2.50	0.43
1:B:151:ASN:C	1:B:151:ASN:ND2	2.72	0.43
1:A:412:LYS:HG3	1:A:412:LYS:HZ3	1.13	0.43
1:B:254:SER:N	1:B:258:ASN:HD21	2.12	0.43
1:B:144:VAL:O	5:B:789:HOH:O	2.21	0.43
1:A:369:LYS:NZ	3:A:630:DG6:HC62	2.33	0.43
1:B:354:ASN:OD1	1:B:356:ASP:CB	2.65	0.43
1:B:473:LYS:HA	1:B:473:LYS:HE2	2.00	0.43
1:A:294:ASN:OD1	1:A:300:THR:HG23	2.18	0.43
1:B:194:ASN:C	1:B:194:ASN:HD22	2.22	0.43
1:B:95:GLN:HE21	1:B:96:THR:N	2.16	0.43
1:A:165:GLU:O	1:A:169:GLN:HG3	2.18	0.43
1:B:82:VAL:HG21	1:B:154:LEU:HD23	2.01	0.43
1:B:322:LYS:HB2	1:B:487:TRP:O	2.18	0.43
1:B:362:ALA:HB1	1:B:364:LYS:HZ3	1.79	0.43
1:B:115:LEU:HD21	1:B:511:GLU:HG3	1.96	0.43
1:A:104:ASN:HD22	1:A:106:PHE:H	1.66	0.43
1:B:276:ALA:O	1:B:277:PRO:C	2.55	0.43
1:B:354:ASN:HB2	1:B:356:ASP:OD2	2.19	0.43
1:B:368:SER:O	1:B:372:SER:HB3	2.19	0.43
1:B:489:LYS:HZ2	3:B:640:DG6:C1	2.32	0.43
1:B:286:ILE:C	1:B:288:GLU:N	2.70	0.43
1:B:454:GLU:O	1:B:457:THR:CG2	2.62	0.43
1:A:528:PHE:HB3	1:A:532:LEU:HD22	2.01	0.43
1:A:318:GLY:CA	1:A:488:LEU:HD22	2.49	0.43
1:A:389:ASN:HD21	1:A:392:LEU:HG	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:THR:HG23	5:A:692:HOH:O	2.14	0.43
1:A:354:ASN:HB2	1:A:356:ASP:OD1	2.19	0.42
1:B:372:SER:CB	5:B:801:HOH:O	2.67	0.42
1:A:502:GLY:O	1:A:503:LEU:C	2.58	0.42
1:A:225:ARG:HG3	1:A:225:ARG:NH2	2.34	0.42
1:A:315:PHE:CE1	1:A:481:LEU:HD21	2.54	0.42
1:B:68:ILE:HD12	1:B:450:LEU:HD13	2.01	0.42
1:B:68:ILE:HG22	1:B:70:LEU:HD13	2.00	0.42
1:B:39:LYS:HD3	1:B:45:PHE:CE2	2.54	0.42
1:B:303:PRO:O	1:B:306:VAL:N	2.52	0.42
1:A:223:ILE:HD12	1:A:281:PHE:CE2	2.54	0.42
1:A:335:PHE:HE1	1:B:503:LEU:HD22	1.83	0.42
1:A:40:THR:HG22	1:A:42:SER:H	1.84	0.42
1:A:217:TRP:CE3	1:A:269:LYS:HG2	2.54	0.42
1:B:29:LYS:HE2	5:B:816:HOH:O	2.19	0.42
1:B:192:ALA:O	1:B:194:ASN:N	2.52	0.42
1:A:69:MET:CG	1:A:69:MET:CE	2.90	0.42
1:A:392:LEU:N	1:A:392:LEU:HD23	2.33	0.42
1:B:352:LEU:HD22	1:B:402:ILE:HD11	2.01	0.42
1:B:261:MET:HG3	1:B:308:LEU:HD23	2.01	0.42
1:B:455:PHE:C	1:B:457:THR:N	2.71	0.42
1:A:497:PHE:CD2	1:B:530:GLU:HG3	2.55	0.42
1:A:39:LYS:HB3	1:A:39:LYS:HE2	1.60	0.42
1:A:354:ASN:ND2	1:A:410:ASP:OD2	2.48	0.42
1:B:480:VAL:HG12	1:B:482:THR:CG2	2.42	0.42
1:A:148:ASP:C	1:A:150:ASN:H	2.22	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD22	1.55	0.42
1:B:325:GLN:HE21	1:B:412:LYS:HE2	1.84	0.42
1:A:225:ARG:HE	1:A:229:ASN:ND2	1.98	0.42
1:A:96:THR:N	1:A:99:GLY:O	2.53	0.42
1:B:40:THR:HG21	1:B:44:ARG:NH1	2.35	0.42
1:B:349:TYR:O	1:B:350:ASN:HB3	2.19	0.42
1:A:322:LYS:HG3	1:A:489:LYS:CA	2.46	0.42
1:B:250:TYR:HA	1:B:299:ASN:ND2	2.34	0.42
1:B:316:ILE:CD1	1:B:316:ILE:C	2.88	0.42
1:B:529:GLU:H	1:B:529:GLU:CD	2.23	0.42
1:B:296:SER:HA	1:B:297:PRO:HD2	1.85	0.42
1:B:297:PRO:HD3	1:B:320:ASP:HB2	2.00	0.42
1:A:315:PHE:CZ	1:A:477:PHE:HB2	2.55	0.42
1:A:377:ILE:HA	1:A:377:ILE:HD13	1.72	0.42
1:A:323:SER:CB	1:A:326:THR:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:VAL:CG2	5:A:728:HOH:O	2.59	0.41
1:A:11:SER:O	1:B:44:ARG:HA	2.20	0.41
1:B:11:SER:CA	5:B:760:HOH:O	2.59	0.41
1:A:77:ASN:HD21	4:A:650:NAI:C7N	2.33	0.41
1:B:191:ILE:HG23	1:B:191:ILE:HD12	1.70	0.41
1:B:292:TYR:O	1:B:316:ILE:HA	2.20	0.41
1:A:163:VAL:CG1	1:A:440:LEU:HD13	2.50	0.41
1:B:55:VAL:O	1:B:461:TYR:HA	2.20	0.41
1:B:165:GLU:O	1:B:169:GLN:HG3	2.20	0.41
1:A:136:MET:HE1	1:A:452:MET:SD	2.60	0.41
1:B:61:LYS:HA	5:B:847:HOH:O	2.20	0.41
1:A:96:THR:CG2	1:A:98:GLU:N	2.81	0.41
1:B:225:ARG:HH21	1:B:225:ARG:HD3	1.72	0.41
1:B:322:LYS:O	1:B:323:SER:C	2.56	0.41
1:B:473:LYS:HG3	1:B:474:PHE:O	2.21	0.41
1:A:530:GLU:HB2	1:B:497:PHE:CE1	2.56	0.41
1:A:73:LEU:HG	1:A:154:LEU:HD11	2.01	0.41
1:B:82:VAL:HG21	1:B:154:LEU:CD2	2.51	0.41
1:B:322:LYS:HD3	1:B:327:LYS:HG3	2.02	0.41
1:B:306:VAL:O	1:B:310:GLU:HG3	2.21	0.41
1:B:116:LYS:CD	1:B:523:GLN:NE2	2.83	0.41
1:A:150:ASN:HB2	1:A:198:ARG:HG2	2.03	0.41
1:A:183:PRO:HA	1:A:201:ASN:O	2.21	0.41
1:A:352:LEU:CD2	1:A:352:LEU:N	2.83	0.41
1:B:392:LEU:N	1:B:392:LEU:HD23	2.35	0.41
1:B:253:VAL:HG22	1:B:302:VAL:HG12	2.02	0.41
1:A:442:ALA:O	1:A:445:LEU:HB3	2.21	0.41
1:B:492:LEU:HD22	1:B:492:LEU:HA	1.51	0.41
1:B:286:ILE:HG22	1:B:308:LEU:HD13	1.97	0.41
1:B:105:TYR:OH	1:B:140:ASN:ND2	2.54	0.41
1:A:291:PRO:CG	5:A:838:HOH:O	2.57	0.41
1:A:197:GLU:CD	1:A:197:GLU:C	2.79	0.41
1:B:501:ASN:HD22	1:B:501:ASN:N	2.19	0.41
1:A:403:LYS:HE3	1:A:403:LYS:HB3	1.74	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.97	0.41
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.21	0.41
1:A:21:TYR:N	1:A:21:TYR:CD1	2.88	0.41
5:A:800:HOH:O	1:B:168:LEU:HD11	2.16	0.40
1:A:276:ALA:O	1:A:279:THR:HB	2.21	0.40
1:B:162:GLN:NE2	5:B:991:HOH:O	2.50	0.40
1:B:109:MET:HE3	1:B:487:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ILE:CG2	5:B:799:HOH:O	2.68	0.40
1:A:447:ILE:O	1:A:451:VAL:HG23	2.21	0.40
1:B:15:VAL:HG13	1:B:15:VAL:H	1.60	0.40
1:A:281:PHE:O	1:A:285:SER:OG	2.37	0.40
1:B:297:PRO:CG	1:B:320:ASP:OD1	2.68	0.40
1:A:24:ASN:HD22	1:A:61:LYS:HB3	1.85	0.40
1:B:307:GLN:O	1:B:310:GLU:N	2.51	0.40
1:A:493:THR:CG2	1:A:494:ARG:N	2.84	0.40
1:B:101:LYS:HA	1:B:101:LYS:HD3	1.76	0.40
1:A:294:ASN:ND2	1:A:295:GLY:N	2.64	0.40
1:B:443:THR:N	1:B:444:PRO:HD2	2.35	0.40
1:B:491:PRO:O	1:B:493:THR:HG23	2.22	0.40
1:B:260:THR:HA	1:B:304:GLY:HA2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:MET:CE	1:A:415:MET:CE[2_555]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	523/533 (98%)	463 (88%)	37 (7%)	23 (4%)	3 1
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	3 1
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	3 1

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
1	A	197	GLU
1	A	198	ARG
1	A	208	LYS
1	A	210	ASN
1	A	319	ASP
1	A	323	SER
1	A	375	SER
1	B	41	ALA
1	B	196	ASP
1	B	197	GLU
1	B	207	GLU
1	B	375	SER
1	B	467	VAL
1	B	469	GLU
1	B	470	ASP
1	B	471	ALA
1	A	374	SER
1	A	469	GLU
1	A	470	ASP
1	A	481	LEU
1	A	495	PRO
1	B	193	ALA
1	B	322	LYS
1	B	361	SER
1	B	496	GLY
1	A	206	ASP
1	A	265	LEU
1	A	361	SER
1	B	22	LYS
1	B	319	ASP
1	B	468	LYS
1	B	495	PRO
1	A	320	ASP
1	B	320	ASP
1	B	473	LYS
1	A	125	ASP
1	A	496	GLY
1	B	106	PHE
1	B	356	ASP
1	B	491	PRO
1	A	502	GLY
1	B	209	GLY

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Mol	Chain	Res	Type
1	B	479	PRO
1	B	480	VAL
1	A	211	VAL
1	A	480	VAL
1	B	447	ILE
1	A	324	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	464/471 (98%)	396 (85%)	68 (15%)	4 3
1	B	463/471 (98%)	381 (82%)	82 (18%)	2 1
All	All	927/942 (98%)	777 (84%)	150 (16%)	3 2

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	16	THR
1	A	50	THR
1	A	58	LEU
1	A	65	LYS
1	A	66	LEU
1	A	70	LEU
1	A	76	ASN
1	A	86	LEU
1	A	92	VAL
1	A	96	THR
1	A	100	VAL
1	A	104	ASN
1	A	122	GLU
1	A	135	PRO
1	A	162	GLN
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	176	MET
1	A	189	ASP
1	A	197	GLU
1	A	200	ASN
1	A	201	ASN
1	A	211	VAL
1	A	220	LEU
1	A	222	ARG
1	A	225	ARG
1	A	236	LEU
1	A	246	ASN
1	A	252	GLU
1	A	258	ASN
1	A	259	ASP
1	A	285	SER
1	A	287	LEU
1	A	294	ASN
1	A	298	GLN
1	A	300	THR
1	A	308	LEU
1	A	319	ASP
1	A	323	SER
1	A	325	GLN
1	A	328	LEU
1	A	330	SER
1	A	332	LEU
1	A	336	LEU
1	A	356	ASP
1	A	364	LYS
1	A	367	ARG
1	A	373	LYS
1	A	374	SER
1	A	377	ILE
1	A	378	ASP
1	A	387	LEU
1	A	391	LYS
1	A	397	ASP
1	A	406	LYS
1	A	412	LYS
1	A	440	LEU
1	A	445	LEU

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Mol	Chain	Res	Type
1	A	453	THR
1	A	483	PHE
1	A	484	LEU
1	A	489	LYS
1	A	497	PHE
1	A	516	LEU
1	A	523	GLN
1	A	532	LEU
1	A	533	LEU
1	B	10	THR
1	B	15	VAL
1	B	16	THR
1	B	17	ASP
1	B	23	ASP
1	B	24	ASN
1	B	29	LYS
1	B	58	LEU
1	B	61	LYS
1	B	62	LYS
1	B	70	LEU
1	B	73	LEU
1	B	79	SER
1	B	80	THR
1	B	95	GLN
1	B	129	PRO
1	B	135	PRO
1	B	144	VAL
1	B	151	ASN
1	B	154	LEU
1	B	162	GLN
1	B	168	LEU
1	B	177	SER
1	B	191	ILE
1	B	194	ASN
1	B	197	GLU
1	B	201	ASN
1	B	207	GLU
1	B	213	THR
1	B	222	ARG
1	B	231	LYS
1	B	233	GLU
1	B	236	LEU

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Mol	Chain	Res	Type
1	B	237	ASP
1	B	257	VAL
1	B	258	ASN
1	B	265	LEU
1	B	273	GLU
1	B	277	PRO
1	B	278	SER
1	B	299	ASN
1	B	315	PHE
1	B	316	ILE
1	B	321	LEU
1	B	323	SER
1	B	325	GLN
1	B	328	LEU
1	B	329	LYS
1	B	330	SER
1	B	332	LEU
1	B	350	ASN
1	B	356	ASP
1	B	361	SER
1	B	364	LYS
1	B	365	GLN
1	B	367	ARG
1	B	371	ILE
1	B	373	LYS
1	B	376	VAL
1	B	387	LEU
1	B	395	LYS
1	B	400	ILE
1	B	415	MET
1	B	441	LEU
1	B	457	THR
1	B	465	ASP
1	B	468	LYS
1	B	473	LYS
1	B	479	PRO
1	B	482	THR
1	B	484	LEU
1	B	488	LEU
1	B	492	LEU
1	B	494	ARG
1	B	497	PHE

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Mol	Chain	Res	Type
1	B	504	ASN
1	B	510	LEU
1	B	514	LEU
1	B	515	ARG
1	B	517	LEU
1	B	522	SER
1	B	532	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	76	ASN
1	A	77	ASN
1	A	88	ASN
1	A	90	HIS
1	A	104	ASN
1	A	124	ASN
1	A	140	ASN
1	A	150	ASN
1	A	151	ASN
1	A	169	GLN
1	A	200	ASN
1	A	201	ASN
1	A	229	ASN
1	A	234	ASN
1	A	246	ASN
1	A	258	ASN
1	A	263	ASN
1	A	266	GLN
1	A	270	ASN
1	A	272	HIS
1	A	294	ASN
1	A	298	GLN
1	A	307	GLN
1	A	325	GLN
1	A	334	GLN
1	A	350	ASN
1	A	359	ASN
1	A	428	ASN
1	A	501	ASN
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	523	GLN
1	B	24	ASN
1	B	91	ASN
1	B	95	GLN
1	B	124	ASN
1	B	140	ASN
1	B	151	ASN
1	B	170	GLN
1	B	194	ASN
1	B	195	GLN
1	B	201	ASN
1	B	219	HIS
1	B	228	GLN
1	B	258	ASN
1	B	263	ASN
1	B	299	ASN
1	B	325	GLN
1	B	334	GLN
1	B	350	ASN
1	B	355	ASN
1	B	398	HIS
1	B	428	ASN
1	B	498	HIS
1	B	501	ASN
1	B	506	GLN
1	B	523	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are modelled with single atom - 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	$\#\|Z\| > 2$
3	DG6	A	630	-	14,14,14	4.33	10 (71%)	15,19,19	1.72	3 (20%)
4	NAI	A	650	-	38,48,48	3.45	23 (60%)	48,73,73	2.19	12 (25%)
3	DG6	B	640	-	14,14,14	3.66	9 (64%)	15,19,19	1.75	3 (20%)
4	NAI	B	660	-	38,48,48	3.83	20 (52%)	48,73,73	2.61	22 (45%)

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
3	DG6	A	630	-	1/1/4/4	0/17/17/17	0/0/0/0
4	NAI	A	650	-	-	0/25/72/72	0/5/5/5
3	DG6	B	640	-	1/1/4/4	0/17/17/17	0/0/0/0
4	NAI	B	660	-	-	0/25/72/72	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	O4B-C1B	-12.85	1.25	1.41
4	A	650	NAI	O2B-C2B	-8.21	1.23	1.43
4	A	650	NAI	O4B-C1B	-7.33	1.31	1.41
4	B	660	NAI	O2B-C2B	-5.74	1.29	1.43
4	A	650	NAI	PA-O1A	-5.40	1.31	1.51
4	A	650	NAI	O3B-C3B	-4.92	1.31	1.43
3	A	630	DG6	P-O1P	-4.49	1.38	1.54
4	B	660	NAI	O3B-C3B	-4.44	1.32	1.43
4	B	660	NAI	PN-O1N	-4.32	1.36	1.54
4	A	650	NAI	C2D-C1D	-4.30	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	650	NAI	PN-O1N	-3.94	1.38	1.54
4	A	650	NAI	C3D-C4D	-3.69	1.43	1.53
3	A	630	DG6	P-O3P	-3.68	1.39	1.51
4	A	650	NAI	C7N-N7N	-3.56	1.22	1.33
3	B	640	DG6	P-O1P	-3.45	1.42	1.54
4	B	660	NAI	C2A-N3A	-3.37	1.26	1.32
4	A	650	NAI	PA-O2A	-3.36	1.40	1.54
4	A	650	NAI	O3D-C3D	-3.34	1.35	1.43
3	A	630	DG6	P-O2P	-3.29	1.42	1.54
4	B	660	NAI	O3D-C3D	-3.20	1.35	1.43
4	B	660	NAI	C4N-C5N	-3.00	1.42	1.49
4	A	650	NAI	O7N-C7N	-2.93	1.17	1.24
4	B	660	NAI	C2B-C3B	-2.92	1.45	1.53
4	A	650	NAI	O5D-C5D	-2.47	1.34	1.44
3	B	640	DG6	P-O3P	-2.23	1.43	1.51
4	A	650	NAI	C4N-C5N	-2.21	1.44	1.49
3	B	640	DG6	P-O2P	-2.10	1.47	1.54
4	A	650	NAI	O4D-C4D	2.03	1.49	1.45
4	B	660	NAI	PA-O5B	2.10	1.68	1.59
4	B	660	NAI	C6A-N6A	2.31	1.42	1.34
3	B	640	DG6	O4-C4	2.38	1.48	1.43
4	A	650	NAI	PN-O2N	2.56	1.60	1.51
3	A	630	DG6	O4-C4	2.58	1.49	1.43
4	A	650	NAI	C5D-C4D	2.65	1.60	1.51
4	B	660	NAI	O2D-C2D	2.91	1.49	1.43
4	B	660	NAI	C8A-N7A	3.10	1.40	1.34
3	A	630	DG6	C2-C1	3.13	1.64	1.51
4	A	650	NAI	O2D-C2D	3.17	1.50	1.43
4	B	660	NAI	C2N-C3N	3.34	1.42	1.34
4	A	650	NAI	C2D-C3D	3.66	1.63	1.53
4	B	660	NAI	C1D-N1N	3.71	1.57	1.46
3	B	640	DG6	C5-C4	3.86	1.61	1.53
4	B	660	NAI	PN-O2N	4.06	1.66	1.51
4	B	660	NAI	C3B-C4B	4.16	1.64	1.53
3	A	630	DG6	C3-C4	4.17	1.62	1.53
4	A	650	NAI	C6N-N1N	4.49	1.50	1.37
4	A	650	NAI	C1D-N1N	4.53	1.59	1.46
3	B	640	DG6	C2-C3	4.56	1.61	1.52
4	A	650	NAI	C8A-N7A	4.56	1.43	1.34
3	B	640	DG6	C3-C4	4.66	1.63	1.53
3	A	630	DG6	C5-C4	4.73	1.63	1.53
4	B	660	NAI	C6N-N1N	4.90	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	C6N-C5N	4.92	1.42	1.33
4	B	660	NAI	O4D-C4D	5.03	1.56	1.45
4	A	650	NAI	C3B-C4B	5.04	1.66	1.53
3	B	640	DG6	P-O6	5.35	1.78	1.60
4	A	650	NAI	C4A-N3A	5.54	1.43	1.35
3	A	630	DG6	C2-C3	6.17	1.64	1.52
3	A	630	DG6	P-O6	6.51	1.82	1.60
3	B	640	DG6	C6-C5	8.32	1.64	1.51
3	A	630	DG6	C6-C5	8.75	1.65	1.51
4	B	660	NAI	C4A-N3A	10.07	1.50	1.35

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	660	NAI	C1B-N9A-C4A	-5.73	118.30	126.94
4	A	650	NAI	O7N-C7N-N7N	-4.95	110.45	122.76
4	A	650	NAI	C1B-N9A-C4A	-4.93	119.51	126.94
4	B	660	NAI	O2D-C2D-C1D	-4.20	95.27	109.94
4	B	660	NAI	C4B-O4B-C1B	-3.97	105.36	109.72
4	B	660	NAI	O3-PN-O5D	-3.45	93.78	102.94
4	B	660	NAI	O7N-C7N-N7N	-3.42	114.27	122.76
4	B	660	NAI	O3-PA-O5B	-3.35	94.06	102.94
4	A	650	NAI	O2D-C2D-C1D	-3.31	98.39	109.94
4	B	660	NAI	C5B-C4B-C3B	-3.20	102.53	115.21
4	B	660	NAI	O3D-C3D-C4D	-3.02	102.00	111.05
4	B	660	NAI	C4N-C5N-C6N	-2.84	117.89	122.58
4	A	650	NAI	C4N-C5N-C6N	-2.83	117.91	122.58
4	B	660	NAI	O4B-C4B-C5B	-2.36	100.89	109.32
4	A	650	NAI	O4B-C4B-C3B	-2.33	100.44	105.15
4	B	660	NAI	O2D-C2D-C3D	-2.18	104.73	111.83
4	A	650	NAI	O5D-PN-O2N	-2.15	101.28	109.62
4	B	660	NAI	O2B-C2B-C3B	-2.07	105.08	111.83
3	A	630	DG6	O2P-P-O6	2.29	113.15	106.56
4	B	660	NAI	C3D-C2D-C1D	2.31	106.05	101.40
4	A	650	NAI	C4B-O4B-C1B	2.48	112.44	109.72
4	A	650	NAI	C2D-C1D-N1N	2.61	120.39	113.34
3	B	640	DG6	O2P-P-O6	2.66	114.22	106.56
4	B	660	NAI	O5D-PN-O2N	2.79	120.44	109.62
4	B	660	NAI	C5N-C4N-C3N	2.86	120.39	112.52
4	B	660	NAI	C2A-N1A-C6A	3.20	124.49	118.77
3	B	640	DG6	O5-C5-C4	3.21	117.09	109.02
4	A	650	NAI	C2A-N1A-C6A	3.27	124.61	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	630	DG6	O5-C5-C4	3.33	117.39	109.02
4	B	660	NAI	O3B-C3B-C4B	3.36	121.13	111.05
4	A	650	NAI	C5N-C4N-C3N	3.62	122.51	112.52
4	B	660	NAI	C2D-C1D-N1N	3.63	123.14	113.34
3	A	630	DG6	O5-C5-C6	4.29	119.55	110.19
4	B	660	NAI	C4A-C5A-N7A	4.51	113.63	109.48
4	B	660	NAI	O2A-PA-O1A	4.54	137.15	112.53
3	B	640	DG6	O5-C5-C6	4.70	120.43	110.19
4	B	660	NAI	O4D-C1D-N1N	5.09	118.82	108.07
4	A	650	NAI	O2A-PA-O1A	5.37	141.64	112.53
4	B	660	NAI	N3A-C2A-N1A	6.48	133.86	128.89
4	A	650	NAI	O4D-C1D-N1N	7.07	123.00	108.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	640	DG6	C5
3	A	630	DG6	C5

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	630	DG6	10	0
4	A	650	NAI	8	0
3	B	640	DG6	17	0
4	B	660	NAI	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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