wwPDB X-ray Structure Validation Summary Report (i)

Mar 20, 2026 – 07:36 AM UTC

PDB ID	:	1L0W / pdb_00001l0w
Title	:	Aspartyl-tRNA synthetase-1 from space-grown crystals
Authors	:	Ng, J.D.; Sauter, C.; Lorber, B.; Kirkland, N.; Arnez, J.; Giege, R.
Deposited on	:	2002-02-14
Resolution	:	2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

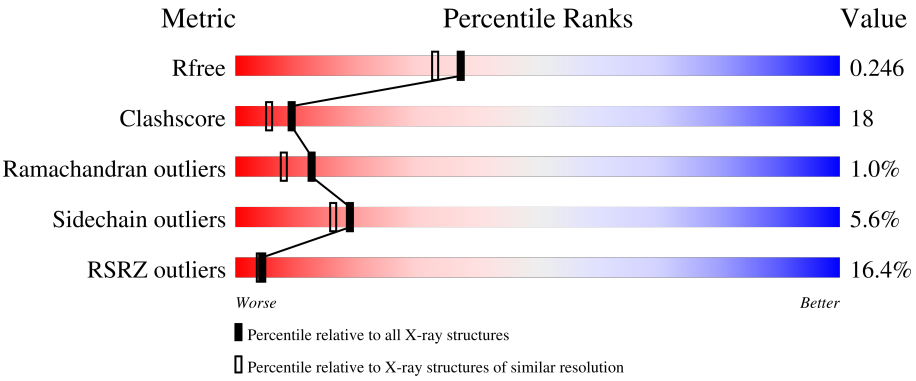
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 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 <=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	580	17% 64% 31%
1	B	580	16% 66% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9521 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 Aspartyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			
1	B	580	Total	C	N	O	S	0	0	0
			4667	2980	840	836	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	109	Total	O	0	0
			109	109		

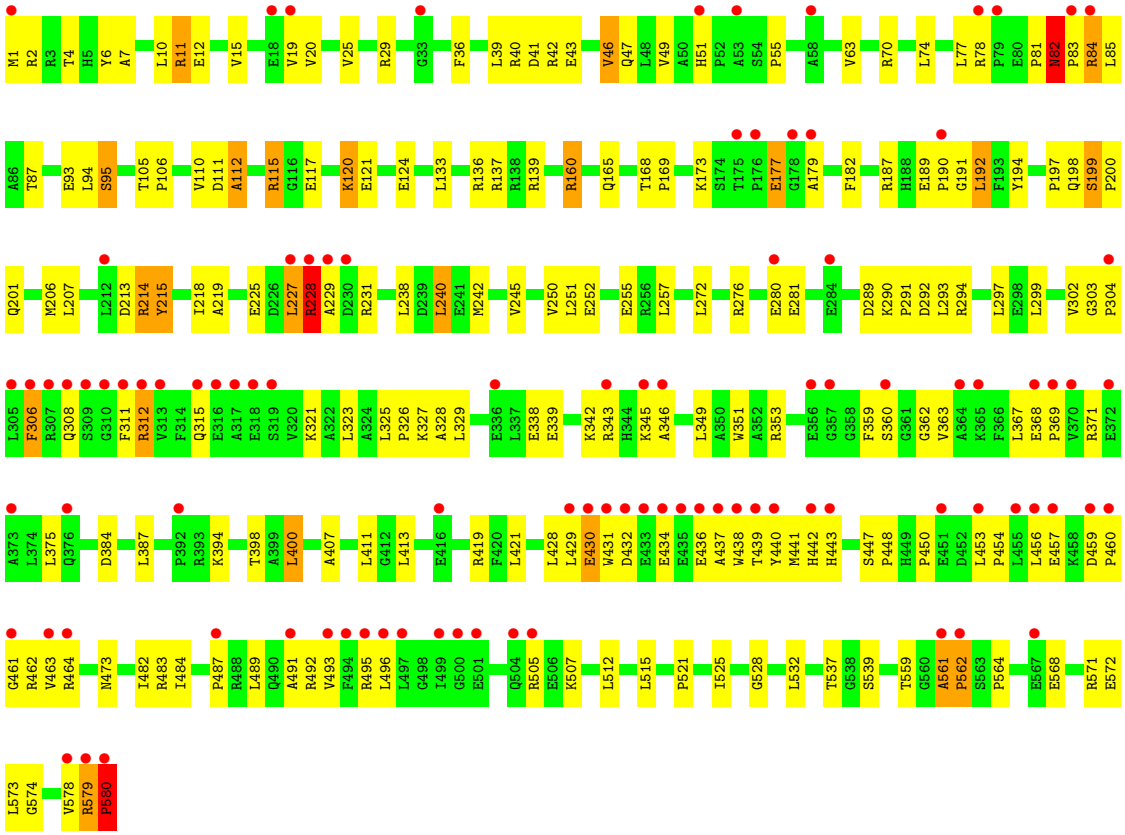
3 Residue-property plots (i)

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: Aspartyl-tRNA synthetase

Chain A:



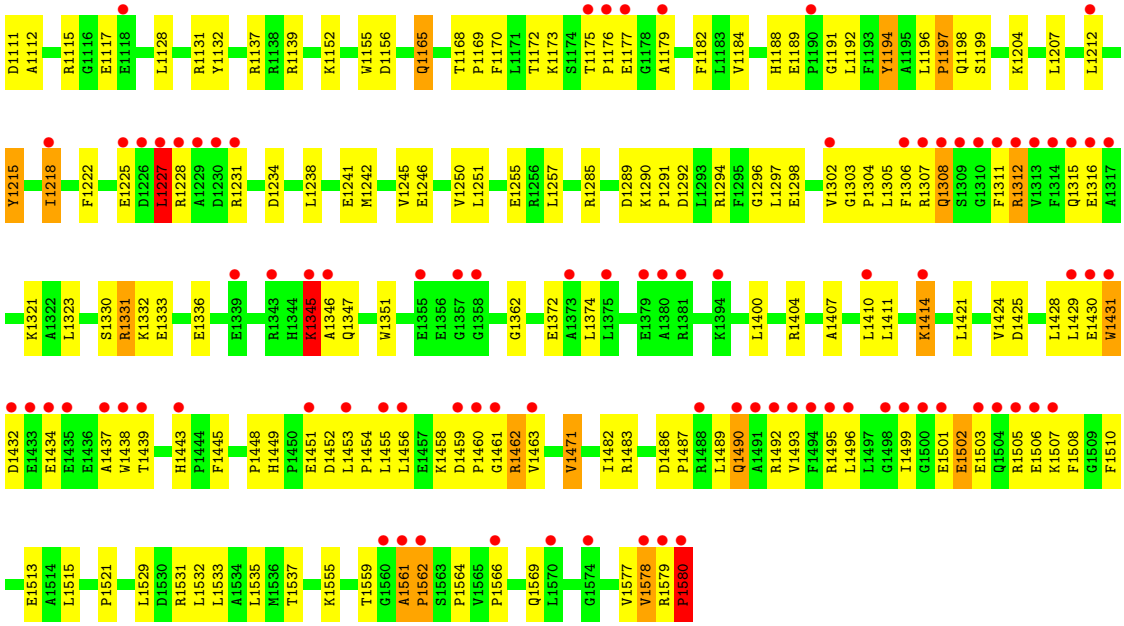


• Molecule 1: Aspartyl-tRNA synthetase

Chain B:






D1111 A1112 R1115 G1116 E1117 E1118 L1128 R1131 Y1132 R1137 R1138 R1139 K1152 W1155 D1156 Q1165 T1168 P1169 F1170 L1171 T1172 K1173 S1174 T1175 P1176 E1177 G1178 A1179 F1182 L1183 V1184 H1188 E1189 P1190 G1191 L1192 F1193 Y1194 A1195 L1196 P1197 Q1198 S1199 K1204 L1207 L1212
Y1215 I1218 F1222 E1225 D1226 L1227 R1228 A1229 D1230 R1231 D1234 L1238 E1241 M1242 V1245 E1246 V1250 L1251 E1255 R1256 L1257 R1285 D1289 K1290 P1291 D1292 L1293 R1294 F1295 G1296 L1297 E1298 V1302 G1303 P1304 L1305 F1306 R1307 Q1308 S1309 G1310 F1311 R1312 V1313 F1314 Q1315 E1316 A1317
K1321 A1322 L1323 S1330 R1331 K1332 E1333 E1336 E1339 R1343 H1344 K1345 A1346 Q1347 W1351 E1355 E1356 G1357 G1358 G1362 E1372 A1373 L1374 L1375 E1379 A1380 R1381 K1394 L1400 R1404 A1407 L1410 L1411 K1414 L1421 V1424 D1425 L1428 L1429 E1430 W1431
D1432 E1433 E1434 E1435 E1436 A1437 W1438 T1439 H1443 P1444 F1445 P1448 H1449 P1450 E1451 D1452 L1453 P1454 L1455 L1456 E1457 K1458 D1459 P1460 G1461 R1462 V1463 V1471 I1482 R1483 D1486 P1487 R1488 L1489 Q1490 A1491 R1492 V1493 F1494 R1495 L1496 L1497 G1498 I1499 G1500 E1501 E1502 E1503 Q1504 R1505 E1506 K1507 F1508 G1509 F1510
E1513 A1514 L1515 P1521 L1529 D1530 R1531 L1532 L1533 A1534 L1535 M1536 T1537 K1555 T1559 G1560 A1561 P1562 S1563 P1564 V1565 P1566 Q1569 L1570 G1574 V1577 V1578 R1579 P1580

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.02Å 156.10Å 177.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	11.98 – 2.01 11.98 – 2.01	Depositor EDS
% Data completeness (in resolution range)	70.7 (11.98-2.01) 70.6 (11.98-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	2438 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.49	0/4779	1.02	31/6467 (0.5%)
1	B	0.53	0/4779	1.31	34/6467 (0.5%)
All	All	0.51	0/9558	1.17	65/12934 (0.5%)

There are no bond length outliers.

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1561	ALA	CA-C-N	47.86	179.67	119.84
1	B	1561	ALA	C-N-CA	47.86	179.67	119.84
1	B	1561	ALA	C-N-CD	-12.63	73.21	125.00
1	A	561	ALA	CA-C-N	10.97	153.34	127.00
1	A	561	ALA	C-N-CA	10.97	153.34	127.00

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	4667	0	4679	193	0
1	B	4667	0	4676	173	0
2	A	78	0	0	1	0
2	B	109	0	0	3	0
All	All	9521	0	9355	339	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 18.

The worst 5 of 339 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:B:1307:ARG:HD3	1:B:1315:GLN:HG2	1.27	1.15
1:A:579:ARG:HB3	1:A:580:PRO:HD2	1.31	1.13
1:A:574:GLY:HA3	1:B:1580:PRO:HG3	1.30	1.13
1:A:306:PHE:HB3	1:A:315:GLN:HE22	1.19	1.04
1:A:160:ARG:HH11	1:A:160:ARG:HB3	1.23	1.03

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	578/580 (100%)	537 (93%)	35 (6%)	6 (1%)	12	8
1	B	578/580 (100%)	538 (93%)	34 (6%)	6 (1%)	12	8
All	All	1156/1160 (100%)	1075 (93%)	69 (6%)	12 (1%)	12	8

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	A	312	ARG
1	B	1084	ARG
1	B	1312	ARG
1	B	1562	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	483/483 (100%)	454 (94%)	29 (6%)	17	14
1	B	483/483 (100%)	458 (95%)	25 (5%)	21	18
All	All	966/966 (100%)	912 (94%)	54 (6%)	19	16

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	580	PRO
1	B	1165	GLN
1	B	1483	ARG
1	B	1010	LEU
1	B	1051	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1143	ASN
1	B	1376	GLN
1	B	1569	GLN
1	B	1504	GLN
1	A	315	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)

There are no ligands in this entry.

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	580/580 (100%)	0.69	97 (16%)	4	4	14, 38, 91, 139	0
1	B	580/580 (100%)	0.56	93 (16%)	5	4	14, 33, 90, 136	0
All	All	1160/1160 (100%)	0.62	190 (16%)	4	4	14, 35, 91, 139	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1580	PRO	12.8
1	A	227	LEU	7.2
1	B	1309	SER	7.2
1	B	1437	ALA	6.9
1	A	580	PRO	6.8

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.