



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 19, 2024 – 04:00 PM EST

PDB ID : 1A3X
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-
PLEXED WITH PG, MN2+ AND K+
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

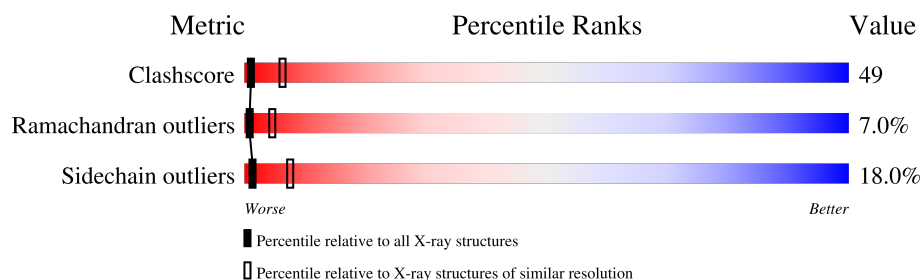
1 Overall quality at a glance

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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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	PGA	B	1006	-	X	-	-

2 Entry composition [i](#)

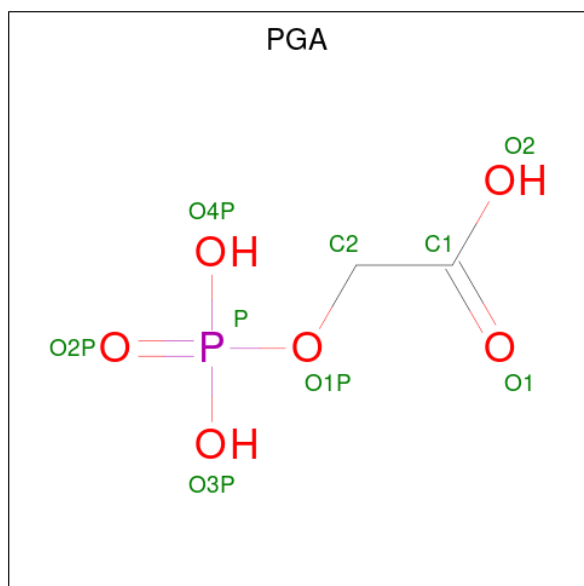
There are 4 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_2H_5O_6P$).



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	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0

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

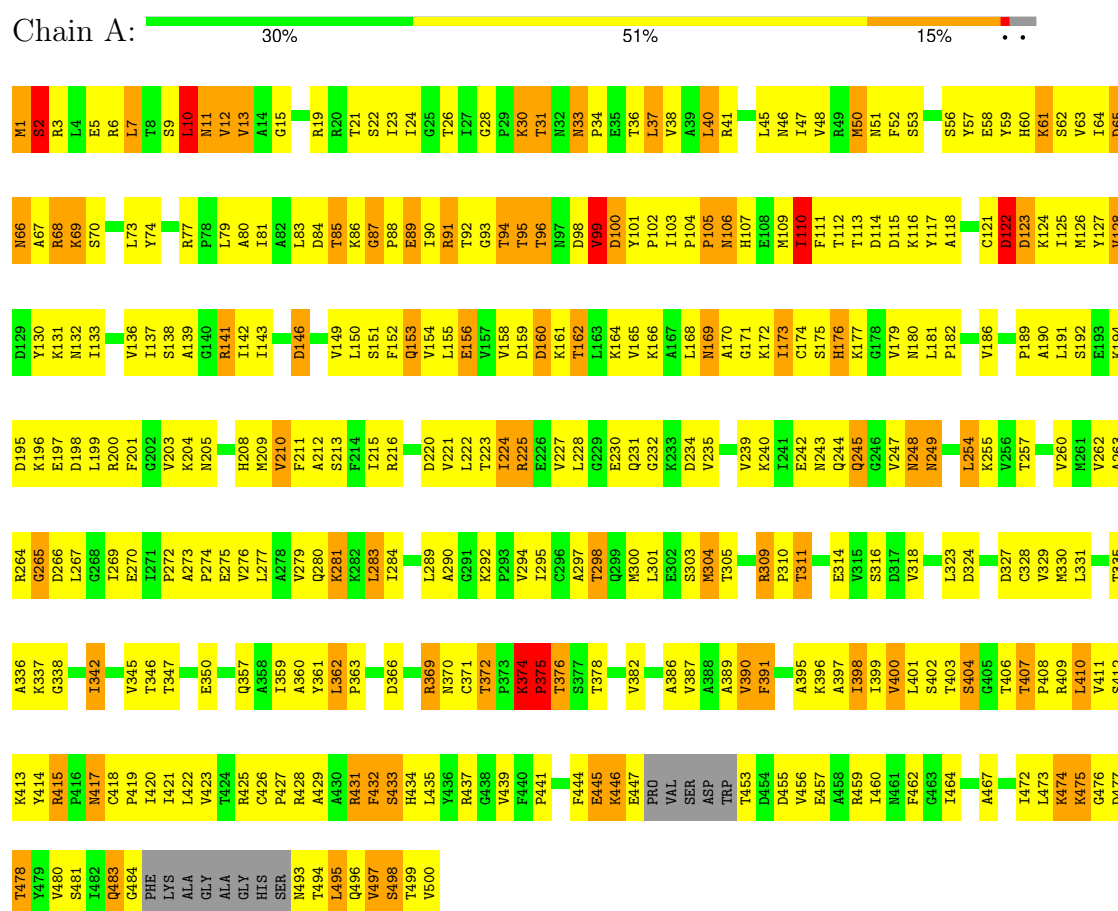
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0

3 Residue-property plots

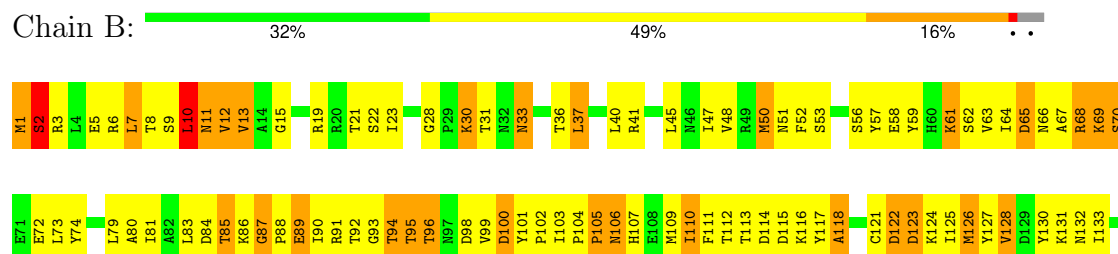
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	I274	E197	V136
LYS	V423	A349	P272	D198	I137
ALA	T424	E350	A273	L199	S138
GLY	R425	Q357	P274	R200	A139
ALA	C426	A358	E275	F201	G140
GLY	P427	I359	V279	H208	R141
HIS	R428	A360	Q280	M209	I142
SER	A429	Y361	K281	V210	I143
M493	A430	L362	K282	F211	Y144
T494	R431	P363	L283	A212	V145
L495	P432	S433	I284	S213	D146
Q496	S433	D366	L289	F214	D147
H434	H434	R369	K292	G148	G148
Q497	L435	N370	P293	I215	V149
S498	Y436	C371	V294	R216	L150
T499	R437	T372	L295	S151	S151
V500	G438	P373	C296	D220	F152
	P441	K374	A297	V221	Q153
		P375	T298	L222	V154
	F444	T376	Q299	T223	L155
	E445	T377	M300	I224	E156
	K446	T378	L301	R225	V157
	E447	V382	E302	E226	V158
	PRO	A386	S303	V227	D159
	VAL	V387	M304	L228	D160
	SER	V388	T305	Q231	K161
	ASP	A388	P308	G232	T162
	TRP	A389	R309	K164	L163
	T453	V390	P310	V235	K165
	D454	F391	T311	V239	K166
	D455	A395	E314	K240	L167
	V456	K396	V315	E241	L168
	E457	I398	S316	N242	M169
	A458	I399	D317	G243	A170
	R459	V400	V318	Q244	G171
	I460	L401	L323	Q245	K172
	R461	S402	D324	G246	I173
	G463	T403		V247	C174
	G465	T404		N248	S175
	K466	S404		N249	H176
	A467	T407	D327	L254	K177
	F468	P408	C328	K255	G178
	E469	R409	V329	V256	V179
		R410	M330	T257	M180
	L473	L410	L331	D258	L181
	K474	V411	A336	G259	G183
	K475	S412	K337	V260	T184
	G476	K413	G338	M261	D185
	D477	Y414		V262	V186
	T478	R415		A263	D187
	Y479	P416	I342	R264	L188
	V480	N417	N343	G265	P189
	S481	C418	K344	D266	A190
	T482	P419	V345	L267	L191
	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, α , β , γ	108.30Å 106.40Å 105.50Å 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 ²)	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	Peptide,Mainchain

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	370	1
1	B	3725	0	3804	375	1
2	A	9	0	2	6	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	745	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 (745) 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:263:ALA:CA	2:A:1005:PGA:O2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:SER:HB2	1:B:496:GLN:HB3	1.62	0.79
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:51:ASN:ND2	1:B:53:SER:HB2	1.99	0.78
1:B:396:LYS:O	1:B:418:CYS:HB2	1.83	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:90:ILE:HB	1:B:179:VAL:HB	1.67	0.75
1:B:496:GLN:HE21	1:B:498:SER:HB2	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:THR:HG22	1:B:372:THR:O	1.87	0.73
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:HD22	1:A:417:ASN:H	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:O	1:A:372:THR:HG22	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:67:ALA:HB1	1:B:79:LEU:HD21	1.74	0.70
1:B:284:ILE:HG23	1:B:294:VAL:HG11	1.73	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:86:LYS:HG2	1:A:89:GLU:OE2	1.93	0.68
1:A:141:ARG:HH12	1:A:181:LEU:HB3	1.58	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:90:ILE:HG23	1:A:130:TYR:HB2	1.75	0.68
1:A:369:ARG:NE	1:A:370:ASN:HD21	1.92	0.68
1:A:499:THR:HG22	1:A:500:VAL:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:C	1:A:249:ASN:H	1.97	0.68
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:53:SER:HA	1:A:86:LYS:HG3	1.77	0.65
1:A:483:GLN:HE21	1:A:483:GLN:N	1.94	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: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:B:369:ARG:NE	1:B:370:ASN:HD21	1.94	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:N	1:B:483:GLN:HE21	1.94	0.65
1:B:211:PHE:O	1:B:240:LYS:HD2	1.97	0.65
1:B:69:LYS:NZ	1:B:73:LEU:HG	2.12	0.64
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:33:ASN:HD21	1:B:36:THR:H	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:HE1	1:A:109:MET:HB3	1.61	0.64
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:9:SER:O	1:A:11:ASN:N	2.31	0.63
1:A:211:PHE:O	1:A:240:LYS:HD2	1.97	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:92:THR:HG22	1:A:177:LYS:H	1.64	0.62
1:A:113:THR:HG22	1:A:128:VAL:O	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:SER:H	1:B:169:ASN:ND2	1.98	0.61
1:B:375:PRO:HB2	1:B:376:THR:HG1	1.66	0.60
1:B:2:SER:HB2	1:B:5:GLU:HB2	1.83	0.60
1:B:141:ARG:HH22	1:B:181:LEU:HA	1.65	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:2:SER:HB2	1:A:5:GLU:HB2	1.82	0.60
1:A:93:GLY:HA3	1:A:127:TYR:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TYR:CE1	1:A:174:CYS:HB3	2.39	0.58
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:HD22	1:B:417:ASN:N	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:101:TYR:CD1	1:A:174:CYS:HA	2.39	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: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:65:ASP:HA	1:B:68:ARG: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: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:84:ASP:OD1	1:A:240:LYS:NZ	2.37	0.56
1:A:92:THR:O	1:A:176:HIS:HD2	1.87	0.56
1:A:141:ARG:HE	1:A:142:ILE:N	2.04	0.56
1:B:180:ASN:O	1:B:182:PRO:HD3	2.05	0.56
1:A:401:LEU:HD12	1:A:401:LEU:N	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:79:LEU:HD12	1:A:80:ALA:H	1.71	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:THR:HA	1:B:161:LYS:O	2.07	0.55
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:HG12	1:A:398:ILE:O	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:57:TYR:O	1:A:61:LYS:HB2	2.08	0.54
1:A:401:LEU:HD23	1:A:459:ARG:HD2	1.89	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:HD23	1:B:495:LEU:C	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:101:TYR:HD2	1:B:172:LYS:HZ1	1.56	0.54
1:B:141:ARG:HH21	1:B:143:ILE:HA	1.73	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:45:LEU:HD21	1:B:48:VAL:CG2	2.38	0.54
1:B:110:ILE:HD11	1:B:112:THR:OG1	2.07	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:52:PHE:CD2	1:A:198:ASP:HB3	2.44	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: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:47:ILE:HG12	1:B:80:ALA:HB3	1.91	0.53
1:B:130:TYR:O	1:B:133:ILE:HG22	2.08	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:HG22	1:A:453:THR:O	2.09	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:B:273:ALA:N	1:B:274:PRO:HD2	2.24	0.53
1:A:478:THR:HG23	1:A:478:THR:O	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:52:PHE:HZ	1:A:201:PHE:CE2	2.27	0.53
1:A:112:THR:CB	1:A:125:ILE:HD11	2.39	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:86:LYS:HZ2	1:B:89:GLU:HG3	1.75	0.52
1:B:476:GLY:N	1:B:500:VAL:HB	2.23	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:95:THR:H	1:B:175:SER:HB3	1.74	0.52
1:B:456:VAL:HG12	1:B:459:ARG:NH2	2.25	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:45:LEU:HD21	1:A:48:VAL:CG2	2.41	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HA	1:A:121:CYS:O	2.09	0.51
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:28:GLY:N	1:B:336:ALA:HA	2.26	0.51
1:B:223:THR:O	1:B:227:VAL:HG23	2.11	0.51
1:A:495:LEU:C	1:A:495:LEU:HD23	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:HD12	1:B:401:LEU:N	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:CD1	1:B:432:PHE:C	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:52:PHE:CD2	1:B:198:ASP:HB3	2.47	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:A:34:PRO:O	1:A:38:VAL:HG23	2.11	0.50
1:A:398:ILE:CG2	1:A:420:ILE:HA	2.40	0.50
1:A:410:LEU:O	1:A:413:LYS:HB3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:GLN:HG2	1:B:484:GLY:N	2.25	0.49
1:A:273:ALA:N	1:A:274:PRO:HD2	2.26	0.49
1:B:57:TYR:O	1:B:61:LYS:HB2	2.12	0.49
1:B:90:ILE:CB	1:B:179:VAL:HB	2.40	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:81:ILE:HD13	1:B:81:ILE:N	2.28	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: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:28:GLY:N	1:A:336:ALA:HA	2.27	0.49
1:A:31:THR:O	1:A:37:LEU:HD22	2.13	0.49
1:A:386:ALA:O	1:A:389:ALA:HB3	2.12	0.49
1:B:85:THR:HG22	1:B:87:GLY:N	2.27	0.49
1:B:103:ILE:HG12	1:B:172:LYS:HB2	1.94	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: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: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:B:247:VAL:HG13	1:B:248:ASN:N	2.28	0.48
1:A:231:GLN:H	1:A:231:GLN:NE2	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:CD	1:B:457:GLU:H	2.17	0.48
1:B:52:PHE:HZ	1:B:201:PHE:CE2	2.32	0.48
1:B:375:PRO:CB	1:B:376:THR:HG1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:VAL:HG23	1:B:13:VAL:HG23	1.94	0.48
1:B:113:THR:CG2	1:B:128:VAL:HG23	2.43	0.48
1:B:114:ASP:OD2	1:B:116:LYS:HG3	2.12	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:94:THR:HG22	1:A:175:SER:HB2	1.95	0.48
1:A:432:PHE:C	1:A:432:PHE:CD1	2.87	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:84:ASP:OD1	1:B:240:LYS:NZ	2.42	0.47
1:B:399:ILE:O	1:B:481:SER:HA	2.15	0.47
1:B:86:LYS:HZ3	1:B:89:GLU:CD	2.17	0.47
1:B:110:ILE:HG13	1:B:162:THR:HG22	1.95	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: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:231:GLN:H	1:B:231:GLN:NE2	2.13	0.47
1:B:415:ARG:NH1	1:B:437:ARG:HB3	2.29	0.47
1:B:130:TYR:CE1	1:B:132:ASN:HB2	2.49	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:A:297:ALA:HB1	1:A:330:MET:HE1	1.96	0.47
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:O	1:B:453:THR:HG22	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:88:PRO:HG3	1:A:189:PRO:O	2.16	0.46
1:A:90:ILE:HB	1:A:179:VAL:HB	1.98	0.46
1:A:115:ASP:HA	1:A:118:ALA:HB2	1.97	0.46
1:A:362:LEU:H	1:A:362:LEU:HD22	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:B:88:PRO:HB2	1:B:188:LEU:HD13	1.96	0.46
1:B:111:PHE:CE2	1:B:126:MET:SD	3.09	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:90:ILE:HD12	1:A:130:TYR:CB	2.39	0.46
1:A:499:THR:CG2	1:A:500:VAL:N	2.77	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:87:GLY:O	1:B:89:GLU:HG2	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HD11	1:A:112:THR:OG1	2.16	0.45
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:85:THR:HG22	1:A:87:GLY:N	2.31	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:B:304:MET:HE1	1:B:343:ASN:CB	2.46	0.45
1:A:50:MET:HE3	1:A:63:VAL:HB	1.98	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: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:88:PRO:HB2	1:B:188:LEU:HB3	1.99	0.45
1:B:103:ILE:HA	1:B:172:LYS:HA	1.98	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:81:ILE:N	1:A:81:ILE:HD13	2.32	0.44
1:A:99:VAL:HG12	1:A:101:TYR:CZ	2.53	0.44
1:A:159:ASP:HB3	1:A:160:ASP:H	1.60	0.44
1:A:204:LYS:HE3	1:A:204:LYS:HB2	1.78	0.44
1:A:444:PHE:HB2	1:A:462:PHE:CD2	2.53	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:B:330:MET:HG3	1:B:331:LEU:H	1.83	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:HG12	1:A:99:VAL:O	2.17	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:B:48:VAL:HG23	1:B:79:LEU:CD1	2.47	0.44
1:B:158:VAL:O	1:B:162:THR:HB	2.18	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:124:LYS:N	1:A:124:LYS:HD2	2.33	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:41:ARG:HD3	1:B:79:LEU:HD22	1.99	0.44
1:B:415:ARG:HH11	1:B:437:ARG:HB3	1.82	0.44
1:A:89:GLU:HG2	1:A:89:GLU:H	1.62	0.44
1:B:94:THR:HG22	1:B:175:SER:HB2	2.00	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: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:91:ARG:HG2	1:B:91:ARG:HH11	1.83	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: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:90:ILE:O	1:B:178:GLY:HA2	2.18	0.43
1:B:115:ASP:HA	1:B:118:ALA:HB2	2.00	0.43
1:A:141:ARG:HH22	1:A:181:LEU:HD23	1.84	0.43
1:A:331:LEU:HD23	1:A:331:LEU:HA	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:37:LEU:HD13	1:B:37:LEU:HA	1.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:ND2	1:A:270:GLU:OE1	2.52	0.43
1:A:493:ASN:OD1	1:A:493:ASN:N	2.51	0.43
1:B:65:ASP:O	1:B:69:LYS:HB2	2.18	0.43
1:B:401:LEU:HD21	1:B:459:ARG:HB2	2.00	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:90:ILE:HG23	1:A:130:TYR:CB	2.48	0.43
1:A:327:ASP:HA	1:A:437:ARG:HB2	2.00	0.43
1:B:88:PRO:HG3	1:B:189:PRO:O	2.19	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:391:PHE:HD1	1:B:391:PHE:HA	1.73	0.43
1:B:496:GLN:HE21	1:B:498:SER:CB	2.24	0.43
1:A:60:HIS:C	1:A:62:SER:N	2.72	0.43
1:A:155:LEU:CB	1:A:164:LYS:HG2	2.39	0.43
1:B:117:TYR:N	1:B:117:TYR:CD1	2.86	0.43
1:B:181:LEU:HB3	1:B:184:THR:HB	2.00	0.43
1:A:30:LYS:HD3	1:A:30:LYS:C	2.40	0.42
1:A:281:LYS:HZ3	1:A:324:ASP:CG	2.22	0.42
1:B:30:LYS:HD3	1:B:30:LYS:C	2.38	0.42
1:B:387:VAL:HG21	1:B:414:TYR:HB2	2.01	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:A:153:GLN:CG	1:A:168:LEU:HD21	2.49	0.42
1:B:8:THR:HG22	1:B:8:THR: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: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:88:PRO:HD3	1:A:190:ALA:O	2.19	0.42
1:A:133:ILE:HD11	1:A:137:ILE:HD12	2.01	0.42
1:A:417:ASN:HD22	1:A:417:ASN:N	2.04	0.42
1:B:56:SER:H	1:B:59:TYR:CB	2.28	0.42
1:B:109:MET:HG3	1:B:110:ILE:N	2.34	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:C	1:B:432:PHE:HD1	2.22	0.42
1:A:276:VAL:O	1:A:280:GLN:N	2.52	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:B:56:SER:OG	1:B:59:TYR:HD1	2.02	0.42
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: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: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:B:89:GLU:HG2	1:B:89:GLU:H	1.62	0.42
1:B:410:LEU:HD12	1:B:410:LEU:HA	1.90	0.42
1:B:432:PHE:O	1:B:435:LEU:HB2	2.20	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:33:ASN:O	1:A:37:LEU:HB2	2.19	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:387:VAL:HG21	1:A:414:TYR:HB2	2.02	0.41
1:B:67:ALA:HA	1:B:70:SER:OG	2.20	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:A:24:ILE:HG12	1:A:47:ILE:HB	2.02	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:472:ILE:HG22	1:A:473:LEU:HD12	2.02	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:B:297:ALA:HB1	1:B:330:MET:HE1	2.03	0.41
1:A:66:ASN:HD22	1:A:66:ASN:HA	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:46:ASN:O	1:A:79:LEU:HD12	2.21	0.41
1:A:100:ASP:OD1	1:A:122:ASP:OD2	2.38	0.41
1:B:239:VAL:HG23	1:B:257:THR:OG1	2.21	0.41
1:A:86:LYS:HD3	1:A:86:LYS:O	2.21	0.41
1:A:132:ASN:O	1:A:133:ILE:C	2.59	0.41
1:B:330:MET:CG	1:B:331:LEU:H	2.34	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:A:215:ILE:HG13	1:A:239:VAL:HG13	2.03	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:B:144:TYR:HB3	1:B:148:GLY:HA2	2.02	0.41
1:B:208:HIS:HA	1:B:428:ARG:HH12	1.86	0.41
1:B:281:LYS:H	1:B:281:LYS:HG3	1.55	0.41
1:B:330:MET:CG	1:B:331:LEU:N	2.84	0.41
1:B:362:LEU:HD13	1:B:362:LEU:H	1.85	0.41
1:B:362:LEU:H	1:B:362:LEU:HD22	1.86	0.41
1:A:234:ASP:OD1	1:A:234:ASP:N	2.53	0.41
1:B:69:LYS:HA	1:B:72:GLU:OE2	2.20	0.41
1:B:342:ILE:HG12	1:B:343:ASN:N	2.36	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:243:ASN:CB	1:B:270:GLU:HG2	2.51	0.40
1:B:262:VAL:O	1:B:264:ARG:N	2.53	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:1:MET:HG2	1:B:2:SER:N	2.36	0.40
1:B:263:ALA:O	2:B:1006:PGA:O1	2.39	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:O	1:A:372:THR:CG2	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:SER:CB	1:B:168:LEU:HB2	2.48	0.40
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	4
1	B	481/500 (96%)	377 (78%)	71 (15%)	33 (7%)	1	5
All	All	962/1000 (96%)	759 (79%)	136 (14%)	67 (7%)	1	4

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

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Mol	Chain	Res	Type
1	A	478	THR
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

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Mol	Chain	Res	Type
1	A	304	MET
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	7
1	B	412/423 (97%)	339 (82%)	73 (18%)	1	8
All	All	824/846 (97%)	676 (82%)	148 (18%)	1	7

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

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Mol	Chain	Res	Type
1	A	31	THR
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

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Mol	Chain	Res	Type
1	A	283	LEU
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

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Mol	Chain	Res	Type
1	B	68	ARG
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

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Mol	Chain	Res	Type
1	B	391	PHE
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

Sometimes 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

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Mol	Chain	Res	Type
1	B	106	ASN
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 oligosaccharides 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	4,3	8,8,8	2.31	3 (37%)	10,11,11	2.98	4 (40%)
2	PGA	A	1005	4,3	8,8,8	3.04	3 (37%)	10,11,11	2.95	4 (40%)

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	4,3	-	4/6/6/6	-
2	PGA	A	1005	4,3	-	2/6/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	PGA	O1P-C2	-6.62	1.36	1.43
2	A	1005	PGA	P-O3P	4.25	1.70	1.54
2	B	1006	PGA	P-O3P	4.12	1.70	1.54
2	B	1006	PGA	O1P-C2	-3.62	1.39	1.43
2	B	1006	PGA	P-O2P	2.34	1.57	1.50
2	A	1005	PGA	P-O2P	2.18	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1006	PGA	O1P-P-O2P	7.23	125.98	106.44
2	A	1005	PGA	O1P-P-O2P	6.90	125.08	106.44
2	B	1006	PGA	O1P-C2-C1	3.78	116.24	110.54
2	A	1005	PGA	O1P-C2-C1	3.66	116.06	110.54
2	A	1005	PGA	O3P-P-O1P	2.96	114.39	106.67
2	B	1006	PGA	O3P-P-O1P	2.42	112.97	106.67
2	A	1005	PGA	O2-C1-O1	-2.40	117.17	123.33
2	B	1006	PGA	O2-C1-O1	-2.23	117.60	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1006	PGA	C2-O1P-P-O3P
2	A	1005	PGA	O2-C1-C2-O1P

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Mol	Chain	Res	Type	Atoms
2	A	1005	PGA	O1-C1-C2-O1P
2	B	1006	PGA	O2-C1-C2-O1P
2	B	1006	PGA	O1-C1-C2-O1P
2	B	1006	PGA	C2-O1P-P-O4P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1006	PGA	2	0
2	A	1005	PGA	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.