



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 PM UTC

PDB ID : 3I7F / pdb_00003i7f
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 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
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

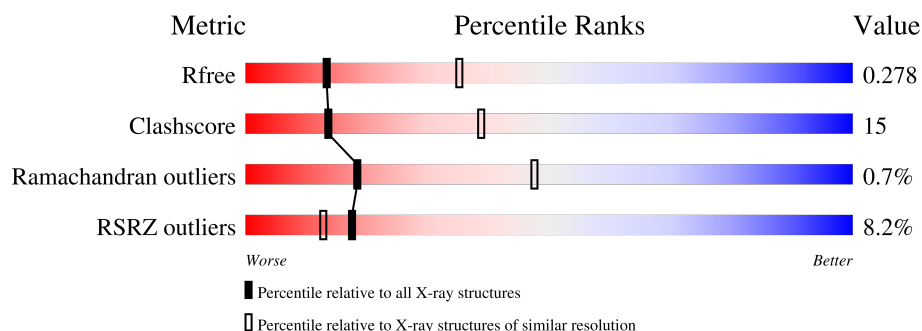
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	548	9% 67% 21% 11%
1	B	548	6% 65% 22% 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		



4 Data and refinement statistics

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 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.80) 99.8 (50.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.237 (Not available) , 0.278	Depositor DCC
R_{free} test set	1601 reflections (5.04%)	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 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	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	0.89	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	0/3929	0.87	0/5322
1	B	0.79	0/3898	0.91	4/5286 (0.1%)
All	All	0.75	0/7827	0.89	4/10608 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	ILE	CB-CA-C	-5.29	105.00	112.14
1	B	407	ASP	N-CA-C	5.07	116.81	111.28
1	B	437	PHE	CA-C-N	5.04	125.28	119.83
1	B	437	PHE	C-N-CA	5.04	125.28	119.83

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	3845	0	3791	115	0
1	B	3814	0	3739	117	0
2	A	36	0	0	14	0
2	B	42	0	0	6	0
All	All	7737	0	7530	222	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 15.

All (222) 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:B:412:THR:CB	2:B:583:HOH:O	2.27	0.83
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:155:MET:HE2	1:B:160:LEU:CD2	2.15	0.76
1:A:350:MET:HE1	1:A:512:CYS:SG	2.26	0.76
1:B:297:TYR:HA	1:B:300:MET:HE3	1.67	0.76
1:A:336:GLU:OE1	1:A:474:ARG:NH1	2.20	0.75
1:A:297:TYR:HA	1:A:300:MET:HE3	1.69	0.75
1:B:155:MET:HE2	1:B:160:LEU:HD21	1.68	0.74
1:A:500:GLU:CD	1:A:503:ARG:HH21	1.96	0.74
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:155:MET:HE2	1:A:160:LEU:CD2	2.20	0.70
1:A:516:LEU:O	1:A:520:THR:HG22	1.91	0.70
1:A:155:MET:HE2	1:A:160:LEU:HD21	1.73	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:B:500:GLU:CD	1:B:503:ARG:HH21	2.00	0.69
1:A:325:ARG:O	2:A:563:HOH:O	2.09	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
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:HD23	1:A:11:LEU:O	1.94	0.66
1:A:507:TRP:CD2	1:B:114:ILE:HD13	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:155:MET:HE1	1:A:160:LEU:HD21	1.78	0.65
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.62	0.64
1:B:469:THR:HG22	1:B:514:ILE:HG23	1.80	0.63
1:B:350:MET:HE1	1:B:512:CYS:SG	2.38	0.63
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.63	0.62
1:B:433:ILE:HG13	1:B:461:VAL:HG22	1.81	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:O	1:B:532:VAL:CG1	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:243:GLN:HG3	1:A:520:THR:HG21	1.83	0.60
1:A:507:TRP:CE3	1:B:114:ILE:HD13	2.36	0.60
1:B:155:MET:HE1	1:B:160:LEU:HD21	1.84	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:155:MET:HE3	1:B:223:ARG:HG3	1.85	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:237:ILE:HD12	1:B:237:ILE:C	2.28	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:346:CYS:O	1:A:350:MET:HG2	2.08	0.54
1:B:156:GLN:HA	1:B:156:GLN:NE2	2.21	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:A:155:MET:HE3	1:A:223:ARG:HG3	1.91	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:NE2	1:A:156:GLN:HA	2.24	0.52
1:B:391:TYR:OH	1:B:409:ASP:O	2.21	0.52
1:B:532:VAL:O	1:B:532:VAL:HG12	2.08	0.52
1:B:243:GLN:HG3	1:B:520:THR:HG21	1.91	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:CG1	1:A:532:VAL:O	2.57	0.52
1:A:350:MET:CE	1:A:512:CYS:SG	2.98	0.51
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
1:B:495:LEU:N	1:B:495:LEU:CD2	2.76	0.49
1:A:328:THR:HG21	1:A:539:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG12	1:B:55:ALA:H	1.76	0.49
1:B:346:CYS:O	1:B:350:MET:HG2	2.13	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:79:LEU:HB2	1:A:90:ALA:HB3	1.95	0.48
1:A:538:ASP:OD1	1:A:541:ARG:N	2.46	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:500:GLU:CD	1:A:503:ARG:NH2	2.69	0.47
1:A:495:LEU:HD23	1:A:495:LEU:N	2.28	0.47
1:B:347:ILE:HA	1:B:350:MET:HG3	1.97	0.47
1:B:495:LEU:HD23	1:B:495:LEU:N	2.30	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:79:LEU:HB2	1:B:90:ALA:HB3	1.96	0.46
1:B:163:PRO:HG2	1:B:166:VAL:HG23	1.97	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:85:ILE:CG2	1:A:237:ILE:HD11	2.38	0.46
1:A:219:SER:O	1:A:221:ASP:N	2.49	0.46
1:B:62:THR:HB	1:B:118:THR:OG1	2.16	0.46
1:A:391:TYR:OH	1:A:409:ASP:O	2.25	0.45
1:A:62:THR:HB	1:A:118:THR:OG1	2.17	0.45
1:A:73:LYS:HD2	1:A:76:MET:HE3	1.97	0.45
1:B:293:SER:C	1:B:295:GLN:H	2.25	0.45
1:A:405:ILE:HD11	1:A:411:PHE:HD1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG13	1:B:54:PRO:CD	2.43	0.45
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:HG2	1:B:350:MET:H	1.63	0.44
1:A:328:THR:HG23	1:A:539:PRO:HD3	1.99	0.44
1:A:243:GLN:NE2	1:A:532:VAL:O	2.50	0.44
1:A:265:PRO:HG2	1:A:297:TYR:CE2	2.52	0.43
1:A:295:GLN:NE2	1:A:445:TYR:CZ	2.86	0.43
1:B:412:THR:C	2:B:583:HOH:O	2.60	0.43
1:B:469:THR:HG21	1:B:514:ILE:HG12	2.00	0.43
1:A:228:MET:HE3	1:B:501:SER:O	2.18	0.43
1:A:341:GLU:HG2	1:B:40:TYR:O	2.18	0.43
1:A:532:VAL:O	1:A:532:VAL:HG12	2.16	0.43
1:B:328:THR:HG23	1:B:539:PRO:HD3	2.00	0.43
1:B:336:GLU:CD	1:B:474:ARG:NH1	2.77	0.43
1:B:469:THR:CG2	1:B:514:ILE:HG12	2.48	0.43
1:A:339:ILE:HD13	1:A:339:ILE:HA	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: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:O	1:A:441:ILE:CG2	2.67	0.42
1:A:63:ILE:HD11	1:A:138:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ILE:HD13	1:B:441:ILE:HA	1.76	0.42
1:B:387:LEU:HD22	1:B:427:TYR:CD2	2.55	0.42
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: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:O	1:B:441:ILE:HG22	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:A:237:ILE:HD12	1:A:237:ILE:C	2.46	0.40
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:A:11:LEU:HD23	1:A:11:LEU:C	2.47	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
1:B:432:TYR:OH	2:B:548:HOH:O	2.22	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%)	16	44
1	B	469/548 (86%)	439 (94%)	27 (6%)	3 (1%)	21	51
All	All	948/1096 (86%)	887 (94%)	54 (6%)	7 (1%)	18	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	VAL
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 [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	485/548 (88%)	0.64	47 (9%)	13 10	14, 19, 24, 40	1 (0%)
1	B	483/548 (88%)	0.34	32 (6%)	24 18	12, 19, 23, 45	0
All	All	968/1096 (88%)	0.49	79 (8%)	17 13	12, 19, 24, 45	1 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	538	ASP	8.4
1	A	211	SER	7.4
1	A	177	VAL	7.1
1	A	209	LYS	6.1
1	A	210	ALA	5.8
1	B	540	ILE	5.2
1	A	322	ASN	5.1
1	A	212	ALA	4.8
1	B	323	THR	4.6
1	B	539	PRO	4.6
1	B	321	SER	4.5
1	B	324	ARG	4.5
1	B	326	HIS	4.3
1	A	327	LEU	4.3
1	B	544	PRO	4.2
1	B	537	ARG	4.2
1	B	541	ARG	4.2
1	B	542	LEU	4.1
1	A	323	THR	4.0
1	A	538	ASP	3.7
1	B	325	ARG	3.7
1	A	218	VAL	3.6
1	A	534	LEU	3.6
1	A	222	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	326	HIS	3.5
1	A	167	PHE	3.4
1	A	176	LYS	3.4
1	A	544	PRO	3.4
1	A	220	GLN	3.4
1	B	224	LEU	3.3
1	A	221	ASP	3.3
1	A	540	ILE	3.2
1	B	293	SER	3.2
1	B	327	LEU	3.2
1	B	176	LYS	3.1
1	A	73	LYS	3.1
1	A	396	GLU	3.1
1	A	166	VAL	3.0
1	B	305	ASP	3.0
1	B	322	ASN	3.0
1	B	212	ALA	3.0
1	B	220	GLN	3.0
1	B	10	GLN	2.9
1	A	293	SER	2.9
1	A	320	ASN	2.9
1	A	217	LYS	2.8
1	A	428	ASN	2.8
1	A	216	VAL	2.8
1	B	210	ALA	2.8
1	A	223	ARG	2.8
1	A	530	ARG	2.7
1	A	367	ASP	2.7
1	A	535	PHE	2.6
1	A	427	TYR	2.5
1	A	321	SER	2.5
1	A	268	ILE	2.5
1	B	209	LYS	2.5
1	B	292	GLN	2.4
1	B	320	ASN	2.4
1	A	306	PHE	2.3
1	A	485	CYS	2.3
1	A	129	GLU	2.3
1	A	336	GLU	2.3
1	B	211	SER	2.3
1	B	301	ALA	2.2
1	A	481	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	543	ASN	2.2
1	A	516	LEU	2.2
1	A	486	ILE	2.2
1	B	125	GLU	2.2
1	A	536	PRO	2.2
1	A	455	TYR	2.2
1	A	380	ASP	2.1
1	A	448	PRO	2.0
1	B	25	GLY	2.0
1	A	426	LYS	2.0
1	A	224	LEU	2.0
1	B	223	ARG	2.0
1	B	102	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.