Full wwPDB X-ray Structure Validation Report

May 15, 2020 – 03:11 pm BST

PDB ID	:	2VG7
Title	:	Crystal structures of HIV-1 reverse transcriptase complexes with thiocarbamate non-nucleoside inhibitors
Authors	:	Spallarossa, A.; Cesarini, S.; Ranise, A.; Ponassi, M.; Unge, T.; Bolognesi, M.
Deposited on	:	2007-11-08
Resolution	:	2.82 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:

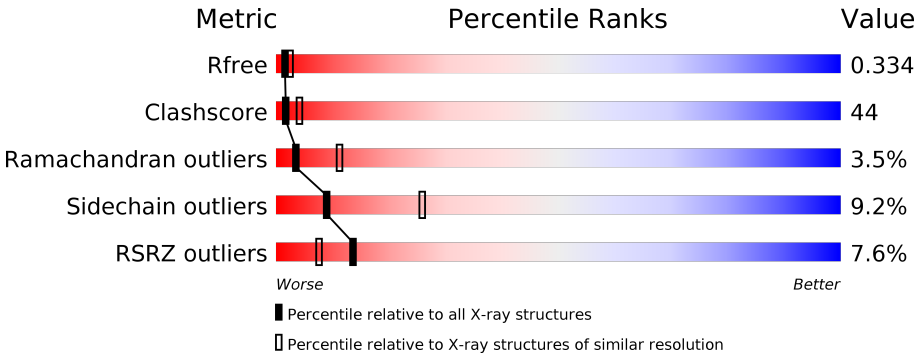
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.82 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	6% 42% 45% 9%
2	B	428	8% 43% 42% 7% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NNI	A	1551	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7782 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.

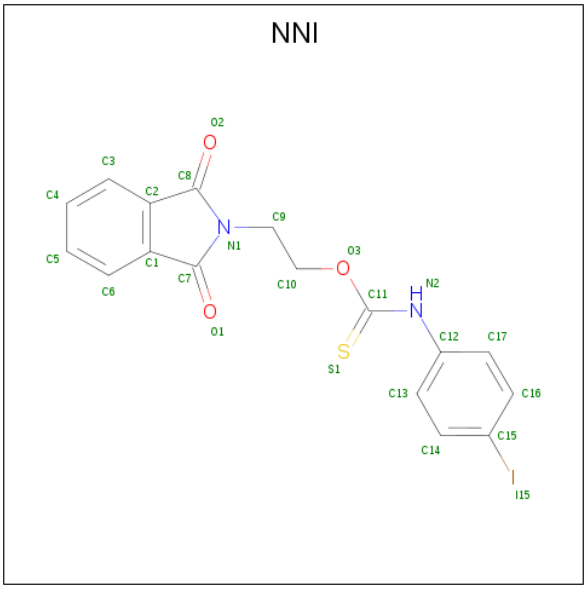
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4436	2873	738	817	8	0	0	1

- Molecule 2 is a protein called P51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	395	3276	2138	536	595	7	0	0	0

- Molecule 3 is O-[2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)ethyl] (4-iodophenyl)thiocarbamate (three-letter code: NNI) (formula: $C_{17}H_{13}IN_2O_3S$).



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

- Molecule 4 is water.

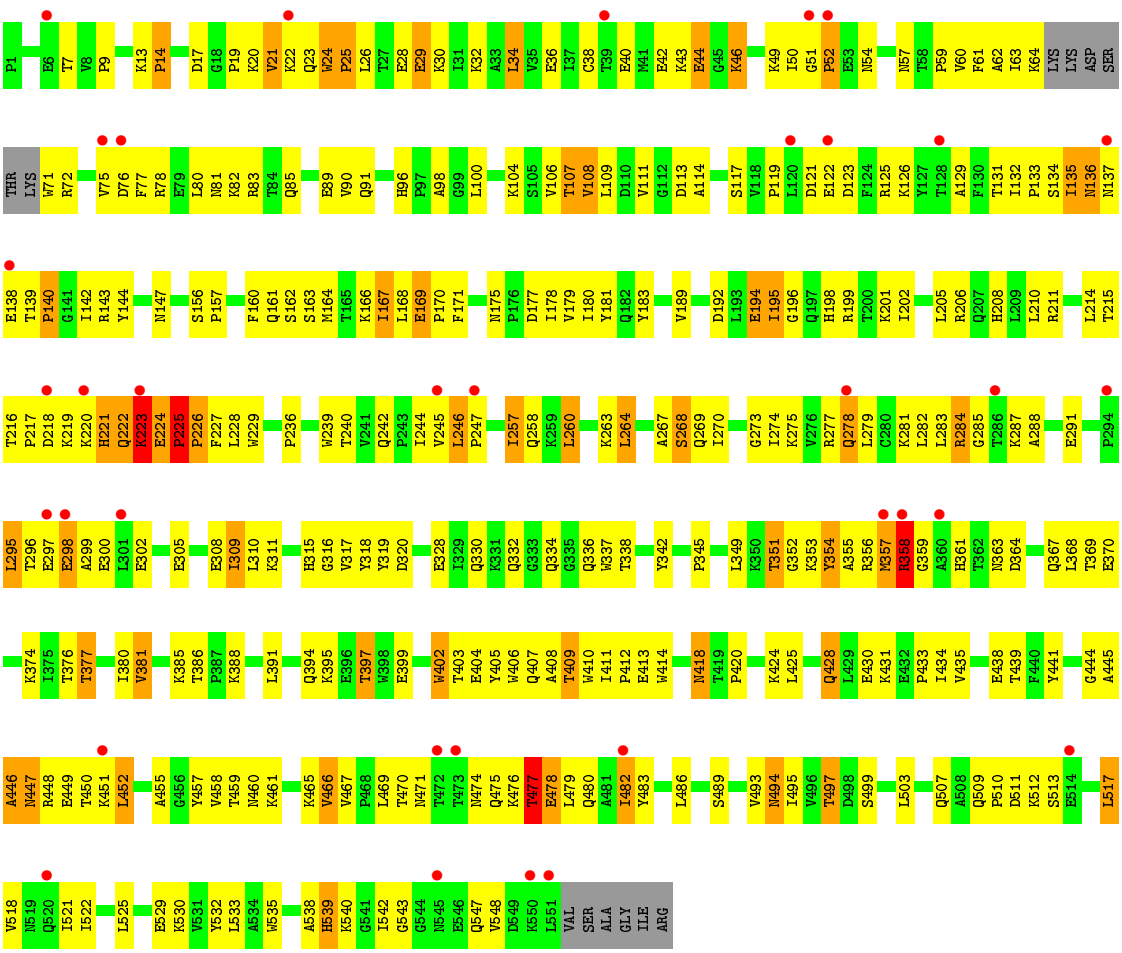
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	23	Total O 23 23	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

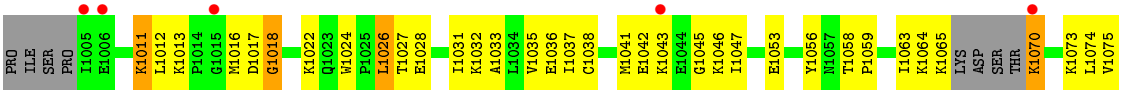
- Molecule 1: REVERSE TRANSCRIPTASE/RIBONUCLEASE H

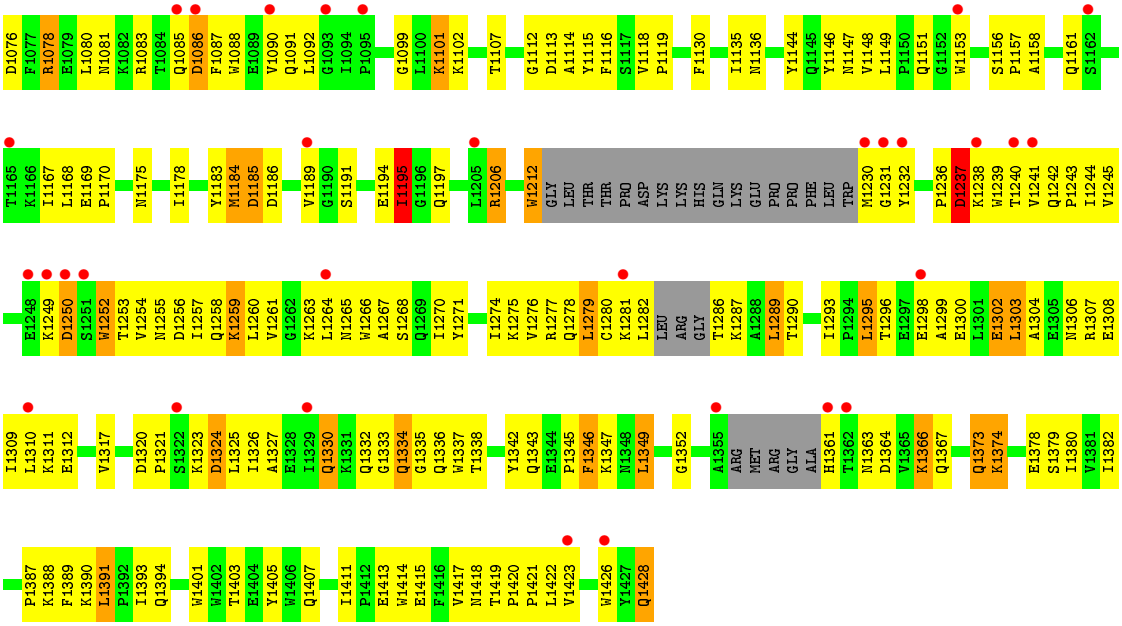
Chain A:



- Molecule 2: P51 RT

Chain B:




D1076 F1077 R1078 E1079 L1080 N1081 K1082 R1083 T1084 Q1085 D1086 F1087 W1088 E1089 Y1090 Q1091 L1092 G1093 I1094 P1095 G1099 L1100 K1101 K1102 T1107 G1112 D1113 A1114 Y1115 F1116 S1117 V1118 P1119 F1130 I1135 N1136 Y1144 Q1145 Y1146 N1147 V1148 L1149 P1150 Q1151 G1152 W1153 S1156 P1157 A1158 Q1161 S1162
T1165 K1166 I1167 L1168 E1169 P1170 N1175 I1178 Y1183 M1184 D1185 D1186 V1189 G1190 S1191 E1194 I1195 G1196 Q1197 L1205 R1206 W1212 GLY LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP M1230 G1231 Y1232 P1236 D1237 K1238 W1239 T1240 V1241 Q1242 P1243 I1244 V1245
E1248 K1249 D1250 S1251 W1252 T1253 V1254 N1255 D1256 I1257 Q1258 K1259 L1260 V1261 G1262 K1263 L1264 N1265 W1266 A1267 S1268 Q1269 I1270 Y1271 I1274 K1275 V1276 R1277 Q1278 L1279 C1280 K1281 L1282 LEU ARG GLY T1286 K1287 A1288 L1289 T1290 I1293 P1294 L1295 T1296 E1297 E1298 A1299 E1300 L1301 E1302 L1303 A1304 E1305 N1306 R1307 E1308
I1309 L1310 K1311 E1312 V1317 D1320 P1321 S1322 K1323 D1324 L1325 I1326 A1327 E1328 I1329 Q1330 K1331 Q1332 G1333 Q1334 G1335 Q1336 W1337 T1338 Y1342 Q1343 E1344 P1345 F1346 K1347 N1348 L1349 G1352 A1355 ARG MET ARG GLY ALA H1361 T1362 N1363 D1364 V1365 K1366 Q1367 Q1373 K1374 E1378 S1379 I1380 V1381 I1382
P1387 K1388 F1389 K1390 L1391 P1392 I1393 Q1394 W1401 W1402 T1403 E1404 Y1405 W1406 Q1407 I1411 P1412 E1413 W1414 E1415 F1416 V1417 N1418 T1419 P1420 P1421 L1422 V1423 W1426 Y1427 Q1428

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.94Å 157.00Å 154.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.82 20.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	81.5 (20.00-2.82) 81.5 (20.00-2.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.333 0.254 , 0.334	Depositor DCC
R_{free} test set	1408 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7782	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.26	1/4553 (0.0%)	0.40	0/6187
2	B	0.23	0/3368	0.40	0/4573
All	All	0.25	1/7921 (0.0%)	0.40	0/10760

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	7.09	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	225	PRO	Peptide

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4436	0	4484	450	0
2	B	3276	0	3297	250	0
3	A	24	0	13	11	0
4	A	23	0	0	5	0
4	B	23	0	0	5	0
All	All	7782	0	7794	683	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 44.

All (683) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CE1	1:A:269:GLN:HE21	1.38	1.41
1:A:465:LYS:O	1:A:466:VAL:CG2	1.70	1.38
2:B:1064:LYS:O	2:B:1065:LYS:HG3	1.38	1.23
1:A:296:THR:O	1:A:300:GLU:HG3	1.43	1.18
1:A:394:GLN:HB2	1:A:397:THR:HG22	1.20	1.17
1:A:278:GLN:OE1	1:A:298:GLU:HB3	1.45	1.15
1:A:511:ASP:O	1:A:512:LYS:HG3	1.42	1.15
2:B:1195:ILE:H	2:B:1195:ILE:HD12	1.09	1.14
1:A:26:LEU:CD2	1:A:133:PRO:HG2	1.79	1.12
2:B:1428:GLN:NE2	2:B:1428:GLN:C	2.02	1.12
1:A:450:THR:CG2	1:A:452:LEU:HD22	1.80	1.12
1:A:394:GLN:HB2	1:A:397:THR:CG2	1.80	1.10
1:A:96:HIS:CE1	1:A:269:GLN:NE2	2.20	1.09
2:B:1266:TRP:CE3	2:B:1426:TRP:CZ3	2.42	1.08
1:A:458:VAL:HG22	1:A:548:VAL:CG2	1.83	1.07
2:B:1263:LYS:HB3	2:B:1426:TRP:CD1	1.92	1.04
1:A:278:GLN:NE2	1:A:281:LYS:HE2	1.73	1.04
1:A:465:LYS:O	1:A:466:VAL:HG23	0.87	1.03
1:A:137:ASN:OD1	4:A:2005:HOH:O	1.75	1.03
1:A:134:SER:O	1:A:136:ASN:N	1.92	1.02
2:B:1428:GLN:O	2:B:1428:GLN:NE2	1.94	1.01
1:A:450:THR:HG22	1:A:452:LEU:HD22	1.39	1.00
2:B:1064:LYS:O	2:B:1065:LYS:CG	2.09	1.00
1:A:96:HIS:HE1	1:A:269:GLN:NE2	1.57	0.98
1:A:40:GLU:OE2	1:A:43:LYS:NZ	1.97	0.98
1:A:278:GLN:OE1	1:A:298:GLU:CB	2.09	0.98
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HD13	2:B:1280:CYS:SG	2.02	0.98
1:A:135:ILE:O	1:A:136:ASN:HB2	1.61	0.96
2:B:1263:LYS:HB3	2:B:1426:TRP:HD1	1.23	0.95
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.49	0.95
2:B:1428:GLN:HE21	2:B:1428:GLN:C	1.65	0.95
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.63	0.95
1:A:356:ARG:NH1	1:A:358:ARG:NH1	2.14	0.94
1:A:458:VAL:HG22	1:A:548:VAL:HG22	1.49	0.93
1:A:465:LYS:C	1:A:466:VAL:HG23	1.88	0.93
2:B:1335:GLY:HA2	2:B:1367:GLN:HE22	1.33	0.93
1:A:334:GLN:OE1	1:A:512:LYS:HE2	1.67	0.92
1:A:23:GLN:HE22	1:A:60:VAL:N	1.65	0.92
2:B:1267:ALA:O	2:B:1270:ILE:O	1.87	0.92
2:B:1278:GLN:HB2	2:B:1302:GLU:HG3	1.52	0.92
1:A:334:GLN:OE1	1:A:512:LYS:CE	2.18	0.91
2:B:1087:PHE:O	2:B:1091:GLN:HB3	1.68	0.91
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.05	0.91
1:A:223:LYS:HD3	1:A:224:GLU:HG3	1.49	0.91
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.13	0.91
2:B:1326:ILE:HG21	2:B:1342:TYR:CZ	2.06	0.91
2:B:1195:ILE:HD12	2:B:1195:ILE:N	1.85	0.90
1:A:26:LEU:HD23	1:A:133:PRO:HG2	1.50	0.90
1:A:57:ASN:HD22	1:A:143:ARG:NH2	1.69	0.89
1:A:223:LYS:HG2	1:A:224:GLU:N	1.86	0.89
2:B:1271:TYR:O	2:B:1274:ILE:HD13	1.72	0.89
1:A:13:LYS:HB3	1:A:14:PRO:HD2	1.54	0.88
1:A:223:LYS:HG2	1:A:224:GLU:H	1.39	0.87
2:B:1255:ASN:HB2	2:B:1289:LEU:HD12	1.56	0.87
1:A:489:SER:HB2	1:A:493:VAL:HG21	1.57	0.87
1:A:25:PRO:HG3	1:A:137:ASN:OD1	1.75	0.86
1:A:356:ARG:HH12	1:A:358:ARG:NH1	1.72	0.86
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.19	0.86
2:B:1013:LYS:HE2	2:B:1086:ASP:H	1.39	0.86
1:A:104:LYS:HB3	1:A:192:ASP:HA	1.58	0.85
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.59	0.85
1:A:542:ILE:CD1	2:B:1280:CYS:SG	2.64	0.85
1:A:518:VAL:O	1:A:522:ILE:HG12	1.77	0.84
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.40	0.84
1:A:332:GLN:O	1:A:336:GLN:HB2	1.78	0.83
1:A:444:GLY:HA3	1:A:477:THR:O	1.78	0.83
1:A:26:LEU:HD22	1:A:133:PRO:HG2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:HE22	1:A:60:VAL:H	1.26	0.83
1:A:336:GLN:OE1	1:A:355:ALA:CB	2.27	0.82
1:A:411:ILE:HG22	1:A:412:PRO:O	1.78	0.82
1:A:493:VAL:HG12	1:A:494:ASN:N	1.94	0.82
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.80	0.82
1:A:450:THR:CG2	1:A:452:LEU:CD2	2.57	0.82
1:A:356:ARG:NH1	1:A:358:ARG:HH12	1.78	0.80
1:A:511:ASP:O	1:A:512:LYS:CG	2.28	0.80
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.63	0.80
1:A:278:GLN:HA	1:A:278:GLN:HE21	1.47	0.79
2:B:1420:PRO:HB2	2:B:1423:VAL:HG23	1.62	0.79
1:A:482:ILE:HD11	1:A:486:LEU:HD11	1.63	0.79
1:A:459:THR:HG22	1:A:461:LYS:H	1.47	0.79
3:A:1551:NNI:O3	3:A:1551:NNI:H13	1.83	0.79
1:A:336:GLN:OE1	1:A:355:ALA:HB2	1.83	0.78
2:B:1064:LYS:O	2:B:1065:LYS:CB	2.32	0.78
1:A:26:LEU:CD2	1:A:133:PRO:CG	2.62	0.78
1:A:108:VAL:H	1:A:223:LYS:HB2	1.48	0.77
2:B:1151:GLN:O	2:B:1185:ASP:OD2	2.02	0.77
2:B:1257:ILE:HD13	2:B:1279:LEU:HD12	1.65	0.77
2:B:1241:VAL:O	2:B:1243:PRO:HD3	1.84	0.77
1:A:134:SER:C	1:A:136:ASN:H	1.87	0.77
1:A:50:ILE:HG12	1:A:54:ASN:ND2	2.00	0.77
1:A:96:HIS:H	2:B:1136:ASN:HD21	1.31	0.77
1:A:44:GLU:HB3	1:A:46:LYS:CD	2.14	0.76
1:A:194:GLU:H	1:A:194:GLU:CD	1.88	0.76
1:A:474:ASN:HB2	4:A:2017:HOH:O	1.85	0.76
1:A:96:HIS:HD2	1:A:98:ALA:H	1.30	0.76
1:A:450:THR:CB	1:A:452:LEU:HD22	2.15	0.76
2:B:1016:MET:SD	4:B:2002:HOH:O	2.44	0.76
2:B:1296:THR:O	2:B:1299:ALA:N	2.18	0.76
2:B:1065:LYS:O	2:B:1407:GLN:HG2	1.86	0.75
1:A:431:LYS:HB3	1:A:431:LYS:NZ	2.01	0.75
1:A:23:GLN:O	1:A:25:PRO:HD3	1.85	0.75
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.68	0.75
1:A:493:VAL:CG1	1:A:494:ASN:N	2.50	0.74
1:A:195:ILE:HG23	1:A:196:GLY:N	2.01	0.74
1:A:297:GLU:HA	1:A:300:GLU:OE1	1.87	0.74
1:A:317:VAL:HG12	1:A:318:TYR:N	2.03	0.74
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.22	0.74
1:A:131:THR:HG22	1:A:143:ARG:HE	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1032:LYS:O	2:B:1035:VAL:HG22	1.88	0.73
2:B:1263:LYS:CB	2:B:1426:TRP:CD1	2.71	0.73
2:B:1018:GLY:HA3	2:B:1056:TYR:CE1	2.23	0.73
2:B:1085:GLN:HA	2:B:1088:TRP:NE1	2.02	0.73
2:B:1345:PRO:O	2:B:1346:PHE:HB2	1.89	0.73
1:A:482:ILE:HD13	1:A:482:ILE:C	2.09	0.73
1:A:278:GLN:HE21	1:A:281:LYS:HE2	1.50	0.72
1:A:29:GLU:HG2	1:A:30:LYS:N	2.05	0.72
1:A:377:THR:O	1:A:381:VAL:HG12	1.88	0.72
1:A:163:SER:O	1:A:167:ILE:HG23	1.89	0.72
1:A:450:THR:HB	1:A:452:LEU:CD2	2.19	0.72
2:B:1309:ILE:O	2:B:1310:LEU:HB2	1.89	0.72
1:A:278:GLN:NE2	1:A:281:LYS:CE	2.53	0.72
1:A:285:GLY:O	1:A:287:LYS:HG2	1.90	0.71
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.19	0.71
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.05	0.71
2:B:1257:ILE:CD1	2:B:1279:LEU:HD12	2.19	0.71
1:A:275:LYS:HD2	1:A:332:GLN:NE2	2.05	0.71
1:A:494:ASN:HB3	1:A:532:TYR:HB3	1.72	0.71
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.72	0.71
1:A:328:GLU:HG3	1:A:330:GLN:HE22	1.55	0.71
1:A:224:GLU:O	1:A:225:PRO:O	2.09	0.71
1:A:278:GLN:HE22	1:A:281:LYS:HE2	1.56	0.71
1:A:223:LYS:O	1:A:224:GLU:HB2	1.89	0.71
1:A:482:ILE:O	1:A:482:ILE:HD13	1.91	0.70
1:A:434:ILE:HD12	1:A:493:VAL:O	1.91	0.70
2:B:1266:TRP:CD2	2:B:1426:TRP:CZ3	2.79	0.70
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.21	0.70
2:B:1156:SER:HB2	2:B:1157:PRO:HD3	1.73	0.70
1:A:317:VAL:CG1	1:A:318:TYR:N	2.55	0.70
2:B:1266:TRP:CZ3	2:B:1426:TRP:CZ3	2.80	0.69
1:A:135:ILE:O	1:A:136:ASN:CB	2.37	0.69
1:A:131:THR:HG23	1:A:143:ARG:HH21	1.58	0.69
1:A:459:THR:HG22	1:A:460:ASN:N	2.05	0.69
1:A:358:ARG:NH1	1:A:358:ARG:HB2	2.07	0.69
2:B:1266:TRP:CE3	2:B:1426:TRP:CH2	2.81	0.68
1:A:195:ILE:CG2	1:A:196:GLY:N	2.55	0.68
2:B:1064:LYS:C	2:B:1065:LYS:HG3	2.13	0.68
2:B:1265:ASN:O	2:B:1268:SER:HB3	1.93	0.68
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.58	0.68
1:A:161:GLN:HB3	4:A:2006:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HB3	1:A:291:GLU:OE1	1.93	0.68
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.16	0.67
1:A:23:GLN:HG3	1:A:131:THR:OG1	1.95	0.67
1:A:356:ARG:HH11	1:A:356:ARG:HB3	1.58	0.67
1:A:428:GLN:HE21	1:A:428:GLN:CA	2.07	0.67
2:B:1183:TYR:O	2:B:1184:MET:O	2.12	0.67
1:A:23:GLN:NE2	1:A:60:VAL:H	1.91	0.67
1:A:23:GLN:NE2	1:A:60:VAL:N	2.39	0.67
2:B:1244:ILE:HD12	2:B:1244:ILE:H	1.59	0.67
1:A:278:GLN:HE22	1:A:281:LYS:CE	2.08	0.67
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.25	0.67
1:A:168:LEU:HD21	1:A:180:ILE:HG21	1.75	0.67
2:B:1282:LEU:HD21	2:B:1295:LEU:HA	1.75	0.67
2:B:1278:GLN:HB2	2:B:1302:GLU:CG	2.24	0.67
1:A:26:LEU:HD23	1:A:133:PRO:CG	2.24	0.67
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.77	0.67
2:B:1335:GLY:HA2	2:B:1367:GLN:NE2	2.06	0.66
1:A:135:ILE:HG22	1:A:135:ILE:O	1.94	0.66
2:B:1266:TRP:CZ3	2:B:1426:TRP:HZ3	2.14	0.66
2:B:1012:LEU:HD21	2:B:1016:MET:HB2	1.76	0.66
2:B:1046:LYS:NZ	2:B:1116:PHE:CE2	2.64	0.66
2:B:1260:LEU:HD13	2:B:1264:LEU:HD12	1.78	0.66
1:A:57:ASN:ND2	1:A:131:THR:HG23	2.11	0.66
1:A:459:THR:HG22	1:A:461:LYS:N	2.09	0.66
2:B:1244:ILE:HD12	2:B:1244:ILE:N	2.10	0.66
1:A:225:PRO:HA	1:A:227:PHE:CE1	2.31	0.66
1:A:273:GLY:O	1:A:309:ILE:HD12	1.95	0.66
1:A:96:HIS:HE1	1:A:269:GLN:HE21	0.72	0.66
1:A:17:ASP:O	1:A:83:ARG:NH1	2.28	0.66
2:B:1279:LEU:HD21	2:B:1303:LEU:HD22	1.78	0.66
1:A:111:VAL:CG1	1:A:214:LEU:HD12	2.26	0.65
1:A:29:GLU:HG2	1:A:30:LYS:H	1.61	0.65
2:B:1041:MET:HE1	2:B:1073:LYS:HD2	1.79	0.65
2:B:1255:ASN:O	2:B:1259:LYS:HG2	1.97	0.65
2:B:1118:VAL:HB	2:B:1149:LEU:CD1	2.26	0.65
2:B:1388:LYS:HG3	2:B:1413:GLU:HB2	1.79	0.65
1:A:267:ALA:C	1:A:269:GLN:H	2.00	0.65
1:A:164:MET:O	1:A:168:LEU:HB2	1.97	0.65
1:A:517:LEU:O	1:A:517:LEU:HD13	1.97	0.65
2:B:1303:LEU:H	2:B:1303:LEU:HD23	1.61	0.65
2:B:1391:LEU:HD23	2:B:1414:TRP:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1017:ASP:O	2:B:1083:ARG:NH1	2.30	0.64
2:B:1022:LYS:N	2:B:1022:LYS:HD2	2.12	0.64
1:A:482:ILE:HD11	1:A:486:LEU:CD1	2.28	0.64
1:A:497:THR:HG22	1:A:499:SER:H	1.62	0.64
2:B:1195:ILE:H	2:B:1195:ILE:CD1	1.89	0.64
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.38	0.64
1:A:20:LYS:HG3	1:A:20:LYS:O	1.98	0.64
1:A:459:THR:CG2	1:A:460:ASN:N	2.61	0.64
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.80	0.63
2:B:1013:LYS:CE	2:B:1086:ASP:H	2.09	0.63
1:A:511:ASP:C	1:A:512:LYS:HG3	2.16	0.63
2:B:1041:MET:HG2	2:B:1046:LYS:HE2	1.80	0.63
2:B:1236:PRO:HA	2:B:1239:TRP:CD2	2.34	0.63
1:A:406:TRP:CE3	2:B:1419:THR:HB	2.33	0.63
1:A:195:ILE:CD1	1:A:199:ARG:HH21	2.11	0.63
1:A:44:GLU:HB3	1:A:46:LYS:HD2	1.81	0.63
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.81	0.63
1:A:357:MET:C	1:A:359:GLY:H	2.01	0.63
1:A:489:SER:HB2	1:A:493:VAL:CG2	2.27	0.63
1:A:163:SER:O	1:A:167:ILE:CG2	2.46	0.63
1:A:441:TYR:O	1:A:548:VAL:HG21	1.99	0.63
2:B:1041:MET:HG2	2:B:1046:LYS:CE	2.28	0.63
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.99	0.63
1:A:458:VAL:CG2	1:A:548:VAL:CG2	2.70	0.62
1:A:221:HIS:C	1:A:223:LYS:N	2.52	0.62
1:A:260:LEU:HD13	1:A:264:LEU:HD22	1.79	0.62
1:A:136:ASN:O	1:A:138:GLU:HG2	1.99	0.62
1:A:195:ILE:CG2	1:A:196:GLY:H	2.13	0.62
1:A:107:THR:OG1	1:A:223:LYS:HG3	1.98	0.62
2:B:1420:PRO:HB2	2:B:1423:VAL:CG2	2.30	0.62
1:A:223:LYS:CG	1:A:224:GLU:N	2.62	0.62
1:A:273:GLY:O	1:A:309:ILE:CD1	2.48	0.62
1:A:330:GLN:HB2	1:A:338:THR:HG22	1.81	0.62
1:A:268:SER:O	1:A:351:THR:HG22	1.99	0.62
1:A:319:TYR:OH	1:A:385:LYS:CE	2.48	0.62
1:A:438:GLU:HG2	1:A:461:LYS:HD2	1.82	0.62
2:B:1363:ASN:OD1	2:B:1366:LYS:HB2	2.00	0.62
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.00	0.61
2:B:1326:ILE:CG2	2:B:1342:TYR:CZ	2.82	0.61
1:A:275:LYS:HD2	1:A:332:GLN:HE21	1.65	0.61
1:A:274:ILE:HD11	1:A:310:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HA	1:A:482:ILE:HG22	1.82	0.61
1:A:297:GLU:HA	1:A:300:GLU:CD	2.20	0.61
1:A:489:SER:CB	1:A:493:VAL:HG21	2.30	0.61
1:A:57:ASN:ND2	1:A:143:ARG:HH21	1.96	0.61
2:B:1183:TYR:CD2	2:B:1380:ILE:HD13	2.35	0.61
2:B:1115:TYR:OH	2:B:1157:PRO:HG3	2.01	0.61
1:A:368:LEU:HD11	1:A:391:LEU:HD13	1.83	0.61
1:A:482:ILE:CD1	1:A:486:LEU:CD1	2.79	0.60
2:B:1240:THR:CG2	2:B:1241:VAL:N	2.64	0.60
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.82	0.60
2:B:1275:LYS:O	2:B:1302:GLU:OE1	2.19	0.60
2:B:1271:TYR:O	2:B:1274:ILE:CD1	2.48	0.60
1:A:107:THR:HG21	1:A:202:ILE:CD1	2.31	0.60
1:A:451:LYS:O	1:A:471:ASN:HA	2.01	0.60
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.01	0.60
1:A:402:TRP:CD1	1:A:403:THR:N	2.70	0.60
2:B:1303:LEU:O	2:B:1307:ARG:HB2	2.02	0.60
1:A:412:PRO:HG3	2:B:1401:TRP:HZ2	1.67	0.60
2:B:1169:GLU:HB3	2:B:1170:PRO:CD	2.28	0.60
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.02	0.59
1:A:82:LYS:CB	1:A:82:LYS:NZ	2.65	0.59
2:B:1363:ASN:OD1	2:B:1366:LYS:N	2.32	0.59
1:A:458:VAL:HG22	1:A:548:VAL:HG23	1.81	0.59
1:A:260:LEU:CD1	1:A:279:LEU:HD13	2.32	0.59
1:A:281:LYS:O	1:A:283:LEU:N	2.35	0.59
1:A:106:VAL:HG11	3:A:1551:NNI:I15	2.72	0.59
1:A:96:HIS:CD2	1:A:98:ALA:H	2.17	0.59
1:A:225:PRO:HG3	1:A:236:PRO:HD3	1.84	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.59
1:A:64:LYS:HB2	1:A:71:TRP:CZ3	2.38	0.59
2:B:1065:LYS:O	2:B:1407:GLN:CG	2.51	0.59
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.38	0.59
1:A:225:PRO:HB2	1:A:226:PRO:CD	2.32	0.59
1:A:202:ILE:O	1:A:206:ARG:HG3	2.02	0.58
1:A:409:THR:O	2:B:1364:ASP:HB2	2.03	0.58
1:A:228:LEU:N	1:A:228:LEU:HD12	2.18	0.58
2:B:1073:LYS:NZ	2:B:1130:PHE:CZ	2.71	0.58
1:A:418:ASN:O	1:A:420:PRO:HD3	2.04	0.58
1:A:221:HIS:C	1:A:223:LYS:H	2.06	0.58
1:A:470:THR:HG22	1:A:471:ASN:ND2	2.18	0.58
1:A:225:PRO:HA	1:A:227:PHE:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LYS:HE2	1:A:413:GLU:OE1	2.03	0.58
2:B:1249:LYS:O	2:B:1250:ASP:HB3	2.03	0.58
1:A:23:GLN:HE22	1:A:60:VAL:HG12	1.67	0.58
1:A:32:LYS:O	1:A:36:GLU:HG3	2.04	0.58
2:B:1330:GLN:HG2	2:B:1338:THR:OG1	2.05	0.57
2:B:1151:GLN:O	2:B:1185:ASP:CG	2.43	0.57
1:A:57:ASN:ND2	1:A:143:ARG:NH2	2.49	0.57
1:A:354:TYR:C	1:A:354:TYR:CD2	2.78	0.57
2:B:1028:GLU:O	2:B:1032:LYS:HG2	2.04	0.57
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.39	0.57
2:B:1266:TRP:CE3	2:B:1426:TRP:HZ3	2.17	0.57
1:A:221:HIS:HB3	1:A:223:LYS:HB3	1.85	0.57
3:A:1551:NNI:O3	3:A:1551:NNI:C13	2.51	0.56
1:A:227:PHE:C	1:A:228:LEU:HD12	2.25	0.56
2:B:1258:GLN:O	2:B:1261:VAL:HG22	2.05	0.56
1:A:44:GLU:HB3	1:A:46:LYS:HD3	1.86	0.56
1:A:113:ASP:HB2	4:A:2004:HOH:O	2.04	0.56
1:A:433:PRO:HG3	2:B:1255:ASN:OD1	2.04	0.56
1:A:476:LYS:C	1:A:478:GLU:H	2.09	0.56
2:B:1391:LEU:CD2	2:B:1414:TRP:HB2	2.35	0.56
2:B:1270:ILE:HG13	2:B:1271:TYR:CD1	2.40	0.56
2:B:1361:HIS:O	2:B:1361:HIS:CG	2.59	0.56
1:A:162:SER:O	1:A:166:LYS:HG3	2.06	0.56
1:A:334:GLN:OE1	1:A:512:LYS:CD	2.52	0.56
1:A:223:LYS:HD3	1:A:224:GLU:CG	2.29	0.56
1:A:298:GLU:H	1:A:298:GLU:CD	2.07	0.56
1:A:428:GLN:NE2	1:A:428:GLN:HA	2.17	0.56
1:A:538:ALA:O	1:A:540:LYS:N	2.39	0.56
1:A:317:VAL:CG1	1:A:318:TYR:H	2.18	0.56
1:A:376:THR:O	1:A:380:ILE:HG12	2.06	0.56
1:A:495:ILE:HB	1:A:533:LEU:HD12	1.88	0.56
1:A:82:LYS:NZ	1:A:82:LYS:HB3	2.21	0.56
1:A:24:TRP:CZ2	1:A:59:PRO:HB3	2.41	0.56
1:A:447:ASN:ND2	1:A:449:GLU:H	2.04	0.56
1:A:206:ARG:NH2	1:A:216:THR:O	2.38	0.56
2:B:1270:ILE:O	2:B:1271:TYR:HB2	2.06	0.55
1:A:357:MET:O	1:A:359:GLY:N	2.38	0.55
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.41	0.55
2:B:1184:MET:O	2:B:1186:ASP:N	2.40	0.55
1:A:278:GLN:OE1	1:A:298:GLU:HB2	2.02	0.55
1:A:465:LYS:HG2	1:A:466:VAL:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1230:MET:HG2	2:B:1231:GLY:H	1.71	0.55
1:A:57:ASN:HA	1:A:129:ALA:O	2.06	0.55
1:A:334:GLN:OE1	1:A:512:LYS:HD3	2.05	0.55
2:B:1058:THR:CG2	2:B:1075:VAL:HG12	2.37	0.55
2:B:1303:LEU:HA	2:B:1306:ASN:HB2	1.89	0.55
1:A:206:ARG:HH21	1:A:216:THR:C	2.10	0.55
1:A:82:LYS:HB3	1:A:82:LYS:HZ3	1.72	0.55
2:B:1035:VAL:HG23	2:B:1036:GLU:N	2.21	0.55
2:B:1230:MET:HA	4:B:2010:HOH:O	2.07	0.55
2:B:1374:LYS:HE2	2:B:1378:GLU:OE2	2.07	0.55
1:A:402:TRP:HD1	1:A:403:THR:HG1	1.53	0.55
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.87	0.55
2:B:1270:ILE:HG23	2:B:1271:TYR:CD1	2.42	0.55
1:A:223:LYS:O	1:A:224:GLU:CB	2.55	0.55
1:A:494:ASN:N	1:A:494:ASN:OD1	2.40	0.55
1:A:431:LYS:HZ3	1:A:431:LYS:HB3	1.72	0.54
1:A:482:ILE:CD1	1:A:486:LEU:HD12	2.37	0.54
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.08	0.54
2:B:1378:GLU:O	2:B:1382:ILE:HG13	2.06	0.54
1:A:356:ARG:NH1	1:A:356:ARG:HB3	2.22	0.54
1:A:493:VAL:CG1	1:A:494:ASN:H	2.18	0.54
1:A:28:GLU:OE1	1:A:135:ILE:CG2	2.55	0.54
1:A:361:HIS:HD2	1:A:513:SER:OG	1.90	0.54
2:B:1326:ILE:HG21	2:B:1342:TYR:CE1	2.41	0.54
1:A:221:HIS:O	1:A:223:LYS:N	2.40	0.54
1:A:26:LEU:HD22	1:A:26:LEU:N	2.22	0.54
2:B:1237:ASP:OD2	2:B:1238:LYS:HD2	2.07	0.54
1:A:450:THR:HG21	1:A:452:LEU:CD2	2.38	0.54
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.22	0.54
2:B:1195:ILE:N	2:B:1195:ILE:CD1	2.57	0.54
1:A:447:ASN:HD22	1:A:448:ARG:N	2.06	0.54
2:B:1012:LEU:HD23	2:B:1013:LYS:N	2.23	0.53
1:A:245:VAL:HG22	1:A:247:PRO:HD3	1.89	0.53
1:A:25:PRO:HG3	1:A:137:ASN:CG	2.29	0.53
1:A:281:LYS:O	1:A:284:ARG:N	2.33	0.53
1:A:479:LEU:HA	1:A:482:ILE:CG2	2.38	0.53
2:B:1317:VAL:HG22	2:B:1347:LYS:HB3	1.89	0.53
1:A:178:ILE:HD11	1:A:201:LYS:CG	2.38	0.53
1:A:450:THR:HB	1:A:452:LEU:HD22	1.80	0.53
2:B:1065:LYS:NZ	2:B:1065:LYS:HB2	2.23	0.53
2:B:1240:THR:HG22	2:B:1241:VAL:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1253:THR:H	2:B:1256:ASP:HB2	1.72	0.53
1:A:108:VAL:CG1	1:A:223:LYS:HA	2.39	0.53
2:B:1244:ILE:CD1	2:B:1244:ILE:H	2.21	0.53
1:A:267:ALA:O	1:A:269:GLN:N	2.42	0.53
1:A:418:ASN:HD22	1:A:418:ASN:C	2.11	0.53
2:B:1239:TRP:CH2	2:B:1378:GLU:HG2	2.44	0.53
1:A:210:LEU:CD1	1:A:215:THR:HG22	2.38	0.53
1:A:229:TRP:CE3	3:A:1551:NNI:H4	2.44	0.52
1:A:467:VAL:O	1:A:467:VAL:HG23	2.08	0.52
2:B:1047:ILE:HD12	2:B:1144:TYR:CD2	2.44	0.52
1:A:319:TYR:OH	1:A:385:LYS:HE3	2.09	0.52
1:A:20:LYS:CG	1:A:20:LYS:O	2.56	0.52
1:A:517:LEU:C	1:A:517:LEU:HD13	2.29	0.52
1:A:51:GLY:O	1:A:52:PRO:O	2.28	0.52
2:B:1242:GLN:HB2	2:B:1352:GLY:HA2	1.91	0.52
1:A:219:LYS:HG3	1:A:219:LYS:O	2.10	0.52
1:A:288:ALA:CB	1:A:291:GLU:OE1	2.57	0.52
2:B:1012:LEU:CD2	2:B:1016:MET:HB2	2.39	0.52
1:A:13:LYS:HB3	1:A:14:PRO:CD	2.36	0.52
2:B:1045:GLY:O	2:B:1147:ASN:OD1	2.27	0.52
1:A:113:ASP:O	1:A:117:SER:OG	2.19	0.52
1:A:222:GLN:O	1:A:223:LYS:O	2.28	0.52
1:A:64:LYS:HB2	1:A:71:TRP:CE3	2.45	0.52
1:A:460:ASN:HA	2:B:1286:THR:O	2.09	0.52
2:B:1101:LYS:O	2:B:1101:LYS:HG2	2.10	0.52
2:B:1320:ASP:OD1	2:B:1320:ASP:C	2.48	0.52
1:A:111:VAL:HG11	1:A:214:LEU:HD12	1.90	0.52
2:B:1309:ILE:HG22	2:B:1310:LEU:H	1.75	0.52
1:A:245:VAL:O	1:A:246:LEU:HD23	2.10	0.52
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.40	0.52
1:A:278:GLN:HA	1:A:278:GLN:NE2	2.22	0.51
2:B:1118:VAL:HB	2:B:1149:LEU:HD11	1.90	0.51
1:A:179:VAL:CG1	3:A:1551:NNI:H9C2	2.40	0.51
2:B:1033:ALA:O	2:B:1037:ILE:HD13	2.10	0.51
1:A:179:VAL:HG11	3:A:1551:NNI:H102	1.93	0.51
1:A:517:LEU:CD1	1:A:517:LEU:C	2.78	0.51
2:B:1151:GLN:O	2:B:1185:ASP:OD1	2.29	0.51
2:B:1276:VAL:HG22	2:B:1276:VAL:O	2.11	0.51
1:A:50:ILE:CG2	1:A:143:ARG:HB3	2.39	0.51
2:B:1337:TRP:HE1	2:B:1367:GLN:NE2	2.08	0.51
1:A:194:GLU:N	1:A:194:GLU:CD	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1282:LEU:CD2	2:B:1295:LEU:HA	2.40	0.51
1:A:302:GLU:HA	1:A:305:GLU:HG2	1.93	0.51
1:A:410:TRP:CE3	2:B:1363:ASN:CB	2.93	0.51
1:A:369:THR:HG21	1:A:409:THR:HG21	1.92	0.51
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.41	0.51
1:A:439:THR:HG23	2:B:1289:LEU:HD23	1.93	0.51
1:A:457:TYR:CD2	1:A:457:TYR:C	2.84	0.51
1:A:17:ASP:O	1:A:83:ARG:HD3	2.10	0.51
2:B:1309:ILE:O	2:B:1310:LEU:CB	2.58	0.51
1:A:50:ILE:HG22	1:A:143:ARG:HB3	1.92	0.51
1:A:227:PHE:CD1	3:A:1551:NNI:I15	3.34	0.50
1:A:328:GLU:HG3	1:A:330:GLN:NE2	2.25	0.50
1:A:43:LYS:NZ	1:A:43:LYS:HB3	2.25	0.50
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.92	0.50
1:A:353:LYS:O	1:A:374:LYS:NZ	2.44	0.50
1:A:179:VAL:HG11	3:A:1551:NNI:C10	2.41	0.50
1:A:469:LEU:CD2	1:A:480:GLN:HG2	2.32	0.50
1:A:394:GLN:O	1:A:397:THR:HG23	2.12	0.50
2:B:1324:ASP:OD1	2:B:1324:ASP:N	2.30	0.50
2:B:1333:GLY:O	2:B:1334:GLN:HB2	2.11	0.50
1:A:351:THR:CG2	1:A:352:GLY:N	2.74	0.50
1:A:24:TRP:HZ3	1:A:61:PHE:HB3	1.76	0.50
2:B:1317:VAL:CG1	2:B:1349:LEU:HD13	2.42	0.50
1:A:104:LYS:HZ2	1:A:194:GLU:HA	1.76	0.50
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.92	0.50
2:B:1337:TRP:HE1	2:B:1367:GLN:HE21	1.58	0.50
1:A:482:ILE:CD1	1:A:482:ILE:C	2.80	0.49
2:B:1296:THR:HG22	2:B:1298:GLU:H	1.77	0.49
1:A:194:GLU:O	1:A:195:ILE:C	2.50	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.93	0.49
1:A:228:LEU:CD1	1:A:228:LEU:N	2.75	0.49
2:B:1107:THR:CG2	4:B:2010:HOH:O	2.60	0.49
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.74	0.49
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.31	0.49
1:A:78:ARG:O	1:A:81:ASN:HB2	2.13	0.49
1:A:302:GLU:HA	1:A:305:GLU:CD	2.33	0.49
1:A:433:PRO:CG	2:B:1255:ASN:OD1	2.60	0.49
1:A:538:ALA:O	1:A:539:HIS:C	2.51	0.49
2:B:1277:ARG:HG3	2:B:1281:LYS:HE3	1.94	0.49
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.94	0.49
1:A:450:THR:CB	1:A:452:LEU:CD2	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1076:ASP:CG	2:B:1078:ARG:HE	2.16	0.49
1:A:317:VAL:HG12	1:A:318:TYR:O	2.13	0.49
1:A:50:ILE:HG12	1:A:54:ASN:HD22	1.74	0.49
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.48	0.49
2:B:1130:PHE:CZ	2:B:1144:TYR:HB2	2.48	0.49
2:B:1178:ILE:HD13	2:B:1191:SER:HB3	1.95	0.49
1:A:216:THR:HB	1:A:217:PRO:HD2	1.94	0.49
1:A:257:ILE:HD11	1:A:279:LEU:O	2.13	0.49
1:A:100:LEU:O	1:A:318:TYR:HB3	2.12	0.49
1:A:445:ALA:O	1:A:446:ALA:HB2	2.12	0.49
1:A:107:THR:HA	1:A:223:LYS:HG3	1.94	0.48
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.35	0.48
2:B:1275:LYS:HE2	2:B:1277:ARG:HH21	1.78	0.48
1:A:336:GLN:NE2	1:A:355:ALA:HB1	2.28	0.48
2:B:1116:PHE:HB2	4:B:2012:HOH:O	2.13	0.48
2:B:1102:LYS:O	2:B:1237:ASP:HB2	2.13	0.48
2:B:1418:ASN:O	2:B:1419:THR:C	2.52	0.48
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.95	0.48
1:A:220:LYS:O	1:A:221:HIS:C	2.49	0.48
1:A:267:ALA:C	1:A:269:GLN:N	2.66	0.48
2:B:1332:GLN:OE1	2:B:1332:GLN:HA	2.14	0.48
1:A:263:LYS:HD3	1:A:263:LYS:HA	1.68	0.48
2:B:1064:LYS:O	2:B:1065:LYS:HB2	2.10	0.48
2:B:1022:LYS:H	2:B:1022:LYS:HD2	1.78	0.48
2:B:1058:THR:HG21	2:B:1075:VAL:HG12	1.94	0.48
2:B:1266:TRP:CD2	2:B:1426:TRP:CE3	3.02	0.48
2:B:1308:GLU:O	2:B:1311:LYS:HG2	2.14	0.48
1:A:475:GLN:O	1:A:478:GLU:HB2	2.13	0.48
2:B:1115:TYR:HB3	2:B:1149:LEU:CB	2.43	0.48
1:A:111:VAL:HG13	1:A:214:LEU:HD12	1.96	0.48
1:A:275:LYS:CD	1:A:332:GLN:NE2	2.76	0.48
1:A:330:GLN:HB2	1:A:338:THR:CG2	2.43	0.48
1:A:431:LYS:HB3	1:A:431:LYS:HZ2	1.75	0.48
1:A:503:LEU:HD12	1:A:533:LEU:HD23	1.95	0.48
2:B:1037:ILE:HG22	2:B:1038:CYS:N	2.29	0.48
1:A:224:GLU:HA	1:A:225:PRO:HD2	1.73	0.47
1:A:402:TRP:HD1	1:A:403:THR:N	2.11	0.47
1:A:351:THR:HG23	1:A:352:GLY:N	2.28	0.47
1:A:459:THR:CG2	1:A:460:ASN:H	2.27	0.47
2:B:1076:ASP:OD2	2:B:1078:ARG:HB2	2.13	0.47
2:B:1286:THR:OG1	2:B:1287:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.30	0.47
2:B:1070:LYS:HB2	2:B:1070:LYS:NZ	2.29	0.47
2:B:1270:ILE:HG23	2:B:1271:TYR:HD1	1.79	0.47
2:B:1428:GLN:CD	2:B:1428:GLN:C	2.69	0.47
1:A:169:GLU:N	1:A:170:PRO:CD	2.78	0.47
1:A:288:ALA:HB3	1:A:291:GLU:CD	2.33	0.47
1:A:399:GLU:HA	1:A:402:TRP:HB3	1.96	0.47
1:A:225:PRO:HB2	1:A:226:PRO:HD2	1.95	0.47
1:A:480:GLN:NE2	1:A:517:LEU:HD21	2.29	0.47
2:B:1018:GLY:CA	2:B:1056:TYR:CE1	2.96	0.47
2:B:1254:VAL:O	2:B:1257:ILE:HG23	2.14	0.47
1:A:108:VAL:HG12	1:A:223:LYS:HA	1.96	0.47
1:A:109:LEU:CD1	1:A:205:LEU:HD23	2.44	0.47
1:A:358:ARG:HH11	1:A:358:ARG:HB2	1.80	0.47
2:B:1090:VAL:HG12	2:B:1090:VAL:O	2.13	0.47
1:A:336:GLN:OE1	1:A:355:ALA:HB1	2.12	0.47
1:A:482:ILE:HD13	1:A:486:LEU:HD12	1.96	0.47
2:B:1389:PHE:O	2:B:1415:GLU:N	2.45	0.47
1:A:354:TYR:OH	1:A:370:GLU:OE2	2.32	0.47
1:A:402:TRP:HD1	1:A:403:THR:OG1	1.97	0.47
2:B:1011:LYS:HD2	2:B:1011:LYS:O	2.15	0.47
1:A:227:PHE:CE1	3:A:1551:NNI:I15	3.38	0.47
1:A:240:THR:HB	1:A:315:HIS:HA	1.97	0.47
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.15	0.47
1:A:357:MET:C	1:A:359:GLY:N	2.68	0.47
1:A:107:THR:HG22	1:A:189:VAL:HB	1.97	0.47
1:A:296:THR:C	1:A:300:GLU:HG3	2.26	0.47
2:B:1013:LYS:HE2	2:B:1086:ASP:N	2.19	0.47
2:B:1296:THR:O	2:B:1299:ALA:HB3	2.15	0.47
2:B:1422:LEU:HB3	2:B:1426:TRP:CH2	2.50	0.47
1:A:167:ILE:O	1:A:208:HIS:HE1	1.98	0.47
1:A:216:THR:HB	1:A:217:PRO:CD	2.45	0.47
1:A:225:PRO:CB	1:A:226:PRO:CD	2.93	0.47
2:B:1147:ASN:O	2:B:1148:VAL:HG13	2.15	0.47
1:A:418:ASN:HD22	1:A:420:PRO:HD3	1.79	0.46
2:B:1326:ILE:HG23	2:B:1327:ALA:N	2.29	0.46
2:B:1420:PRO:HA	2:B:1421:PRO:HD3	1.81	0.46
1:A:223:LYS:NZ	1:A:224:GLU:HG2	2.30	0.46
2:B:1081:ASN:ND2	2:B:1153:TRP:HD1	2.13	0.46
2:B:1035:VAL:CG2	2:B:1036:GLU:N	2.79	0.46
2:B:1175:ASN:HB3	2:B:1178:ILE:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1194:GLU:HB2	2:B:1197:GLN:OE1	2.14	0.46
2:B:1028:GLU:HB2	2:B:1135:ILE:HD11	1.97	0.46
1:A:529:GLU:O	1:A:530:LYS:HG3	2.16	0.46
2:B:1277:ARG:O	2:B:1281:LYS:HG3	2.15	0.46
1:A:142:ILE:HG22	1:A:144:TYR:CE2	2.50	0.46
1:A:368:LEU:CD1	1:A:391:LEU:HD13	2.46	0.46
1:A:43:LYS:HZ2	1:A:43:LYS:HB3	1.79	0.46
2:B:1042:GLU:HG3	2:B:1043:LYS:N	2.30	0.46
1:A:410:TRP:CE3	2:B:1363:ASN:HB2	2.50	0.46
2:B:1419:THR:HA	2:B:1420:PRO:HD2	1.77	0.46
1:A:195:ILE:HD11	1:A:199:ARG:HH21	1.80	0.46
2:B:1092:LEU:HB2	2:B:1158:ALA:HB1	1.98	0.46
1:A:107:THR:HA	1:A:223:LYS:CG	2.46	0.46
1:A:90:VAL:HG12	1:A:90:VAL:O	2.16	0.46
1:A:125:ARG:HD3	1:A:147:ASN:HD22	1.81	0.45
1:A:302:GLU:HA	1:A:305:GLU:CG	2.46	0.45
1:A:96:HIS:H	2:B:1136:ASN:ND2	2.07	0.45
2:B:1058:THR:HG23	2:B:1059:PRO:HD2	1.98	0.45
1:A:206:ARG:NE	1:A:216:THR:OG1	2.50	0.45
1:A:281:LYS:C	1:A:283:LEU:N	2.69	0.45
2:B:1334:GLN:HA	2:B:1334:GLN:HE21	1.81	0.45
1:A:26:LEU:HD23	1:A:133:PRO:CD	2.46	0.45
1:A:480:GLN:O	1:A:483:TYR:HB3	2.17	0.45
1:A:51:GLY:O	1:A:52:PRO:C	2.55	0.45
2:B:1028:GLU:CB	2:B:1135:ILE:HD11	2.47	0.45
2:B:1027:THR:O	2:B:1031:ILE:HG13	2.16	0.45
2:B:1261:VAL:HB	2:B:1276:VAL:HG21	1.98	0.45
2:B:1323:LYS:HG2	2:B:1343:GLN:HB3	1.98	0.45
2:B:1063:ILE:HD13	2:B:1074:LEU:HD22	1.98	0.45
2:B:1270:ILE:O	2:B:1271:TYR:CB	2.64	0.45
2:B:1263:LYS:HA	2:B:1426:TRP:CD1	2.52	0.45
1:A:171:PHE:C	1:A:171:PHE:CD2	2.90	0.45
1:A:177:ASP:N	1:A:177:ASP:OD2	2.49	0.45
1:A:245:VAL:HG22	1:A:246:LEU:N	2.31	0.45
1:A:402:TRP:CD1	1:A:402:TRP:C	2.90	0.45
1:A:470:THR:O	1:A:471:ASN:HB2	2.17	0.44
1:A:28:GLU:OE1	1:A:135:ILE:HG23	2.17	0.44
1:A:503:LEU:HG	1:A:507:GLN:HE21	1.79	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.44
1:A:425:LEU:H	1:A:425:LEU:HD22	1.82	0.44
1:A:408:ALA:HB1	2:B:1364:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.99	0.44
1:A:405:TYR:CE1	1:A:407:GLN:HB3	2.53	0.44
1:A:89:GLU:OE1	1:A:91:GLN:NE2	2.43	0.44
2:B:1236:PRO:HA	2:B:1239:TRP:CE2	2.53	0.44
2:B:1012:LEU:O	2:B:1013:LYS:C	2.54	0.44
2:B:1293:ILE:HG13	2:B:1293:ILE:O	2.18	0.44
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.32	0.44
2:B:1334:GLN:HE21	2:B:1334:GLN:CA	2.30	0.44
1:A:356:ARG:C	1:A:357:MET:HG3	2.38	0.44
1:A:476:LYS:O	1:A:478:GLU:N	2.51	0.44
1:A:25:PRO:CG	1:A:137:ASN:HD21	2.30	0.43
2:B:1090:VAL:CG1	2:B:1090:VAL:O	2.66	0.43
1:A:295:LEU:HD23	1:A:299:ALA:HB3	1.99	0.43
2:B:1078:ARG:HD2	2:B:1411:ILE:O	2.18	0.43
2:B:1257:ILE:O	2:B:1261:VAL:HG13	2.17	0.43
2:B:1257:ILE:HD11	2:B:1279:LEU:HD12	2.00	0.43
1:A:109:LEU:HD23	1:A:221:HIS:CD2	2.54	0.43
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.43
2:B:1037:ILE:HG21	2:B:1073:LYS:HB2	2.00	0.43
2:B:1266:TRP:CZ2	2:B:1346:PHE:CZ	3.06	0.43
1:A:195:ILE:HG12	1:A:199:ARG:NH2	2.32	0.43
1:A:239:TRP:O	1:A:316:GLY:N	2.51	0.43
1:A:542:ILE:O	1:A:543:GLY:C	2.56	0.43
2:B:1184:MET:C	2:B:1186:ASP:H	2.22	0.43
2:B:1374:LYS:CE	2:B:1378:GLU:OE2	2.67	0.43
1:A:77:PHE:O	1:A:78:ARG:C	2.56	0.43
1:A:439:THR:CG2	2:B:1289:LEU:HD23	2.48	0.43
2:B:1420:PRO:CG	2:B:1423:VAL:HG21	2.49	0.43
1:A:281:LYS:C	1:A:283:LEU:H	2.21	0.43
1:A:358:ARG:CZ	1:A:358:ARG:HB2	2.48	0.43
2:B:1013:LYS:NZ	2:B:1085:GLN:HB3	2.33	0.43
2:B:1157:PRO:O	2:B:1161:GLN:HG3	2.18	0.43
1:A:13:LYS:CB	1:A:14:PRO:HD2	2.32	0.43
1:A:395:LYS:O	1:A:399:GLU:HG2	2.19	0.43
2:B:1428:GLN:OXT	2:B:1428:GLN:NE2	2.46	0.43
2:B:1312:GLU:OE2	2:B:1312:GLU:HA	2.18	0.43
1:A:49:LYS:HE2	1:A:142:ILE:HG23	2.01	0.43
2:B:1168:LEU:O	2:B:1169:GLU:C	2.57	0.43
2:B:1194:GLU:O	2:B:1195:ILE:C	2.57	0.43
1:A:363:ASN:O	1:A:364:ASP:C	2.57	0.42
2:B:1373:GLN:HB2	2:B:1373:GLN:HE21	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:C	1:A:136:ASN:N	2.52	0.42
1:A:135:ILE:CG2	1:A:135:ILE:O	2.65	0.42
1:A:142:ILE:CG2	1:A:144:TYR:CE2	3.02	0.42
1:A:450:THR:HG22	1:A:450:THR:O	2.18	0.42
1:A:60:VAL:HG23	1:A:75:VAL:HG22	2.00	0.42
1:A:356:ARG:HB3	1:A:358:ARG:HH12	1.84	0.42
2:B:1255:ASN:HB2	2:B:1289:LEU:CD1	2.38	0.42
1:A:270:ILE:HG13	1:A:270:ILE:O	2.19	0.42
2:B:1112:GLY:O	2:B:1114:ALA:N	2.47	0.42
1:A:122:GLU:CA	1:A:125:ARG:HG3	2.43	0.42
1:A:466:VAL:O	1:A:466:VAL:HG12	2.18	0.42
1:A:511:ASP:C	1:A:511:ASP:OD2	2.57	0.42
2:B:1011:LYS:HD2	2:B:1011:LYS:C	2.39	0.42
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.42
2:B:1047:ILE:HG22	2:B:1146:TYR:HA	2.00	0.42
1:A:435:VAL:HG22	2:B:1290:THR:HG21	2.00	0.42
2:B:1304:ALA:O	2:B:1307:ARG:HB3	2.19	0.42
2:B:1388:LYS:HB2	2:B:1388:LYS:HE3	1.86	0.42
1:A:129:ALA:HA	1:A:144:TYR:O	2.19	0.42
1:A:336:GLN:HE22	1:A:355:ALA:HB1	1.85	0.42
1:A:455:ALA:HB3	1:A:469:LEU:HD11	2.02	0.42
1:A:63:ILE:CG2	1:A:72:ARG:HG3	2.50	0.42
1:A:479:LEU:CA	1:A:482:ILE:HG22	2.48	0.42
2:B:1295:LEU:HD13	2:B:1300:GLU:OE2	2.20	0.42
1:A:240:THR:CG2	1:A:315:HIS:CD2	3.03	0.42
2:B:1260:LEU:HD13	2:B:1260:LEU:C	2.39	0.42
2:B:1336:GLN:HB3	2:B:1336:GLN:HE21	1.64	0.42
2:B:1325:LEU:HD23	2:B:1343:GLN:HG3	2.02	0.42
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.50	0.42
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.34	0.42
1:A:458:VAL:HG11	1:A:547:GLN:HG3	2.01	0.42
2:B:1169:GLU:CB	2:B:1170:PRO:HD3	2.28	0.42
2:B:1326:ILE:CG2	2:B:1327:ALA:N	2.81	0.42
1:A:24:TRP:O	1:A:25:PRO:C	2.57	0.41
1:A:452:LEU:HD23	1:A:452:LEU:O	2.20	0.41
2:B:1024:TRP:O	2:B:1026:LEU:HD13	2.19	0.41
2:B:1081:ASN:ND2	2:B:1153:TRP:CD1	2.88	0.41
2:B:1260:LEU:HD13	2:B:1264:LEU:CD1	2.48	0.41
1:A:106:VAL:HG21	3:A:1551:NNI:I15	2.90	0.41
1:A:195:ILE:HG12	1:A:199:ARG:NE	2.34	0.41
1:A:220:LYS:O	1:A:222:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1206:ARG:CA	2:B:1206:ARG:HE	2.32	0.41
1:A:131:THR:CG2	1:A:143:ARG:HE	2.28	0.41
1:A:308:GLU:O	1:A:311:LYS:CB	2.68	0.41
1:A:28:GLU:OE1	1:A:135:ILE:HG21	2.19	0.41
2:B:1099:GLY:HA3	4:B:2009:HOH:O	2.19	0.41
1:A:521:ILE:O	1:A:525:LEU:HG	2.20	0.41
1:A:125:ARG:HH11	1:A:147:ASN:ND2	2.19	0.41
1:A:410:TRP:CZ3	2:B:1363:ASN:HB3	2.55	0.41
2:B:1167:ILE:HG12	2:B:1212:TRP:CD2	2.56	0.41
1:A:59:PRO:HB2	1:A:76:ASP:HB3	2.03	0.41
2:B:1274:ILE:HD12	2:B:1274:ILE:N	2.35	0.41
2:B:1320:ASP:HA	2:B:1321:PRO:HD3	1.87	0.41
2:B:1366:LYS:HG2	2:B:1405:TYR:CD1	2.56	0.41
1:A:308:GLU:O	1:A:311:LYS:HB2	2.20	0.41
1:A:425:LEU:N	1:A:425:LEU:HD22	2.36	0.41
2:B:1118:VAL:HA	2:B:1119:PRO:HD3	1.86	0.41
2:B:1390:LYS:HD3	2:B:1417:VAL:HG11	2.03	0.41
1:A:20:LYS:HD2	1:A:20:LYS:C	2.41	0.41
1:A:25:PRO:HG3	1:A:137:ASN:ND2	2.36	0.41
1:A:217:PRO:O	1:A:221:HIS:CD2	2.74	0.41
1:A:431:LYS:HE3	4:A:2014:HOH:O	2.20	0.41
1:A:43:LYS:NZ	1:A:44:GLU:OE2	2.54	0.41
1:A:46:LYS:HD2	1:A:46:LYS:N	2.36	0.41
1:A:85:GLN:NE2	2:B:1053:GLU:O	2.50	0.41
2:B:1296:THR:O	2:B:1299:ALA:CB	2.69	0.41
2:B:1263:LYS:CA	2:B:1426:TRP:CD1	3.03	0.41
1:A:195:ILE:HG22	1:A:196:GLY:H	1.84	0.40
1:A:244:ILE:O	1:A:244:ILE:HG23	2.21	0.40
1:A:274:ILE:HD11	1:A:310:LEU:CD1	2.50	0.40
1:A:277:ARG:HB3	1:A:277:ARG:NH1	2.36	0.40
2:B:1307:ARG:O	2:B:1309:ILE:O	2.39	0.40
2:B:1249:LYS:O	2:B:1250:ASP:CB	2.67	0.40
1:A:107:THR:OG1	1:A:223:LYS:CG	2.66	0.40
1:A:227:PHE:HD1	3:A:1551:NNI:I15	2.74	0.40
1:A:320:ASP:C	1:A:320:ASP:OD2	2.60	0.40
1:A:357:MET:N	1:A:357:MET:HE2	2.36	0.40
2:B:1317:VAL:CG2	2:B:1347:LYS:HB3	2.50	0.40
1:A:447:ASN:HB3	1:A:450:THR:HB	2.04	0.40
2:B:1017:ASP:O	2:B:1018:GLY:O	2.39	0.40
2:B:1012:LEU:HD22	2:B:1016:MET:O	2.22	0.40
2:B:1379:SER:CB	2:B:1387:PRO:HD3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	541/557 (97%)	465 (86%)	54 (10%)	22 (4%)	3 8
2	B	385/428 (90%)	329 (86%)	46 (12%)	10 (3%)	5 17
All	All	926/985 (94%)	794 (86%)	100 (11%)	32 (4%)	3 11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	135	ILE
1	A	136	ASN
1	A	195	ILE
1	A	223	LYS
1	A	225	PRO
1	A	226	PRO
1	A	466	VAL
1	A	539	HIS
2	B	1184	MET
2	B	1195	ILE
2	B	1250	ASP
1	A	14	PRO
1	A	218	ASP
1	A	221	HIS
1	A	222	GLN
1	A	268	SER
1	A	282	LEU
1	A	477	THR
1	A	140	PRO
2	B	1018	GLY
2	B	1237	ASP

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Mol	Chain	Res	Type
2	B	1252	TRP
1	A	224	GLU
1	A	358	ARG
1	A	446	ALA
2	B	1302	GLU
1	A	345	PRO
2	B	1346	PHE
2	B	1113	ASP
2	B	1185	ASP
1	A	25	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	486/497 (98%)	438 (90%)	48 (10%)	8 22
2	B	361/390 (93%)	331 (92%)	30 (8%)	11 31
All	All	847/887 (96%)	769 (91%)	78 (9%)	9 26

All (78) 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	29	GLU
1	A	34	LEU
1	A	44	GLU
1	A	46	LYS
1	A	107	THR
1	A	108	VAL
1	A	123	ASP
1	A	126	LYS
1	A	167	ILE
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	194	GLU
1	A	211	ARG
1	A	223	LYS
1	A	242	GLN
1	A	246	LEU
1	A	257	ILE
1	A	258	GLN
1	A	260	LEU
1	A	264	LEU
1	A	278	GLN
1	A	284	ARG
1	A	295	LEU
1	A	298	GLU
1	A	309	ILE
1	A	351	THR
1	A	354	TYR
1	A	357	MET
1	A	358	ARG
1	A	377	THR
1	A	381	VAL
1	A	386	THR
1	A	397	THR
1	A	402	TRP
1	A	404	GLU
1	A	409	THR
1	A	418	ASN
1	A	424	LYS
1	A	428	GLN
1	A	447	ASN
1	A	452	LEU
1	A	477	THR
1	A	482	ILE
1	A	494	ASN
1	A	497	THR
1	A	517	LEU
2	B	1011	LYS
2	B	1026	LEU
2	B	1070	LYS
2	B	1078	ARG
2	B	1080	LEU
2	B	1086	ASP
2	B	1101	LYS

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Mol	Chain	Res	Type
2	B	1189	VAL
2	B	1195	ILE
2	B	1206	ARG
2	B	1212	TRP
2	B	1232	TYR
2	B	1237	ASP
2	B	1245	VAL
2	B	1252	TRP
2	B	1259	LYS
2	B	1279	LEU
2	B	1289	LEU
2	B	1295	LEU
2	B	1303	LEU
2	B	1324	ASP
2	B	1330	GLN
2	B	1334	GLN
2	B	1349	LEU
2	B	1366	LYS
2	B	1373	GLN
2	B	1374	LYS
2	B	1391	LEU
2	B	1403	THR
2	B	1428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	96	HIS
1	A	136	ASN
1	A	147	ASN
1	A	151	GLN
1	A	161	GLN
1	A	208	HIS
1	A	242	GLN
1	A	255	ASN
1	A	269	GLN
1	A	278	GLN
1	A	315	HIS
1	A	332	GLN
1	A	340	GLN

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Mol	Chain	Res	Type
1	A	361	HIS
1	A	367	GLN
1	A	418	ASN
1	A	428	GLN
1	A	447	ASN
1	A	464	GLN
1	A	471	ASN
1	A	507	GLN
1	A	520	GLN
1	A	524	GLN
2	B	1081	ASN
2	B	1136	ASN
2	B	1147	ASN
2	B	1151	GLN
2	B	1182	GLN
2	B	1265	ASN
2	B	1269	GLN
2	B	1334	GLN
2	B	1336	GLN
2	B	1340	GLN
2	B	1367	GLN
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	NNI	A	1551	-	26,26,26	2.42	6 (23%)	36,36,36	2.89	12 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NNI	A	1551	-	-	0/10/26/26	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	NNI	C2-C8	-5.97	1.39	1.48
3	A	1551	NNI	C1-C7	-5.78	1.39	1.48
3	A	1551	NNI	C7-N1	-5.36	1.33	1.39
3	A	1551	NNI	C8-N1	-5.12	1.33	1.39
3	A	1551	NNI	C12-N2	-4.03	1.33	1.41
3	A	1551	NNI	O3-C11	2.58	1.36	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1551	NNI	C10-O3-C11	-9.85	111.10	119.11
3	A	1551	NNI	O3-C11-S1	-7.67	119.86	125.10
3	A	1551	NNI	C2-C8-N1	5.00	109.43	105.88
3	A	1551	NNI	C1-C7-N1	4.88	109.34	105.88
3	A	1551	NNI	O3-C11-N2	4.32	120.99	111.94
3	A	1551	NNI	C12-N2-C11	-3.94	122.95	130.00
3	A	1551	NNI	C7-N1-C8	-3.92	108.83	112.03
3	A	1551	NNI	C6-C1-C7	2.44	133.62	129.63
3	A	1551	NNI	C1-C2-C8	-2.40	106.18	108.26
3	A	1551	NNI	C2-C1-C7	-2.36	106.21	108.26
3	A	1551	NNI	C3-C2-C8	2.19	133.21	129.63
3	A	1551	NNI	O2-C8-C2	-2.14	124.51	128.68

There are no chirality outliers.

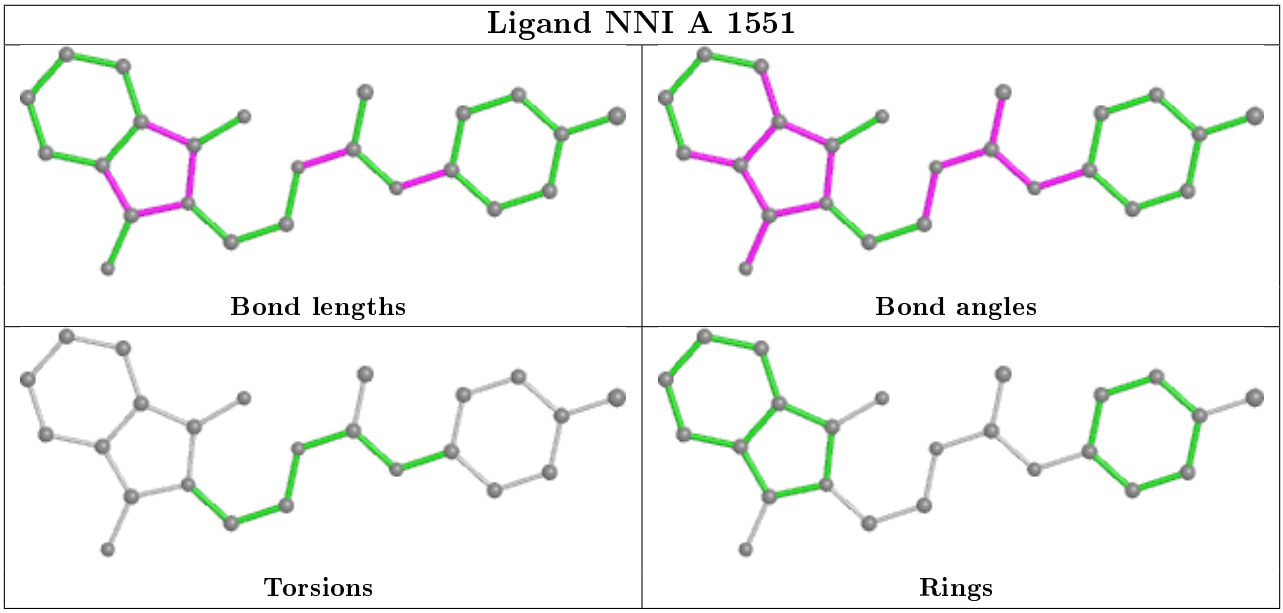
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	NNI	11	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 then 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	545/557 (97%)	0.42	35 (6%) 19 12	33, 54, 78, 89	0
2	B	395/428 (92%)	0.36	36 (9%) 9 5	31, 51, 87, 95	0
All	All	940/985 (95%)	0.39	71 (7%) 13 7	31, 53, 85, 95	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	ASN	7.7
1	A	551	LEU	7.5
2	B	1231	GLY	5.5
2	B	1090	VAL	5.3
2	B	1248	GLU	5.1
2	B	1162	SER	5.0
2	B	1240	THR	4.4
1	A	286	THR	4.1
1	A	52	PRO	3.7
1	A	138	GLU	3.7
2	B	1362	THR	3.7
1	A	128	THR	3.6
2	B	1015	GLY	3.5
2	B	1093	GLY	3.5
1	A	514	GLU	3.4
1	A	301	LEU	3.3
2	B	1250	ASP	3.3
2	B	1322	SER	3.2
2	B	1251	SER	3.2
1	A	223	LYS	3.1
2	B	1095	PRO	3.1
2	B	1361	HIS	3.1
2	B	1241	VAL	3.0
1	A	451	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLY	3.0
1	A	22	LYS	3.0
2	B	1230	MET	3.0
1	A	122	GLU	2.9
2	B	1238	LYS	2.9
2	B	1249	LYS	2.8
1	A	520	GLN	2.7
1	A	76	ASP	2.7
1	A	218	ASP	2.7
1	A	298	GLU	2.6
1	A	357	MET	2.6
2	B	1423	VAL	2.6
2	B	1153	TRP	2.6
1	A	294	PRO	2.6
1	A	360	ALA	2.6
1	A	473	THR	2.5
2	B	1232	TYR	2.5
1	A	550	LYS	2.5
2	B	1426	TRP	2.5
1	A	545	ASN	2.5
2	B	1298	GLU	2.5
2	B	1329	ILE	2.5
1	A	120	LEU	2.5
1	A	482	ILE	2.5
2	B	1005	ILE	2.4
1	A	245	VAL	2.4
2	B	1070	LYS	2.4
2	B	1043	LYS	2.4
1	A	297	GLU	2.3
2	B	1006	GLU	2.3
1	A	278	GLN	2.3
1	A	220	LYS	2.2
2	B	1205	LEU	2.2
2	B	1310	LEU	2.2
1	A	247	PRO	2.2
1	A	472	THR	2.2
2	B	1264	LEU	2.1
2	B	1281	LYS	2.1
2	B	1355	ALA	2.1
2	B	1189	VAL	2.1
1	A	75	VAL	2.1
1	A	39	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	6	GLU	2.1
2	B	1086	ASP	2.0
1	A	358	ARG	2.0
2	B	1165	THR	2.0
2	B	1085	GLN	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)

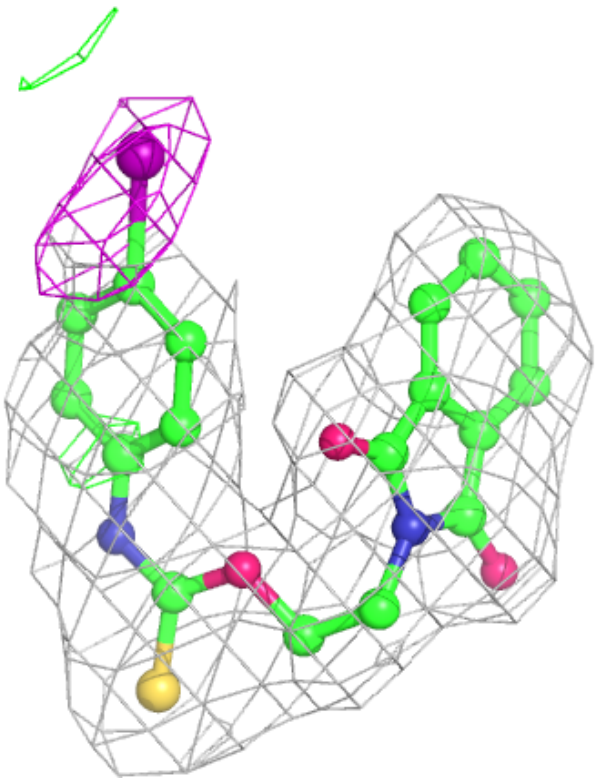
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

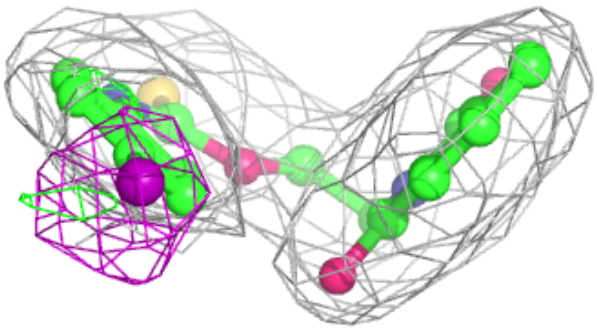
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NNI	A	1551	24/24	0.95	0.20	37,40,72,81	0

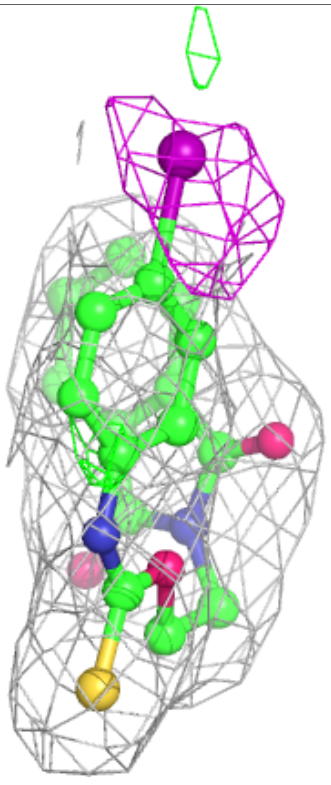
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NNI A 1551:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.