Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:11 am BST

PDB ID	:	3I7F
Title	:	Aspartyl tRNA synthetase from Entamoeba histolytica
Authors	:	Arakaki, T.; Merritt, E.A.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on	:	2009-07-08
Resolution	:	2.80 Å(reported)

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

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

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

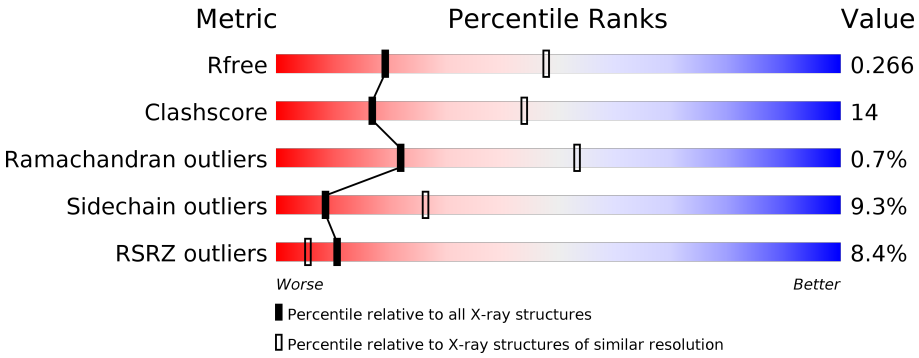
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	548	7% 65% 19% • 11%
1	B	548	8% 64% 18% 5% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7737 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	485	Total	C	N	O	S	0	0	0
			3845	2479	634	708	24			
1	B	483	Total	C	N	O	S	0	0	0
			3814	2463	620	707	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	PDB 3I7F
A	-2	PRO	-	EXPRESSION TAG	PDB 3I7F
A	-1	GLY	-	EXPRESSION TAG	PDB 3I7F
A	0	SER	-	EXPRESSION TAG	PDB 3I7F
B	-3	GLY	-	EXPRESSION TAG	PDB 3I7F
B	-2	PRO	-	EXPRESSION TAG	PDB 3I7F
B	-1	GLY	-	EXPRESSION TAG	PDB 3I7F
B	0	SER	-	EXPRESSION TAG	PDB 3I7F

- Molecule 2 is water.

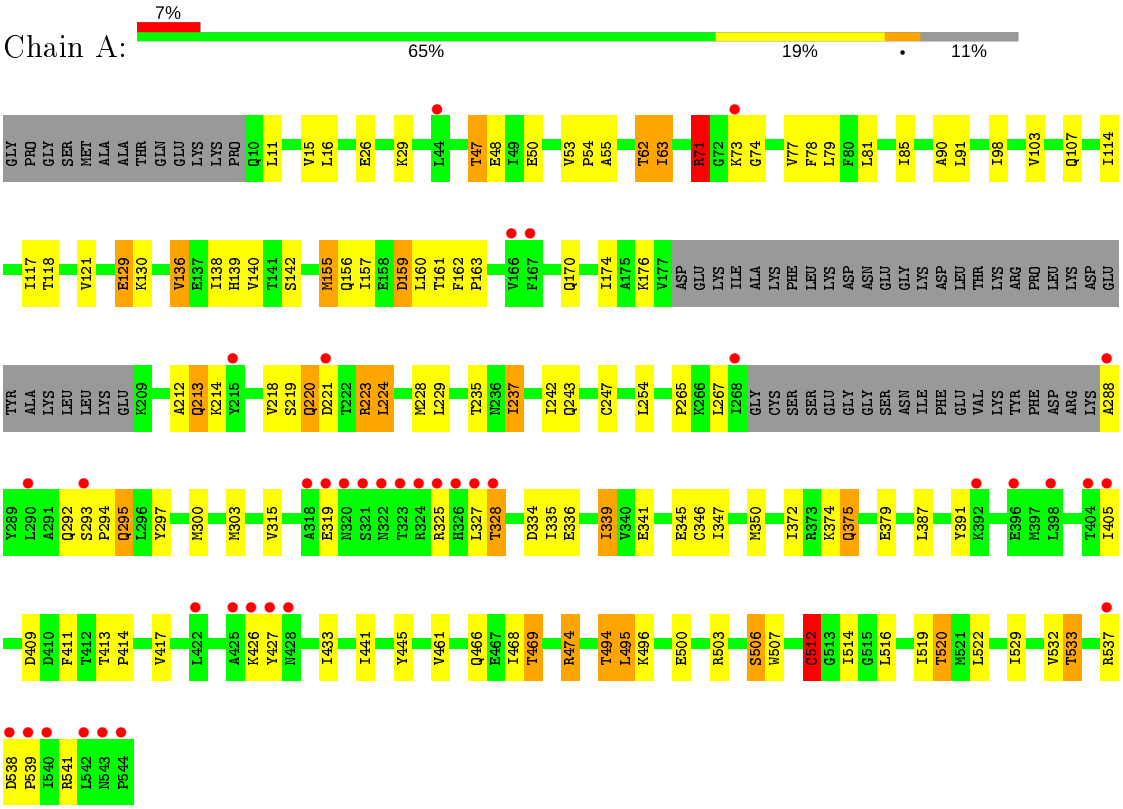
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		
2	B	42	Total	O	0	0
			42	42		

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.

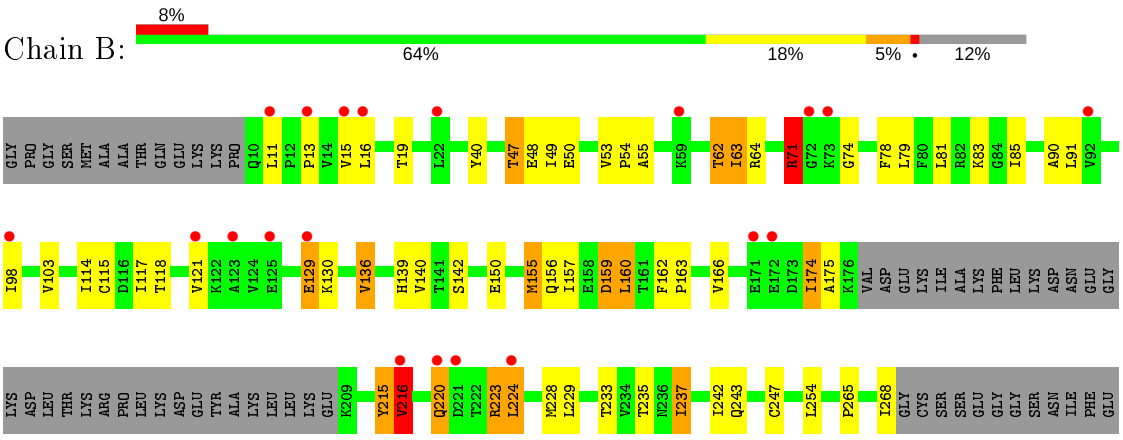
- Molecule 1: Aspartyl-tRNA synthetase

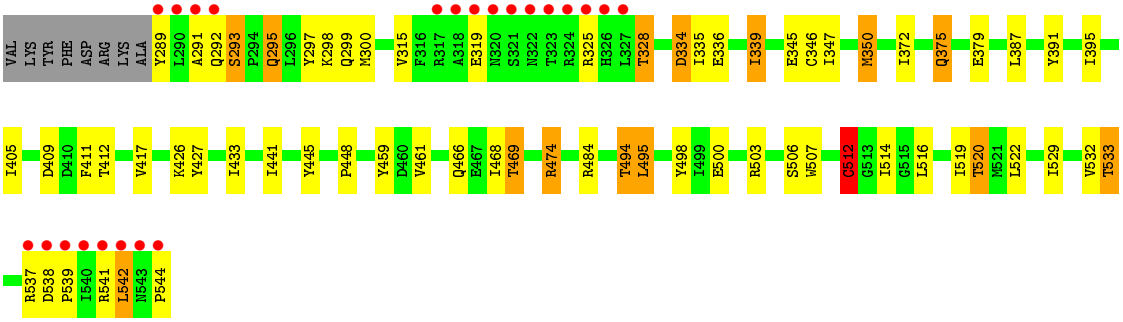
Chain A:



- Molecule 1: Aspartyl-tRNA synthetase

Chain B:




VAL LYS TYR PHE ASP ARG LYS ALA Y289 L290 A291 Q292 S293 P294 Q295 L296 Y297 K298 Q299 M300 V315 F316 R317 A318 E319 N320 S321 N322 T323 R324 R325 H326 L327 T328 D334 I335 E336 I339 E345 C346 I347 M350 I372 Q375 E379 L387 Y391 I395
I405 D409 D410 F411 T412 V417 K426 Y427 I433 I441 Y445 P448 Y459 D460 V461 Q466 E467 I468 T469 R474 R484 T494 L495 Y498 I499 E500 R503 S506 W507 C512 G513 I514 G515 L516 I519 T520 M521 L522 I529 V532 T533
R537 D538 P539 I540 R541 L542 N543 P544

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	247.85Å 247.85Å 56.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 40.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.80) 99.8 (40.90-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.237 0.237 , 0.266	Depositor DCC
R_{free} test set	1594 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.851 for H, K, L 0.149 for K, H, -L	Depositor
Outliers	0 of 31681 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7737	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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	0.58	2/3929 (0.1%)	0.68	1/5322 (0.0%)
1	B	0.64	1/3898 (0.0%)	0.71	1/5286 (0.0%)
All	All	0.61	3/7827 (0.0%)	0.69	2/10608 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	CYS	CB-SG	-9.65	1.65	1.82
1	A	512	CYS	CB-SG	-7.98	1.68	1.82
1	A	26	GLU	CG-CD	5.39	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	71	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	71	ARG	NE-CZ-NH1	6.82	123.71	120.30

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	3845	0	3791	110	0
1	B	3814	0	3739	112	0
2	A	36	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	42	0	0	4	0
All	All	7737	0	7530	213	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 14.

All (213) 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:254:LEU:HD11	1:A:335:ILE:HD11	1.52	0.90
1:B:254:LEU:HD11	1:B:335:ILE:HD11	1.53	0.90
1:A:538:ASP:N	2:A:572:HOH:O	2.03	0.87
1:A:85:ILE:HG23	1:A:237:ILE:HD11	1.58	0.85
1:A:155:MET:HE2	1:A:160:LEU:HD21	1.58	0.83
1:B:412:THR:CB	2:B:583:HOH:O	2.27	0.83
1:A:155:MET:HE2	1:A:160:LEU:CD2	2.09	0.82
1:B:155:MET:CE	1:B:160:LEU:HD21	2.12	0.80
1:A:155:MET:CE	1:A:160:LEU:HD21	2.11	0.80
1:A:541:ARG:O	2:A:572:HOH:O	1.99	0.80
1:A:170:GLN:CB	2:A:577:HOH:O	2.30	0.80
1:A:73:LYS:HA	2:A:578:HOH:O	1.83	0.79
1:B:336:GLU:OE1	1:B:474:ARG:NH1	2.15	0.79
1:B:297:TYR:HA	1:B:300:MET:HE3	1.65	0.78
1:B:155:MET:HE2	1:B:160:LEU:CD2	2.14	0.78
1:B:155:MET:HE2	1:B:160:LEU:HD21	1.66	0.76
1:A:297:TYR:HA	1:A:300:MET:HE3	1.67	0.75
1:A:336:GLU:OE1	1:A:474:ARG:NH1	2.20	0.75
1:A:350:MET:SD	2:A:571:HOH:O	2.44	0.73
1:B:78:PHE:CE2	1:B:91:LEU:HD13	2.24	0.72
1:B:85:ILE:HG23	1:B:237:ILE:HD11	1.73	0.71
1:A:159:ASP:OD2	2:A:556:HOH:O	2.09	0.71
1:A:516:LEU:O	1:A:520:THR:HG22	1.91	0.70
1:A:295:GLN:OE1	1:A:474:ARG:NH1	2.24	0.70
1:B:295:GLN:OE1	1:B:474:ARG:NH1	2.25	0.69
1:A:325:ARG:O	2:A:563:HOH:O	2.09	0.69
1:A:500:GLU:CD	1:A:503:ARG:HH21	1.96	0.69
1:B:468:ILE:HG13	1:B:469:THR:HG23	1.73	0.69
1:A:78:PHE:CE2	1:A:91:LEU:HD13	2.28	0.69
1:B:47:THR:O	1:B:63:ILE:HG22	1.94	0.68
1:B:53:VAL:HG13	1:B:54:PRO:HD2	1.74	0.68
1:A:468:ILE:HG13	1:A:469:THR:HG23	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:HG13	1:A:461:VAL:HG22	1.77	0.67
1:A:235:THR:OG1	1:A:375:GLN:HG3	1.95	0.66
1:A:11:LEU:O	1:A:11:LEU:HD23	1.94	0.66
1:A:507:TRP:CD2	1:B:114:ILE:HD13	2.30	0.66
1:B:347:ILE:HD12	1:B:433:ILE:CD1	2.26	0.66
1:A:295:GLN:NE2	1:A:445:TYR:CE1	2.64	0.65
1:B:500:GLU:CD	1:B:503:ARG:HH21	2.00	0.65
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.62	0.64
1:B:469:THR:HG22	1:B:514:ILE:HG23	1.80	0.63
1:B:433:ILE:HG13	1:B:461:VAL:HG22	1.81	0.62
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.63	0.62
1:A:469:THR:HG22	1:A:514:ILE:HG23	1.81	0.62
1:B:215:TYR:O	1:B:216:VAL:HG12	2.00	0.62
1:A:426:LYS:HD3	1:A:427:TYR:CE2	2.34	0.62
1:A:288:ALA:CB	1:B:542:LEU:HD11	2.31	0.61
1:B:532:VAL:CG1	1:B:532:VAL:O	2.48	0.61
1:B:295:GLN:NE2	1:B:445:TYR:CE1	2.69	0.61
1:B:484:ARG:NH1	2:B:576:HOH:O	2.33	0.61
1:A:507:TRP:CE3	1:B:114:ILE:HD13	2.36	0.60
1:A:243:GLN:HG3	1:A:520:THR:HG21	1.83	0.60
1:B:298:LYS:HD2	1:B:334:ASP:HB3	1.84	0.59
1:B:235:THR:OG1	1:B:375:GLN:HG3	2.02	0.59
1:B:292:GLN:O	1:B:315:VAL:HG13	2.01	0.59
1:A:214:LYS:CB	2:A:577:HOH:O	2.49	0.59
1:B:350:MET:SD	1:B:512:CYS:SG	3.00	0.59
1:B:155:MET:HE1	1:B:160:LEU:HD21	1.85	0.58
1:A:220:GLN:O	1:A:224:LEU:HB2	2.03	0.58
1:A:53:VAL:HG13	1:A:54:PRO:HD2	1.84	0.58
1:B:155:MET:HE3	1:B:223:ARG:HG3	1.86	0.58
1:B:347:ILE:HG23	1:B:433:ILE:HD12	1.86	0.57
1:A:47:THR:O	1:A:63:ILE:HG22	2.02	0.57
1:A:163:PRO:HB3	1:A:374:LYS:O	2.04	0.57
1:A:494:THR:HG22	1:A:495:LEU:HD22	1.86	0.57
1:A:288:ALA:HB2	1:B:542:LEU:HD11	1.86	0.57
1:A:292:GLN:O	1:A:315:VAL:HG13	2.05	0.57
1:B:49:ILE:HD12	1:B:83:LYS:HB3	1.88	0.56
1:B:129:GLU:OE2	1:B:130:LYS:N	2.39	0.56
1:B:174:ILE:O	1:B:174:ILE:HG22	2.04	0.56
1:B:347:ILE:HD12	1:B:433:ILE:HD11	1.87	0.56
1:A:220:GLN:HA	1:A:223:ARG:HD3	1.89	0.56
1:A:496:LYS:NZ	1:B:13:PRO:O	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ILE:HG22	1:A:522:LEU:HD12	1.87	0.55
1:B:220:GLN:HA	1:B:223:ARG:HD3	1.87	0.55
1:A:537:ARG:HA	2:A:572:HOH:O	2.05	0.55
1:B:220:GLN:O	1:B:224:LEU:HB2	2.06	0.55
1:A:91:LEU:HD23	1:A:139:HIS:CD2	2.41	0.55
1:B:405:ILE:HD11	1:B:411:PHE:CD1	2.41	0.54
1:B:441:ILE:CG2	1:B:441:ILE:O	2.56	0.54
1:B:516:LEU:O	1:B:520:THR:HG22	2.07	0.54
1:B:426:LYS:HD3	1:B:427:TYR:CE2	2.43	0.54
1:B:156:GLN:NE2	1:B:156:GLN:HA	2.21	0.54
1:A:346:CYS:O	1:A:350:MET:HG2	2.08	0.54
1:B:237:ILE:C	1:B:237:ILE:HD12	2.28	0.54
1:A:114:ILE:HD13	1:B:507:TRP:CD2	2.43	0.53
1:A:339:ILE:CD1	1:A:345:GLU:HB2	2.38	0.53
1:A:15:VAL:O	1:A:16:LEU:HD23	2.08	0.53
1:B:325:ARG:NH1	1:B:466:GLN:OE1	2.42	0.53
1:B:74:GLY:O	1:B:103:VAL:HG11	2.08	0.53
1:A:114:ILE:HD13	1:B:507:TRP:CE3	2.44	0.52
1:A:156:GLN:HA	1:A:156:GLN:NE2	2.24	0.52
1:B:391:TYR:OH	1:B:409:ASP:O	2.21	0.52
1:B:532:VAL:HG12	1:B:532:VAL:O	2.08	0.52
1:B:243:GLN:HG3	1:B:520:THR:HG21	1.91	0.52
1:A:350:MET:CE	1:A:512:CYS:SG	2.98	0.52
1:A:129:GLU:OE2	1:A:130:LYS:N	2.43	0.52
1:A:155:MET:CE	1:A:160:LEU:HD11	2.39	0.52
1:A:532:VAL:O	1:A:532:VAL:CG1	2.57	0.52
1:B:62:THR:HA	1:B:117:ILE:O	2.09	0.51
1:A:405:ILE:HD11	1:A:411:PHE:CD1	2.45	0.51
1:B:11:LEU:O	1:B:11:LEU:HD23	2.10	0.51
1:A:74:GLY:O	1:A:103:VAL:HG11	2.12	0.50
1:A:325:ARG:NH1	1:A:466:GLN:OE1	2.44	0.50
1:A:495:LEU:HD23	1:A:495:LEU:H	1.76	0.50
1:B:155:MET:CE	1:B:160:LEU:HD11	2.41	0.50
1:B:495:LEU:HD23	1:B:495:LEU:H	1.76	0.50
1:B:529:ILE:O	1:B:533:THR:HG23	2.12	0.50
1:B:405:ILE:HD11	1:B:411:PHE:HD1	1.77	0.50
1:B:494:THR:HG22	1:B:495:LEU:HD22	1.93	0.50
1:B:91:LEU:HD23	1:B:139:HIS:CD2	2.47	0.49
1:A:350:MET:SD	1:A:512:CYS:SG	3.04	0.49
1:A:516:LEU:O	1:A:519:ILE:HG22	2.11	0.49
1:A:529:ILE:O	1:A:533:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:CD2	1:B:495:LEU:N	2.76	0.49
1:A:328:THR:HG21	1:A:539:PRO:HG3	1.95	0.49
1:B:346:CYS:O	1:B:350:MET:HG2	2.13	0.49
1:B:53:VAL:HG12	1:B:55:ALA:H	1.76	0.49
1:A:155:MET:HE1	1:A:160:LEU:HD21	1.93	0.49
1:A:294:PRO:CG	2:A:579:HOH:O	2.60	0.49
1:B:298:LYS:HE3	1:B:336:GLU:OE1	2.12	0.49
1:A:538:ASP:OD1	1:A:541:ARG:N	2.46	0.48
1:A:79:LEU:HB2	1:A:90:ALA:HB3	1.95	0.48
1:A:218:VAL:HG12	1:A:219:SER:H	1.78	0.48
1:A:267:LEU:O	1:B:542:LEU:HD21	2.14	0.48
1:B:242:ILE:HD12	1:B:372:ILE:CD1	2.43	0.48
1:B:538:ASP:OD1	1:B:541:ARG:N	2.46	0.48
1:A:55:ALA:HB2	2:A:561:HOH:O	2.14	0.48
1:B:159:ASP:HA	1:B:162:PHE:CD2	2.49	0.48
1:B:339:ILE:CD1	1:B:345:GLU:HB2	2.43	0.48
1:B:98:ILE:HD11	1:B:140:VAL:O	2.14	0.48
1:A:62:THR:HA	1:A:117:ILE:O	2.13	0.47
1:A:81:LEU:HD21	1:A:117:ILE:CD1	2.45	0.47
1:B:242:ILE:HD12	1:B:372:ILE:HD11	1.96	0.47
1:A:347:ILE:HA	1:A:350:MET:HG3	1.95	0.47
1:A:495:LEU:HD23	1:A:495:LEU:N	2.28	0.47
1:B:495:LEU:HD23	1:B:495:LEU:N	2.30	0.47
1:B:347:ILE:HA	1:B:350:MET:HG3	1.97	0.47
1:B:516:LEU:O	1:B:519:ILE:HG22	2.14	0.47
1:A:495:LEU:N	1:A:495:LEU:CD2	2.77	0.47
1:A:73:LYS:O	1:A:73:LYS:HD3	2.15	0.47
1:B:163:PRO:HG2	1:B:166:VAL:HG23	1.97	0.46
1:B:79:LEU:HB2	1:B:90:ALA:HB3	1.96	0.46
1:A:327:LEU:HD22	1:A:538:ASP:HB3	1.96	0.46
1:B:64:ARG:HA	1:B:115:CYS:O	2.15	0.46
1:B:121:VAL:HG13	1:B:136:VAL:HG13	1.96	0.46
1:B:537:ARG:CZ	1:B:542:LEU:O	2.63	0.46
1:A:77:VAL:HG21	1:A:107:GLN:HG3	1.97	0.46
1:B:328:THR:HG21	1:B:539:PRO:HG3	1.97	0.46
1:A:219:SER:O	1:A:221:ASP:N	2.49	0.46
1:A:85:ILE:CG2	1:A:237:ILE:HD11	2.38	0.46
1:B:62:THR:HB	1:B:118:THR:OG1	2.16	0.46
1:A:62:THR:HB	1:A:118:THR:OG1	2.17	0.45
1:A:405:ILE:HD11	1:A:411:PHE:HD1	1.82	0.45
1:B:53:VAL:HG13	1:B:54:PRO:CD	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:HD21	1:B:117:ILE:CD1	2.46	0.45
1:A:121:VAL:HG13	1:A:136:VAL:HG13	1.99	0.45
1:A:224:LEU:HD13	2:A:546:HOH:O	2.15	0.45
1:B:339:ILE:HA	1:B:339:ILE:HD13	1.63	0.45
1:A:516:LEU:O	1:A:520:THR:CG2	2.62	0.45
1:B:350:MET:CE	1:B:512:CYS:SG	3.05	0.45
1:B:468:ILE:HG22	1:B:522:LEU:HD12	1.97	0.45
1:A:212:ALA:HA	1:A:213:GLN:CB	2.47	0.45
1:B:15:VAL:O	1:B:16:LEU:HD23	2.16	0.44
1:B:224:LEU:HD22	1:B:544:PRO:HD3	1.99	0.44
1:B:254:LEU:CD1	1:B:335:ILE:HD11	2.38	0.44
1:B:350:MET:H	1:B:350:MET:HG2	1.63	0.44
1:A:328:THR:HG23	1:A:539:PRO:HD3	1.99	0.44
1:A:391:TYR:OH	1:A:409:ASP:O	2.25	0.44
1:A:243:GLN:NE2	1:A:532:VAL:O	2.50	0.44
1:A:295:GLN:NE2	1:A:445:TYR:CZ	2.86	0.43
1:A:265:PRO:HG2	1:A:297:TYR:CE2	2.52	0.43
1:B:469:THR:HG21	1:B:514:ILE:HG12	2.00	0.43
1:A:341:GLU:HG2	1:B:40:TYR:O	2.18	0.43
1:A:532:VAL:HG12	1:A:532:VAL:O	2.16	0.43
1:B:328:THR:HG23	1:B:539:PRO:HD3	2.00	0.43
1:B:469:THR:CG2	1:B:514:ILE:HG12	2.48	0.43
1:A:339:ILE:HA	1:A:339:ILE:HD13	1.68	0.43
1:B:448:PRO:HB3	2:B:576:HOH:O	2.18	0.43
1:A:294:PRO:HG2	2:A:579:HOH:O	2.19	0.43
1:B:233:THR:O	1:B:237:ILE:HG23	2.19	0.43
1:B:19:THR:HG23	1:B:150:GLU:HG2	2.01	0.43
1:B:268:ILE:N	1:B:289:TYR:O	2.51	0.43
1:A:53:VAL:HG12	1:A:55:ALA:H	1.84	0.43
1:B:265:PRO:HG2	1:B:297:TYR:CE2	2.54	0.43
1:A:500:GLU:CD	1:A:503:ARG:NH2	2.69	0.43
1:A:98:ILE:HD11	1:A:140:VAL:O	2.19	0.42
1:A:294:PRO:HB2	2:A:579:HOH:O	2.18	0.42
1:A:242:ILE:HD12	1:A:372:ILE:HD11	2.02	0.42
1:B:19:THR:HG22	1:B:150:GLU:HA	2.02	0.42
1:A:303:MET:SD	1:A:506:SER:OG	2.65	0.42
1:B:47:THR:O	1:B:63:ILE:CG2	2.65	0.42
1:A:441:ILE:CG2	1:A:441:ILE:O	2.67	0.42
1:A:63:ILE:HD11	1:A:138:ILE:HD11	2.01	0.42
1:B:441:ILE:HA	1:B:441:ILE:HD13	1.76	0.42
1:B:387:LEU:HD22	1:B:427:TYR:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HG22	1:A:161:THR:O	2.19	0.41
1:A:242:ILE:HD12	1:A:372:ILE:CD1	2.50	0.41
1:B:299:GLN:NE2	1:B:498:TYR:OH	2.52	0.41
1:A:155:MET:HE3	1:A:223:ARG:HG3	2.03	0.41
1:B:175:ALA:HB3	2:B:546:HOH:O	2.20	0.41
1:A:387:LEU:HD22	1:A:427:TYR:CD2	2.56	0.41
1:A:159:ASP:HA	1:A:162:PHE:CD2	2.55	0.41
1:A:469:THR:CG2	1:A:514:ILE:HG12	2.51	0.41
1:B:441:ILE:HG22	1:B:441:ILE:O	2.21	0.41
1:A:413:THR:HB	1:A:414:PRO:HD3	2.03	0.41
1:B:268:ILE:HD11	1:B:291:ALA:HB2	2.03	0.41
1:B:293:SER:C	1:B:295:GLN:H	2.25	0.41
1:B:19:THR:CG2	1:B:150:GLU:HG2	2.51	0.40
1:B:395:ILE:HG23	1:B:405:ILE:HG21	2.02	0.40
1:B:347:ILE:HD11	1:B:459:TYR:CD2	2.56	0.40
1:A:53:VAL:HG13	1:A:54:PRO:CD	2.51	0.40
1:A:63:ILE:HD11	1:A:138:ILE:CD1	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	479/548 (87%)	448 (94%)	27 (6%)	4 (1%)	19	49
1	B	477/548 (87%)	447 (94%)	27 (6%)	3 (1%)	25	56
All	All	956/1096 (87%)	895 (94%)	54 (6%)	7 (1%)	22	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	213	GLN
1	A	220	GLN
1	B	220	GLN
1	A	176	LYS
1	A	174	ILE
1	B	174	ILE

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	412/490 (84%)	376 (91%)	36 (9%)	10 30
1	B	408/490 (83%)	368 (90%)	40 (10%)	8 24
All	All	820/980 (84%)	744 (91%)	76 (9%)	9 26

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	47	THR
1	A	48	GLU
1	A	50	GLU
1	A	62	THR
1	A	63	ILE
1	A	71	ARG
1	A	129	GLU
1	A	136	VAL
1	A	142	SER
1	A	155	MET
1	A	157	ILE
1	A	159	ASP
1	A	223	ARG
1	A	224	LEU
1	A	228	MET
1	A	229	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	237	ILE
1	A	247	CYS
1	A	293	SER
1	A	295	GLN
1	A	319	GLU
1	A	328	THR
1	A	334	ASP
1	A	339	ILE
1	A	375	GLN
1	A	379	GLU
1	A	417	VAL
1	A	469	THR
1	A	474	ARG
1	A	494	THR
1	A	495	LEU
1	A	506	SER
1	A	512	CYS
1	A	520	THR
1	A	533	THR
1	B	47	THR
1	B	48	GLU
1	B	50	GLU
1	B	62	THR
1	B	63	ILE
1	B	71	ARG
1	B	129	GLU
1	B	136	VAL
1	B	142	SER
1	B	155	MET
1	B	157	ILE
1	B	159	ASP
1	B	160	LEU
1	B	215	TYR
1	B	216	VAL
1	B	223	ARG
1	B	224	LEU
1	B	228	MET
1	B	229	LEU
1	B	237	ILE
1	B	247	CYS
1	B	293	SER
1	B	295	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	319	GLU
1	B	328	THR
1	B	334	ASP
1	B	339	ILE
1	B	350	MET
1	B	375	GLN
1	B	379	GLU
1	B	417	VAL
1	B	469	THR
1	B	474	ARG
1	B	494	THR
1	B	495	LEU
1	B	506	SER
1	B	512	CYS
1	B	520	THR
1	B	533	THR
1	B	542	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	299	GLN
1	B	156	GLN
1	B	299	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

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	485/548 (88%)	0.28	38 (7%) 13 7	14, 19, 24, 40	1 (0%)
1	B	483/548 (88%)	0.22	43 (8%) 9 5	12, 19, 23, 45	0
All	All	968/1096 (88%)	0.25	81 (8%) 11 5	12, 19, 24, 45	1 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	SER	9.9
1	B	323	THR	9.9
1	B	324	ARG	8.9
1	A	322	ASN	8.3
1	B	326	HIS	7.7
1	B	325	ARG	7.2
1	A	327	LEU	7.0
1	B	322	ASN	7.0
1	B	538	ASP	6.2
1	B	539	PRO	5.6
1	A	326	HIS	5.6
1	B	540	ILE	5.3
1	B	327	LEU	5.2
1	B	537	ARG	4.8
1	A	540	ILE	4.8
1	B	544	PRO	4.7
1	A	544	PRO	4.2
1	B	121	VAL	4.2
1	B	73	LYS	4.1
1	B	541	ARG	4.1
1	A	543	ASN	4.0
1	A	321	SER	3.9
1	A	320	ASN	3.9
1	A	290	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	542	LEU	3.9
1	B	125	GLU	3.8
1	A	73	LYS	3.7
1	A	268	ILE	3.6
1	B	290	LEU	3.6
1	B	543	ASN	3.5
1	A	323	THR	3.5
1	B	220	GLN	3.5
1	A	426	LYS	3.4
1	A	539	PRO	3.3
1	B	16	LEU	3.2
1	A	405	ILE	3.2
1	A	325	ARG	3.1
1	A	293	SER	3.0
1	B	72	GLY	3.0
1	B	319	GLU	3.0
1	B	11	LEU	2.9
1	A	538	ASP	2.9
1	A	221	ASP	2.9
1	A	215	TYR	2.8
1	A	319	GLU	2.8
1	B	98	ILE	2.8
1	A	166	VAL	2.8
1	A	428	ASN	2.7
1	B	320	ASN	2.6
1	B	289	TYR	2.6
1	B	59	LYS	2.6
1	A	44	LEU	2.6
1	B	171	GLU	2.5
1	A	392	LYS	2.5
1	A	404	THR	2.5
1	A	425	ALA	2.5
1	A	328	THR	2.4
1	B	292	GLN	2.3
1	B	123	ALA	2.3
1	A	288	ALA	2.3
1	A	318	ALA	2.3
1	B	318	ALA	2.3
1	B	15	VAL	2.3
1	B	221	ASP	2.3
1	A	427	TYR	2.3
1	B	172	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	422	LEU	2.2
1	B	22	LEU	2.2
1	B	224	LEU	2.2
1	B	92	VAL	2.2
1	A	398	LEU	2.2
1	A	542	LEU	2.2
1	A	324	ARG	2.2
1	B	129	GLU	2.1
1	B	291	ALA	2.1
1	B	216	VAL	2.1
1	B	317	ARG	2.1
1	A	167	PHE	2.1
1	A	537	ARG	2.1
1	A	396	GLU	2.0
1	B	13	PRO	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.