



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:12 PM UTC

PDB ID : 2VG7 / pdb_00002vg7
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 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

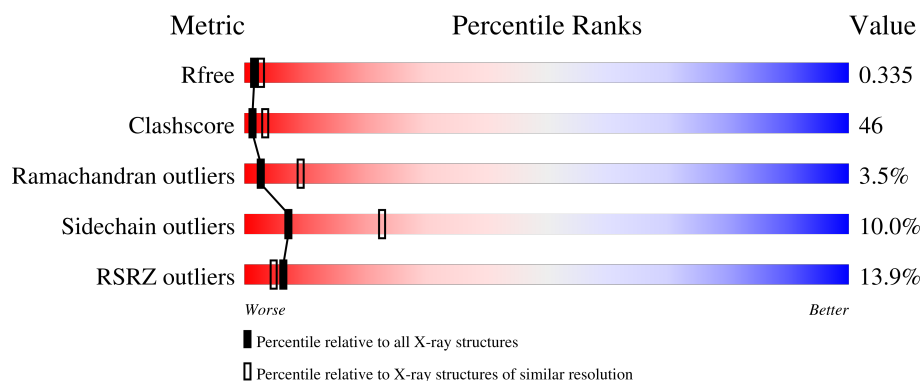
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 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	NNI	A	1551	-	-	X	-

2 Entry composition [i](#)

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.

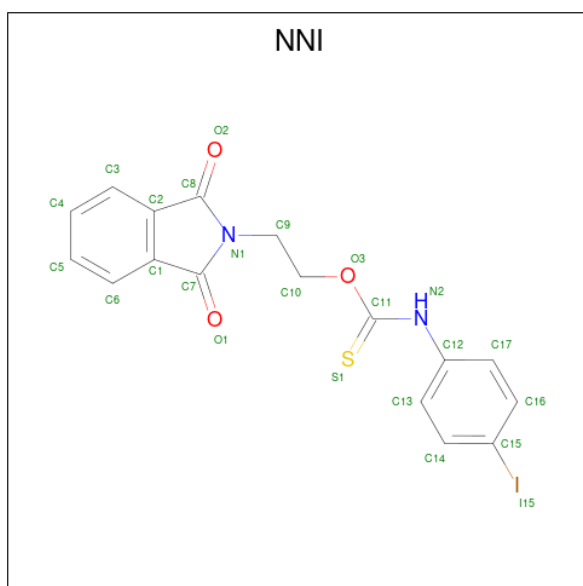
- Molecule 1 is a protein called REVERSE TRANSCRIPTASE/RIBONUCLEASE H.

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

- Molecule 2 is a protein called P51 RT.

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

- Molecule 3 is O-[2-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)ethyl] (4-iodophenyl)thiocarbamate (CCD ID: NNI) (formula: C₁₇H₁₃IN₂O₃S).



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

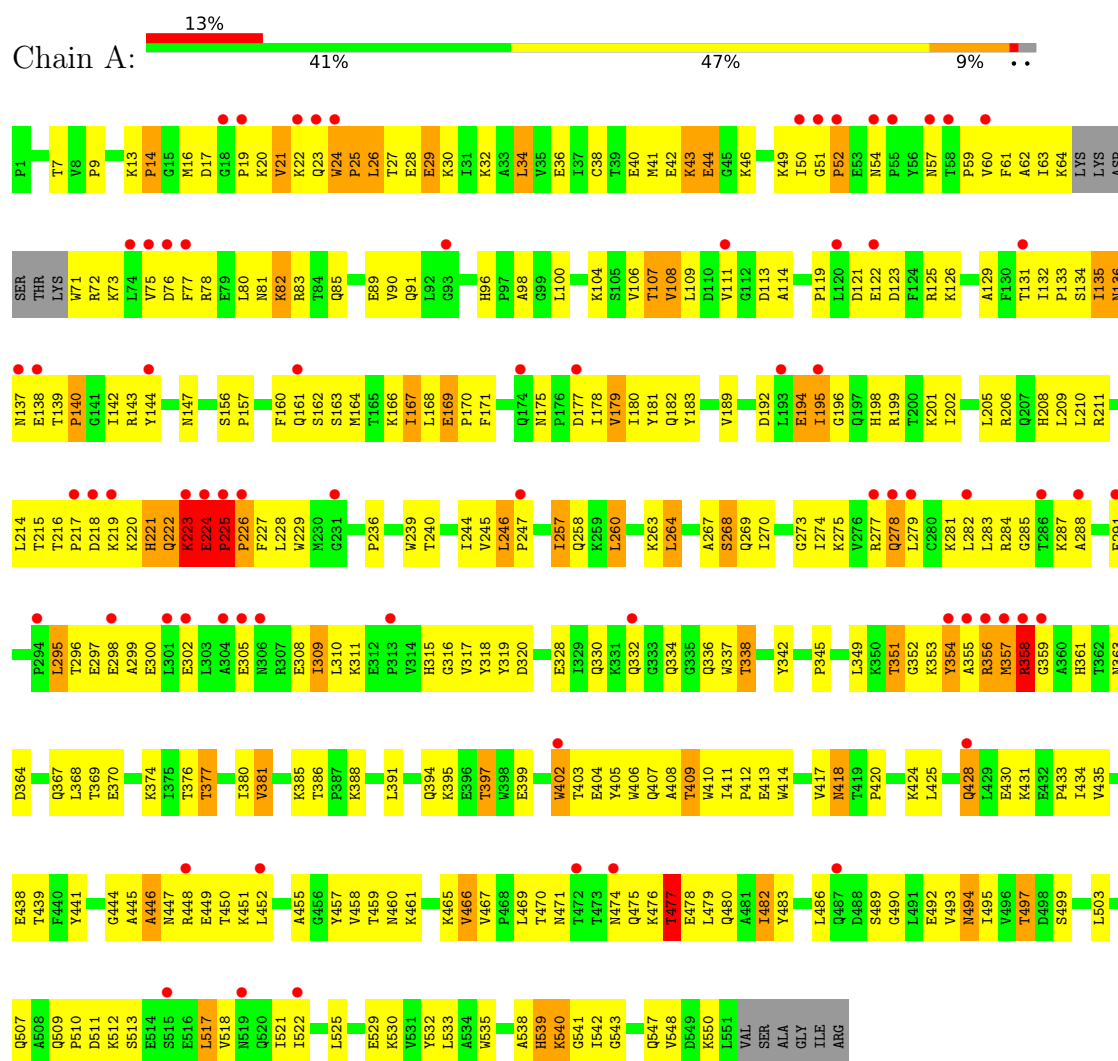
- Molecule 4 is water.

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

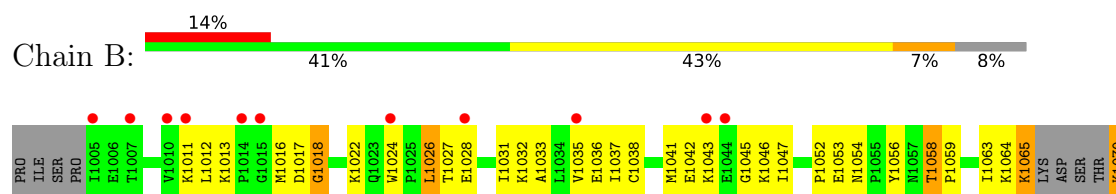
3 Residue-property plots [i](#)

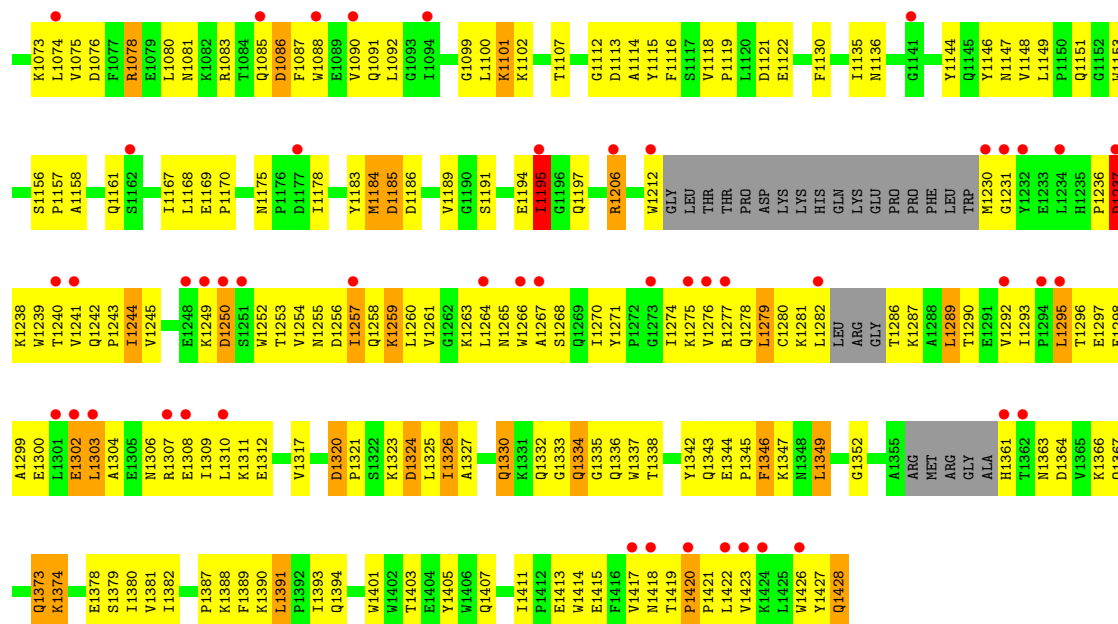
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





4 Data and refinement statistics

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) 81.2 (20.00-2.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.255 , 0.333 0.254 , 0.335	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)	0.43 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

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: 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	0.31	1/4553 (0.0%)	0.70	3/6187 (0.0%)
2	B	0.28	0/3368	0.69	4/4573 (0.1%)
All	All	0.30	1/7921 (0.0%)	0.69	7/10760 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	550	LYS	C-N	-6.86	1.23	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	CA-C-N	8.53	129.17	120.38
1	A	224	GLU	C-N-CA	8.53	129.17	120.38
2	B	1320	ASP	CA-C-N	5.97	125.67	119.82
2	B	1320	ASP	C-N-CA	5.97	125.67	119.82
1	A	225	PRO	N-CA-C	5.30	117.17	110.70
2	B	1420	PRO	CA-C-N	5.17	125.22	119.32
2	B	1420	PRO	C-N-CA	5.17	125.22	119.32

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	471	0
2	B	3276	0	3297	261	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	715	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 (715) 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
2:B:1428:GLN:C	2:B:1428:GLN:NE2	2.02	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:HD12	2:B:1195:ILE:H	1.09	1.14
1:A:26:LEU:CD2	1:A:133:PRO:HG2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1428:GLN:C	2:B:1428:GLN:HE21	1.65	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
1:A:542:ILE:HD13	2:B:1280:CYS:SG	2.02	0.98
1:A:465:LYS:C	1:A:466:VAL:HG23	1.88	0.97
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:NE2	2:B:1428:GLN:O	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:134:SER:C	1:A:136:ASN:H	1.87	0.81
1:A:194:GLU:CD	1:A:194:GLU:H	1.88	0.81
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:HE21	1:A:278:GLN:HA	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
1:A:482:ILE:HD13	1:A:482:ILE:C	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1065:LYS:O	2:B:1407:GLN:HG2	1.86	0.75
1:A:431:LYS:NZ	1:A:431:LYS:HB3	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
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:1064:LYS:C	2:B:1065:LYS:HG3	2.13	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:29:GLU:HG2	1:A:30:LYS:N	2.05	0.72
1:A:278:GLN:HE21	1:A:281:LYS:HE2	1.50	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:511:ASP:C	1:A:512:LYS:HG3	2.16	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:434:ILE:HD12	1:A:493:VAL:O	1.91	0.70
1:A:482:ILE:HD13	1:A:482:ILE: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
2:B:1041:MET:HE1	2:B:1073:LYS:HD2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:CG1	1:A:318:TYR:N	2.55	0.70
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.74	0.69
2:B:1266:TRP:CZ3	2:B:1426:TRP:CZ3	2.80	0.69
1:A:267:ALA:C	1:A:269:GLN:H	2.00	0.69
1:A:135:ILE:O	1:A:136:ASN:CB	2.37	0.69
1:A:337:TRP:NE1	1:A:367:GLN:HE21	1.89	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: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
1:A:288:ALA:HB3	1:A:291:GLU:OE1	1.93	0.68
1:A:357:MET:C	1:A:359:GLY:H	2.01	0.68
1:A:23:GLN:HG3	1:A:131:THR:OG1	1.95	0.67
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.16	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:1278:GLN:HB2	2:B:1302:GLU:CG	2.24	0.67
2:B:1282:LEU:HD21	2:B:1295:LEU:HA	1.75	0.67
1:A:221:HIS:C	1:A:223:LYS:N	2.52	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:O	1:A:135:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:GLU:HA	1:A:300:GLU:CD	2.20	0.66
1:A:17:ASP:O	1:A:83:ARG:NH1	2.28	0.66
1:A:96:HIS:HE1	1:A:269:GLN:HE21	0.72	0.66
2:B:1279:LEU:HD21	2:B:1303:LEU:HD22	1.78	0.66
1:A:402:TRP:CD1	1:A:403:THR:HG1	2.14	0.65
1:A:29:GLU:HG2	1:A:30:LYS:H	1.61	0.65
1:A:111:VAL:CG1	1:A:214:LEU:HD12	2.26	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:164:MET:O	1:A:168:LEU:HB2	1.97	0.65
1:A:517:LEU:HD13	1:A:517:LEU:O	1.97	0.65
2:B:1303:LEU:HD23	2:B:1303:LEU:H	1.61	0.65
2:B:1391:LEU:HD23	2:B:1414:TRP:HB2	1.79	0.64
2:B:1017:ASP:O	2:B:1083:ARG:NH1	2.30	0.64
2:B:1022:LYS:HD2	2:B:1022:LYS:N	2.12	0.64
1:A:41:MET:HE1	1:A:73:LYS:NZ	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:406:TRP:CE3	2:B:1419:THR:HB	2.33	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: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: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:260:LEU:HD13	1:A:264:LEU:HD22	1.79	0.62
1:A:107:THR:OG1	1:A:223:LYS:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:1151:GLN:O	2:B:1185:ASP:CG	2.43	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:354:TYR:C	1:A:354:TYR:CD2	2.78	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:221:HIS:C	1:A:223:LYS:H	2.06	0.61
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
1:A:479:LEU:HA	1:A:482:ILE:HG22	1.82	0.61
1:A:227:PHE:C	1:A:228:LEU:HD12	2.25	0.61
1:A:489:SER:CB	1:A:493:VAL:HG21	2.30	0.61
1:A:476:LYS:C	1:A:478:GLU:H	2.09	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:1037:ILE:CG2	2:B:1041:MET:HE2	2.30	0.61
1:A:298:GLU:H	1:A:298:GLU:CD	2.07	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
1:A:134:SER:C	1:A:136:ASN:N	2.52	0.60
1:A:206:ARG:HH21	1:A:216:THR:C	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.02	0.59
1:A:82:LYS:NZ	1:A:82:LYS:CB	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:96:HIS:CD2	1:A:98:ALA:H	2.17	0.59
1:A:106:VAL:HG11	3:A:1551:NNI:I15	2.72	0.59
1:A:225:PRO:HG3	1:A:236:PRO:HD3	1.84	0.59
1:A:64:LYS:HB2	1:A:71:TRP:CZ3	2.38	0.59
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	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:HD12	1:A:228:LEU:N	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:418:ASN:C	1:A:418:ASN:HD22	2.11	0.58
1:A:25:PRO:HG3	1:A:137:ASN:CG	2.29	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
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
1:A:57:ASN:ND2	1:A:143:ARG:NH2	2.49	0.57
1:A:296:THR:C	1:A:300:GLU:HG3	2.26	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
1:A:517:LEU:HD13	1:A:517:LEU:C	2.29	0.57
3:A:1551:NNI:O3	3:A:1551:NNI:C13	2.51	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:517:LEU:C	1:A:517:LEU:CD1	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1270:ILE:HG13	2:B:1271:TYR:CD1	2.40	0.56
2:B:1361:HIS:CG	2:B:1361:HIS:O	2.59	0.56
2:B:1391:LEU:CD2	2:B:1414:TRP:HB2	2.35	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: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:82:LYS:NZ	1:A:82:LYS:HB3	2.21	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: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:194:GLU:CD	1:A:194:GLU:N	2.62	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
2:B:1320:ASP:OD1	2:B:1320:ASP:C	2.48	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
1:A:457:TYR:C	1:A:457:TYR:CD2	2.84	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
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: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:HB3	1:A:431:LYS:HZ3	1.72	0.54
1:A:430:GLU:OE2	1:A:530:LYS:HG2	2.08	0.54
1:A:482:ILE:CD1	1:A:486:LEU:HD12	2.37	0.54
2:B:1378:GLU:O	2:B:1382:ILE:HG13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:O	1:A:195:ILE:C	2.50	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:26:LEU:HD22	1:A:26:LEU:N	2.22	0.54
1:A:221:HIS:O	1:A:223:LYS:N	2.40	0.54
1:A:302:GLU:HA	1:A:305:GLU:CD	2.33	0.54
1:A:538:ALA:O	1:A:539:HIS:C	2.51	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:1076:ASP:CG	2:B:1078:ARG:HE	2.16	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: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
2:B:1418:ASN:O	2:B:1419:THR:C	2.52	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
1:A:220:LYS:O	1:A:221:HIS:C	2.49	0.53
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:H	2:B:1244:ILE:CD1	2.21	0.53
1:A:267:ALA:O	1:A:269:GLN:N	2.42	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
2:B:1428:GLN:C	2:B:1428:GLN:CD	2.69	0.53
1:A:229:TRP:CE3	3:A:1551:NNI:H4	2.44	0.52
1:A:467:VAL:HG23	1:A:467:VAL:O	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:O	1:A:20:LYS:CG	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:O	1:A:219:LYS:HG3	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:64:LYS:HB2	1:A:71:TRP:CE3	2.45	0.52
1:A:222:GLN:O	1:A:223:LYS:O	2.28	0.52
1:A:288:ALA:HB3	1:A:291:GLU:CD	2.33	0.52
1:A:460:ASN:HA	2:B:1286:THR:O	2.09	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:NE2	1:A:278:GLN:HA	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
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
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:357:MET:C	1:A:359:GLY:N	2.68	0.51
1:A:369:THR:HG21	1:A:409:THR:HG21	1.92	0.51
1:A:439:THR:HG23	2:B:1289:LEU:HD23	1.93	0.51
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.41	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:43:LYS:NZ	1:A:43:LYS:HB3	2.25	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TRP:HZ3	1:A:61:PHE:HB3	1.76	0.50
1:A:351:THR:CG2	1:A:352:GLY:N	2.74	0.50
2:B:1317:VAL:CG1	2:B:1349:LEU:HD13	2.42	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:281:LYS:C	1:A:283:LEU:N	2.69	0.50
1:A:51:GLY:O	1:A:52:PRO:C	2.55	0.49
2:B:1296:THR:HG22	2:B:1298:GLU:H	1.77	0.49
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.93	0.49
1:A:104:LYS:HZ2	1:A:194:GLU:HA	1.77	0.49
1:A:171:PHE:C	1:A:171:PHE:CD2	2.90	0.49
1:A:228:LEU:N	1:A:228:LEU:CD1	2.75	0.49
2:B:1107:THR:CG2	4:B:2010:HOH:O	2.60	0.49
1:A:78:ARG:O	1:A:81:ASN:HB2	2.13	0.49
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.74	0.49
1:A:402:TRP:CD1	1:A:402:TRP:C	2.90	0.49
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.31	0.49
1:A:433:PRO:CG	2:B:1255:ASN:OD1	2.60	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
1:A:50:ILE:HG12	1:A:54:ASN:HD22	1.74	0.49
1:A:317:VAL:HG12	1:A:318:TYR:O	2.13	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:482:ILE:C	1:A:482:ILE:CD1	2.80	0.49
2:B:1012:LEU:O	2:B:1013:LYS:C	2.54	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
2:B:1333:GLY:O	2:B:1334:GLN:HB2	2.11	0.49
1:A:16:MET:HE2	1:A:83:ARG:HG2	1.94	0.48
1:A:107:THR:HA	1:A:223:LYS:HG3	1.94	0.48
1:A:356:ARG:C	1:A:357:MET:HG3	2.38	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:1102:LYS:O	2:B:1237:ASP:HB2	2.13	0.48
2:B:1116:PHE:HB2	4:B:2012:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.95	0.48
2:B:1332:GLN:HA	2:B:1332:GLN:OE1	2.14	0.48
1:A:263:LYS:HA	1:A:263:LYS:HD3	1.68	0.48
2:B:1064:LYS:O	2:B:1065:LYS:HB2	2.10	0.48
1:A:542:ILE:O	1:A:543:GLY:C	2.56	0.48
2:B:1022:LYS:HD2	2:B:1022:LYS:H	1.78	0.48
2:B:1058:THR:HG21	2:B:1075:VAL:HG12	1.94	0.48
2:B:1184:MET:C	2:B:1186:ASP:H	2.22	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:77:PHE:O	1:A:78:ARG:C	2.56	0.48
1:A:267:ALA:C	1:A:269:GLN:N	2.66	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:281:LYS:C	1:A:283:LEU:H	2.21	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: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:1168:LEU:O	2:B:1169:GLU:C	2.57	0.47
2:B:1270:ILE:HG23	2:B:1271:TYR:HD1	1.79	0.47
1:A:41:MET:HE1	1:A:73:LYS:HZ1	1.79	0.47
1:A:169:GLU:N	1:A:170:PRO:CD	2.78	0.47
1:A:363:ASN:O	1:A:364:ASP:C	2.57	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:HB2	1:A:358:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1090:VAL:HG12	2:B:1090:VAL:O	2.13	0.47
2:B:1101:LYS:O	2:B:1101:LYS:HG2	2.10	0.47
2:B:1194:GLU:O	2:B:1195:ILE:C	2.57	0.47
1:A:336:GLN:OE1	1:A:355:ALA:HB1	2.12	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
1:A:482:ILE:HD13	1:A:486:LEU:HD12	1.96	0.47
1:A:511:ASP:C	1:A:511:ASP:OD2	2.57	0.47
2:B:1011:LYS:HD2	2:B:1011:LYS:O	2.15	0.47
2:B:1389:PHE:O	2:B:1415:GLU:N	2.45	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:OE2	1:A:308:GLU:HA	2.15	0.47
1:A:428:GLN:HA	1:A:428:GLN:NE2	2.17	0.47
2:B:1011:LYS:HD2	2:B:1011:LYS:C	2.39	0.47
1:A:107:THR:HG22	1:A:189:VAL:HB	1.97	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:1286:THR:OG1	2:B:1287:LYS:N	2.47	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:24:TRP:O	1:A:25:PRO:C	2.57	0.46
1:A:41:MET:HE1	1:A:73:LYS:HZ2	1.80	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:1260:LEU:HD13	2:B:1260:LEU:C	2.39	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
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:410:TRP:CE3	2:B:1363:ASN:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:GLU:C	2:B:1169:GLU:CD	2.83	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:1037:ILE:HG23	2:B:1041:MET:HE2	1.97	0.46
2:B:1092:LEU:HB2	2:B:1158:ALA:HB1	1.98	0.46
1:A:90:VAL:HG12	1:A:90:VAL:O	2.16	0.46
1:A:107:THR:HA	1:A:223:LYS:CG	2.46	0.46
1:A:20:LYS:HD2	1:A:20:LYS:C	2.41	0.45
1:A:96:HIS:H	2:B:1136:ASN:ND2	2.07	0.45
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
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
2:B:1334:GLN:HE21	2:B:1334:GLN:HA	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
2:B:1027:THR:O	2:B:1031:ILE:HG13	2.16	0.45
2:B:1028:GLU:CB	2:B:1135:ILE:HD11	2.47	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:1042:GLU:HG3	2:B:1043:LYS:N	2.30	0.45
2:B:1263:LYS:HA	2:B:1426:TRP:CD1	2.52	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:336:GLN:CD	1:A:355:ALA:HB1	2.42	0.45
1:A:490:GLY:C	1:A:492:GLU:H	2.25	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:492:GLU:C	1:A:493:VAL:HG23	2.42	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:408:ALA:HB1	2:B:1364:ASP:HB3	1.98	0.44
1:A:425:LEU:H	1:A:425:LEU:HD22	1.82	0.44
1:A:89:GLU:OE1	1:A:91:GLN:NE2	2.43	0.44
1:A:320:ASP:OD2	1:A:320:ASP:C	2.60	0.44
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
2:B:1236:PRO:HA	2:B:1239:TRP:CE2	2.53	0.44
1:A:13:LYS:O	1:A:14:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1293:ILE:O	2:B:1293:ILE:HG13	2.18	0.44
1:A:198:HIS:NE2	1:A:202:ILE:HD11	2.32	0.44
1:A:476:LYS:C	1:A:478:GLU:N	2.74	0.44
2:B:1334:GLN:HE21	2:B:1334:GLN:CA	2.30	0.44
1:A:136:ASN:O	1:A:137:ASN:C	2.61	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:O	2:B:1090:VAL:CG1	2.66	0.43
2:B:1121:ASP:O	2:B:1122:GLU:C	2.61	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:1099:GLY:O	2:B:1100:LEU:C	2.61	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
2:B:1374:LYS:CE	2:B:1378:GLU:OE2	2.67	0.43
1:A:439:THR:CG2	2:B:1289:LEU:HD23	2.48	0.43
2:B:1183:TYR:O	2:B:1184:MET:C	2.62	0.43
2:B:1420:PRO:CG	2:B:1423:VAL:HG21	2.49	0.43
1:A:139:THR:O	1:A:140:PRO:C	2.61	0.43
1:A:357:MET:HE2	1:A:357:MET:N	2.33	0.43
1:A:358:ARG:HB2	1:A:358:ARG:CZ	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:1312:GLU:HA	2:B:1312:GLU:OE2	2.18	0.43
1:A:49:LYS:HE2	1:A:142:ILE:HG23	2.01	0.43
1:A:355:ALA:C	1:A:356:ARG:HG2	2.44	0.43
2:B:1373:GLN:HE21	2:B:1373:GLN:HB2	1.55	0.42
1:A:60:VAL:HG23	1:A:75:VAL:HG22	2.00	0.42
1:A:135:ILE:O	1:A:135:ILE:CG2	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
2:B:1012:LEU:HD23	2:B:1012:LEU:C	2.44	0.42
2:B:1052:PRO:C	2:B:1054:ASN:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:435:VAL:HG22	2:B:1290:THR:HG21	2.00	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
2:B:1304:ALA:O	2:B:1307:ARG:HB3	2.19	0.42
2:B:1388:LYS:HE3	2:B:1388:LYS:HB2	1.86	0.42
1:A:63:ILE:CG2	1:A:72:ARG:HG3	2.50	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:466:VAL:HG12	1:A:466:VAL:O	2.18	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:1325:LEU:HD23	2:B:1343:GLN:HG3	2.02	0.42
2:B:1336:GLN:HE21	2:B:1336:GLN:HB3	1.64	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:452:LEU:HD23	1:A:452:LEU:O	2.20	0.41
1:A:480:GLN:CD	1:A:517:LEU:HD21	2.45	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
2:B:1206:ARG:CA	2:B:1206:ARG:HE	2.32	0.41
2:B:1236:PRO:O	2:B:1237:ASP:C	2.63	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
1:A:206:ARG:NH2	1:A:217:PRO:C	2.79	0.41
2:B:1099:GLY:HA3	4:B:2009:HOH:O	2.19	0.41
1:A:447:ASN:HD22	1:A:447:ASN:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1427:TYR:O	2:B:1428:GLN:C	2.63	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
1:A:121:ASP:OD1	1:A:121:ASP:C	2.63	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:25:PRO:HG3	1:A:137:ASN:ND2	2.36	0.41
1:A:27:THR:O	1:A:28:GLU:C	2.62	0.41
1:A:308:GLU:O	1:A:311:LYS:HB2	2.20	0.41
1:A:425:LEU:HD22	1:A:425:LEU:N	2.36	0.41
2:B:1118:VAL:HA	2:B:1119:PRO:HD3	1.86	0.41
2:B:1296:THR:O	2:B:1297:GLU:C	2.63	0.41
2:B:1390:LYS:HD3	2:B:1417:VAL:HG11	2.03	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
1:A:217:PRO:O	1:A:221:HIS:CD2	2.74	0.41
1:A:336:GLN:CD	1:A:355:ALA:CB	2.93	0.41
1:A:431:LYS:HE3	4:A:2014:HOH:O	2.20	0.41
2:B:1263:LYS:CA	2:B:1426:TRP:CD1	3.03	0.41
2:B:1296:THR:O	2:B:1299:ALA:CB	2.69	0.41
2:B:1336:GLN:C	2:B:1337:TRP:CD1	2.99	0.41
1:A:195:ILE:HG22	1:A:196:GLY:H	1.84	0.40
1:A:274:ILE:HD11	1:A:310:LEU:CD1	2.50	0.40
1:A:277:ARG:NH1	1:A:277:ARG:HB3	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:222:GLN:C	1:A:223:LYS:O	2.63	0.40
1:A:227:PHE:HD1	3:A:1551:NNI:I15	2.74	0.40
2:B:1317:VAL:CG2	2:B:1347:LYS:HB3	2.50	0.40
1:A:244:ILE:O	1:A:244:ILE:HG23	2.21	0.40
1:A:447:ASN:HB3	1:A:450:THR:HB	2.04	0.40
1:A:540:LYS:O	1:A:541:GLY:C	2.65	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%)	2	7
2	B	385/428 (90%)	329 (86%)	46 (12%)	10 (3%)	4	14
All	All	926/985 (94%)	794 (86%)	100 (11%)	32 (4%)	3	9

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%)	434 (89%)	52 (11%)	6	20
2	B	361/390 (93%)	328 (91%)	33 (9%)	9	27
All	All	847/887 (96%)	762 (90%)	85 (10%)	7	23

All (85) 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	26	LEU
1	A	29	GLU
1	A	34	LEU
1	A	43	LYS
1	A	44	GLU
1	A	82	LYS
1	A	107	THR
1	A	108	VAL
1	A	123	ASP
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	167	ILE
1	A	169	GLU
1	A	179	VAL
1	A	182	GLN
1	A	194	GLU
1	A	209	LEU
1	A	211	ARG
1	A	223	LYS
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	295	LEU
1	A	309	ILE
1	A	338	THR
1	A	351	THR
1	A	354	TYR
1	A	356	ARG
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	417	VAL
1	A	418	ASN
1	A	424	LYS
1	A	428	GLN
1	A	477	THR
1	A	482	ILE
1	A	494	ASN
1	A	497	THR
1	A	517	LEU
1	A	540	LYS
2	B	1026	LEU
2	B	1058	THR
2	B	1065	LYS

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Mol	Chain	Res	Type
2	B	1070	LYS
2	B	1078	ARG
2	B	1080	LEU
2	B	1086	ASP
2	B	1101	LYS
2	B	1189	VAL
2	B	1195	ILE
2	B	1206	ARG
2	B	1237	ASP
2	B	1244	ILE
2	B	1245	VAL
2	B	1257	ILE
2	B	1259	LYS
2	B	1279	LEU
2	B	1289	LEU
2	B	1292	VAL
2	B	1295	LEU
2	B	1303	LEU
2	B	1324	ASP
2	B	1326	ILE
2	B	1330	GLN
2	B	1334	GLN
2	B	1344	GLU
2	B	1349	LEU
2	B	1373	GLN
2	B	1374	LYS
2	B	1381	VAL
2	B	1391	LEU
2	B	1403	THR
2	B	1428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) 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	207	GLN

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Mol	Chain	Res	Type
1	A	208	HIS
1	A	255	ASN
1	A	269	GLN
1	A	278	GLN
1	A	315	HIS
1	A	332	GLN
1	A	340	GLN
1	A	361	HIS
1	A	367	GLN
1	A	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	539	HIS
1	A	545	ASN
2	B	1081	ASN
2	B	1136	ASN
2	B	1147	ASN
2	B	1151	GLN
2	B	1182	GLN
2	B	1235	HIS
2	B	1242	GLN
2	B	1265	ASN
2	B	1334	GLN
2	B	1336	GLN
2	B	1340	GLN
2	B	1367	GLN
2	B	1394	GLN
2	B	1428	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	NNI	A	1551	-	26,26,26	2.43	6 (23%)	36,36,36	2.82	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	-6.04	1.39	1.48
3	A	1551	NNI	C1-C7	-5.84	1.39	1.48
3	A	1551	NNI	C7-N1	-5.35	1.33	1.39
3	A	1551	NNI	C8-N1	-5.11	1.33	1.39
3	A	1551	NNI	C12-N2	-4.04	1.33	1.41
3	A	1551	NNI	O3-C11	2.37	1.36	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1551	NNI	C10-O3-C11	-10.13	111.10	119.04
3	A	1551	NNI	O3-C11-S1	-6.48	119.86	125.07
3	A	1551	NNI	C2-C8-N1	4.80	109.43	105.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1551	NNI	C1-C7-N1	4.68	109.34	105.88
3	A	1551	NNI	O3-C11-N2	4.50	120.99	112.20
3	A	1551	NNI	C12-N2-C11	-4.12	122.95	130.07
3	A	1551	NNI	C7-N1-C8	-3.73	108.83	112.02
3	A	1551	NNI	C6-C1-C7	2.40	133.62	129.59
3	A	1551	NNI	C1-C2-C8	-2.37	106.18	108.26
3	A	1551	NNI	C2-C1-C7	-2.34	106.21	108.26
3	A	1551	NNI	C3-C2-C8	2.16	133.21	129.59
3	A	1551	NNI	O2-C8-C2	-2.14	124.51	128.66

There are no chirality outliers.

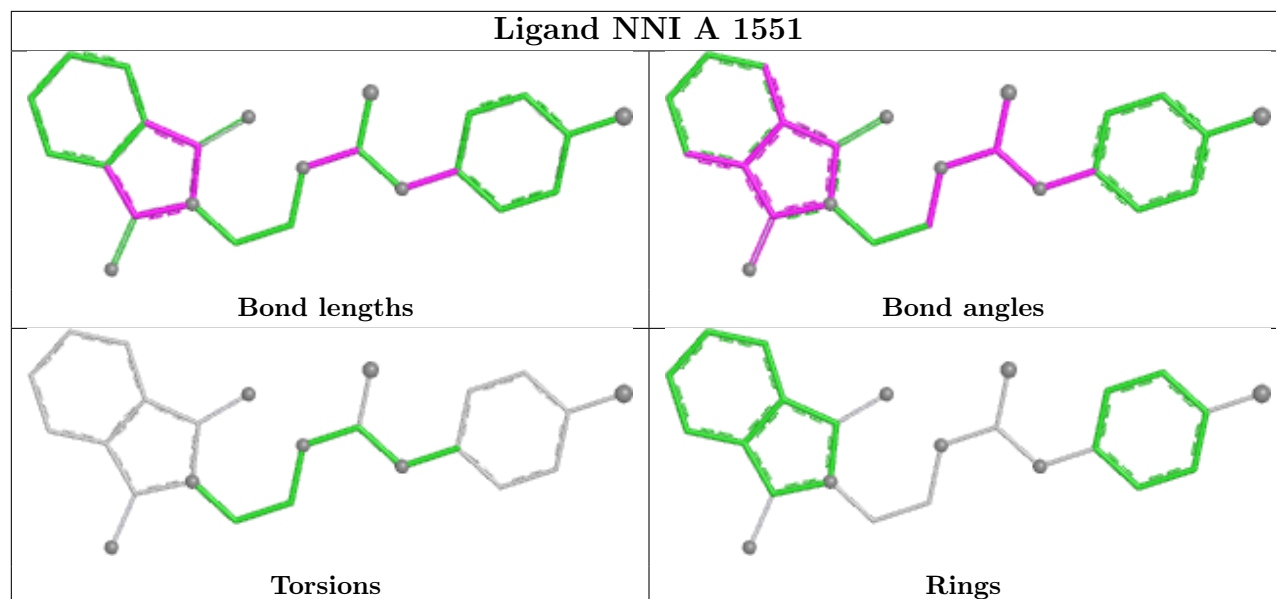
There are no torsion outliers.

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 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	545/557 (97%)	0.86	71 (13%) 7 5	33, 54, 78, 89	0
2	B	395/428 (92%)	0.87	60 (15%) 5 4	31, 51, 87, 95	0
All	All	940/985 (95%)	0.87	131 (13%) 6 5	31, 53, 85, 95	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	ASN	6.3
2	B	1231	GLY	6.1
1	A	75	VAL	5.8
1	A	218	ASP	4.8
2	B	1301	LEU	4.7
1	A	76	ASP	4.6
2	B	1240	THR	4.5
1	A	122	GLU	4.3
2	B	1251	SER	4.3
1	A	294	PRO	4.3
2	B	1426	TRP	4.1
1	A	224	GLU	4.1
2	B	1248	GLU	4.0
2	B	1310	LEU	4.0
2	B	1162	SER	4.0
2	B	1422	LEU	3.9
1	A	301	LEU	3.9
2	B	1090	VAL	3.9
2	B	1014	PRO	3.9
2	B	1418	ASN	3.9
2	B	1423	VAL	3.8
1	A	358	ARG	3.7
2	B	1420	PRO	3.7
1	A	219	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	1028	GLU	3.6
1	A	60	VAL	3.6
1	A	354	TYR	3.5
1	A	50	ILE	3.4
1	A	225	PRO	3.4
1	A	144	TYR	3.3
2	B	1257	ILE	3.3
2	B	1266	TRP	3.3
1	A	519	ASN	3.2
1	A	93	GLY	3.2
1	A	131	THR	3.2
1	A	359	GLY	3.2
1	A	278	GLN	3.1
1	A	51	GLY	3.1
1	A	288	ALA	3.1
1	A	472	THR	3.1
1	A	515	SER	3.1
1	A	226	PRO	3.1
1	A	231	GLY	3.0
2	B	1303	LEU	3.0
1	A	298	GLU	3.0
1	A	111	VAL	3.0
2	B	1250	ASP	3.0
2	B	1015	GLY	2.9
1	A	138	GLU	2.9
1	A	161	GLN	2.9
1	A	24	TRP	2.8
2	B	1282	LEU	2.8
1	A	522	ILE	2.8
1	A	77	PHE	2.8
1	A	304	ALA	2.8
2	B	1264	LEU	2.8
2	B	1292	VAL	2.7
2	B	1232	TYR	2.7
2	B	1362	THR	2.7
2	B	1010	VAL	2.7
2	B	1011	LYS	2.7
2	B	1249	LYS	2.7
1	A	306	ASN	2.7
1	A	174	GLN	2.6
1	A	223	LYS	2.6
1	A	52	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1275	LYS	2.6
2	B	1085	GLN	2.6
1	A	355	ALA	2.6
1	A	279	LEU	2.5
1	A	177	ASP	2.5
1	A	357	MET	2.5
2	B	1302	GLU	2.5
1	A	487	GLN	2.5
2	B	1237	ASP	2.5
2	B	1230	MET	2.5
2	B	1273	GLY	2.5
1	A	277	ARG	2.5
1	A	54	ASN	2.5
2	B	1044	GLU	2.5
2	B	1195	ILE	2.4
2	B	1007	THR	2.4
1	A	120	LEU	2.4
1	A	18	GLY	2.4
2	B	1267	ALA	2.4
2	B	1361	HIS	2.4
1	A	217	PRO	2.4
2	B	1295	LEU	2.4
1	A	448	ARG	2.3
1	A	428	GLN	2.3
1	A	402	TRP	2.3
2	B	1024	TRP	2.3
1	A	193	LEU	2.3
2	B	1206	ARG	2.3
2	B	1417	VAL	2.3
1	A	474	ASN	2.3
2	B	1241	VAL	2.3
1	A	332	GLN	2.3
1	A	356	ARG	2.3
2	B	1276	VAL	2.3
1	A	74	LEU	2.2
2	B	1424	LYS	2.2
2	B	1277	ARG	2.2
1	A	286	THR	2.2
1	A	291	GLU	2.2
1	A	23	GLN	2.2
1	A	247	PRO	2.2
1	A	302	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1074	LEU	2.2
1	A	313	PRO	2.2
2	B	1088	TRP	2.2
1	A	22	LYS	2.2
1	A	305	GLU	2.2
1	A	195	ILE	2.2
1	A	282	LEU	2.2
1	A	452	LEU	2.2
2	B	1234	LEU	2.2
2	B	1094	ILE	2.1
2	B	1177	ASP	2.1
1	A	58	THR	2.1
2	B	1307	ARG	2.1
2	B	1212	TRP	2.1
1	A	19	PRO	2.1
2	B	1141	GLY	2.1
1	A	57	ASN	2.1
2	B	1005	ILE	2.1
2	B	1043	LYS	2.0
2	B	1035	VAL	2.0
1	A	55	PRO	2.0
2	B	1294	PRO	2.0
2	B	1308	GLU	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.

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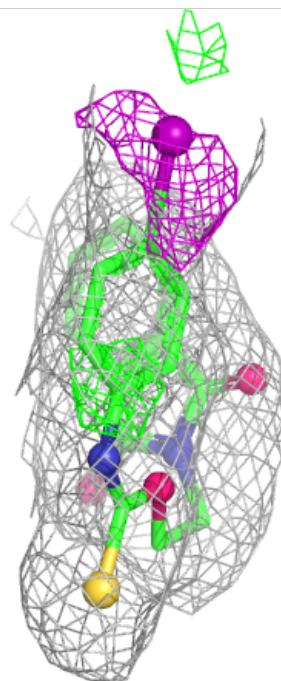
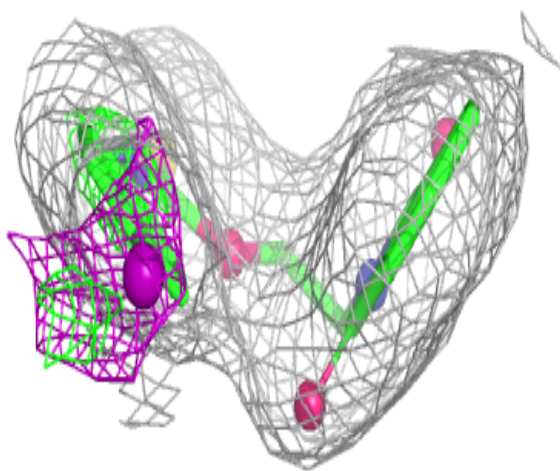
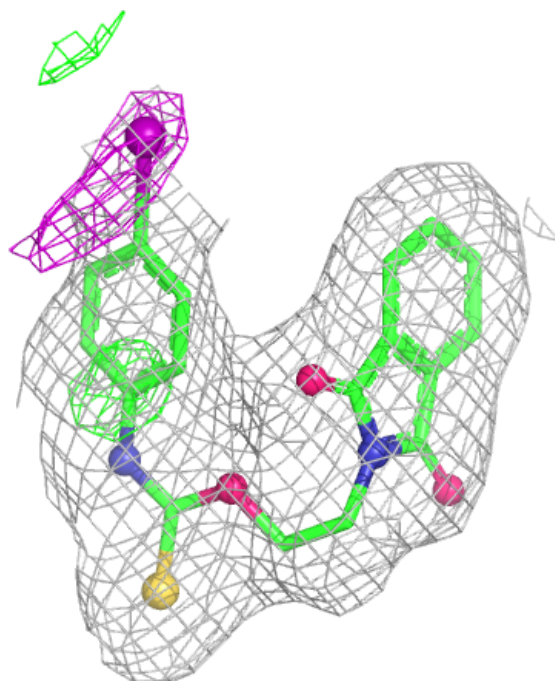
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NNI	A	1551	24/24	0.94	0.12	37,40,72,81	0

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.