



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:55 PM UTC

PDB ID : 9JE9 / pdb_00009je9
Title : Crystal structure of a amidase that can hydrolase PU plastic
Authors : Li, Z.S.; Fang, S.T.; Zheng, Z.R.; Xia, W.; Zhou, H.Y.; Li, W.S.; You, S.; Han, X.; Liu, W.D.
Deposited on : 2024-09-02
Resolution : 2.41 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

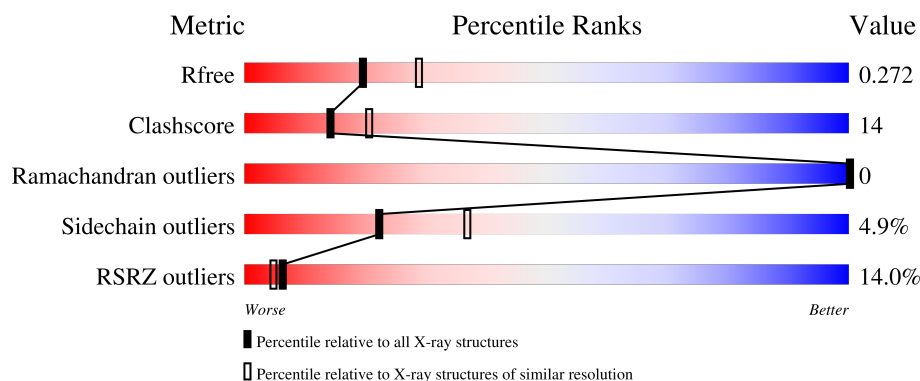
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	461	10% 64% 23% • 12%
1	B	461	15% 65% 25% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6299 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 Amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3036	1918	539	572	7			
1	B	423	Total	C	N	O	S	0	0	0
			3163	1996	563	597	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0A2T7VCT5
A	-21	HIS	-	expression tag	UNP A0A2T7VCT5
A	-20	HIS	-	expression tag	UNP A0A2T7VCT5
A	-19	HIS	-	expression tag	UNP A0A2T7VCT5
A	-18	HIS	-	expression tag	UNP A0A2T7VCT5
A	-17	HIS	-	expression tag	UNP A0A2T7VCT5
A	-16	HIS	-	expression tag	UNP A0A2T7VCT5
A	-15	GLU	-	expression tag	UNP A0A2T7VCT5
A	-14	ASN	-	expression tag	UNP A0A2T7VCT5
A	-13	LEU	-	expression tag	UNP A0A2T7VCT5
A	-12	TYR	-	expression tag	UNP A0A2T7VCT5
A	-11	PHE	-	expression tag	UNP A0A2T7VCT5
A	-10	GLN	-	expression tag	UNP A0A2T7VCT5
A	-9	GLY	-	expression tag	UNP A0A2T7VCT5
A	-8	ALA	-	expression tag	UNP A0A2T7VCT5
A	-7	GLY	-	expression tag	UNP A0A2T7VCT5
A	-6	ALA	-	expression tag	UNP A0A2T7VCT5
A	-5	GLY	-	expression tag	UNP A0A2T7VCT5
A	-4	ALA	-	expression tag	UNP A0A2T7VCT5
A	-3	GLY	-	expression tag	UNP A0A2T7VCT5
A	-2	ALA	-	expression tag	UNP A0A2T7VCT5
A	-1	GLY	-	expression tag	UNP A0A2T7VCT5
A	0	ALA	-	expression tag	UNP A0A2T7VCT5
B	-22	MET	-	initiating methionine	UNP A0A2T7VCT5
B	-21	HIS	-	expression tag	UNP A0A2T7VCT5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP A0A2T7VCT5
B	-19	HIS	-	expression tag	UNP A0A2T7VCT5
B	-18	HIS	-	expression tag	UNP A0A2T7VCT5
B	-17	HIS	-	expression tag	UNP A0A2T7VCT5
B	-16	HIS	-	expression tag	UNP A0A2T7VCT5
B	-15	GLU	-	expression tag	UNP A0A2T7VCT5
B	-14	ASN	-	expression tag	UNP A0A2T7VCT5
B	-13	LEU	-	expression tag	UNP A0A2T7VCT5
B	-12	TYR	-	expression tag	UNP A0A2T7VCT5
B	-11	PHE	-	expression tag	UNP A0A2T7VCT5
B	-10	GLN	-	expression tag	UNP A0A2T7VCT5
B	-9	GLY	-	expression tag	UNP A0A2T7VCT5
B	-8	ALA	-	expression tag	UNP A0A2T7VCT5
B	-7	GLY	-	expression tag	UNP A0A2T7VCT5
B	-6	ALA	-	expression tag	UNP A0A2T7VCT5
B	-5	GLY	-	expression tag	UNP A0A2T7VCT5
B	-4	ALA	-	expression tag	UNP A0A2T7VCT5
B	-3	GLY	-	expression tag	UNP A0A2T7VCT5
B	-2	ALA	-	expression tag	UNP A0A2T7VCT5
B	-1	GLY	-	expression tag	UNP A0A2T7VCT5
B	0	ALA	-	expression tag	UNP A0A2T7VCT5

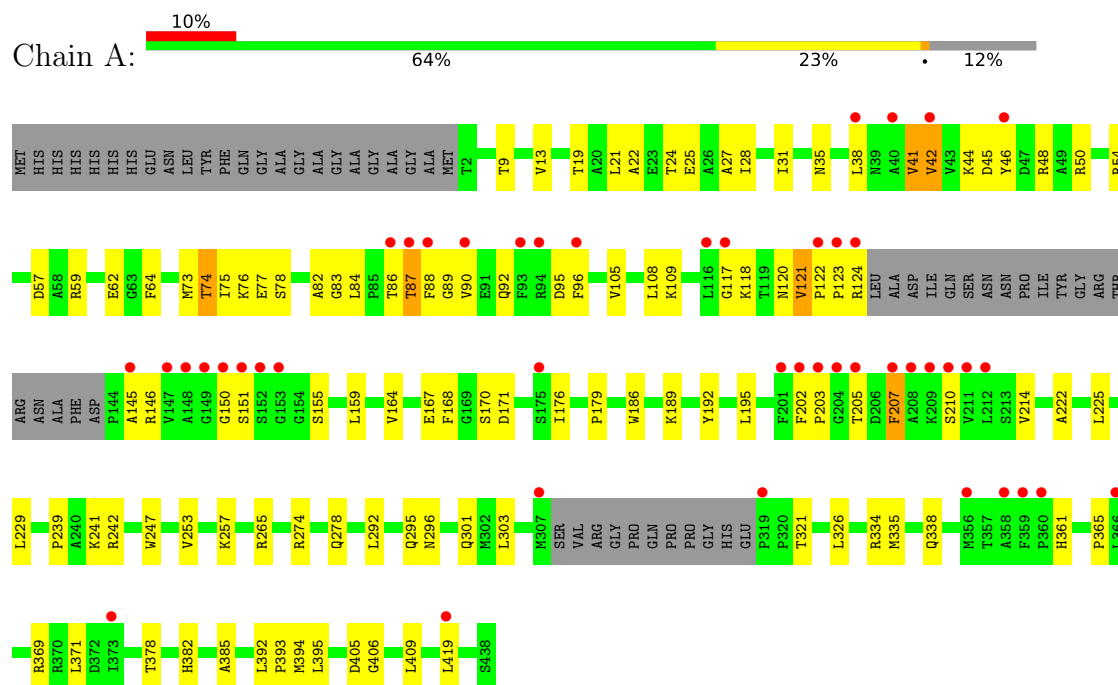
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	44	Total	O	0	0
			44	44		

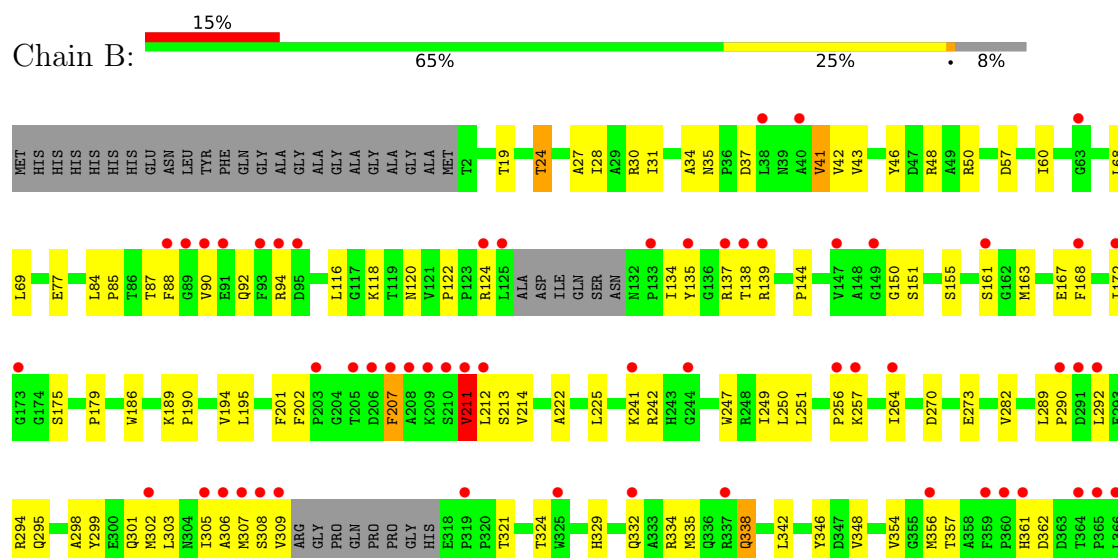
3 Residue-property plots

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: Amidase



• Molecule 1: Amidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	92.82Å 92.82Å 135.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.82 – 2.41 92.82 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.8 (92.82-2.41) 98.8 (92.82-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.218 , 0.273 0.223 , 0.272	Depositor DCC
R_{free} test set	2056 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6299	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.44	0/3104	0.69	2/4239 (0.0%)
1	B	0.46	0/3234	0.74	1/4418 (0.0%)
All	All	0.45	0/6338	0.72	3/8657 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	VAL	N-CA-CB	-6.62	103.47	111.21
1	B	211	VAL	CA-C-O	-5.18	116.89	121.97
1	A	207	PHE	CA-CB-CG	5.14	118.94	113.80

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	3036	0	2990	80	0
1	B	3163	0	3103	97	0
2	A	56	0	0	5	0
2	B	44	0	0	2	0
All	All	6299	0	6093	175	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 (175) 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:31:ILE:HA	1:B:163:MET:HE2	1.47	0.96
1:A:296:ASN:HD21	1:A:385:ALA:CB	1.83	0.91
1:A:155:SER:HB3	1:A:167:GLU:HG2	1.54	0.88
1:A:73:MET:HE1	1:A:108:LEU:HD13	1.56	0.87
1:B:172:ILE:HD12	1:B:213:SER:HB3	1.58	0.85
1:B:368:HIS:HA	1:B:380:PHE:H	1.40	0.83
1:A:395:LEU:HD23	1:A:419:LEU:HD12	1.60	0.83
1:A:405:ASP:OD2	1:A:406:GLY:N	2.13	0.82
1:B:290:PRO:HB3	1:B:338:GLN:HB3	1.61	0.81
1:B:321:THR:HG23	1:B:324:THR:H	1.47	0.79
1:A:167:GLU:HG3	1:A:168:PHE:N	2.03	0.73
1:B:294:ARG:HH22	1:B:334:ARG:HH11	1.37	0.72
1:B:122:PRO:HG2	1:B:150:GLY:O	1.90	0.72
1:B:257:LYS:O	1:B:382:HIS:ND1	2.23	0.71
1:A:50:ARG:O	1:A:54:ARG:HG3	1.91	0.71
1:A:87:THR:HG23	1:A:89:GLY:H	1.56	0.69
1:B:404:ARG:HG3	1:B:410:PRO:HA	1.76	0.68
1:B:124:ARG:HH22	1:B:175:SER:HB2	1.59	0.67
1:B:90:VAL:HA	1:B:134:ILE:HD11	1.74	0.66
1:B:137:ARG:NH1	1:B:138:THR:O	2.28	0.66
1:A:77:GLU:HA	1:A:118:LYS:HE3	1.76	0.66
1:B:77:GLU:HA	1:B:118:LYS:HE3	1.78	0.66
1:A:27:ALA:O	1:A:31:ILE:HG13	1.96	0.65
1:B:27:ALA:O	1:B:31:ILE:HG13	1.97	0.65
1:A:24:THR:O	1:A:28:ILE:HD12	1.97	0.64
1:B:294:ARG:HH22	1:B:334:ARG:HD3	1.60	0.64
1:B:294:ARG:NH2	1:B:334:ARG:HD3	2.13	0.64
1:A:214:VAL:HA	2:A:508:HOH:O	1.97	0.63
1:A:296:ASN:HD21	1:A:385:ALA:HB1	1.62	0.62
1:B:189:LYS:NZ	1:B:395:LEU:O	2.29	0.62
1:B:294:ARG:HH12	1:B:334:ARG:NH1	1.98	0.62
1:A:105:VAL:O	1:A:109:LYS:HG3	2.01	0.61
1:B:168:PHE:HZ	1:B:195:LEU:HD23	1.66	0.60
1:B:257:LYS:HB3	1:B:382:HIS:CE1	2.37	0.60
1:B:87:THR:HG21	1:B:134:ILE:HG13	1.84	0.60
1:A:296:ASN:HD21	1:A:385:ALA:HB2	1.66	0.60
1:A:186:TRP:HB3	1:A:225:LEU:HD11	1.84	0.58
1:A:96:PHE:CD2	1:A:96:PHE:N	2.72	0.58
1:B:295:GLN:HG3	1:B:392:LEU:HD22	1.86	0.57
1:A:155:SER:HB3	1:A:167:GLU:CG	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LEU:HD22	1:B:381:LEU:H	1.69	0.57
1:B:118:LYS:NZ	2:B:503:HOH:O	2.37	0.56
1:B:85:PRO:HG3	1:B:94:ARG:NH2	2.19	0.56
1:B:308:SER:OG	1:B:309:VAL:N	2.38	0.55
1:A:19:THR:OG1	1:A:57:ASP:OD2	2.23	0.55
1:A:202:PHE:HB3	1:A:205:THR:HG21	1.87	0.55
1:B:189:LYS:HG2	1:B:214:VAL:HG21	1.88	0.55
1:A:21:LEU:HD13	1:A:25:GLU:HG3	1.89	0.55
1:B:298:ALA:O	1:B:302:MET:HG3	2.05	0.55
1:A:44:LYS:HD3	1:A:46:TYR:OH	2.07	0.55
1:B:124:ARG:NH2	1:B:175:SER:HB2	2.22	0.54
1:A:31:ILE:O	1:A:35:ASN:HB2	2.07	0.54
1:A:59:ARG:HA	1:A:62:GLU:HG2	1.89	0.54
1:A:123:PRO:O	1:A:124:ARG:C	2.50	0.54
1:B:48:ARG:HH21	1:B:84:LEU:HD13	1.72	0.54
1:A:19:THR:HG23	1:A:22:ALA:H	1.72	0.54
1:A:296:ASN:ND2	1:A:385:ALA:HB1	2.23	0.54
1:B:299:TYR:CE2	1:B:303:LEU:HD11	2.43	0.54
1:A:48:ARG:HH21	1:A:84:LEU:HD11	1.73	0.54
1:A:76:LYS:NZ	1:A:170:SER:OG	2.41	0.53
1:B:294:ARG:HH22	1:B:334:ARG:NH1	2.05	0.53
1:B:303:LEU:O	1:B:307:MET:HG2	2.08	0.53
1:A:171:ASP:HB2	1:A:176:ILE:HD12	1.90	0.53
1:A:392:LEU:HB3	1:A:393:PRO:HD3	1.89	0.53
1:B:46:TYR:O	1:B:50:ARG:HG3	2.08	0.53
1:B:211:VAL:O	1:B:212:LEU:HB2	2.07	0.53
1:B:150:GLY:HA3	1:B:179:PRO:HG3	1.90	0.53
1:B:251:LEU:HD21	1:B:282:VAL:HG12	1.91	0.53
1:B:335:MET:HA	1:B:335:MET:HE2	1.91	0.53
1:B:31:ILE:HG12	1:B:163:MET:HB3	1.90	0.52
1:A:296:ASN:ND2	1:A:385:ALA:CB	2.62	0.52
1:A:186:TRP:CZ3	1:A:222:ALA:HB2	2.45	0.51
1:B:250:LEU:HB2	1:B:346:TYR:CE2	2.45	0.51
1:A:48:ARG:NH2	1:A:82:ALA:O	2.41	0.51
1:A:371:LEU:O	1:A:378:THR:N	2.41	0.51
1:B:28:ILE:HG13	1:B:116:LEU:HD13	1.93	0.51
1:B:139:ARG:HE	1:B:144:PRO:HB3	1.76	0.51
1:B:60:ILE:HG12	1:B:69:LEU:HD21	1.93	0.50
1:A:86:THR:HG22	1:A:118:LYS:NZ	2.26	0.50
1:B:289:LEU:HD12	1:B:290:PRO:HD2	1.92	0.50
1:A:192:TYR:CB	1:A:394:MET:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HH21	1:A:84:LEU:CD1	2.24	0.50
1:A:326:LEU:HB3	1:B:207:PHE:HE2	1.76	0.50
1:A:395:LEU:HD23	1:A:419:LEU:CD1	2.37	0.50
1:B:37:ASP:O	1:B:139:ARG:HD3	2.12	0.50
1:A:74:THR:HG22	1:A:117:GLY:O	2.12	0.49
1:B:122:PRO:O	1:B:151:SER:HA	2.12	0.49
1:B:124:ARG:NH2	1:B:172:ILE:HG22	2.27	0.49
1:B:92:GLN:OE1	1:B:92:GLN:HA	2.11	0.49
1:B:264:ILE:HG12	1:B:411:ILE:HG23	1.94	0.49
1:B:302:MET:HA	1:B:305:ILE:HB	1.93	0.49
1:A:335:MET:HE2	1:A:335:MET:HA	1.95	0.48
1:B:24:THR:HG22	1:B:116:LEU:HD21	1.94	0.48
1:A:42:VAL:HG13	1:A:120:ASN:HB2	1.95	0.48
1:B:42:VAL:HG23	1:B:43:VAL:HG23	1.96	0.48
1:B:294:ARG:NH2	1:B:334:ARG:HH11	2.08	0.48
1:B:393:PRO:HB2	1:B:395:LEU:HG	1.95	0.48
1:A:393:PRO:HB2	1:A:395:LEU:HG	1.97	0.47
1:B:202:PHE:CE1	1:B:213:SER:HB2	2.49	0.47
1:A:326:LEU:HB3	1:B:207:PHE:CE2	2.50	0.47
1:A:28:ILE:HG23	1:A:46:TYR:CZ	2.49	0.47
1:B:249:ILE:HG23	1:B:348:VAL:HG23	1.95	0.47
1:A:95:ASP:HB2	1:A:96:PHE:CE2	2.49	0.47
1:A:150:GLY:HA3	1:A:179:PRO:HG3	1.96	0.47
1:B:90:VAL:HG13	1:B:134:ILE:HD11	1.96	0.47
1:B:368:HIS:HA	1:B:380:PHE:HB2	1.96	0.47
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.96	0.47
1:B:380:PHE:O	1:B:381:LEU:C	2.56	0.46
1:A:334:ARG:O	1:A:338:GLN:HG3	2.15	0.46
1:A:9:THR:O	1:A:13:VAL:HG23	2.15	0.46
1:B:42:VAL:HG11	1:B:135:TYR:HB3	1.96	0.46
1:A:145:ALA:O	1:A:361:HIS:NE2	2.49	0.46
1:B:194:VAL:HG23	1:B:195:LEU:HD12	1.97	0.46
1:B:306:ALA:HB3	1:B:307:MET:HE2	1.96	0.46
1:B:30:ARG:NH2	2:B:502:HOH:O	2.30	0.46
1:A:73:MET:HE2	1:A:75:ILE:HG23	1.97	0.46
1:B:34:ALA:HB3	1:B:163:MET:HE3	1.97	0.46
1:B:186:TRP:HB3	1:B:225:LEU:HD11	1.96	0.46
1:A:192:TYR:CD2	1:A:394:MET:HE2	2.51	0.45
1:A:146:ARG:HB2	2:A:550:HOH:O	2.17	0.45
1:B:190:PRO:HG2	1:B:195:LEU:HD22	1.98	0.45
1:A:121:VAL:HA	1:A:151:SER:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:HA	1:B:60:ILE:HD12	1.99	0.44
1:A:146:ARG:HG2	1:A:409:LEU:HD11	2.00	0.44
1:B:42:VAL:CG1	1:B:120:ASN:HB2	2.47	0.44
1:B:294:ARG:HH22	1:B:334:ARG:CD	2.29	0.44
1:A:274:ARG:O	1:A:278:GLN:HG2	2.18	0.44
1:B:368:HIS:HA	1:B:380:PHE:N	2.22	0.44
1:A:83:GLY:C	1:A:84:LEU:HD12	2.44	0.43
1:A:159:LEU:HD23	1:A:164:VAL:O	2.18	0.43
1:B:35:ASN:ND2	1:B:41:VAL:HG22	2.33	0.43
1:A:74:THR:HG22	1:A:117:GLY:C	2.43	0.43
1:B:356:MET:HE2	1:B:383:GLN:OE1	2.19	0.43
1:B:31:ILE:O	1:B:35:ASN:HB2	2.19	0.43
1:B:241:LYS:HD3	1:B:421:GLN:OE1	2.19	0.43
1:B:92:GLN:OE1	1:B:134:ILE:HD12	2.19	0.42
1:A:75:ILE:HG22	1:A:168:PHE:HB2	2.02	0.42
1:A:292:LEU:HA	1:A:295:GLN:HB3	2.01	0.42
1:A:257:LYS:O	1:A:382:HIS:HB3	2.19	0.42
1:B:42:VAL:HB	1:B:135:TYR:CD1	2.55	0.42
1:A:195:LEU:HD21	1:A:229:LEU:HD12	2.02	0.42
1:A:239:PRO:O	2:A:502:HOH:O	2.22	0.42
1:A:393:PRO:O	1:A:394:MET:HB2	2.19	0.42
1:B:386:PHE:HA	1:B:389:LEU:HD12	2.02	0.42
1:B:241:LYS:O	1:B:241:LYS:HG2	2.20	0.42
1:B:321:THR:O	1:B:324:THR:OG1	2.33	0.42
1:B:256:PRO:HD3	1:B:292:LEU:HB2	2.02	0.42
1:A:35:ASN:HD21	1:A:41:VAL:HB	1.85	0.42
1:A:87:THR:HG23	1:A:89:GLY:N	2.29	0.42
1:B:290:PRO:HD2	1:B:342:LEU:HD22	2.02	0.42
1:B:354:VAL:HG13	1:B:356:MET:HE3	2.02	0.42
1:A:59:ARG:O	1:A:64:PHE:HB3	2.20	0.41
1:A:45:ASP:OD1	1:A:84:LEU:HD11	2.20	0.41
1:A:214:VAL:CA	2:A:508:HOH:O	2.63	0.41
1:B:329:HIS:O	1:B:332:GLN:HG3	2.20	0.41
1:A:122:PRO:HD2	1:A:150:GLY:O	2.21	0.41
1:B:42:VAL:HG13	1:B:120:ASN:HB2	2.01	0.41
1:B:354:VAL:CG1	1:B:356:MET:HE3	2.50	0.41
1:B:356:MET:HG3	1:B:357:THR:O	2.20	0.41
1:B:88:PHE:HA	1:B:201:PHE:CE2	2.56	0.41
1:B:155:SER:OG	1:B:167:GLU:OE2	2.34	0.41
1:B:242:ARG:HD3	1:B:247:TRP:CE3	2.55	0.41
1:B:301:GLN:H	1:B:301:GLN:HG2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:NZ	2:A:515:HOH:O	2.53	0.41
1:A:365:PRO:O	1:A:369:ARG:N	2.50	0.41
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.89	0.41
1:B:186:TRP:CZ3	1:B:222:ALA:HB2	2.55	0.41
1:B:305:ILE:HD13	1:B:305:ILE:HA	1.87	0.41
1:A:78:SER:HA	1:A:88:PHE:CE1	2.56	0.40
1:A:242:ARG:HD3	1:A:247:TRP:CD2	2.55	0.40
1:B:405:ASP:OD1	1:B:409:LEU:N	2.54	0.40
1:A:296:ASN:HD21	1:A:385:ALA:CA	2.31	0.40
1:A:257:LYS:HB3	1:A:382:HIS:CE1	2.55	0.40
1:A:202:PHE:HA	1:A:203:PRO:HD3	1.78	0.40
1:A:253:VAL:HG11	1:A:265:ARG:HG3	2.02	0.40

There are no symmetry-related clashes.

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	401/461 (87%)	393 (98%)	8 (2%)	0	100	100
1	B	417/461 (90%)	399 (96%)	18 (4%)	0	100	100
All	All	818/922 (89%)	792 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	302/345 (88%)	289 (96%)	13 (4%)	26	42
1	B	315/345 (91%)	298 (95%)	17 (5%)	20	33
All	All	617/690 (89%)	587 (95%)	30 (5%)	22	37

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	42	VAL
1	A	74	THR
1	A	87	THR
1	A	90	VAL
1	A	92	GLN
1	A	121	VAL
1	A	189	LYS
1	A	207	PHE
1	A	210	SER
1	A	301	GLN
1	A	303	LEU
1	A	321	THR
1	B	19	THR
1	B	24	THR
1	B	41	VAL
1	B	161	SER
1	B	207	PHE
1	B	211	VAL
1	B	270	ASP
1	B	273	GLU
1	B	338	GLN
1	B	361	HIS
1	B	362	ASP
1	B	368	HIS
1	B	376	GLU
1	B	378	THR
1	B	380	PHE
1	B	400	VAL
1	B	407	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	296	ASN
1	A	301	GLN
1	A	304	ASN
1	A	327	HIS
1	A	332	GLN
1	A	336	GLN
1	B	246	GLN
1	B	327	HIS

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	407/461 (88%)	0.87	45 (11%) 10 8	46, 76, 125, 156	0
1	B	423/461 (91%)	1.05	71 (16%) 4 3	48, 79, 142, 169	0
All	All	830/922 (90%)	0.96	116 (13%) 6 5	46, 78, 132, 169	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	VAL	6.3
1	A	150	GLY	5.4
1	B	208	ALA	5.3
1	B	125	LEU	5.3
1	A	208	ALA	5.3
1	B	367	PRO	5.3
1	B	359	PHE	4.6
1	B	210	SER	4.6
1	A	151	SER	4.5
1	A	152	SER	4.4
1	A	148	ALA	4.4
1	A	359	PHE	4.4
1	B	93	PHE	4.3
1	A	153	GLY	4.2
1	B	368	HIS	4.1
1	A	149	GLY	4.0
1	B	309	VAL	4.0
1	A	203	PRO	3.9
1	A	211	VAL	3.9
1	B	135	TYR	3.9
1	B	203	PRO	3.9
1	A	88	PHE	3.8
1	B	137	ARG	3.8
1	A	42	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	LEU	3.7
1	B	205	THR	3.7
1	A	366	LEU	3.6
1	B	206	ASP	3.6
1	B	292	LEU	3.6
1	B	149	GLY	3.6
1	B	360	PRO	3.6
1	B	305	ILE	3.5
1	B	207	PHE	3.5
1	B	325	TRP	3.3
1	A	38	LEU	3.3
1	B	365	PRO	3.3
1	B	211	VAL	3.3
1	B	319	PRO	3.3
1	A	210	SER	3.2
1	B	124	ARG	3.2
1	A	205	THR	3.2
1	B	209	LYS	3.1
1	B	361	HIS	3.1
1	A	212	LEU	3.1
1	A	147	VAL	3.0
1	A	209	LYS	2.9
1	B	380	PHE	2.9
1	B	364	THR	2.9
1	A	207	PHE	2.9
1	A	307	MET	2.9
1	A	356	MET	2.8
1	B	38	LEU	2.8
1	A	86	THR	2.8
1	B	370	ARG	2.8
1	B	89	GLY	2.7
1	B	264	ILE	2.7
1	A	201	PHE	2.6
1	A	360	PRO	2.6
1	B	256	PRO	2.6
1	A	40	ALA	2.6
1	B	307	MET	2.6
1	B	369	ARG	2.6
1	B	308	SER	2.6
1	B	378	THR	2.6
1	A	358	ALA	2.6
1	B	133	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	212	LEU	2.5
1	A	319	PRO	2.5
1	B	244	GLY	2.5
1	A	93	PHE	2.5
1	A	419	LEU	2.5
1	B	408	GLY	2.5
1	B	302	MET	2.5
1	A	123	PRO	2.4
1	B	406	GLY	2.4
1	B	373	ILE	2.4
1	B	95	ASP	2.4
1	B	147	VAL	2.4
1	A	87	THR	2.4
1	B	290	PRO	2.3
1	B	173	GLY	2.3
1	B	306	ALA	2.3
1	B	376	GLU	2.3
1	A	117	GLY	2.3
1	A	116	LEU	2.3
1	B	377	ASP	2.3
1	A	202	PHE	2.3
1	B	337	ARG	2.3
1	B	168	PHE	2.3
1	B	94	ARG	2.3
1	A	124	ARG	2.2
1	B	139	ARG	2.2
1	B	63	GLY	2.2
1	B	437	TRP	2.2
1	B	384	PHE	2.2
1	A	46	TYR	2.2
1	B	332	GLN	2.2
1	A	373	ILE	2.2
1	A	96	PHE	2.2
1	A	90	VAL	2.1
1	B	241	LYS	2.1
1	A	145	ALA	2.1
1	B	40	ALA	2.1
1	A	94	ARG	2.1
1	B	88	PHE	2.1
1	B	138	THR	2.1
1	A	175	SER	2.1
1	B	291	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	356	MET	2.1
1	B	371	LEU	2.1
1	B	172	ILE	2.0
1	B	257	LYS	2.0
1	A	122	PRO	2.0
1	B	161	SER	2.0
1	B	91	GLU	2.0
1	A	204	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 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.