



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:49 pm BST

PDB ID : 1A3X  
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-  
PLEXED WITH PG, MN<sup>2+</sup> AND K<sup>+</sup>  
Authors : Jurica, M.S.; Mesecar, A.; Heath, P.J.; Shi, W.; Nowak, T.; Stoddard, B.L.  
Deposited on : 1998-01-26  
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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

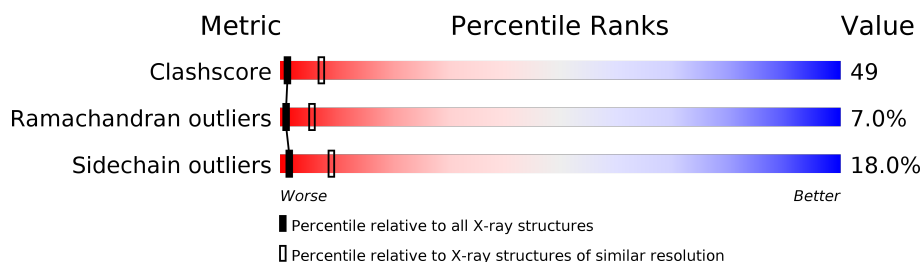
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGA	A	1005	-	-	X	-

## 2 Entry composition [i](#)

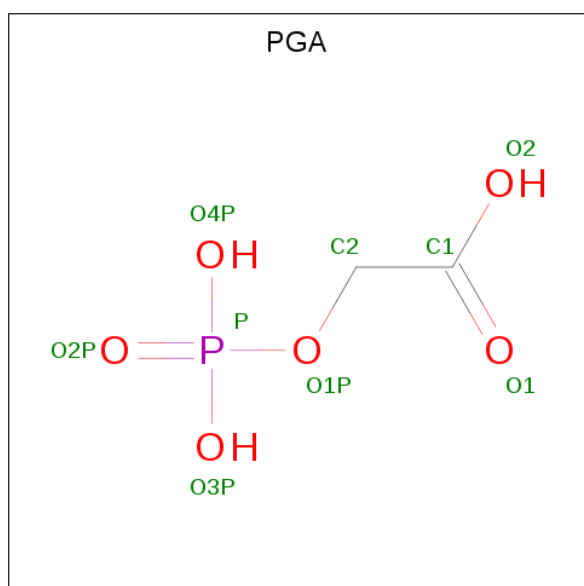
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			
1	B	487	Total	C	N	O	S	0	0	0
			3725	2347	642	718	18			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: C<sub>2</sub>H<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

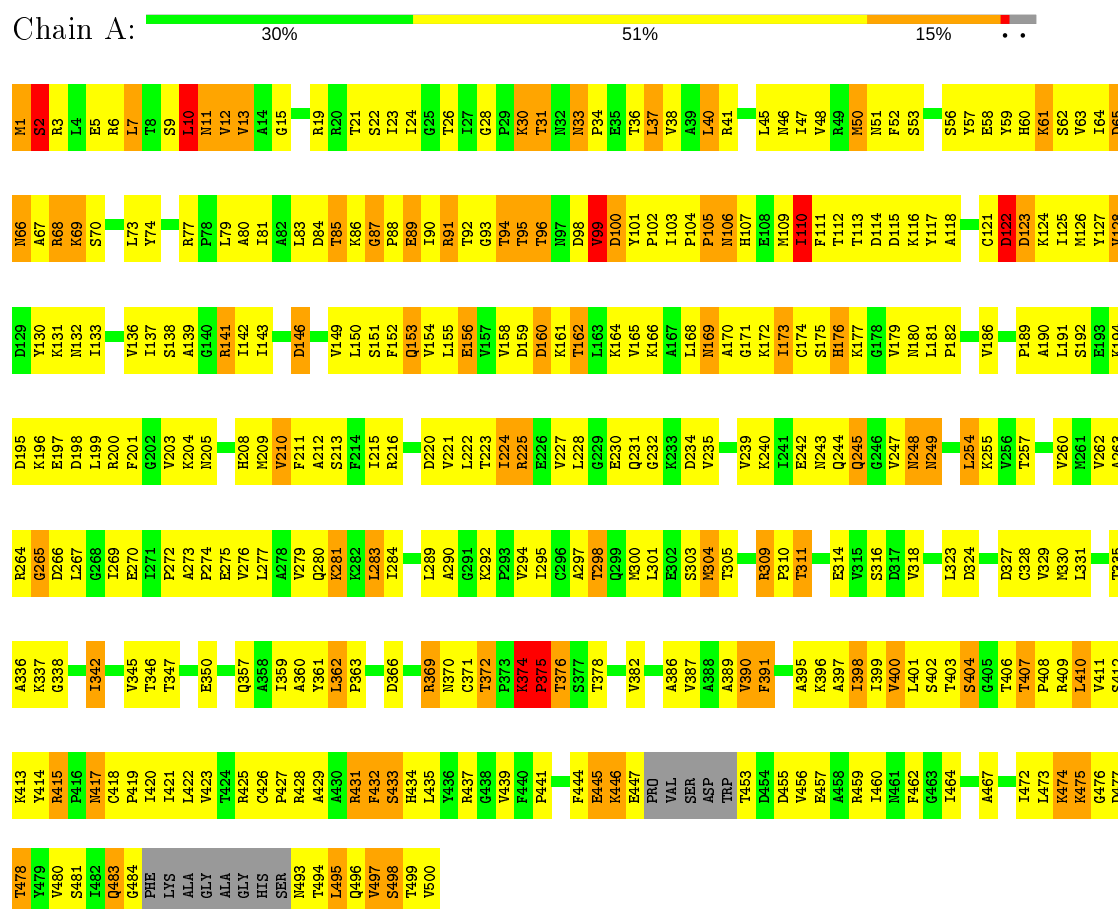
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0

### 3 Residue-property plots

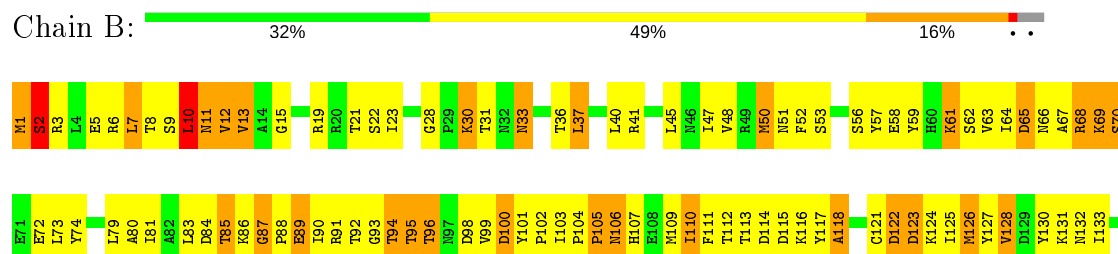
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: PYRUVATE KINASE



#### • Molecule 1: PYRUVATE KINASE



PHE	L422	M348	I271	E197	V136
LYS	V423	A349	P272	D198	I137
ALA	T424	E350	A273	L199	S138
GLY	R425		P274	R200	A139
ALA	C426	Q357	E275	F201	G140
GLY	P427	A358			R141
HIS	R428	I359	V279	H208	I142
SER	A429	A360	Q280	M209	I143
	A430	Y361	R281	V210	Y144
T494	R431	L362	K282	F211	V145
L495	P432	P363	L283	A212	D146
Q496	S433		I284	S213	D147
V497	H434	D366	P214	G148	G148
S498	L435		L289	I215	V149
T499	Y436	R369		R216	L150
V500	R370	N370	K292		S151
	G438	C371	P293	D220	F152
	V439	T372	V294	V221	Q153
	P440	P373	I295	L222	V154
	P441	K374	C296	T223	L155
		P375	A297	I224	E156
F444		T376	T298	R225	V157
E445		S377	Q299	E226	V158
K446		T378	M300	V227	D159
E447			L301	L228	D160
PRO		V382	E302		K161
VAL		A386	S303	Q231	T162
SER		V387	M304	G232	L163
ASP		A387	T305		K164
TRP		A388		V235	V165
T453		A389	P308		K166
D454		V390	R309	V239	A167
D455		F391	F310	K240	L168
V456			T311	E241	M169
E457		A395	E314	E242	A170
A458		K396	V315	N243	G171
R459		A397	S316	Q244	K172
I460		I398	S316	Q245	I173
M461		I399	D317	G246	C174
P462		V400	V318	V247	S175
G463		L401		N248	H176
I464		S402	L323		K177
E465		T403	D324	N249	G178
K466		S404			V179
A467			D327	L254	M180
E468		T407	C328	K255	L181
E469		P408	V329	V256	P182
		R409	M330	T257	G183
L473		L410	L331	D258	T184
K474		V411		G259	D185
K475		S412	A336	V260	V186
G476		K413	R337	M261	D187
D477		Y414	G338	V262	L188
T478		R415		A263	P189
Y479		P416	I342	R264	
V480		M417	N343	G265	A190
S481		C418	K344	D266	L191
I482		P419	V345	L267	
Q483		I420	T346	G268	K194
G484		I421	T347	I269	D195
				E270	K196

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.30 Å   106.40 Å   105.50 Å 90.00°   110.80°   90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	85.0 (100.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.227 , 0.341	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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: K, MN, PGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	2/3781 (0.1%)	0.88	4/5124 (0.1%)
1	B	0.41	0/3781	1.03	7/5124 (0.1%)
All	All	0.51	2/7562 (0.0%)	0.96	11/10248 (0.1%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	LYS	C-N	-26.09	0.84	1.34
1	A	375	PRO	C-N	5.31	1.46	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	PRO	O-C-N	-31.91	71.64	122.70
1	B	375	PRO	CA-C-N	-31.09	48.81	117.20
1	A	375	PRO	O-C-N	-25.38	82.10	122.70
1	A	375	PRO	CA-C-N	-24.09	64.20	117.20
1	B	374	LYS	O-C-N	-21.78	79.71	121.10
1	B	374	LYS	C-N-CD	-21.33	73.68	120.60
1	A	374	LYS	C-N-CD	-20.82	74.79	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	LYS	CA-C-N	14.60	157.98	117.10
1	B	375	PRO	C-N-CA	-7.56	102.79	121.70
1	A	374	LYS	C-N-CA	-7.31	91.29	122.00
1	B	374	LYS	C-N-CA	-5.03	100.89	122.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	374	LYS	Peptide
1	A	375	PRO	Mainchain
1	B	374	LYS	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

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	3725	0	3804	369	1
1	B	3725	0	3804	375	1
2	A	9	0	2	5	0
2	B	9	0	2	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	7472	0	7612	744	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 49.

All (744) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:HG2	1:A:375:PRO:HD3	1.25	1.11
1:B:186:VAL:HG23	1:B:216:ARG:HE	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:PRO:HB2	1:A:275:GLU:HG3	1.28	1.06
1:B:272:PRO:HB2	1:B:275:GLU:HG3	1.37	1.05
1:A:390:VAL:HB	1:A:395:ALA:HB3	1.37	1.02
1:A:378:THR:HG22	1:A:493:ASN:HD21	1.18	1.01
1:A:263:ALA:HB1	2:A:1005:PGA:O2	1.58	1.00
1:A:374:LYS:HG2	1:A:375:PRO:CD	1.89	1.00
1:B:378:THR:HG22	1:B:493:ASN:HD21	1.21	0.98
1:B:375:PRO:HB2	1:B:376:THR:OG1	1.61	0.98
1:B:390:VAL:HB	1:B:395:ALA:HB3	1.45	0.96
1:A:263:ALA:CB	2:A:1005:PGA:O2	2.14	0.96
1:A:220:ASP:O	1:A:224:ILE:HG22	1.63	0.95
1:B:374:LYS:H	1:B:375:PRO:HB3	1.31	0.95
1:B:374:LYS:N	1:B:375:PRO:HB3	1.82	0.94
1:B:220:ASP:O	1:B:224:ILE:HG22	1.69	0.93
1:B:342:ILE:HD13	1:B:342:ILE:H	1.33	0.91
1:A:374:LYS:CG	1:A:375:PRO:HD3	2.03	0.89
1:A:342:ILE:HD13	1:A:342:ILE:H	1.36	0.89
1:B:375:PRO:CB	1:B:376:THR:OG1	2.19	0.89
1:A:369:ARG:HE	1:A:370:ASN:HD21	1.22	0.87
1:B:310:PRO:HG3	1:B:347:THR:HG21	1.58	0.86
1:A:264:ARG:HH21	1:A:280:GLN:HE22	1.24	0.84
1:B:395:ALA:HA	1:B:478:THR:HG23	1.57	0.84
1:A:224:ILE:O	1:A:228:LEU:HD23	1.78	0.84
1:A:265:GLY:N	2:A:1005:PGA:O1	2.12	0.83
1:A:378:THR:HG22	1:A:493:ASN:ND2	1.93	0.83
1:A:395:ALA:HA	1:A:478:THR:HG23	1.61	0.83
1:B:224:ILE:O	1:B:228:LEU:HD23	1.79	0.83
1:A:310:PRO:HG3	1:A:347:THR:HG21	1.61	0.83
1:B:369:ARG:HE	1:B:370:ASN:HD21	1.24	0.82
1:B:378:THR:HG22	1:B:493:ASN:ND2	1.95	0.82
1:B:51:ASN:HD21	1:B:53:SER:HB2	1.44	0.82
1:A:106:ASN:HD21	1:A:166:LYS:NZ	1.78	0.81
1:B:153:GLN:HB2	1:B:168:LEU:HD21	1.60	0.81
1:A:151:SER:H	1:A:169:ASN:HD21	1.25	0.81
1:A:158:VAL:HB	1:A:162:THR:HB	1.60	0.81
1:A:155:LEU:HB2	1:A:164:LYS:HG2	1.62	0.81
1:B:216:ARG:HB3	1:B:245:GLN:HG2	1.61	0.81
1:A:56:SER:N	1:A:59:TYR:HB2	1.97	0.80
1:B:309:ARG:HD3	1:B:309:ARG:N	1.93	0.80
1:B:104:PRO:HD2	1:B:171:GLY:O	1.82	0.79
1:B:481:SER:HB2	1:B:496:GLN:HB3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HB	1:B:162:THR:HB	1.64	0.79
1:A:254:LEU:O	1:A:292:LYS:HE3	1.83	0.79
1:B:56:SER:N	1:B:59:TYR:HB2	1.98	0.79
1:A:151:SER:N	1:A:169:ASN:HD21	1.80	0.79
1:B:90:ILE:HD12	1:B:130:TYR:HB2	1.64	0.79
1:B:52:PHE:O	1:B:86:LYS:HB2	1.82	0.78
1:A:369:ARG:HE	1:A:370:ASN:ND2	1.80	0.78
1:B:366:ASP:O	1:B:369:ARG:HG3	1.83	0.78
1:A:481:SER:HB2	1:A:496:GLN:HB3	1.65	0.78
1:B:396:LYS:O	1:B:418:CYS:HB2	1.83	0.78
1:B:51:ASN:ND2	1:B:53:SER:HB2	1.99	0.78
1:B:254:LEU:O	1:B:292:LYS:HE3	1.82	0.77
1:A:51:ASN:HD21	1:A:53:SER:HB2	1.49	0.77
1:A:90:ILE:HD12	1:A:130:TYR:HB2	1.65	0.77
1:B:139:ALA:HA	1:B:154:VAL:HG12	1.67	0.77
1:B:141:ARG:HH12	1:B:181:LEU:HB3	1.50	0.76
1:B:408:PRO:HG3	1:B:422:LEU:HD13	1.66	0.76
1:A:284:ILE:HG23	1:A:294:VAL:HG11	1.66	0.76
1:A:275:GLU:O	1:A:279:VAL:HG23	1.86	0.75
1:A:295:ILE:HG12	1:A:328:CYS:HB2	1.68	0.75
1:A:33:ASN:HD21	1:A:36:THR:H	1.32	0.75
1:B:496:GLN:HE21	1:B:498:SER:HB2	1.50	0.75
1:B:90:ILE:HB	1:B:179:VAL:HB	1.67	0.75
1:B:189:PRO:HB2	1:B:191:LEU:O	1.87	0.75
1:A:216:ARG:HB3	1:A:245:GLN:HG2	1.68	0.75
1:A:51:ASN:ND2	1:A:53:SER:HB2	2.02	0.74
1:A:52:PHE:O	1:A:86:LYS:HB2	1.87	0.74
1:A:125:ILE:HG12	1:A:126:MET:H	1.53	0.74
1:A:117:TYR:O	1:A:121:CYS:HB3	1.88	0.74
1:A:408:PRO:HG3	1:A:422:LEU:HD13	1.69	0.74
1:A:263:ALA:HA	2:A:1005:PGA:O2	1.87	0.74
1:B:151:SER:H	1:B:169:ASN:HD21	1.36	0.74
1:B:369:ARG:HE	1:B:370:ASN:ND2	1.85	0.74
1:A:366:ASP:O	1:A:369:ARG:HG3	1.88	0.74
1:A:496:GLN:HG3	1:A:497:VAL:N	2.02	0.73
1:A:346:THR:O	1:A:350:GLU:HG3	1.87	0.73
1:B:117:TYR:O	1:B:121:CYS:HB3	1.89	0.73
1:B:151:SER:N	1:B:169:ASN:HD21	1.86	0.73
1:B:155:LEU:HB2	1:B:164:LYS:HG2	1.71	0.73
1:B:496:GLN:HG3	1:B:497:VAL:H	1.53	0.73
1:B:372:THR:O	1:B:372:THR:HG22	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ILE:HG23	1:B:420:ILE:HA	1.71	0.72
1:B:496:GLN:HG3	1:B:497:VAL:N	2.04	0.72
1:B:417:ASN:HD22	1:B:417:ASN:H	1.36	0.72
1:A:396:LYS:O	1:A:418:CYS:HB2	1.88	0.72
1:A:423:VAL:HG11	1:A:459:ARG:HB3	1.72	0.72
1:A:151:SER:H	1:A:169:ASN:ND2	1.88	0.72
1:B:295:ILE:HG12	1:B:328:CYS:HB2	1.70	0.72
1:B:125:ILE:HG12	1:B:126:MET:H	1.55	0.72
1:A:311:THR:OG1	1:A:314:GLU:HG3	1.90	0.71
1:A:398:ILE:HG23	1:A:420:ILE:HA	1.71	0.71
1:B:213:SER:HA	1:B:240:LYS:HD3	1.73	0.71
1:A:417:ASN:H	1:A:417:ASN:HD22	1.39	0.71
1:B:86:LYS:HG2	1:B:89:GLU:OE2	1.91	0.71
1:A:125:ILE:HG12	1:A:126:MET:N	2.06	0.71
1:A:372:THR:HG22	1:A:372:THR:O	1.88	0.71
1:A:496:GLN:HG3	1:A:497:VAL:H	1.55	0.71
1:B:346:THR:O	1:B:350:GLU:HG3	1.91	0.70
1:B:499:THR:HG22	1:B:500:VAL:N	2.07	0.70
1:B:79:LEU:HD12	1:B:80:ALA:H	1.55	0.70
1:A:263:ALA:C	2:A:1005:PGA:O2	2.29	0.70
1:A:153:GLN:HB2	1:A:168:LEU:HD21	1.74	0.70
1:B:456:VAL:O	1:B:460:ILE:HG13	1.92	0.70
1:A:496:GLN:HE21	1:A:498:SER:HB2	1.56	0.70
1:A:121:CYS:O	1:A:122:ASP:HB3	1.92	0.70
1:A:476:GLY:H	1:A:500:VAL:HB	1.57	0.70
1:B:284:ILE:HG23	1:B:294:VAL:HG11	1.73	0.70
1:B:67:ALA:HB1	1:B:79:LEU:HD21	1.74	0.70
1:A:48:VAL:HG23	1:A:79:LEU:HD11	1.72	0.69
1:A:106:ASN:HD21	1:A:166:LYS:HZ3	1.41	0.69
1:B:209:MET:O	1:B:210:VAL:HG23	1.91	0.69
1:B:243:ASN:HA	1:B:270:GLU:HG2	1.75	0.69
1:B:499:THR:HG22	1:B:500:VAL:H	1.56	0.69
1:A:104:PRO:HD2	1:A:171:GLY:O	1.93	0.69
1:A:141:ARG:HH12	1:A:181:LEU:HB3	1.58	0.68
1:A:86:LYS:HG2	1:A:89:GLU:OE2	1.93	0.68
1:A:101:TYR:HD2	1:A:172:LYS:HZ1	1.40	0.68
1:A:499:THR:HG22	1:A:500:VAL:H	1.59	0.68
1:A:369:ARG:NE	1:A:370:ASN:HD21	1.92	0.68
1:A:90:ILE:HG23	1:A:130:TYR:HB2	1.75	0.68
1:A:499:THR:HG22	1:A:500:VAL:N	2.08	0.68
1:A:247:VAL:C	1:A:249:ASN:H	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:NE2	1:A:431:ARG:HD3	2.10	0.67
1:B:125:ILE:HG12	1:B:126:MET:N	2.09	0.67
1:B:264:ARG:HH21	1:B:280:GLN:HE22	1.40	0.67
1:A:213:SER:HA	1:A:240:LYS:HD3	1.77	0.67
1:A:304:MET:HG3	1:A:310:PRO:HB3	1.76	0.67
1:B:301:LEU:HD23	1:B:314:GLU:HB3	1.75	0.67
1:B:124:LYS:N	1:B:124:LYS:HD2	2.10	0.67
1:B:311:THR:OG1	1:B:314:GLU:HG3	1.95	0.67
1:B:476:GLY:H	1:B:500:VAL:HB	1.59	0.67
1:A:243:ASN:HA	1:A:270:GLU:HG2	1.76	0.67
1:B:53:SER:HA	1:B:86:LYS:CG	2.24	0.66
1:B:475:LYS:HA	1:B:500:VAL:HB	1.78	0.66
1:B:360:ALA:HB1	1:B:363:PRO:HG2	1.78	0.66
1:B:133:ILE:HA	1:B:136:VAL:HG22	1.76	0.66
1:B:275:GLU:O	1:B:279:VAL:HG23	1.95	0.66
1:A:53:SER:HA	1:A:86:LYS:CG	2.24	0.66
1:A:84:ASP:CG	1:A:240:LYS:HZ2	1.98	0.66
1:A:33:ASN:ND2	1:A:36:THR:H	1.93	0.66
1:B:216:ARG:HG2	1:B:243:ASN:HD21	1.61	0.66
1:A:56:SER:H	1:A:59:TYR:HB2	1.60	0.65
1:A:216:ARG:HG2	1:A:243:ASN:HD21	1.61	0.65
1:B:53:SER:HA	1:B:86:LYS:HG3	1.77	0.65
1:A:3:ARG:HG2	1:A:7:LEU:HD22	1.77	0.65
1:A:483:GLN:HE21	1:A:483:GLN:N	1.94	0.65
1:A:53:SER:HA	1:A:86:LYS:HG3	1.77	0.65
1:A:360:ALA:HB1	1:A:363:PRO:HG2	1.79	0.65
1:B:139:ALA:HA	1:B:154:VAL:CG1	2.26	0.65
1:A:107:HIS:CE1	1:A:109:MET:HB3	2.32	0.65
1:A:390:VAL:CB	1:A:395:ALA:HB3	2.21	0.65
1:B:369:ARG:NE	1:B:370:ASN:HD21	1.94	0.65
1:B:56:SER:H	1:B:59:TYR:HB2	1.60	0.65
1:B:64:ILE:HG12	1:B:81:ILE:HG21	1.79	0.65
1:A:475:LYS:HA	1:A:500:VAL:HB	1.79	0.65
1:B:423:VAL:HG11	1:B:459:ARG:HB3	1.78	0.65
1:B:483:GLN:HE21	1:B:483:GLN:N	1.94	0.65
1:B:211:PHE:O	1:B:240:LYS:HD2	1.97	0.65
1:B:308:PRO:C	1:B:309:ARG:HD3	2.18	0.64
1:B:387:VAL:O	1:B:390:VAL:HG13	1.97	0.64
1:B:69:LYS:NZ	1:B:73:LEU:HG	2.12	0.64
1:B:33:ASN:HD21	1:B:36:THR:H	1.45	0.64
1:A:107:HIS:HE1	1:A:109:MET:HB3	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:O	1:A:133:ILE:HG22	1.97	0.64
1:B:112:THR:HG23	1:B:161:LYS:O	1.98	0.64
1:B:260:VAL:HG13	1:B:294:VAL:HG23	1.79	0.64
1:B:263:ALA:C	2:B:1006:PGA:O1	2.36	0.64
1:A:67:ALA:HB1	1:A:79:LEU:HD21	1.80	0.64
1:A:133:ILE:HA	1:A:136:VAL:HG22	1.79	0.63
1:A:196:LYS:HB3	1:A:200:ARG:HH21	1.63	0.63
1:B:247:VAL:C	1:B:249:ASN:H	2.02	0.63
1:B:208:HIS:NE2	1:B:431:ARG:HD3	2.13	0.63
1:A:375:PRO:O	1:A:376:THR:C	2.36	0.63
1:B:297:ALA:O	1:B:298:THR:HB	1.98	0.63
1:A:211:PHE:O	1:A:240:LYS:HD2	1.97	0.63
1:A:9:SER:O	1:A:11:ASN:N	2.31	0.63
1:B:398:ILE:HD13	1:B:411:VAL:HG11	1.80	0.63
1:B:3:ARG:HG2	1:B:7:LEU:HD22	1.78	0.63
1:A:64:ILE:HG12	1:A:81:ILE:HG21	1.80	0.63
1:B:107:HIS:HE1	1:B:109:MET:HB3	1.63	0.63
1:B:304:MET:HG3	1:B:310:PRO:HB3	1.79	0.63
1:A:257:THR:O	1:A:292:LYS:HD3	1.99	0.63
1:B:257:THR:O	1:B:292:LYS:HD3	1.98	0.63
1:A:429:ALA:HA	1:A:432:PHE:CZ	2.33	0.63
1:B:429:ALA:HA	1:B:432:PHE:CZ	2.34	0.63
1:A:209:MET:O	1:A:210:VAL:HG23	1.99	0.62
1:B:186:VAL:CG2	1:B:216:ARG:HE	2.06	0.62
1:A:113:THR:HG22	1:A:128:VAL:O	1.98	0.62
1:A:92:THR:HG22	1:A:177:LYS:H	1.64	0.62
1:A:141:ARG:HH22	1:A:181:LEU:HA	1.63	0.62
1:B:101:TYR:CD1	1:B:174:CYS:HA	2.33	0.62
1:B:92:THR:HG22	1:B:177:LYS:H	1.65	0.62
1:A:112:THR:HG23	1:A:161:LYS:O	1.99	0.62
1:A:110:ILE:HD11	1:A:162:THR:HG23	1.82	0.62
1:B:111:PHE:CZ	1:B:126:MET:SD	2.93	0.61
1:B:232:GLY:O	1:B:235:VAL:HG22	2.00	0.61
1:A:101:TYR:HB3	1:A:172:LYS:HG3	1.82	0.61
1:A:12:VAL:O	1:A:13:VAL:HB	2.00	0.61
1:A:180:ASN:O	1:A:182:PRO:HD3	2.01	0.61
1:B:113:THR:HG22	1:B:128:VAL:O	2.00	0.61
1:B:375:PRO:HB3	1:B:376:THR:OG1	1.99	0.61
1:B:9:SER:O	1:B:11:ASN:N	2.33	0.61
1:B:56:SER:O	1:B:59:TYR:HB2	2.01	0.61
1:B:151:SER:H	1:B:169:ASN:ND2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:PRO:HB2	1:B:376:THR:HG1	1.66	0.60
1:B:141:ARG:HH22	1:B:181:LEU:HA	1.65	0.60
1:B:2:SER:HB2	1:B:5:GLU:HB2	1.83	0.60
1:B:362:LEU:HB2	1:B:363:PRO:CD	2.31	0.60
1:A:301:LEU:HD23	1:A:314:GLU:HB3	1.82	0.60
1:B:398:ILE:HG12	1:B:398:ILE:O	2.01	0.60
1:A:93:GLY:HA3	1:A:127:TYR:HB3	1.82	0.60
1:A:2:SER:HB2	1:A:5:GLU:HB2	1.82	0.60
1:B:102:PRO:HB3	1:B:123:ASP:OD2	2.01	0.60
1:A:297:ALA:O	1:A:298:THR:HB	2.02	0.60
1:A:112:THR:HB	1:A:125:ILE:HD11	1.82	0.60
1:A:403:THR:HG23	1:A:426:CYS:HB2	1.83	0.60
1:B:107:HIS:CE1	1:B:109:MET:HB3	2.37	0.60
1:B:141:ARG:HH12	1:B:181:LEU:CB	2.14	0.60
1:A:409:ARG:O	1:A:412:SER:HB3	2.01	0.60
1:A:474:LYS:O	1:A:475:LYS:HB3	2.00	0.60
1:B:396:LYS:O	1:B:419:PRO:HD2	2.02	0.60
1:B:242:GLU:HA	1:B:267:LEU:HD13	1.84	0.59
1:B:475:LYS:HA	1:B:500:VAL:CG1	2.32	0.59
1:B:48:VAL:HG23	1:B:79:LEU:HD11	1.83	0.59
1:B:151:SER:HB2	1:B:168:LEU:HB2	1.84	0.59
1:A:65:ASP:HA	1:A:68:ARG:HB2	1.84	0.59
1:A:41:ARG:NH2	1:A:74:TYR:O	2.36	0.59
1:B:95:THR:HA	1:B:121:CYS:O	2.03	0.59
1:A:56:SER:O	1:A:59:TYR:HB2	2.03	0.59
1:A:242:GLU:HA	1:A:267:LEU:HD13	1.84	0.59
1:A:300:MET:O	1:A:314:GLU:HB3	2.03	0.59
1:B:15:GLY:H	1:B:357:GLN:HE22	1.51	0.59
1:A:139:ALA:HA	1:A:154:VAL:HG12	1.85	0.58
1:A:398:ILE:HD13	1:A:411:VAL:HG11	1.83	0.58
1:A:15:GLY:H	1:A:357:GLN:HE22	1.52	0.58
1:A:387:VAL:O	1:A:390:VAL:HG13	2.03	0.58
1:B:156:GLU:HB2	1:B:164:LYS:HE2	1.86	0.58
1:A:151:SER:HB2	1:A:168:LEU:HB2	1.85	0.58
1:B:121:CYS:O	1:B:122:ASP:HB3	2.03	0.58
1:B:474:LYS:O	1:B:475:LYS:HB3	2.04	0.58
1:A:12:VAL:HG23	1:A:13:VAL:HG23	1.85	0.58
1:B:151:SER:HB3	1:B:168:LEU:HD12	1.85	0.58
1:B:195:ASP:HA	1:B:198:ASP:OD2	2.03	0.58
1:B:477:ASP:O	1:B:478:THR:HB	2.03	0.58
1:A:101:TYR:CE1	1:A:174:CYS:HB3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:THR:HA	1:B:175:SER:HB2	1.85	0.58
1:A:69:LYS:NZ	1:A:73:LEU:HG	2.18	0.58
1:A:94:THR:HA	1:A:175:SER:HB2	1.84	0.57
1:B:105:PRO:HD2	1:B:107:HIS:CD2	2.39	0.57
1:B:417:ASN:N	1:B:417:ASN:HD22	2.01	0.57
1:A:303:SER:C	1:A:305:THR:H	2.07	0.57
1:A:91:ARG:HH11	1:A:91:ARG:HG2	1.69	0.57
1:B:69:LYS:HZ2	1:B:73:LEU:HG	1.68	0.57
1:A:475:LYS:HA	1:A:500:VAL:CG1	2.34	0.57
1:B:110:ILE:HD11	1:B:162:THR:HG23	1.86	0.57
1:B:264:ARG:HB2	1:B:297:ALA:O	2.05	0.57
1:B:480:VAL:HG13	1:B:496:GLN:O	2.03	0.57
1:A:106:ASN:ND2	1:A:166:LYS:NZ	2.50	0.57
1:A:112:THR:HA	1:A:161:LYS:O	2.05	0.57
1:A:101:TYR:CD1	1:A:174:CYS:HA	2.39	0.57
1:A:189:PRO:HB2	1:A:191:LEU:O	2.05	0.57
1:B:403:THR:HG23	1:B:426:CYS:HB2	1.87	0.57
1:B:112:THR:HB	1:B:125:ILE:HD11	1.87	0.57
1:B:431:ARG:O	1:B:434:HIS:HD2	1.88	0.57
1:B:65:ASP:HA	1:B:68:ARG:HB2	1.87	0.57
1:A:456:VAL:O	1:A:460:ILE:HG13	2.05	0.57
1:A:141:ARG:HH12	1:A:181:LEU:CB	2.16	0.56
1:B:33:ASN:ND2	1:B:36:THR:H	2.02	0.56
1:B:409:ARG:O	1:B:412:SER:HB3	2.05	0.56
1:A:141:ARG:HE	1:A:142:ILE:N	2.04	0.56
1:A:92:THR:O	1:A:176:HIS:HD2	1.87	0.56
1:A:84:ASP:OD1	1:A:240:LYS:NZ	2.37	0.56
1:B:180:ASN:O	1:B:182:PRO:HD3	2.05	0.56
1:A:401:LEU:N	1:A:401:LEU:HD12	2.21	0.56
1:B:110:ILE:HD13	1:B:125:ILE:HG13	1.87	0.56
1:A:101:TYR:HD2	1:A:172:LYS:NZ	2.03	0.55
1:A:110:ILE:HD13	1:A:125:ILE:HG13	1.88	0.55
1:A:247:VAL:O	1:A:249:ASN:N	2.39	0.55
1:A:264:ARG:HB2	1:A:297:ALA:O	2.06	0.55
1:A:153:GLN:HG3	1:A:168:LEU:HD21	1.88	0.55
1:A:232:GLY:O	1:A:235:VAL:HG22	2.05	0.55
1:A:396:LYS:O	1:A:419:PRO:HD2	2.06	0.55
1:A:79:LEU:HD12	1:A:80:ALA:H	1.71	0.55
1:B:362:LEU:HB2	1:B:363:PRO:HD3	1.87	0.55
1:A:480:VAL:HG13	1:A:496:GLN:O	2.05	0.55
1:B:112:THR:HA	1:B:161:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:HB1	1:B:79:LEU:CD2	2.36	0.55
1:B:141:ARG:HE	1:B:142:ILE:N	2.05	0.55
1:B:300:MET:O	1:B:314:GLU:HB3	2.06	0.55
1:B:153:GLN:CB	1:B:168:LEU:HD21	2.32	0.55
1:A:67:ALA:HB1	1:A:79:LEU:CD2	2.36	0.55
1:A:195:ASP:HA	1:A:198:ASP:OD2	2.07	0.55
1:A:444:PHE:CE2	1:A:459:ARG:HG2	2.42	0.55
1:B:12:VAL:O	1:B:13:VAL:HB	2.06	0.55
1:B:79:LEU:HD12	1:B:80:ALA:N	2.22	0.55
1:A:114:ASP:O	1:A:115:ASP:HB2	2.06	0.54
1:A:208:HIS:CE1	1:A:431:ARG:HD3	2.43	0.54
1:A:398:ILE:O	1:A:398:ILE:HG12	2.07	0.54
1:A:477:ASP:O	1:A:478:THR:HB	2.07	0.54
1:B:102:PRO:O	1:B:173:ILE:HG22	2.06	0.54
1:A:401:LEU:HD23	1:A:459:ARG:HD2	1.89	0.54
1:A:57:TYR:O	1:A:61:LYS:HB2	2.08	0.54
1:B:460:ILE:O	1:B:464:ILE:HG13	2.08	0.54
1:B:399:ILE:HA	1:B:421:ILE:O	2.07	0.54
1:B:495:LEU:C	1:B:495:LEU:HD23	2.28	0.54
1:B:41:ARG:NH2	1:B:74:TYR:O	2.40	0.54
1:B:86:LYS:NZ	1:B:89:GLU:HG3	2.22	0.54
1:A:476:GLY:N	1:A:500:VAL:HB	2.21	0.54
1:B:141:ARG:HH21	1:B:143:ILE:HA	1.73	0.54
1:B:101:TYR:HD2	1:B:172:LYS:HZ1	1.56	0.54
1:B:208:HIS:CE1	1:B:431:ARG:HD3	2.43	0.54
1:A:47:ILE:HG12	1:A:80:ALA:HB3	1.89	0.54
1:B:110:ILE:HD11	1:B:112:THR:OG1	2.07	0.54
1:B:45:LEU:HD21	1:B:48:VAL:CG2	2.38	0.54
1:B:402:SER:HB3	1:B:422:LEU:HD11	1.89	0.54
1:A:362:LEU:HB2	1:A:363:PRO:CD	2.38	0.53
1:A:146:ASP:OD1	1:A:177:LYS:HD2	2.08	0.53
1:A:431:ARG:O	1:A:434:HIS:HD2	1.90	0.53
1:A:52:PHE:CD2	1:A:198:ASP:HB3	2.44	0.53
1:B:159:ASP:HB2	1:B:162:THR:OG1	2.09	0.53
1:B:444:PHE:CE2	1:B:459:ARG:HG2	2.43	0.53
1:B:130:TYR:O	1:B:133:ILE:HG22	2.08	0.53
1:B:47:ILE:HG12	1:B:80:ALA:HB3	1.91	0.53
1:A:399:ILE:HA	1:A:421:ILE:O	2.09	0.53
1:A:427:PRO:O	1:A:431:ARG:HG3	2.09	0.53
1:A:453:THR:O	1:A:453:THR:HG22	2.09	0.53
1:B:273:ALA:N	1:B:274:PRO:HD2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD21	1:B:48:VAL:HG22	1.91	0.53
1:A:478:THR:O	1:A:478:THR:HG23	2.09	0.53
1:B:196:LYS:HB3	1:B:200:ARG:HH21	1.74	0.53
1:B:445:GLU:O	1:B:446:LYS:CB	2.56	0.53
1:A:69:LYS:HZ2	1:A:73:LEU:HG	1.73	0.53
1:B:114:ASP:O	1:B:115:ASP:HB2	2.08	0.53
1:A:112:THR:CB	1:A:125:ILE:HD11	2.39	0.53
1:A:52:PHE:HZ	1:A:201:PHE:CE2	2.27	0.53
1:A:496:GLN:CG	1:A:497:VAL:H	2.22	0.52
1:B:153:GLN:HG3	1:B:168:LEU:HD21	1.91	0.52
1:B:303:SER:C	1:B:305:THR:H	2.11	0.52
1:B:362:LEU:HD13	1:B:362:LEU:N	2.24	0.52
1:A:45:LEU:HD21	1:A:48:VAL:HG22	1.91	0.52
1:B:476:GLY:N	1:B:500:VAL:HB	2.23	0.52
1:B:86:LYS:HZ2	1:B:89:GLU:HG3	1.75	0.52
1:A:102:PRO:HB3	1:A:123:ASP:OD2	2.09	0.52
1:B:10:LEU:O	1:B:11:ASN:C	2.47	0.52
1:B:427:PRO:O	1:B:431:ARG:HG3	2.09	0.52
1:B:84:ASP:CG	1:B:240:LYS:HZ2	2.12	0.52
1:A:1:MET:O	1:A:3:ARG:N	2.43	0.52
1:A:247:VAL:C	1:A:249:ASN:N	2.63	0.52
1:B:496:GLN:CG	1:B:497:VAL:H	2.19	0.52
1:B:105:PRO:CD	1:B:107:HIS:HD2	2.23	0.52
1:B:123:ASP:HB3	1:B:124:LYS:HD2	1.92	0.52
1:B:425:ARG:HA	1:B:444:PHE:O	2.10	0.52
1:A:103:ILE:HA	1:A:172:LYS:HA	1.92	0.52
1:B:6:ARG:NE	1:B:360:ALA:HB2	2.25	0.52
1:B:398:ILE:HG22	1:B:419:PRO:O	2.10	0.52
1:A:6:ARG:NE	1:A:360:ALA:HB2	2.24	0.52
1:B:456:VAL:HG12	1:B:459:ARG:NH2	2.25	0.52
1:B:95:THR:H	1:B:175:SER:HB3	1.74	0.52
1:A:111:PHE:CD1	1:A:165:VAL:HG21	2.45	0.52
1:A:151:SER:HB3	1:A:168:LEU:HD12	1.91	0.52
1:B:1:MET:O	1:B:3:ARG:N	2.43	0.52
1:B:429:ALA:HA	1:B:432:PHE:CE2	2.45	0.52
1:A:105:PRO:HD2	1:A:107:HIS:CD2	2.45	0.51
1:A:264:ARG:HE	1:A:280:GLN:NE2	2.08	0.51
1:A:362:LEU:HB2	1:A:363:PRO:HD3	1.91	0.51
1:A:425:ARG:HA	1:A:444:PHE:O	2.09	0.51
1:A:45:LEU:HD21	1:A:48:VAL:CG2	2.41	0.51
1:A:95:THR:HA	1:A:121:CYS:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASP:HB2	1:A:162:THR:OG1	2.10	0.51
1:A:223:THR:O	1:A:227:VAL:HG23	2.10	0.51
1:B:410:LEU:O	1:B:413:LYS:HB3	2.10	0.51
1:B:496:GLN:CG	1:B:497:VAL:N	2.73	0.51
1:A:52:PHE:HZ	1:A:201:PHE:HE2	1.59	0.51
1:B:213:SER:CA	1:B:240:LYS:HD3	2.41	0.51
1:A:86:LYS:HZ2	1:A:89:GLU:HG3	1.74	0.51
1:A:361:TYR:CG	1:A:417:ASN:HB3	2.45	0.51
1:B:122:ASP:O	1:B:124:LYS:N	2.42	0.51
1:A:496:GLN:CG	1:A:497:VAL:N	2.73	0.51
1:B:223:THR:O	1:B:227:VAL:HG23	2.11	0.51
1:B:28:GLY:N	1:B:336:ALA:HA	2.26	0.51
1:A:495:LEU:HD23	1:A:495:LEU:C	2.31	0.51
1:B:106:ASN:HD21	1:B:166:LYS:NZ	2.09	0.51
1:A:446:LYS:O	1:A:447:GLU:CB	2.58	0.50
1:A:19:ARG:NH1	1:A:21:THR:O	2.42	0.50
1:A:429:ALA:HA	1:A:432:PHE:CE2	2.45	0.50
1:B:382:VAL:HG21	1:B:493:ASN:ND2	2.26	0.50
1:B:401:LEU:N	1:B:401:LEU:HD12	2.26	0.50
1:A:432:PHE:O	1:A:435:LEU:HB2	2.12	0.50
1:B:279:VAL:HG12	1:B:279:VAL:O	2.10	0.50
1:B:432:PHE:C	1:B:432:PHE:CD1	2.84	0.50
1:A:156:GLU:HB2	1:A:164:LYS:HE2	1.94	0.50
1:A:247:VAL:HG13	1:A:248:ASN:N	2.26	0.50
1:A:445:GLU:O	1:A:446:LYS:CB	2.60	0.50
1:B:23:ILE:HG21	1:B:345:VAL:HG13	1.94	0.50
1:B:359:ILE:HG22	1:B:360:ALA:N	2.26	0.50
1:B:475:LYS:HA	1:B:500:VAL:CB	2.40	0.50
1:B:52:PHE:CD2	1:B:198:ASP:HB3	2.47	0.50
1:A:34:PRO:O	1:A:38:VAL:HG23	2.11	0.50
1:A:410:LEU:O	1:A:413:LYS:HB3	2.12	0.50
1:A:398:ILE:CG2	1:A:420:ILE:HA	2.40	0.50
1:B:398:ILE:CG2	1:B:420:ILE:HA	2.39	0.50
1:A:399:ILE:O	1:A:481:SER:HA	2.11	0.49
1:B:361:TYR:CG	1:B:417:ASN:HB3	2.46	0.49
1:B:374:LYS:N	1:B:375:PRO:CB	2.67	0.49
1:B:141:ARG:NH2	1:B:143:ILE:HA	2.28	0.49
1:B:390:VAL:CB	1:B:395:ALA:HB3	2.29	0.49
1:B:439:VAL:O	1:B:441:PRO:HD3	2.12	0.49
1:A:425:ARG:HH21	1:A:447:GLU:N	2.09	0.49
1:B:483:GLN:HG2	1:B:484:GLY:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:N	1:A:274:PRO:HD2	2.26	0.49
1:B:90:ILE:CB	1:B:179:VAL:HB	2.40	0.49
1:B:57:TYR:O	1:B:61:LYS:HB2	2.12	0.49
1:A:279:VAL:O	1:A:283:LEU:HD22	2.12	0.49
1:A:457:GLU:H	1:A:457:GLU:CD	2.16	0.49
1:B:93:GLY:HA3	1:B:127:TYR:HB3	1.95	0.49
1:B:425:ARG:HH21	1:B:447:GLU:N	2.10	0.49
1:B:81:ILE:N	1:B:81:ILE:HD13	2.28	0.49
1:A:141:ARG:HH21	1:A:143:ILE:HA	1.76	0.49
1:B:112:THR:CB	1:B:125:ILE:HD11	2.42	0.49
1:B:188:LEU:HD23	1:B:189:PRO:HD2	1.94	0.49
1:B:266:ASP:O	1:B:269:ILE:N	2.41	0.49
1:B:499:THR:CG2	1:B:500:VAL:N	2.75	0.49
1:A:31:THR:O	1:A:37:LEU:HD22	2.13	0.49
1:A:28:GLY:N	1:A:336:ALA:HA	2.27	0.49
1:A:386:ALA:O	1:A:389:ALA:HB3	2.12	0.49
1:B:103:ILE:HG12	1:B:172:LYS:HB2	1.94	0.49
1:B:85:THR:HG22	1:B:87:GLY:N	2.27	0.49
1:A:122:ASP:O	1:A:124:LYS:N	2.43	0.49
1:B:146:ASP:O	1:B:149:VAL:HG13	2.12	0.49
1:B:264:ARG:HE	1:B:280:GLN:NE2	2.11	0.49
1:B:499:THR:CG2	1:B:500:VAL:H	2.25	0.49
1:A:212:ALA:O	1:A:240:LYS:HB2	2.12	0.49
1:A:460:ILE:O	1:A:464:ILE:HG13	2.13	0.49
1:B:105:PRO:HD2	1:B:107:HIS:HD2	1.78	0.49
1:A:141:ARG:HH12	1:A:181:LEU:CA	2.26	0.48
1:A:266:ASP:O	1:A:269:ILE:N	2.45	0.48
1:A:305:THR:HG23	1:A:338:GLY:HA2	1.95	0.48
1:A:86:LYS:NZ	1:A:89:GLU:HG3	2.27	0.48
1:A:89:GLU:O	1:A:90:ILE:HD13	2.12	0.48
1:B:247:VAL:HG13	1:B:248:ASN:N	2.28	0.48
1:A:231:GLN:NE2	1:A:231:GLN:H	2.11	0.48
1:B:258:ASP:O	1:B:293:PRO:HD2	2.13	0.48
1:A:139:ALA:HA	1:A:154:VAL:CG1	2.43	0.48
1:B:400:VAL:O	1:B:422:LEU:HA	2.14	0.48
1:B:457:GLU:H	1:B:457:GLU:CD	2.17	0.48
1:B:375:PRO:CB	1:B:376:THR:HG1	2.23	0.48
1:B:52:PHE:HZ	1:B:201:PHE:CE2	2.32	0.48
1:A:301:LEU:O	1:A:304:MET:HB2	2.13	0.48
1:A:475:LYS:HA	1:A:500:VAL:CB	2.42	0.48
1:B:113:THR:CG2	1:B:128:VAL:HG23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ASP:OD2	1:B:116:LYS:HG3	2.12	0.48
1:B:12:VAL:HG23	1:B:13:VAL:HG23	1.94	0.48
1:B:422:LEU:HD23	1:B:441:PRO:HB3	1.94	0.48
1:B:186:VAL:HG23	1:B:216:ARG:NE	2.05	0.48
1:B:305:THR:HG23	1:B:338:GLY:HA2	1.96	0.48
1:B:386:ALA:O	1:B:389:ALA:HB3	2.14	0.48
1:B:477:ASP:O	1:B:478:THR:CB	2.61	0.48
1:A:432:PHE:CD1	1:A:432:PHE:C	2.87	0.48
1:A:94:THR:HG22	1:A:175:SER:HB2	1.95	0.48
1:B:342:ILE:H	1:B:342:ILE:CD1	2.10	0.48
1:B:401:LEU:HD23	1:B:459:ARG:HD2	1.94	0.48
1:A:175:SER:O	1:A:177:LYS:HG2	2.14	0.48
1:B:100:ASP:OD1	1:B:122:ASP:OD2	2.31	0.48
1:B:141:ARG:HH12	1:B:181:LEU:CA	2.27	0.48
1:B:478:THR:HG23	1:B:478:THR:O	2.13	0.48
1:A:146:ASP:O	1:A:149:VAL:HG22	2.14	0.47
1:A:279:VAL:O	1:A:279:VAL:HG12	2.13	0.47
1:B:399:ILE:O	1:B:481:SER:HA	2.15	0.47
1:B:84:ASP:OD1	1:B:240:LYS:NZ	2.42	0.47
1:B:110:ILE:HG13	1:B:162:THR:HG22	1.95	0.47
1:B:86:LYS:HZ3	1:B:89:GLU:CD	2.17	0.47
1:A:95:THR:H	1:A:175:SER:HB3	1.79	0.47
1:A:402:SER:HB3	1:A:422:LEU:HD11	1.96	0.47
1:B:188:LEU:CD2	1:B:189:PRO:HD2	2.44	0.47
1:A:361:TYR:HB3	1:A:391:PHE:CZ	2.49	0.47
1:A:425:ARG:NH2	1:A:447:GLU:N	2.62	0.47
1:B:215:ILE:HG13	1:B:239:VAL:HG13	1.95	0.47
1:B:314:GLU:O	1:B:318:VAL:HG23	2.14	0.47
1:A:456:VAL:HG12	1:A:459:ARG:NH2	2.29	0.47
1:B:247:VAL:C	1:B:249:ASN:N	2.67	0.47
1:B:247:VAL:O	1:B:249:ASN:N	2.45	0.47
1:A:10:LEU:O	1:A:11:ASN:C	2.52	0.47
1:B:231:GLN:NE2	1:B:231:GLN:H	2.13	0.47
1:B:415:ARG:NH1	1:B:437:ARG:HB3	2.29	0.47
1:A:153:GLN:CB	1:A:168:LEU:HD21	2.43	0.47
1:A:404:SER:HB2	1:A:406:THR:OG1	2.15	0.47
1:B:141:ARG:HE	1:B:142:ILE:H	1.63	0.47
1:B:156:GLU:OE1	1:B:164:LYS:NZ	2.48	0.47
1:B:130:TYR:CE1	1:B:132:ASN:HB2	2.49	0.47
1:A:297:ALA:HB1	1:A:330:MET:HE1	1.96	0.47
1:A:48:VAL:HG23	1:A:79:LEU:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:NH1	1:B:21:THR:O	2.41	0.47
1:B:33:ASN:O	1:B:37:LEU:HB2	2.15	0.47
1:A:91:ARG:HG2	1:A:91:ARG:NH1	2.29	0.47
1:B:175:SER:O	1:B:177:LYS:HG2	2.15	0.47
1:B:247:VAL:CG1	1:B:248:ASN:N	2.78	0.47
1:B:467:ALA:HB1	1:B:473:LEU:HD13	1.96	0.47
1:B:425:ARG:NH2	1:B:447:GLU:N	2.63	0.46
1:A:400:VAL:O	1:A:422:LEU:HA	2.15	0.46
1:A:114:ASP:C	1:A:116:LYS:H	2.18	0.46
1:B:453:THR:HG22	1:B:453:THR:O	2.15	0.46
1:A:106:ASN:ND2	1:A:106:ASN:O	2.48	0.46
1:A:361:TYR:HB3	1:A:391:PHE:HZ	1.80	0.46
1:B:92:THR:O	1:B:176:HIS:HD2	1.99	0.46
1:A:110:ILE:HD13	1:A:110:ILE:O	2.15	0.46
1:A:415:ARG:NH1	1:A:437:ARG:HB3	2.31	0.46
1:B:41:ARG:HA	1:B:45:LEU:HB3	1.98	0.46
1:A:115:ASP:HA	1:A:118:ALA:HB2	1.97	0.46
1:A:90:ILE:HB	1:A:179:VAL:HB	1.98	0.46
1:A:362:LEU:HD22	1:A:362:LEU:H	1.81	0.46
1:A:382:VAL:HG21	1:A:493:ASN:ND2	2.31	0.46
1:A:401:LEU:HD21	1:A:459:ARG:HB2	1.97	0.46
1:A:456:VAL:HG12	1:A:459:ARG:CZ	2.46	0.46
1:A:88:PRO:HG3	1:A:189:PRO:O	2.16	0.46
1:B:111:PHE:CE2	1:B:126:MET:SD	3.09	0.46
1:B:88:PRO:HB2	1:B:188:LEU:HD13	1.96	0.46
1:B:329:VAL:HB	1:B:348:MET:SD	2.55	0.46
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.80	0.46
1:A:499:THR:CG2	1:A:500:VAL:N	2.77	0.46
1:A:90:ILE:HD12	1:A:130:TYR:CB	2.39	0.46
1:B:112:THR:HG22	1:B:113:THR:N	2.31	0.46
1:A:192:SER:H	1:A:195:ASP:HB2	1.81	0.45
1:A:359:ILE:HG22	1:A:360:ALA:N	2.32	0.45
1:B:110:ILE:CD1	1:B:112:THR:OG1	2.64	0.45
1:B:446:LYS:O	1:B:447:GLU:CB	2.63	0.45
1:B:87:GLY:O	1:B:89:GLU:HG2	2.15	0.45
1:A:126:MET:HE1	1:A:173:ILE:HG13	1.98	0.45
1:B:133:ILE:O	1:B:137:ILE:HB	2.17	0.45
1:B:156:GLU:HB2	1:B:164:LYS:CE	2.46	0.45
1:B:185:ASP:OD1	1:B:245:GLN:NE2	2.49	0.45
1:B:327:ASP:HA	1:B:437:ARG:HB2	1.98	0.45
1:A:110:ILE:HD11	1:A:112:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:NH2	1:A:143:ILE:HA	2.32	0.45
1:B:243:ASN:HA	1:B:270:GLU:CG	2.43	0.45
1:B:484:GLY:HA2	1:B:493:ASN:HA	1.99	0.45
1:A:216:ARG:HD3	1:A:245:GLN:NE2	2.31	0.45
1:A:221:VAL:O	1:A:224:ILE:HG23	2.16	0.45
1:A:247:VAL:CG1	1:A:248:ASN:N	2.79	0.45
1:A:439:VAL:O	1:A:441:PRO:HD3	2.16	0.45
1:A:85:THR:HG22	1:A:87:GLY:N	2.31	0.45
1:B:304:MET:HE1	1:B:343:ASN:CB	2.46	0.45
1:A:213:SER:CA	1:A:240:LYS:HD3	2.44	0.45
1:A:362:LEU:N	1:A:362:LEU:HD13	2.32	0.45
1:A:50:MET:HE3	1:A:63:VAL:HB	1.98	0.45
1:B:102:PRO:CG	1:B:122:ASP:OD2	2.65	0.45
1:A:86:LYS:HZ3	1:A:89:GLU:CD	2.19	0.45
1:B:90:ILE:CD1	1:B:130:TYR:HB2	2.41	0.45
1:A:141:ARG:HE	1:A:142:ILE:H	1.64	0.45
1:A:243:ASN:HA	1:A:270:GLU:CG	2.45	0.45
1:B:103:ILE:HA	1:B:172:LYS:HA	1.98	0.45
1:B:88:PRO:HB2	1:B:188:LEU:HB3	1.99	0.45
1:A:113:THR:CG2	1:A:128:VAL:HG23	2.46	0.45
1:B:50:MET:HE3	1:B:63:VAL:HB	1.98	0.45
1:A:260:VAL:HG13	1:A:294:VAL:HG23	1.98	0.44
1:B:105:PRO:O	1:B:106:ASN:HB2	2.17	0.44
1:B:158:VAL:CB	1:B:162:THR:HB	2.43	0.44
1:B:153:GLN:CG	1:B:168:LEU:HD21	2.47	0.44
1:A:159:ASP:HB3	1:A:160:ASP:H	1.60	0.44
1:A:204:LYS:HB2	1:A:204:LYS:HE3	1.78	0.44
1:A:444:PHE:HB2	1:A:462:PHE:CD2	2.53	0.44
1:A:81:ILE:HD13	1:A:81:ILE:N	2.32	0.44
1:A:99:VAL:HG12	1:A:101:TYR:CZ	2.53	0.44
1:B:330:MET:HG3	1:B:331:LEU:H	1.83	0.44
1:B:28:GLY:HA3	1:B:336:ALA:O	2.17	0.44
1:B:45:LEU:HD11	1:B:47:ILE:O	2.18	0.44
1:A:141:ARG:NH2	1:A:181:LEU:HA	2.32	0.44
1:A:397:ALA:HB2	1:A:473:LEU:HD11	1.99	0.44
1:A:56:SER:H	1:A:59:TYR:CB	2.27	0.44
1:A:87:GLY:O	1:A:89:GLU:HG2	2.17	0.44
1:A:99:VAL:O	1:A:99:VAL:HG12	2.17	0.44
1:B:158:VAL:O	1:B:162:THR:HB	2.18	0.44
1:B:48:VAL:HG23	1:B:79:LEU:CD1	2.47	0.44
1:A:124:LYS:N	1:A:124:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:HG12	1:A:172:LYS:HB2	2.00	0.44
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.32	0.44
1:A:477:ASP:O	1:A:478:THR:CB	2.66	0.44
1:B:415:ARG:HH11	1:B:437:ARG:HB3	1.82	0.44
1:B:41:ARG:HD3	1:B:79:LEU:HD22	1.99	0.44
1:A:89:GLU:H	1:A:89:GLU:HG2	1.62	0.44
1:B:145:VAL:O	1:B:149:VAL:HG22	2.17	0.44
1:B:456:VAL:HG12	1:B:459:ARG:CZ	2.48	0.44
1:B:94:THR:HG22	1:B:175:SER:HB2	2.00	0.44
1:B:216:ARG:HD3	1:B:245:GLN:NE2	2.33	0.44
1:B:407:THR:N	1:B:408:PRO:HD2	2.32	0.44
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.81	0.44
1:A:483:GLN:HG2	1:A:484:GLY:N	2.33	0.44
1:B:301:LEU:O	1:B:304:MET:HB2	2.18	0.44
1:B:398:ILE:CD1	1:B:411:VAL:HG11	2.47	0.44
1:B:91:ARG:HH11	1:B:91:ARG:HG2	1.83	0.44
1:A:133:ILE:O	1:A:137:ILE:HB	2.17	0.43
1:A:263:ALA:O	1:A:267:LEU:HB2	2.18	0.43
1:B:444:PHE:HB2	1:B:462:PHE:CD2	2.53	0.43
1:A:158:VAL:O	1:A:162:THR:HB	2.18	0.43
1:A:242:GLU:HA	1:A:267:LEU:HB2	1.99	0.43
1:B:191:LEU:HD22	1:B:195:ASP:HB3	1.98	0.43
1:B:62:SER:OG	1:B:63:VAL:N	2.51	0.43
1:A:112:THR:HG22	1:A:113:THR:N	2.33	0.43
1:A:208:HIS:HA	1:A:428:ARG:HH12	1.84	0.43
1:A:467:ALA:HB1	1:A:473:LEU:HD13	2.00	0.43
1:B:115:ASP:HA	1:B:118:ALA:HB2	2.00	0.43
1:B:90:ILE:O	1:B:178:GLY:HA2	2.18	0.43
1:A:141:ARG:HH22	1:A:181:LEU:HD23	1.84	0.43
1:A:331:LEU:HA	1:A:331:LEU:HD23	1.90	0.43
1:A:398:ILE:HG22	1:A:419:PRO:O	2.18	0.43
1:A:423:VAL:HG21	1:A:459:ARG:O	2.19	0.43
1:A:425:ARG:HG2	1:A:444:PHE:O	2.19	0.43
1:B:122:ASP:OD1	1:B:122:ASP:C	2.56	0.43
1:B:156:GLU:HB2	1:B:164:LYS:NZ	2.34	0.43
1:B:242:GLU:HA	1:B:267:LEU:HB2	2.01	0.43
1:B:304:MET:HG3	1:B:310:PRO:CB	2.48	0.43
1:B:37:LEU:HA	1:B:37:LEU:HD13	1.77	0.43
1:A:102:PRO:O	1:A:173:ILE:HG22	2.19	0.43
1:B:279:VAL:O	1:B:283:LEU:HD22	2.19	0.43
1:A:180:ASN:ND2	1:A:270:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ASN:N	1:A:493:ASN:OD1	2.51	0.43
1:B:401:LEU:HD21	1:B:459:ARG:HB2	2.00	0.43
1:B:65:ASP:O	1:B:69:LYS:HB2	2.18	0.43
1:A:484:GLY:HA2	1:A:493:ASN:HA	2.01	0.43
1:B:222:LEU:O	1:B:225:ARG:HB3	2.18	0.43
1:B:243:ASN:CA	1:B:270:GLU:HG2	2.44	0.43
1:A:327:ASP:HA	1:A:437:ARG:HB2	2.00	0.43
1:A:90:ILE:HG23	1:A:130:TYR:CB	2.48	0.43
1:B:113:THR:HG22	1:B:128:VAL:HG23	2.00	0.43
1:B:133:ILE:O	1:B:137:ILE:N	2.47	0.43
1:B:146:ASP:O	1:B:149:VAL:HG22	2.19	0.43
1:B:88:PRO:HG3	1:B:189:PRO:O	2.19	0.43
1:B:391:PHE:HA	1:B:391:PHE:HD1	1.73	0.43
1:B:496:GLN:HE21	1:B:498:SER:CB	2.24	0.43
1:A:155:LEU:CB	1:A:164:LYS:HG2	2.39	0.43
1:A:60:HIS:C	1:A:62:SER:N	2.72	0.43
1:B:117:TYR:CD1	1:B:117:TYR:N	2.86	0.43
1:B:181:LEU:HB3	1:B:184:THR:HB	2.00	0.43
1:A:281:LYS:HZ3	1:A:324:ASP:CG	2.22	0.42
1:A:30:LYS:C	1:A:30:LYS:HD3	2.40	0.42
1:B:30:LYS:C	1:B:30:LYS:HD3	2.38	0.42
1:B:387:VAL:HG21	1:B:414:TYR:HB2	2.01	0.42
1:A:153:GLN:CG	1:A:168:LEU:HD21	2.49	0.42
1:A:41:ARG:HA	1:A:45:LEU:HB3	2.01	0.42
1:A:45:LEU:HD11	1:A:47:ILE:O	2.19	0.42
1:B:115:ASP:OD1	1:B:131:LYS:HE3	2.19	0.42
1:B:496:GLN:HG3	1:B:498:SER:H	1.84	0.42
1:B:8:THR:HG22	1:B:8:THR:O	2.19	0.42
1:A:65:ASP:O	1:A:69:LYS:HB2	2.19	0.42
1:B:466:LYS:HZ2	1:B:469:GLU:CD	2.21	0.42
1:A:133:ILE:HD11	1:A:137:ILE:HD12	2.01	0.42
1:A:417:ASN:N	1:A:417:ASN:HD22	2.04	0.42
1:A:88:PRO:HD3	1:A:190:ALA:O	2.19	0.42
1:B:109:MET:HG3	1:B:110:ILE:N	2.34	0.42
1:B:56:SER:H	1:B:59:TYR:CB	2.28	0.42
1:A:314:GLU:O	1:A:318:VAL:HG23	2.18	0.42
1:B:194:LYS:O	1:B:197:GLU:HB2	2.20	0.42
1:B:432:PHE:HD1	1:B:432:PHE:C	2.22	0.42
1:A:276:VAL:O	1:A:280:GLN:N	2.52	0.42
1:B:56:SER:OG	1:B:59:TYR:HD1	2.02	0.42
1:B:7:LEU:HA	1:B:10:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:SER:C	1:A:435:LEU:H	2.23	0.42
1:B:361:TYR:HB3	1:B:391:PHE:CZ	2.54	0.42
1:A:110:ILE:HG13	1:A:162:THR:HG22	2.01	0.42
1:A:143:ILE:HB	1:A:152:PHE:HB2	2.02	0.42
1:A:244:GLN:HA	1:A:247:VAL:HG12	2.01	0.42
1:A:499:THR:CG2	1:A:500:VAL:H	2.27	0.42
1:B:407:THR:N	1:B:408:PRO:CD	2.82	0.42
1:A:23:ILE:HG21	1:A:345:VAL:HG13	2.02	0.42
1:A:342:ILE:H	1:A:342:ILE:CD1	2.12	0.42
1:A:361:TYR:CD1	1:A:417:ASN:HB3	2.55	0.42
1:A:37:LEU:HD13	1:A:37:LEU:HA	1.79	0.42
1:A:41:ARG:HG2	1:A:45:LEU:HD23	2.02	0.42
1:B:410:LEU:HA	1:B:410:LEU:HD12	1.90	0.42
1:B:432:PHE:O	1:B:435:LEU:HB2	2.20	0.42
1:B:89:GLU:H	1:B:89:GLU:HG2	1.62	0.42
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.90	0.42
1:B:497:VAL:O	1:B:497:VAL:HG22	2.20	0.42
1:A:106:ASN:HD21	1:A:166:LYS:HZ1	1.60	0.41
1:A:243:ASN:CA	1:A:270:GLU:HG2	2.46	0.41
1:A:110:ILE:HD11	1:A:162:THR:CG2	2.50	0.41
1:A:113:THR:HB	1:A:131:LYS:NZ	2.35	0.41
1:A:180:ASN:OD1	1:A:269:ILE:HG21	2.20	0.41
1:A:481:SER:CB	1:A:496:GLN:HB3	2.42	0.41
1:B:132:ASN:O	1:B:133:ILE:C	2.58	0.41
1:A:304:MET:HG3	1:A:310:PRO:CB	2.48	0.41
1:A:407:THR:N	1:A:408:PRO:HD2	2.35	0.41
1:A:12:VAL:O	1:A:13:VAL:CB	2.68	0.41
1:A:194:LYS:O	1:A:197:GLU:HB2	2.20	0.41
1:A:199:LEU:O	1:A:203:VAL:HG23	2.21	0.41
1:A:254:LEU:HD13	1:A:290:ALA:HB2	2.02	0.41
1:A:33:ASN:O	1:A:37:LEU:HB2	2.19	0.41
1:A:387:VAL:HG21	1:A:414:TYR:HB2	2.02	0.41
1:B:153:GLN:HB2	1:B:168:LEU:CD2	2.41	0.41
1:B:263:ALA:O	1:B:267:LEU:HB2	2.21	0.41
1:B:67:ALA:HA	1:B:70:SER:OG	2.20	0.41
1:A:122:ASP:OD1	1:A:122:ASP:C	2.58	0.41
1:A:130:TYR:CE1	1:A:132:ASN:HB2	2.56	0.41
1:A:24:ILE:HG12	1:A:47:ILE:HB	2.02	0.41
1:A:472:ILE:HG22	1:A:473:LEU:HD12	2.02	0.41
1:B:297:ALA:HB1	1:B:330:MET:HE1	2.03	0.41
1:B:88:PRO:CB	1:B:188:LEU:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:HA	1:A:66:ASN:HD22	1.64	0.41
1:B:144:TYR:HA	1:B:150:LEU:O	2.21	0.41
1:B:416:PRO:CG	1:B:420:ILE:HD11	2.51	0.41
1:A:100:ASP:OD1	1:A:122:ASP:OD2	2.38	0.41
1:A:46:ASN:O	1:A:79:LEU:HD12	2.21	0.41
1:B:239:VAL:HG23	1:B:257:THR:OG1	2.21	0.41
1:A:132:ASN:O	1:A:133:ILE:C	2.59	0.41
1:A:86:LYS:HD3	1:A:86:LYS:O	2.21	0.41
1:B:330:MET:CG	1:B:331:LEU:H	2.34	0.41
1:A:215:ILE:HG13	1:A:239:VAL:HG13	2.03	0.41
1:B:144:TYR:HB3	1:B:148:GLY:HA2	2.02	0.41
1:B:281:LYS:HG3	1:B:281:LYS:H	1.55	0.41
1:A:180:ASN:C	1:A:182:PRO:HD3	2.42	0.41
1:A:195:ASP:O	1:A:199:LEU:HG	2.20	0.41
1:B:208:HIS:HA	1:B:428:ARG:HH12	1.86	0.41
1:B:330:MET:CG	1:B:331:LEU:N	2.84	0.41
1:B:362:LEU:H	1:B:362:LEU:HD13	1.85	0.41
1:B:362:LEU:HD22	1:B:362:LEU:H	1.86	0.41
1:B:41:ARG:HG2	1:B:45:LEU:HD23	2.02	0.41
1:B:52:PHE:HZ	1:B:201:PHE:HE2	1.67	0.41
1:A:234:ASP:N	1:A:234:ASP:OD1	2.53	0.41
1:B:342:ILE:HG12	1:B:343:ASN:N	2.36	0.41
1:B:69:LYS:HA	1:B:72:GLU:OE2	2.20	0.41
1:A:125:ILE:CG1	1:A:126:MET:N	2.82	0.40
1:A:276:VAL:O	1:A:277:LEU:C	2.59	0.40
1:B:262:VAL:O	1:B:264:ARG:N	2.53	0.40
1:B:243:ASN:CB	1:B:270:GLU:HG2	2.51	0.40
1:A:26:THR:O	1:A:335:THR:HB	2.20	0.40
1:A:289:LEU:HD11	1:A:371:CYS:CB	2.52	0.40
1:A:303:SER:C	1:A:305:THR:N	2.73	0.40
1:A:415:ARG:HH11	1:A:437:ARG:HB3	1.86	0.40
1:B:47:ILE:HG22	1:B:48:VAL:N	2.36	0.40
1:B:493:ASN:N	1:B:493:ASN:OD1	2.54	0.40
1:A:28:GLY:HA3	1:A:336:ALA:O	2.21	0.40
1:A:496:GLN:HG3	1:A:498:SER:H	1.86	0.40
1:B:263:ALA:O	2:B:1006:PGA:O1	2.39	0.40
1:B:1:MET:HG2	1:B:2:SER:N	2.36	0.40
1:B:361:TYR:CD1	1:B:417:ASN:HB3	2.56	0.40
1:A:222:LEU:O	1:A:225:ARG:HB3	2.22	0.40
1:A:372:THR:CG2	1:A:372:THR:O	2.60	0.40
1:B:151:SER:CB	1:B:168:LEU:HB2	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD22	1:A:195:ASP:HB3	2.04	0.40
1:A:201:PHE:O	1:A:205:ASN:ND2	2.52	0.40
1:B:102:PRO:HG2	1:B:122:ASP:OD2	2.22	0.40
1:B:220:ASP:O	1:B:224:ILE:CG2	2.56	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:309:ARG:NH2	1:B:268:GLY:O[1_545]	2.06	0.14

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/500 (96%)	382 (79%)	65 (14%)	34 (7%)	1	5
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	6
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	6

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	12	VAL
1	A	96	THR
1	A	99	VAL
1	A	106	ASN
1	A	375	PRO
1	A	398	ILE
1	A	446	LYS
1	A	478	THR

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Mol	Chain	Res	Type
1	A	497	VAL
1	B	10	LEU
1	B	96	THR
1	B	99	VAL
1	B	106	ASN
1	B	374	LYS
1	B	375	PRO
1	B	398	ILE
1	B	446	LYS
1	B	478	THR
1	B	497	VAL
1	A	2	SER
1	A	85	THR
1	A	87	GLY
1	A	123	ASP
1	A	146	ASP
1	A	176	HIS
1	A	265	GLY
1	A	374	LYS
1	B	2	SER
1	B	12	VAL
1	B	85	THR
1	B	123	ASP
1	B	146	ASP
1	B	176	HIS
1	B	265	GLY
1	A	11	ASN
1	A	248	ASN
1	A	249	ASN
1	A	494	THR
1	B	11	ASN
1	B	87	GLY
1	B	248	ASN
1	B	249	ASN
1	B	494	THR
1	B	495	LEU
1	A	13	VAL
1	A	105	PRO
1	A	122	ASP
1	A	170	ALA
1	A	298	THR
1	A	304	MET

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Mol	Chain	Res	Type
1	B	13	VAL
1	B	105	PRO
1	B	118	ALA
1	B	255	LYS
1	B	298	THR
1	A	255	LYS
1	A	475	LYS
1	A	495	LEU
1	B	170	ALA
1	B	304	MET
1	B	475	LYS
1	A	110	ILE
1	A	210	VAL
1	A	372	THR
1	B	372	THR
1	B	210	VAL

### 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	412/423 (97%)	337 (82%)	75 (18%)	1	9
1	B	412/423 (97%)	339 (82%)	73 (18%)	2	9
All	All	824/846 (97%)	676 (82%)	148 (18%)	1	9

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	SER
1	A	7	LEU
1	A	10	LEU
1	A	22	SER
1	A	30	LYS
1	A	31	THR

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Mol	Chain	Res	Type
1	A	33	ASN
1	A	37	LEU
1	A	40	LEU
1	A	50	MET
1	A	58	GLU
1	A	61	LYS
1	A	65	ASP
1	A	66	ASN
1	A	68	ARG
1	A	69	LYS
1	A	70	SER
1	A	77	ARG
1	A	83	LEU
1	A	89	GLU
1	A	91	ARG
1	A	94	THR
1	A	95	THR
1	A	96	THR
1	A	98	ASP
1	A	99	VAL
1	A	100	ASP
1	A	110	ILE
1	A	122	ASP
1	A	128	VAL
1	A	138	SER
1	A	141	ARG
1	A	150	LEU
1	A	153	GLN
1	A	156	GLU
1	A	160	ASP
1	A	162	THR
1	A	169	ASN
1	A	173	ILE
1	A	186	VAL
1	A	224	ILE
1	A	225	ARG
1	A	230	GLU
1	A	245	GLN
1	A	254	LEU
1	A	262	VAL
1	A	281	LYS
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	309	ARG
1	A	311	THR
1	A	316	SER
1	A	323	LEU
1	A	329	VAL
1	A	337	LYS
1	A	342	ILE
1	A	362	LEU
1	A	369	ARG
1	A	376	THR
1	A	390	VAL
1	A	391	PHE
1	A	400	VAL
1	A	404	SER
1	A	407	THR
1	A	410	LEU
1	A	415	ARG
1	A	417	ASN
1	A	431	ARG
1	A	432	PHE
1	A	433	SER
1	A	445	GLU
1	A	455	ASP
1	A	474	LYS
1	A	483	GLN
1	A	498	SER
1	B	1	MET
1	B	2	SER
1	B	7	LEU
1	B	10	LEU
1	B	22	SER
1	B	30	LYS
1	B	31	THR
1	B	33	ASN
1	B	37	LEU
1	B	40	LEU
1	B	50	MET
1	B	58	GLU
1	B	61	LYS
1	B	65	ASP
1	B	66	ASN
1	B	68	ARG

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Mol	Chain	Res	Type
1	B	69	LYS
1	B	70	SER
1	B	83	LEU
1	B	89	GLU
1	B	94	THR
1	B	95	THR
1	B	96	THR
1	B	98	ASP
1	B	100	ASP
1	B	110	ILE
1	B	122	ASP
1	B	126	MET
1	B	128	VAL
1	B	138	SER
1	B	141	ARG
1	B	150	LEU
1	B	153	GLN
1	B	156	GLU
1	B	160	ASP
1	B	162	THR
1	B	169	ASN
1	B	173	ILE
1	B	186	VAL
1	B	224	ILE
1	B	225	ARG
1	B	245	GLN
1	B	254	LEU
1	B	281	LYS
1	B	283	LEU
1	B	309	ARG
1	B	311	THR
1	B	316	SER
1	B	323	LEU
1	B	324	ASP
1	B	329	VAL
1	B	337	LYS
1	B	342	ILE
1	B	362	LEU
1	B	369	ARG
1	B	376	THR
1	B	390	VAL
1	B	391	PHE

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Mol	Chain	Res	Type
1	B	400	VAL
1	B	404	SER
1	B	407	THR
1	B	410	LEU
1	B	415	ARG
1	B	417	ASN
1	B	428	ARG
1	B	431	ARG
1	B	432	PHE
1	B	433	SER
1	B	445	GLU
1	B	455	ASP
1	B	474	LYS
1	B	483	GLN
1	B	498	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	60	HIS
1	A	66	ASN
1	A	106	ASN
1	A	169	ASN
1	A	176	HIS
1	A	231	GLN
1	A	243	ASN
1	A	244	GLN
1	A	245	GLN
1	A	280	GLN
1	A	343	ASN
1	A	357	GLN
1	A	370	ASN
1	A	417	ASN
1	A	434	HIS
1	A	483	GLN
1	A	493	ASN
1	A	496	GLN
1	B	33	ASN
1	B	60	HIS
1	B	66	ASN
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	132	ASN
1	B	169	ASN
1	B	176	HIS
1	B	231	GLN
1	B	243	ASN
1	B	244	GLN
1	B	280	GLN
1	B	343	ASN
1	B	357	GLN
1	B	370	ASN
1	B	417	ASN
1	B	434	HIS
1	B	483	GLN
1	B	493	ASN
1	B	496	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
2	PGA	B	1006	3,4	5,8,8	2.31	2 (40%)	6,11,11	3.24	2 (33%)
2	PGA	A	1005	1,3,4	5,8,8	2.49	3 (60%)	6,11,11	3.21	2 (33%)

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
2	PGA	B	1006	3,4	-	2/4/6/6	-
2	PGA	A	1005	1,3,4	-	0/4/6/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	P-O3P	4.09	1.70	1.54
2	B	1006	PGA	P-O3P	3.97	1.70	1.54
2	B	1006	PGA	P-O2P	2.24	1.57	1.50
2	A	1005	PGA	O1P-C2	-2.20	1.36	1.45
2	A	1005	PGA	P-O2P	2.08	1.57	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O1P-P-O2P	6.95	125.98	106.47
2	A	1005	PGA	O1P-P-O2P	6.63	125.08	106.47
2	A	1005	PGA	O3P-P-O1P	2.88	114.39	106.73
2	B	1006	PGA	O3P-P-O1P	2.35	112.97	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1006	PGA	C2-O1P-P-O3P
2	B	1006	PGA	C2-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1006	PGA	2	0
2	A	1005	PGA	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	374:LYS	C	375:PRO	N	0.84

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.