



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:45 PM UTC

PDB ID : 2VG5 / pdb_00002vg5
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 : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

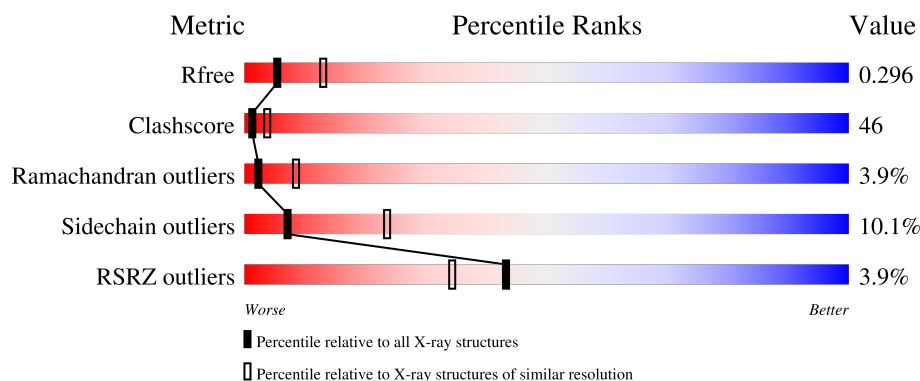
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	B	428	

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	NNC	A	1551	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7872 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.

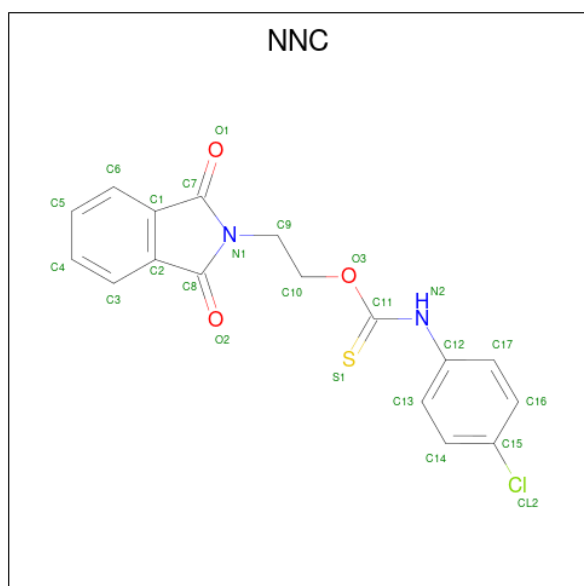
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4475	2898	744	825	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-chlorophenyl)thiocarbamate (CCD ID: NNC) (formula: C₁₇H₁₃ClN₂O₃S).



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

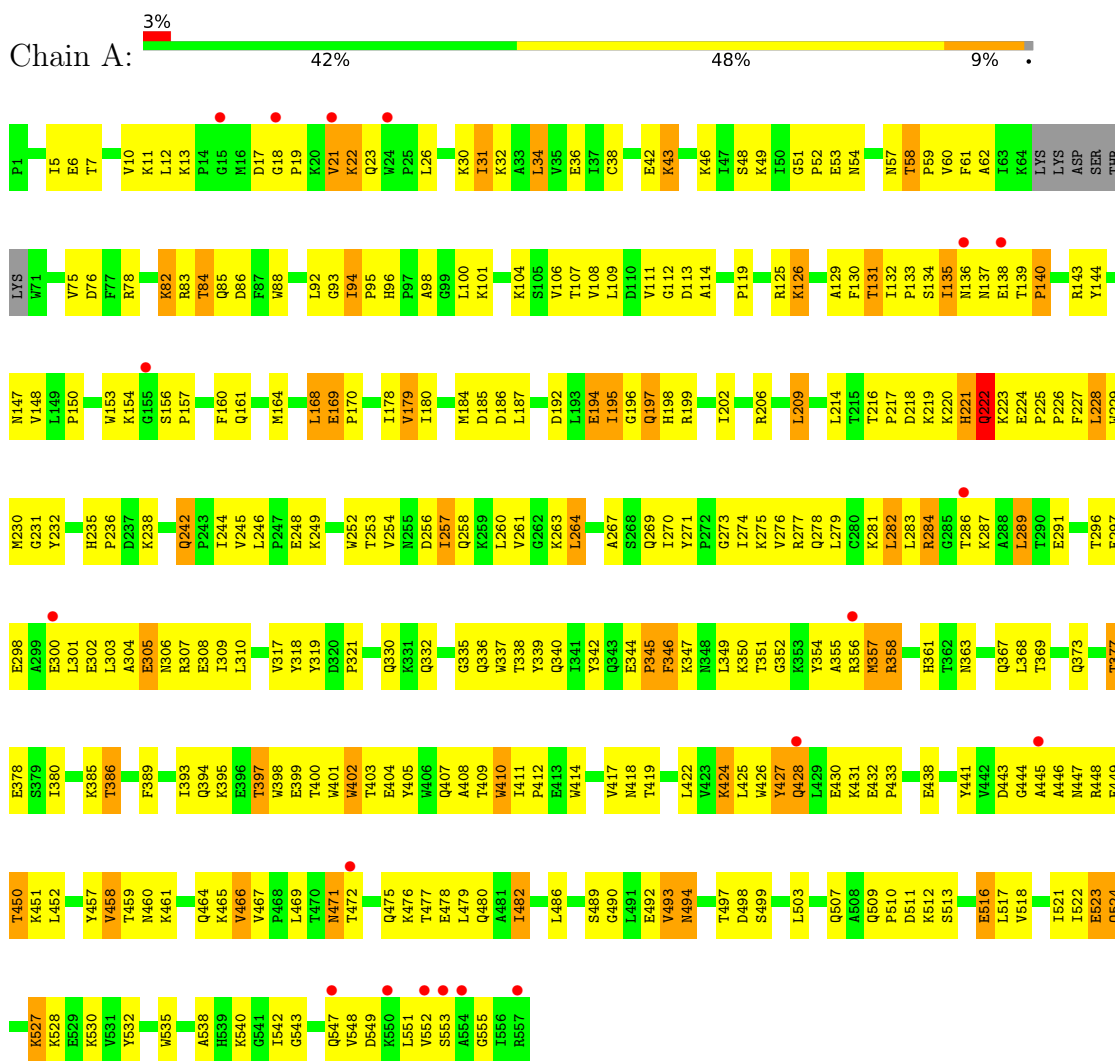
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	25	Total 25	O 25	0	0

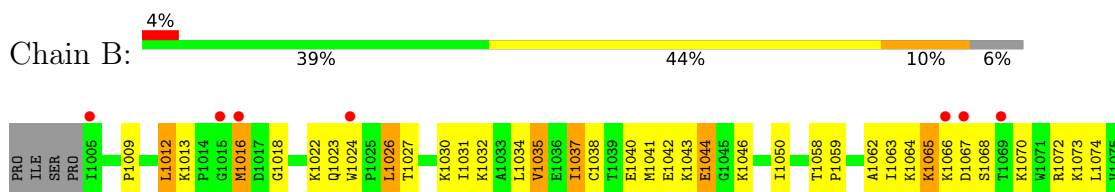
3 Residue-property plots

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



D1076	G1152	W1230	P1294	H1361
F1077	W1153	G1231	L1295	T1362
E1078	K1154	Y1232	T1296	N1363
E1079	G1155	E1233	E1297	D1364
L1080	S1156	L1234	E1298	V1365
N1081	P1157	H1235	A1299	K1366
K1082	A1158	P1236	E1300	Q1367
R1083	I1159	D1237	L1301	L1368
T1084	F1160	K1238	E1302	T1369
D1086	Q1161	W1239	L1303	A1370
Q1085	K1166	T1240	A1304	A1371
F1087	F1087	V1241	E1305	V1372
W1088	I1167	Q1242	N1306	I1375
E1089	L1168	P1243	R1307	I1380
V1090	E1169	I1244	E1308	V1381
Q1091	P1170	V1245	I1309	I1382
L1092	N1175	L1246	L1310	K1385
G1093	I1178	P1247	K1311	K1388
I1094	V1179	E1248	E1312	F1389
F1095	I1180	K1249	P1313	K1390
H1096	Y1181	D1250	V1314	L1391
K1101	Y1183	T1253	V1317	F1392
K1104	M1184	V1254	Y1318	I1393
S1105	D1185	N1255	Y1319	Q1394
V1106	D1186	D1256	D1320	K1395
T1107	L1187	I1257	K1323	E1396
L1108	Y1188	Q1258	D1324	T1397
V1109	V1189	K1259	L1325	W1398
L1109	G1190	L1260	I1326	W1401
D1110	S1191	V1261	Q1330	W1402
V1111	G1192	G1262	K1331	T1403
G1112	I1195	K1263	Q1332	E1404
D1113	A1114	L1264	G1333	Y1405
Y1115	I1202	N1265	Q1334	W1406
F1116	L1205	W1266	G1335	Q1407
S1117	R1206	A1267	Q1336	E1413
V1118	Q1207	S1268	W1337	W1414
D1121	Q1207	Q1269	T1338	N1418
E1122	R1211	Y1271	Y1342	T1419
R1125	W1212	I1274	Q1343	P1420
K1126	G1213	K1275	E1344	L1421
F1130	L1214	V1276	P1345	L1422
T1131	THR	R1277	F1346	V1423
I1132	PRO	Q1278	K1347	K1424
L1133	ASP	L1279	N1348	L1425
L1136	LYS	C1280	L1349	W1426
N1137	LYS	K1281	K1350	Y1427
Y1144	HIS	L1282	T1351	Q1428
Q1145	GLN	LEU	Y1354	
V1148	LYS	GLY	A1355	
L1149	GLU	T1286	ARG	
P1150	PRO	K1287	MET	
Q1151	PRO	A1288	ARG	
	LEU	L1289	GLY	
	TRP	I1293	ALA	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.86Å 156.13Å 154.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.0 (20.00-2.80) 88.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.237 , 0.297 0.235 , 0.296	Depositor DCC
R_{free} test set	1589 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7872	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NNC

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	0.30	0/4592	0.69	0/6240
2	B	0.29	0/3411	0.66	0/4632
All	All	0.29	0/8003	0.68	0/10872

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4475	0	4521	442	0
2	B	3318	0	3341	301	0
3	A	24	0	13	12	0
4	A	30	0	0	9	0
4	B	25	0	0	6	0
All	All	7872	0	7875	728	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 46.

All (728) 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:107:THR:HG21	1:A:202:ILE:CD1	1.42	1.44
1:A:450:THR:CG2	1:A:452:LEU:HD22	1.51	1.38
1:A:357:MET:HE3	1:A:357:MET:N	1.37	1.33
1:A:357:MET:H	1:A:357:MET:CE	1.51	1.24
1:A:450:THR:HG21	1:A:452:LEU:HD22	1.22	1.18
2:B:1428:GLN:NE2	2:B:1428:GLN:O	1.77	1.17
1:A:107:THR:CG2	1:A:202:ILE:HD11	1.73	1.16
1:A:107:THR:HG21	1:A:202:ILE:HD13	1.30	1.14
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.31	1.12
1:A:523:GLU:HG2	4:A:2030:HOH:O	1.47	1.11
1:A:489:SER:HB2	1:A:493:VAL:HG11	1.13	1.10
2:B:1087:PHE:O	2:B:1091:GLN:HB3	1.53	1.09
1:A:394:GLN:HB2	1:A:397:THR:HG22	1.16	1.09
2:B:1241:VAL:O	2:B:1243:PRO:HD3	1.52	1.08
2:B:1065:LYS:HG3	2:B:1066:LYS:H	0.91	1.07
2:B:1267:ALA:O	2:B:1270:ILE:O	1.72	1.07
1:A:277:ARG:HB2	1:A:336:GLN:NE2	1.70	1.06
1:A:450:THR:HG22	1:A:452:LEU:HD22	1.32	1.05
2:B:1195:ILE:H	2:B:1195:ILE:HD12	0.88	1.04
1:A:289:LEU:HD23	1:A:289:LEU:H	1.19	1.04
1:A:459:THR:HG22	1:A:461:LYS:H	1.21	1.03
2:B:1065:LYS:HG3	2:B:1066:LYS:N	1.64	1.03
2:B:1195:ILE:HD12	2:B:1195:ILE:N	1.74	1.03
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.04	1.03
2:B:1263:LYS:HB3	2:B:1426:TRP:CD1	1.94	1.03
1:A:107:THR:HG21	1:A:202:ILE:HD11	1.04	1.02
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.40	1.02
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.42	1.01
2:B:1237:ASP:OD1	2:B:1238:LYS:HD2	1.59	1.01
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.60	1.01
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.39	1.01
1:A:96:HIS:CE1	1:A:269:GLN:HE21	1.80	0.99
1:A:357:MET:N	1:A:357:MET:CE	2.13	0.99
1:A:96:HIS:H	2:B:1136:ASN:HD21	1.07	0.99
2:B:1065:LYS:CG	2:B:1066:LYS:H	1.74	0.98
2:B:1195:ILE:H	2:B:1195:ILE:CD1	1.68	0.98
2:B:1335:GLY:HA2	2:B:1367:GLN:HE22	1.27	0.98
1:A:445:ALA:O	1:A:477:THR:HG21	1.62	0.98
3:A:1551:NNC:H13	3:A:1551:NNC:O3	1.63	0.98
2:B:1323:LYS:O	2:B:1343:GLN:NE2	1.97	0.98
2:B:1206:ARG:NH2	2:B:1214:LEU:HD12	1.78	0.98
2:B:1271:TYR:O	2:B:1274:ILE:HD13	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLY:HA3	1:A:477:THR:O	1.63	0.97
1:A:466:VAL:HG12	1:A:466:VAL:O	1.63	0.97
1:A:356:ARG:HB3	1:A:358:ARG:HH22	1.29	0.96
2:B:1265:ASN:O	2:B:1268:SER:HB3	1.66	0.96
2:B:1244:ILE:HD12	2:B:1244:ILE:H	1.30	0.96
1:A:351:THR:HG22	1:A:352:GLY:N	1.78	0.96
1:A:277:ARG:HB2	1:A:336:GLN:HE22	1.30	0.95
1:A:107:THR:CG2	1:A:202:ILE:CD1	2.36	0.94
1:A:277:ARG:HD3	1:A:336:GLN:NE2	1.81	0.93
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.50	0.93
2:B:1266:TRP:CE3	2:B:1426:TRP:CZ3	2.56	0.93
1:A:548:VAL:O	1:A:552:VAL:HG23	1.68	0.92
1:A:471:ASN:HD22	1:A:471:ASN:H	1.15	0.92
1:A:137:ASN:O	1:A:138:GLU:HB3	1.68	0.92
1:A:277:ARG:HD3	1:A:336:GLN:HE21	1.32	0.92
1:A:450:THR:HG21	1:A:452:LEU:CD2	2.00	0.92
1:A:469:LEU:CD2	1:A:480:GLN:HG2	1.97	0.91
1:A:486:LEU:HB3	1:A:524:GLN:HG2	1.52	0.91
1:A:138:GLU:O	1:A:138:GLU:HG3	1.71	0.91
1:A:96:HIS:HD2	1:A:98:ALA:H	1.17	0.91
1:A:305:GLU:O	1:A:308:GLU:N	2.04	0.91
2:B:1041:MET:HE1	2:B:1073:LYS:HZ2	1.35	0.90
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.00	0.90
2:B:1263:LYS:HB3	2:B:1426:TRP:HD1	1.30	0.90
2:B:1354:TYR:OH	2:B:1370:GLU:OE1	1.90	0.90
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.08	0.89
1:A:287:LYS:HD2	1:A:291:GLU:OE1	1.71	0.89
1:A:297:GLU:HA	1:A:300:GLU:OE1	1.73	0.88
1:A:60:VAL:HG23	1:A:75:VAL:HG22	1.54	0.88
1:A:228:LEU:HD12	1:A:228:LEU:N	1.87	0.88
1:A:450:THR:CG2	1:A:452:LEU:CD2	2.47	0.88
1:A:125:ARG:HD3	1:A:147:ASN:HD22	1.37	0.87
2:B:1086:ASP:O	2:B:1090:VAL:HG22	1.72	0.87
2:B:1309:ILE:O	2:B:1310:LEU:HB2	1.74	0.87
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.73	0.86
2:B:1391:LEU:CD2	2:B:1414:TRP:HB2	2.05	0.86
1:A:394:GLN:HB2	1:A:397:THR:CG2	2.03	0.86
1:A:464:GLN:OE1	1:A:551:LEU:HD22	1.74	0.86
1:A:227:PHE:C	1:A:228:LEU:HD12	2.00	0.86
1:A:179:VAL:CG1	3:A:1551:NNC:H9C2	2.05	0.85
2:B:1293:ILE:HG23	2:B:1294:PRO:HD2	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG22	1:A:499:SER:H	1.39	0.85
1:A:444:GLY:CA	1:A:477:THR:O	2.23	0.85
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.39	0.85
2:B:1314:VAL:HG11	2:B:1317:VAL:CG2	2.05	0.85
1:A:273:GLY:O	1:A:275:LYS:HD3	1.77	0.85
1:A:332:GLN:O	1:A:336:GLN:HB2	1.77	0.85
1:A:492:GLU:HG3	1:A:530:LYS:HB2	1.59	0.85
2:B:1085:GLN:HA	2:B:1088:TRP:NE1	1.92	0.85
1:A:351:THR:CG2	1:A:352:GLY:H	1.88	0.84
1:A:179:VAL:HG11	3:A:1551:NNC:C10	2.06	0.84
2:B:1303:LEU:N	2:B:1303:LEU:HD23	1.91	0.84
1:A:125:ARG:HH11	1:A:147:ASN:ND2	1.76	0.84
2:B:1277:ARG:O	2:B:1280:CYS:N	2.09	0.84
1:A:355:ALA:O	1:A:357:MET:HE2	1.77	0.84
2:B:1420:PRO:HG2	2:B:1423:VAL:HG21	1.58	0.84
1:A:540:LYS:HB2	1:A:542:ILE:CD1	2.08	0.83
1:A:351:THR:CG2	1:A:352:GLY:N	2.39	0.83
1:A:106:VAL:CG1	1:A:227:PHE:HE2	1.90	0.83
1:A:228:LEU:N	1:A:228:LEU:CD1	2.42	0.83
1:A:356:ARG:HG2	4:A:2018:HOH:O	1.76	0.83
2:B:1428:GLN:NE2	2:B:1428:GLN:C	2.36	0.83
1:A:93:GLY:HA3	2:B:1137:ASN:ND2	1.94	0.82
2:B:1107:THR:HA	2:B:1232:TYR:O	1.78	0.82
1:A:469:LEU:HD21	1:A:480:GLN:CG	1.99	0.82
2:B:1064:LYS:O	2:B:1065:LYS:O	1.98	0.82
2:B:1087:PHE:HD2	4:B:2001:HOH:O	1.62	0.82
1:A:286:THR:O	1:A:287:LYS:HG2	1.79	0.81
1:A:161:GLN:HB3	4:A:2007:HOH:O	1.79	0.81
1:A:518:VAL:O	1:A:522:ILE:HG12	1.81	0.81
1:A:277:ARG:HH11	1:A:336:GLN:NE2	1.79	0.81
2:B:1303:LEU:HD23	2:B:1303:LEU:H	1.46	0.81
1:A:471:ASN:HD22	1:A:471:ASN:N	1.78	0.80
1:A:179:VAL:HG11	3:A:1551:NNC:H102	1.60	0.80
1:A:96:HIS:HE1	1:A:269:GLN:HE21	1.25	0.80
1:A:319:TYR:OH	1:A:385:LYS:HE3	1.81	0.80
1:A:85:GLN:O	1:A:154:LYS:NZ	2.13	0.80
1:A:466:VAL:O	1:A:466:VAL:CG1	2.30	0.79
1:A:17:ASP:O	1:A:83:ARG:NH1	2.15	0.79
1:A:96:HIS:H	2:B:1136:ASN:ND2	1.80	0.79
1:A:351:THR:HG22	1:A:352:GLY:H	1.46	0.79
1:A:196:GLY:O	1:A:197:GLN:CB	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:CB	1:A:336:GLN:NE2	2.45	0.78
1:A:475:GLN:HG3	4:A:2028:HOH:O	1.81	0.78
1:A:356:ARG:HA	1:A:357:MET:HE2	1.64	0.78
2:B:1032:LYS:HE2	2:B:1032:LYS:HA	1.65	0.78
2:B:1303:LEU:H	2:B:1303:LEU:CD2	1.96	0.78
1:A:84:THR:HG22	1:A:85:GLN:N	1.98	0.78
1:A:289:LEU:H	1:A:289:LEU:CD2	1.95	0.78
1:A:441:TYR:O	1:A:548:VAL:HG21	1.84	0.77
2:B:1113:ASP:HB2	4:B:2008:HOH:O	1.82	0.77
1:A:287:LYS:CD	1:A:291:GLU:OE1	2.32	0.77
1:A:549:ASP:O	1:A:553:SER:OG	2.00	0.77
2:B:1156:SER:HB2	2:B:1157:PRO:HD3	1.66	0.77
1:A:489:SER:CB	1:A:493:VAL:HG11	2.06	0.77
1:A:471:ASN:H	1:A:471:ASN:ND2	1.80	0.76
2:B:1296:THR:HG22	2:B:1298:GLU:H	1.49	0.76
2:B:1012:LEU:HD23	2:B:1013:LYS:H	1.49	0.76
1:A:22:LYS:H	1:A:22:LYS:HD2	1.49	0.76
2:B:1266:TRP:CZ2	2:B:1346:PHE:HZ	2.03	0.76
2:B:1365:VAL:O	2:B:1369:THR:OG1	2.05	0.75
2:B:1249:LYS:O	2:B:1250:ASP:HB3	1.87	0.75
1:A:287:LYS:CG	1:A:291:GLU:OE1	2.35	0.75
1:A:449:GLU:O	1:A:450:THR:HB	1.85	0.75
2:B:1345:PRO:O	2:B:1346:PHE:HB2	1.86	0.75
1:A:46:LYS:HD2	1:A:46:LYS:N	2.00	0.74
2:B:1244:ILE:HD12	2:B:1244:ILE:N	2.02	0.74
2:B:1335:GLY:HA2	2:B:1367:GLN:NE2	2.02	0.74
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.18	0.74
1:A:34:LEU:CD1	1:A:62:ALA:HB2	2.17	0.74
2:B:1244:ILE:H	2:B:1244:ILE:CD1	2.00	0.74
1:A:361:HIS:HD2	1:A:513:SER:OG	1.70	0.74
2:B:1266:TRP:CZ2	2:B:1346:PHE:CZ	2.76	0.74
1:A:96:HIS:CD2	1:A:98:ALA:H	2.02	0.74
2:B:1336:GLN:HE21	2:B:1336:GLN:HA	1.52	0.74
1:A:26:LEU:HD23	1:A:133:PRO:HG3	1.68	0.74
1:A:34:LEU:HD11	1:A:62:ALA:HB2	1.70	0.73
2:B:1314:VAL:HG11	2:B:1317:VAL:HB	1.70	0.73
1:A:23:GLN:NE2	1:A:60:VAL:H	1.86	0.73
2:B:1151:GLN:HG3	4:B:2014:HOH:O	1.87	0.73
1:A:131:THR:HG23	1:A:143:ARG:HH21	1.53	0.73
2:B:1344:GLU:OE1	2:B:1344:GLU:HA	1.87	0.73
3:A:1551:NNC:O3	3:A:1551:NNC:C13	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1263:LYS:CB	2:B:1426:TRP:CD1	2.72	0.73
1:A:134:SER:CB	1:A:139:THR:HB	2.19	0.73
2:B:1278:GLN:HB2	2:B:1302:GLU:HG3	1.68	0.73
2:B:1363:ASN:OD1	2:B:1366:LYS:N	2.16	0.72
2:B:1391:LEU:HD23	2:B:1414:TRP:HB2	1.69	0.72
1:A:23:GLN:HE21	1:A:60:VAL:H	1.37	0.72
1:A:459:THR:HG22	1:A:461:LYS:N	2.01	0.72
1:A:106:VAL:HG12	1:A:227:PHE:CE2	2.25	0.72
1:A:277:ARG:CB	1:A:336:GLN:HE22	2.01	0.72
1:A:317:VAL:HG12	1:A:318:TYR:N	2.04	0.72
2:B:1175:ASN:HB3	2:B:1178:ILE:HG13	1.72	0.72
2:B:1338:THR:HG21	2:B:1427:TYR:O	1.88	0.72
2:B:1158:ALA:O	2:B:1161:GLN:HG3	1.90	0.72
1:A:278:GLN:HB2	1:A:302:GLU:OE1	1.90	0.71
1:A:356:ARG:HB3	1:A:358:ARG:NH2	2.03	0.71
2:B:1279:LEU:O	2:B:1282:LEU:HB3	1.89	0.71
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.36	0.71
2:B:1366:LYS:HG2	2:B:1405:TYR:CD1	2.24	0.71
1:A:195:ILE:HG21	1:A:199:ARG:HH21	1.56	0.71
1:A:260:LEU:HD13	1:A:264:LEU:HD22	1.73	0.71
2:B:1366:LYS:O	2:B:1370:GLU:HG3	1.91	0.70
2:B:1040:GLU:O	2:B:1044:GLU:HG2	1.91	0.70
2:B:1270:ILE:O	2:B:1271:TYR:HB2	1.90	0.70
1:A:53:GLU:N	1:A:53:GLU:OE1	2.24	0.70
1:A:356:ARG:HA	1:A:357:MET:CE	2.21	0.70
2:B:1277:ARG:O	2:B:1278:GLN:C	2.35	0.70
1:A:106:VAL:HG11	1:A:227:PHE:HE2	1.57	0.70
1:A:409:THR:HG22	1:A:410:TRP:N	2.07	0.70
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.18	0.70
2:B:1420:PRO:HG2	2:B:1423:VAL:CG2	2.22	0.70
1:A:277:ARG:CD	1:A:336:GLN:HE21	2.03	0.69
1:A:332:GLN:O	1:A:332:GLN:HG3	1.91	0.69
1:A:194:GLU:CD	1:A:194:GLU:H	2.00	0.69
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.25	0.69
1:A:76:ASP:OD1	1:A:76:ASP:C	2.35	0.69
1:A:106:VAL:CG1	1:A:227:PHE:CE2	2.75	0.69
1:A:289:LEU:HD23	1:A:289:LEU:N	2.02	0.69
1:A:449:GLU:O	1:A:450:THR:CB	2.40	0.69
2:B:1280:CYS:O	2:B:1282:LEU:N	2.26	0.69
1:A:196:GLY:O	1:A:197:GLN:HB3	1.93	0.69
1:A:179:VAL:HG13	3:A:1551:NNC:H9C2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.56	0.69
2:B:1266:TRP:CD2	2:B:1426:TRP:CE3	2.81	0.68
2:B:1270:ILE:HG23	2:B:1271:TYR:CD1	2.29	0.68
2:B:1255:ASN:HB2	2:B:1289:LEU:CD1	2.23	0.68
1:A:412:PRO:HG3	2:B:1401:TRP:HZ2	1.59	0.68
2:B:1278:GLN:HB2	2:B:1302:GLU:CG	2.23	0.68
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.57	0.67
1:A:244:ILE:HG12	1:A:263:LYS:HD2	1.75	0.67
1:A:497:THR:HG22	1:A:498:ASP:N	2.09	0.67
1:A:139:THR:O	1:A:140:PRO:C	2.35	0.67
1:A:517:LEU:C	1:A:517:LEU:HD13	2.18	0.67
2:B:1253:THR:O	2:B:1257:ILE:CG2	2.43	0.67
2:B:1314:VAL:HG11	2:B:1317:VAL:CB	2.23	0.67
1:A:179:VAL:CG1	3:A:1551:NNC:C9	2.73	0.67
1:A:464:GLN:CD	1:A:551:LEU:HD22	2.19	0.67
2:B:1266:TRP:CD2	2:B:1426:TRP:CZ3	2.83	0.67
2:B:1314:VAL:CG1	2:B:1317:VAL:HB	2.24	0.67
2:B:1118:VAL:HB	2:B:1149:LEU:CD1	2.25	0.66
1:A:409:THR:HG22	1:A:410:TRP:H	1.59	0.66
1:A:373:GLN:O	1:A:377:THR:HG22	1.95	0.66
2:B:1065:LYS:CG	2:B:1066:LYS:N	2.43	0.66
2:B:1309:ILE:O	2:B:1310:LEU:CB	2.43	0.66
2:B:1064:LYS:HE3	2:B:1068:SER:O	1.96	0.66
2:B:1237:ASP:OD1	2:B:1237:ASP:C	2.39	0.66
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.23	0.66
2:B:1368:LEU:O	2:B:1372:VAL:HG23	1.95	0.66
1:A:260:LEU:HD12	1:A:279:LEU:HD13	1.78	0.65
1:A:426:TRP:O	1:A:427:TYR:HB3	1.96	0.65
2:B:1388:LYS:HG3	2:B:1413:GLU:HB2	1.77	0.65
2:B:1337:TRP:HE1	2:B:1367:GLN:NE2	1.93	0.65
1:A:195:ILE:CG2	1:A:199:ARG:HH21	2.10	0.65
1:A:228:LEU:HD23	4:A:2012:HOH:O	1.96	0.65
1:A:465:LYS:O	1:A:466:VAL:HG23	1.96	0.65
1:A:394:GLN:CB	1:A:397:THR:HG22	2.10	0.65
1:A:356:ARG:CA	1:A:357:MET:HE2	2.26	0.65
2:B:1206:ARG:HH22	2:B:1214:LEU:HA	1.61	0.65
2:B:1303:LEU:HA	2:B:1306:ASN:HB2	1.77	0.65
1:A:443:ASP:OD2	1:A:444:GLY:N	2.30	0.64
1:A:42:GLU:OE2	1:A:49:LYS:HE3	1.97	0.64
1:A:433:PRO:HG3	2:B:1255:ASN:OD1	1.98	0.64
2:B:1169:GLU:HB3	2:B:1170:PRO:CD	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.78	0.64
2:B:1065:LYS:HD2	2:B:1072:ARG:HH21	1.62	0.64
2:B:1279:LEU:HD22	2:B:1302:GLU:HG3	1.80	0.64
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.23	0.63
1:A:57:ASN:HB2	1:A:143:ARG:NH2	2.11	0.63
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.32	0.63
2:B:1393:ILE:HG12	2:B:1394:GLN:H	1.64	0.62
1:A:438:GLU:OE2	1:A:459:THR:CG2	2.43	0.62
1:A:17:ASP:OD1	1:A:18:GLY:N	2.30	0.62
1:A:395:LYS:O	1:A:399:GLU:HG2	2.00	0.62
2:B:1151:GLN:HB3	2:B:1185:ASP:OD2	2.00	0.62
1:A:548:VAL:O	1:A:552:VAL:CG2	2.45	0.62
1:A:85:GLN:HG3	1:A:86:ASP:N	2.14	0.62
1:A:497:THR:HG22	1:A:499:SER:N	2.13	0.62
2:B:1104:LYS:HA	2:B:1237:ASP:OD2	1.99	0.62
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.81	0.62
1:A:277:ARG:CD	1:A:336:GLN:NE2	2.59	0.61
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	1.81	0.61
2:B:1309:ILE:HG13	2:B:1310:LEU:N	2.15	0.61
1:A:100:LEU:O	1:A:318:TYR:HB3	2.00	0.61
1:A:438:GLU:HG2	1:A:461:LYS:HD2	1.82	0.61
1:A:338:THR:OG1	4:A:2016:HOH:O	2.13	0.61
2:B:1122:GLU:HG2	2:B:1125:ARG:CZ	2.30	0.61
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.82	0.61
1:A:84:THR:HG22	1:A:85:GLN:H	1.63	0.61
1:A:78:ARG:O	1:A:82:LYS:HG3	1.99	0.61
1:A:450:THR:HG22	1:A:452:LEU:CD2	2.22	0.61
2:B:1085:GLN:O	2:B:1087:PHE:N	2.33	0.61
2:B:1183:TYR:CD2	2:B:1380:ILE:HD13	2.36	0.61
2:B:1085:GLN:O	2:B:1086:ASP:C	2.44	0.60
2:B:1253:THR:O	2:B:1257:ILE:HG23	2.01	0.60
1:A:317:VAL:CG1	1:A:318:TYR:N	2.64	0.60
1:A:497:THR:HG22	1:A:498:ASP:H	1.65	0.60
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.82	0.60
2:B:1037:ILE:HG22	2:B:1041:MET:HE2	1.82	0.60
1:A:363:ASN:HA	1:A:511:ASP:OD2	2.02	0.60
2:B:1041:MET:HE1	2:B:1073:LYS:NZ	2.13	0.60
2:B:1337:TRP:HE1	2:B:1367:GLN:HE21	1.49	0.60
1:A:283:LEU:O	1:A:284:ARG:C	2.44	0.60
1:A:494:ASN:N	1:A:494:ASN:OD1	2.34	0.60
2:B:1296:THR:O	2:B:1299:ALA:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:CD1	1:A:279:LEU:HD13	2.32	0.60
1:A:448:ARG:O	1:A:451:LYS:HD2	2.00	0.60
1:A:402:TRP:CD1	1:A:402:TRP:C	2.79	0.59
2:B:1296:THR:O	2:B:1299:ALA:N	2.34	0.59
2:B:1023:GLN:OE1	2:B:1059:PRO:HA	2.02	0.59
1:A:57:ASN:HA	1:A:129:ALA:O	2.03	0.59
1:A:527:LYS:HE3	1:A:527:LYS:HA	1.83	0.59
2:B:1278:GLN:HA	2:B:1278:GLN:OE1	2.02	0.59
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.18	0.59
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.83	0.59
2:B:1012:LEU:HD23	2:B:1013:LYS:N	2.15	0.59
2:B:1333:GLY:O	2:B:1334:GLN:HB2	2.03	0.59
1:A:96:HIS:CE1	1:A:269:GLN:NE2	2.63	0.58
2:B:1428:GLN:C	2:B:1428:GLN:CD	2.71	0.58
1:A:408:ALA:O	2:B:1393:ILE:HG13	2.03	0.58
2:B:1065:LYS:HD2	2:B:1072:ARG:NH2	2.19	0.58
1:A:125:ARG:NH1	1:A:147:ASN:ND2	2.50	0.58
1:A:301:LEU:O	1:A:304:ALA:HB3	2.04	0.58
1:A:361:HIS:CD2	1:A:513:SER:OG	2.55	0.58
2:B:1153:TRP:CZ2	2:B:1155:GLY:HA3	2.38	0.58
2:B:1277:ARG:O	2:B:1279:LEU:N	2.37	0.58
1:A:195:ILE:O	1:A:199:ARG:HG3	2.04	0.58
1:A:551:LEU:C	1:A:551:LEU:HD12	2.28	0.58
2:B:1024:TRP:O	2:B:1026:LEU:HD13	2.04	0.58
2:B:1371:ALA:O	2:B:1375:ILE:HG13	2.02	0.58
1:A:273:GLY:O	1:A:275:LYS:CD	2.51	0.57
1:A:411:ILE:HG22	1:A:412:PRO:O	2.03	0.57
2:B:1249:LYS:O	2:B:1250:ASP:CB	2.52	0.57
2:B:1312:GLU:HA	2:B:1312:GLU:OE2	2.04	0.57
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.40	0.57
1:A:438:GLU:CG	1:A:461:LYS:HD2	2.34	0.57
2:B:1106:VAL:N	2:B:1234:LEU:O	2.27	0.57
2:B:1032:LYS:O	2:B:1035:VAL:HG22	2.04	0.57
2:B:1153:TRP:CE2	2:B:1155:GLY:HA3	2.39	0.57
2:B:1064:LYS:O	2:B:1065:LYS:C	2.48	0.57
2:B:1206:ARG:HH21	2:B:1214:LEU:HD12	1.65	0.57
2:B:1130:PHE:CZ	2:B:1144:TYR:HB2	2.39	0.57
1:A:305:GLU:O	1:A:306:ASN:C	2.48	0.57
1:A:447:ASN:HD22	1:A:448:ARG:N	2.03	0.57
2:B:1255:ASN:HB2	2:B:1289:LEU:HD13	1.86	0.57
2:B:1309:ILE:HG13	2:B:1310:LEU:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.44	0.57
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.35	0.57
2:B:1013:LYS:HB2	2:B:1016:MET:CG	2.35	0.57
2:B:1116:PHE:HZ	2:B:1151:GLN:HE21	1.53	0.56
2:B:1085:GLN:HA	2:B:1088:TRP:CD1	2.40	0.56
1:A:179:VAL:CG1	3:A:1551:NNC:C10	2.82	0.56
1:A:221:HIS:O	1:A:222:GLN:O	2.23	0.56
1:A:246:LEU:HD22	1:A:260:LEU:CD2	2.36	0.56
2:B:1030:LYS:O	2:B:1034:LEU:HG	2.06	0.56
2:B:1270:ILE:HG23	2:B:1271:TYR:HD1	1.71	0.56
2:B:1246:LEU:HD21	2:B:1310:LEU:CD1	2.36	0.56
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.88	0.56
1:A:451:LYS:HG2	4:A:2025:HOH:O	2.06	0.56
2:B:1314:VAL:HG11	2:B:1317:VAL:HG23	1.87	0.56
2:B:1031:ILE:O	2:B:1035:VAL:HG13	2.06	0.56
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.88	0.55
2:B:1080:LEU:CD2	2:B:1084:THR:HG21	2.36	0.55
1:A:356:ARG:HH12	1:A:358:ARG:NH1	2.04	0.55
2:B:1293:ILE:CG2	2:B:1294:PRO:HD2	2.33	0.55
1:A:445:ALA:O	1:A:477:THR:CG2	2.47	0.55
1:A:129:ALA:HA	1:A:144:TYR:O	2.06	0.55
2:B:1253:THR:O	2:B:1257:ILE:HG22	2.06	0.55
1:A:107:THR:HG22	1:A:202:ILE:HD11	1.80	0.55
1:A:195:ILE:HG22	1:A:199:ARG:HE	1.72	0.55
1:A:43:LYS:HZ3	1:A:43:LYS:HB3	1.72	0.55
2:B:1080:LEU:CD2	2:B:1084:THR:CG2	2.85	0.55
1:A:357:MET:HE3	1:A:357:MET:H	0.58	0.55
1:A:447:ASN:HD22	1:A:447:ASN:C	2.14	0.55
1:A:179:VAL:CG1	3:A:1551:NNC:H102	2.36	0.55
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.54	0.55
1:A:438:GLU:CD	1:A:461:LYS:HD2	2.32	0.55
1:A:517:LEU:HD11	1:A:521:ILE:HD11	1.89	0.55
1:A:540:LYS:HB2	1:A:542:ILE:HD13	1.87	0.55
2:B:1107:THR:HG22	2:B:1109:LEU:HD13	1.88	0.55
1:A:179:VAL:HG13	3:A:1551:NNC:C9	2.35	0.54
1:A:444:GLY:HA2	1:A:477:THR:O	2.06	0.54
1:A:356:ARG:NH1	1:A:358:ARG:NH1	2.55	0.54
2:B:1084:THR:O	2:B:1085:GLN:C	2.51	0.54
1:A:214:LEU:N	1:A:214:LEU:HD22	2.22	0.54
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.73	0.54
2:B:1266:TRP:CZ3	2:B:1426:TRP:HZ3	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:C	1:A:186:ASP:H	2.16	0.54
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.90	0.54
1:A:287:LYS:HB3	1:A:291:GLU:OE1	2.08	0.54
1:A:344:GLU:O	1:A:345:PRO:C	2.49	0.54
2:B:1101:LYS:O	2:B:1101:LYS:HG2	2.08	0.53
2:B:1391:LEU:HD21	2:B:1414:TRP:HB2	1.89	0.53
1:A:257:ILE:HD12	1:A:261:VAL:HG23	1.89	0.53
2:B:1080:LEU:HD23	2:B:1080:LEU:O	2.07	0.53
2:B:1388:LYS:HA	2:B:1413:GLU:O	2.08	0.53
1:A:386:THR:HG21	4:A:2019:HOH:O	2.09	0.53
1:A:31:ILE:HD13	1:A:133:PRO:HG2	1.91	0.53
1:A:95:PRO:HA	2:B:1136:ASN:O	2.08	0.53
1:A:380:ILE:HD12	2:B:1027:THR:HG22	1.91	0.53
1:A:106:VAL:HG11	3:A:1551:NNC:CL2	2.46	0.53
2:B:1168:LEU:CD1	2:B:1180:ILE:HG21	2.37	0.53
2:B:1266:TRP:CZ3	2:B:1426:TRP:CZ3	2.96	0.53
1:A:57:ASN:HD22	1:A:143:ARG:HH21	1.55	0.53
1:A:335:GLY:HA2	1:A:512:LYS:HZ1	1.74	0.53
1:A:7:THR:CG2	1:A:119:PRO:HB2	2.37	0.53
1:A:418:ASN:HD22	1:A:422:LEU:HD21	1.74	0.53
1:A:465:LYS:O	1:A:466:VAL:CG2	2.57	0.53
1:A:275:LYS:HG3	1:A:332:GLN:OE1	2.09	0.53
1:A:267:ALA:C	1:A:269:GLN:H	2.17	0.52
1:A:270:ILE:HG23	1:A:271:TYR:CD2	2.44	0.52
2:B:1236:PRO:HA	2:B:1239:TRP:CD2	2.44	0.52
2:B:1418:ASN:O	2:B:1420:PRO:HD3	2.09	0.52
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.90	0.52
1:A:43:LYS:HB3	1:A:43:LYS:NZ	2.23	0.52
1:A:475:GLN:O	1:A:478:GLU:HB2	2.09	0.52
2:B:1260:LEU:HD13	2:B:1264:LEU:HD12	1.91	0.52
2:B:1277:ARG:HG3	4:B:2021:HOH:O	2.09	0.52
2:B:1342:TYR:HB3	2:B:1348:ASN:HB3	1.91	0.52
1:A:507:GLN:HE21	2:B:1421:PRO:HB3	1.73	0.52
2:B:1336:GLN:NE2	2:B:1355:ALA:HB2	2.23	0.52
2:B:1065:LYS:HB3	2:B:1068:SER:OG	2.08	0.52
2:B:1391:LEU:HD21	2:B:1414:TRP:CB	2.40	0.52
2:B:1027:THR:O	2:B:1031:ILE:HG13	2.09	0.52
2:B:1156:SER:HB2	2:B:1157:PRO:CD	2.39	0.52
1:A:131:THR:HG23	1:A:143:ARG:NH2	2.22	0.52
1:A:287:LYS:HG3	1:A:291:GLU:OE1	2.07	0.52
2:B:1391:LEU:CD2	2:B:1414:TRP:CB	2.85	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:O	1:A:34:LEU:HD22	2.09	0.52
1:A:194:GLU:CD	1:A:194:GLU:N	2.66	0.52
1:A:134:SER:OG	1:A:139:THR:HB	2.10	0.52
1:A:465:LYS:C	1:A:466:VAL:HG23	2.35	0.52
2:B:1295:LEU:HD13	2:B:1300:GLU:OE2	2.09	0.52
2:B:1342:TYR:HB3	2:B:1348:ASN:HA	1.92	0.52
1:A:26:LEU:HD23	1:A:133:PRO:CG	2.40	0.51
1:A:517:LEU:C	1:A:517:LEU:CD1	2.83	0.51
1:A:410:TRP:CE3	2:B:1363:ASN:HB2	2.45	0.51
1:A:428:GLN:HE21	1:A:428:GLN:CA	2.24	0.51
2:B:1213:GLY:O	2:B:1214:LEU:C	2.53	0.51
2:B:1254:VAL:HG21	2:B:1288:ALA:O	2.11	0.51
2:B:1308:GLU:HA	2:B:1311:LYS:HE2	1.92	0.51
1:A:5:ILE:HG13	1:A:6:GLU:N	2.25	0.51
2:B:1270:ILE:O	2:B:1271:TYR:CB	2.57	0.51
2:B:1118:VAL:HB	2:B:1149:LEU:HD12	1.93	0.51
2:B:1153:TRP:O	2:B:1155:GLY:N	2.43	0.51
2:B:1246:LEU:O	2:B:1307:ARG:NH1	2.43	0.51
2:B:1254:VAL:O	2:B:1258:GLN:HG3	2.10	0.51
1:A:274:ILE:HD11	1:A:310:LEU:CD1	2.41	0.51
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.45	0.51
2:B:1303:LEU:O	2:B:1304:ALA:C	2.53	0.51
1:A:153:TRP:CD2	1:A:154:LYS:O	2.64	0.51
1:A:510:PRO:O	1:A:522:ILE:HD12	2.11	0.51
1:A:197:GLN:HG2	4:A:2011:HOH:O	2.10	0.50
1:A:466:VAL:O	1:A:467:VAL:C	2.54	0.50
2:B:1363:ASN:OD1	2:B:1366:LYS:HB2	2.11	0.50
1:A:131:THR:HG23	1:A:143:ARG:HE	1.75	0.50
2:B:1046:LYS:HD3	2:B:1116:PHE:HB3	1.93	0.50
2:B:1307:ARG:O	2:B:1309:ILE:O	2.29	0.50
1:A:184:MET:O	1:A:186:ASP:N	2.44	0.50
1:A:277:ARG:CG	1:A:336:GLN:HE21	2.25	0.50
1:A:308:GLU:OE2	1:A:308:GLU:HA	2.11	0.50
2:B:1247:PRO:HB2	2:B:1249:LYS:HG2	1.94	0.50
1:A:131:THR:CG2	1:A:143:ARG:HE	2.23	0.50
1:A:459:THR:HG22	1:A:460:ASN:N	2.26	0.50
1:A:482:ILE:HD13	1:A:482:ILE:C	2.37	0.50
1:A:53:GLU:O	1:A:54:ASN:C	2.54	0.50
1:A:254:VAL:HB	1:A:289:LEU:HA	1.93	0.50
1:A:257:ILE:HG12	1:A:283:LEU:HD21	1.94	0.50
2:B:1326:ILE:HD11	2:B:1390:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:HD22	1:A:26:LEU:N	2.27	0.50
1:A:216:THR:HB	1:A:217:PRO:HD2	1.94	0.50
2:B:1013:LYS:HB2	2:B:1016:MET:HG2	1.94	0.50
2:B:1096:HIS:CE1	2:B:1382:ILE:O	2.65	0.50
1:A:51:GLY:C	1:A:53:GLU:OE1	2.55	0.50
1:A:356:ARG:CA	1:A:357:MET:CE	2.88	0.50
2:B:1112:GLY:C	2:B:1114:ALA:H	2.20	0.50
1:A:125:ARG:HD3	1:A:147:ASN:ND2	2.18	0.49
1:A:478:GLU:O	1:A:482:ILE:HG22	2.12	0.49
2:B:1240:THR:HG23	2:B:1241:VAL:N	2.27	0.49
1:A:516:GLU:CD	1:A:516:GLU:H	2.16	0.49
1:A:337:TRP:NE1	1:A:367:GLN:HE21	2.06	0.49
1:A:425:LEU:N	1:A:425:LEU:HD22	2.28	0.49
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.42	0.49
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.94	0.49
2:B:1396:GLU:CD	2:B:1396:GLU:H	2.20	0.49
2:B:1122:GLU:HA	2:B:1125:ARG:HG3	1.95	0.49
2:B:1255:ASN:O	2:B:1259:LYS:HG2	2.12	0.49
2:B:1246:LEU:N	2:B:1246:LEU:HD22	2.28	0.49
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.47	0.48
1:A:317:VAL:CG1	1:A:318:TYR:H	2.26	0.48
1:A:194:GLU:O	1:A:195:ILE:C	2.55	0.48
1:A:218:ASP:O	1:A:219:LYS:C	2.56	0.48
1:A:355:ALA:O	1:A:357:MET:HG3	2.13	0.48
2:B:1271:TYR:HB3	2:B:1274:ILE:HD11	1.94	0.48
2:B:1299:ALA:O	2:B:1300:GLU:C	2.55	0.48
1:A:38:CYS:O	1:A:42:GLU:HB2	2.13	0.48
1:A:51:GLY:C	1:A:53:GLU:H	2.21	0.48
1:A:109:LEU:O	1:A:187:LEU:N	2.37	0.48
1:A:196:GLY:O	1:A:197:GLN:HB2	2.10	0.48
1:A:458:VAL:HG21	1:A:547:GLN:CG	2.44	0.48
2:B:1092:LEU:HB2	2:B:1158:ALA:HB1	1.96	0.48
2:B:1336:GLN:C	2:B:1337:TRP:CD1	2.92	0.48
1:A:277:ARG:HH11	1:A:336:GLN:HE22	1.55	0.48
1:A:476:LYS:C	1:A:478:GLU:H	2.21	0.48
1:A:48:SER:O	1:A:144:TYR:HA	2.14	0.48
1:A:278:GLN:CG	1:A:298:GLU:HB3	2.29	0.48
1:A:356:ARG:C	1:A:357:MET:CE	2.83	0.48
1:A:425:LEU:HD22	1:A:425:LEU:H	1.78	0.48
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.96	0.48
1:A:61:PHE:CD1	1:A:61:PHE:N	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:LEU:CD2	2:B:1080:LEU:C	2.86	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.14	0.48
1:A:342:TYR:HA	1:A:349:LEU:CD1	2.43	0.48
2:B:1326:ILE:HG23	2:B:1342:TYR:O	2.14	0.48
1:A:134:SER:O	1:A:135:ILE:C	2.57	0.47
1:A:351:THR:HG23	1:A:352:GLY:H	1.72	0.47
2:B:1266:TRP:CG	2:B:1426:TRP:CE3	3.02	0.47
2:B:1302:GLU:O	2:B:1305:GLU:N	2.45	0.47
1:A:21:VAL:CG1	1:A:59:PRO:CD	2.83	0.47
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.80	0.47
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.95	0.47
1:A:517:LEU:HD13	1:A:517:LEU:O	2.14	0.47
1:A:401:TRP:O	1:A:402:TRP:C	2.56	0.47
1:A:457:TYR:C	1:A:457:TYR:CD2	2.92	0.47
2:B:1038:CYS:SG	2:B:1132:ILE:HD11	2.55	0.47
2:B:1276:VAL:HG22	2:B:1276:VAL:O	2.14	0.47
1:A:106:VAL:HG11	1:A:227:PHE:CE2	2.42	0.47
1:A:367:GLN:OE1	1:A:512:LYS:HE3	2.13	0.47
1:A:287:LYS:CB	1:A:291:GLU:OE1	2.62	0.47
1:A:231:GLY:O	1:A:242:GLN:HB2	2.15	0.47
1:A:354:TYR:C	1:A:354:TYR:CD2	2.93	0.47
1:A:443:ASP:HB3	1:A:548:VAL:HG12	1.96	0.47
1:A:458:VAL:HG21	1:A:547:GLN:HG2	1.97	0.47
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.44	0.47
1:A:551:LEU:HD12	1:A:552:VAL:N	2.30	0.47
2:B:1306:ASN:O	2:B:1309:ILE:O	2.33	0.47
1:A:344:GLU:O	1:A:346:PHE:N	2.48	0.47
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.27	0.47
1:A:507:GLN:NE2	2:B:1421:PRO:HB3	2.29	0.46
2:B:1058:THR:HG23	2:B:1076:ASP:O	2.15	0.46
1:A:46:LYS:HD2	1:A:46:LYS:H	1.78	0.46
1:A:286:THR:O	1:A:287:LYS:CG	2.57	0.46
1:A:32:LYS:O	1:A:36:GLU:HG3	2.14	0.46
1:A:405:TYR:CE1	1:A:407:GLN:HB2	2.50	0.46
1:A:431:LYS:NZ	1:A:431:LYS:HB3	2.30	0.46
2:B:1332:GLN:O	2:B:1333:GLY:O	2.33	0.46
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.31	0.46
1:A:317:VAL:HG12	1:A:318:TYR:H	1.80	0.46
2:B:1246:LEU:HD21	2:B:1310:LEU:HD12	1.97	0.46
1:A:369:THR:CG2	1:A:398:TRP:HH2	2.28	0.46
1:A:548:VAL:HG12	1:A:552:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1317:VAL:HG22	2:B:1347:LYS:HB3	1.97	0.46
1:A:84:THR:CG2	1:A:85:GLN:N	2.68	0.46
1:A:245:VAL:HG13	1:A:245:VAL:O	2.14	0.46
2:B:1022:LYS:HD2	2:B:1022:LYS:N	2.31	0.46
2:B:1126:LYS:HG2	4:B:2011:HOH:O	2.14	0.46
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.79	0.46
2:B:1013:LYS:HB2	2:B:1016:MET:HG3	1.97	0.46
2:B:1195:ILE:N	2:B:1195:ILE:CD1	2.47	0.46
1:A:94:ILE:HD13	1:A:94:ILE:HA	1.72	0.46
1:A:260:LEU:CD1	1:A:264:LEU:HD22	2.45	0.46
2:B:1085:GLN:O	2:B:1088:TRP:N	2.49	0.46
2:B:1108:VAL:HB	2:B:1232:TYR:CB	2.45	0.46
2:B:1423:VAL:O	2:B:1424:LYS:C	2.58	0.46
1:A:10:VAL:HG12	1:A:11:LYS:N	2.31	0.46
1:A:139:THR:O	1:A:140:PRO:O	2.34	0.45
2:B:1030:LYS:HB3	2:B:1062:ALA:HB3	1.97	0.45
2:B:1108:VAL:HB	2:B:1232:TYR:HB2	1.98	0.45
2:B:1207:GLN:O	2:B:1211:ARG:HD3	2.14	0.45
1:A:57:ASN:HD22	1:A:143:ARG:NH2	2.15	0.45
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.45
1:A:345:PRO:O	1:A:346:PHE:HB2	2.16	0.45
2:B:1080:LEU:CD2	2:B:1080:LEU:O	2.63	0.45
2:B:1394:GLN:O	2:B:1395:LYS:C	2.57	0.45
1:A:107:THR:CG2	1:A:202:ILE:HD13	2.22	0.45
1:A:253:THR:O	1:A:257:ILE:CG2	2.65	0.45
2:B:1255:ASN:ND2	2:B:1259:LYS:HD3	2.31	0.45
1:A:126:LYS:H	1:A:126:LYS:HD2	1.82	0.45
1:A:156:SER:N	1:A:157:PRO:CD	2.79	0.45
2:B:1326:ILE:CG2	2:B:1342:TYR:O	2.65	0.45
1:A:112:GLY:O	1:A:113:ASP:C	2.59	0.45
1:A:409:THR:CG2	1:A:410:TRP:N	2.77	0.45
2:B:1079:GLU:O	2:B:1083:ARG:HG3	2.16	0.45
1:A:281:LYS:C	1:A:283:LEU:N	2.74	0.45
1:A:257:ILE:CG1	1:A:283:LEU:HD21	2.46	0.45
1:A:516:GLU:CD	1:A:516:GLU:N	2.74	0.45
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.47	0.45
2:B:1330:GLN:HG2	2:B:1338:THR:OG1	2.17	0.45
1:A:148:VAL:O	1:A:150:PRO:HD3	2.17	0.45
2:B:1088:TRP:CZ3	2:B:1154:LYS:HD3	2.51	0.45
2:B:1295:LEU:HD12	2:B:1295:LEU:O	2.17	0.45
1:A:424:LYS:HE3	1:A:426:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:VAL:O	1:A:467:VAL:HG23	2.17	0.45
2:B:1261:VAL:HA	2:B:1264:LEU:HB2	1.99	0.45
2:B:1260:LEU:HD13	2:B:1260:LEU:C	2.41	0.45
2:B:1326:ILE:HD12	2:B:1388:LYS:O	2.17	0.45
1:A:267:ALA:C	1:A:269:GLN:N	2.74	0.44
1:A:282:LEU:HD21	1:A:296:THR:H	1.82	0.44
1:A:367:GLN:NE2	1:A:512:LYS:HZ1	2.15	0.44
2:B:1022:LYS:HD2	2:B:1022:LYS:H	1.82	0.44
2:B:1187:LEU:HD23	2:B:1187:LEU:HA	1.88	0.44
2:B:1422:LEU:HB3	2:B:1426:TRP:CH2	2.52	0.44
1:A:13:LYS:HG3	1:A:84:THR:O	2.18	0.44
2:B:1077:PHE:O	2:B:1078:ARG:C	2.58	0.44
2:B:1166:LYS:HE3	2:B:1166:LYS:HB2	1.85	0.44
2:B:1303:LEU:O	2:B:1307:ARG:N	2.30	0.44
1:A:94:ILE:HD12	1:A:229:TRP:CZ2	2.52	0.44
1:A:96:HIS:HD2	1:A:98:ALA:N	1.98	0.44
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.99	0.44
1:A:433:PRO:CG	2:B:1255:ASN:OD1	2.64	0.44
2:B:1013:LYS:CB	2:B:1016:MET:HG2	2.47	0.44
2:B:1175:ASN:HB3	2:B:1178:ILE:CG1	2.45	0.44
1:A:94:ILE:O	1:A:94:ILE:HG22	2.18	0.44
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.00	0.44
1:A:410:TRP:CE3	2:B:1363:ASN:CB	3.01	0.44
2:B:1081:ASN:ND2	2:B:1153:TRP:HD1	2.15	0.44
1:A:393:ILE:HG12	1:A:397:THR:HG23	1.98	0.44
2:B:1151:GLN:O	2:B:1185:ASP:OD1	2.36	0.44
2:B:1156:SER:CB	2:B:1157:PRO:HD3	2.43	0.44
1:A:19:PRO:HG2	1:A:58:THR:HG22	1.99	0.44
1:A:303:LEU:HG	1:A:307:ARG:NH1	2.33	0.44
1:A:402:TRP:CD1	1:A:403:THR:N	2.85	0.44
1:A:402:TRP:HD1	1:A:403:THR:N	2.16	0.44
1:A:459:THR:CG2	1:A:460:ASN:N	2.81	0.44
2:B:1111:VAL:O	2:B:1111:VAL:HG13	2.18	0.44
1:A:76:ASP:OD2	1:A:78:ARG:NH1	2.51	0.44
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.72	0.44
1:A:350:LYS:HD3	1:A:378:GLU:OE2	2.17	0.44
1:A:355:ALA:O	1:A:357:MET:CE	2.58	0.44
1:A:497:THR:CG2	1:A:499:SER:H	2.22	0.44
2:B:1042:GLU:HG3	2:B:1043:LYS:N	2.33	0.44
1:A:497:THR:CG2	1:A:498:ASP:N	2.78	0.44
1:A:517:LEU:HD13	1:A:521:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:HD21	1:A:180:ILE:HG21	1.99	0.43
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.64	0.43
1:A:319:TYR:OH	1:A:385:LYS:CE	2.61	0.43
1:A:169:GLU:CB	1:A:170:PRO:CD	2.87	0.43
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.74	0.43
2:B:1067:ASP:HB2	2:B:1407:GLN:NE2	2.33	0.43
2:B:1326:ILE:HG23	2:B:1342:TYR:CD1	2.53	0.43
1:A:252:TRP:CE3	1:A:256:ASP:HB3	2.53	0.43
1:A:330:GLN:NE2	1:A:340:GLN:HE22	2.14	0.43
2:B:1153:TRP:C	2:B:1155:GLY:N	2.76	0.43
2:B:1259:LYS:HD3	4:B:2020:HOH:O	2.18	0.43
1:A:219:LYS:O	1:A:220:LYS:C	2.61	0.43
2:B:1393:ILE:HG21	2:B:1398:TRP:HB2	2.01	0.43
2:B:1184:MET:O	2:B:1185:ASP:HB2	2.19	0.43
2:B:1258:GLN:O	2:B:1261:VAL:HG22	2.19	0.43
2:B:1271:TYR:HB3	2:B:1274:ILE:CD1	2.48	0.43
2:B:1296:THR:O	2:B:1299:ALA:CB	2.64	0.43
2:B:1319:TYR:OH	2:B:1385:LYS:HD3	2.17	0.43
2:B:1363:ASN:CG	2:B:1366:LYS:HB2	2.44	0.43
1:A:168:LEU:HA	1:A:168:LEU:HD12	1.78	0.43
1:A:229:TRP:O	1:A:230:MET:C	2.62	0.43
1:A:278:GLN:NE2	1:A:298:GLU:HB2	2.33	0.43
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.43
2:B:1299:ALA:O	2:B:1302:GLU:N	2.47	0.43
1:A:125:ARG:HH11	1:A:147:ASN:HD22	1.61	0.43
2:B:1422:LEU:HB3	2:B:1426:TRP:CZ2	2.54	0.43
1:A:93:GLY:CA	2:B:1137:ASN:ND2	2.75	0.42
1:A:96:HIS:HE1	1:A:269:GLN:NE2	2.05	0.42
1:A:130:PHE:CD1	1:A:130:PHE:N	2.87	0.42
1:A:432:GLU:HB2	1:A:433:PRO:HD2	2.00	0.42
1:A:471:ASN:N	1:A:471:ASN:ND2	2.46	0.42
2:B:1240:THR:CG2	2:B:1241:VAL:N	2.80	0.42
1:A:93:GLY:HA3	2:B:1137:ASN:HD21	1.79	0.42
1:A:94:ILE:O	1:A:95:PRO:C	2.62	0.42
1:A:296:THR:O	1:A:300:GLU:HG3	2.19	0.42
1:A:367:GLN:NE2	1:A:512:LYS:NZ	2.68	0.42
2:B:1080:LEU:HD23	2:B:1084:THR:HG23	2.02	0.42
2:B:1266:TRP:HZ2	2:B:1346:PHE:HZ	1.59	0.42
1:A:287:LYS:HD2	1:A:291:GLU:CD	2.41	0.42
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.47	0.42
1:A:472:THR:HB	1:A:476:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:LEU:CD2	2:B:1084:THR:HG23	2.49	0.42
2:B:1085:GLN:C	2:B:1087:PHE:N	2.77	0.42
2:B:1121:ASP:O	2:B:1122:GLU:C	2.62	0.42
1:A:184:MET:C	1:A:186:ASP:N	2.76	0.42
1:A:356:ARG:CB	1:A:358:ARG:HH22	2.16	0.42
2:B:1234:LEU:HD12	2:B:1234:LEU:HA	1.88	0.42
1:A:101:LYS:HE2	1:A:101:LYS:HB2	1.69	0.42
1:A:424:LYS:HE3	1:A:426:TRP:CZ2	2.55	0.42
2:B:1279:LEU:HD22	2:B:1302:GLU:CG	2.49	0.42
1:A:12:LEU:HD23	1:A:84:THR:HA	2.01	0.42
1:A:94:ILE:HG13	1:A:230:MET:HE2	2.02	0.42
1:A:447:ASN:C	1:A:447:ASN:ND2	2.78	0.42
2:B:1279:LEU:CD2	2:B:1302:GLU:CB	2.98	0.42
1:A:235:HIS:HB3	1:A:236:PRO:HD2	2.02	0.41
2:B:1063:ILE:HD13	2:B:1074:LEU:HD22	2.02	0.41
1:A:106:VAL:HG23	1:A:236:PRO:HB3	2.02	0.41
1:A:229:TRP:CE3	3:A:1551:NNC:H5	2.55	0.41
1:A:277:ARG:CG	1:A:336:GLN:NE2	2.82	0.41
1:A:447:ASN:CG	1:A:449:GLU:O	2.63	0.41
1:A:466:VAL:HG22	1:A:551:LEU:HD13	2.02	0.41
2:B:1267:ALA:O	2:B:1268:SER:C	2.63	0.41
2:B:1320:ASP:OD1	2:B:1320:ASP:C	2.63	0.41
2:B:1325:LEU:HD12	2:B:1385:LYS:HG3	2.02	0.41
1:A:195:ILE:HG22	1:A:199:ARG:NE	2.35	0.41
1:A:399:GLU:O	1:A:400:THR:C	2.63	0.41
2:B:1178:ILE:HD13	2:B:1191:SER:HB3	2.01	0.41
2:B:1428:GLN:NE2	2:B:1428:GLN:CA	2.83	0.41
1:A:106:VAL:HG12	1:A:227:PHE:CZ	2.55	0.41
1:A:479:LEU:HA	1:A:482:ILE:HG22	2.02	0.41
2:B:1159:ILE:O	2:B:1159:ILE:HG22	2.21	0.41
2:B:1169:GLU:OE2	2:B:1169:GLU:C	2.63	0.41
2:B:1266:TRP:CZ2	2:B:1346:PHE:CE2	3.09	0.41
1:A:281:LYS:O	1:A:283:LEU:N	2.54	0.41
2:B:1153:TRP:C	2:B:1155:GLY:H	2.29	0.41
2:B:1335:GLY:O	2:B:1355:ALA:HA	2.20	0.41
1:A:54:ASN:ND2	1:A:54:ASN:H	2.18	0.41
1:A:319:TYR:CZ	1:A:321:PRO:HA	2.56	0.41
2:B:1148:VAL:O	2:B:1149:LEU:C	2.62	0.41
1:A:88:TRP:CZ2	1:A:92:LEU:HD11	2.56	0.41
1:A:134:SER:HB3	1:A:139:THR:HB	1.98	0.41
1:A:248:GLU:C	1:A:249:LYS:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:OE2	1:A:347:LYS:HD2	2.20	0.41
2:B:1105:SER:HA	2:B:1234:LEU:O	2.20	0.41
2:B:1423:VAL:O	2:B:1425:LEU:N	2.53	0.41
1:A:23:GLN:NE2	1:A:60:VAL:HG12	2.36	0.41
1:A:95:PRO:HB3	2:B:1136:ASN:O	2.21	0.41
1:A:138:GLU:O	1:A:138:GLU:CG	2.53	0.41
1:A:281:LYS:C	1:A:283:LEU:H	2.28	0.41
1:A:389:PHE:O	1:A:414:TRP:HA	2.21	0.41
2:B:1092:LEU:O	2:B:1161:GLN:NE2	2.53	0.41
2:B:1094:ILE:HD12	2:B:1094:ILE:N	2.35	0.41
2:B:1178:ILE:HD13	2:B:1191:SER:CB	2.51	0.41
2:B:1202:ILE:O	2:B:1205:LEU:HB3	2.21	0.41
2:B:1350:LYS:HG2	2:B:1351:THR:N	2.36	0.41
2:B:1418:ASN:O	2:B:1420:PRO:CD	2.68	0.41
2:B:1420:PRO:HB2	2:B:1423:VAL:HG23	2.02	0.41
2:B:1088:TRP:CH2	2:B:1154:LYS:HD3	2.56	0.41
1:A:134:SER:O	1:A:136:ASN:O	2.39	0.40
1:A:369:THR:OG1	1:A:398:TRP:HZ3	2.04	0.40
1:A:490:GLY:C	1:A:492:GLU:H	2.29	0.40
1:A:367:GLN:CD	1:A:512:LYS:HZ1	2.29	0.40
1:A:111:VAL:HG11	1:A:214:LEU:HD12	2.03	0.40
1:A:274:ILE:HD11	1:A:310:LEU:HD13	2.02	0.40
1:A:369:THR:OG1	1:A:398:TRP:CZ3	2.73	0.40
2:B:1271:TYR:CB	2:B:1274:ILE:CD1	3.00	0.40
2:B:1388:LYS:HG3	2:B:1413:GLU:CB	2.49	0.40
1:A:195:ILE:CG2	1:A:199:ARG:NH2	2.81	0.40
1:A:235:HIS:HB2	1:A:238:LYS:O	2.22	0.40
2:B:1031:ILE:O	2:B:1032:LYS:C	2.65	0.40
2:B:1042:GLU:O	2:B:1043:LYS:C	2.64	0.40
2:B:1044:GLU:HG2	2:B:1044:GLU:H	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	547/557 (98%)	480 (88%)	48 (9%)	19 (4%)	3	10
2	B	393/428 (92%)	331 (84%)	44 (11%)	18 (5%)	2	6
All	All	940/985 (95%)	811 (86%)	92 (10%)	37 (4%)	2	8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	140	PRO
1	A	222	GLN
2	B	1065	LYS
2	B	1085	GLN
2	B	1086	ASP
2	B	1277	ARG
2	B	1278	GLN
2	B	1281	LYS
2	B	1302	GLU
1	A	197	GLN
1	A	345	PRO
1	A	346	PHE
1	A	466	VAL
2	B	1250	ASP
2	B	1280	CYS
2	B	1310	LEU
2	B	1333	GLY
1	A	185	ASP
1	A	282	LEU
1	A	427	TYR
1	A	450	THR
1	A	528	LYS
2	B	1154	LYS
2	B	1424	LYS
1	A	284	ARG
1	A	543	GLY
2	B	1184	MET
1	A	555	GLY
2	B	1009	PRO
1	A	410	TRP
2	B	1231	GLY
2	B	1242	GLN

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Mol	Chain	Res	Type
2	B	1018	GLY
1	A	135	ILE
1	A	52	PRO
1	A	169	GLU

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	489/497 (98%)	441 (90%)	48 (10%)	7	25
2	B	366/390 (94%)	328 (90%)	38 (10%)	7	22
All	All	855/887 (96%)	769 (90%)	86 (10%)	7	23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	22	LYS
1	A	31	ILE
1	A	34	LEU
1	A	43	LYS
1	A	58	THR
1	A	82	LYS
1	A	94	ILE
1	A	108	VAL
1	A	126	LYS
1	A	131	THR
1	A	168	LEU
1	A	178	ILE
1	A	179	VAL
1	A	194	GLU
1	A	195	ILE
1	A	209	LEU
1	A	221	HIS
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	228	LEU
1	A	242	GLN
1	A	257	ILE
1	A	258	GLN
1	A	264	LEU
1	A	289	LEU
1	A	305	GLU
1	A	309	ILE
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	377	THR
1	A	386	THR
1	A	397	THR
1	A	402	TRP
1	A	404	GLU
1	A	417	VAL
1	A	419	THR
1	A	424	LYS
1	A	428	GLN
1	A	458	VAL
1	A	471	ASN
1	A	482	ILE
1	A	493	VAL
1	A	494	ASN
1	A	516	GLU
1	A	523	GLU
1	A	524	GLN
1	A	527	LYS
2	B	1012	LEU
2	B	1016	MET
2	B	1026	LEU
2	B	1035	VAL
2	B	1037	ILE
2	B	1044	GLU
2	B	1070	LYS
2	B	1078	ARG
2	B	1080	LEU
2	B	1090	VAL
2	B	1101	LYS
2	B	1109	LEU
2	B	1113	ASP

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Mol	Chain	Res	Type
2	B	1178	ILE
2	B	1189	VAL
2	B	1195	ILE
2	B	1237	ASP
2	B	1240	THR
2	B	1244	ILE
2	B	1245	VAL
2	B	1246	LEU
2	B	1257	ILE
2	B	1259	LYS
2	B	1280	CYS
2	B	1289	LEU
2	B	1295	LEU
2	B	1303	LEU
2	B	1314	VAL
2	B	1326	ILE
2	B	1330	GLN
2	B	1334	GLN
2	B	1336	GLN
2	B	1344	GLU
2	B	1349	LEU
2	B	1369	THR
2	B	1403	THR
2	B	1425	LEU
2	B	1428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	54	ASN
1	A	57	ASN
1	A	85	GLN
1	A	96	HIS
1	A	147	ASN
1	A	161	GLN
1	A	258	GLN
1	A	269	GLN
1	A	315	HIS
1	A	336	GLN
1	A	340	GLN
1	A	361	HIS

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Mol	Chain	Res	Type
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	509	GLN
1	A	524	GLN
1	A	545	ASN
2	B	1081	ASN
2	B	1096	HIS
2	B	1136	ASN
2	B	1137	ASN
2	B	1174	GLN
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 oligosaccharides 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	NNC	A	1551	-	26,26,26	2.45	6 (23%)	36,36,36	3.05	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	NNC	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	NNC	C1-C7	-5.95	1.39	1.48
3	A	1551	NNC	C2-C8	-5.83	1.39	1.48
3	A	1551	NNC	C8-N1	-5.43	1.33	1.39
3	A	1551	NNC	C7-N1	-5.14	1.33	1.39
3	A	1551	NNC	C12-N2	-4.09	1.33	1.41
3	A	1551	NNC	O3-C11	2.42	1.36	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1551	NNC	C10-O3-C11	-12.11	109.55	119.04
3	A	1551	NNC	O3-C11-S1	-6.45	119.88	125.07
3	A	1551	NNC	C12-N2-C11	-5.41	120.73	130.07
3	A	1551	NNC	C1-C7-N1	4.55	109.25	105.88
3	A	1551	NNC	C2-C8-N1	4.52	109.22	105.88
3	A	1551	NNC	O3-C11-N2	4.40	120.81	112.20
3	A	1551	NNC	C8-N1-C7	-3.46	109.07	112.02
3	A	1551	NNC	C3-C2-C8	2.40	133.61	129.59
3	A	1551	NNC	C2-C1-C7	-2.36	106.19	108.26
3	A	1551	NNC	C1-C2-C8	-2.29	106.25	108.26
3	A	1551	NNC	C6-C1-C7	2.22	133.32	129.59
3	A	1551	NNC	C10-C9-N1	-2.15	108.71	112.26

There are no chirality outliers.

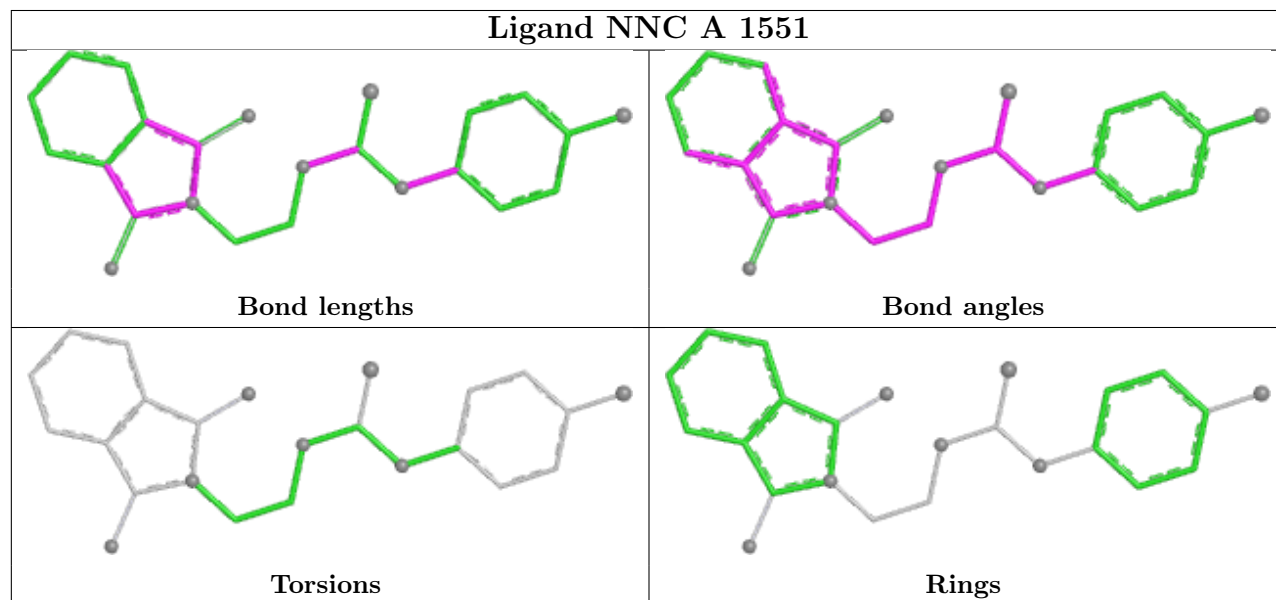
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1551	NNC	12	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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	551/557 (98%)	0.21	19 (3%) 48 39	20, 44, 67, 85	0
2	B	401/428 (93%)	0.10	18 (4%) 38 30	23, 40, 75, 90	0
All	All	952/985 (96%)	0.16	37 (3%) 43 34	20, 43, 72, 90	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	TRP	5.7
1	A	472	THR	5.1
2	B	1066	LYS	4.1
1	A	136	ASN	3.6
1	A	356	ARG	3.4
2	B	1231	GLY	3.2
2	B	1289	LEU	3.2
1	A	553	SER	3.1
1	A	300	GLU	2.9
2	B	1295	LEU	2.9
1	A	552	VAL	2.8
1	A	547	GLN	2.8
1	A	15	GLY	2.7
1	A	445	ALA	2.7
1	A	550	LYS	2.7
2	B	1362	THR	2.7
1	A	286	THR	2.6
2	B	1069	THR	2.6
2	B	1288	ALA	2.6
2	B	1005	ILE	2.5
2	B	1418	ASN	2.5
2	B	1232	TYR	2.5
2	B	1067	ASP	2.4
2	B	1282	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	554	ALA	2.4
2	B	1230	MET	2.4
2	B	1286	THR	2.4
1	A	21	VAL	2.4
2	B	1024	TRP	2.3
2	B	1361	HIS	2.2
1	A	557	ARG	2.2
2	B	1016	MET	2.1
1	A	18	GLY	2.0
2	B	1015	GLY	2.0
1	A	138	GLU	2.0
1	A	428	GLN	2.0
1	A	155	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

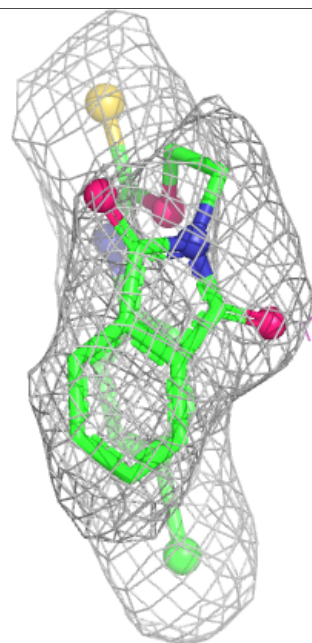
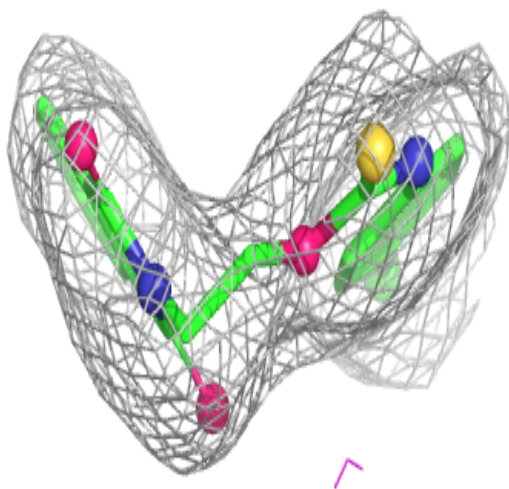
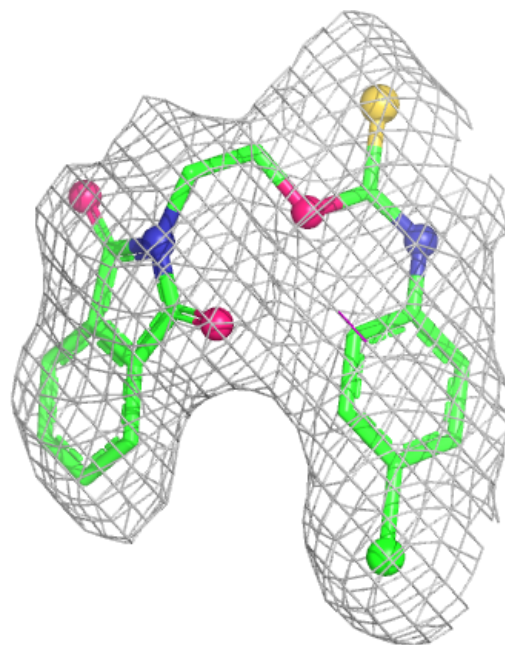
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NNC	A	1551	24/24	0.97	0.06	26,29,36,38	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 NNC 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.