Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:18 pm BST

PDB ID	:	1N9W
Title	:	Crystal structure of the non-discriminating and archaeal-type aspartyl-tRNA synthetase from Thermus thermophilus
Authors	:	Charron, C.; Roy, H.; Blaise, M.; Giege, R.; Kern, D.
Deposited on	:	2002-11-26
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

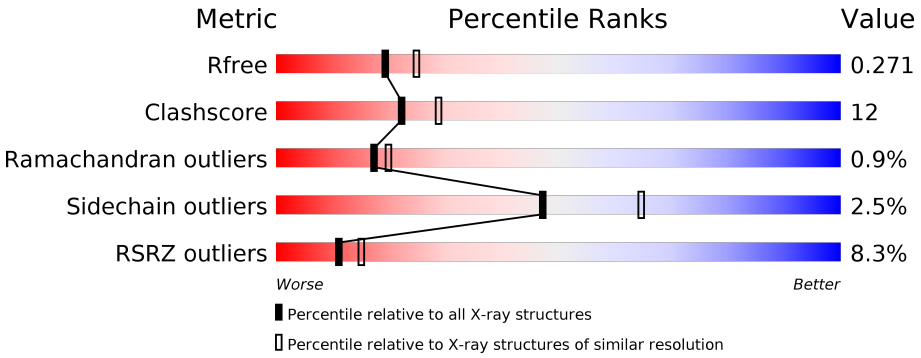
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	4% 64% 19% • 16%
1	B	422	10% 61% 23% • 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5921 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2869	1843	500	519	7			
1	B	359	Total	C	N	O	S	0	0	0
			2893	1859	503	524	7			

- Molecule 2 is water.

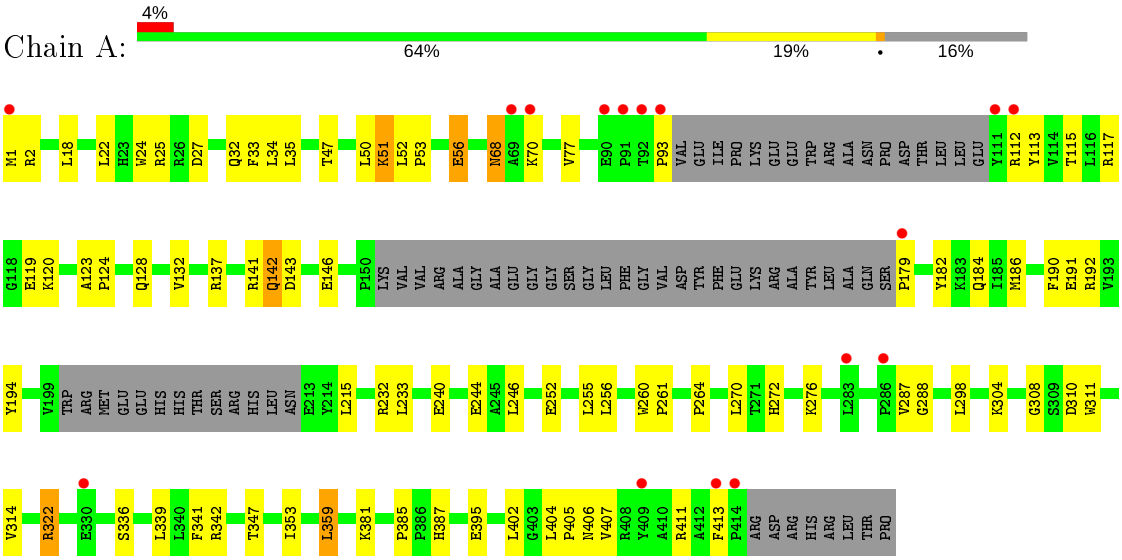
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	70	Total	O	0	0
			70	70		

3 Residue-property plots (i)

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

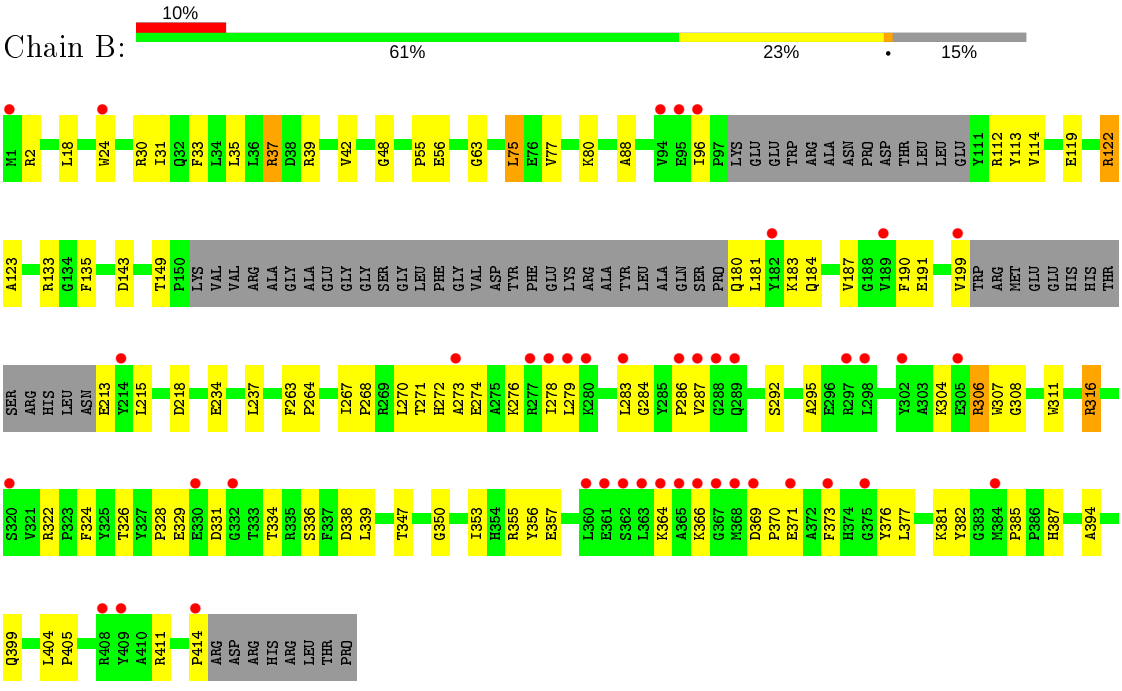
- Molecule 1: aspartyl-tRNA synthetase 2

Chain A:



- Molecule 1: aspartyl-tRNA synthetase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.36Å 122.55Å 167.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 32.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.30) 98.2 (32.56-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	4.89 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.262 0.240 , 0.271	Depositor DCC
R_{free} test set	3717 reflections (7.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5921	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	0.41	1/2932 (0.0%)	0.62	0/3962
1	B	0.39	1/2956 (0.0%)	0.61	2/3996 (0.1%)
All	All	0.40	2/5888 (0.0%)	0.61	2/7958 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	LYS	CE-NZ	-6.31	1.33	1.49
1	B	381	LYS	CE-NZ	-5.94	1.34	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	ARG	CG-CD-NE	-5.65	99.93	111.80
1	B	381	LYS	CD-CE-NZ	5.35	124.00	111.70

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	2869	0	2887	62	0
1	B	2893	0	2912	75	0
2	A	89	0	0	2	0
2	B	70	0	0	3	0
All	All	5921	0	5799	135	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 12.

All (135) 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:96:ILE:HD11	1:B:114:VAL:HG22	1.54	0.89
1:B:37:ARG:HB3	1:B:42:VAL:HG12	1.61	0.83
1:B:24:TRP:NE1	1:B:35:LEU:HD22	1.95	0.81
1:B:292:SER:H	1:B:295:ALA:HB3	1.51	0.75
1:B:279:LEU:HD23	1:B:283:LEU:HD12	1.69	0.74
1:B:339:LEU:HB3	1:B:347:THR:HB	1.68	0.74
1:A:406:ASN:ND2	1:A:407:VAL:H	1.89	0.71
1:A:18:LEU:HD11	1:A:77:VAL:HG21	1.74	0.69
1:A:353:ILE:HB	1:A:359:LEU:HD13	1.74	0.69
1:A:339:LEU:HB3	1:A:347:THR:HB	1.74	0.69
1:B:271:THR:HG22	1:B:273:ALA:H	1.56	0.69
1:A:112:ARG:HA	1:A:115:THR:HG22	1.76	0.68
1:B:183:LYS:HE2	1:B:218:ASP:OD1	1.94	0.67
1:B:355:ARG:HB3	1:B:355:ARG:NH1	2.13	0.63
1:B:63:GLY:HA2	1:B:80:LYS:HG2	1.79	0.63
1:B:37:ARG:CB	1:B:42:VAL:HG12	2.28	0.62
1:B:276:LYS:HG3	1:B:287:VAL:HG21	1.81	0.62
1:A:27:ASP:HA	1:A:32:GLN:HB3	1.82	0.62
1:A:24:TRP:HB3	1:A:35:LEU:HD12	1.80	0.62
1:B:119:GLU:HA	1:B:122:ARG:HD2	1.84	0.60
1:A:119:GLU:HB3	1:A:255:LEU:HD11	1.82	0.60
1:A:128:GLN:HE22	1:A:395:GLU:HG3	1.67	0.59
1:B:411:ARG:HB3	1:B:414:PRO:HG3	1.83	0.59
1:B:18:LEU:HD11	1:B:77:VAL:HG21	1.84	0.59
1:B:122:ARG:HD3	2:B:426:HOH:O	2.02	0.59
1:A:123:ALA:HB3	1:A:124:PRO:HD3	1.84	0.58
1:B:199:VAL:O	1:B:213:GLU:HA	2.03	0.58
1:B:122:ARG:HG2	1:B:123:ALA:N	2.16	0.58
1:A:1:MET:CE	1:A:2:ARG:H	2.16	0.57
1:B:274:GLU:O	1:B:278:ILE:HG13	2.05	0.56
1:A:264:PRO:HG3	1:A:311:TRP:CZ2	2.40	0.56
1:A:32:GLN:HG2	1:A:47:THR:OG1	2.06	0.56
1:A:272:HIS:CE1	1:A:276:LYS:HD2	2.41	0.55
1:A:322:ARG:HH11	1:A:336:SER:HB2	1.70	0.55
1:B:328:PRO:HD3	1:B:353:ILE:HD11	1.89	0.54
1:A:146:GLU:HB2	1:A:194:TYR:CZ	2.43	0.54
1:B:213:GLU:HG2	1:B:411:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASP:CG	1:A:342:ARG:HH11	2.11	0.53
1:B:355:ARG:HH12	1:B:357:GLU:HB2	1.74	0.53
1:B:399:GLN:HA	1:B:404:LEU:HD12	1.90	0.53
1:B:271:THR:HB	1:B:274:GLU:HG3	1.91	0.53
1:B:31:ILE:HD12	1:B:33:PHE:CE2	2.44	0.53
1:A:32:GLN:NE2	1:A:50:LEU:H	2.06	0.53
1:B:324:PHE:HB3	1:B:366:LYS:HD2	1.90	0.53
1:A:120:LYS:HG2	1:A:255:LEU:HD22	1.91	0.53
1:B:373:PHE:O	1:B:377:LEU:HG	2.09	0.53
1:A:51:LYS:HZ2	1:A:51:LYS:H	1.57	0.52
1:B:355:ARG:HH12	1:B:357:GLU:H	1.57	0.52
1:A:51:LYS:CE	1:A:51:LYS:H	2.22	0.52
1:A:68:ASN:ND2	1:A:70:LYS:H	2.07	0.52
1:A:56:GLU:HG3	1:A:117:ARG:NH1	2.25	0.51
1:A:385:PRO:O	1:A:387:HIS:HD2	1.92	0.51
1:B:24:TRP:CZ2	1:B:35:LEU:HD13	2.45	0.51
1:A:33:PHE:C	1:A:34:LEU:HD12	2.31	0.51
1:A:184:GLN:OE1	1:A:387:HIS:HE1	1.93	0.51
1:A:142:GLN:HG3	2:A:432:HOH:O	2.11	0.51
1:B:24:TRP:HE1	1:B:35:LEU:HD22	1.73	0.51
1:A:141:ARG:NH2	1:A:240:GLU:OE1	2.44	0.50
1:A:25:ARG:HH11	1:A:25:ARG:HG2	1.76	0.50
1:A:22:LEU:HD21	1:A:25:ARG:HD2	1.94	0.49
1:B:270:LEU:HD21	1:B:278:ILE:HD12	1.95	0.49
1:B:364:LYS:HZ1	1:B:370:PRO:HG2	1.78	0.49
1:A:128:GLN:O	1:A:132:VAL:HG23	2.12	0.49
1:A:68:ASN:C	1:A:68:ASN:HD22	2.16	0.49
1:B:180:GLN:O	1:B:184:GLN:HG3	2.13	0.48
1:A:233:LEU:C	1:A:233:LEU:HD23	2.33	0.48
1:A:406:ASN:ND2	1:A:407:VAL:N	2.59	0.48
1:A:1:MET:HE2	1:A:2:ARG:H	1.78	0.48
1:B:322:ARG:NH2	1:B:338:ASP:OD1	2.45	0.48
1:B:356:TYR:HE1	1:B:377:LEU:HB3	1.78	0.48
1:B:355:ARG:HB3	1:B:355:ARG:HH11	1.76	0.48
1:B:306:ARG:HG2	1:B:307:TRP:CE2	2.49	0.48
1:B:271:THR:HG23	1:B:316:ARG:HB2	1.95	0.47
1:B:183:LYS:O	1:B:187:VAL:HG23	2.14	0.47
1:B:279:LEU:HD23	1:B:283:LEU:CD1	2.43	0.47
1:A:50:LEU:HD12	1:A:51:LYS:HZ2	1.79	0.47
1:B:37:ARG:O	1:B:37:ARG:HG3	2.15	0.47
1:A:32:GLN:HB2	1:A:52:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:NH2	2:B:481:HOH:O	2.45	0.46
1:B:181:LEU:HD13	1:B:376:TYR:CD1	2.51	0.46
1:A:304:LYS:O	1:A:308:GLY:HA2	2.15	0.46
1:B:385:PRO:O	1:B:387:HIS:HD2	1.98	0.46
1:A:310:ASP:CG	1:A:342:ARG:NH1	2.68	0.46
1:A:413:PHE:HE2	1:B:149:THR:HG22	1.81	0.46
1:A:252:GLU:H	1:A:252:GLU:CD	2.18	0.46
1:A:287:VAL:HG22	1:A:288:GLY:N	2.30	0.46
1:B:279:LEU:O	1:B:284:GLY:N	2.49	0.45
1:A:179:PRO:HA	1:A:182:TYR:HD2	1.81	0.45
1:B:272:HIS:O	1:B:276:LYS:HB2	2.15	0.45
1:B:31:ILE:HG13	1:B:31:ILE:O	2.16	0.45
1:A:260:TRP:HA	1:A:261:PRO:HD3	1.80	0.45
1:A:261:PRO:HG3	1:A:342:ARG:NH2	2.32	0.45
1:A:190:PHE:O	1:A:191:GLU:HB2	2.17	0.44
1:B:304:LYS:O	1:B:308:GLY:HA2	2.17	0.44
1:B:55:PRO:O	1:B:56:GLU:HB2	2.18	0.44
1:A:246:LEU:HD13	1:A:260:TRP:CZ2	2.53	0.44
1:B:264:PRO:HG3	1:B:311:TRP:CZ2	2.53	0.44
1:B:263:PHE:HA	1:B:264:PRO:HD3	1.82	0.43
1:A:52:LEU:HA	1:A:53:PRO:HD3	1.85	0.43
1:A:93:PRO:HD3	1:B:382:TYR:OH	2.17	0.43
1:A:51:LYS:NZ	1:A:51:LYS:H	2.15	0.43
1:A:270:LEU:O	1:A:314:VAL:HA	2.18	0.43
1:B:279:LEU:HA	1:B:283:LEU:HD12	2.01	0.43
1:B:88:ALA:HA	2:B:429:HOH:O	2.19	0.43
1:B:75:LEU:HA	1:B:75:LEU:HD13	1.78	0.43
1:A:404:LEU:HA	1:A:405:PRO:HD3	1.89	0.43
1:A:137:ARG:NH1	1:A:244:GLU:OE1	2.52	0.42
1:B:306:ARG:HH11	1:B:306:ARG:HG3	1.84	0.42
1:A:50:LEU:HD12	1:A:51:LYS:NZ	2.34	0.42
1:B:234:GLU:OE1	1:B:347:THR:HG21	2.20	0.42
1:B:369:ASP:HA	1:B:370:PRO:HD3	1.83	0.42
1:B:369:ASP:OD2	1:B:371:GLU:HB3	2.19	0.42
1:A:233:LEU:HD23	1:A:233:LEU:O	2.20	0.42
1:A:261:PRO:HG2	1:A:341:PHE:HZ	1.84	0.42
1:B:336:SER:HA	1:B:350:GLY:HA3	2.02	0.42
1:B:267:ILE:HA	1:B:268:PRO:HD3	1.94	0.42
1:B:276:LYS:O	1:B:287:VAL:HG11	2.20	0.42
1:B:356:TYR:CE1	1:B:377:LEU:HB3	2.54	0.42
1:A:32:GLN:HE22	1:A:50:LEU:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD22	1:A:407:VAL:H	1.66	0.41
1:B:215:LEU:HB3	1:B:394:ALA:HB3	2.02	0.41
1:B:326:THR:HG22	1:B:334:THR:HB	2.02	0.41
1:B:30:ARG:O	1:B:48:GLY:HA3	2.20	0.41
1:A:232:ARG:NH2	2:A:461:HOH:O	2.54	0.41
1:B:112:ARG:O	1:B:114:VAL:N	2.54	0.41
1:B:292:SER:N	1:B:295:ALA:HB3	2.29	0.41
1:B:276:LYS:HG3	1:B:287:VAL:CG2	2.49	0.41
1:B:213:GLU:HG2	1:B:411:ARG:HH22	1.85	0.41
1:B:2:ARG:HH12	1:B:39:ARG:HH12	1.69	0.41
1:A:142:GLN:O	1:A:143:ASP:HB2	2.22	0.40
1:B:135:PHE:CE1	1:B:237:LEU:HD21	2.56	0.40
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.21	0.40
1:A:256:LEU:CD1	1:A:402:LEU:HD13	2.51	0.40
1:B:190:PHE:O	1:B:191:GLU:HB2	2.20	0.40
1:A:68:ASN:HD22	1:A:70:LYS:H	1.70	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	348/422 (82%)	335 (96%)	12 (3%)	1 (0%)	41	50
1	B	351/422 (83%)	326 (93%)	20 (6%)	5 (1%)	11	11
All	All	699/844 (83%)	661 (95%)	32 (5%)	6 (1%)	17	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	113	TYR
1	B	331	ASP

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Mol	Chain	Res	Type
1	A	113	TYR
1	B	316	ARG
1	B	405	PRO
1	B	286	PRO

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	299/355 (84%)	288 (96%)	11 (4%)	34 48
1	B	302/355 (85%)	298 (99%)	4 (1%)	69 82
All	All	601/710 (85%)	586 (98%)	15 (2%)	47 65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	56	GLU
1	A	68	ASN
1	A	142	GLN
1	A	186	MET
1	A	192	ARG
1	A	215	LEU
1	A	298	LEU
1	A	322	ARG
1	A	359	LEU
1	A	411	ARG
1	B	75	LEU
1	B	122	ARG
1	B	143	ASP
1	B	306	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	32	GLN
1	A	68	ASN
1	A	78	GLN
1	A	128	GLN
1	A	184	GLN
1	A	354	HIS
1	A	387	HIS
1	A	406	ASN
1	B	11	HIS
1	B	184	GLN
1	B	387	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	356/422 (84%)	0.19	16 (4%) 33 40	13, 32, 53, 75	0
1	B	359/422 (85%)	0.68	43 (11%) 4 6	17, 38, 78, 95	0
All	All	715/844 (84%)	0.43	59 (8%) 11 15	13, 34, 69, 95	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	MET	9.2
1	B	367	GLY	6.6
1	B	1	MET	5.1
1	A	93	PRO	4.9
1	A	1	MET	4.8
1	B	364	LYS	4.8
1	B	289	GLN	4.5
1	B	366	LYS	4.4
1	B	330	GLU	4.4
1	B	286	PRO	4.3
1	A	179	PRO	3.9
1	B	283	LEU	3.9
1	B	361	GLU	3.7
1	B	365	ALA	3.6
1	B	94	VAL	3.5
1	A	112	ARG	3.5
1	A	414	PRO	3.5
1	A	91	PRO	3.4
1	B	369	ASP	3.4
1	A	111	TYR	3.4
1	B	298	LEU	3.3
1	B	363	LEU	3.3
1	B	278	ILE	3.3
1	B	371	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	3.1
1	B	320	SER	3.1
1	B	199	VAL	3.1
1	B	408	ARG	3.0
1	A	92	THR	3.0
1	B	373	PHE	3.0
1	B	409	TYR	3.0
1	B	332	GLY	2.9
1	B	360	LEU	2.8
1	B	280	LYS	2.7
1	B	24	TRP	2.7
1	A	70	LYS	2.7
1	B	279	LEU	2.7
1	A	413	PHE	2.6
1	B	273	ALA	2.5
1	B	288	GLY	2.5
1	B	362	SER	2.5
1	A	286	PRO	2.4
1	B	189	VAL	2.4
1	B	182	TYR	2.3
1	B	287	VAL	2.3
1	A	90	GLU	2.3
1	A	330	GLU	2.3
1	B	96	ILE	2.3
1	A	283	LEU	2.2
1	B	305	GLU	2.2
1	B	297	ARG	2.1
1	A	409	TYR	2.1
1	B	302	TYR	2.1
1	B	384	MET	2.1
1	B	214	TYR	2.1
1	B	277	ARG	2.1
1	A	69	ALA	2.1
1	B	414	PRO	2.0
1	B	375	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.