



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 05:41 pm BST

PDB ID : 1JZQ  
Title : Isoleucyl-tRNA synthetase Complexed with Isoleucyl-adenylate analogue  
Authors : Nakama, T.; Nureki, O.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2001-09-17  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

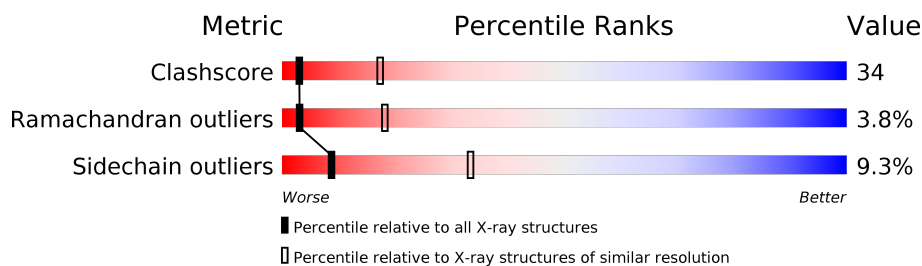
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	821	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6731 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.

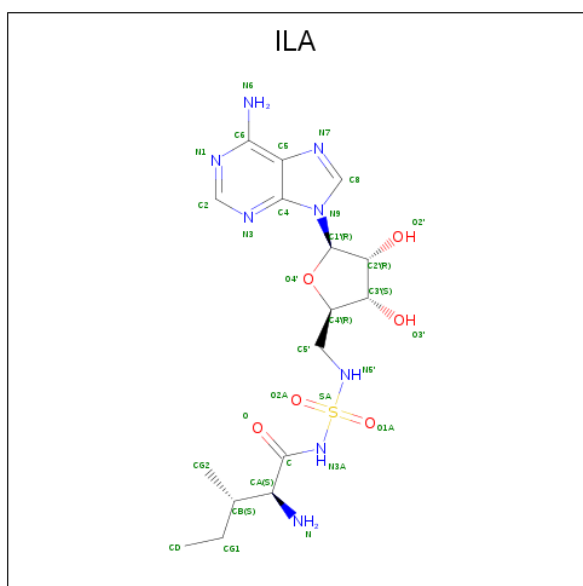
- Molecule 1 is a protein called Isoleucyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	821	Total	C	N	O	S	0	0	0
			6698	4334	1144	1200	20			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is N-[ISOLEUCINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (three-letter code: ILA) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>8</sub>O<sub>6</sub>S).

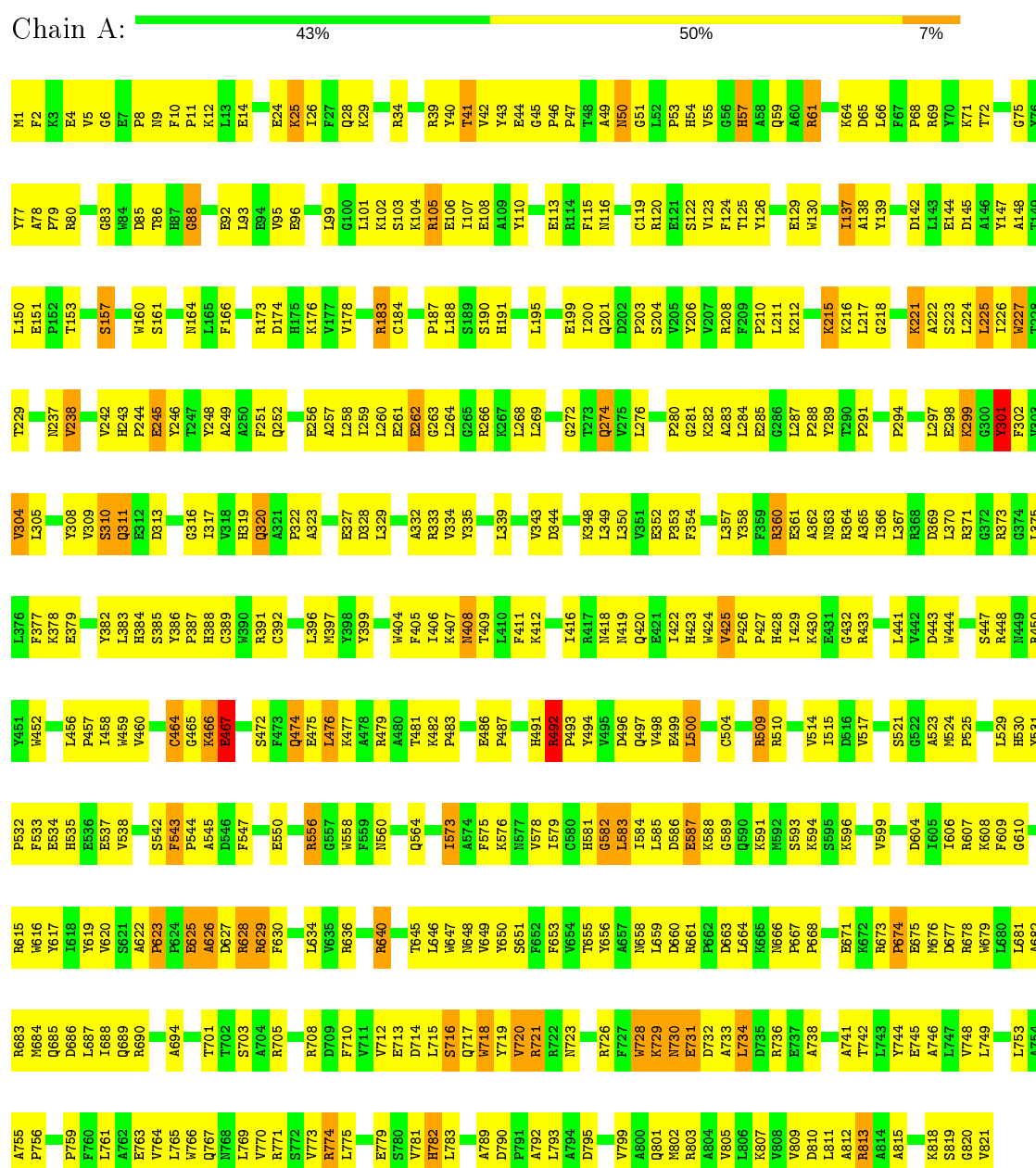


### 3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Isoleucyl-tRNA synthetase



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.47Å 95.19Å 126.21Å 90.00° 126.22° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 5 Model quality [i](#)

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

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

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	0.39	0/6901	0.67	3/9386 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	88	GLY	N-CA-C	5.89	127.83	113.10
1	A	137	ILE	N-CA-C	-5.58	95.94	111.00
1	A	529	LEU	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6698	0	6573	455	1
2	A	2	0	0	0	0
3	A	31	0	26	3	0
All	All	6731	0	6599	455	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (455) 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:370:LEU:HD22	1:A:375:LEU:HD11	1.42	1.02
1:A:425:VAL:HG21	1:A:579:ILE:HG12	1.43	1.01
1:A:676:MET:HG2	1:A:723:ASN:HD21	1.31	0.92
1:A:5:VAL:HG23	1:A:6:GLY:H	1.36	0.89
1:A:694:ALA:HB3	1:A:703:SER:HB3	1.56	0.87
1:A:629:ARG:NH1	1:A:629:ARG:H	1.73	0.86
1:A:408:ASN:H	1:A:408:ASN:HD22	1.21	0.84
1:A:629:ARG:HH11	1:A:629:ARG:HB2	1.41	0.84
1:A:408:ASN:HD21	1:A:443:ASP:HA	1.43	0.83
1:A:426:PRO:HB3	1:A:625:GLU:HG2	1.61	0.82
1:A:199:GLU:HA	1:A:385:SER:HA	1.62	0.81
1:A:712:VAL:HG12	1:A:716:SER:HB2	1.63	0.81
1:A:215:LYS:HZ2	1:A:215:LYS:HB2	1.45	0.81
1:A:767:GLN:O	1:A:771:ARG:HB2	1.81	0.80
1:A:726:ARG:O	1:A:731:GLU:HG3	1.82	0.80
1:A:252:GLN:HB2	1:A:276:LEU:HD21	1.63	0.79
1:A:729:LYS:HD2	1:A:730:ASN:N	1.97	0.79
1:A:25:LYS:NZ	1:A:25:LYS:HB3	1.98	0.78
1:A:675:GLU:HA	1:A:678:ARG:NH1	1.99	0.78
1:A:408:ASN:N	1:A:408:ASN:HD22	1.79	0.78
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.47	0.77
1:A:755:ALA:HB3	1:A:756:PRO:HD3	1.67	0.76
1:A:148:ALA:O	1:A:151:GLU:HG3	1.85	0.76
1:A:138:ALA:HB3	1:A:759:PRO:HG3	1.69	0.75
1:A:65:ASP:O	1:A:68:PRO:HD2	1.87	0.75
1:A:34:ARG:HD2	1:A:75:GLY:HA2	1.67	0.75
1:A:412:LYS:O	1:A:416:ILE:HG13	1.85	0.74
1:A:509:ARG:HH11	1:A:509:ARG:HB3	1.52	0.74
1:A:674:PRO:HB2	1:A:726:ARG:HH22	1.52	0.74
1:A:418:ASN:HB3	1:A:573:ILE:HG22	1.70	0.74
1:A:50:ASN:HD22	1:A:51:GLY:N	1.85	0.74
1:A:543:PHE:HB3	1:A:544:PRO:HD3	1.68	0.74
1:A:221:LYS:HE3	1:A:222:ALA:N	2.03	0.73
1:A:370:LEU:HD22	1:A:375:LEU:CD1	2.17	0.73
1:A:582:GLY:HA3	1:A:626:ALA:O	1.89	0.72
1:A:674:PRO:CB	1:A:726:ARG:HH22	2.02	0.72
1:A:801:GLN:O	1:A:805:VAL:HG23	1.90	0.72
1:A:59:GLN:NE2	1:A:581:HIS:HD2	1.87	0.72
1:A:54:HIS:O	1:A:57:HIS:HB2	1.88	0.71
1:A:681:LEU:HD13	1:A:793:LEU:HD23	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:OD1	1:A:12:LYS:HD3	1.90	0.71
1:A:717:GLN:O	1:A:718:TRP:HE3	1.73	0.71
1:A:715:LEU:HD13	1:A:716:SER:N	2.06	0.70
1:A:731:GLU:OE2	1:A:736:ARG:HB3	1.92	0.70
1:A:237:ASN:HB2	1:A:319:HIS:CE1	2.27	0.70
1:A:353:PRO:HG2	1:A:354:PHE:CD1	2.27	0.69
1:A:460:VAL:HG13	1:A:466:LYS:HB3	1.74	0.69
1:A:64:LYS:O	1:A:64:LYS:HD3	1.92	0.69
1:A:675:GLU:HA	1:A:678:ARG:HH12	1.55	0.69
1:A:675:GLU:HG3	1:A:678:ARG:HH22	1.57	0.69
1:A:408:ASN:ND2	1:A:443:ASP:HA	2.07	0.69
1:A:456:LEU:HG	1:A:458:ILE:HD12	1.72	0.69
1:A:456:LEU:HD13	1:A:515:ILE:HD11	1.75	0.69
1:A:45:GLY:HA3	3:A:1301:ILA:HD2	1.74	0.68
1:A:668:PRO:HB2	1:A:673:ARG:CZ	2.23	0.68
1:A:690:ARG:HH21	1:A:803:ARG:NH2	1.91	0.67
1:A:64:LYS:HD2	1:A:139:TYR:CE1	2.29	0.67
1:A:608:LYS:HB3	1:A:608:LYS:NZ	2.09	0.67
1:A:712:VAL:CG1	1:A:716:SER:HB2	2.25	0.67
1:A:459:TRP:CE2	1:A:510:ARG:HB3	2.29	0.67
1:A:629:ARG:H	1:A:629:ARG:CZ	2.07	0.67
1:A:715:LEU:HD22	1:A:720:VAL:HG11	1.77	0.67
1:A:408:ASN:H	1:A:408:ASN:ND2	1.94	0.66
1:A:42:VAL:HG12	1:A:64:LYS:HE2	1.78	0.66
1:A:673:ARG:HH12	1:A:738:ALA:HB3	1.60	0.66
1:A:95:VAL:HG21	1:A:119:CYS:HA	1.77	0.66
1:A:10:PHE:O	1:A:14:GLU:HG3	1.96	0.66
1:A:645:THR:HG23	1:A:715:LEU:HG	1.77	0.65
1:A:587:GLU:O	1:A:588:LYS:HG2	1.95	0.65
1:A:25:LYS:HB3	1:A:25:LYS:HZ3	1.61	0.65
1:A:64:LYS:HD2	1:A:139:TYR:HE1	1.61	0.65
1:A:532:PRO:HG2	1:A:533:PHE:CD1	2.31	0.65
1:A:608:LYS:HB3	1:A:608:LYS:HZ3	1.60	0.65
1:A:215:LYS:H	1:A:215:LYS:HE3	1.60	0.65
1:A:486:GLU:HB2	1:A:487:PRO:HD3	1.78	0.64
1:A:464:CYS:SG	1:A:465:GLY:N	2.68	0.64
1:A:728:TRP:HA	1:A:728:TRP:CE3	2.32	0.64
1:A:585:LEU:HB2	1:A:629:ARG:HA	1.78	0.64
1:A:262:GLU:HG2	1:A:263:GLY:N	2.12	0.64
1:A:101:LEU:HD23	1:A:107:ILE:HG13	1.80	0.64
1:A:386:TYR:CD1	1:A:387:PRO:HD2	2.33	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:CD1	1:A:287:LEU:HD11	2.28	0.64
1:A:456:LEU:HG	1:A:458:ILE:CD1	2.27	0.64
1:A:583:LEU:HD23	1:A:584:ILE:N	2.13	0.64
1:A:425:VAL:CG2	1:A:579:ILE:HG12	2.22	0.63
1:A:715:LEU:CD2	1:A:720:VAL:HG11	2.28	0.63
1:A:676:MET:CG	1:A:723:ASN:HD21	2.08	0.63
1:A:728:TRP:HE3	1:A:728:TRP:HA	1.63	0.63
1:A:8:PRO:HG3	1:A:647:TRP:CD1	2.34	0.63
1:A:684:MET:O	1:A:688:ILE:HG13	1.98	0.63
1:A:426:PRO:HG2	1:A:429:ILE:HG13	1.79	0.63
1:A:5:VAL:HG23	1:A:6:GLY:N	2.11	0.63
1:A:291:PRO:O	1:A:294:PRO:HD3	1.99	0.63
1:A:543:PHE:O	1:A:544:PRO:C	2.34	0.63
1:A:244:PRO:HB3	1:A:305:LEU:HD22	1.82	0.62
1:A:238:VAL:HG12	1:A:297:LEU:HD11	1.82	0.62
1:A:354:PHE:O	1:A:357:LEU:HD23	1.99	0.62
1:A:99:LEU:HD13	1:A:110:TYR:CZ	2.35	0.62
1:A:456:LEU:CD1	1:A:515:ILE:HD11	2.30	0.62
1:A:5:VAL:HG11	1:A:651:SER:HA	1.81	0.62
1:A:793:LEU:H	1:A:793:LEU:HD12	1.64	0.61
1:A:425:VAL:HG12	1:A:426:PRO:N	2.14	0.61
1:A:212:LYS:HE3	1:A:288:PRO:HB2	1.81	0.61
1:A:61:ARG:HG2	1:A:61:ARG:NH1	2.15	0.61
1:A:677:ASP:HB3	1:A:742:THR:HG21	1.82	0.61
1:A:41:THR:HG21	1:A:542:SER:HA	1.82	0.60
1:A:263:GLY:HA2	1:A:266:ARG:HG2	1.84	0.60
1:A:243:HIS:HB2	1:A:309:VAL:HG22	1.83	0.60
1:A:221:LYS:O	1:A:256:GLU:HB2	2.02	0.60
1:A:524:MET:HB3	1:A:525:PRO:HD3	1.82	0.60
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.14	0.60
1:A:604:ASP:HA	1:A:607:ARG:NH1	2.17	0.60
1:A:120:ARG:O	1:A:123:VAL:HG22	2.02	0.60
1:A:805:VAL:O	1:A:809:VAL:HG23	2.02	0.60
1:A:650:TYR:HE1	1:A:769:LEU:HD11	1.67	0.59
1:A:370:LEU:CD2	1:A:375:LEU:HD11	2.24	0.59
1:A:93:LEU:HD22	1:A:391:ARG:HB3	1.84	0.59
1:A:211:LEU:HD11	1:A:287:LEU:HD11	1.85	0.59
1:A:679:TRP:CE2	1:A:802:MET:HG2	2.38	0.59
1:A:718:TRP:HA	1:A:718:TRP:CE3	2.35	0.59
1:A:583:LEU:HD23	1:A:584:ILE:H	1.68	0.59
1:A:92:GLU:HG2	1:A:115:PHE:CE2	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:CG1	1:A:64:LYS:HE2	2.32	0.58
1:A:262:GLU:HG2	1:A:263:GLY:H	1.68	0.58
1:A:243:HIS:HD2	1:A:244:PRO:HD2	1.68	0.58
1:A:543:PHE:O	1:A:545:ALA:N	2.36	0.58
1:A:221:LYS:C	1:A:221:LYS:HE3	2.23	0.58
1:A:243:HIS:CD2	1:A:244:PRO:HD2	2.38	0.58
1:A:793:LEU:N	1:A:793:LEU:HD12	2.19	0.58
1:A:629:ARG:HH11	1:A:629:ARG:CB	2.16	0.58
1:A:645:THR:HG23	1:A:715:LEU:CG	2.34	0.58
1:A:753:LEU:O	1:A:756:PRO:HD2	2.02	0.57
1:A:532:PRO:HG2	1:A:533:PHE:CE1	2.39	0.57
1:A:715:LEU:CD1	1:A:716:SER:N	2.67	0.57
1:A:530:HIS:HB3	1:A:534:GLU:HB2	1.86	0.57
1:A:807:LYS:O	1:A:811:LEU:HD23	2.03	0.57
1:A:187:PRO:O	1:A:188:LEU:HD23	2.05	0.57
1:A:77:TYR:O	1:A:79:PRO:HD3	2.05	0.57
1:A:45:GLY:HA3	3:A:1301:ILA:CD	2.34	0.57
1:A:251:PHE:CD2	1:A:269:LEU:HD12	2.40	0.57
1:A:795:ASP:O	1:A:799:VAL:HG23	2.05	0.57
1:A:676:MET:HG2	1:A:723:ASN:ND2	2.12	0.57
1:A:298:GLU:CD	1:A:298:GLU:H	2.09	0.56
1:A:655:THR:O	1:A:659:LEU:HD23	2.05	0.56
1:A:42:VAL:HG21	1:A:68:PRO:HG3	1.87	0.56
1:A:92:GLU:HG2	1:A:115:PHE:HE2	1.70	0.56
1:A:43:TYR:HB3	1:A:524:MET:HE1	1.87	0.56
1:A:560:ASN:ND2	1:A:564:GLN:HE21	2.03	0.56
1:A:215:LYS:CE	1:A:215:LYS:H	2.18	0.56
1:A:88:GLY:HA3	1:A:517:VAL:CG1	2.36	0.56
1:A:104:LYS:O	1:A:108:GLU:HG3	2.05	0.55
1:A:215:LYS:HZ1	1:A:216:LYS:H	1.53	0.55
1:A:50:ASN:C	1:A:50:ASN:HD22	2.08	0.55
1:A:663:ASP:OD1	1:A:666:ASN:HB2	2.06	0.55
1:A:543:PHE:HB3	1:A:544:PRO:CD	2.36	0.55
1:A:629:ARG:NH1	1:A:629:ARG:N	2.49	0.55
1:A:204:SER:HG	1:A:227:TRP:HZ3	1.53	0.55
1:A:649:VAL:HG23	1:A:720:VAL:HG21	1.88	0.55
1:A:674:PRO:HD2	1:A:677:ASP:OD2	2.07	0.55
1:A:285:GLU:OE2	1:A:305:LEU:HD12	2.04	0.55
1:A:733:ALA:O	1:A:734:LEU:C	2.46	0.55
1:A:284:LEU:N	1:A:284:LEU:HD12	2.22	0.55
1:A:764:VAL:CG2	1:A:765:LEU:N	2.70	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD12	1:A:301:TYR:CE1	2.42	0.54
1:A:673:ARG:HA	1:A:673:ARG:NE	2.22	0.54
1:A:103:SER:OG	1:A:105:ARG:HG3	2.07	0.54
1:A:419:ASN:ND2	1:A:424:TRP:HE1	2.06	0.54
1:A:622:ALA:O	1:A:628:ARG:NH2	2.40	0.54
1:A:620:VAL:HG23	1:A:705:ARG:HG2	1.88	0.54
1:A:104:LYS:HD2	1:A:184:CYS:O	2.08	0.54
1:A:333:ARG:HA	1:A:333:ARG:NE	2.21	0.54
1:A:790:ASP:OD2	1:A:792:ALA:HB3	2.08	0.54
1:A:258:LEU:O	1:A:260:LEU:HD23	2.07	0.54
1:A:215:LYS:HB2	1:A:215:LYS:NZ	2.20	0.53
1:A:710:PHE:HA	1:A:713:GLU:HG2	1.89	0.53
1:A:212:LYS:HE2	1:A:289:TYR:O	2.08	0.53
1:A:59:GLN:CD	1:A:581:HIS:HD2	2.11	0.53
1:A:589:GLY:H	1:A:629:ARG:HG2	1.74	0.53
1:A:668:PRO:HG2	1:A:673:ARG:NH1	2.22	0.53
1:A:775:LEU:N	1:A:775:LEU:HD23	2.24	0.53
1:A:353:PRO:HG2	1:A:354:PHE:CE1	2.43	0.53
1:A:694:ALA:CB	1:A:703:SER:HB3	2.34	0.53
1:A:766:TRP:CE3	1:A:770:VAL:HG21	2.44	0.53
1:A:544:PRO:HB2	1:A:576:LYS:HE3	1.90	0.53
1:A:609:PHE:CE2	1:A:636:ARG:HB2	2.43	0.53
1:A:623:PRO:HA	1:A:701:THR:HG21	1.89	0.53
1:A:486:GLU:HB2	1:A:487:PRO:CD	2.39	0.53
1:A:55:VAL:HG11	1:A:630:PHE:CE2	2.44	0.53
1:A:774:ARG:HG2	1:A:774:ARG:HH11	1.74	0.53
1:A:50:ASN:C	1:A:50:ASN:ND2	2.62	0.52
1:A:419:ASN:HD21	1:A:424:TRP:HE1	1.56	0.52
1:A:646:LEU:HD23	1:A:761:LEU:HD21	1.91	0.52
1:A:766:TRP:CB	1:A:781:VAL:HG22	2.39	0.52
1:A:200:ILE:HG12	1:A:201:GLN:N	2.24	0.52
1:A:678:ARG:HB2	1:A:678:ARG:NH1	2.25	0.52
1:A:208:ARG:HH11	1:A:375:LEU:HA	1.75	0.52
1:A:587:GLU:OE2	1:A:634:LEU:HD13	2.10	0.52
1:A:712:VAL:O	1:A:716:SER:HB3	2.09	0.52
1:A:153:THR:HB	1:A:530:HIS:CD2	2.45	0.52
1:A:322:PRO:HB3	1:A:332:ALA:HB2	1.92	0.51
1:A:640:ARG:HG3	1:A:640:ARG:HH11	1.74	0.51
1:A:102:LYS:HE3	1:A:106:GLU:OE2	2.10	0.51
1:A:358:TYR:CD2	1:A:360:ARG:HB2	2.45	0.51
1:A:367:LEU:HD23	1:A:379:GLU:OE1	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ASP:HB3	1:A:793:LEU:HD13	1.91	0.51
1:A:46:PRO:O	1:A:85:ASP:HB2	2.10	0.51
1:A:142:ASP:HB3	1:A:145:ASP:OD1	2.10	0.51
1:A:224:LEU:HD22	1:A:317:ILE:HD13	1.93	0.51
1:A:575:PHE:CD1	1:A:578:VAL:HG22	2.45	0.51
1:A:708:ARG:O	1:A:712:VAL:HG23	2.10	0.51
1:A:364:ARG:HG3	1:A:365:ALA:N	2.25	0.51
1:A:499:GLU:HG2	1:A:509:ARG:HD2	1.92	0.51
1:A:262:GLU:O	1:A:264:LEU:N	2.34	0.51
1:A:86:THR:O	1:A:452:TRP:NE1	2.43	0.51
1:A:429:ILE:HG23	1:A:433:ARG:HB2	1.93	0.51
1:A:620:VAL:HG23	1:A:705:ARG:CG	2.41	0.51
1:A:68:PRO:O	1:A:72:THR:HG23	2.11	0.50
1:A:616:TRP:HZ2	1:A:708:ARG:HB2	1.75	0.50
1:A:161:SER:O	1:A:164:ASN:HB3	2.11	0.50
1:A:284:LEU:H	1:A:284:LEU:HD12	1.75	0.50
1:A:93:LEU:HG	1:A:183:ARG:NH2	2.27	0.50
1:A:765:LEU:O	1:A:769:LEU:HB2	2.11	0.50
1:A:377:PHE:HD1	1:A:378:LYS:HB2	1.77	0.50
1:A:304:VAL:HG13	1:A:335:TYR:CE1	2.47	0.49
1:A:404:TRP:HH2	1:A:467:GLU:HG2	1.78	0.49
1:A:560:ASN:HD21	1:A:564:GLN:HE21	1.58	0.49
1:A:586:ASP:O	1:A:629:ARG:HB3	2.12	0.49
1:A:25:LYS:O	1:A:29:LYS:HD3	2.12	0.49
1:A:674:PRO:CB	1:A:726:ARG:NH2	2.74	0.49
1:A:57:HIS:CE1	1:A:130:TRP:HH2	2.29	0.49
1:A:573:ILE:H	1:A:573:ILE:HD13	1.77	0.49
1:A:763:GLU:OE1	1:A:781:VAL:HG23	2.12	0.49
1:A:116:ASN:ND2	1:A:493:PRO:HD3	2.27	0.49
1:A:497:GLN:NE2	1:A:497:GLN:HA	2.28	0.49
1:A:649:VAL:HG22	1:A:649:VAL:O	2.13	0.49
1:A:200:ILE:HG12	1:A:201:GLN:H	1.78	0.49
1:A:425:VAL:HG23	1:A:578:VAL:O	2.13	0.49
1:A:820:GLY:O	1:A:821:VAL:HB	2.13	0.49
1:A:263:GLY:CA	1:A:266:ARG:HG2	2.42	0.49
1:A:43:TYR:HB3	1:A:524:MET:CE	2.43	0.49
1:A:243:HIS:HD2	1:A:244:PRO:CD	2.26	0.48
1:A:653:PHE:CZ	1:A:744:TYR:HB2	2.48	0.48
1:A:206:TYR:HD1	1:A:378:LYS:HB3	1.77	0.48
1:A:479:ARG:HB3	1:A:500:LEU:HB3	1.94	0.48
1:A:714:ASP:O	1:A:720:VAL:HB	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:VAL:HG23	1:A:765:LEU:N	2.28	0.48
1:A:425:VAL:O	1:A:427:PRO:N	2.46	0.48
1:A:49:ALA:O	1:A:126:TYR:HB2	2.13	0.48
1:A:24:GLU:OE1	1:A:779:GLU:OE2	2.31	0.48
1:A:298:GLU:O	1:A:299:LYS:HB2	2.14	0.48
1:A:426:PRO:HG2	1:A:429:ILE:CG1	2.43	0.48
1:A:685:GLN:O	1:A:689:GLN:HG3	2.12	0.48
1:A:708:ARG:C	1:A:708:ARG:HD3	2.34	0.48
1:A:291:PRO:HG3	1:A:301:TYR:CE2	2.48	0.48
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.79	0.48
1:A:477:LYS:CE	1:A:483:PRO:HA	2.44	0.48
1:A:535:HIS:HA	1:A:537:GLU:OE2	2.14	0.48
1:A:728:TRP:O	1:A:731:GLU:HB2	2.14	0.48
1:A:242:VAL:HB	1:A:248:TYR:CZ	2.48	0.48
1:A:280:PRO:HG2	1:A:283:ALA:HB2	1.95	0.48
1:A:333:ARG:HD3	1:A:333:ARG:O	2.14	0.48
1:A:425:VAL:HG12	1:A:426:PRO:CD	2.43	0.48
1:A:586:ASP:C	1:A:588:LYS:N	2.66	0.48
1:A:377:PHE:C	1:A:377:PHE:CD1	2.87	0.48
1:A:492:ARG:HD2	1:A:492:ARG:HA	1.44	0.48
1:A:5:VAL:CG2	1:A:6:GLY:H	2.18	0.48
1:A:781:VAL:C	1:A:783:LEU:H	2.16	0.48
1:A:217:LEU:HD22	1:A:217:LEU:N	2.29	0.48
1:A:215:LYS:O	1:A:218:GLY:N	2.32	0.48
1:A:606:ILE:O	1:A:610:GLY:HA2	2.14	0.48
1:A:65:ASP:CG	1:A:615:ARG:HH22	2.15	0.48
1:A:10:PHE:HB2	1:A:11:PRO:HD3	1.95	0.47
1:A:40:TYR:CD1	1:A:71:LYS:HG2	2.49	0.47
1:A:535:HIS:HB3	1:A:538:VAL:HB	1.95	0.47
1:A:766:TRP:CG	1:A:781:VAL:HG22	2.49	0.47
1:A:173:ARG:NH2	1:A:467:GLU:OE2	2.48	0.47
1:A:361:GLU:C	1:A:363:ASN:N	2.68	0.47
1:A:472:SER:OG	1:A:475:GLU:HG3	2.14	0.47
1:A:43:TYR:CE2	1:A:545:ALA:HB2	2.49	0.47
1:A:645:THR:HG23	1:A:715:LEU:CD1	2.45	0.47
1:A:648:ASN:C	1:A:650:TYR:H	2.18	0.47
1:A:83:GLY:HA2	1:A:147:TYR:O	2.15	0.47
1:A:226:ILE:HG22	1:A:227:TRP:N	2.29	0.47
1:A:408:ASN:ND2	1:A:408:ASN:N	2.52	0.47
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.74	0.47
1:A:221:LYS:CA	1:A:221:LYS:HE3	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LYS:O	1:A:477:LYS:HD3	2.15	0.46
1:A:284:LEU:O	1:A:287:LEU:HB3	2.14	0.46
1:A:344:ASP:OD1	1:A:348:LYS:HE3	2.16	0.46
1:A:29:LYS:HB3	1:A:783:LEU:HD21	1.97	0.46
1:A:77:TYR:C	1:A:79:PRO:HD3	2.36	0.46
1:A:246:TYR:O	1:A:280:PRO:HA	2.14	0.46
1:A:45:GLY:O	1:A:47:PRO:HD3	2.16	0.46
1:A:674:PRO:HG2	1:A:726:ARG:NH2	2.31	0.46
1:A:248:TYR:HD2	1:A:261:GLU:N	2.13	0.46
1:A:304:VAL:CG1	1:A:305:LEU:N	2.78	0.46
1:A:116:ASN:HD22	1:A:493:PRO:HD3	1.80	0.46
1:A:645:THR:HG23	1:A:715:LEU:HD12	1.97	0.46
1:A:586:ASP:O	1:A:588:LYS:N	2.49	0.46
1:A:57:HIS:O	1:A:61:ARG:HD3	2.16	0.46
1:A:673:ARG:NH1	1:A:738:ALA:HB3	2.29	0.46
1:A:206:TYR:HB3	1:A:225:LEU:HD21	1.97	0.46
1:A:248:TYR:CD2	1:A:261:GLU:N	2.84	0.46
1:A:113:GLU:HG3	1:A:494:TYR:OH	2.16	0.46
1:A:720:VAL:HG13	1:A:720:VAL:O	2.15	0.46
1:A:222:ALA:HB2	1:A:257:ALA:HB3	1.98	0.46
1:A:464:CYS:HB3	1:A:504:CYS:SG	2.56	0.46
1:A:476:LEU:HD22	1:A:498:VAL:HG11	1.98	0.46
1:A:575:PHE:HE1	1:A:578:VAL:HG21	1.80	0.46
1:A:655:THR:HG22	1:A:656:TYR:HD2	1.80	0.46
1:A:687:LEU:HD13	1:A:710:PHE:HB2	1.98	0.46
1:A:775:LEU:CD2	1:A:775:LEU:H	2.28	0.46
1:A:492:ARG:NE	1:A:496:ASP:OD2	2.27	0.45
1:A:59:GLN:CD	1:A:581:HIS:CD2	2.89	0.45
1:A:715:LEU:HD22	1:A:720:VAL:CG1	2.45	0.45
1:A:251:PHE:CD1	1:A:251:PHE:N	2.84	0.45
1:A:496:ASP:OD1	1:A:510:ARG:NH1	2.49	0.45
1:A:650:TYR:HE1	1:A:769:LEU:CD1	2.29	0.45
1:A:203:PRO:O	1:A:229:THR:HA	2.17	0.45
1:A:389:CYS:N	1:A:396:LEU:CD1	2.80	0.45
1:A:809:VAL:O	1:A:813:ARG:HD2	2.15	0.45
1:A:678:ARG:HH11	1:A:678:ARG:CB	2.29	0.45
1:A:741:ALA:HB1	1:A:745:GLU:OE2	2.16	0.45
1:A:280:PRO:O	1:A:281:GLY:C	2.55	0.45
1:A:668:PRO:HB2	1:A:673:ARG:NE	2.30	0.45
1:A:24:GLU:O	1:A:29:LYS:NZ	2.45	0.45
1:A:302:PHE:CE2	1:A:304:VAL:HG23	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:TRP:HA	1:A:510:ARG:HA	1.98	0.45
1:A:744:TYR:O	1:A:748:VAL:HG23	2.16	0.45
1:A:775:LEU:HD23	1:A:775:LEU:H	1.82	0.45
1:A:92:GLU:HB3	1:A:450:ARG:HH21	1.81	0.45
1:A:178:VAL:HG21	1:A:187:PRO:HB3	1.98	0.45
1:A:684:MET:HE3	1:A:749:LEU:HD22	1.99	0.45
1:A:448:ARG:HB2	1:A:514:VAL:O	2.17	0.45
1:A:746:ALA:O	1:A:749:LEU:N	2.49	0.45
1:A:226:ILE:HG21	1:A:319:HIS:HB2	1.98	0.44
1:A:404:TRP:HB2	1:A:447:SER:HB3	1.99	0.44
1:A:767:GLN:HA	1:A:771:ARG:HG3	1.99	0.44
1:A:389:CYS:N	1:A:396:LEU:HD13	2.32	0.44
1:A:389:CYS:HB3	1:A:392:CYS:O	2.17	0.44
1:A:420:GLN:HA	1:A:430:LYS:HD3	1.98	0.44
1:A:660:ASP:O	1:A:661:ARG:C	2.55	0.44
1:A:671:GLU:CD	1:A:671:GLU:H	2.21	0.44
1:A:148:ALA:N	1:A:151:GLU:OE2	2.49	0.44
1:A:25:LYS:HB3	1:A:25:LYS:HZ2	1.78	0.44
1:A:362:ALA:O	1:A:366:ILE:HG13	2.17	0.44
1:A:588:LYS:HD3	1:A:588:LYS:HA	1.84	0.44
1:A:124:PHE:O	1:A:126:TYR:N	2.51	0.44
1:A:425:VAL:HB	1:A:579:ILE:HA	1.99	0.44
1:A:251:PHE:O	1:A:257:ALA:HA	2.17	0.44
1:A:343:VAL:HG22	1:A:349:LEU:HD22	2.00	0.44
1:A:88:GLY:HA3	1:A:517:VAL:HG11	1.98	0.44
1:A:392:CYS:SG	1:A:392:CYS:O	2.74	0.44
1:A:191:HIS:HB2	1:A:556:ARG:O	2.17	0.44
1:A:668:PRO:CB	1:A:673:ARG:CZ	2.93	0.44
1:A:719:TYR:C	1:A:721:ARG:N	2.71	0.44
1:A:452:TRP:CZ3	1:A:491:HIS:CD2	3.05	0.44
1:A:533:PHE:O	1:A:534:GLU:HG3	2.18	0.44
1:A:59:GLN:NE2	1:A:581:HIS:CD2	2.77	0.44
1:A:719:TYR:C	1:A:721:ARG:H	2.19	0.44
1:A:9:ASN:CG	1:A:12:LYS:HD3	2.38	0.44
1:A:369:ASP:O	1:A:373:ARG:HG3	2.18	0.43
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.33	0.43
1:A:821:VAL:HG22	1:A:821:VAL:OXT	2.18	0.43
1:A:93:LEU:HG	1:A:183:ARG:HH21	1.83	0.43
1:A:430:LYS:HB2	1:A:430:LYS:NZ	2.33	0.43
1:A:481:THR:O	1:A:482:LYS:HD2	2.18	0.43
1:A:40:TYR:CG	1:A:71:LYS:HG2	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:O	1:A:96:GLU:HB2	2.17	0.43
1:A:690:ARG:HH21	1:A:803:ARG:HH22	1.63	0.43
1:A:243:HIS:ND1	1:A:246:TYR:CE2	2.87	0.43
1:A:262:GLU:C	1:A:264:LEU:H	2.20	0.43
1:A:425:VAL:HG12	1:A:426:PRO:HD3	2.00	0.43
1:A:492:ARG:HB3	1:A:493:PRO:CD	2.49	0.43
1:A:66:LEU:HD12	1:A:66:LEU:O	2.18	0.43
1:A:40:TYR:CE1	1:A:71:LYS:HG2	2.54	0.43
1:A:211:LEU:HD12	1:A:287:LEU:HD11	1.98	0.43
1:A:274:GLN:N	1:A:274:GLN:OE1	2.33	0.43
1:A:607:ARG:HG3	1:A:608:LYS:N	2.32	0.43
1:A:1:MET:HE3	1:A:661:ARG:HD2	2.00	0.43
1:A:397:MET:CE	1:A:399:TYR:CD1	3.02	0.43
1:A:425:VAL:O	1:A:426:PRO:C	2.54	0.43
1:A:405:PHE:HA	1:A:444:TRP:O	2.19	0.43
1:A:137:ILE:O	1:A:139:TYR:N	2.45	0.43
1:A:280:PRO:O	1:A:283:ALA:HB3	2.18	0.43
1:A:308:TYR:OH	1:A:320:GLN:OE1	2.37	0.43
1:A:157:SER:O	1:A:160:TRP:HB3	2.17	0.43
1:A:766:TRP:CZ3	1:A:770:VAL:HG21	2.54	0.43
1:A:523:ALA:O	1:A:524:MET:C	2.58	0.42
1:A:211:LEU:HD21	1:A:259:ILE:HD12	2.01	0.42
1:A:208:ARG:HG3	1:A:208:ARG:O	2.19	0.42
1:A:237:ASN:CA	1:A:319:HIS:HE1	2.31	0.42
1:A:667:PRO:HA	1:A:668:PRO:HD3	1.91	0.42
1:A:682:ALA:HB1	1:A:795:ASP:H	1.84	0.42
1:A:210:PRO:HA	1:A:223:SER:OG	2.19	0.42
1:A:53:PRO:HA	1:A:57:HIS:ND1	2.35	0.42
1:A:2:PHE:HZ	1:A:664:LEU:CD1	2.31	0.42
1:A:261:GLU:HB2	1:A:316:GLY:HA3	2.02	0.42
1:A:323:ALA:HB2	1:A:339:LEU:CD1	2.49	0.42
1:A:474:GLN:HG3	1:A:475:GLU:N	2.34	0.42
1:A:550:GLU:HB3	3:A:1301:ILA:O3'	2.20	0.42
1:A:8:PRO:HG3	1:A:647:TRP:NE1	2.34	0.42
1:A:137:ILE:HG13	1:A:137:ILE:O	2.20	0.42
1:A:249:ALA:HB3	1:A:251:PHE:CE1	2.54	0.42
1:A:425:VAL:O	1:A:427:PRO:CD	2.66	0.42
1:A:477:LYS:HE2	1:A:483:PRO:HA	2.02	0.42
1:A:524:MET:HE2	1:A:558:TRP:HZ2	1.85	0.42
1:A:648:ASN:C	1:A:650:TYR:N	2.72	0.42
1:A:812:ALA:O	1:A:815:ALA:HB3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:C	1:A:396:LEU:HD13	2.39	0.42
1:A:39:ARG:HG3	1:A:40:TYR:N	2.34	0.42
1:A:673:ARG:CA	1:A:673:ARG:NE	2.82	0.42
1:A:681:LEU:O	1:A:685:GLN:HG2	2.20	0.42
1:A:24:GLU:OE2	1:A:779:GLU:OE2	2.37	0.42
1:A:591:LYS:HB2	1:A:591:LYS:HE3	1.95	0.41
1:A:659:LEU:O	1:A:661:ARG:N	2.51	0.41
1:A:124:PHE:C	1:A:126:TYR:H	2.24	0.41
1:A:304:VAL:HG13	1:A:305:LEU:N	2.35	0.41
1:A:406:ILE:O	1:A:408:ASN:N	2.52	0.41
1:A:719:TYR:O	1:A:723:ASN:HB2	2.21	0.41
1:A:732:ASP:OD2	1:A:732:ASP:C	2.59	0.41
1:A:262:GLU:CG	1:A:263:GLY:N	2.79	0.41
1:A:425:VAL:O	1:A:427:PRO:HD3	2.20	0.41
1:A:573:ILE:HD13	1:A:573:ILE:N	2.35	0.41
1:A:593:SER:O	1:A:599:VAL:HG13	2.20	0.41
1:A:50:ASN:HA	1:A:122:SER:O	2.20	0.41
1:A:262:GLU:CG	1:A:263:GLY:H	2.32	0.41
1:A:775:LEU:CD2	1:A:775:LEU:N	2.84	0.41
1:A:243:HIS:NE2	1:A:245:GLU:HG3	2.35	0.41
1:A:683:ARG:HH11	1:A:686:ASP:HB3	1.85	0.41
1:A:260:LEU:O	1:A:261:GLU:C	2.59	0.41
1:A:456:LEU:HD13	1:A:515:ILE:CD1	2.46	0.41
1:A:291:PRO:HG3	1:A:301:TYR:CZ	2.56	0.41
1:A:405:PHE:N	1:A:405:PHE:CD1	2.89	0.41
1:A:383:LEU:C	1:A:383:LEU:HD13	2.41	0.41
1:A:138:ALA:CB	1:A:759:PRO:HG3	2.46	0.41
1:A:650:TYR:CE1	1:A:769:LEU:HD11	2.52	0.41
1:A:617:TYR:O	1:A:619:TYR:N	2.54	0.41
1:A:409:THR:C	1:A:411:PHE:H	2.24	0.40
1:A:675:GLU:HA	1:A:678:ARG:CZ	2.48	0.40
1:A:685:GLN:OE1	1:A:789:ALA:HA	2.21	0.40
1:A:773:VAL:HG12	1:A:774:ARG:HG3	2.03	0.40
1:A:54:HIS:O	1:A:55:VAL:C	2.57	0.40
1:A:658:ASN:C	1:A:661:ARG:HE	2.25	0.40
1:A:717:GLN:O	1:A:717:GLN:HG2	2.22	0.40
1:A:174:ASP:OD2	1:A:176:LYS:HD2	2.20	0.40
1:A:678:ARG:NH1	1:A:678:ARG:CB	2.85	0.40
1:A:69:ARG:NH1	1:A:782:HIS:CD2	2.89	0.40
1:A:422:ILE:HG22	1:A:423:HIS:N	2.37	0.40
1:A:547:PHE:CD1	1:A:547:PHE:C	2.95	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:CG2	1:A:78:ALA:HB3	2.50	0.40
1:A:102:LYS:HB2	1:A:106:GLU:OE2	2.22	0.40
1:A:166:PHE:CZ	1:A:467:GLU:HB3	2.57	0.40
1:A:310:SER:OG	1:A:311:GLN:N	2.54	0.40
1:A:237:ASN:CB	1:A:319:HIS:CE1	3.01	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:NE2	1:A:28:GLN:NE2[2_454]	1.91	0.29

## 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	819/821 (100%)	692 (84%)	96 (12%)	31 (4%)	3 18

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	TYR
1	A	310	SER
1	A	467	GLU
1	A	531	TYR
1	A	543	PHE
1	A	716	SER
1	A	125	THR
1	A	352	GLU
1	A	464	CYS
1	A	466	LYS
1	A	492	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	311	GLN
1	A	407	LYS
1	A	425	VAL
1	A	432	GLY
1	A	582	GLY
1	A	626	ALA
1	A	734	LEU
1	A	819	SER
1	A	262	GLU
1	A	272	GLY
1	A	282	LYS
1	A	299	LYS
1	A	428	HIS
1	A	457	PRO
1	A	587	GLU
1	A	782	HIS
1	A	238	VAL
1	A	623	PRO
1	A	674	PRO
1	A	334	VAL

### 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	698/698 (100%)	633 (91%)	65 (9%)	9 33

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	25	LYS
1	A	26	ILE
1	A	41	THR
1	A	44	GLU
1	A	50	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	57	HIS
1	A	61	ARG
1	A	80	ARG
1	A	105	ARG
1	A	129	GLU
1	A	144	GLU
1	A	150	LEU
1	A	157	SER
1	A	183	ARG
1	A	190	SER
1	A	195	LEU
1	A	215	LYS
1	A	221	LYS
1	A	225	LEU
1	A	227	TRP
1	A	245	GLU
1	A	268	LEU
1	A	274	GLN
1	A	301	TYR
1	A	304	VAL
1	A	313	ASP
1	A	320	GLN
1	A	327	GLU
1	A	328	ASP
1	A	329	LEU
1	A	350	LEU
1	A	360	ARG
1	A	382	TYR
1	A	384	HIS
1	A	408	ASN
1	A	441	LEU
1	A	467	GLU
1	A	474	GLN
1	A	476	LEU
1	A	492	ARG
1	A	500	LEU
1	A	509	ARG
1	A	521	SER
1	A	556	ARG
1	A	573	ILE
1	A	583	LEU
1	A	594	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	596	LYS
1	A	625	GLU
1	A	627	ASP
1	A	628	ARG
1	A	629	ARG
1	A	640	ARG
1	A	718	TRP
1	A	720	VAL
1	A	721	ARG
1	A	728	TRP
1	A	729	LYS
1	A	730	ASN
1	A	731	GLU
1	A	774	ARG
1	A	810	ASP
1	A	813	ARG
1	A	818	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	59	GLN
1	A	117	GLN
1	A	164	ASN
1	A	191	HIS
1	A	237	ASN
1	A	311	GLN
1	A	320	GLN
1	A	408	ASN
1	A	419	ASN
1	A	474	GLN
1	A	497	GLN
1	A	560	ASN
1	A	564	GLN
1	A	581	HIS
1	A	717	GLN
1	A	723	ASN
1	A	730	ASN
1	A	782	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	ILA	A	1301	-	29,33,33	3.70	10 (34%)	31,49,49	2.14	9 (29%)

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	ILA	A	1301	-	-	0/21/41/41	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	ILA	CA-C	11.66	1.64	1.53
3	A	1301	ILA	SA-N5'	9.90	1.73	1.61
3	A	1301	ILA	O1A-SA	8.68	1.56	1.43
3	A	1301	ILA	O4'-C1'	5.48	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	ILA	O2A-SA	4.15	1.49	1.43
3	A	1301	ILA	C4-N3	3.01	1.39	1.35
3	A	1301	ILA	C-N3A	-2.34	1.33	1.37
3	A	1301	ILA	C3'-C2'	-2.30	1.47	1.53
3	A	1301	ILA	O4'-C4'	2.22	1.50	1.45
3	A	1301	ILA	C2-N3	2.05	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	ILA	N3A-SA-N5'	-5.48	97.42	110.88
3	A	1301	ILA	C-CA-N	4.59	117.29	110.28
3	A	1301	ILA	O1A-SA-N5'	4.06	113.89	106.73
3	A	1301	ILA	C3'-C2'-C1'	3.96	106.94	100.98
3	A	1301	ILA	C1'-N9-C4	-3.30	120.84	126.64
3	A	1301	ILA	O4'-C1'-C2'	-3.18	102.28	106.93
3	A	1301	ILA	O2A-SA-N5'	-2.69	101.99	106.73
3	A	1301	ILA	O-C-N3A	2.28	127.39	123.00
3	A	1301	ILA	C4'-C5'-N5'	-2.07	108.37	112.51

There are no chirality outliers.

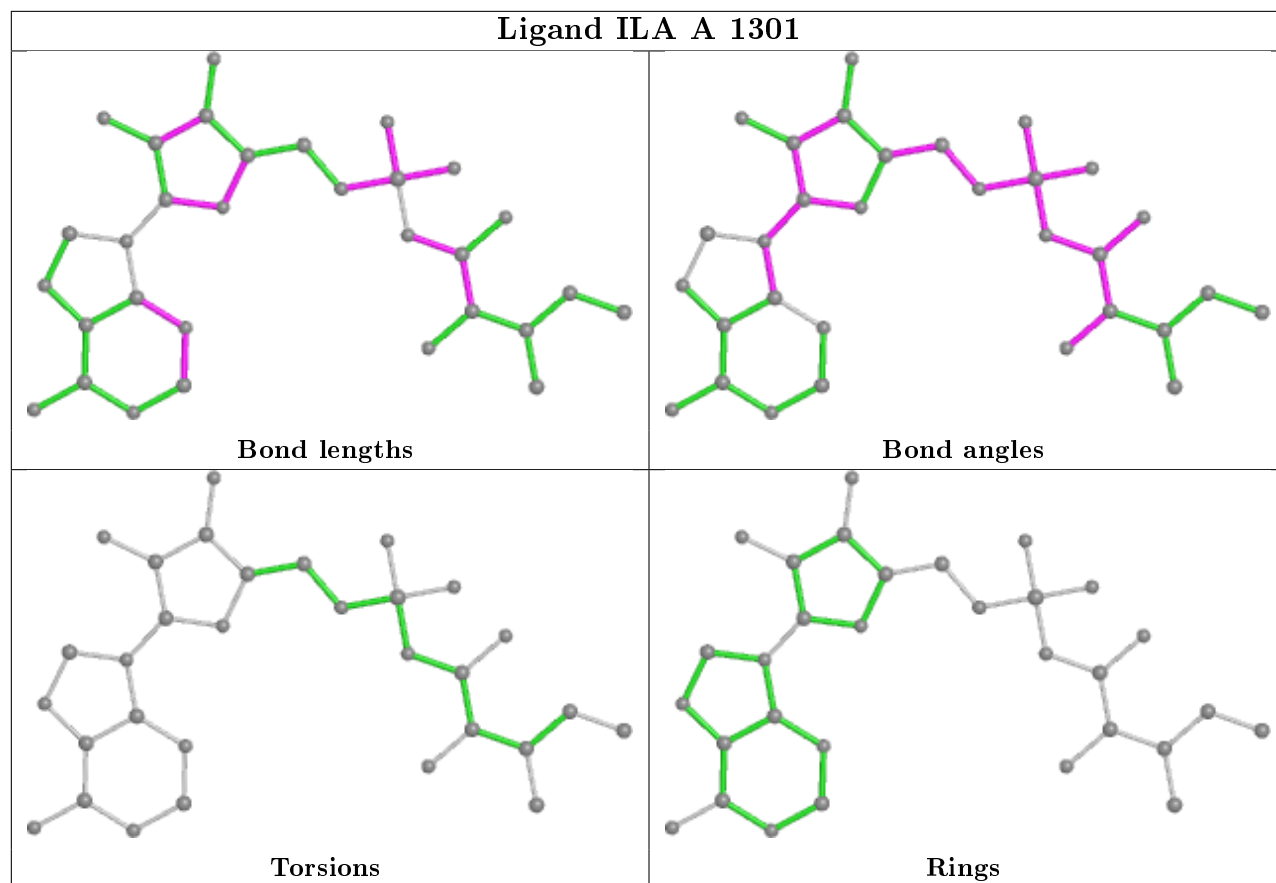
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1301	ILA	3	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 ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.