



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VG6  
Title : CRYSTAL STRUCTURES OF HIV-1 REVERSE TRANSCRIPTASE COM-  
PLEXES WITH THIOCARBAMATE NON-NUCLEOSIDE INHIBITORS  
Authors : Spallarossa, A.; Cesarini, S.; Ranise, A.; Ponassi, M.; Unge, T.; Bolognesi, M.  
Deposited on : 2007-11-08  
Resolution : 3.01 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

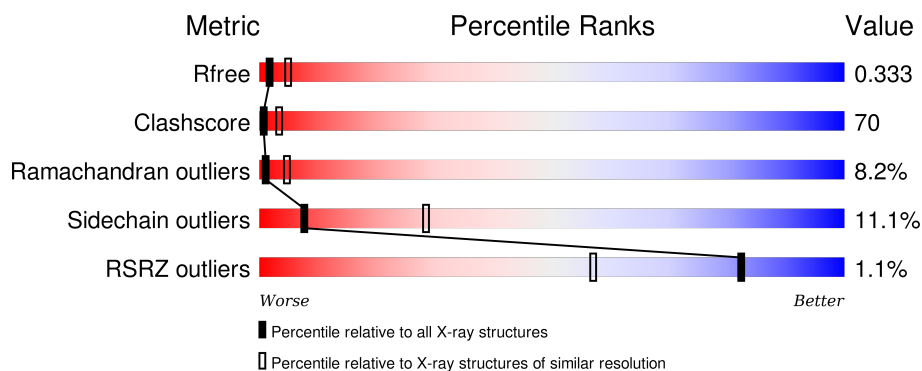
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
$R_{free}$	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div></div> <div>31% 53% 15% .</div> </div>
2	B	428	<div> <div></div> <div>27% 55% 11% • 6%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7856 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.

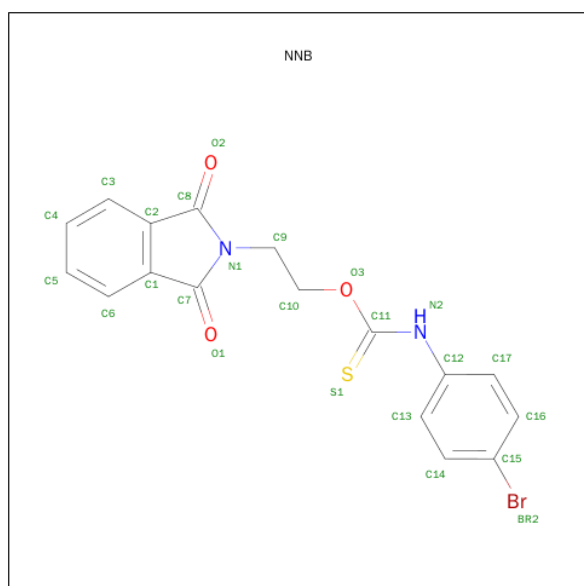
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	1
			4468	2893	745	822	8			

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3318	2163	543	605	7			

- Molecule 3 is O-[2-(1,3-DIOXO-1,3-DIHYDRO-2H-ISOINDOL-2-YL)ETHYL] (4-BROMO PHENYL)THIOCARBAMATE (three-letter code: NNB) (formula: C<sub>17</sub>H<sub>13</sub>BrN<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	S	0	0
			24	1	17	2	3	1		

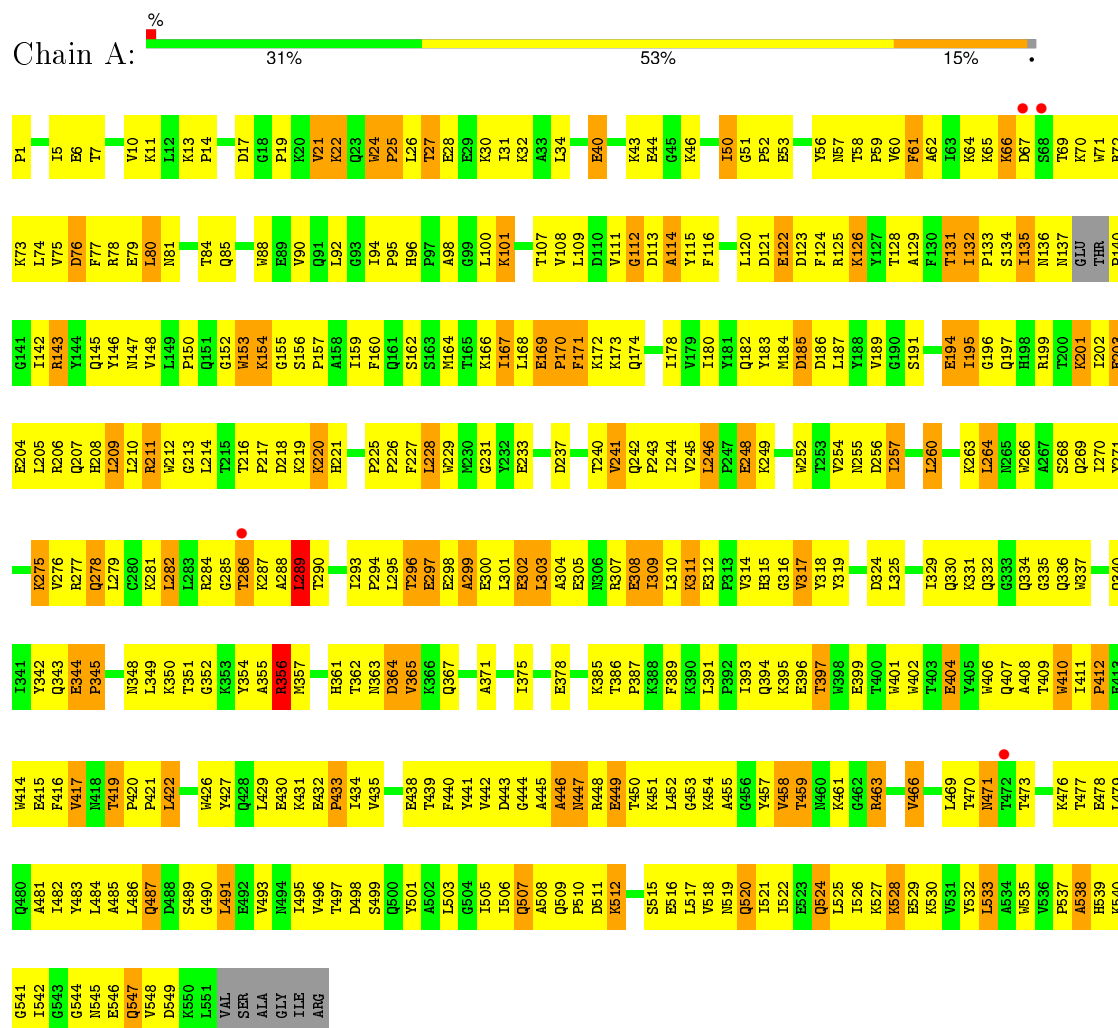
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	24	Total 24	O 24	0	0

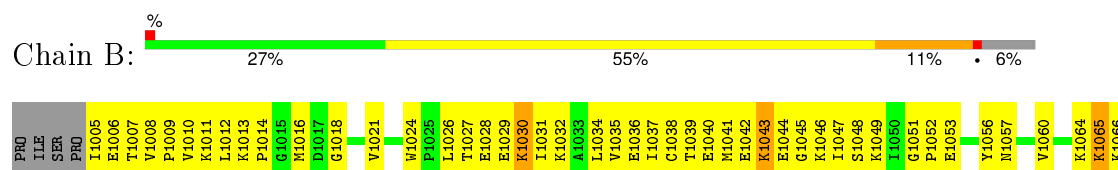
### 3 Residue-property plots

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

#### • Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H



#### • Molecule 2: P51 RT



E1399	G1333	I1270	L1209	Q1145	D1067
E1400	Q1334	Y1271	L1210	Y1146	S1068
W1401	G1335	P1272	M1211	M1147	T1069
W1402	Q1336	G1273	W1212	V1148	
L1403	W1337	I1274	G1213	L1149	R1072
E1404	T1338	K1275	L1214	P1150	K1073
Y1405	Y1339	V1276	THR	Q1151	L1074
W1406	Q1340	M1277	THR	G1152	V1075
W1407	I1341	Q1278	PRO	W1153	D1076
	Y1342	L1279	ASP	K1154	F1077
	Q1343	C1280	LYS	G1155	R1078
W1410	E1344	K1281	LYS	S1156	E1079
	P1345	L1282	HIS	P1157	L1080
E1414	F1346	LEU	GLN	A1158	N1081
E1415	F1347	ARG	LYS	G1159	K1082
F1416	M1348	GLY	GLU	F1160	R1083
Y1417	K1349	T1286	PRO	S1162	Q1084
N1418	K1350	K1287	PRO	S1163	Q1085
T1419	T1351	A1288	PHE	M1164	D1086
P1420	G1352	L1289	LEU		F1087
P1421		T1290	TRP		W1088
L1422	A1355	E1291	M1230	I1167	E1089
Y1423	ARG	V1292	G1231	L1168	V1090
K1424	MET	I1293	Y1232	E1169	Q1091
L1425	ARG	P1294	E1233	P1170	L1092
W1426	GLY	L1295	L1234	F1171	G1093
Y1427	ALA	T1296	H1235	K1172	I1094
Q1428	H1361	E1297	P1236	K1173	
	T1362	E1298		Q1182	V1111
	N1363	A1299	W1239	Y1183	G1112
D1364	D1364	E1300	T1240	M1184	D1113
V1365	V1365	L1301	V1241	D1186	A1114
K1366	K1366	E1302	Q1242	D1187	V1115
Q1367	Q1367	L1303	P1243	L1187	F1116
		A1304	I1244	Y1188	S1117
		E1305	V1245	V1189	V1118
		N1306	L1246	G1190	P1119
		R1307	P1247	S1191	L1120
	K1374	E1308	E1248	D1192	D1121
	I1375	I1309	K1249	L1193	E1122
	T1376	L1310	D1250	E1194	D1123
	T1377	K1311	S1251	I1195	F1124
	E1378	E1312	W1252	G1196	R1125
	S1379	P1313	T1253	Q1197	K1126
	I1380	W1314	V1254	H1198	
	V1381		M1255	R1199	F1130
	I1382	V1317	D1256	T1200	I1135
	W1383		I1257	K1201	N1136
	G1384		Q1258	I1202	
	K1385		K1259	E1203	
			L1260	R1206	
	K1388		V1261		
	F1389		G1262		
	K1390		K1263		
	L1391		L1264		
	P1392		N1265		
	I1393		W1266		
	Q1394		A1267		
	K1395		S1268		
			Q1269		
	W1398				

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.59Å 157.18Å 154.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 19.93 – 3.01	Depositor EDS
% Data completeness (in resolution range)	83.8 (20.00-3.01) 83.8 (19.93-3.01)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.244 , 0.335 0.237 , 0.333	Depositor DCC
$R_{free}$ test set	1236 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 24341 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.28	1/4585 (0.0%)	0.43	0/6226
2	B	0.24	0/3411	0.41	0/4632
All	All	0.26	1/7996 (0.0%)	0.42	0/10858

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	GLU	CD-OE2	7.34	1.33	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	419	THR	Peptide

### 5.2 Too-close contacts [i](#)

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4468	0	4527	624	1
2	B	3318	0	3341	499	0
3	A	24	0	13	2	0
4	A	22	0	0	9	1
4	B	24	0	0	10	0
All	All	7856	0	7881	1099	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 70.

All (1099) 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)
2:B:1266:TRP:CH2	2:B:1346:PHE:HZ	1.25	1.49
2:B:1266:TRP:CH2	2:B:1346:PHE:CZ	1.99	1.48
1:A:450:THR:CG2	1:A:452:LEU:HD22	1.51	1.40
1:A:344:GLU:HB3	1:A:345:PRO:CD	1.49	1.36
2:B:1282:LEU:O	2:B:1287:LYS:NZ	1.67	1.26
1:A:486:LEU:HB3	1:A:524:GLN:CG	1.66	1.25
2:B:1195:ILE:CD1	2:B:1195:ILE:H	1.39	1.22
1:A:410:TRP:CE3	2:B:1363:ASN:HB2	1.76	1.20
1:A:50:ILE:HD12	1:A:51:GLY:N	1.54	1.20
1:A:206:ARG:NH1	1:A:217:PRO:O	1.77	1.17
2:B:1195:ILE:HD12	2:B:1195:ILE:N	1.47	1.16
1:A:76:ASP:O	1:A:76:ASP:OD2	1.63	1.16
2:B:1323:LYS:HE2	2:B:1324:ASP:OD1	1.43	1.16
1:A:486:LEU:CB	1:A:524:GLN:HG2	1.76	1.16
2:B:1303:LEU:HD12	2:B:1304:ALA:N	1.62	1.14
2:B:1323:LYS:CE	2:B:1324:ASP:OD1	1.95	1.14
1:A:278:GLN:HA	1:A:278:GLN:HE21	0.97	1.12
1:A:263:LYS:CA	1:A:263:LYS:HE2	1.79	1.11
1:A:218:ASP:HB3	1:A:221:HIS:HB2	1.23	1.11
2:B:1087:PHE:O	2:B:1091:GLN:HB3	1.47	1.10
1:A:278:GLN:HE22	1:A:281:LYS:HD2	1.00	1.10
1:A:263:LYS:HA	1:A:263:LYS:HE2	1.22	1.10
2:B:1012:LEU:HD23	2:B:1013:LYS:H	1.04	1.10
2:B:1391:LEU:CD2	2:B:1414:TRP:HB2	1.83	1.09
2:B:1005:ILE:HG22	2:B:1006:GLU:H	0.99	1.09
1:A:120:LEU:HD12	1:A:121:ASP:H	1.11	1.08
1:A:450:THR:HG22	1:A:452:LEU:HD22	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1266:TRP:CZ3	2:B:1346:PHE:HZ	1.70	1.07
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.33	1.07
1:A:220:LYS:H	1:A:220:LYS:HD3	1.20	1.06
1:A:497:THR:HG22	1:A:498:ASP:O	1.54	1.06
1:A:84:THR:HG22	1:A:85:GLN:H	1.18	1.06
1:A:451:LYS:O	1:A:470:THR:O	1.71	1.06
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.06	1.06
1:A:450:THR:HG21	1:A:452:LEU:HD22	1.37	1.06
2:B:1324:ASP:OD2	2:B:1388:LYS:HE3	1.54	1.06
1:A:278:GLN:NE2	1:A:281:LYS:HD2	1.72	1.05
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.38	1.04
2:B:1246:LEU:O	2:B:1307:ARG:NH1	1.91	1.04
2:B:1317:VAL:HG22	2:B:1347:LYS:HG3	1.35	1.03
1:A:305:GLU:O	1:A:309:ILE:HG23	1.57	1.03
1:A:344:GLU:CB	1:A:345:PRO:HD2	1.89	1.03
1:A:410:TRP:CE3	2:B:1363:ASN:CB	2.40	1.02
1:A:344:GLU:HB3	1:A:345:PRO:HD2	1.05	1.02
2:B:1005:ILE:HG22	2:B:1006:GLU:N	1.71	1.01
2:B:1266:TRP:CZ2	2:B:1346:PHE:CE2	2.49	1.01
1:A:286:THR:HG22	1:A:286:THR:O	1.59	1.01
1:A:344:GLU:CB	1:A:345:PRO:CD	2.39	1.01
1:A:395:LYS:O	1:A:399:GLU:HG2	1.61	1.01
2:B:1266:TRP:O	2:B:1269:GLN:HB2	1.60	1.01
1:A:356:ARG:HA	1:A:356:ARG:HE	1.24	1.01
1:A:395:LYS:HE2	1:A:396:GLU:OE2	1.60	1.00
2:B:1275:LYS:HA	2:B:1275:LYS:HE3	1.44	1.00
1:A:342:TYR:HA	1:A:349:LEU:CD1	1.90	1.00
1:A:94:ILE:CG2	1:A:229:TRP:HH2	1.75	1.00
2:B:1249:LYS:O	2:B:1250:ASP:CG	2.00	1.00
1:A:524:GLN:HA	1:A:524:GLN:HE21	1.24	0.99
1:A:394:GLN:HB2	1:A:397:THR:HG22	1.45	0.99
2:B:1391:LEU:HD21	2:B:1414:TRP:HB2	1.42	0.99
2:B:1266:TRP:CZ2	2:B:1346:PHE:CZ	2.50	0.99
2:B:1335:GLY:HA2	2:B:1367:GLN:HE22	1.27	0.98
1:A:94:ILE:CG2	1:A:229:TRP:CH2	2.46	0.98
1:A:278:GLN:HE22	1:A:281:LYS:CD	1.76	0.98
1:A:450:THR:CG2	1:A:452:LEU:CD2	2.42	0.97
2:B:1326:ILE:HG22	2:B:1342:TYR:O	1.62	0.97
1:A:458:VAL:O	1:A:459:THR:OG1	1.81	0.97
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.01	0.96
2:B:1081:ASN:HD21	2:B:1154:LYS:H	1.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:GLU:HG2	1:A:461:LYS:HD3	1.46	0.94
1:A:134:SER:CB	1:A:140:PRO:HD2	1.97	0.94
2:B:1293:ILE:HB	2:B:1294:PRO:CD	1.96	0.94
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.29	0.94
1:A:337:TRP:NE1	1:A:367:GLN:HG2	1.83	0.93
1:A:435:VAL:HG22	2:B:1290:THR:HG21	1.48	0.93
1:A:459:THR:HG22	1:A:461:LYS:H	1.33	0.93
1:A:278:GLN:HA	1:A:278:GLN:NE2	1.80	0.93
1:A:297:GLU:HA	1:A:300:GLU:OE1	1.68	0.93
1:A:231:GLY:O	1:A:242:GLN:HG3	1.67	0.93
1:A:371:ALA:O	1:A:375:ILE:HG13	1.68	0.93
1:A:50:ILE:HD12	1:A:51:GLY:H	1.20	0.92
1:A:309:ILE:HD12	1:A:309:ILE:C	1.89	0.92
1:A:486:LEU:HD13	1:A:524:GLN:HB3	1.49	0.92
2:B:1005:ILE:CG2	2:B:1006:GLU:H	1.82	0.92
2:B:1012:LEU:HD23	2:B:1013:LYS:N	1.85	0.92
1:A:203:GLU:OE2	1:A:219:LYS:HD3	1.70	0.91
1:A:218:ASP:HB3	1:A:221:HIS:CB	1.99	0.91
2:B:1311:LYS:HE2	4:B:2018:HOH:O	1.70	0.91
1:A:479:LEU:O	1:A:517:LEU:HD11	1.69	0.91
1:A:344:GLU:HB3	1:A:345:PRO:HD3	1.52	0.90
1:A:410:TRP:CZ3	2:B:1363:ASN:HB3	2.06	0.90
1:A:335:GLY:HA2	1:A:367:GLN:NE2	1.86	0.90
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.00	0.90
2:B:1076:ASP:OD2	2:B:1078:ARG:HB2	1.69	0.90
1:A:84:THR:HG22	1:A:85:GLN:N	1.83	0.90
1:A:248:GLU:O	1:A:249:LYS:HG2	1.70	0.90
1:A:178:ILE:HD11	1:A:191:SER:HB3	1.55	0.89
1:A:248:GLU:HA	1:A:248:GLU:OE2	1.71	0.89
2:B:1296:THR:HB	2:B:1299:ALA:HB3	1.54	0.89
1:A:216:THR:HB	1:A:217:PRO:HD2	1.54	0.89
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.52	0.89
2:B:1270:ILE:HG23	2:B:1271:TYR:CD2	2.08	0.88
1:A:162:SER:HB2	2:B:1052:PRO:HG3	1.54	0.88
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.72	0.88
3:A:1551:NNB:H13	3:A:1551:NNB:O3	1.73	0.88
2:B:1105:SER:HB3	2:B:1235:HIS:ND1	1.87	0.88
1:A:26:LEU:CD2	1:A:133:PRO:HG2	2.03	0.88
2:B:1161:GLN:OE1	2:B:1161:GLN:C	2.11	0.88
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.54	0.88
2:B:1021:VAL:O	2:B:1057:ASN:ND2	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1170:PRO:O	2:B:1174:GLN:HG3	1.74	0.87
1:A:241:VAL:HG12	1:A:266:TRP:NE1	1.90	0.87
1:A:411:ILE:HG22	1:A:412:PRO:O	1.75	0.87
1:A:120:LEU:HD12	1:A:121:ASP:N	1.89	0.86
2:B:1183:TYR:O	2:B:1184:MET:O	1.92	0.86
2:B:1254:VAL:HG12	2:B:1258:GLN:OE1	1.75	0.86
1:A:288:ALA:O	1:A:290:THR:N	2.08	0.86
1:A:287:LYS:HD2	1:A:293:ILE:HD11	1.57	0.86
1:A:263:LYS:HA	1:A:263:LYS:CE	2.04	0.86
2:B:1249:LYS:HE2	2:B:1256:ASP:OD1	1.75	0.86
2:B:1293:ILE:HB	2:B:1294:PRO:HD2	1.57	0.86
1:A:540:LYS:HB3	1:A:542:ILE:HD13	1.57	0.85
2:B:1086:ASP:OD1	2:B:1087:PHE:N	2.09	0.85
1:A:240:THR:HG22	1:A:241:VAL:N	1.91	0.85
2:B:1167:ILE:HG12	2:B:1212:TRP:CD1	2.12	0.85
1:A:539:HIS:HD2	1:A:549:ASP:OD1	1.60	0.85
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.75	0.85
1:A:278:GLN:CA	1:A:278:GLN:HE21	1.87	0.84
1:A:107:THR:HG21	1:A:202:ILE:CD1	2.08	0.84
2:B:1270:ILE:HG23	2:B:1271:TYR:HD2	1.40	0.84
2:B:1199:ARG:HD2	2:B:1230:MET:HB3	1.58	0.84
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.57	0.84
2:B:1323:LYS:HE3	2:B:1324:ASP:OD1	1.78	0.84
1:A:228:LEU:N	1:A:228:LEU:HD22	1.92	0.84
1:A:84:THR:CG2	1:A:85:GLN:H	1.90	0.84
1:A:136:ASN:O	1:A:137:ASN:O	1.96	0.84
1:A:361:HIS:CE1	1:A:505:ILE:HD13	2.13	0.84
1:A:178:ILE:CD1	1:A:191:SER:HB3	2.07	0.84
2:B:1374:LYS:HD3	2:B:1374:LYS:C	1.97	0.84
1:A:107:THR:HB	4:A:2007:HOH:O	1.76	0.84
1:A:282:LEU:HD21	1:A:296:THR:HG23	1.57	0.84
1:A:355:ALA:O	1:A:357:MET:N	2.11	0.84
1:A:447:ASN:HD22	1:A:449:GLU:H	1.26	0.83
2:B:1012:LEU:CD2	2:B:1013:LYS:H	1.87	0.83
2:B:1169:GLU:HB3	2:B:1170:PRO:CD	2.06	0.83
1:A:134:SER:O	1:A:136:ASN:N	2.12	0.82
2:B:1087:PHE:O	2:B:1091:GLN:CB	2.27	0.82
1:A:431:LYS:HE2	1:A:431:LYS:HA	1.61	0.82
1:A:231:GLY:C	1:A:242:GLN:HG3	2.00	0.82
1:A:96:HIS:H	2:B:1136:ASN:HD21	1.27	0.82
1:A:458:VAL:HG11	1:A:547:GLN:HG3	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HD2	1:A:66:LYS:H	1.43	0.81
2:B:1031:ILE:O	2:B:1035:VAL:HG13	1.80	0.81
1:A:50:ILE:CD1	1:A:51:GLY:N	2.42	0.81
2:B:1266:TRP:CZ3	2:B:1346:PHE:CZ	2.54	0.81
2:B:1317:VAL:HG22	2:B:1347:LYS:CG	2.11	0.80
1:A:395:LYS:CE	1:A:396:GLU:OE2	2.29	0.80
2:B:1326:ILE:HG21	2:B:1342:TYR:CE1	2.16	0.80
2:B:1266:TRP:CH2	2:B:1346:PHE:CE2	2.65	0.80
1:A:69:THR:HG23	1:A:69:THR:O	1.80	0.80
2:B:1271:TYR:HB3	2:B:1274:ILE:CD1	2.12	0.80
1:A:263:LYS:N	1:A:263:LYS:HE2	1.97	0.80
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.81	0.79
2:B:1013:LYS:NZ	2:B:1085:GLN:HB3	1.98	0.79
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.63	0.79
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.16	0.78
2:B:1425:LEU:HD23	2:B:1425:LEU:C	2.03	0.78
1:A:286:THR:O	1:A:286:THR:CG2	2.30	0.78
2:B:1317:VAL:CG2	2:B:1347:LYS:HG3	2.12	0.78
2:B:1171:PHE:HA	2:B:1174:GLN:HE21	1.46	0.78
1:A:94:ILE:HG21	1:A:229:TRP:CH2	2.16	0.78
1:A:473:THR:H	1:A:476:LYS:HE3	1.49	0.78
1:A:112:GLY:HA2	4:A:2003:HOH:O	1.81	0.78
2:B:1195:ILE:HD12	2:B:1195:ILE:H	0.62	0.78
2:B:1303:LEU:HD12	2:B:1304:ALA:H	1.43	0.78
1:A:537:PRO:O	1:A:538:ALA:O	2.02	0.78
1:A:76:ASP:C	1:A:76:ASP:OD2	2.20	0.78
1:A:26:LEU:HD23	1:A:133:PRO:HG2	1.66	0.78
1:A:447:ASN:ND2	1:A:449:GLU:H	1.82	0.78
2:B:1374:LYS:HD3	2:B:1374:LYS:O	1.84	0.77
1:A:126:LYS:HA	1:A:145:GLN:OE1	1.82	0.77
1:A:409:THR:HG22	1:A:410:TRP:N	1.99	0.77
2:B:1151:GLN:O	2:B:1153:TRP:N	2.17	0.77
1:A:458:VAL:HG23	1:A:459:THR:N	1.99	0.77
1:A:65:LYS:HD3	1:A:66:LYS:HD2	1.66	0.77
2:B:1391:LEU:HD21	2:B:1414:TRP:CB	2.13	0.77
1:A:162:SER:CB	2:B:1052:PRO:HG3	2.15	0.77
1:A:227:PHE:C	1:A:228:LEU:HD22	2.05	0.77
2:B:1067:ASP:H	2:B:1407:GLN:HE22	1.29	0.77
2:B:1299:ALA:O	2:B:1302:GLU:HB2	1.85	0.77
1:A:453:GLY:O	1:A:454:LYS:HG3	1.85	0.77
2:B:1332:GLN:O	2:B:1333:GLY:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TRP:CE2	1:A:367:GLN:HG2	2.20	0.77
2:B:1298:GLU:OE2	2:B:1298:GLU:HA	1.85	0.77
2:B:1067:ASP:H	2:B:1407:GLN:NE2	1.83	0.76
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.83	0.76
1:A:13:LYS:HE3	1:A:84:THR:O	1.83	0.76
1:A:184:MET:O	1:A:186:ASP:N	2.18	0.76
2:B:1270:ILE:O	2:B:1271:TYR:HB2	1.86	0.76
2:B:1169:GLU:OE2	2:B:1169:GLU:CA	2.33	0.75
2:B:1400:THR:HG22	2:B:1401:TRP:CD1	2.21	0.75
2:B:1267:ALA:O	2:B:1270:ILE:O	2.04	0.75
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.86	0.75
2:B:1266:TRP:CE3	2:B:1426:TRP:CZ3	2.74	0.75
1:A:450:THR:HG21	1:A:452:LEU:CD2	2.10	0.75
2:B:1151:GLN:HB3	2:B:1185:ASP:OD1	1.87	0.75
2:B:1066:LYS:HE3	4:B:2006:HOH:O	1.87	0.75
2:B:1105:SER:CB	2:B:1235:HIS:ND1	2.50	0.75
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.68	0.75
2:B:1013:LYS:CE	2:B:1085:GLN:HB3	2.17	0.75
1:A:66:LYS:CD	1:A:66:LYS:H	1.98	0.74
1:A:435:VAL:CG2	2:B:1290:THR:HG21	2.17	0.74
1:A:520:GLN:HA	1:A:520:GLN:OE1	1.86	0.74
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.23	0.74
1:A:486:LEU:HD13	1:A:524:GLN:CB	2.16	0.74
1:A:53:GLU:N	1:A:53:GLU:OE1	2.12	0.74
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.22	0.74
1:A:275:LYS:HE2	1:A:332:GLN:CD	2.08	0.74
1:A:447:ASN:HD22	1:A:447:ASN:C	1.90	0.74
2:B:1169:GLU:OE2	2:B:1169:GLU:HA	1.88	0.74
1:A:246:LEU:HD12	1:A:307:ARG:HG2	1.69	0.74
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.68	0.74
1:A:410:TRP:CE3	2:B:1363:ASN:HB3	2.23	0.74
1:A:518:VAL:O	1:A:522:ILE:HG12	1.88	0.74
1:A:491:LEU:HD12	1:A:491:LEU:N	2.03	0.73
2:B:1253:THR:HG22	2:B:1292:VAL:HA	1.70	0.73
1:A:441:TYR:O	1:A:548:VAL:HG21	1.88	0.73
1:A:6:GLU:HG3	1:A:7:THR:N	2.03	0.73
1:A:61:PHE:CZ	1:A:74:LEU:HD22	2.24	0.73
1:A:540:LYS:HG2	1:A:541:GLY:H	1.54	0.73
2:B:1034:LEU:HA	2:B:1037:ILE:HG22	1.71	0.73
2:B:1008:VAL:O	2:B:1010:VAL:N	2.21	0.73
1:A:539:HIS:CD2	1:A:549:ASP:OD1	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG12	1:A:397:THR:HG23	1.71	0.73
1:A:241:VAL:HG12	1:A:266:TRP:HE1	1.52	0.73
2:B:1122:GLU:HG2	2:B:1125:ARG:CZ	2.19	0.73
2:B:1260:LEU:HG	2:B:1279:LEU:HD21	1.70	0.73
2:B:1067:ASP:N	2:B:1407:GLN:HE22	1.87	0.73
2:B:1135:ILE:HD12	2:B:1135:ILE:O	1.89	0.73
2:B:1122:GLU:O	2:B:1125:ARG:HG3	1.88	0.72
2:B:1262:GLY:O	2:B:1265:ASN:HB3	1.89	0.72
1:A:61:PHE:CE1	1:A:74:LEU:HD22	2.24	0.72
1:A:10:VAL:HG12	1:A:11:LYS:N	2.04	0.72
2:B:1034:LEU:O	2:B:1037:ILE:HG22	1.88	0.72
1:A:356:ARG:HA	1:A:356:ARG:NE	2.03	0.72
1:A:337:TRP:HE1	1:A:367:GLN:HG2	1.53	0.72
1:A:66:LYS:HD2	1:A:66:LYS:N	2.04	0.72
2:B:1251:SER:O	2:B:1252:TRP:HB2	1.88	0.72
2:B:1086:ASP:O	2:B:1090:VAL:HG22	1.89	0.72
1:A:547:GLN:O	1:A:547:GLN:OE1	2.06	0.72
2:B:1311:LYS:HG2	4:B:2018:HOH:O	1.90	0.72
1:A:506:ILE:O	1:A:508:ALA:N	2.22	0.72
2:B:1266:TRP:CE2	2:B:1346:PHE:HE2	2.08	0.71
1:A:260:LEU:HD22	1:A:264:LEU:HD22	1.72	0.71
2:B:1347:LYS:HA	2:B:1347:LYS:HE3	1.73	0.71
1:A:185:ASP:HB2	4:A:2005:HOH:O	1.90	0.71
2:B:1027:THR:OG1	2:B:1030:LYS:HD3	1.90	0.71
2:B:1184:MET:O	2:B:1186:ASP:N	2.22	0.71
2:B:1254:VAL:O	2:B:1258:GLN:HB2	1.90	0.71
1:A:195:ILE:HG12	1:A:199:ARG:HH21	1.54	0.71
1:A:430:GLU:OE2	1:A:530:LYS:HG2	1.90	0.71
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.71	0.71
2:B:1277:ARG:HH11	2:B:1278:GLN:NE2	1.89	0.71
2:B:1081:ASN:ND2	2:B:1154:LYS:HB2	2.06	0.71
1:A:334:GLN:HA	1:A:334:GLN:OE1	1.91	0.71
2:B:1425:LEU:HD23	2:B:1425:LEU:O	1.91	0.70
1:A:271:TYR:CD1	1:A:309:ILE:CD1	2.75	0.70
1:A:275:LYS:HE2	1:A:332:GLN:NE2	2.07	0.70
2:B:1013:LYS:HE3	2:B:1085:GLN:CB	2.20	0.70
2:B:1103:LYS:NZ	2:B:1179:VAL:CG2	2.54	0.70
2:B:1241:VAL:HG13	2:B:1351:THR:HG23	1.72	0.70
1:A:220:LYS:N	1:A:220:LYS:HD3	2.00	0.70
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.73	0.70
1:A:167:ILE:O	1:A:208:HIS:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.21	0.70
2:B:1332:GLN:OE1	2:B:1424:LYS:O	2.10	0.70
2:B:1156:SER:HB2	2:B:1157:PRO:HD3	1.74	0.70
2:B:1161:GLN:OE1	2:B:1161:GLN:O	2.09	0.70
2:B:1086:ASP:CA	2:B:1090:VAL:HG22	2.21	0.69
1:A:46:LYS:HE3	1:A:116:PHE:O	1.92	0.69
1:A:289:LEU:HD23	1:A:289:LEU:N	2.07	0.69
2:B:1103:LYS:HZ3	2:B:1179:VAL:CG2	2.04	0.69
2:B:1282:LEU:HD22	2:B:1296:THR:OG1	1.92	0.69
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.40	0.69
1:A:276:VAL:O	1:A:276:VAL:HG23	1.93	0.69
2:B:1080:LEU:HD23	2:B:1080:LEU:O	1.93	0.69
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.22	0.69
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.74	0.69
1:A:120:LEU:CD1	1:A:121:ASP:H	1.97	0.69
1:A:511:ASP:O	1:A:512:LYS:HB3	1.91	0.69
2:B:1013:LYS:NZ	2:B:1085:GLN:CB	2.56	0.69
1:A:27:THR:HG23	1:A:30:LYS:HD3	1.74	0.69
1:A:241:VAL:CG1	1:A:266:TRP:NE1	2.55	0.69
1:A:489:SER:HB2	1:A:493:VAL:HG12	1.75	0.69
1:A:26:LEU:HD22	1:A:133:PRO:HG2	1.75	0.68
2:B:1271:TYR:HB3	2:B:1274:ILE:HD13	1.75	0.68
2:B:1335:GLY:CA	2:B:1367:GLN:HE22	2.04	0.68
2:B:1366:LYS:HG3	2:B:1405:TYR:CD1	2.28	0.68
1:A:520:GLN:OE1	1:A:520:GLN:CA	2.42	0.68
2:B:1005:ILE:CG2	2:B:1006:GLU:N	2.46	0.68
2:B:1362:THR:O	2:B:1362:THR:HG23	1.93	0.68
2:B:1271:TYR:O	2:B:1274:ILE:HD13	1.93	0.68
1:A:240:THR:CG2	1:A:241:VAL:N	2.57	0.68
1:A:96:HIS:HD2	1:A:98:ALA:H	1.39	0.68
2:B:1199:ARG:O	2:B:1202:ILE:HG22	1.93	0.68
2:B:1064:LYS:O	2:B:1065:LYS:O	2.12	0.68
1:A:155:GLY:O	1:A:159:ILE:HG12	1.92	0.68
1:A:486:LEU:HD13	1:A:524:GLN:CG	2.24	0.68
1:A:254:VAL:HB	1:A:289:LEU:HA	1.75	0.68
1:A:195:ILE:O	1:A:199:ARG:HG3	1.94	0.68
2:B:1269:GLN:HA	2:B:1269:GLN:OE1	1.92	0.67
2:B:1088:TRP:CH2	2:B:1154:LYS:HD3	2.29	0.67
2:B:1270:ILE:HD11	2:B:1347:LYS:CE	2.25	0.67
1:A:409:THR:O	2:B:1364:ASP:HB2	1.95	0.67
2:B:1323:LYS:HE2	2:B:1324:ASP:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HA	1:A:226:PRO:C	2.15	0.67
1:A:506:ILE:C	1:A:508:ALA:H	1.98	0.67
1:A:271:TYR:HD1	1:A:309:ILE:CD1	2.08	0.67
2:B:1276:VAL:O	2:B:1276:VAL:HG22	1.94	0.67
1:A:524:GLN:HA	1:A:524:GLN:NE2	2.05	0.67
1:A:96:HIS:HE1	1:A:269:GLN:HE21	1.43	0.67
2:B:1252:TRP:HD1	2:B:1295:LEU:CD2	2.08	0.67
1:A:203:GLU:HA	1:A:203:GLU:OE1	1.95	0.67
2:B:1271:TYR:CB	2:B:1274:ILE:HD13	2.25	0.67
1:A:337:TRP:HE1	1:A:367:GLN:CG	2.07	0.67
2:B:1249:LYS:O	2:B:1250:ASP:OD1	2.13	0.67
2:B:1270:ILE:CD1	2:B:1347:LYS:NZ	2.58	0.66
2:B:1169:GLU:C	2:B:1169:GLU:OE2	2.33	0.66
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.75	0.66
2:B:1266:TRP:HH2	2:B:1346:PHE:CZ	2.04	0.66
1:A:220:LYS:CD	1:A:220:LYS:H	1.99	0.66
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.30	0.66
2:B:1151:GLN:C	2:B:1153:TRP:H	1.97	0.66
2:B:1293:ILE:CB	2:B:1294:PRO:CD	2.73	0.66
2:B:1346:PHE:O	2:B:1347:LYS:HE3	1.95	0.66
1:A:134:SER:HB3	1:A:140:PRO:HD2	1.77	0.66
3:A:1551:NNB:O3	3:A:1551:NNB:C13	2.41	0.66
2:B:1234:LEU:HD11	2:B:1239:TRP:HZ2	1.59	0.66
2:B:1084:THR:HG1	2:B:1088:TRP:HD1	1.42	0.66
2:B:1086:ASP:HA	2:B:1090:VAL:HG22	1.78	0.65
1:A:64:LYS:HE3	1:A:69:THR:HA	1.78	0.65
2:B:1420:PRO:HG2	2:B:1423:VAL:HG21	1.78	0.65
2:B:1320:ASP:H	2:B:1343:GLN:NE2	1.94	0.65
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.26	0.65
2:B:1175:ASN:O	2:B:1177:ASP:N	2.29	0.65
1:A:319:TYR:OH	1:A:385:LYS:HE2	1.96	0.65
2:B:1202:ILE:HD13	2:B:1202:ILE:C	2.16	0.65
1:A:64:LYS:CE	1:A:69:THR:HA	2.26	0.65
2:B:1103:LYS:NZ	2:B:1179:VAL:HG21	2.10	0.65
2:B:1266:TRP:CE2	2:B:1346:PHE:CE2	2.83	0.65
1:A:471:ASN:HD22	1:A:471:ASN:H	1.45	0.65
1:A:153:TRP:CG	1:A:154:LYS:N	2.64	0.65
2:B:1012:LEU:CD2	2:B:1013:LYS:N	2.54	0.65
2:B:1111:VAL:O	2:B:1111:VAL:HG13	1.96	0.65
1:A:455:ALA:HB2	1:A:469:LEU:HD11	1.78	0.65
2:B:1088:TRP:CZ3	2:B:1154:LYS:HD3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:O	1:A:233:GLU:HA	1.96	0.65
1:A:88:TRP:CE2	2:B:1143:ARG:HD2	2.31	0.65
1:A:458:VAL:HG23	1:A:459:THR:H	1.58	0.65
1:A:309:ILE:HD12	1:A:310:LEU:N	2.12	0.65
1:A:260:LEU:CD2	1:A:264:LEU:HD22	2.27	0.65
2:B:1080:LEU:HD23	2:B:1084:THR:HG23	1.78	0.65
2:B:1042:GLU:O	2:B:1045:GLY:N	2.24	0.65
2:B:1296:THR:HB	2:B:1299:ALA:CB	2.25	0.64
2:B:1234:LEU:HD11	2:B:1239:TRP:CZ2	2.33	0.64
2:B:1060:VAL:HG12	2:B:1075:VAL:HG13	1.77	0.64
1:A:228:LEU:CD2	1:A:228:LEU:N	2.60	0.64
1:A:57:ASN:HA	1:A:129:ALA:O	1.97	0.64
2:B:1330:GLN:OE1	2:B:1340:GLN:NE2	2.30	0.64
1:A:497:THR:HG22	1:A:498:ASP:N	2.12	0.64
1:A:122:GLU:HA	1:A:125:ARG:HE	1.61	0.64
2:B:1043:LYS:HE3	2:B:1043:LYS:O	1.98	0.64
1:A:438:GLU:HG2	1:A:461:LYS:CD	2.23	0.64
1:A:248:GLU:CA	1:A:248:GLU:OE2	2.42	0.63
1:A:6:GLU:HG3	1:A:7:THR:H	1.63	0.63
2:B:1270:ILE:HD11	2:B:1347:LYS:HE2	1.78	0.63
1:A:419:THR:O	1:A:421:PRO:HD2	1.99	0.63
2:B:1013:LYS:HZ1	2:B:1085:GLN:HB3	1.64	0.63
1:A:81:ASN:ND2	1:A:153:TRP:O	2.31	0.63
1:A:302:GLU:O	1:A:304:ALA:N	2.31	0.63
1:A:115:TYR:CE1	4:A:2004:HOH:O	2.50	0.63
1:A:51:GLY:C	1:A:53:GLU:OE1	2.36	0.63
2:B:1391:LEU:HD23	2:B:1414:TRP:HB2	1.78	0.63
2:B:1337:TRP:HE1	2:B:1367:GLN:NE2	1.96	0.63
2:B:1161:GLN:C	2:B:1161:GLN:CD	2.57	0.63
1:A:136:ASN:O	1:A:137:ASN:C	2.37	0.63
1:A:134:SER:C	1:A:136:ASN:N	2.51	0.63
2:B:1066:LYS:HB2	4:B:2005:HOH:O	1.98	0.63
2:B:1333:GLY:O	2:B:1334:GLN:HB2	1.97	0.63
1:A:34:LEU:HD21	1:A:60:VAL:HG22	1.80	0.63
2:B:1363:ASN:OD1	2:B:1363:ASN:O	2.17	0.62
2:B:1296:THR:O	2:B:1297:GLU:C	2.37	0.62
1:A:521:ILE:HG22	1:A:521:ILE:O	1.97	0.62
1:A:206:ARG:CZ	1:A:217:PRO:O	2.46	0.62
2:B:1374:LYS:C	2:B:1374:LYS:CD	2.66	0.62
2:B:1080:LEU:CD2	2:B:1153:TRP:HE1	2.12	0.62
2:B:1271:TYR:HB3	2:B:1274:ILE:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1290:THR:O	2:B:1290:THR:HG22	1.98	0.62
2:B:1142:ILE:HD12	2:B:1142:ILE:H	1.65	0.62
2:B:1428:GLN:HE21	2:B:1428:GLN:HA	1.65	0.62
1:A:180:ILE:CD1	1:A:189:VAL:HG13	2.29	0.62
1:A:107:THR:CG2	1:A:202:ILE:HD11	2.29	0.62
2:B:1275:LYS:CE	2:B:1275:LYS:HA	2.27	0.61
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.33	0.61
1:A:540:LYS:HD3	1:A:542:ILE:HD11	1.82	0.61
1:A:489:SER:OG	1:A:493:VAL:HG11	2.00	0.61
2:B:1366:LYS:HG3	2:B:1405:TYR:CG	2.36	0.61
2:B:1013:LYS:HE3	2:B:1085:GLN:HB3	1.82	0.61
1:A:240:THR:HG22	1:A:241:VAL:H	1.65	0.61
1:A:51:GLY:HA3	1:A:53:GLU:OE1	2.00	0.61
2:B:1326:ILE:HD11	2:B:1390:LYS:HE3	1.81	0.61
2:B:1013:LYS:CE	2:B:1085:GLN:CB	2.78	0.61
1:A:5:ILE:HD13	1:A:167:ILE:HG13	1.83	0.61
1:A:491:LEU:HD12	1:A:491:LEU:H	1.65	0.61
1:A:197:GLN:O	1:A:201:LYS:HB2	2.01	0.61
1:A:527:LYS:O	1:A:528:LYS:O	2.19	0.61
2:B:1080:LEU:HD22	2:B:1153:TRP:NE1	2.15	0.61
1:A:546:GLU:O	1:A:549:ASP:HB2	2.01	0.61
1:A:96:HIS:N	2:B:1136:ASN:HD21	1.95	0.61
1:A:65:LYS:HD2	1:A:67:ASP:HB3	1.83	0.61
1:A:61:PHE:H	1:A:61:PHE:HD1	1.49	0.61
1:A:10:VAL:CG1	1:A:11:LYS:N	2.64	0.61
1:A:441:TYR:CE2	1:A:544:GLY:HA3	2.36	0.60
2:B:1073:LYS:NZ	2:B:1075:VAL:CG2	2.64	0.60
2:B:1169:GLU:CB	2:B:1170:PRO:HD3	2.22	0.60
1:A:337:TRP:NE1	1:A:367:GLN:CG	2.61	0.60
2:B:1326:ILE:CG2	2:B:1342:TYR:CE1	2.85	0.60
1:A:120:LEU:H	1:A:148:VAL:HA	1.64	0.60
1:A:438:GLU:CG	1:A:461:LYS:HD3	2.24	0.60
1:A:134:SER:C	1:A:136:ASN:H	2.03	0.60
1:A:517:LEU:HD13	1:A:517:LEU:C	2.21	0.60
1:A:100:LEU:O	1:A:318:TYR:HB3	1.99	0.60
1:A:395:LYS:HG3	1:A:396:GLU:N	2.15	0.60
2:B:1203:GLU:O	2:B:1206:ARG:HB2	2.01	0.60
1:A:275:LYS:CE	1:A:332:GLN:NE2	2.65	0.60
1:A:450:THR:CB	1:A:452:LEU:HD22	2.28	0.60
2:B:1115:TYR:C	2:B:1117:SER:H	2.05	0.60
2:B:1302:GLU:OE1	2:B:1302:GLU:HA	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1293:ILE:HB	2:B:1294:PRO:HD3	1.82	0.60
2:B:1420:PRO:HB2	2:B:1423:VAL:HG23	1.84	0.60
1:A:135:ILE:O	1:A:136:ASN:ND2	2.34	0.60
2:B:1032:LYS:O	2:B:1035:VAL:HG22	2.02	0.60
2:B:1029:GLU:HG3	2:B:1030:LYS:HD2	1.84	0.60
2:B:1249:LYS:O	2:B:1250:ASP:CB	2.50	0.60
2:B:1323:LYS:HE2	2:B:1324:ASP:N	2.17	0.60
2:B:1310:LEU:C	2:B:1312:GLU:H	2.05	0.60
2:B:1085:GLN:O	2:B:1087:PHE:N	2.34	0.60
2:B:1261:VAL:HG23	2:B:1262:GLY:N	2.16	0.60
1:A:122:GLU:HA	1:A:125:ARG:NE	2.17	0.60
2:B:1314:VAL:CG1	2:B:1317:VAL:HG23	2.32	0.60
2:B:1425:LEU:CD2	2:B:1425:LEU:C	2.70	0.60
1:A:410:TRP:CZ3	2:B:1363:ASN:CB	2.73	0.60
2:B:1301:LEU:HD23	2:B:1305:GLU:HB2	1.83	0.59
1:A:459:THR:HG22	1:A:461:LYS:N	2.11	0.59
2:B:1239:TRP:CH2	2:B:1378:GLU:HG2	2.37	0.59
2:B:1034:LEU:HA	2:B:1037:ILE:CG2	2.32	0.59
1:A:218:ASP:OD1	1:A:219:LYS:N	2.36	0.59
2:B:1103:LYS:HZ3	2:B:1179:VAL:HG21	1.64	0.59
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.85	0.59
1:A:132:ILE:HB	1:A:142:ILE:HG23	1.84	0.59
2:B:1195:ILE:CD1	2:B:1195:ILE:N	2.20	0.59
1:A:438:GLU:OE1	1:A:463:ARG:NH1	2.35	0.59
1:A:497:THR:CG2	1:A:498:ASP:O	2.42	0.59
1:A:17:ASP:OD1	1:A:17:ASP:N	2.34	0.59
2:B:1332:GLN:HE22	2:B:1338:THR:CG2	2.15	0.59
2:B:1080:LEU:HD22	2:B:1153:TRP:HE1	1.67	0.59
2:B:1314:VAL:HG11	2:B:1317:VAL:CG2	2.32	0.59
1:A:335:GLY:CA	1:A:367:GLN:HE22	2.10	0.59
1:A:484:LEU:HD12	1:A:487:GLN:HE21	1.66	0.59
2:B:1320:ASP:H	2:B:1343:GLN:HE22	1.51	0.58
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.37	0.58
1:A:508:ALA:O	1:A:509:GLN:C	2.41	0.58
1:A:350:LYS:HD3	1:A:378:GLU:OE2	2.03	0.58
1:A:52:PRO:N	1:A:53:GLU:OE1	2.36	0.58
1:A:271:TYR:HD1	1:A:309:ILE:HD13	1.66	0.58
1:A:94:ILE:HG23	1:A:95:PRO:HD2	1.84	0.58
2:B:1374:LYS:HE3	2:B:1378:GLU:CG	2.33	0.58
1:A:445:ALA:O	1:A:446:ALA:HB2	2.03	0.58
1:A:113:ASP:O	1:A:114:ALA:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1419:THR:HG22	2:B:1420:PRO:O	2.03	0.58
2:B:1324:ASP:OD2	2:B:1388:LYS:CE	2.42	0.58
1:A:309:ILE:HD11	1:A:310:LEU:HD12	1.85	0.58
2:B:1124:PHE:CD2	2:B:1124:PHE:O	2.56	0.58
1:A:449:GLU:OE2	1:A:449:GLU:HA	2.04	0.58
2:B:1271:TYR:CB	2:B:1274:ILE:CD1	2.80	0.58
2:B:1246:LEU:HD21	2:B:1310:LEU:HD12	1.85	0.58
2:B:1028:GLU:O	2:B:1032:LYS:HG2	2.03	0.58
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.34	0.58
2:B:1042:GLU:HG3	2:B:1043:LYS:N	2.19	0.58
1:A:205:LEU:HG	1:A:209:LEU:HD22	1.86	0.58
1:A:455:ALA:CB	1:A:469:LEU:HD11	2.33	0.58
1:A:410:TRP:CD2	2:B:1363:ASN:HB2	2.33	0.58
2:B:1255:ASN:HB2	2:B:1289:LEU:CD1	2.34	0.58
1:A:438:GLU:OE2	1:A:459:THR:CG2	2.51	0.58
1:A:420:PRO:HA	1:A:422:LEU:HD22	1.86	0.58
1:A:426:TRP:O	1:A:427:TYR:HB3	2.03	0.58
1:A:207:GLN:HA	1:A:207:GLN:OE1	2.04	0.58
2:B:1367:GLN:HA	2:B:1370:GLU:OE1	2.03	0.58
1:A:27:THR:O	1:A:31:ILE:HG13	2.03	0.58
2:B:1043:LYS:CA	2:B:1043:LYS:HE3	2.34	0.57
1:A:356:ARG:CA	1:A:356:ARG:HE	2.08	0.57
2:B:1270:ILE:HD13	2:B:1347:LYS:NZ	2.19	0.57
2:B:1012:LEU:O	2:B:1014:PRO:HD3	2.04	0.57
2:B:1084:THR:O	2:B:1085:GLN:C	2.42	0.57
1:A:393:ILE:O	1:A:416:PHE:HD1	1.88	0.57
1:A:94:ILE:HG22	1:A:229:TRP:HH2	1.62	0.57
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.38	0.57
1:A:471:ASN:ND2	1:A:471:ASN:H	2.02	0.57
1:A:409:THR:HG22	1:A:410:TRP:H	1.66	0.57
1:A:64:LYS:HE3	1:A:69:THR:CA	2.35	0.57
1:A:13:LYS:HG3	1:A:84:THR:O	2.04	0.57
1:A:288:ALA:C	1:A:289:LEU:HD23	2.25	0.57
2:B:1314:VAL:HG11	2:B:1317:VAL:HG21	1.87	0.57
1:A:547:GLN:C	1:A:547:GLN:OE1	2.42	0.57
1:A:50:ILE:HG13	1:A:51:GLY:O	2.05	0.57
1:A:302:GLU:O	1:A:305:GLU:HG2	2.05	0.57
2:B:1254:VAL:O	2:B:1258:GLN:N	2.32	0.57
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.86	0.57
1:A:154:LYS:HG3	1:A:155:GLY:N	2.19	0.56
1:A:409:THR:CG2	1:A:410:TRP:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:H	2:B:1136:ASN:ND2	1.98	0.56
1:A:171:PHE:HA	1:A:174:GLN:CG	2.36	0.56
1:A:473:THR:HG23	1:A:476:LYS:HE2	1.86	0.56
1:A:516:GLU:O	1:A:519:ASN:HB2	2.05	0.56
2:B:1253:THR:HG22	2:B:1292:VAL:CA	2.36	0.56
2:B:1047:ILE:HD12	2:B:1144:TYR:CG	2.41	0.56
2:B:1164:MET:O	2:B:1168:LEU:HG	2.06	0.56
2:B:1337:TRP:HE1	2:B:1367:GLN:HE21	1.53	0.56
2:B:1374:LYS:HE3	2:B:1378:GLU:HG3	1.86	0.56
2:B:1296:THR:HG21	2:B:1299:ALA:HB2	1.88	0.56
1:A:497:THR:CG2	1:A:498:ASP:N	2.69	0.56
1:A:442:VAL:CG2	1:A:497:THR:OG1	2.54	0.56
1:A:240:THR:CG2	1:A:241:VAL:H	2.18	0.56
1:A:218:ASP:CB	1:A:221:HIS:CB	2.79	0.56
2:B:1081:ASN:HD21	2:B:1154:LYS:N	1.95	0.56
2:B:1253:THR:O	2:B:1257:ILE:CG2	2.54	0.56
1:A:241:VAL:HG11	1:A:266:TRP:CD1	2.41	0.56
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.23	0.56
2:B:1080:LEU:HD23	2:B:1080:LEU:C	2.26	0.55
2:B:1242:GLN:HB3	2:B:1351:THR:O	2.06	0.55
2:B:1242:GLN:HG3	2:B:1242:GLN:O	2.06	0.55
1:A:180:ILE:HD12	1:A:189:VAL:HG22	1.88	0.55
1:A:507:GLN:O	1:A:507:GLN:HG3	2.06	0.55
1:A:391:LEU:C	1:A:417:VAL:HG23	2.26	0.55
2:B:1103:LYS:NZ	2:B:1179:VAL:HG23	2.21	0.55
1:A:305:GLU:O	1:A:309:ILE:CG2	2.46	0.55
2:B:1199:ARG:O	2:B:1202:ILE:CG2	2.53	0.55
1:A:171:PHE:HA	1:A:174:GLN:HG2	1.87	0.55
1:A:506:ILE:C	1:A:508:ALA:N	2.59	0.55
2:B:1040:GLU:O	2:B:1043:LYS:HB3	2.05	0.55
2:B:1160:PHE:O	2:B:1161:GLN:C	2.45	0.55
1:A:310:LEU:O	1:A:311:LYS:C	2.44	0.55
1:A:489:SER:CB	1:A:493:VAL:HG11	2.37	0.55
2:B:1347:LYS:HA	2:B:1347:LYS:CE	2.37	0.55
2:B:1320:ASP:N	2:B:1343:GLN:HE22	2.05	0.55
1:A:282:LEU:CD2	1:A:296:THR:HG23	2.34	0.55
2:B:1122:GLU:HA	2:B:1125:ARG:HG3	1.89	0.55
1:A:342:TYR:CA	1:A:349:LEU:CD1	2.78	0.55
1:A:439:THR:CG2	1:A:441:TYR:CE1	2.89	0.55
1:A:171:PHE:CA	1:A:174:GLN:HG2	2.37	0.55
2:B:1314:VAL:CG1	2:B:1317:VAL:CG2	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1423:VAL:O	2:B:1425:LEU:N	2.41	0.54
1:A:443:ASP:OD2	1:A:444:GLY:N	2.40	0.54
2:B:1065:LYS:HB2	2:B:1065:LYS:HZ2	1.72	0.54
2:B:1047:ILE:HD12	2:B:1144:TYR:CD2	2.42	0.54
1:A:410:TRP:HB3	2:B:1365:VAL:CG2	2.38	0.54
1:A:128:THR:OG1	1:A:146:TYR:HB2	2.08	0.54
2:B:1323:LYS:CE	2:B:1324:ASP:H	2.19	0.54
1:A:65:LYS:HG3	1:A:72:ARG:HE	1.71	0.54
2:B:1303:LEU:CD1	2:B:1304:ALA:N	2.53	0.54
2:B:1309:ILE:O	2:B:1309:ILE:CG2	2.56	0.54
1:A:287:LYS:NZ	1:A:293:ILE:HG12	2.22	0.54
2:B:1103:LYS:HZ3	2:B:1179:VAL:HG23	1.72	0.54
1:A:524:GLN:HE21	1:A:524:GLN:CA	2.05	0.54
2:B:1325:LEU:HD13	2:B:1383:TRP:CE3	2.42	0.54
1:A:389:PHE:O	1:A:414:TRP:HA	2.08	0.54
2:B:1270:ILE:CD1	2:B:1347:LYS:CE	2.86	0.54
2:B:1390:LYS:HA	2:B:1415:GLU:O	2.08	0.54
1:A:479:LEU:HB3	1:A:517:LEU:CD1	2.38	0.54
2:B:1065:LYS:NZ	4:B:2005:HOH:O	2.40	0.54
1:A:10:VAL:CG1	1:A:11:LYS:H	2.20	0.54
2:B:1347:LYS:CA	2:B:1347:LYS:HE3	2.36	0.54
2:B:1303:LEU:HD12	2:B:1304:ALA:CA	2.37	0.54
1:A:263:LYS:CA	1:A:263:LYS:CE	2.63	0.54
2:B:1169:GLU:OE2	2:B:1169:GLU:O	2.26	0.54
1:A:302:GLU:O	1:A:303:LEU:C	2.45	0.54
1:A:394:GLN:CB	1:A:397:THR:HG22	2.29	0.54
2:B:1239:TRP:O	2:B:1240:THR:HG23	2.08	0.54
1:A:51:GLY:CA	1:A:53:GLU:OE1	2.55	0.54
2:B:1007:THR:CG2	2:B:1119:PRO:O	2.56	0.53
2:B:1115:TYR:O	2:B:1117:SER:N	2.42	0.53
1:A:298:GLU:OE1	1:A:298:GLU:N	2.31	0.53
1:A:183:TYR:N	4:A:2006:HOH:O	2.41	0.53
2:B:1261:VAL:O	2:B:1265:ASN:N	2.32	0.53
2:B:1034:LEU:CA	2:B:1037:ILE:HG22	2.38	0.53
1:A:10:VAL:HG12	1:A:11:LYS:H	1.73	0.53
2:B:1268:SER:HA	2:B:1274:ILE:HB	1.90	0.53
1:A:329:ILE:HG22	1:A:330:GLN:N	2.24	0.53
1:A:511:ASP:OD2	1:A:511:ASP:C	2.47	0.53
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.08	0.53
1:A:203:GLU:O	1:A:207:GLN:HG2	2.08	0.53
1:A:335:GLY:HA3	1:A:357:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:OG	1:A:140:PRO:HD2	2.08	0.53
1:A:96:HIS:HE1	1:A:269:GLN:NE2	2.06	0.53
2:B:1267:ALA:O	2:B:1268:SER:C	2.47	0.53
2:B:1270:ILE:CD1	2:B:1347:LYS:HZ3	2.22	0.53
1:A:447:ASN:HD22	1:A:448:ARG:N	2.06	0.53
1:A:170:PRO:O	1:A:173:LYS:N	2.42	0.53
1:A:218:ASP:CB	1:A:221:HIS:HB2	2.17	0.53
1:A:244:ILE:CD1	1:A:263:LYS:HB3	2.39	0.53
1:A:22:LYS:H	1:A:22:LYS:HD2	1.73	0.53
1:A:470:THR:OG1	1:A:471:ASN:ND2	2.39	0.52
1:A:483:TYR:HB2	1:A:521:ILE:HD11	1.90	0.52
1:A:271:TYR:CZ	1:A:314:VAL:HG12	2.44	0.52
1:A:25:PRO:HG3	1:A:137:ASN:OD1	2.09	0.52
2:B:1255:ASN:O	2:B:1259:LYS:HG3	2.09	0.52
1:A:486:LEU:CD1	1:A:524:GLN:HG2	2.39	0.52
2:B:1115:TYR:HB3	2:B:1149:LEU:CB	2.32	0.52
1:A:96:HIS:CD2	1:A:98:ALA:H	2.25	0.52
2:B:1209:LEU:O	2:B:1210:LEU:C	2.46	0.52
2:B:1270:ILE:HD11	2:B:1347:LYS:NZ	2.24	0.52
1:A:308:GLU:O	1:A:311:LYS:N	2.42	0.52
1:A:61:PHE:N	1:A:61:PHE:CD1	2.77	0.52
1:A:447:ASN:C	1:A:447:ASN:ND2	2.62	0.52
2:B:1348:ASN:N	2:B:1348:ASN:HD22	2.08	0.52
1:A:450:THR:HB	1:A:452:LEU:CD2	2.40	0.52
1:A:26:LEU:HD23	1:A:133:PRO:CG	2.38	0.52
2:B:1212:TRP:O	2:B:1214:LEU:N	2.37	0.52
2:B:1423:VAL:O	2:B:1424:LYS:C	2.47	0.52
1:A:349:LEU:H	1:A:349:LEU:HD12	1.74	0.52
2:B:1325:LEU:HD23	2:B:1343:GLN:HG2	1.91	0.52
1:A:166:LYS:O	1:A:169:GLU:N	2.42	0.52
1:A:482:ILE:O	1:A:483:TYR:C	2.48	0.52
2:B:1086:ASP:C	2:B:1086:ASP:OD1	2.48	0.52
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.91	0.52
1:A:202:ILE:C	1:A:204:GLU:N	2.62	0.52
1:A:443:ASP:N	1:A:481:ALA:HB1	2.25	0.52
1:A:94:ILE:HG22	1:A:95:PRO:O	2.09	0.52
1:A:134:SER:HB2	1:A:140:PRO:HD2	1.90	0.51
1:A:170:PRO:O	1:A:172:LYS:N	2.43	0.51
2:B:1243:PRO:C	2:B:1244:ILE:HD12	2.31	0.51
1:A:440:PHE:HE2	1:A:457:TYR:CE2	2.29	0.51
1:A:471:ASN:N	1:A:471:ASN:HD22	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1286:THR:OG1	2:B:1287:LYS:N	2.43	0.51
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.88	0.51
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.92	0.51
2:B:1252:TRP:CD1	2:B:1295:LEU:HD22	2.45	0.51
2:B:1142:ILE:CG2	2:B:1144:TYR:CE1	2.93	0.51
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.92	0.51
1:A:410:TRP:CB	2:B:1365:VAL:HG23	2.41	0.51
1:A:540:LYS:HG2	1:A:541:GLY:N	2.23	0.51
1:A:420:PRO:N	1:A:421:PRO:CD	2.73	0.51
2:B:1314:VAL:HG12	2:B:1317:VAL:HG23	1.92	0.51
2:B:1257:ILE:HD13	2:B:1279:LEU:HD11	1.93	0.51
2:B:1086:ASP:C	2:B:1090:VAL:HG22	2.31	0.51
1:A:537:PRO:O	1:A:538:ALA:C	2.49	0.51
2:B:1202:ILE:HG23	2:B:1203:GLU:N	2.24	0.51
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.24	0.51
2:B:1080:LEU:HD22	2:B:1153:TRP:CD1	2.45	0.51
1:A:391:LEU:O	1:A:417:VAL:HG23	2.10	0.51
2:B:1044:GLU:HA	2:B:1044:GLU:OE2	2.11	0.51
2:B:1415:GLU:HG2	2:B:1415:GLU:O	2.11	0.51
2:B:1301:LEU:HD23	2:B:1301:LEU:O	2.11	0.51
1:A:166:LYS:O	1:A:168:LEU:N	2.44	0.51
1:A:115:TYR:CD1	4:A:2004:HOH:O	2.64	0.51
1:A:180:ILE:HD13	1:A:189:VAL:HG13	1.92	0.51
1:A:503:LEU:HD12	1:A:507:GLN:HB2	1.93	0.51
2:B:1081:ASN:ND2	2:B:1154:LYS:H	1.96	0.51
2:B:1317:VAL:HG22	2:B:1347:LYS:CD	2.41	0.50
1:A:393:ILE:CG1	1:A:397:THR:HG23	2.41	0.50
1:A:248:GLU:O	1:A:249:LYS:CG	2.51	0.50
1:A:406:TRP:CH2	2:B:1418:ASN:HA	2.47	0.50
2:B:1277:ARG:HG3	2:B:1278:GLN:H	1.76	0.50
1:A:351:THR:HG22	1:A:352:GLY:N	2.26	0.50
1:A:241:VAL:CG1	1:A:266:TRP:CD1	2.94	0.50
1:A:96:HIS:CE1	1:A:269:GLN:NE2	2.79	0.50
2:B:1178:ILE:HD13	2:B:1191:SER:HB2	1.93	0.50
1:A:489:SER:CB	1:A:493:VAL:CG1	2.90	0.50
2:B:1082:LYS:O	2:B:1085:GLN:HB2	2.11	0.50
1:A:183:TYR:O	1:A:186:ASP:HB2	2.11	0.50
2:B:1043:LYS:HA	2:B:1043:LYS:HE3	1.93	0.50
1:A:450:THR:CB	1:A:452:LEU:CD2	2.87	0.50
1:A:337:TRP:HE1	1:A:367:GLN:CD	2.15	0.50
1:A:135:ILE:O	1:A:136:ASN:CG	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:O	1:A:365:VAL:C	2.49	0.50
1:A:420:PRO:N	1:A:421:PRO:HD3	2.26	0.50
2:B:1043:LYS:CE	2:B:1043:LYS:O	2.59	0.50
2:B:1270:ILE:HD13	2:B:1347:LYS:HZ1	1.76	0.50
2:B:1282:LEU:C	2:B:1287:LYS:NZ	2.59	0.50
1:A:225:PRO:HD3	1:A:227:PHE:CZ	2.46	0.50
2:B:1039:THR:O	2:B:1042:GLU:HG2	2.10	0.50
2:B:1147:ASN:O	2:B:1148:VAL:HG13	2.10	0.50
2:B:1422:LEU:O	2:B:1425:LEU:HB3	2.11	0.50
1:A:483:TYR:HB2	1:A:521:ILE:CD1	2.42	0.50
2:B:1252:TRP:CD1	2:B:1295:LEU:CD2	2.92	0.50
2:B:1296:THR:HG22	2:B:1299:ALA:N	2.27	0.50
2:B:1326:ILE:CD1	2:B:1390:LYS:HE3	2.42	0.49
2:B:1115:TYR:C	2:B:1117:SER:N	2.66	0.49
1:A:164:MET:O	1:A:168:LEU:HB2	2.12	0.49
1:A:293:ILE:HG22	1:A:294:PRO:O	2.11	0.49
1:A:195:ILE:HG22	1:A:196:GLY:N	2.28	0.49
1:A:529:GLU:O	1:A:530:LYS:HG3	2.13	0.49
1:A:257:ILE:HD11	1:A:279:LEU:O	2.12	0.49
1:A:244:ILE:HD13	1:A:263:LYS:HB3	1.93	0.49
1:A:337:TRP:CZ2	1:A:367:GLN:HG2	2.47	0.49
1:A:309:ILE:CD1	1:A:310:LEU:N	2.76	0.49
1:A:70:LYS:HD3	4:A:2001:HOH:O	2.13	0.49
2:B:1255:ASN:HD21	2:B:1259:LYS:NZ	2.11	0.49
2:B:1341:ILE:HB	2:B:1350:LYS:HB2	1.94	0.49
2:B:1344:GLU:O	2:B:1345:PRO:C	2.50	0.49
1:A:470:THR:OG1	1:A:471:ASN:N	2.45	0.49
2:B:1080:LEU:CD2	2:B:1153:TRP:NE1	2.75	0.49
1:A:40:GLU:HA	1:A:43:LYS:HZ2	1.78	0.49
1:A:237:ASP:N	1:A:237:ASP:OD1	2.46	0.49
1:A:349:LEU:N	1:A:349:LEU:HD12	2.28	0.49
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.78	0.49
2:B:1042:GLU:CG	2:B:1043:LYS:N	2.76	0.49
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.94	0.49
1:A:77:PHE:O	1:A:78:ARG:C	2.49	0.49
2:B:1246:LEU:HD21	2:B:1310:LEU:CD1	2.43	0.49
1:A:498:ASP:O	1:A:499:SER:OG	2.30	0.49
1:A:314:VAL:HG22	1:A:315:HIS:H	1.78	0.49
1:A:170:PRO:O	1:A:171:PHE:C	2.51	0.49
2:B:1037:ILE:HD11	4:B:2007:HOH:O	2.11	0.49
2:B:1122:GLU:HG2	2:B:1125:ARG:NH2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1278:GLN:HA	2:B:1278:GLN:OE1	2.12	0.49
1:A:285:GLY:O	1:A:287:LYS:N	2.41	0.49
1:A:473:THR:O	1:A:477:THR:HG23	2.12	0.49
1:A:70:LYS:HD3	1:A:71:TRP:H	1.78	0.49
1:A:458:VAL:HG11	1:A:547:GLN:CG	2.37	0.48
2:B:1253:THR:HG22	2:B:1292:VAL:HB	1.94	0.48
2:B:1234:LEU:HD12	4:B:2017:HOH:O	2.13	0.48
1:A:473:THR:H	1:A:476:LYS:CE	2.22	0.48
1:A:40:GLU:HG3	1:A:43:LYS:NZ	2.28	0.48
2:B:1008:VAL:O	2:B:1010:VAL:HG23	2.12	0.48
1:A:120:LEU:CD1	1:A:121:ASP:N	2.67	0.48
1:A:245:VAL:C	1:A:246:LEU:HD23	2.32	0.48
2:B:1178:ILE:HD13	2:B:1191:SER:CB	2.44	0.48
2:B:1425:LEU:O	2:B:1428:GLN:HB2	2.13	0.48
2:B:1080:LEU:HD23	2:B:1084:THR:CG2	2.43	0.48
1:A:443:ASP:HB3	1:A:548:VAL:HG12	1.94	0.48
2:B:1296:THR:CG2	2:B:1299:ALA:HB2	2.44	0.48
1:A:410:TRP:HB3	2:B:1365:VAL:HG23	1.95	0.48
2:B:1325:LEU:CD1	2:B:1383:TRP:CE3	2.96	0.48
1:A:297:GLU:HG3	1:A:301:LEU:HD23	1.96	0.48
1:A:308:GLU:O	1:A:309:ILE:C	2.50	0.48
1:A:5:ILE:HD13	1:A:167:ILE:CG1	2.42	0.48
1:A:519:ASN:O	1:A:522:ILE:HB	2.14	0.48
1:A:419:THR:C	1:A:421:PRO:CD	2.81	0.48
2:B:1007:THR:HG21	2:B:1119:PRO:O	2.13	0.48
2:B:1422:LEU:HB2	2:B:1426:TRP:CH2	2.48	0.48
1:A:297:GLU:HG3	1:A:301:LEU:CD2	2.43	0.48
2:B:1085:GLN:O	2:B:1086:ASP:C	2.52	0.48
2:B:1042:GLU:CG	2:B:1043:LYS:H	2.27	0.48
1:A:125:ARG:HB3	1:A:146:TYR:O	2.13	0.48
1:A:495:ILE:HG22	1:A:496:VAL:N	2.29	0.48
2:B:1423:VAL:O	2:B:1426:TRP:N	2.47	0.48
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.49	0.48
2:B:1086:ASP:O	2:B:1090:VAL:CG2	2.60	0.48
2:B:1151:GLN:C	2:B:1153:TRP:N	2.61	0.48
2:B:1202:ILE:HD13	2:B:1202:ILE:O	2.14	0.48
1:A:268:SER:O	1:A:351:THR:HB	2.13	0.48
1:A:309:ILE:O	1:A:309:ILE:HD12	2.14	0.48
2:B:1118:VAL:HB	2:B:1149:LEU:CD1	2.44	0.48
2:B:1362:THR:CG2	2:B:1362:THR:O	2.62	0.48
2:B:1420:PRO:HB2	2:B:1423:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1236:PRO:HA	2:B:1239:TRP:CD2	2.49	0.47
1:A:166:LYS:C	1:A:168:LEU:N	2.66	0.47
1:A:482:ILE:O	1:A:485:ALA:N	2.47	0.47
2:B:1336:GLN:C	2:B:1337:TRP:CD1	2.87	0.47
2:B:1043:LYS:C	2:B:1043:LYS:HE3	2.33	0.47
1:A:432:GLU:HB2	1:A:433:PRO:CD	2.43	0.47
1:A:486:LEU:CD1	1:A:524:GLN:CG	2.92	0.47
2:B:1085:GLN:HB3	2:B:1086:ASP:H	1.51	0.47
1:A:65:LYS:HD3	1:A:66:LYS:N	2.29	0.47
1:A:404:GLU:HG2	4:A:2019:HOH:O	2.14	0.47
2:B:1170:PRO:O	2:B:1174:GLN:CG	2.56	0.47
2:B:1105:SER:HA	2:B:1235:HIS:HA	1.97	0.47
1:A:194:GLU:O	1:A:195:ILE:C	2.53	0.47
2:B:1332:GLN:HE22	2:B:1338:THR:HG23	1.80	0.47
2:B:1363:ASN:OD1	2:B:1366:LYS:HB2	2.14	0.47
1:A:218:ASP:H	1:A:221:HIS:HB3	1.80	0.47
1:A:296:THR:O	1:A:297:GLU:C	2.51	0.47
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.33	0.47
2:B:1105:SER:HB2	2:B:1235:HIS:ND1	2.29	0.47
1:A:540:LYS:HD3	2:B:1280:CYS:SG	2.54	0.47
2:B:1420:PRO:CG	2:B:1423:VAL:HG21	2.44	0.47
2:B:1013:LYS:HE2	2:B:1086:ASP:HB3	1.97	0.47
1:A:394:GLN:O	1:A:395:LYS:C	2.51	0.47
2:B:1254:VAL:HG21	2:B:1288:ALA:O	2.15	0.47
1:A:511:ASP:O	1:A:512:LYS:CB	2.61	0.47
1:A:210:LEU:O	1:A:213:GLY:N	2.22	0.47
2:B:1079:GLU:HG3	2:B:1083:ARG:HE	1.79	0.47
1:A:19:PRO:HD2	1:A:56:TYR:HB3	1.97	0.47
1:A:309:ILE:C	1:A:309:ILE:CD1	2.62	0.47
1:A:404:GLU:CG	4:A:2019:HOH:O	2.62	0.47
2:B:1253:THR:O	2:B:1254:VAL:C	2.53	0.47
1:A:453:GLY:C	1:A:454:LYS:HG3	2.34	0.47
2:B:1051:GLY:HA3	2:B:1053:GLU:OE1	2.14	0.47
2:B:1013:LYS:HE3	2:B:1085:GLN:HB2	1.97	0.47
1:A:61:PHE:N	1:A:61:PHE:HD1	2.10	0.47
2:B:1042:GLU:O	2:B:1043:LYS:C	2.54	0.47
1:A:466:VAL:O	1:A:466:VAL:HG13	2.15	0.47
2:B:1199:ARG:C	2:B:1202:ILE:HG22	2.34	0.46
2:B:1073:LYS:HZ2	2:B:1075:VAL:CG2	2.28	0.46
2:B:1142:ILE:HG21	2:B:1144:TYR:CE1	2.50	0.46
1:A:1:PRO:HG2	1:A:213:GLY:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:CD1	1:A:524:GLN:HB3	2.33	0.46
2:B:1308:GLU:O	2:B:1310:LEU:N	2.48	0.46
2:B:1183:TYR:CD2	2:B:1380:ILE:HD13	2.50	0.46
1:A:287:LYS:CD	1:A:293:ILE:HD11	2.38	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.98	0.46
1:A:483:TYR:HB2	1:A:521:ILE:CG1	2.44	0.46
1:A:202:ILE:O	1:A:204:GLU:N	2.49	0.46
2:B:1326:ILE:HG13	2:B:1388:LYS:HB2	1.96	0.46
2:B:1329:ILE:O	2:B:1392:PRO:HG3	2.15	0.46
2:B:1183:TYR:O	2:B:1184:MET:C	2.53	0.46
1:A:277:ARG:HG3	1:A:336:GLN:HE21	1.80	0.46
1:A:94:ILE:CG2	1:A:95:PRO:HD2	2.44	0.46
1:A:134:SER:O	1:A:135:ILE:C	2.53	0.46
1:A:430:GLU:O	1:A:532:TYR:HD1	1.99	0.46
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.97	0.46
2:B:1092:LEU:HB2	2:B:1158:ALA:HB1	1.96	0.46
1:A:354:TYR:C	1:A:354:TYR:CD2	2.88	0.46
1:A:217:PRO:HB2	1:A:221:HIS:O	2.15	0.46
2:B:1309:ILE:O	2:B:1312:GLU:HB2	2.16	0.46
1:A:281:LYS:O	1:A:284:ARG:HB2	2.15	0.46
2:B:1170:PRO:O	2:B:1173:LYS:HB3	2.16	0.46
1:A:5:ILE:HG13	1:A:6:GLU:N	2.31	0.46
2:B:1296:THR:HG22	2:B:1299:ALA:H	1.80	0.46
1:A:344:GLU:O	1:A:345:PRO:C	2.52	0.46
1:A:79:GLU:O	1:A:81:ASN:N	2.49	0.46
2:B:1261:VAL:HA	2:B:1264:LEU:HB2	1.97	0.46
1:A:266:TRP:O	1:A:269:GLN:HG3	2.15	0.46
2:B:1142:ILE:HG22	2:B:1144:TYR:CE1	2.51	0.46
1:A:351:THR:HG22	1:A:352:GLY:H	1.80	0.46
1:A:324:ASP:O	1:A:343:GLN:HG2	2.15	0.46
1:A:240:THR:HG22	1:A:241:VAL:O	2.15	0.46
2:B:1332:GLN:O	2:B:1333:GLY:C	2.54	0.46
2:B:1253:THR:HG22	2:B:1292:VAL:CB	2.46	0.46
2:B:1292:VAL:CG2	2:B:1293:ILE:N	2.79	0.46
1:A:287:LYS:HZ3	1:A:293:ILE:HG12	1.81	0.46
1:A:450:THR:O	1:A:451:LYS:HB2	2.16	0.45
1:A:295:LEU:O	1:A:296:THR:C	2.53	0.45
1:A:297:GLU:O	1:A:298:GLU:C	2.53	0.45
2:B:1212:TRP:C	2:B:1214:LEU:H	2.18	0.45
1:A:503:LEU:O	1:A:507:GLN:CB	2.64	0.45
1:A:309:ILE:CG1	1:A:310:LEU:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HG21	1:A:414:TRP:CD1	2.51	0.45
2:B:1184:MET:C	2:B:1186:ASP:H	2.17	0.45
1:A:363:ASN:O	1:A:364:ASP:C	2.53	0.45
2:B:1266:TRP:CE3	2:B:1426:TRP:CE3	3.04	0.45
2:B:1013:LYS:HZ2	2:B:1085:GLN:CB	2.28	0.45
2:B:1035:VAL:CG2	2:B:1036:GLU:N	2.80	0.45
1:A:108:VAL:O	1:A:109:LEU:HD23	2.15	0.45
2:B:1161:GLN:O	2:B:1162:SER:C	2.55	0.45
1:A:152:GLY:O	1:A:153:TRP:O	2.35	0.45
1:A:154:LYS:HB2	1:A:154:LYS:HE3	1.80	0.45
2:B:1239:TRP:CZ2	2:B:1378:GLU:HG2	2.52	0.45
1:A:65:LYS:CD	1:A:67:ASP:H	2.29	0.45
2:B:1034:LEU:C	2:B:1037:ILE:HG22	2.37	0.45
1:A:529:GLU:HG2	1:A:529:GLU:O	2.16	0.45
1:A:410:TRP:HE3	2:B:1363:ASN:HB2	1.64	0.45
1:A:546:GLU:O	1:A:549:ASP:CB	2.65	0.45
1:A:479:LEU:HB3	1:A:517:LEU:HD12	1.98	0.45
1:A:255:ASN:O	1:A:256:ASP:C	2.55	0.45
2:B:1422:LEU:HB3	2:B:1426:TRP:CZ2	2.51	0.45
1:A:80:LEU:O	1:A:84:THR:OG1	2.20	0.45
1:A:166:LYS:C	1:A:168:LEU:H	2.19	0.45
1:A:430:GLU:O	1:A:532:TYR:CD1	2.70	0.45
1:A:40:GLU:HG3	1:A:43:LYS:HZ1	1.81	0.45
2:B:1345:PRO:O	2:B:1346:PHE:HB2	2.17	0.45
1:A:483:TYR:O	1:A:486:LEU:HB2	2.17	0.45
2:B:1324:ASP:CG	2:B:1388:LYS:HE3	2.34	0.45
1:A:393:ILE:HG12	1:A:397:THR:CG2	2.45	0.45
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.99	0.45
1:A:65:LYS:HE3	1:A:67:ASP:HB2	1.99	0.45
1:A:169:GLU:O	1:A:172:LYS:HB2	2.15	0.45
2:B:1193:LEU:O	2:B:1194:GLU:C	2.55	0.45
2:B:1201:LYS:HD2	2:B:1201:LYS:HA	1.60	0.45
2:B:1261:VAL:O	2:B:1262:GLY:C	2.55	0.45
1:A:406:TRP:O	2:B:1331:LYS:HB3	2.17	0.45
2:B:1242:GLN:HB3	2:B:1352:GLY:HA2	1.99	0.45
1:A:210:LEU:O	1:A:211:ARG:C	2.54	0.45
2:B:1261:VAL:HG23	2:B:1262:GLY:H	1.82	0.45
1:A:88:TRP:CZ2	1:A:92:LEU:HD11	2.52	0.45
2:B:1047:ILE:CD1	2:B:1144:TYR:CD2	3.00	0.45
1:A:206:ARG:CZ	1:A:216:THR:OG1	2.65	0.45
1:A:254:VAL:HB	1:A:289:LEU:CA	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:CD1	1:A:491:LEU:N	2.74	0.45
1:A:31:ILE:O	1:A:32:LYS:C	2.56	0.45
1:A:317:VAL:HG23	1:A:348:ASN:O	2.18	0.44
1:A:264:LEU:HA	1:A:264:LEU:HD12	1.80	0.44
2:B:1276:VAL:CG2	2:B:1276:VAL:O	2.63	0.44
2:B:1271:TYR:O	2:B:1272:PRO:C	2.55	0.44
1:A:458:VAL:CG1	1:A:547:GLN:HG3	2.40	0.44
2:B:1255:ASN:HB2	2:B:1289:LEU:HD11	1.97	0.44
1:A:447:ASN:HB3	1:A:452:LEU:HD23	2.00	0.44
1:A:248:GLU:OE2	1:A:249:LYS:N	2.49	0.44
1:A:391:LEU:HD12	1:A:414:TRP:CD2	2.52	0.44
2:B:1065:LYS:HB2	2:B:1065:LYS:NZ	2.33	0.44
2:B:1024:TRP:O	2:B:1026:LEU:HD13	2.18	0.44
1:A:441:TYR:HB2	1:A:458:VAL:HG22	1.98	0.44
1:A:520:GLN:C	1:A:522:ILE:H	2.21	0.44
1:A:52:PRO:CD	1:A:53:GLU:OE1	2.66	0.44
2:B:1065:LYS:HZ2	2:B:1068:SER:HB3	1.82	0.44
2:B:1422:LEU:CB	2:B:1426:TRP:CZ2	3.01	0.44
2:B:1150:PRO:HG2	2:B:1153:TRP:CB	2.47	0.44
2:B:1168:LEU:O	2:B:1169:GLU:C	2.55	0.44
1:A:547:GLN:O	1:A:549:ASP:N	2.49	0.44
2:B:1047:ILE:HD12	2:B:1144:TYR:HB3	1.99	0.44
1:A:521:ILE:O	1:A:525:LEU:HG	2.17	0.44
2:B:1323:LYS:HA	2:B:1323:LYS:HD2	1.64	0.44
2:B:1282:LEU:HD12	2:B:1282:LEU:C	2.38	0.44
1:A:299:ALA:O	1:A:300:GLU:C	2.57	0.44
1:A:79:GLU:C	1:A:81:ASN:N	2.72	0.44
2:B:1261:VAL:CG2	2:B:1262:GLY:N	2.80	0.44
2:B:1264:LEU:CD1	2:B:1279:LEU:HD23	2.47	0.44
1:A:503:LEU:O	1:A:507:GLN:HB2	2.18	0.44
2:B:1232:TYR:HD1	2:B:1232:TYR:C	2.22	0.44
1:A:101:LYS:HE2	1:A:101:LYS:H	1.82	0.44
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.18	0.44
2:B:1081:ASN:HB3	4:B:2013:HOH:O	2.17	0.44
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.53	0.44
1:A:114:ALA:O	1:A:115:TYR:C	2.56	0.44
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.52	0.44
1:A:419:THR:O	1:A:421:PRO:CD	2.64	0.44
2:B:1266:TRP:CD2	2:B:1426:TRP:CE3	3.06	0.43
2:B:1323:LYS:O	2:B:1343:GLN:OE1	2.36	0.43
1:A:171:PHE:CE2	1:A:205:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLU:HG3	1:A:520:GLN:NE2	2.33	0.43
1:A:429:LEU:H	1:A:509:GLN:HE21	1.66	0.43
1:A:84:THR:HB	1:A:154:LYS:HD3	2.00	0.43
2:B:1094:ILE:HD13	2:B:1182:GLN:O	2.18	0.43
2:B:1428:GLN:HE21	2:B:1428:GLN:CA	2.28	0.43
2:B:1428:GLN:NE2	2:B:1428:GLN:CA	2.82	0.43
1:A:216:THR:HB	1:A:217:PRO:CD	2.37	0.43
2:B:1326:ILE:CG2	2:B:1342:TYR:CD1	3.01	0.43
2:B:1080:LEU:CD2	2:B:1084:THR:CG2	2.95	0.43
2:B:1398:TRP:HB3	2:B:1416:PHE:CE2	2.54	0.43
1:A:295:LEU:O	1:A:300:GLU:OE2	2.36	0.43
1:A:84:THR:HB	1:A:154:LYS:CD	2.48	0.43
1:A:479:LEU:HB3	1:A:517:LEU:HD11	2.00	0.43
1:A:446:ALA:HA	1:A:453:GLY:HA3	1.99	0.43
2:B:1251:SER:O	2:B:1252:TRP:CB	2.62	0.43
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.00	0.43
1:A:271:TYR:CD1	1:A:309:ILE:HD13	2.48	0.43
1:A:309:ILE:HG13	1:A:310:LEU:N	2.33	0.43
1:A:394:GLN:O	1:A:396:GLU:N	2.51	0.43
1:A:195:ILE:HG23	1:A:199:ARG:HE	1.83	0.43
1:A:363:ASN:OD1	1:A:363:ASN:O	2.36	0.43
2:B:1130:PHE:CZ	2:B:1144:TYR:HB2	2.53	0.43
1:A:101:LYS:N	1:A:101:LYS:HD3	2.34	0.43
1:A:298:GLU:CD	1:A:298:GLU:H	2.19	0.43
2:B:1311:LYS:HG2	2:B:1311:LYS:O	2.17	0.43
1:A:65:LYS:HD3	1:A:67:ASP:H	1.84	0.43
2:B:1034:LEU:O	2:B:1038:CYS:HB2	2.18	0.43
2:B:1232:TYR:CD1	2:B:1232:TYR:C	2.92	0.43
2:B:1257:ILE:CD1	2:B:1279:LEU:HD11	2.49	0.43
1:A:210:LEU:C	1:A:212:TRP:N	2.71	0.43
2:B:1046:LYS:CD	2:B:1116:PHE:HB3	2.49	0.43
2:B:1126:LYS:HA	2:B:1145:GLN:OE1	2.19	0.43
1:A:395:LYS:O	1:A:399:GLU:CG	2.50	0.43
1:A:122:GLU:O	1:A:125:ARG:HG3	2.19	0.43
2:B:1046:LYS:HD2	2:B:1116:PHE:HB3	2.00	0.43
2:B:1271:TYR:HB2	2:B:1274:ILE:HD13	2.00	0.43
1:A:521:ILE:CG2	1:A:521:ILE:O	2.65	0.43
1:A:406:TRP:CZ3	1:A:407:GLN:CG	3.02	0.43
1:A:77:PHE:CZ	1:A:150:PRO:HB3	2.53	0.43
2:B:1203:GLU:HA	2:B:1206:ARG:HG3	2.00	0.43
1:A:169:GLU:CB	1:A:170:PRO:CD	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CE3	1:A:407:GLN:N	2.87	0.43
1:A:246:LEU:HD12	1:A:307:ARG:CG	2.42	0.43
1:A:430:GLU:HA	1:A:430:GLU:OE1	2.19	0.43
2:B:1197:GLN:O	2:B:1200:THR:HB	2.19	0.43
2:B:1270:ILE:HD11	2:B:1347:LYS:HZ3	1.84	0.42
2:B:1332:GLN:HE21	2:B:1332:GLN:HB2	1.51	0.42
1:A:65:LYS:HG3	1:A:72:ARG:NE	2.33	0.42
2:B:1066:LYS:C	2:B:1068:SER:H	2.22	0.42
2:B:1363:ASN:OD1	2:B:1366:LYS:CB	2.68	0.42
1:A:547:GLN:C	1:A:549:ASP:N	2.71	0.42
1:A:252:TRP:HE3	1:A:256:ASP:HB3	1.84	0.42
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.49	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
2:B:1398:TRP:C	2:B:1400:THR:H	2.22	0.42
2:B:1270:ILE:HG13	2:B:1271:TYR:H	1.84	0.42
1:A:202:ILE:O	1:A:203:GLU:C	2.58	0.42
2:B:1161:GLN:O	2:B:1164:MET:N	2.53	0.42
2:B:1260:LEU:CG	2:B:1279:LEU:HD21	2.45	0.42
2:B:1065:LYS:CB	2:B:1065:LYS:NZ	2.82	0.42
1:A:275:LYS:HE2	1:A:332:GLN:CG	2.48	0.42
2:B:1007:THR:HG22	2:B:1119:PRO:O	2.18	0.42
1:A:43:LYS:O	1:A:43:LYS:HG2	2.18	0.42
1:A:325:LEU:CB	1:A:387:PRO:HB3	2.49	0.42
1:A:210:LEU:O	1:A:212:TRP:N	2.53	0.42
2:B:1388:LYS:HB3	4:B:2023:HOH:O	2.18	0.42
1:A:288:ALA:HA	1:A:289:LEU:HD23	2.01	0.42
1:A:473:THR:HG23	1:A:476:LYS:CE	2.48	0.42
1:A:518:VAL:O	1:A:519:ASN:C	2.58	0.42
1:A:334:GLN:CA	1:A:334:GLN:OE1	2.65	0.42
1:A:22:LYS:N	1:A:22:LYS:HD2	2.33	0.42
1:A:22:LYS:HE3	1:A:22:LYS:HB3	1.87	0.42
1:A:278:GLN:HE22	1:A:281:LYS:CE	2.31	0.42
1:A:24:TRP:HD1	1:A:25:PRO:HD2	1.85	0.42
1:A:167:ILE:O	1:A:208:HIS:CE1	2.63	0.42
1:A:471:ASN:N	1:A:471:ASN:ND2	2.66	0.42
1:A:458:VAL:CG2	1:A:459:THR:H	2.23	0.42
2:B:1042:GLU:HG3	2:B:1043:LYS:H	1.81	0.42
1:A:410:TRP:HB3	2:B:1365:VAL:HG21	2.02	0.42
2:B:1300:GLU:O	2:B:1303:LEU:HG	2.19	0.42
2:B:1290:THR:O	2:B:1290:THR:CG2	2.66	0.42
2:B:1103:LYS:HZ1	2:B:1179:VAL:CG2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:C	1:A:124:PHE:H	2.23	0.42
2:B:1243:PRO:O	2:B:1244:ILE:HD12	2.19	0.42
1:A:443:ASP:H	1:A:481:ALA:HB1	1.84	0.42
1:A:201:LYS:HE3	1:A:201:LYS:HA	2.02	0.42
2:B:1245:VAL:C	2:B:1246:LEU:HD13	2.40	0.42
1:A:498:ASP:CG	1:A:538:ALA:HA	2.40	0.42
2:B:1121:ASP:O	2:B:1122:GLU:C	2.57	0.42
1:A:445:ALA:O	1:A:446:ALA:CB	2.68	0.41
2:B:1270:ILE:HA	2:B:1270:ILE:HD12	1.86	0.41
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.41
1:A:506:ILE:HG21	1:A:533:LEU:HD12	2.02	0.41
1:A:109:LEU:O	1:A:187:LEU:N	2.41	0.41
2:B:1268:SER:O	2:B:1269:GLN:C	2.57	0.41
2:B:1324:ASP:HA	2:B:1385:LYS:NZ	2.35	0.41
2:B:1013:LYS:O	2:B:1016:MET:HG3	2.20	0.41
1:A:498:ASP:OD1	1:A:545:ASN:OD1	2.38	0.41
1:A:355:ALA:O	1:A:356:ARG:C	2.55	0.41
2:B:1292:VAL:HG22	2:B:1293:ILE:N	2.34	0.41
1:A:450:THR:HG22	1:A:452:LEU:CD2	2.17	0.41
2:B:1310:LEU:C	2:B:1312:GLU:N	2.71	0.41
1:A:336:GLN:OE1	1:A:355:ALA:HB2	2.20	0.41
1:A:335:GLY:CA	1:A:367:GLN:NE2	2.71	0.41
2:B:1199:ARG:HG2	2:B:1199:ARG:H	1.64	0.41
2:B:1395:LYS:HB2	2:B:1416:PHE:CD1	2.56	0.41
1:A:443:ASP:C	1:A:481:ALA:HB2	2.41	0.41
1:A:302:GLU:O	1:A:305:GLU:N	2.53	0.41
2:B:1400:THR:CG2	2:B:1401:TRP:CD1	2.98	0.41
2:B:1073:LYS:HZ2	2:B:1075:VAL:HG23	1.85	0.41
2:B:1083:ARG:HG2	2:B:1083:ARG:H	1.74	0.41
2:B:1332:GLN:NE2	2:B:1338:THR:HG23	2.36	0.41
2:B:1391:LEU:HA	2:B:1392:PRO:HD2	1.91	0.41
1:A:506:ILE:CG2	1:A:533:LEU:HD12	2.50	0.41
2:B:1424:LYS:HE2	2:B:1424:LYS:HB3	1.74	0.41
2:B:1306:ASN:O	2:B:1307:ARG:C	2.59	0.41
1:A:184:MET:HB3	1:A:185:ASP:H	1.77	0.41
1:A:331:LYS:HB3	1:A:421:PRO:HB2	2.02	0.41
1:A:409:THR:CG2	1:A:410:TRP:H	2.29	0.41
2:B:1085:GLN:N	2:B:1088:TRP:NE1	2.69	0.41
1:A:547:GLN:C	1:A:549:ASP:H	2.22	0.41
2:B:1378:GLU:O	2:B:1382:ILE:HG13	2.20	0.41
1:A:60:VAL:HB	1:A:75:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:CD1	1:A:344:GLU:O	2.74	0.41
2:B:1303:LEU:O	2:B:1307:ARG:HB2	2.21	0.41
1:A:439:THR:CG2	1:A:441:TYR:HE1	2.33	0.41
1:A:26:LEU:CD2	1:A:133:PRO:CG	2.89	0.41
1:A:473:THR:O	1:A:476:LYS:N	2.44	0.41
1:A:408:ALA:HB3	2:B:1393:ILE:HB	2.03	0.41
1:A:440:PHE:CE2	1:A:457:TYR:CE2	3.09	0.41
2:B:1100:LEU:O	2:B:1102:LYS:N	2.54	0.41
2:B:1101:LYS:HE3	4:B:2022:HOH:O	2.20	0.41
2:B:1268:SER:N	2:B:1274:ILE:HG21	2.36	0.41
1:A:499:SER:OG	1:A:499:SER:O	2.39	0.41
1:A:84:THR:CG2	1:A:85:GLN:N	2.54	0.41
2:B:1066:LYS:O	2:B:1067:ASP:HB3	2.21	0.41
2:B:1393:ILE:HD13	2:B:1398:TRP:HB2	2.03	0.41
2:B:1277:ARG:CG	2:B:1278:GLN:H	2.34	0.41
2:B:1314:VAL:HG11	2:B:1317:VAL:HG23	2.00	0.40
1:A:486:LEU:HD12	1:A:521:ILE:HG23	2.02	0.40
1:A:410:TRP:HB2	2:B:1365:VAL:HG23	2.03	0.40
2:B:1320:ASP:OD2	2:B:1322:SER:N	2.45	0.40
1:A:407:GLN:HG2	2:B:1393:ILE:HA	2.02	0.40
1:A:520:GLN:C	1:A:522:ILE:N	2.74	0.40
1:A:434:ILE:HD12	1:A:493:VAL:O	2.20	0.40
2:B:1041:MET:CE	2:B:1073:LYS:HE3	2.51	0.40
2:B:1112:GLY:C	2:B:1114:ALA:H	2.24	0.40
2:B:1188:TYR:CD2	2:B:1188:TYR:N	2.89	0.40
2:B:1376:THR:HB	2:B:1410:TRP:CH2	2.56	0.40
2:B:1422:LEU:O	2:B:1423:VAL:C	2.59	0.40
2:B:1064:LYS:HB3	2:B:1068:SER:O	2.21	0.40
1:A:520:GLN:OE1	1:A:520:GLN:N	2.54	0.40
1:A:520:GLN:O	1:A:522:ILE:N	2.54	0.40
1:A:34:LEU:HD11	1:A:73:LYS:HG3	2.03	0.40
1:A:111:VAL:HG13	1:A:214:LEU:HD12	2.03	0.40
2:B:1150:PRO:O	2:B:1156:SER:OG	2.24	0.40
1:A:159:ILE:HG12	1:A:159:ILE:H	1.58	0.40
1:A:311:LYS:NZ	1:A:312:GLU:OE1	2.55	0.40
2:B:1035:VAL:HG23	2:B:1036:GLU:N	2.36	0.40
2:B:1175:ASN:N	2:B:1175:ASN:ND2	2.69	0.40
2:B:1209:LEU:HD23	2:B:1209:LEU:HA	1.89	0.40
2:B:1018:GLY:HA3	2:B:1056:TYR:CE1	2.57	0.40
1:A:50:ILE:C	1:A:50:ILE:CD1	2.88	0.40
2:B:1301:LEU:HA	2:B:1304:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:LEU:O	2:B:1084:THR:HG23	2.20	0.40
2:B:1013:LYS:O	2:B:1016:MET:CG	2.70	0.40
2:B:1080:LEU:CD2	2:B:1080:LEU:C	2.90	0.40
1:A:220:LYS:N	1:A:220:LYS:CD	2.68	0.40
1:A:426:TRP:O	1:A:526:ILE:HG12	2.20	0.40
2:B:1410:TRP:O	2:B:1410:TRP:CE3	2.74	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:289:LEU:CD2	4:A:2013:HOH:O[3_555]	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	545/557 (98%)	390 (72%)	110 (20%)	45 (8%)	<b>1</b>	<b>4</b>
2	B	393/428 (92%)	293 (75%)	68 (17%)	32 (8%)	<b>1</b>	<b>5</b>
All	All	938/985 (95%)	683 (73%)	178 (19%)	77 (8%)	<b>1</b>	<b>5</b>

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	28	GLU
1	A	114	ALA
1	A	135	ILE
1	A	153	TRP
1	A	185	ASP
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	289	LEU
1	A	302	GLU
1	A	303	LEU
1	A	345	PRO
1	A	356	ARG
1	A	507	GLN
1	A	528	LYS
1	A	538	ALA
2	B	1065	LYS
2	B	1085	GLN
2	B	1184	MET
2	B	1250	ASP
2	B	1333	GLY
2	B	1423	VAL
1	A	112	GLY
1	A	365	VAL
1	A	466	VAL
1	A	512	LYS
1	A	515	SER
2	B	1049	LYS
2	B	1086	ASP
2	B	1116	PHE
2	B	1152	GLY
2	B	1161	GLN
2	B	1185	ASP
2	B	1297	GLU
2	B	1308	GLU
2	B	1424	LYS
1	A	154	LYS
1	A	171	PHE
1	A	203	GLU
1	A	286	THR
1	A	297	GLU
1	A	412	PRO
1	A	422	LEU
1	A	433	PRO
1	A	446	ALA
1	A	458	VAL
1	A	459	THR
1	A	463	ARG
2	B	1009	PRO
2	B	1121	ASP

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Mol	Chain	Res	Type
2	B	1194	GLU
1	A	167	ILE
1	A	170	PRO
1	A	282	LEU
1	A	311	LYS
1	A	344	GLU
1	A	364	ASP
2	B	1210	LEU
2	B	1311	LYS
1	A	80	LEU
1	A	308	GLU
1	A	410	TRP
2	B	1169	GLU
2	B	1254	VAL
2	B	1268	SER
2	B	1334	GLN
2	B	1399	GLU
1	A	299	ALA
2	B	1176	PRO
2	B	1309	ILE
2	B	1314	VAL
2	B	1421	PRO
2	B	1213	GLY
2	B	1247	PRO
2	B	1345	PRO
1	A	25	PRO
1	A	243	PRO
1	A	490	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/497 (99%)	434 (89%)	56 (11%)	7	27
2	B	366/390 (94%)	327 (89%)	39 (11%)	8	30
All	All	856/887 (96%)	761 (89%)	95 (11%)	8	28

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	22	LYS
1	A	24	TRP
1	A	27	THR
1	A	40	GLU
1	A	44	GLU
1	A	50	ILE
1	A	58	THR
1	A	61	PHE
1	A	66	LYS
1	A	76	ASP
1	A	90	VAL
1	A	101	LYS
1	A	122	GLU
1	A	123	ASP
1	A	126	LYS
1	A	131	THR
1	A	132	ILE
1	A	143	ARG
1	A	169	GLU
1	A	182	GLN
1	A	194	GLU
1	A	201	LYS
1	A	209	LEU
1	A	211	ARG
1	A	220	LYS
1	A	228	LEU
1	A	241	VAL
1	A	246	LEU
1	A	248	GLU
1	A	257	ILE
1	A	260	LEU
1	A	264	LEU
1	A	275	LYS
1	A	278	GLN
1	A	289	LEU
1	A	296	THR
1	A	309	ILE
1	A	317	VAL
1	A	356	ARG
1	A	362	THR
1	A	386	THR

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Mol	Chain	Res	Type
1	A	397	THR
1	A	402	TRP
1	A	404	GLU
1	A	415	GLU
1	A	417	VAL
1	A	447	ASN
1	A	449	GLU
1	A	471	ASN
1	A	487	GLN
1	A	491	LEU
1	A	520	GLN
1	A	524	GLN
1	A	533	LEU
1	A	547	GLN
2	B	1011	LYS
2	B	1030	LYS
2	B	1043	LYS
2	B	1048	SER
2	B	1072	ARG
2	B	1073	LYS
2	B	1078	ARG
2	B	1086	ASP
2	B	1094	ILE
2	B	1161	GLN
2	B	1169	GLU
2	B	1175	ASN
2	B	1185	ASP
2	B	1189	VAL
2	B	1191	SER
2	B	1195	ILE
2	B	1199	ARG
2	B	1201	LYS
2	B	1202	ILE
2	B	1232	TYR
2	B	1242	GLN
2	B	1246	LEU
2	B	1257	ILE
2	B	1275	LYS
2	B	1277	ARG
2	B	1289	LEU
2	B	1323	LYS
2	B	1330	GLN

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Mol	Chain	Res	Type
2	B	1332	GLN
2	B	1334	GLN
2	B	1347	LYS
2	B	1351	THR
2	B	1361	HIS
2	B	1374	LYS
2	B	1381	VAL
2	B	1400	THR
2	B	1403	THR
2	B	1415	GLU
2	B	1428	GLN

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

Mol	Chain	Res	Type
1	A	57	ASN
1	A	96	HIS
1	A	136	ASN
1	A	182	GLN
1	A	208	HIS
1	A	222	GLN
1	A	269	GLN
1	A	278	GLN
1	A	315	HIS
1	A	332	GLN
1	A	340	GLN
1	A	361	HIS
1	A	367	GLN
1	A	447	ASN
1	A	464	GLN
1	A	471	ASN
1	A	487	GLN
1	A	500	GLN
1	A	539	HIS
1	A	545	ASN
2	B	1081	ASN
2	B	1096	HIS
2	B	1136	ASN
2	B	1137	ASN
2	B	1147	ASN
2	B	1174	GLN
2	B	1182	GLN

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Mol	Chain	Res	Type
2	B	1255	ASN
2	B	1278	GLN
2	B	1330	GLN
2	B	1332	GLN
2	B	1340	GLN
2	B	1343	GLN
2	B	1348	ASN
2	B	1367	GLN
2	B	1407	GLN
2	B	1418	ASN
2	B	1428	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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
3	NNB	A	1551	-	26,26,26	2.45	6 (23%)	36,36,36	3.13	13 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NNB	A	1551	-	-	0/9/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1551	NNB	C1-C7	-6.25	1.38	1.48
3	A	1551	NNB	C2-C8	-5.87	1.39	1.48
3	A	1551	NNB	C7-N1	-5.12	1.33	1.39
3	A	1551	NNB	C8-N1	-5.00	1.33	1.39
3	A	1551	NNB	C12-N2	-4.39	1.33	1.41
3	A	1551	NNB	O3-C11	2.36	1.36	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1551	NNB	C10-O3-C11	-11.88	109.05	119.09
3	A	1551	NNB	O3-C11-S1	-7.46	119.76	125.06
3	A	1551	NNB	C12-N2-C11	-5.86	120.71	130.04
3	A	1551	NNB	C8-N1-C7	-3.34	109.16	111.95
3	A	1551	NNB	C10-C9-N1	-2.94	108.38	112.37
3	A	1551	NNB	C2-C1-C7	-2.56	106.09	108.27
3	A	1551	NNB	C1-C2-C8	-2.40	106.23	108.27
3	A	1551	NNB	C9-N1-C7	2.05	125.77	123.89
3	A	1551	NNB	C6-C1-C7	2.27	133.17	129.67
3	A	1551	NNB	C3-C2-C8	2.48	133.51	129.67
3	A	1551	NNB	O3-C11-N2	3.83	120.63	111.57
3	A	1551	NNB	C2-C8-N1	4.51	109.03	105.88
3	A	1551	NNB	C1-C7-N1	5.14	109.48	105.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	NNB	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	549/557 (98%)	-0.41	4 (0%) 89 70	16, 41, 62, 79	0
2	B	401/428 (93%)	-0.43	6 (1%) 76 48	18, 37, 74, 85	0
All	All	950/985 (96%)	-0.42	10 (1%) 82 57	16, 40, 67, 85	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	3.6
2	B	1361	HIS	3.0
2	B	1068	SER	2.6
2	B	1069	THR	2.5
1	A	472	THR	2.4
1	A	68	SER	2.3
2	B	1067	ASP	2.2
2	B	1213	GLY	2.2
1	A	286	THR	2.1
2	B	1277	ARG	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NNB	A	1551	24/24	0.98	0.14	-0.99	23,27,40,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.