



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:02 am BST

PDB ID : 1IYL
Title : Crystal Structure of Candida albicans N-myristoyltransferase with Non-peptidic Inhibitor
Authors : Sogabe, S.; Fukami, T.A.; Morikami, K.; Shiratori, Y.; Aoki, Y.; D'Arcy, A.; Winkler, F.K.; Banner, D.W.; Ohtsuka, T.
Deposited on : 2002-08-29
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
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

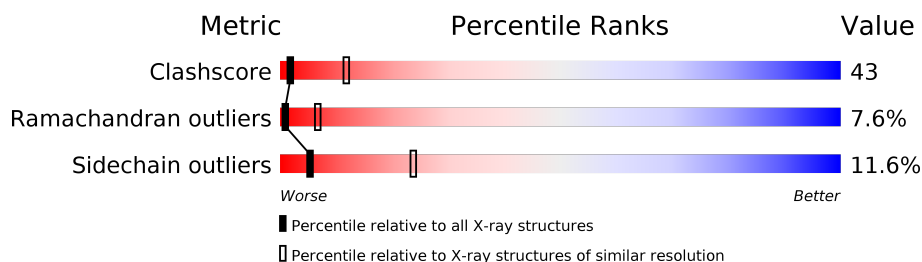
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	392	50% 40% 6% ..
1	B	392	34% 48% 14% ..
1	C	392	51% 38% 8% ..
1	D	392	27% 52% 16% ..

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	R64	B	452	-	-	X	-

2 Entry composition [i](#)

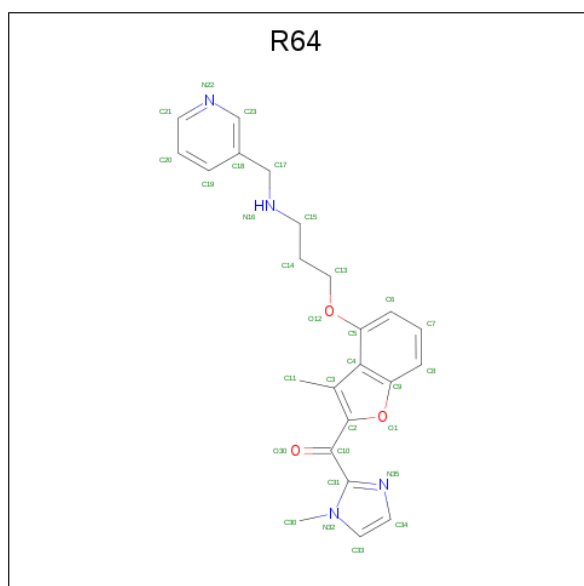
There are 2 unique types of molecules in this entry. The entry contains 12597 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myristoyl-CoA:Protein N-Myristoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3148	2039	514	586	9			
1	B	380	Total	C	N	O	S	0	0	0
			3117	2021	510	577	9			
1	C	381	Total	C	N	O	S	0	0	0
			3125	2025	511	580	9			
1	D	380	Total	C	N	O	S	0	0	0
			3117	2021	510	577	9			

- Molecule 2 is (1-METHYL-1H-IMIDAZOL-2-YL)-(3-METHYL-4-{3-[(PYRIDIN-3-YL METHYL)-AMINO]-PROPOXY}-BENZOFURAN-2-YL)-METHANONE (three-letter code: R64) (formula: C₂₃H₂₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	23	4	3		

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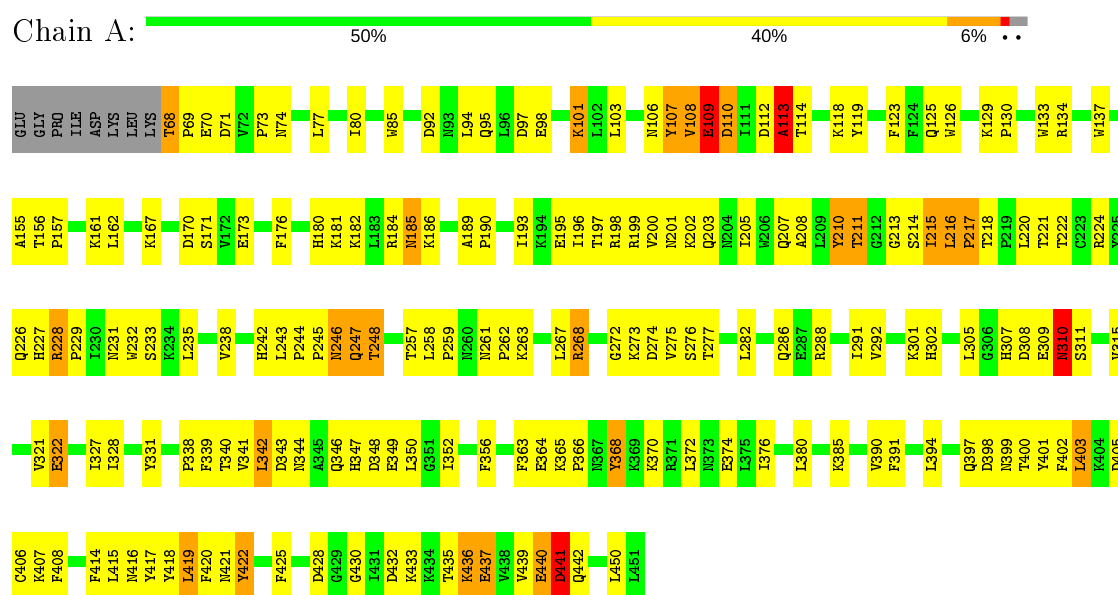
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			30	23	4	3		
2	C	1	Total	C	N	O	0	0
			30	23	4	3		

3 Residue-property plots

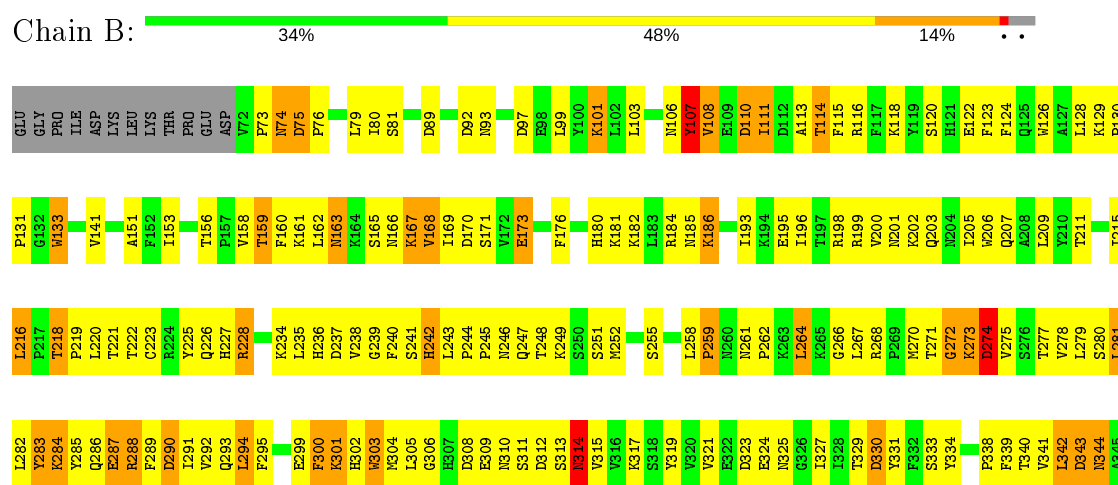
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

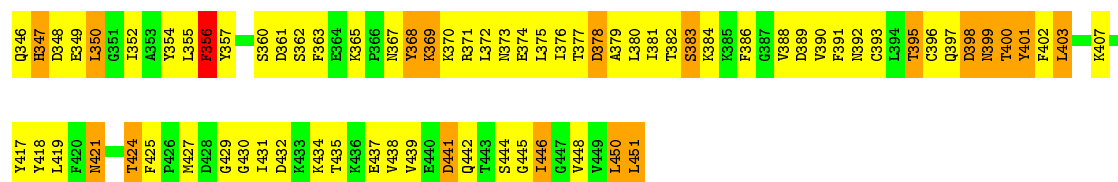
Note EDS was not executed.

• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase



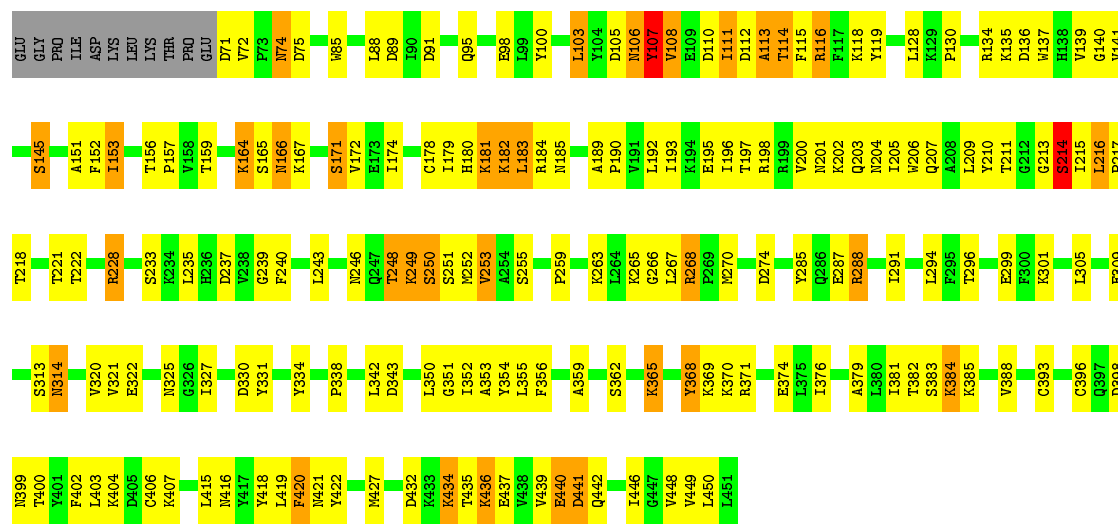
• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase





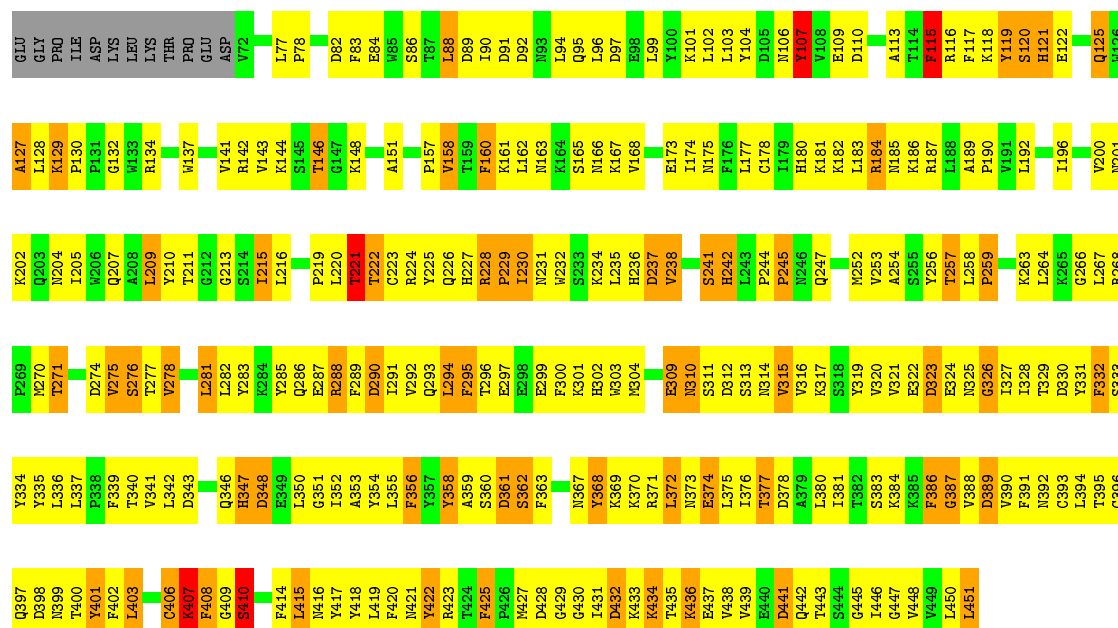
• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase

Chain C: 51% 38% 8% ..



• Molecule 1: Myristoyl-CoA:Protein N-Myristoyltransferase

Chain D: 27% 52% 16% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.28 Å 96.89 Å 269.28 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20	Depositor
% Data completeness (in resolution range)	98.8 (40.00-3.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.284 , 0.366	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12597	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: R64

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	1/3233 (0.0%)	0.70	3/4389 (0.1%)
1	B	0.54	1/3201 (0.0%)	0.65	1/4344 (0.0%)
1	C	0.52	1/3209 (0.0%)	0.68	1/4355 (0.0%)
1	D	0.55	0/3201	0.63	0/4344
All	All	0.55	3/12844 (0.0%)	0.67	5/17432 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	TYR	C-N	-15.78	0.97	1.34
1	B	113	ALA	C-N	-7.78	1.16	1.34
1	C	113	ALA	C-N	-5.13	1.22	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ALA	O-C-N	-9.51	107.48	122.70
1	A	113	ALA	C-N-CA	8.64	143.29	121.70
1	C	107	TYR	CA-C-N	-6.40	103.11	117.20
1	B	107	TYR	O-C-N	5.96	132.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	113	ALA	CA-C-N	5.93	130.24	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	TYR	Mainchain
1	D	107	TYR	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	3148	0	3098	162	0
1	B	3117	0	3074	290	0
1	C	3125	0	3078	188	0
1	D	3117	0	3075	449	0
2	A	30	0	24	3	0
2	B	30	0	24	10	0
2	C	30	0	24	0	0
All	All	12597	0	12397	1070	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (1070) 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:D:228:ARG:HH11	1:D:380:LEU:HB3	1.09	1.16
1:D:184:ARG:HB2	1:D:184:ARG:HH11	1.06	1.12
1:D:451:LEU:HD12	1:D:451:LEU:H	1.23	1.03
1:D:264:LEU:HG	1:D:374:GLU:HB3	1.41	1.02
1:D:226:GLN:HA	1:D:410:SER:HA	1.41	1.00
1:D:399:ASN:O	1:D:403:LEU:HB2	1.62	0.98
1:A:365:LYS:HE3	1:A:366:PRO:HD2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG12	1:A:109:GLU:H	1.31	0.92
1:B:74:ASN:HD22	1:B:75:ASP:H	1.05	0.92
1:D:238:VAL:HB	1:D:341:VAL:HG11	1.52	0.92
1:C:215:ILE:HG13	1:C:216:LEU:H	1.37	0.90
1:D:228:ARG:NH1	1:D:380:LEU:HB3	1.86	0.90
1:D:211:THR:HB	1:D:415:LEU:HD11	1.53	0.90
1:A:68:THR:HG22	1:A:69:PRO:HA	1.53	0.89
1:D:209:LEU:HD12	1:D:210:TYR:N	1.86	0.88
1:D:289:PHE:HA	1:D:445:GLY:HA2	1.55	0.88
1:D:184:ARG:HB2	1:D:184:ARG:NH1	1.88	0.88
1:D:216:LEU:HB2	1:D:418:TYR:HE2	1.39	0.88
1:B:314:ASN:ND2	1:B:314:ASN:H	1.72	0.87
1:A:210:TYR:OH	1:A:420:PHE:HB2	1.73	0.87
1:A:189:ALA:HB3	1:A:190:PRO:HD3	1.54	0.87
1:D:442:GLN:HE21	1:D:443:THR:H	1.18	0.87
1:B:161:LYS:HB2	1:B:294:LEU:HD11	1.54	0.87
1:D:235:LEU:O	1:D:238:VAL:HG22	1.75	0.87
1:D:224:ARG:NH1	1:D:410:SER:HB3	1.90	0.86
1:B:285:TYR:O	1:B:288:ARG:HD2	1.76	0.86
1:B:171:SER:HB2	1:B:207:GLN:O	1.76	0.86
1:C:211:THR:HG23	1:C:450:LEU:HD22	1.57	0.86
1:D:106:ASN:ND2	1:D:181:LYS:H	1.76	0.84
1:B:451:LEU:HD23	1:B:451:LEU:H	1.42	0.84
1:B:74:ASN:HD22	1:B:75:ASP:N	1.75	0.83
1:C:74:ASN:HD22	1:C:74:ASN:H	1.24	0.83
1:D:362:SER:HB2	1:D:371:ARG:HB3	1.61	0.83
1:D:175:ASN:ND2	1:D:450:LEU:HD23	1.94	0.83
1:B:74:ASN:ND2	1:B:75:ASP:H	1.77	0.82
1:D:221:THR:HG23	1:D:429:GLY:HA2	1.60	0.82
1:D:431:ILE:HG22	1:D:439:VAL:HG22	1.59	0.82
1:D:372:LEU:O	1:D:376:ILE:HG12	1.80	0.82
1:B:110:ASP:OD1	1:B:115:PHE:HB2	1.80	0.81
1:D:278:VAL:HA	1:D:281:LEU:CD2	2.10	0.81
1:D:184:ARG:CB	1:D:184:ARG:HH11	1.90	0.81
1:D:259:PRO:HG2	1:D:263:LYS:NZ	1.96	0.81
1:D:161:LYS:HB2	1:D:294:LEU:HD13	1.64	0.80
1:D:162:LEU:HB2	1:D:167:LYS:HB3	1.63	0.80
1:B:162:LEU:HB3	1:B:165:SER:HB2	1.62	0.80
1:C:114:THR:HA	1:C:342:LEU:HD12	1.63	0.79
1:D:226:GLN:HG2	1:D:410:SER:OG	1.81	0.79
1:C:130:PRO:HG3	1:C:156:THR:HG23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ARG:HH11	1:D:380:LEU:CB	1.94	0.79
1:D:321:VAL:HB	1:D:330:ASP:HB2	1.64	0.79
1:D:228:ARG:HH12	1:D:258:LEU:HD11	1.49	0.78
1:B:99:LEU:HG	1:B:103:LEU:HD13	1.66	0.78
1:B:161:LYS:CB	1:B:294:LEU:HD11	2.13	0.78
1:D:362:SER:CB	1:D:371:ARG:HB3	2.14	0.78
1:D:399:ASN:HB3	1:D:403:LEU:HD12	1.66	0.77
1:B:115:PHE:O	1:B:116:ARG:HD3	1.83	0.77
1:D:220:LEU:HD22	1:D:419:LEU:HD11	1.67	0.77
1:D:316:VAL:O	1:D:317:LYS:HD3	1.85	0.77
1:D:316:VAL:HA	1:D:335:TYR:HA	1.65	0.77
1:B:273:LYS:HG3	1:B:274:ASP:H	1.49	0.77
1:B:281:LEU:O	1:B:284:LYS:HG3	1.85	0.77
1:D:376:ILE:O	1:D:380:LEU:HG	1.83	0.77
1:D:235:LEU:HD11	1:D:389:ASP:O	1.85	0.77
1:C:434:LYS:HE2	1:C:434:LYS:O	1.83	0.76
1:D:290:ASP:H	1:D:445:GLY:CA	1.98	0.76
1:D:337:LEU:O	1:D:337:LEU:HD12	1.84	0.76
1:C:369:LYS:HE3	1:C:441:ASP:OD2	1.85	0.76
1:C:196:ILE:O	1:C:200:VAL:HG23	1.85	0.76
1:B:264:LEU:HD11	1:B:374:GLU:HB3	1.68	0.75
1:C:213:GLY:O	1:C:215:ILE:HG12	1.87	0.75
1:B:450:LEU:H	1:B:450:LEU:HD12	1.48	0.75
1:D:228:ARG:HB2	1:D:408:PHE:CB	2.17	0.75
1:D:290:ASP:CG	1:D:445:GLY:HA3	2.07	0.75
1:B:131:PRO:HG2	1:B:299:GLU:HG2	1.69	0.74
1:D:383:SER:C	1:D:388:VAL:HB	2.07	0.74
1:B:321:VAL:CG2	1:B:330:ASP:HB2	2.17	0.74
1:A:68:THR:HA	1:A:70:GLU:HG3	1.69	0.74
1:D:216:LEU:HB2	1:D:418:TYR:CE2	2.22	0.74
1:A:171:SER:HA	1:A:205:ILE:CG2	2.18	0.73
1:A:222:THR:OG1	1:A:416:ASN:ND2	2.21	0.73
1:A:228:ARG:HH12	1:A:258:LEU:HD21	1.53	0.73
1:B:271:THR:O	1:B:275:VAL:HG23	1.87	0.73
1:B:216:LEU:HD22	1:B:216:LEU:H	1.54	0.73
1:C:439:VAL:HG23	1:C:442:GLN:HB2	1.71	0.73
1:A:186:LYS:O	1:B:80:ILE:HD12	1.87	0.73
1:D:160:PHE:H	1:D:160:PHE:HD2	1.37	0.73
1:B:355:LEU:HD23	1:B:399:ASN:ND2	2.03	0.73
1:A:130:PRO:HG3	1:A:156:THR:HG23	1.71	0.73
1:B:308:ASP:HB3	1:B:311:SER:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:HD21	1:D:402:PHE:CD2	2.24	0.73
1:A:180:HIS:HD2	1:A:182:LYS:H	1.35	0.72
1:B:341:VAL:HG23	1:B:349:GLU:O	1.90	0.72
1:D:362:SER:O	1:D:368:TYR:HA	1.89	0.72
1:B:355:LEU:HD23	1:B:399:ASN:HD21	1.53	0.72
1:D:341:VAL:CG2	1:D:350:LEU:HD22	2.19	0.72
1:D:228:ARG:HB2	1:D:408:PHE:HB3	1.71	0.72
1:A:267:LEU:HD12	1:A:321:VAL:HG22	1.71	0.72
1:C:171:SER:HB2	1:C:207:GLN:O	1.90	0.72
1:D:268:ARG:HH11	1:D:268:ARG:HG2	1.54	0.72
1:C:215:ILE:HG13	1:C:216:LEU:N	2.04	0.72
1:C:436:LYS:HZ3	1:C:436:LYS:HB2	1.55	0.72
1:A:107:TYR:O	1:A:108:VAL:O	2.07	0.71
1:D:367:ASN:HB2	1:D:370:LYS:HB3	1.70	0.71
1:C:301:LYS:NZ	1:C:309:GLU:HB3	2.04	0.71
1:C:118:LYS:HB3	1:C:338:PRO:HG2	1.72	0.71
1:C:439:VAL:O	1:C:439:VAL:HG23	1.90	0.71
1:A:436:LYS:HZ3	1:A:436:LYS:HB2	1.55	0.71
1:A:92:ASP:OD2	1:A:94:LEU:HB2	1.89	0.71
1:C:107:TYR:CE1	1:C:108:VAL:HG23	2.25	0.71
1:C:268:ARG:HH22	1:C:274:ASP:CG	1.93	0.71
1:A:110:ASP:OD1	1:A:112:ASP:HB2	1.91	0.71
1:B:262:PRO:HB3	1:B:267:LEU:HD23	1.71	0.71
1:C:174:ILE:HB	1:C:210:TYR:HB3	1.72	0.71
1:D:380:LEU:HD11	1:D:406:CYS:SG	2.31	0.71
1:B:432:ASP:OD1	1:B:435:THR:HG23	1.90	0.71
1:D:431:ILE:HG22	1:D:439:VAL:H	1.53	0.71
1:B:246:ASN:O	1:B:247:GLN:HG2	1.90	0.71
1:B:268:ARG:HH11	1:B:268:ARG:HG2	1.56	0.70
1:D:369:LYS:NZ	1:D:373:ASN:HD21	1.89	0.70
1:D:220:LEU:O	1:D:427:MET:HB2	1.91	0.70
1:D:122:GLU:HA	1:D:125:GLN:CD	2.11	0.70
1:B:215:ILE:H	1:B:215:ILE:HD12	1.56	0.70
1:B:321:VAL:HB	1:B:330:ASP:OD1	1.91	0.70
1:D:383:SER:CA	1:D:388:VAL:HB	2.22	0.70
1:D:436:LYS:HZ2	1:D:436:LYS:HB2	1.55	0.70
1:C:415:LEU:C	1:C:416:ASN:HD22	1.94	0.69
1:B:314:ASN:ND2	1:B:314:ASN:N	2.39	0.69
1:C:402:PHE:O	1:C:406:CYS:HB2	1.91	0.69
1:C:116:ARG:HH21	1:C:116:ARG:HG2	1.58	0.69
1:D:228:ARG:HD3	1:D:229:PRO:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:LYS:O	1:C:374:GLU:HG3	1.92	0.69
1:D:97:ASP:O	1:D:101:LYS:HG3	1.92	0.69
1:D:275:VAL:HG12	1:D:297:GLU:HG2	1.73	0.69
1:C:184:ARG:HG2	1:C:184:ARG:HH11	1.58	0.69
1:C:351:GLY:C	1:C:352:ILE:HD12	2.13	0.69
1:D:235:LEU:CD1	1:D:390:VAL:HB	2.23	0.69
1:A:184:ARG:HH11	1:A:184:ARG:HG2	1.58	0.69
1:D:270:MET:HG2	1:D:320:VAL:HG13	1.74	0.68
1:B:267:LEU:HD22	1:B:378:ASP:OD1	1.94	0.68
1:D:175:ASN:HD21	1:D:450:LEU:HD23	1.59	0.68
1:D:187:ARG:O	1:D:190:PRO:HD2	1.92	0.68
1:D:339:PHE:CD2	1:D:352:ILE:HD12	2.27	0.68
1:D:340:THR:HA	1:D:348:ASP:O	1.94	0.68
1:C:200:VAL:HG12	1:C:205:ILE:HB	1.75	0.67
1:C:228:ARG:HG2	1:C:407:LYS:O	1.94	0.67
1:D:291:ILE:HG22	1:D:445:GLY:O	1.94	0.67
1:C:115:PHE:O	1:C:116:ARG:HD2	1.95	0.67
1:A:327:ILE:HD11	1:C:135:LYS:HE2	1.75	0.67
1:D:288:ARG:HG3	1:D:443:THR:HG21	1.76	0.67
1:D:116:ARG:HG3	1:D:117:PHE:H	1.59	0.67
1:B:289:PHE:HB3	1:B:445:GLY:O	1.95	0.67
1:D:372:LEU:HD21	1:D:402:PHE:HD2	1.58	0.67
1:A:327:ILE:CD1	1:C:135:LYS:HE2	2.25	0.66
1:C:400:THR:HA	1:C:403:LEU:HG	1.77	0.66
1:D:259:PRO:HG2	1:D:263:LYS:HZ2	1.60	0.66
1:D:268:ARG:HG2	1:D:268:ARG:NH1	2.10	0.66
1:D:274:ASP:O	1:D:278:VAL:HG22	1.95	0.66
1:D:372:LEU:HD11	1:D:402:PHE:CD2	2.30	0.66
1:B:161:LYS:HE3	1:B:163:ASN:OD1	1.96	0.66
1:D:283:TYR:HE1	1:D:294:LEU:HA	1.61	0.66
1:D:432:ASP:OD1	1:D:435:THR:HG23	1.96	0.66
1:B:114:THR:HG23	1:B:343:ASP:N	2.10	0.66
1:D:223:CYS:SG	1:D:396:CYS:HB3	2.36	0.66
1:D:118:LYS:O	1:D:118:LYS:HD3	1.96	0.66
1:D:266:GLY:O	1:D:321:VAL:HA	1.96	0.66
1:D:277:THR:HG21	1:D:328:ILE:HB	1.77	0.66
1:A:301:LYS:HG3	1:A:305:LEU:HD12	1.78	0.66
1:C:259:PRO:HD2	1:C:381:ILE:HD11	1.78	0.66
1:D:174:ILE:HB	1:D:210:TYR:HB3	1.78	0.66
1:A:257:THR:O	1:A:258:LEU:HD23	1.95	0.65
1:B:186:LYS:HZ2	1:B:186:LYS:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:HIS:O	1:B:244:PRO:HD3	1.95	0.65
1:A:85:TRP:CZ2	1:B:79:LEU:HD21	2.31	0.65
1:C:209:LEU:HD23	1:C:210:TYR:N	2.12	0.65
1:D:106:ASN:HD22	1:D:181:LYS:H	1.43	0.65
1:D:285:TYR:CD2	1:D:359:ALA:HA	2.31	0.65
1:D:394:LEU:HD11	1:D:415:LEU:HD23	1.75	0.65
1:B:323:ASP:OD2	1:B:327:ILE:HB	1.96	0.65
1:B:363:PHE:HA	1:B:368:TYR:CD2	2.32	0.65
1:D:224:ARG:O	1:D:395:THR:HG23	1.97	0.65
1:D:341:VAL:HG21	1:D:350:LEU:HD22	1.77	0.65
1:D:221:THR:HG21	1:D:446:ILE:HG13	1.77	0.65
1:D:451:LEU:CD1	1:D:451:LEU:H	2.00	0.65
1:B:228:ARG:HG2	1:B:407:LYS:O	1.96	0.65
1:D:224:ARG:HB3	1:D:395:THR:HG21	1.79	0.65
1:A:130:PRO:HG3	1:A:156:THR:CG2	2.27	0.65
1:A:198:ARG:HD2	1:B:73:PRO:O	1.96	0.65
1:D:189:ALA:HB3	1:D:190:PRO:HD3	1.78	0.65
1:A:435:THR:C	1:A:436:LYS:HZ3	2.00	0.65
1:C:314:ASN:N	1:C:314:ASN:HD22	1.94	0.65
1:D:278:VAL:HA	1:D:281:LEU:HD21	1.77	0.64
1:B:128:LEU:HD21	1:B:176:PHE:CD2	2.33	0.64
1:B:225:TYR:CE2	2:B:452:R64:C3	2.80	0.64
1:D:293:GLN:HB3	1:D:295:PHE:HE1	1.62	0.64
1:D:346:GLN:HG3	1:D:347:HIS:CD2	2.33	0.64
1:D:290:ASP:HB2	1:D:427:MET:CE	2.26	0.64
1:D:293:GLN:HB3	1:D:295:PHE:CE1	2.32	0.64
1:D:228:ARG:HE	1:D:380:LEU:HD22	1.61	0.64
1:B:321:VAL:HG21	1:B:330:ASP:HB2	1.80	0.64
1:C:301:LYS:HZ2	1:C:309:GLU:HB3	1.61	0.64
1:C:252:MET:O	1:C:255:SER:N	2.31	0.64
1:C:107:TYR:CZ	1:C:108:VAL:HG23	2.32	0.64
1:D:435:THR:C	1:D:437:GLU:H	2.01	0.64
1:A:210:TYR:CD1	1:A:418:TYR:HB2	2.33	0.64
1:D:228:ARG:HB2	1:D:408:PHE:CA	2.28	0.64
1:B:222:THR:HG22	1:B:431:ILE:HD11	1.80	0.63
1:B:225:TYR:HE2	2:B:452:R64:C3	2.11	0.63
1:C:301:LYS:HG2	1:C:305:LEU:HD12	1.80	0.63
1:D:419:LEU:HD23	1:D:419:LEU:N	2.14	0.63
1:C:171:SER:OG	1:C:172:VAL:N	2.30	0.63
1:C:268:ARG:CZ	1:C:320:VAL:HG21	2.28	0.63
1:A:185:ASN:N	1:A:185:ASN:HD22	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:HB2	1:B:391:PHE:HE2	1.64	0.63
1:D:432:ASP:HB3	1:D:435:THR:HG23	1.80	0.63
1:B:225:TYR:CD2	2:B:452:R64:C9	2.82	0.63
1:A:228:ARG:NH1	1:A:258:LEU:HD21	2.13	0.63
1:B:400:THR:HA	1:B:403:LEU:HD12	1.79	0.63
1:D:395:THR:HG21	1:D:438:VAL:HG22	1.80	0.63
1:B:234:LYS:HE3	1:B:347:HIS:CG	2.34	0.62
1:A:68:THR:CG2	1:A:69:PRO:HA	2.26	0.62
1:D:259:PRO:HB2	1:D:381:ILE:HD13	1.82	0.62
1:D:401:TYR:HA	1:D:441:ASP:HA	1.81	0.62
1:D:290:ASP:H	1:D:445:GLY:HA3	1.63	0.62
1:C:211:THR:HG23	1:C:450:LEU:CD2	2.26	0.62
1:C:259:PRO:HB2	1:C:381:ILE:HD13	1.81	0.62
1:D:339:PHE:CG	1:D:352:ILE:HD12	2.33	0.62
1:B:128:LEU:HD21	1:B:176:PHE:CE2	2.34	0.62
1:C:189:ALA:HB3	1:C:190:PRO:HD3	1.81	0.62
1:C:365:LYS:CD	1:C:365:LYS:H	2.13	0.62
1:D:442:GLN:NE2	1:D:443:THR:H	1.93	0.62
1:B:235:LEU:HD21	1:B:389:ASP:O	2.00	0.62
1:C:321:VAL:HB	1:C:330:ASP:HB2	1.81	0.62
1:D:362:SER:OG	1:D:371:ARG:HB3	2.00	0.62
1:B:346:GLN:HE21	1:B:347:HIS:CD2	2.18	0.61
1:B:329:THR:O	1:B:360:SER:HA	2.00	0.61
1:D:211:THR:HG23	1:D:450:LEU:HD22	1.81	0.61
1:B:349:GLU:O	1:B:350:LEU:HB2	1.99	0.61
1:B:290:ASP:H	1:B:445:GLY:HA2	1.65	0.61
1:D:339:PHE:O	1:D:340:THR:HG23	2.00	0.61
1:D:227:HIS:O	1:D:409:GLY:HA3	2.00	0.61
1:B:186:LYS:HA	1:B:186:LYS:NZ	2.15	0.61
1:D:220:LEU:CD1	1:D:427:MET:HG3	2.31	0.61
1:D:97:ASP:CG	1:D:101:LYS:HE3	2.20	0.61
1:A:199:ARG:O	1:A:202:LYS:HB2	1.99	0.61
1:B:395:THR:HG21	1:B:431:ILE:HG23	1.81	0.61
1:D:99:LEU:HD12	1:D:103:LEU:HD13	1.83	0.61
1:B:200:VAL:HG12	1:B:205:ILE:HB	1.82	0.61
1:B:235:LEU:HB2	1:B:241:SER:OG	2.00	0.61
1:C:171:SER:HA	1:C:205:ILE:HG23	1.81	0.61
1:C:442:GLN:HA	1:C:442:GLN:HE21	1.64	0.61
1:D:286:GLN:HB3	1:D:292:VAL:CG1	2.31	0.61
1:B:180:HIS:CD2	1:B:182:LYS:H	2.19	0.61
1:B:273:LYS:HG3	1:B:274:ASP:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:LYS:HE2	1:D:436:LYS:HE3	1.82	0.61
1:A:341:VAL:HG12	1:A:344:ASN:HB2	1.83	0.61
1:C:365:LYS:HD2	1:C:365:LYS:H	1.66	0.61
1:B:167:LYS:O	1:B:169:ILE:HG13	2.01	0.61
1:D:230:ILE:CG2	1:D:384:LYS:HG3	2.31	0.60
1:D:200:VAL:HG12	1:D:205:ILE:HB	1.82	0.60
1:A:107:TYR:O	1:A:108:VAL:C	2.33	0.60
1:A:232:TRP:HA	1:A:235:LEU:HD12	1.82	0.60
1:D:232:TRP:CE2	1:D:236:HIS:HB2	2.36	0.60
1:A:196:ILE:O	1:A:200:VAL:HG23	2.01	0.60
1:C:209:LEU:HD23	1:C:210:TYR:H	1.67	0.60
1:D:235:LEU:HD21	1:D:389:ASP:HB2	1.83	0.60
1:D:109:GLU:OE2	1:D:342:LEU:HD21	2.01	0.60
1:C:106:ASN:HD22	1:C:181:LYS:HG3	1.66	0.60
1:C:72:VAL:HG23	1:D:202:LYS:HE2	1.84	0.60
1:D:187:ARG:HH12	1:D:190:PRO:HG2	1.65	0.60
1:B:244:PRO:HD2	1:B:252:MET:CE	2.32	0.60
1:D:232:TRP:NE1	1:D:236:HIS:HB2	2.17	0.60
1:D:383:SER:O	1:D:388:VAL:HB	2.02	0.60
1:D:226:GLN:HB2	1:D:393:CYS:SG	2.42	0.60
1:D:317:LYS:O	1:D:333:SER:HA	2.00	0.60
1:D:180:HIS:CD2	1:D:182:LYS:HB2	2.37	0.59
1:C:110:ASP:CG	1:C:115:PHE:H	2.06	0.59
1:D:334:TYR:HB2	1:D:354:TYR:O	2.02	0.59
1:D:300:PHE:O	1:D:304:MET:HG2	2.01	0.59
1:D:369:LYS:HZ2	1:D:373:ASN:HD21	1.50	0.59
1:B:340:THR:HA	1:B:349:GLU:HA	1.85	0.59
1:A:435:THR:HG23	1:A:437:GLU:H	1.67	0.59
1:A:80:ILE:CD1	1:B:186:LYS:HB3	2.33	0.59
1:B:160:PHE:CE2	1:B:169:ILE:HB	2.37	0.59
1:B:349:GLU:HG2	1:B:350:LEU:H	1.67	0.59
1:B:93:ASN:O	1:B:97:ASP:HB2	2.02	0.59
1:D:127:ALA:C	1:D:128:LEU:HD12	2.22	0.59
1:A:118:LYS:NZ	1:A:349:GLU:OE1	2.35	0.59
1:B:222:THR:O	1:B:429:GLY:HA3	2.03	0.59
1:B:431:ILE:HG22	1:B:438:VAL:HA	1.83	0.59
1:B:193:ILE:O	1:B:196:ILE:HG22	2.02	0.59
1:B:325:ASN:O	1:B:327:ILE:HG13	2.00	0.59
1:B:184:ARG:O	1:B:185:ASN:HB2	2.03	0.59
1:B:219:PRO:HB3	1:B:418:TYR:CZ	2.38	0.59
1:B:323:ASP:C	1:B:325:ASN:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LEU:CD1	1:C:95:GLN:HB3	2.31	0.59
1:D:442:GLN:HE21	1:D:443:THR:N	1.96	0.59
1:D:291:ILE:CG2	1:D:446:ILE:HA	2.33	0.59
1:D:451:LEU:HD12	1:D:451:LEU:N	2.07	0.59
1:D:317:LYS:HB2	1:D:334:TYR:CZ	2.38	0.59
1:A:186:LYS:HB3	1:B:80:ILE:HD12	1.84	0.58
1:D:141:VAL:HB	1:D:151:ALA:HB3	1.85	0.58
1:D:271:THR:HG23	1:D:274:ASP:OD2	2.02	0.58
1:D:372:LEU:HD12	1:D:372:LEU:O	2.02	0.58
1:A:118:LYS:HB3	1:A:338:PRO:HG2	1.86	0.58
1:B:393:CYS:HB2	1:B:399:ASN:ND2	2.18	0.58
1:D:228:ARG:NE	1:D:380:LEU:HD22	2.18	0.58
1:D:339:PHE:CD1	1:D:352:ILE:HB	2.38	0.58
1:D:224:ARG:NH1	1:D:410:SER:O	2.36	0.58
1:A:226:GLN:HE21	1:A:403:LEU:HD22	1.68	0.58
1:D:116:ARG:CG	1:D:117:PHE:H	2.17	0.58
1:D:283:TYR:CE1	1:D:294:LEU:HA	2.39	0.58
1:A:129:LYS:HG2	1:A:133:TRP:CE2	2.38	0.58
1:B:225:TYR:CE2	2:B:452:R64:C4	2.86	0.58
1:C:197:THR:HG22	1:C:201:ASN:OD1	2.03	0.58
1:D:315:VAL:C	1:D:336:LEU:H	2.07	0.58
1:B:308:ASP:HB3	1:B:311:SER:CB	2.33	0.58
1:C:107:TYR:CE1	1:C:108:VAL:CG2	2.86	0.58
1:D:267:LEU:HD11	1:D:332:PHE:HE2	1.68	0.58
1:B:329:THR:HB	1:B:361:ASP:OD2	2.04	0.58
1:B:401:TYR:CD1	1:B:441:ASP:HA	2.39	0.58
1:B:244:PRO:HD2	1:B:252:MET:HE1	1.86	0.58
1:D:436:LYS:N	1:D:436:LYS:HD3	2.17	0.58
1:D:229:PRO:O	1:D:230:ILE:HG12	2.03	0.58
1:B:432:ASP:HB3	1:B:435:THR:OG1	2.04	0.57
1:D:121:HIS:O	1:D:125:GLN:NE2	2.37	0.57
1:D:173:GLU:CD	1:D:450:LEU:HG	2.24	0.57
1:D:315:VAL:HG23	1:D:316:VAL:H	1.67	0.57
1:A:272:GLY:HA3	1:A:309:GLU:OE2	2.04	0.57
1:A:171:SER:HA	1:A:205:ILE:HG23	1.85	0.57
1:C:381:ILE:O	1:C:384:LYS:HG3	2.04	0.57
1:A:224:ARG:HD2	1:A:414:PHE:CE2	2.39	0.57
1:B:279:LEU:HD13	1:B:300:PHE:CD1	2.39	0.57
1:D:222:THR:HA	1:D:416:ASN:HA	1.85	0.57
1:A:247:GLN:O	1:A:248:THR:HG23	2.04	0.57
1:C:111:ILE:HG23	1:C:112:ASP:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HB3	1:B:80:ILE:CD1	2.35	0.57
1:D:220:LEU:HD22	1:D:419:LEU:CD1	2.35	0.57
1:D:244:PRO:HG2	1:D:252:MET:CE	2.34	0.57
1:C:314:ASN:ND2	1:C:314:ASN:N	2.53	0.57
1:D:296:THR:O	1:D:299:GLU:N	2.31	0.57
1:D:339:PHE:CE1	1:D:352:ILE:HB	2.39	0.57
1:D:372:LEU:CD2	1:D:402:PHE:HB3	2.35	0.57
1:A:112:ASP:O	1:A:113:ALA:HB3	2.05	0.56
1:D:432:ASP:HB3	1:D:435:THR:CG2	2.35	0.56
1:D:442:GLN:HG3	1:D:443:THR:N	2.19	0.56
1:B:107:TYR:O	1:B:108:VAL:C	2.44	0.56
1:B:270:MET:HA	1:B:274:ASP:OD2	2.06	0.56
1:B:278:VAL:O	1:B:281:LEU:HB3	2.04	0.56
1:D:268:ARG:NH1	1:D:320:VAL:HG23	2.20	0.56
1:C:268:ARG:NH2	1:C:274:ASP:OD2	2.38	0.56
1:D:400:THR:O	1:D:401:TYR:O	2.23	0.56
1:B:176:PHE:CD1	2:B:452:R64:HC21	2.39	0.56
1:D:270:MET:HG2	1:D:320:VAL:CG1	2.35	0.56
1:A:161:LYS:HG2	1:A:162:LEU:N	2.20	0.56
1:B:294:LEU:HD12	1:B:294:LEU:H	1.68	0.56
1:B:266:GLY:O	1:B:321:VAL:HA	2.06	0.56
1:D:270:MET:CE	1:D:278:VAL:HG21	2.35	0.56
1:D:286:GLN:HB3	1:D:292:VAL:HG11	1.86	0.56
1:C:404:LYS:HE2	1:C:440:GLU:OE1	2.06	0.56
1:D:302:HIS:O	1:D:304:MET:N	2.39	0.56
1:B:303:TRP:HA	1:B:303:TRP:CE3	2.41	0.56
1:B:301:LYS:HG3	1:B:305:LEU:HD12	1.88	0.56
1:C:249:LYS:HD2	1:C:250:SER:H	1.71	0.56
1:C:434:LYS:HD3	1:C:435:THR:HG23	1.88	0.56
1:B:273:LYS:O	1:B:275:VAL:N	2.38	0.56
1:D:173:GLU:OE2	1:D:450:LEU:HG	2.06	0.56
1:D:309:GLU:HG3	1:D:310:ASN:H	1.71	0.56
1:D:331:TYR:HE2	1:D:359:ALA:HB3	1.70	0.56
1:C:110:ASP:OD2	1:C:113:ALA:N	2.38	0.56
1:C:204:ASN:HA	1:C:206:TRP:HE1	1.70	0.56
1:C:434:LYS:HE2	1:C:434:LYS:C	2.26	0.56
1:D:270:MET:CG	1:D:320:VAL:HG13	2.36	0.56
1:D:381:ILE:O	1:D:383:SER:N	2.37	0.56
1:D:90:ILE:HB	1:D:96:LEU:HD13	1.88	0.56
1:D:230:ILE:HG23	1:D:384:LYS:NZ	2.21	0.56
1:D:220:LEU:CD2	1:D:419:LEU:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ARG:HD3	1:D:228:ARG:O	2.05	0.56
1:B:118:LYS:HB3	1:B:338:PRO:HG2	1.88	0.55
1:B:129:LYS:HE3	1:B:133:TRP:CZ2	2.41	0.55
1:B:223:CYS:SG	1:B:396:CYS:HB3	2.46	0.55
1:B:329:THR:HB	1:B:361:ASP:CG	2.27	0.55
1:C:153:ILE:HG23	1:C:153:ILE:O	2.06	0.55
1:C:442:GLN:HA	1:C:442:GLN:NE2	2.20	0.55
1:C:72:VAL:HG23	1:C:72:VAL:O	2.06	0.55
1:D:315:VAL:HG12	1:D:336:LEU:O	2.06	0.55
1:D:235:LEU:HD13	1:D:390:VAL:HB	1.87	0.55
1:D:431:ILE:HG21	1:D:438:VAL:HA	1.88	0.55
1:C:141:VAL:HB	1:C:151:ALA:HB3	1.87	0.55
1:D:395:THR:CG2	1:D:438:VAL:HG22	2.36	0.55
1:D:263:LYS:HB2	1:D:377:THR:HG21	1.88	0.55
1:B:361:ASP:OD2	1:B:362:SER:N	2.40	0.55
1:D:278:VAL:HA	1:D:281:LEU:HD23	1.89	0.55
1:D:222:THR:HG23	1:D:416:ASN:ND2	2.22	0.55
1:A:227:HIS:O	1:A:229:PRO:HD3	2.06	0.55
1:D:271:THR:N	1:D:274:ASP:OD2	2.31	0.55
1:C:352:ILE:HD12	1:C:352:ILE:N	2.22	0.55
1:D:386:PHE:CD1	1:D:386:PHE:N	2.71	0.55
1:A:370:LYS:O	1:A:374:GLU:HG3	2.06	0.55
1:A:156:THR:HG23	1:A:157:PRO:HD2	1.88	0.55
1:B:245:PRO:O	1:B:246:ASN:OD1	2.24	0.55
1:B:268:ARG:NH1	1:B:268:ARG:HG2	2.21	0.55
1:C:268:ARG:NH1	1:C:322:GLU:OE1	2.37	0.55
1:D:259:PRO:HB2	1:D:381:ILE:CD1	2.37	0.55
1:B:309:GLU:HG3	1:B:310:ASN:OD1	2.07	0.55
1:D:220:LEU:HD22	1:D:419:LEU:HD21	1.89	0.55
1:D:297:GLU:O	1:D:301:LYS:HB2	2.07	0.55
1:A:103:LEU:HB3	1:A:119:TYR:CE1	2.42	0.54
1:A:243:LEU:HD23	1:A:244:PRO:O	2.07	0.54
1:A:441:ASP:N	1:A:441:ASP:OD2	2.40	0.54
1:D:268:ARG:O	1:D:320:VAL:HG22	2.07	0.54
1:C:202:LYS:C	1:C:203:GLN:HG2	2.28	0.54
1:D:132:GLY:O	1:D:157:PRO:HG3	2.07	0.54
1:D:228:ARG:NH1	1:D:380:LEU:HD13	2.21	0.54
1:D:355:LEU:HD12	1:D:355:LEU:N	2.22	0.54
1:D:230:ILE:HG22	1:D:384:LYS:HG3	1.90	0.54
1:A:430:GLY:O	1:A:439:VAL:HG22	2.07	0.54
1:B:272:GLY:O	1:B:275:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:MET:HG2	1:B:305:LEU:HD21	1.88	0.54
1:C:111:ILE:HG13	1:C:112:ASP:OD2	2.08	0.54
1:D:207:GLN:NE2	1:D:421:ASN:ND2	2.55	0.54
1:A:185:ASN:N	1:A:185:ASN:ND2	2.56	0.54
1:A:176:PHE:CE1	2:A:452:R64:HC21	2.43	0.54
1:D:120:SER:OG	1:D:121:HIS:N	2.41	0.54
1:D:241:SER:OG	1:D:242:HIS:N	2.40	0.54
1:B:101:LYS:HE3	1:B:101:LYS:O	2.06	0.54
1:C:110:ASP:OD1	1:C:113:ALA:HA	2.07	0.54
1:C:180:HIS:HD2	1:C:182:LYS:HB2	1.73	0.54
1:D:89:ASP:OD2	1:D:91:ASP:HB2	2.08	0.54
1:D:115:PHE:HE2	1:D:341:VAL:HG22	1.73	0.54
1:D:201:ASN:HD22	1:D:201:ASN:N	2.04	0.54
1:B:355:LEU:HB2	1:B:391:PHE:CE2	2.43	0.54
1:D:372:LEU:HD21	1:D:402:PHE:HB3	1.89	0.54
1:C:116:ARG:NH2	1:C:116:ARG:HG2	2.24	0.53
1:C:95:GLN:O	1:C:98:GLU:HB2	2.08	0.53
1:D:129:LYS:N	1:D:130:PRO:CD	2.71	0.53
1:D:165:SER:O	1:D:166:ASN:HB3	2.08	0.53
1:D:180:HIS:HE2	1:D:182:LYS:HD2	1.73	0.53
1:D:362:SER:HB2	1:D:371:ARG:CB	2.36	0.53
1:A:184:ARG:O	1:A:185:ASN:HB2	2.08	0.53
1:A:213:GLY:C	1:A:215:ILE:H	2.11	0.53
1:B:383:SER:HA	1:B:386:PHE:CD1	2.43	0.53
1:C:100:TYR:HE1	1:C:119:TYR:O	1.91	0.53
1:D:97:ASP:OD2	1:D:101:LYS:HE3	2.09	0.53
1:A:108:VAL:HG12	1:A:109:GLU:N	2.13	0.53
1:B:376:ILE:O	1:B:379:ALA:HB3	2.08	0.53
1:C:432:ASP:OD1	1:C:435:THR:HG23	2.08	0.53
1:A:184:ARG:CG	1:A:184:ARG:HH11	2.21	0.53
1:B:271:THR:O	1:B:272:GLY:C	2.47	0.53
1:B:339:PHE:CG	1:B:352:ILE:HD12	2.43	0.53
1:C:105:ASP:O	1:C:181:LYS:HE3	2.08	0.53
1:C:165:SER:O	1:C:166:ASN:C	2.47	0.53
1:D:234:LYS:HD2	1:D:347:HIS:NE2	2.23	0.53
1:A:106:ASN:ND2	1:A:181:LYS:H	2.07	0.53
1:B:237:ASP:O	1:B:239:GLY:N	2.41	0.53
1:C:130:PRO:HG3	1:C:156:THR:CG2	2.36	0.53
1:D:189:ALA:HA	1:D:192:LEU:HD12	1.91	0.53
1:D:281:LEU:HG	1:D:282:LEU:N	2.24	0.53
1:D:288:ARG:HG2	1:D:289:PHE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PHE:CA	1:D:445:GLY:HA2	2.34	0.53
1:B:234:LYS:HE3	1:B:347:HIS:CD2	2.43	0.53
1:C:215:ILE:HG13	1:C:216:LEU:CD2	2.39	0.53
1:C:88:LEU:HD11	1:C:95:GLN:HB3	1.90	0.53
1:D:417:TYR:HE2	1:D:448:VAL:HG23	1.73	0.53
1:D:369:LYS:C	1:D:369:LYS:HD3	2.29	0.53
1:D:230:ILE:HG21	1:D:383:SER:OG	2.09	0.53
1:C:211:THR:HA	1:C:416:ASN:O	2.08	0.53
1:D:369:LYS:HD3	1:D:373:ASN:HD21	1.74	0.53
1:A:301:LYS:HG3	1:A:305:LEU:CD1	2.39	0.52
1:B:129:LYS:HE3	1:B:133:TRP:CE2	2.45	0.52
1:D:268:ARG:O	1:D:319:TYR:HA	2.09	0.52
1:A:171:SER:HA	1:A:205:ILE:HG21	1.89	0.52
1:B:215:ILE:N	1:B:215:ILE:HD12	2.21	0.52
1:C:178:CYS:C	1:C:179:ILE:HD12	2.29	0.52
1:C:296:THR:HG23	1:C:299:GLU:OE2	2.09	0.52
1:D:213:GLY:O	1:D:215:ILE:HG13	2.08	0.52
1:D:296:THR:OG1	1:D:299:GLU:HG3	2.10	0.52
1:A:235:LEU:O	1:A:238:VAL:HG22	2.09	0.52
1:A:220:LEU:HD11	1:A:419:LEU:HB2	1.92	0.52
1:B:272:GLY:O	1:B:275:VAL:CG2	2.58	0.52
1:B:209:LEU:CD1	1:B:450:LEU:HD23	2.40	0.52
1:D:226:GLN:HA	1:D:410:SER:CA	2.29	0.52
1:D:275:VAL:HG12	1:D:276:SER:N	2.23	0.52
1:D:376:ILE:HG13	1:D:402:PHE:CE1	2.44	0.52
1:A:352:ILE:HG12	1:A:390:VAL:HG12	1.91	0.52
1:A:95:GLN:HA	1:A:98:GLU:HG3	1.92	0.52
1:C:128:LEU:O	1:C:130:PRO:HD2	2.10	0.52
1:C:248:THR:HG23	1:C:251:SER:OG	2.09	0.52
1:B:342:LEU:O	1:B:344:ASN:N	2.43	0.52
1:A:85:TRP:CH2	1:B:79:LEU:HD21	2.45	0.52
1:C:362:SER:HA	1:C:365:LYS:HD3	1.92	0.52
1:C:355:LEU:HD23	1:C:399:ASN:HD21	1.75	0.52
1:D:324:GLU:CD	1:D:324:GLU:H	2.14	0.52
1:D:224:ARG:CZ	1:D:410:SER:HB3	2.40	0.52
1:A:74:ASN:HA	1:B:202:LYS:HE3	1.92	0.52
1:D:232:TRP:HE1	1:D:236:HIS:HD2	1.57	0.52
1:A:73:PRO:HG2	1:B:198:ARG:HD2	1.92	0.52
1:D:361:ASP:C	1:D:363:PHE:H	2.12	0.52
1:D:224:ARG:HA	1:D:414:PHE:HA	1.91	0.52
1:B:300:PHE:O	1:B:301:LYS:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASN:HD22	1:B:314:ASN:N	2.07	0.52
1:B:395:THR:HB	1:B:429:GLY:O	2.10	0.52
1:D:275:VAL:O	1:D:276:SER:C	2.47	0.52
1:D:209:LEU:HB2	1:D:419:LEU:HD22	1.92	0.52
1:B:401:TYR:CE1	1:B:441:ASP:HB3	2.45	0.51
1:C:249:LYS:C	1:C:251:SER:H	2.14	0.51
1:D:369:LYS:HD3	1:D:369:LYS:O	2.10	0.51
1:D:436:LYS:NZ	1:D:436:LYS:HB2	2.22	0.51
1:A:193:ILE:O	1:A:196:ILE:HG22	2.10	0.51
1:B:396:CYS:HB2	1:B:446:ILE:HB	1.92	0.51
1:C:263:LYS:O	1:C:265:LYS:HD3	2.10	0.51
1:D:315:VAL:O	1:D:317:LYS:HE2	2.11	0.51
1:D:228:ARG:HB2	1:D:408:PHE:HA	1.91	0.51
1:D:290:ASP:H	1:D:445:GLY:HA2	1.70	0.51
1:C:368:TYR:O	1:C:369:LYS:C	2.48	0.51
1:B:350:LEU:O	1:B:352:ILE:HG13	2.11	0.51
1:B:339:PHE:CD1	1:B:352:ILE:HD12	2.45	0.51
1:A:327:ILE:HG12	1:C:135:LYS:HE2	1.93	0.51
1:C:156:THR:HG23	1:C:157:PRO:HD2	1.92	0.51
1:B:180:HIS:HD2	1:B:182:LYS:H	1.58	0.51
1:C:215:ILE:CG1	1:C:216:LEU:H	2.17	0.51
1:B:289:PHE:HD2	1:B:444:SER:O	1.92	0.51
1:B:290:ASP:N	1:B:290:ASP:OD2	2.43	0.51
1:B:376:ILE:HG13	1:B:402:PHE:CD1	2.46	0.51
1:C:379:ALA:O	1:C:382:THR:OG1	2.27	0.51
1:D:116:ARG:CG	1:D:117:PHE:N	2.74	0.51
1:D:127:ALA:O	1:D:128:LEU:HD12	2.10	0.51
1:D:210:TYR:O	1:D:418:TYR:HB2	2.11	0.51
1:D:295:PHE:HD1	1:D:295:PHE:H	1.59	0.51
1:B:176:PHE:CE1	2:B:452:R64:HC21	2.46	0.51
1:C:135:LYS:C	1:C:137:TRP:H	2.14	0.51
1:C:439:VAL:CG2	1:C:439:VAL:O	2.58	0.51
1:D:275:VAL:O	1:D:278:VAL:HG23	2.11	0.51
1:D:374:GLU:HA	1:D:377:THR:CG2	2.39	0.51
1:A:372:LEU:HD23	1:A:401:TYR:HB2	1.93	0.51
1:B:209:LEU:HD12	1:B:209:LEU:O	2.11	0.51
1:B:349:GLU:CG	1:B:350:LEU:H	2.23	0.51
1:C:221:THR:HG23	1:C:222:THR:N	2.24	0.51
1:D:314:ASN:HA	1:D:317:LYS:HZ1	1.75	0.51
1:A:186:LYS:HD3	1:B:80:ILE:HD13	1.93	0.51
1:C:204:ASN:HA	1:C:206:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LEU:O	1:D:106:ASN:HB2	2.10	0.51
1:D:115:PHE:CE2	1:D:341:VAL:HG13	2.46	0.51
1:D:128:LEU:C	1:D:130:PRO:HD2	2.31	0.51
1:A:220:LEU:CD1	1:A:419:LEU:HB2	2.41	0.51
1:C:115:PHE:C	1:C:116:ARG:HD2	2.31	0.51
1:C:249:LYS:CD	1:C:250:SER:H	2.24	0.51
1:C:221:THR:HG21	1:C:446:ILE:HG13	1.93	0.51
1:D:231:ASN:HB3	1:D:389:ASP:HB3	1.93	0.51
1:D:372:LEU:HD11	1:D:402:PHE:CE2	2.44	0.51
1:D:235:LEU:HD11	1:D:390:VAL:HB	1.91	0.51
1:A:433:LYS:NZ	1:A:433:LYS:HB3	2.26	0.50
1:B:384:LYS:C	1:B:386:PHE:H	2.13	0.50
1:C:376:ILE:O	1:C:379:ALA:HB3	2.11	0.50
1:C:74:ASN:HD22	1:C:74:ASN:N	2.01	0.50
1:D:253:VAL:O	1:D:256:TYR:N	2.43	0.50
1:D:267:LEU:HA	1:D:320:VAL:O	2.10	0.50
1:B:160:PHE:HB2	1:B:292:VAL:O	2.11	0.50
1:B:159:THR:HG23	1:B:170:ASP:CG	2.32	0.50
1:B:289:PHE:CD2	1:B:444:SER:O	2.64	0.50
1:B:123:PHE:HD1	1:B:315:VAL:HG11	1.76	0.50
1:C:106:ASN:ND2	1:C:181:LYS:H	2.08	0.50
1:D:220:LEU:HD22	1:D:419:LEU:CG	2.41	0.50
1:D:232:TRP:HE1	1:D:236:HIS:CD2	2.29	0.50
1:B:370:LYS:HA	1:B:373:ASN:HD22	1.75	0.50
1:D:291:ILE:O	1:D:291:ILE:HG23	2.11	0.50
1:D:332:PHE:CD2	1:D:332:PHE:N	2.80	0.50
1:D:264:LEU:CG	1:D:374:GLU:HB3	2.26	0.50
1:A:435:THR:C	1:A:436:LYS:NZ	2.64	0.50
1:B:234:LYS:C	1:B:236:HIS:H	2.13	0.50
1:B:357:TYR:OH	1:B:448:VAL:HA	2.12	0.50
1:C:285:TYR:CD2	1:C:359:ALA:HA	2.47	0.50
1:C:368:TYR:O	1:C:371:ARG:N	2.45	0.50
1:D:278:VAL:O	1:D:282:LEU:CB	2.60	0.50
1:A:286:GLN:HB3	1:A:292:VAL:HG11	1.92	0.50
1:A:210:TYR:CZ	1:A:420:PHE:HB2	2.47	0.50
1:C:214:SER:HA	1:C:416:ASN:OD1	2.12	0.50
1:D:301:LYS:NZ	1:D:301:LYS:HB3	2.27	0.50
1:D:309:GLU:HG3	1:D:310:ASN:N	2.27	0.50
1:D:277:THR:O	1:D:281:LEU:HD23	2.11	0.50
1:D:346:GLN:HB2	1:D:347:HIS:CE1	2.46	0.50
1:A:195:GLU:OE1	1:A:199:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:HB2	1:B:340:THR:HG23	1.94	0.49
1:B:206:TRP:O	1:B:207:GLN:NE2	2.45	0.49
1:D:314:ASN:O	1:D:315:VAL:HG13	2.12	0.49
1:D:336:LEU:HD23	1:D:352:ILE:O	2.11	0.49
1:A:85:TRP:CD1	1:B:76:PRO:HB2	2.47	0.49
1:B:344:ASN:CG	1:B:346:GLN:H	2.15	0.49
1:C:107:TYR:CG	1:C:108:VAL:N	2.80	0.49
1:C:134:ARG:HH21	1:C:203:GLN:NE2	2.09	0.49
1:D:142:ARG:HA	1:D:148:LYS:O	2.12	0.49
1:D:425:PHE:CD2	1:D:425:PHE:N	2.80	0.49
1:A:309:GLU:C	1:A:311:SER:H	2.14	0.49
1:B:323:ASP:O	1:B:325:ASN:N	2.45	0.49
1:C:180:HIS:CD2	1:C:182:LYS:H	2.31	0.49
1:C:270:MET:HB2	1:C:320:VAL:HG13	1.94	0.49
1:C:334:TYR:HB2	1:C:354:TYR:O	2.13	0.49
1:B:427:MET:HG2	1:B:445:GLY:HA3	1.95	0.49
1:A:180:HIS:CD2	1:A:182:LYS:H	2.24	0.49
1:A:342:LEU:O	1:A:344:ASN:N	2.43	0.49
1:B:141:VAL:HB	1:B:151:ALA:HB3	1.94	0.49
1:D:317:LYS:HB2	1:D:334:TYR:CE2	2.46	0.49
1:A:277:THR:HG21	1:A:328:ILE:HD12	1.95	0.49
1:B:156:THR:O	1:B:173:GLU:N	2.45	0.49
1:B:308:ASP:OD2	1:B:311:SER:HB2	2.13	0.49
1:A:327:ILE:CG1	1:C:135:LYS:HE2	2.42	0.49
1:D:223:CYS:O	1:D:415:LEU:N	2.46	0.49
1:D:232:TRP:HA	1:D:235:LEU:HD12	1.94	0.49
1:D:377:THR:HG23	1:D:378:ASP:H	1.77	0.49
1:D:221:THR:CG2	1:D:446:ILE:HG13	2.43	0.49
1:A:245:PRO:C	1:A:246:ASN:OD1	2.51	0.49
1:A:421:ASN:O	1:A:422:TYR:HB2	2.13	0.49
1:C:268:ARG:HG3	1:C:320:VAL:HG23	1.95	0.49
1:B:221:THR:OG1	1:B:222:THR:N	2.44	0.49
1:D:285:TYR:CG	1:D:359:ALA:HA	2.48	0.49
1:D:290:ASP:OD1	1:D:445:GLY:HA3	2.11	0.49
1:D:295:PHE:CD2	1:D:300:PHE:HA	2.48	0.49
1:A:288:ARG:NH2	1:A:368:TYR:OH	2.46	0.49
1:A:439:VAL:HG23	1:A:439:VAL:O	2.13	0.49
1:C:416:ASN:HB3	1:C:418:TYR:CE1	2.47	0.49
1:D:157:PRO:O	1:D:158:VAL:HB	2.13	0.49
1:D:161:LYS:HB2	1:D:294:LEU:CD1	2.40	0.49
1:B:181:LYS:HA	1:B:184:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:HB3	1:D:110:ASP:OD1	2.13	0.48
1:B:258:LEU:O	1:B:259:PRO:O	2.31	0.48
1:B:279:LEU:HD12	1:B:282:LEU:HD23	1.95	0.48
1:B:333:SER:OG	1:B:356:PHE:HB3	2.12	0.48
1:B:399:ASN:O	1:B:403:LEU:HG	2.12	0.48
1:C:178:CYS:O	1:C:179:ILE:HD12	2.12	0.48
1:D:183:LEU:O	1:D:186:LYS:HB2	2.14	0.48
1:A:211:THR:HA	1:A:416:ASN:O	2.12	0.48
1:B:248:THR:O	1:B:251:SER:N	2.46	0.48
1:D:268:ARG:O	1:D:319:TYR:CA	2.61	0.48
1:A:130:PRO:HA	1:A:302:HIS:CD2	2.47	0.48
1:D:268:ARG:O	1:D:320:VAL:N	2.46	0.48
1:D:290:ASP:HB2	1:D:427:MET:SD	2.53	0.48
1:A:216:LEU:H	1:A:216:LEU:CD2	2.26	0.48
1:A:210:TYR:HH	1:A:420:PHE:HB2	1.72	0.48
1:B:399:ASN:HA	1:B:402:PHE:CE2	2.49	0.48
1:D:315:VAL:O	1:D:336:LEU:N	2.47	0.48
1:D:435:THR:C	1:D:437:GLU:N	2.66	0.48
1:A:232:TRP:O	1:A:235:LEU:HB2	2.14	0.48
1:B:106:ASN:ND2	1:B:181:LYS:H	2.12	0.48
1:D:302:HIS:C	1:D:304:MET:H	2.16	0.48
1:D:291:ILE:HD12	1:D:419:LEU:HD11	1.94	0.48
1:A:339:PHE:CD2	1:A:352:ILE:HD12	2.48	0.48
1:A:110:ASP:HB2	2:A:452:R64:C30	2.43	0.48
1:C:252:MET:O	1:C:253:VAL:C	2.52	0.48
1:D:355:LEU:HD12	1:D:355:LEU:H	1.79	0.48
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.33	0.48
1:A:173:GLU:HG3	1:A:450:LEU:HD23	1.95	0.48
1:C:180:HIS:HB3	1:C:183:LEU:HD23	1.96	0.48
1:C:95:GLN:HA	1:C:98:GLU:HG3	1.94	0.48
1:D:209:LEU:HD12	1:D:210:TYR:H	1.75	0.48
1:D:230:ILE:HG23	1:D:384:LYS:HZ3	1.77	0.48
1:D:383:SER:HA	1:D:388:VAL:HB	1.95	0.48
1:A:68:THR:HA	1:A:69:PRO:C	2.34	0.48
1:C:184:ARG:CG	1:C:184:ARG:HH11	2.27	0.48
1:C:215:ILE:HG13	1:C:216:LEU:HD22	1.95	0.48
1:C:399:ASN:HA	1:C:402:PHE:CE2	2.48	0.48
1:D:360:SER:HB2	1:D:375:LEU:CD2	2.43	0.48
1:A:399:ASN:HA	1:A:402:PHE:CE2	2.49	0.48
1:B:173:GLU:OE2	1:B:450:LEU:HB3	2.14	0.48
1:B:270:MET:HG3	1:B:274:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HG12	1:C:140:GLY:N	2.29	0.47
1:D:270:MET:HA	1:D:320:VAL:CG1	2.44	0.47
1:C:322:GLU:HA	1:C:327:ILE:O	2.15	0.47
1:D:177:LEU:HD12	1:D:178:CYS:N	2.29	0.47
1:A:282:LEU:O	1:A:286:GLN:HG3	2.15	0.47
1:D:296:THR:O	1:D:297:GLU:C	2.53	0.47
1:D:375:LEU:O	1:D:376:ILE:HD13	2.15	0.47
1:B:361:ASP:HA	1:B:363:PHE:CE2	2.50	0.47
1:D:267:LEU:HD21	1:D:332:PHE:HZ	1.79	0.47
1:A:207:GLN:HA	1:A:420:PHE:O	2.14	0.47
1:B:341:VAL:N	1:B:348:ASP:O	2.47	0.47
1:B:264:LEU:HD21	1:B:374:GLU:OE1	2.13	0.47
1:C:110:ASP:OD1	1:C:114:THR:N	2.48	0.47
1:C:195:GLU:HA	1:D:77:LEU:HD23	1.96	0.47
1:A:363:PHE:CE1	1:A:364:GLU:HG3	2.49	0.47
1:B:323:ASP:CG	1:B:327:ILE:HB	2.35	0.47
1:C:202:LYS:O	1:C:203:GLN:HG2	2.14	0.47
1:D:116:ARG:HB2	1:D:342:LEU:HD23	1.97	0.47
1:D:207:GLN:HE22	1:D:421:ASN:ND2	2.13	0.47
1:B:201:ASN:ND2	1:B:205:ILE:O	2.43	0.47
1:C:193:ILE:HA	1:C:196:ILE:HG22	1.96	0.47
1:D:398:ASP:O	1:D:401:TYR:HB2	2.15	0.47
1:A:394:LEU:HD13	1:A:417:TYR:OH	2.15	0.47
1:B:300:PHE:CZ	1:B:304:MET:HG3	2.49	0.47
1:C:434:LYS:NZ	1:C:435:THR:HG22	2.29	0.47
1:D:184:ARG:O	1:D:185:ASN:HB2	2.14	0.47
1:D:321:VAL:CB	1:D:330:ASP:HB2	2.42	0.47
1:D:389:ASP:N	1:D:389:ASP:OD2	2.48	0.47
1:D:224:ARG:N	1:D:395:THR:OG1	2.40	0.47
1:A:221:THR:HG23	1:A:222:THR:N	2.29	0.47
1:A:268:ARG:NH2	1:A:274:ASP:OD2	2.48	0.47
1:A:436:LYS:NZ	1:A:436:LYS:HB2	2.25	0.47
1:B:252:MET:O	1:B:255:SER:N	2.47	0.47
1:B:252:MET:O	1:B:255:SER:OG	2.20	0.47
1:B:273:LYS:HG3	1:B:274:ASP:N	2.25	0.47
1:B:368:TYR:O	1:B:369:LYS:C	2.53	0.47
1:C:179:ILE:HD11	1:C:192:LEU:HD12	1.97	0.47
1:C:435:THR:HB	1:C:437:GLU:OE1	2.15	0.47
1:C:89:ASP:C	1:C:89:ASP:OD2	2.51	0.47
1:D:116:ARG:HB3	1:D:340:THR:OG1	2.15	0.47
1:D:278:VAL:O	1:D:282:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:LYS:CD	1:D:373:ASN:HD21	2.27	0.47
1:D:441:ASP:OD2	1:D:441:ASP:N	2.48	0.47
1:B:161:LYS:HA	1:B:168:VAL:HA	1.97	0.46
1:B:284:LYS:HA	1:B:287:GLU:OE1	2.14	0.46
1:D:282:LEU:HA	1:D:359:ALA:CB	2.45	0.46
1:D:231:ASN:HB2	1:D:384:LYS:HG2	1.96	0.46
1:A:257:THR:C	1:A:258:LEU:HD23	2.35	0.46
1:B:377:THR:HA	1:B:380:LEU:HD12	1.98	0.46
1:D:118:LYS:O	1:D:119:TYR:C	2.53	0.46
1:D:245:PRO:C	1:D:247:GLN:H	2.17	0.46
1:D:270:MET:HE1	1:D:278:VAL:HG21	1.96	0.46
1:D:275:VAL:CG1	1:D:297:GLU:HG2	2.43	0.46
1:D:268:ARG:HG2	1:D:320:VAL:HG23	1.97	0.46
1:D:289:PHE:CE2	1:D:443:THR:HG23	2.51	0.46
1:A:110:ASP:OD1	1:A:113:ALA:N	2.49	0.46
1:A:210:TYR:OH	1:A:420:PHE:CD1	2.68	0.46
1:B:294:LEU:HD12	1:B:294:LEU:N	2.30	0.46
1:B:317:LYS:HB2	1:B:334:TYR:CE1	2.51	0.46
1:C:448:VAL:HG12	1:C:449:VAL:N	2.30	0.46
1:B:120:SER:C	1:B:122:GLU:H	2.18	0.46
1:C:325:ASN:O	1:C:327:ILE:HG13	2.16	0.46
1:D:313:SER:O	1:D:317:LYS:NZ	2.46	0.46
1:D:432:ASP:CB	1:D:435:THR:HG23	2.44	0.46
1:D:361:ASP:O	1:D:363:PHE:N	2.48	0.46
1:B:221:THR:CG2	1:B:446:ILE:HD11	2.46	0.46
1:B:376:ILE:HG13	1:B:402:PHE:CG	2.50	0.46
1:D:286:GLN:HA	1:D:289:PHE:CE1	2.50	0.46
1:D:315:VAL:HA	1:D:336:LEU:O	2.15	0.46
1:D:417:TYR:O	1:D:418:TYR:CD1	2.68	0.46
1:D:221:THR:HG1	1:D:427:MET:HB2	1.81	0.46
1:A:137:TRP:HB3	1:A:155:ALA:HB3	1.97	0.46
1:A:268:ARG:HH11	1:A:322:GLU:CD	2.19	0.46
1:B:162:LEU:O	1:B:166:ASN:N	2.49	0.46
1:D:319:TYR:HB2	1:D:332:PHE:CE2	2.51	0.46
1:D:369:LYS:HD3	1:D:373:ASN:ND2	2.30	0.46
1:D:434:LYS:HA	1:D:434:LYS:HE2	1.98	0.46
1:D:200:VAL:CG1	1:D:205:ILE:HB	2.45	0.46
1:D:228:ARG:NH1	1:D:230:ILE:HD11	2.31	0.46
1:D:336:LEU:HD21	1:D:353:ALA:HB2	1.97	0.46
1:B:201:ASN:C	1:B:203:GLN:H	2.19	0.46
1:D:189:ALA:O	1:D:192:LEU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:THR:HG21	1:C:446:ILE:CG1	2.46	0.46
1:C:439:VAL:HG23	1:C:442:GLN:CB	2.42	0.46
1:D:184:ARG:HG3	1:D:185:ASN:ND2	2.31	0.46
1:B:319:TYR:CE2	1:B:382:THR:HG21	2.51	0.45
1:C:107:TYR:O	1:C:108:VAL:C	2.55	0.45
1:C:88:LEU:HD12	1:C:95:GLN:HB3	1.96	0.45
1:D:282:LEU:HA	1:D:359:ALA:HB2	1.98	0.45
1:D:315:VAL:HA	1:D:336:LEU:H	1.81	0.45
1:D:319:TYR:O	1:D:320:VAL:HG13	2.16	0.45
1:B:118:LYS:NZ	1:B:340:THR:HG22	2.31	0.45
1:B:80:ILE:HG12	1:B:81:SER:N	2.30	0.45
1:D:175:ASN:HD21	1:D:450:LEU:CD2	2.28	0.45
1:D:286:GLN:HG2	1:D:289:PHE:CE1	2.52	0.45
1:A:365:LYS:HB3	1:A:366:PRO:HD2	1.98	0.45
1:B:201:ASN:C	1:B:203:GLN:N	2.69	0.45
1:B:216:LEU:HB2	1:B:418:TYR:CE2	2.52	0.45
1:C:184:ARG:HG2	1:C:184:ARG:NH1	2.30	0.45
1:C:352:ILE:CD1	1:C:352:ILE:N	2.80	0.45
1:A:101:LYS:HB2	1:A:101:LYS:NZ	2.32	0.45
1:B:243:LEU:HG	1:B:243:LEU:O	2.16	0.45
1:B:293:GLN:NE2	1:B:295:PHE:CZ	2.85	0.45
1:B:377:THR:O	1:B:380:LEU:HB2	2.15	0.45
1:D:163:ASN:ND2	1:D:287:GLU:HA	2.32	0.45
1:D:323:ASP:CG	1:D:325:ASN:H	2.19	0.45
1:D:369:LYS:CE	1:D:373:ASN:HD21	2.29	0.45
1:B:288:ARG:HH21	1:B:288:ARG:HG3	1.81	0.45
1:D:376:ILE:HG21	1:D:402:PHE:CE1	2.52	0.45
1:D:434:LYS:C	1:D:436:LYS:HE3	2.36	0.45
1:B:432:ASP:CG	1:B:434:LYS:H	2.20	0.45
1:C:134:ARG:NH2	1:C:203:GLN:NE2	2.65	0.45
1:C:434:LYS:HD3	1:C:435:THR:CG2	2.47	0.45
1:B:245:PRO:O	1:B:246:ASN:CG	2.55	0.45
1:B:346:GLN:HG2	1:B:347:HIS:N	2.32	0.45
1:B:399:ASN:HA	1:B:402:PHE:CZ	2.51	0.45
1:B:74:ASN:O	1:B:75:ASP:O	2.34	0.45
1:C:206:TRP:N	1:C:206:TRP:CD1	2.84	0.45
1:C:266:GLY:O	1:C:268:ARG:HG2	2.17	0.45
1:D:160:PHE:CD2	1:D:160:PHE:N	2.84	0.45
1:D:331:TYR:CD1	1:D:332:PHE:N	2.85	0.45
1:D:369:LYS:NZ	1:D:373:ASN:ND2	2.59	0.45
1:B:323:ASP:C	1:B:325:ASN:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:HH21	1:C:203:GLN:HE21	1.65	0.45
1:C:74:ASN:ND2	1:C:74:ASN:H	2.02	0.45
1:D:129:LYS:N	1:D:130:PRO:HD2	2.32	0.45
1:D:291:ILE:HG22	1:D:446:ILE:HA	1.98	0.45
1:A:210:TYR:CE1	1:A:418:TYR:HB2	2.52	0.45
1:B:299:GLU:O	1:B:302:HIS:HB3	2.17	0.45
1:B:334:TYR:OH	1:B:386:PHE:HE1	2.00	0.45
1:B:226:GLN:O	1:B:392:ASN:HA	2.17	0.45
1:C:103:LEU:HD12	1:C:178:CYS:SG	2.57	0.45
1:C:216:LEU:HB3	1:C:217:PRO:HD2	1.99	0.45
1:D:264:LEU:HD12	1:D:378:ASP:OD1	2.17	0.45
1:D:431:ILE:HB	1:D:439:VAL:HG13	1.98	0.45
1:D:223:CYS:HA	1:D:395:THR:OG1	2.17	0.45
1:B:106:ASN:HD22	1:B:181:LYS:H	1.64	0.44
1:B:321:VAL:CB	1:B:330:ASP:OD1	2.64	0.44
1:B:334:TYR:HB2	1:B:354:TYR:O	2.17	0.44
1:B:207:GLN:HE21	1:B:421:ASN:HB3	1.81	0.44
1:C:182:LYS:N	1:C:182:LYS:HE3	2.32	0.44
1:D:125:GLN:HG2	1:D:125:GLN:H	1.43	0.44
1:D:267:LEU:HD21	1:D:332:PHE:CZ	2.52	0.44
1:A:215:ILE:HG13	1:A:216:LEU:H	1.83	0.44
1:B:200:VAL:CG1	1:B:205:ILE:HB	2.45	0.44
1:B:279:LEU:HG	1:B:283:TYR:CE2	2.52	0.44
1:B:397:GLN:HB3	1:B:398:ASP:H	1.50	0.44
1:D:315:VAL:CA	1:D:336:LEU:H	2.30	0.44
1:B:215:ILE:CD1	1:B:215:ILE:H	2.26	0.44
1:D:289:PHE:HE2	1:D:443:THR:HG23	1.83	0.44
1:D:309:GLU:CG	1:D:310:ASN:N	2.81	0.44
1:D:253:VAL:O	1:D:257:THR:N	2.50	0.44
1:D:161:LYS:HB3	1:D:292:VAL:CG2	2.47	0.44
1:D:360:SER:HB2	1:D:375:LEU:HD21	2.00	0.44
1:D:291:ILE:HG23	1:D:447:GLY:H	1.82	0.44
1:A:161:LYS:HG3	1:A:167:LYS:O	2.17	0.44
1:A:245:PRO:O	1:A:246:ASN:O	2.36	0.44
1:A:308:ASP:OD2	1:A:310:ASN:N	2.50	0.44
1:D:236:HIS:C	1:D:238:VAL:H	2.21	0.44
1:B:372:LEU:HD21	1:B:402:PHE:HD2	1.83	0.44
1:C:416:ASN:N	1:C:416:ASN:HD22	2.12	0.44
1:D:89:ASP:HB3	1:D:95:GLN:NE2	2.32	0.44
1:A:108:VAL:CG1	1:A:109:GLU:H	2.10	0.44
1:B:161:LYS:HB2	1:B:168:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:SER:O	1:D:362:SER:N	2.51	0.44
1:B:242:HIS:ND1	1:B:242:HIS:N	2.64	0.44
1:B:286:GLN:HB3	1:B:292:VAL:HG11	1.98	0.44
1:B:378:ASP:HA	1:B:381:ILE:HD12	1.99	0.44
1:B:372:LEU:CD2	1:B:402:PHE:HD2	2.30	0.44
1:D:221:THR:OG1	1:D:427:MET:HB2	2.18	0.44
1:D:286:GLN:HB3	1:D:292:VAL:HG12	1.98	0.44
1:D:333:SER:OG	1:D:356:PHE:HD2	2.01	0.44
1:D:88:LEU:HD23	1:D:89:ASP:H	1.83	0.44
1:B:378:ASP:OD2	1:B:381:ILE:HD12	2.18	0.44
1:D:302:HIS:C	1:D:304:MET:N	2.71	0.44
1:D:323:ASP:OD2	1:D:325:ASN:ND2	2.51	0.44
1:B:362:SER:HA	1:B:365:LYS:HG2	1.99	0.43
1:B:451:LEU:O	2:B:452:R64:HC19	2.18	0.43
1:C:171:SER:HA	1:C:205:ILE:CG2	2.48	0.43
1:C:207:GLN:HG3	1:C:421:ASN:O	2.17	0.43
1:D:115:PHE:CD2	1:D:341:VAL:HA	2.53	0.43
1:B:279:LEU:O	1:B:280:SER:C	2.56	0.43
1:B:365:LYS:HB2	1:B:367:ASN:OD1	2.18	0.43
1:D:226:GLN:HG2	1:D:410:SER:CB	2.47	0.43
1:D:300:PHE:CE2	1:D:304:MET:HG3	2.53	0.43
1:D:354:TYR:HA	1:D:392:ASN:O	2.18	0.43
1:A:184:ARG:NH1	1:A:184:ARG:CG	2.80	0.43
1:A:217:PRO:O	1:A:218:THR:OG1	2.35	0.43
1:B:114:THR:HG23	1:B:343:ASP:H	1.81	0.43
1:B:264:LEU:HB2	1:B:378:ASP:OD1	2.19	0.43
1:D:370:LYS:O	1:D:373:ASN:HB2	2.17	0.43
1:D:438:VAL:HG12	1:D:439:VAL:O	2.18	0.43
1:B:110:ASP:CG	1:B:111:ILE:H	2.21	0.43
1:B:395:THR:HG21	1:B:431:ILE:CG2	2.46	0.43
1:D:234:LYS:O	1:D:237:ASP:HB2	2.18	0.43
1:D:294:LEU:O	1:D:295:PHE:O	2.37	0.43
1:D:315:VAL:HG23	1:D:316:VAL:N	2.32	0.43
1:B:110:ASP:O	1:B:111:ILE:HB	2.18	0.43
1:B:169:ILE:HG21	1:B:207:GLN:HG2	2.00	0.43
1:B:439:VAL:HG23	1:B:439:VAL:O	2.18	0.43
1:D:162:LEU:HD23	1:D:162:LEU:HA	1.79	0.43
1:D:162:LEU:CB	1:D:167:LYS:HB3	2.40	0.43
1:A:432:ASP:OD1	1:A:435:THR:HG22	2.19	0.43
1:B:334:TYR:HA	1:B:356:PHE:HB2	2.00	0.43
1:C:153:ILE:CG2	1:C:153:ILE:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TRP:HH2	1:D:205:ILE:HD12	1.84	0.43
1:D:428:ASP:C	1:D:430:GLY:H	2.21	0.43
1:A:308:ASP:CG	1:A:309:GLU:N	2.71	0.43
1:B:248:THR:O	1:B:249:LYS:C	2.56	0.43
1:B:303:TRP:HA	1:B:303:TRP:HE3	1.81	0.43
1:B:388:VAL:HG12	1:B:390:VAL:H	1.83	0.43
1:C:291:ILE:CG2	1:C:446:ILE:HA	2.49	0.43
1:D:270:MET:HG3	1:D:319:TYR:O	2.18	0.43
1:A:208:ALA:HB3	1:A:420:PHE:HB3	2.00	0.43
1:A:376:ILE:HG13	1:A:402:PHE:CD2	2.54	0.43
1:B:165:SER:O	1:B:167:LYS:HE2	2.19	0.43
1:B:424:THR:OG1	1:B:425:PHE:N	2.51	0.43
1:D:180:HIS:HE2	1:D:182:LYS:CD	2.32	0.43
1:D:210:TYR:HE2	1:D:420:PHE:HB2	1.83	0.43
1:D:436:LYS:CB	1:D:436:LYS:HZ2	2.29	0.43
1:D:435:THR:O	1:D:437:GLU:N	2.51	0.43
1:B:130:PRO:HB2	1:B:131:PRO:HD2	2.01	0.43
1:B:275:VAL:HG22	1:B:305:LEU:HD11	2.00	0.43
1:C:180:HIS:CD2	1:C:182:LYS:HB2	2.51	0.43
1:C:435:THR:C	1:C:436:LYS:HZ3	2.22	0.43
1:A:184:ARG:O	1:A:185:ASN:CB	2.66	0.43
1:B:234:LYS:C	1:B:236:HIS:N	2.72	0.43
1:B:401:TYR:HD1	1:B:441:ASP:HA	1.82	0.43
1:C:135:LYS:O	1:C:137:TRP:N	2.52	0.43
1:A:134:ARG:HH21	1:A:203:GLN:NE2	2.17	0.42
1:A:228:ARG:HB2	1:A:408:PHE:CE2	2.54	0.42
1:A:228:ARG:HB2	1:A:408:PHE:CZ	2.53	0.42
1:B:258:LEU:CD2	1:B:259:PRO:HD2	2.49	0.42
1:C:164:LYS:C	1:C:166:ASN:H	2.22	0.42
1:D:355:LEU:HD13	1:D:393:CYS:HA	2.01	0.42
1:A:196:ILE:HG23	1:A:197:THR:N	2.34	0.42
2:A:452:R64:O12	2:A:452:R64:H111	2.19	0.42
1:D:143:VAL:CG1	1:D:146:THR:HG23	2.49	0.42
1:B:279:LEU:HD21	1:B:295:PHE:HB2	2.02	0.42
1:B:344:ASN:OD1	1:B:346:GLN:N	2.49	0.42
1:B:349:GLU:O	1:B:350:LEU:CB	2.67	0.42
1:C:237:ASP:C	1:C:239:GLY:H	2.22	0.42
1:C:249:LYS:O	1:C:251:SER:N	2.52	0.42
1:C:291:ILE:HG22	1:C:446:ILE:HA	2.01	0.42
1:D:142:ARG:HG2	1:D:142:ARG:HH21	1.83	0.42
1:D:274:ASP:OD2	1:D:320:VAL:HG11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:CB	1:A:190:PRO:HD3	2.39	0.42
1:A:275:VAL:O	1:A:276:SER:C	2.57	0.42
1:B:225:TYR:HD2	2:B:452:R64:C9	2.29	0.42
1:B:234:LYS:HE3	1:B:347:HIS:CE1	2.54	0.42
1:B:285:TYR:HH	1:B:368:TYR:HH	1.68	0.42
1:B:362:SER:CB	1:B:371:ARG:HG2	2.50	0.42
1:C:107:TYR:O	1:C:108:VAL:O	2.38	0.42
1:C:139:VAL:O	1:C:152:PHE:CD1	2.73	0.42
1:C:352:ILE:HG22	1:C:353:ALA:N	2.34	0.42
1:D:209:LEU:HD12	1:D:209:LEU:C	2.37	0.42
1:D:245:PRO:C	1:D:247:GLN:N	2.72	0.42
1:D:290:ASP:HB2	1:D:427:MET:HE3	1.99	0.42
1:D:77:LEU:HD13	1:D:77:LEU:HA	1.89	0.42
1:A:376:ILE:O	1:A:380:LEU:HG	2.20	0.42
1:A:77:LEU:HD12	1:A:77:LEU:C	2.40	0.42
1:B:184:ARG:O	1:B:185:ASN:CB	2.66	0.42
1:B:300:PHE:O	1:B:303:TRP:N	2.52	0.42
1:D:109:GLU:CD	1:D:342:LEU:HD21	2.39	0.42
1:D:118:LYS:HB2	1:D:340:THR:HG23	2.01	0.42
1:D:237:ASP:C	1:D:238:VAL:HG13	2.40	0.42
1:D:286:GLN:O	1:D:289:PHE:CD1	2.72	0.42
1:D:168:VAL:HG22	1:D:294:LEU:HD22	2.02	0.42
1:A:106:ASN:HD22	1:A:181:LYS:HB2	1.83	0.42
1:B:235:LEU:HD22	1:B:350:LEU:HD11	2.01	0.42
1:C:180:HIS:HD2	1:C:182:LYS:H	1.67	0.42
1:C:385:LYS:HD2	1:C:385:LYS:O	2.20	0.42
1:D:103:LEU:O	1:D:107:TYR:HB2	2.20	0.42
1:D:430:GLY:O	1:D:439:VAL:HG22	2.20	0.42
1:A:170:ASP:O	1:A:205:ILE:HG23	2.20	0.42
1:A:213:GLY:O	1:A:215:ILE:N	2.52	0.42
1:A:235:LEU:HD23	1:A:350:LEU:HD11	2.01	0.42
1:D:196:ILE:O	1:D:200:VAL:HG23	2.19	0.42
1:D:315:VAL:H	1:D:317:LYS:HZ3	1.67	0.42
1:B:196:ILE:O	1:B:200:VAL:HG23	2.20	0.42
1:B:227:HIS:HA	1:B:392:ASN:OD1	2.20	0.42
1:B:118:LYS:HZ2	1:B:340:THR:CG2	2.32	0.42
1:D:99:LEU:O	1:D:102:LEU:HB3	2.20	0.42
1:D:288:ARG:HG3	1:D:443:THR:CG2	2.45	0.42
1:D:322:GLU:HG3	1:D:322:GLU:O	2.19	0.42
1:D:347:HIS:HB2	1:D:348:ASP:H	1.41	0.42
1:D:92:ASP:OD2	1:D:94:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ILE:O	1:D:96:LEU:HB2	2.19	0.42
1:A:210:TYR:OH	1:A:420:PHE:CB	2.57	0.42
1:B:221:THR:HG21	1:B:446:ILE:CG1	2.49	0.42
1:B:344:ASN:HD21	1:B:346:GLN:HB3	1.85	0.42
1:D:275:VAL:HG21	1:D:301:LYS:HG3	2.02	0.42
1:D:371:ARG:HG3	1:D:375:LEU:CD1	2.50	0.42
1:D:434:LYS:O	1:D:436:LYS:HE3	2.20	0.42
1:D:371:ARG:HG3	1:D:375:LEU:HD11	2.02	0.42
1:A:291:ILE:HG23	1:A:291:ILE:O	2.20	0.41
1:D:339:PHE:HB3	1:D:340:THR:H	1.73	0.41
1:A:436:LYS:HZ3	1:A:436:LYS:CB	2.28	0.41
1:B:131:PRO:HG3	1:B:299:GLU:HA	2.02	0.41
1:B:321:VAL:HB	1:B:330:ASP:CB	2.50	0.41
1:B:321:VAL:CG1	1:B:330:ASP:OD1	2.66	0.41
1:B:395:THR:O	1:B:430:GLY:HA3	2.21	0.41
1:B:431:ILE:HA	1:B:437:GLU:O	2.20	0.41
1:B:352:ILE:HD13	2:B:452:R64:C34	2.50	0.41
1:C:166:ASN:C	1:C:166:ASN:HD22	2.23	0.41
1:D:295:PHE:HD2	1:D:300:PHE:HA	1.84	0.41
1:D:339:PHE:CE2	1:D:352:ILE:HD12	2.54	0.41
1:A:406:CYS:O	1:A:407:LYS:HB2	2.19	0.41
1:A:435:THR:HG23	1:A:437:GLU:HB2	2.02	0.41
1:A:85:TRP:CZ2	1:B:79:LEU:CD2	3.02	0.41
1:B:108:VAL:O	1:B:108:VAL:HG12	2.20	0.41
1:B:118:LYS:HZ2	1:B:340:THR:HG22	1.84	0.41
1:B:398:ASP:O	1:B:400:THR:N	2.52	0.41
1:D:216:LEU:CD2	1:D:216:LEU:N	2.83	0.41
1:D:288:ARG:HG2	1:D:289:PHE:H	1.85	0.41
1:D:396:CYS:O	1:D:397:GLN:HB2	2.19	0.41
1:D:219:PRO:HB2	1:D:416:ASN:OD1	2.19	0.41
1:B:261:ASN:HA	1:B:262:PRO:HD3	1.93	0.41
1:B:277:THR:O	1:B:280:SER:N	2.54	0.41
1:B:291:ILE:HG22	1:B:427:MET:HE2	2.03	0.41
1:B:417:TYR:CE2	1:B:450:LEU:HD11	2.55	0.41
1:C:111:ILE:HG23	1:C:112:ASP:H	1.86	0.41
1:C:72:VAL:HG11	1:D:201:ASN:HB3	2.02	0.41
1:D:106:ASN:ND2	1:D:180:HIS:ND1	2.68	0.41
1:D:317:LYS:N	1:D:334:TYR:O	2.53	0.41
1:D:335:TYR:CZ	1:D:451:LEU:HA	2.55	0.41
1:D:387:GLY:O	1:D:389:ASP:OD2	2.39	0.41
1:D:442:GLN:CG	1:D:443:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ARG:HD3	1:D:77:LEU:CD2	2.50	0.41
1:A:123:PHE:HA	1:A:315:VAL:HG21	2.02	0.41
1:A:380:LEU:HD23	1:A:391:PHE:CD1	2.55	0.41
1:B:181:LYS:HA	1:B:184:ARG:HH11	1.85	0.41
1:B:361:ASP:HA	1:B:363:PHE:CD2	2.55	0.41
1:A:432:ASP:O	1:A:436:LYS:N	2.53	0.41
1:B:450:LEU:CD1	1:B:450:LEU:H	2.13	0.41
1:C:441:ASP:OD2	1:C:441:ASP:N	2.54	0.41
1:D:406:CYS:C	1:D:407:LYS:HD2	2.40	0.41
1:B:221:THR:HG21	1:B:446:ILE:HD11	2.03	0.41
1:B:89:ASP:OD1	1:B:92:ASP:HB2	2.21	0.41
1:D:431:ILE:CG2	1:D:439:VAL:H	2.26	0.41
1:D:77:LEU:HD12	1:D:78:PRO:HD2	2.03	0.41
1:A:216:LEU:HD22	1:A:216:LEU:N	2.35	0.41
1:A:301:LYS:CG	1:A:305:LEU:HD12	2.48	0.41
1:A:363:PHE:HA	1:A:368:TYR:CD2	2.55	0.41
1:A:440:GLU:O	1:A:441:ASP:C	2.59	0.41
1:B:173:GLU:OE1	1:B:450:LEU:HB3	2.21	0.41
1:B:195:GLU:OE1	1:B:199:ARG:NH2	2.44	0.41
1:C:368:TYR:O	1:C:370:LYS:N	2.54	0.41
1:D:211:THR:CG2	1:D:450:LEU:HD13	2.51	0.41
1:D:354:TYR:CE2	1:D:392:ASN:HB2	2.56	0.41
1:A:402:PHE:O	1:A:406:CYS:HB2	2.20	0.41
1:B:123:PHE:O	1:B:124:PHE:C	2.58	0.41
1:B:225:TYR:CD2	2:B:452:R64:C4	3.04	0.41
1:B:131:PRO:CG	1:B:299:GLU:HA	2.51	0.41
1:B:74:ASN:O	1:B:75:ASP:HB3	2.21	0.41
1:C:235:LEU:HD23	1:C:350:LEU:HD11	2.03	0.41
1:C:222:THR:HG23	1:C:416:ASN:ND2	2.36	0.41
1:D:201:ASN:ND2	1:D:201:ASN:N	2.69	0.41
1:D:222:THR:HG23	1:D:416:ASN:CG	2.41	0.41
1:D:232:TRP:O	1:D:235:LEU:N	2.54	0.41
1:D:287:GLU:O	1:D:288:ARG:C	2.59	0.41
1:D:429:GLY:C	1:D:431:ILE:H	2.25	0.41
1:B:279:LEU:HA	1:B:279:LEU:HD12	1.85	0.41
1:D:118:LYS:HB2	1:D:339:PHE:O	2.21	0.41
1:D:281:LEU:HG	1:D:282:LEU:H	1.86	0.41
1:D:334:TYR:CB	1:D:354:TYR:O	2.68	0.41
1:D:428:ASP:CG	1:D:430:GLY:H	2.24	0.41
1:C:135:LYS:C	1:C:137:TRP:N	2.75	0.41
1:C:301:LYS:CE	1:C:309:GLU:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ILE:CG2	1:C:353:ALA:N	2.84	0.41
1:D:353:ALA:O	1:D:392:ASN:HB2	2.21	0.41
1:A:261:ASN:HA	1:A:262:PRO:HD3	1.87	0.40
1:B:158:VAL:HG13	1:B:158:VAL:O	2.20	0.40
1:B:255:SER:HB2	1:B:407:LYS:NZ	2.36	0.40
1:C:383:SER:HB2	1:C:388:VAL:HB	2.02	0.40
1:D:143:VAL:HG11	1:D:146:THR:HG23	2.04	0.40
1:B:330:ASP:HB3	1:B:375:LEU:HD22	2.03	0.40
1:B:383:SER:HA	1:B:386:PHE:HD1	1.84	0.40
1:C:180:HIS:O	1:C:182:LYS:N	2.54	0.40
1:C:210:TYR:HE2	1:C:420:PHE:HB2	1.85	0.40
1:C:313:SER:C	1:C:314:ASN:HD22	2.24	0.40
1:D:270:MET:HA	1:D:320:VAL:HG13	2.02	0.40
1:D:331:TYR:CD1	1:D:331:TYR:C	2.94	0.40
1:D:376:ILE:HG22	1:D:380:LEU:HG	2.02	0.40
1:D:403:LEU:HD21	1:D:408:PHE:HB2	2.03	0.40
1:D:451:LEU:CD1	1:D:451:LEU:N	2.77	0.40
1:A:126:TRP:CE3	1:A:315:VAL:HG11	2.56	0.40
1:A:201:ASN:HD22	1:A:201:ASN:N	2.18	0.40
1:A:397:GLN:HB3	1:A:398:ASP:H	1.72	0.40
1:C:288:ARG:HG3	1:C:288:ARG:HH21	1.86	0.40
1:C:85:TRP:CH2	1:C:195:GLU:HG2	2.57	0.40
1:D:270:MET:CG	1:D:319:TYR:O	2.70	0.40
1:D:84:GLU:OE1	1:D:144:LYS:HG2	2.22	0.40
1:A:112:ASP:O	1:A:113:ALA:CB	2.70	0.40
1:A:231:ASN:O	1:A:232:TRP:C	2.60	0.40
1:B:126:TRP:HD1	1:B:306:GLY:HA2	1.87	0.40
1:C:442:GLN:CA	1:C:442:GLN:NE2	2.83	0.40
1:D:83:PHE:CE2	1:D:183:LEU:HD21	2.57	0.40
1:D:267:LEU:HD13	1:D:321:VAL:HG22	2.04	0.40
1:D:336:LEU:CD2	1:D:353:ALA:HB2	2.50	0.40
1:B:218:THR:HA	1:B:219:PRO:HD2	1.96	0.40
1:B:295:PHE:HB3	1:B:300:PHE:HB2	2.03	0.40
1:D:142:ARG:NH2	1:D:142:ARG:HG2	2.37	0.40
1:D:210:TYR:CZ	1:D:418:TYR:HB3	2.57	0.40
1:D:326:GLY:C	1:D:327:ILE:HD12	2.41	0.40
1:D:400:THR:C	1:D:441:ASP:H	2.25	0.40
1:D:289:PHE:HB3	1:D:445:GLY:O	2.22	0.40

There are no symmetry-related clashes.

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	382/392 (97%)	315 (82%)	49 (13%)	18 (5%)	2	17
1	B	378/392 (96%)	263 (70%)	78 (21%)	37 (10%)	0	3
1	C	379/392 (97%)	310 (82%)	48 (13%)	21 (6%)	2	14
1	D	378/392 (96%)	247 (65%)	91 (24%)	40 (11%)	0	2
All	All	1517/1568 (97%)	1135 (75%)	266 (18%)	116 (8%)	1	7

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	109	GLU
1	A	114	THR
1	A	246	ASN
1	A	342	LEU
1	B	108	VAL
1	B	111	ILE
1	B	259	PRO
1	B	312	ASP
1	B	343	ASP
1	B	350	LEU
1	B	369	LYS
1	B	446	ILE
1	C	108	VAL
1	C	145	SER
1	C	214	SER
1	D	104	TYR
1	D	230	ILE
1	D	275	VAL
1	D	295	PHE
1	D	315	VAL
1	D	348	ASP

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Mol	Chain	Res	Type
1	D	401	TYR
1	D	408	PHE
1	A	215	ILE
1	A	343	ASP
1	A	368	TYR
1	A	441	ASP
1	B	114	THR
1	B	238	VAL
1	B	240	PHE
1	B	272	GLY
1	B	274	ASP
1	B	300	PHE
1	B	324	GLU
1	B	399	ASN
1	B	441	ASP
1	C	153	ILE
1	C	250	SER
1	C	287	GLU
1	C	343	ASP
1	C	441	ASP
1	D	215	ILE
1	D	237	ASP
1	D	241	SER
1	D	254	ALA
1	D	356	PHE
1	D	361	ASP
1	D	362	SER
1	D	407	LYS
1	D	410	SER
1	A	214	SER
1	A	307	HIS
1	A	403	LEU
1	A	422	TYR
1	A	440	GLU
1	B	75	ASP
1	B	163	ASN
1	B	264	LEU
1	B	313	SER
1	B	314	ASN
1	B	403	LEU
1	B	442	GLN
1	C	136	ASP

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Mol	Chain	Res	Type
1	C	164	LYS
1	C	181	LYS
1	C	240	PHE
1	C	253	VAL
1	C	368	TYR
1	D	115	PHE
1	D	119	TYR
1	D	127	ALA
1	D	158	VAL
1	D	221	THR
1	D	245	PRO
1	D	259	PRO
1	D	276	SER
1	D	303	TRP
1	D	415	LEU
1	D	422	TYR
1	A	113	ALA
1	B	110	ASP
1	B	133	TRP
1	B	273	LYS
1	B	281	LEU
1	B	347	HIS
1	B	368	TYR
1	C	233	SER
1	C	396	CYS
1	C	422	TYR
1	D	113	ALA
1	D	121	HIS
1	D	311	SER
1	D	358	TYR
1	D	372	LEU
1	A	247	GLN
1	B	107	TYR
1	B	220	LEU
1	B	301	LYS
1	B	356	PHE
1	C	111	ILE
1	C	216	LEU
1	C	218	THR
1	D	120	SER
1	D	238	VAL
1	A	310	ASN

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Mol	Chain	Res	Type
1	B	168	VAL
1	C	440	GLU
1	B	153	ILE
1	A	259	PRO
1	B	218	THR
1	D	129	LYS
1	D	326	GLY
1	D	351	GLY
1	D	387	GLY
1	D	229	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/360 (98%)	315 (89%)	38 (11%)	6	27
1	B	349/360 (97%)	314 (90%)	35 (10%)	7	30
1	C	350/360 (97%)	312 (89%)	38 (11%)	6	26
1	D	349/360 (97%)	297 (85%)	52 (15%)	3	14
All	All	1401/1440 (97%)	1238 (88%)	163 (12%)	5	24

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	71	ASP
1	A	97	ASP
1	A	101	LYS
1	A	109	GLU
1	A	110	ASP
1	A	125	GLN
1	A	185	ASN
1	A	210	TYR
1	A	211	THR
1	A	216	LEU

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Mol	Chain	Res	Type
1	A	217	PRO
1	A	228	ARG
1	A	233	SER
1	A	242	HIS
1	A	248	THR
1	A	263	LYS
1	A	268	ARG
1	A	273	LYS
1	A	310	ASN
1	A	322	GLU
1	A	331	TYR
1	A	340	THR
1	A	346	GLN
1	A	347	HIS
1	A	348	ASP
1	A	356	PHE
1	A	385	LYS
1	A	400	THR
1	A	405	ASP
1	A	415	LEU
1	A	419	LEU
1	A	425	PHE
1	A	428	ASP
1	A	436	LYS
1	A	437	GLU
1	A	441	ASP
1	A	442	GLN
1	B	74	ASN
1	B	101	LYS
1	B	159	THR
1	B	167	LYS
1	B	173	GLU
1	B	186	LYS
1	B	211	THR
1	B	216	LEU
1	B	228	ARG
1	B	242	HIS
1	B	274	ASP
1	B	283	TYR
1	B	284	LYS
1	B	287	GLU
1	B	288	ARG

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Mol	Chain	Res	Type
1	B	290	ASP
1	B	294	LEU
1	B	303	TRP
1	B	314	ASN
1	B	330	ASP
1	B	331	TYR
1	B	342	LEU
1	B	344	ASN
1	B	356	PHE
1	B	378	ASP
1	B	383	SER
1	B	395	THR
1	B	398	ASP
1	B	400	THR
1	B	401	TYR
1	B	419	LEU
1	B	421	ASN
1	B	424	THR
1	B	450	LEU
1	B	451	LEU
1	C	71	ASP
1	C	74	ASN
1	C	75	ASP
1	C	91	ASP
1	C	103	LEU
1	C	106	ASN
1	C	114	THR
1	C	116	ARG
1	C	145	SER
1	C	159	THR
1	C	166	ASN
1	C	167	LYS
1	C	171	SER
1	C	182	LYS
1	C	183	LEU
1	C	185	ASN
1	C	214	SER
1	C	228	ARG
1	C	243	LEU
1	C	246	ASN
1	C	248	THR
1	C	249	LYS

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Mol	Chain	Res	Type
1	C	267	LEU
1	C	268	ARG
1	C	288	ARG
1	C	294	LEU
1	C	314	ASN
1	C	331	TYR
1	C	356	PHE
1	C	365	LYS
1	C	384	LYS
1	C	393	CYS
1	C	398	ASP
1	C	419	LEU
1	C	420	PHE
1	C	427	MET
1	C	434	LYS
1	C	436	LYS
1	D	82	ASP
1	D	86	SER
1	D	88	LEU
1	D	107	TYR
1	D	115	PHE
1	D	125	GLN
1	D	134	ARG
1	D	146	THR
1	D	160	PHE
1	D	184	ARG
1	D	204	ASN
1	D	209	LEU
1	D	221	THR
1	D	222	THR
1	D	225	TYR
1	D	228	ARG
1	D	242	HIS
1	D	257	THR
1	D	271	THR
1	D	278	VAL
1	D	281	LEU
1	D	288	ARG
1	D	290	ASP
1	D	294	LEU
1	D	309	GLU
1	D	310	ASN

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Mol	Chain	Res	Type
1	D	312	ASP
1	D	323	ASP
1	D	329	THR
1	D	332	PHE
1	D	343	ASP
1	D	347	HIS
1	D	358	TYR
1	D	368	TYR
1	D	374	GLU
1	D	377	THR
1	D	386	PHE
1	D	389	ASP
1	D	391	PHE
1	D	403	LEU
1	D	406	CYS
1	D	407	LYS
1	D	410	SER
1	D	422	TYR
1	D	423	ARG
1	D	425	PHE
1	D	432	ASP
1	D	433	LYS
1	D	434	LYS
1	D	436	LYS
1	D	441	ASP
1	D	451	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	125	GLN
1	A	180	HIS
1	A	185	ASN
1	A	201	ASN
1	A	203	GLN
1	A	227	HIS
1	A	307	HIS
1	A	310	ASN
1	A	416	ASN
1	B	74	ASN
1	B	106	ASN

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Mol	Chain	Res	Type
1	B	125	GLN
1	B	166	ASN
1	B	180	HIS
1	B	185	ASN
1	B	207	GLN
1	B	226	GLN
1	B	307	HIS
1	B	314	ASN
1	B	373	ASN
1	C	74	ASN
1	C	106	ASN
1	C	166	ASN
1	C	180	HIS
1	C	185	ASN
1	C	203	GLN
1	C	307	HIS
1	C	314	ASN
1	C	416	ASN
1	C	442	GLN
1	D	106	ASN
1	D	138	HIS
1	D	175	ASN
1	D	185	ASN
1	D	201	ASN
1	D	236	HIS
1	D	325	ASN
1	D	421	ASN
1	D	442	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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	R64	A	452	-	27,33,33	1.14	3 (11%)	30,45,45	1.53	7 (23%)
2	R64	B	452	-	27,33,33	1.19	4 (14%)	30,45,45	1.69	7 (23%)
2	R64	C	452	-	27,33,33	0.85	1 (3%)	30,45,45	1.19	4 (13%)

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	R64	A	452	-	-	0/9/17/17	0/4/4/4
2	R64	B	452	-	-	1/9/17/17	0/4/4/4
2	R64	C	452	-	-	0/9/17/17	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	452	R64	C17-C18	-3.17	1.44	1.51
2	B	452	R64	C4-C9	-3.12	1.36	1.43
2	A	452	R64	C4-C9	-2.93	1.37	1.43
2	A	452	R64	C2-C10	-2.70	1.44	1.50
2	B	452	R64	C17-C18	-2.40	1.46	1.51
2	B	452	R64	C7-C6	2.23	1.43	1.38
2	B	452	R64	C2-C10	-2.09	1.45	1.50
2	C	452	R64	C4-C9	-2.07	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	R64	C33-N32-C31	-3.87	104.15	108.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	R64	O30-C10-C2	3.61	125.04	118.58
2	A	452	R64	C33-N32-C31	-3.26	104.85	108.56
2	B	452	R64	O30-C10-C31	2.99	123.45	118.44
2	B	452	R64	C3-C4-C9	-2.99	105.43	110.65
2	B	452	R64	C8-C9-C4	2.87	122.60	117.84
2	B	452	R64	O12-C5-C6	-2.79	118.31	124.46
2	A	452	R64	C30-N32-C31	2.76	130.30	126.39
2	C	452	R64	C8-C9-C4	2.67	122.27	117.84
2	B	452	R64	C30-N32-C31	2.67	130.17	126.39
2	A	452	R64	C3-C4-C9	-2.61	106.08	110.65
2	C	452	R64	C33-N32-C31	-2.44	105.78	108.56
2	A	452	R64	C17-N16-C15	-2.39	105.21	113.41
2	C	452	R64	C21-N22-C23	2.16	120.58	116.85
2	A	452	R64	O30-C10-C2	2.10	122.34	118.58
2	C	452	R64	C3-C4-C9	-2.09	107.00	110.65
2	A	452	R64	C19-C18-C23	2.04	120.09	117.10
2	A	452	R64	C15-C14-C13	-2.03	106.39	113.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	452	R64	N16-C17-C18-C23

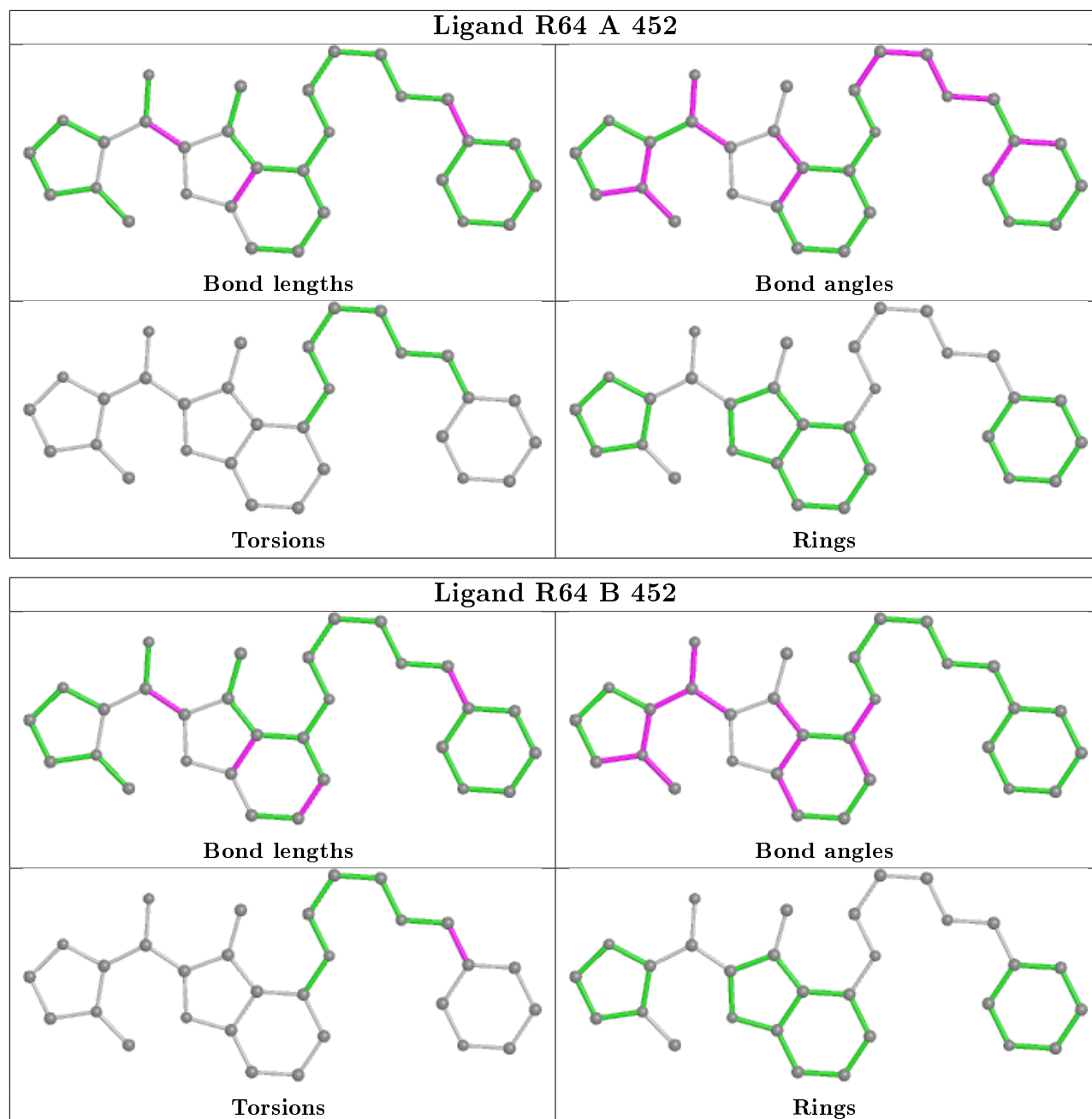
There are no ring outliers.

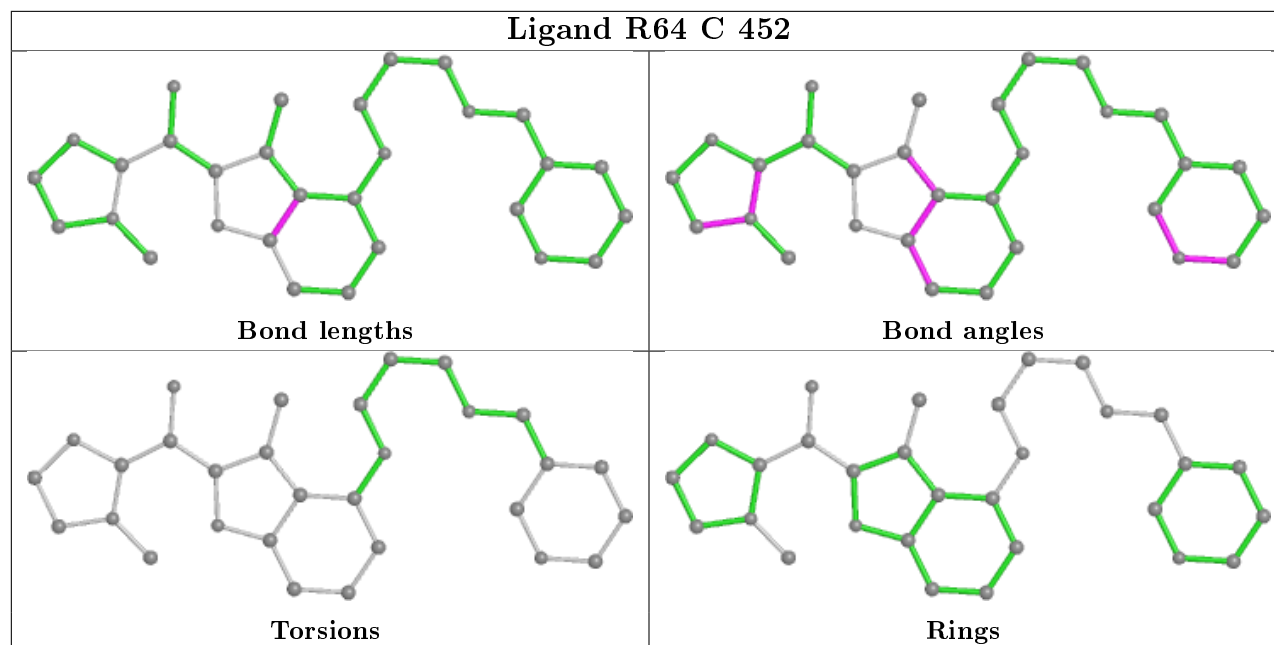
2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	452	R64	3	0
2	B	452	R64	10	0

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

equivalents in the CSD to analyse the geometry.





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	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	113:ALA	C	114:THR	N	1.16
1	A	107:TYR	C	108:VAL	N	0.97

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.