



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:04 AM UTC

PDB ID : 5EJF / pdb_00005ejf
Title : Crystal structure of NAD kinase P101A mutant from *Listeria monocytogenes*
Authors : Poncet-Montange, G.; Assairi, L.; Gelin, M.; Pochet, S.; Labesse, G.
Deposited on : 2015-11-01
Resolution : 2.12 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

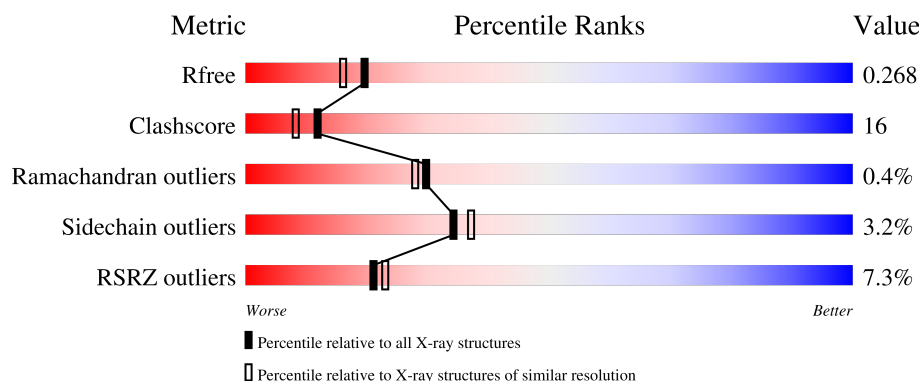
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	272	4% 69% 23% 7%
1	B	272	9% 74% 18% 7%
1	C	272	7% 65% 24% 8%
1	D	272	7% 61% 29% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8378 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 NAD kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	1	0
			2012	1291	334	378	9			
1	B	253	Total	C	N	O	S	0	0	0
			1967	1266	329	364	8			
1	C	251	Total	C	N	O	S	0	0	0
			1946	1250	321	366	9			
1	D	250	Total	C	N	O	S	0	0	0
			1945	1249	326	361	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	ALA	PRO	conflict	UNP Q8Y8D7
A	265	LEU	-	expression tag	UNP Q8Y8D7
A	266	GLU	-	expression tag	UNP Q8Y8D7
A	267	HIS	-	expression tag	UNP Q8Y8D7
A	268	HIS	-	expression tag	UNP Q8Y8D7
A	269	HIS	-	expression tag	UNP Q8Y8D7
A	270	HIS	-	expression tag	UNP Q8Y8D7
A	271	HIS	-	expression tag	UNP Q8Y8D7
A	272	HIS	-	expression tag	UNP Q8Y8D7
B	101	ALA	PRO	conflict	UNP Q8Y8D7
B	265	LEU	-	expression tag	UNP Q8Y8D7
B	266	GLU	-	expression tag	UNP Q8Y8D7
B	267	HIS	-	expression tag	UNP Q8Y8D7
B	268	HIS	-	expression tag	UNP Q8Y8D7
B	269	HIS	-	expression tag	UNP Q8Y8D7
B	270	HIS	-	expression tag	UNP Q8Y8D7
B	271	HIS	-	expression tag	UNP Q8Y8D7
B	272	HIS	-	expression tag	UNP Q8Y8D7
C	101	ALA	PRO	conflict	UNP Q8Y8D7
C	265	LEU	-	expression tag	UNP Q8Y8D7
C	266	GLU	-	expression tag	UNP Q8Y8D7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP Q8Y8D7
C	268	HIS	-	expression tag	UNP Q8Y8D7
C	269	HIS	-	expression tag	UNP Q8Y8D7
C	270	HIS	-	expression tag	UNP Q8Y8D7
C	271	HIS	-	expression tag	UNP Q8Y8D7
C	272	HIS	-	expression tag	UNP Q8Y8D7
D	101	ALA	PRO	conflict	UNP Q8Y8D7
D	265	LEU	-	expression tag	UNP Q8Y8D7
D	266	GLU	-	expression tag	UNP Q8Y8D7
D	267	HIS	-	expression tag	UNP Q8Y8D7
D	268	HIS	-	expression tag	UNP Q8Y8D7
D	269	HIS	-	expression tag	UNP Q8Y8D7
D	270	HIS	-	expression tag	UNP Q8Y8D7
D	271	HIS	-	expression tag	UNP Q8Y8D7
D	272	HIS	-	expression tag	UNP Q8Y8D7

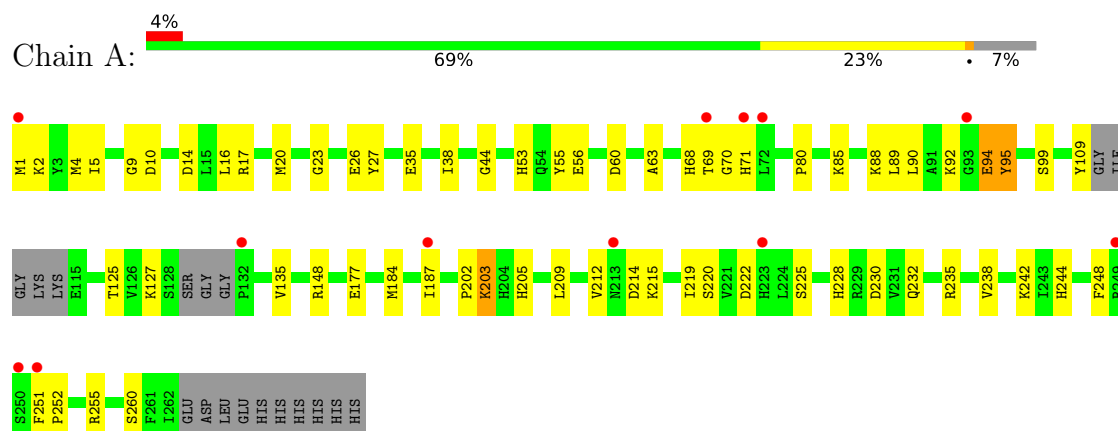
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	147	Total O 147 147	0	0
2	B	131	Total O 131 131	0	0
2	C	118	Total O 118 118	0	0
2	D	112	Total O 112 112	0	0

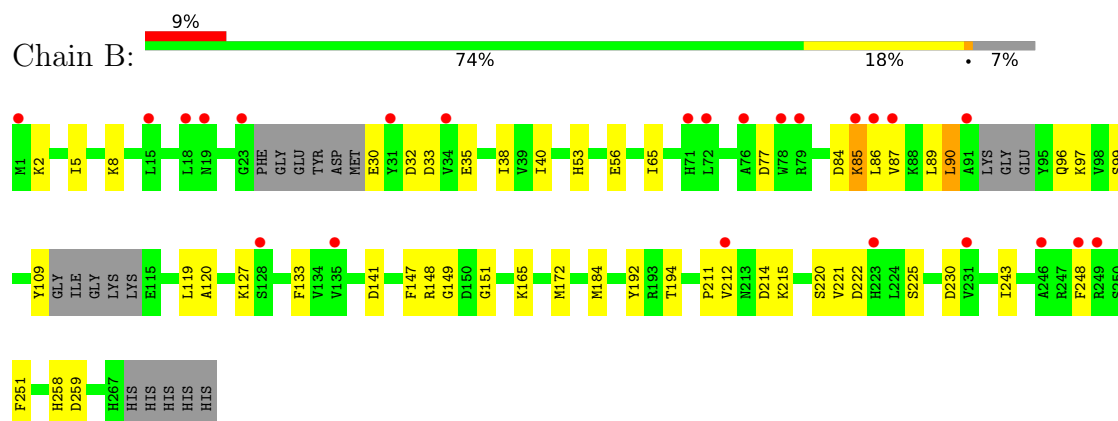
3 Residue-property plots [i](#)

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.

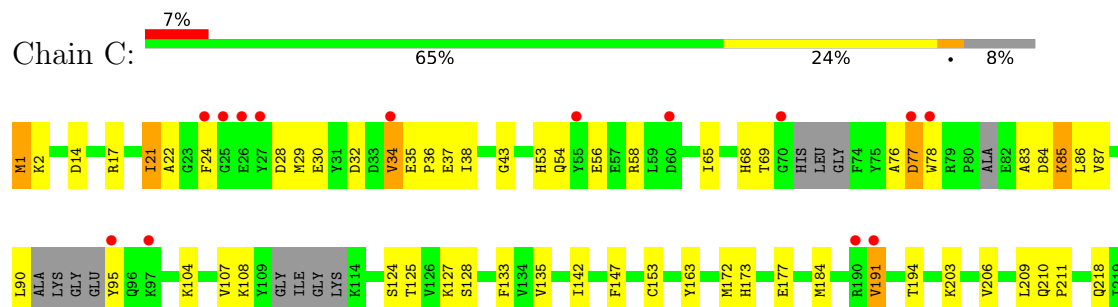
• Molecule 1: NAD kinase 1

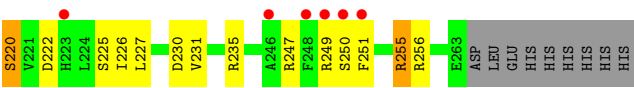


• Molecule 1: NAD kinase 1

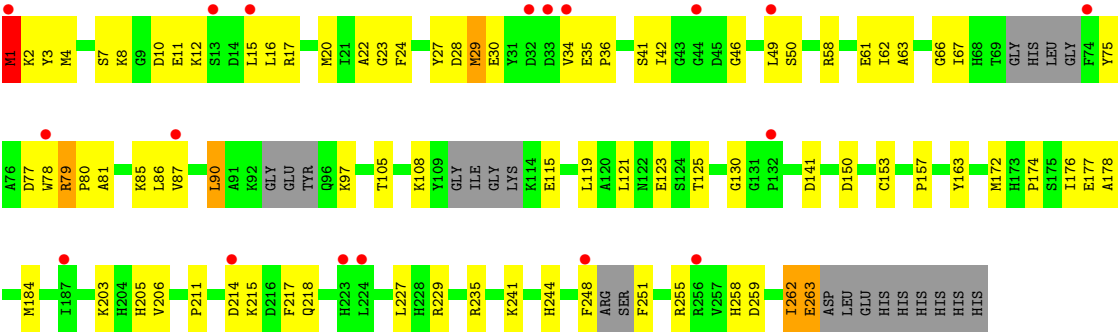


• Molecule 1: NAD kinase 1





● Molecule 1: NAD kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.04Å 119.17Å 67.59Å 90.00° 100.98° 90.00°	Depositor
Resolution (Å)	34.78 – 2.12 34.78 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.78-2.12) 99.4 (34.78-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.269 0.214 , 0.268	Depositor DCC
R_{free} test set	2981 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8378	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.00% 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

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	0/2063	0.75	0/2789
1	B	0.46	0/2012	0.70	0/2725
1	C	0.47	0/1990	0.72	0/2696
1	D	0.50	0/1987	0.76	3/2685 (0.1%)
All	All	0.51	0/8052	0.73	3/10895 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	MET	CG-SD-CE	-10.29	78.25	100.90
1	D	1	MET	CG-SD-CE	-6.27	87.11	100.90
1	D	29	MET	CA-CB-CG	-5.91	102.28	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	191	VAL	Peptide
1	D	262	ILE	Peptide

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	2012	0	1944	58	0
1	B	1967	0	1903	41	0
1	C	1946	0	1845	74	1
1	D	1945	0	1877	75	1
2	A	147	0	0	14	1
2	B	131	0	0	11	0
2	C	118	0	0	28	0
2	D	112	0	0	16	0
All	All	8378	0	7569	244	2

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 16.

All (244) 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:177:GLU:HB3	1:A:203:LYS:HE3	1.28	1.09
1:A:235:ARG:NH2	2:A:302:HOH:O	1.90	1.02
1:D:28:ASP:C	1:D:29:MET:HG2	1.84	0.99
1:A:230:ASP:OD2	2:A:301:HOH:O	1.82	0.97
1:B:30:GLU:N	2:B:305:HOH:O	2.01	0.93
1:C:108:LYS:O	2:C:301:HOH:O	1.86	0.93
1:D:203:LYS:O	2:D:301:HOH:O	1.85	0.93
1:A:44:GLY:HA2	1:A:68:HIS:HD1	1.33	0.91
1:D:46:GLY:O	2:D:302:HOH:O	1.88	0.91
1:B:109:TYR:HB3	2:B:319:HOH:O	1.71	0.91
1:D:1:MET:HE1	1:D:90:LEU:HD22	1.55	0.89
1:D:1:MET:SD	1:D:3:TYR:HB3	2.14	0.88
1:C:184:MET:SD	2:C:397:HOH:O	2.36	0.84
1:A:230:ASP:O	2:A:303:HOH:O	1.93	0.84
1:B:141:ASP:OD1	2:B:301:HOH:O	1.96	0.82
1:B:35:GLU:O	2:B:302:HOH:O	1.96	0.82
1:D:11:GLU:O	2:D:303:HOH:O	1.98	0.82
1:A:177:GLU:CB	1:A:203:LYS:HE3	2.10	0.81
1:C:43:GLY:O	2:C:302:HOH:O	1.97	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TYR:O	2:B:304:HOH:O	2.00	0.80
1:B:211:PRO:O	2:B:303:HOH:O	2.00	0.79
1:A:69:THR:OG1	2:A:304:HOH:O	2.01	0.79
1:C:104:LYS:NZ	2:C:308:HOH:O	2.09	0.78
1:A:44:GLY:HA2	1:A:68:HIS:ND1	1.98	0.78
1:A:177:GLU:HB3	1:A:203:LYS:CE	2.13	0.78
1:D:105:THR:OG1	2:D:304:HOH:O	2.01	0.78
1:C:24:PHE:O	2:C:305:HOH:O	2.03	0.77
1:D:251:PHE:N	2:D:311:HOH:O	2.17	0.77
1:A:255:ARG:NH2	2:A:309:HOH:O	2.16	0.77
1:C:32:ASP:O	2:C:306:HOH:O	2.03	0.76
1:C:220:SER:OG	2:C:303:HOH:O	1.98	0.76
1:C:85:LYS:NZ	2:C:310:HOH:O	2.16	0.76
1:D:27:TYR:HB2	1:D:29:MET:HG3	1.68	0.76
1:A:235:ARG:NH1	2:A:310:HOH:O	2.19	0.74
1:D:119:LEU:HD11	1:D:241:LYS:HD2	1.70	0.73
1:A:14:ASP:OD1	2:A:305:HOH:O	2.05	0.73
1:C:85:LYS:NZ	2:C:312:HOH:O	2.22	0.72
1:C:255:ARG:HG3	1:C:255:ARG:HH21	1.53	0.72
1:C:14:ASP:OD2	2:C:307:HOH:O	2.07	0.72
1:D:174:PRO:O	2:D:306:HOH:O	2.08	0.72
1:D:229:ARG:NH1	2:D:313:HOH:O	2.23	0.71
1:D:77:ASP:OD1	1:D:78:TRP:N	2.24	0.71
1:A:9:GLY:O	2:A:306:HOH:O	2.09	0.71
1:D:123:GLU:OE2	2:D:307:HOH:O	2.09	0.70
1:D:141:ASP:OD2	2:D:308:HOH:O	2.09	0.70
1:D:108:LYS:NZ	1:D:115:GLU:OE1	2.23	0.70
1:C:53:HIS:ND1	1:C:56:GLU:OE2	2.24	0.69
1:D:58:ARG:NH2	1:D:62:ILE:HD11	2.08	0.69
1:A:222:ASP:O	2:A:307:HOH:O	2.10	0.68
1:A:127:LYS:HE3	1:A:184:MET:HE1	1.77	0.68
1:B:127:LYS:HE3	1:B:184:MET:HE1	1.76	0.68
1:C:128:SER:HB3	1:C:133:PHE:HB2	1.75	0.67
1:A:5:ILE:HB	1:A:17:ARG:HH11	1.59	0.67
1:C:77:ASP:HB3	2:C:322:HOH:O	1.95	0.67
1:A:230:ASP:OD1	2:A:308:HOH:O	2.11	0.66
1:A:203:LYS:HD3	1:A:238:VAL:HG11	1.77	0.66
1:D:125:THR:HB	1:D:184:MET:HE1	1.77	0.65
1:B:84:ASP:HA	1:B:87:VAL:HG22	1.79	0.65
1:D:163:TYR:HE2	1:D:184:MET:HE2	1.60	0.65
1:C:54:GLN:OE1	2:C:309:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLU:N	2:C:311:HOH:O	2.29	0.65
1:B:133:PHE:CE2	1:B:151:GLY:HA2	2.31	0.65
1:A:89:LEU:HD22	1:A:94:GLU:OE2	1.98	0.64
1:A:135:VAL:HG21	1:A:209:LEU:HB3	1.80	0.64
1:C:250:SER:O	1:C:250:SER:OG	2.14	0.64
1:C:177:GLU:HB3	1:C:203:LYS:HZ3	1.62	0.63
1:D:28:ASP:C	1:D:29:MET:CG	2.68	0.63
1:C:218:GLN:NE2	1:C:227:LEU:HB2	2.14	0.63
1:D:24:PHE:CD1	1:D:29:MET:CE	2.82	0.63
1:D:24:PHE:HD1	1:D:29:MET:CE	2.11	0.63
1:C:36:PRO:HD2	1:C:58:ARG:NH1	2.14	0.63
1:C:65:ILE:HD11	1:C:78:TRP:NE1	2.12	0.63
1:C:249:ARG:N	2:C:319:HOH:O	2.32	0.62
1:A:92:LYS:HD2	1:A:92:LYS:O	1.98	0.62
1:B:90:LEU:HD13	1:B:248:PHE:HZ	1.64	0.62
1:D:78:TRP:HD1	1:D:86:LEU:HD22	1.65	0.62
1:B:215:LYS:HB2	1:B:230:ASP:HA	1.83	0.61
1:D:78:TRP:CD1	1:D:86:LEU:HD22	2.35	0.61
1:D:42:ILE:HG12	1:D:67:ILE:HG13	1.83	0.60
1:D:79:ARG:HG3	1:D:80:PRO:HD2	1.82	0.60
1:D:24:PHE:CD1	1:D:87:VAL:HG13	2.36	0.60
1:C:77:ASP:OD1	1:C:78:TRP:CD1	2.56	0.59
1:B:53:HIS:ND1	1:B:56:GLU:OE2	2.30	0.59
1:B:38:ILE:HG21	1:B:90:LEU:HD21	1.84	0.58
1:A:109:TYR:OH	1:A:228:HIS:ND1	2.30	0.58
1:A:26:GLU:HG3	1:A:27:TYR:CE2	2.39	0.58
1:C:36:PRO:HD2	1:C:58:ARG:HH12	1.68	0.58
1:C:77:ASP:OD1	1:C:78:TRP:CG	2.58	0.57
1:C:107:VAL:HG12	2:C:301:HOH:O	2.04	0.57
1:B:2:LYS:HD3	1:B:32:ASP:OD2	2.04	0.57
1:C:153:CYS:HB2	1:C:184:MET:HE3	1.85	0.57
1:C:38:ILE:HD13	1:C:90:LEU:HD22	1.86	0.56
1:B:2:LYS:HD2	2:B:302:HOH:O	2.04	0.56
1:C:1:MET:HB2	1:C:37:GLU:OE1	2.05	0.56
1:D:77:ASP:OD1	1:D:78:TRP:CG	2.59	0.56
1:B:133:PHE:CD2	1:B:151:GLY:HA2	2.41	0.56
1:D:42:ILE:HA	1:D:67:ILE:HB	1.87	0.56
1:D:206:VAL:HG11	1:D:235:ARG:NH2	2.21	0.56
1:A:38:ILE:HG21	1:A:90:LEU:HD21	1.89	0.55
1:C:21:ILE:HG13	1:C:22:ALA:N	2.22	0.55
1:C:36:PRO:HD3	2:C:311:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:HG21	1:C:209:LEU:HB3	1.87	0.55
1:D:36:PRO:O	1:D:58:ARG:NH1	2.38	0.55
1:C:83:ALA:O	1:C:86:LEU:HB3	2.07	0.55
1:A:95:TYR:HB3	1:A:248:PHE:CE2	2.41	0.55
1:C:35:GLU:HA	1:C:58:ARG:CZ	2.37	0.54
1:D:177:GLU:OE1	1:D:203:LYS:HE3	2.07	0.54
1:C:1:MET:HG2	1:C:29:MET:HE3	1.87	0.54
1:D:49:LEU:HD23	1:D:121:LEU:HD23	1.89	0.54
1:D:86:LEU:O	1:D:90:LEU:HB2	2.07	0.54
1:D:206:VAL:HG11	1:D:235:ARG:CZ	2.38	0.54
1:D:77:ASP:OD1	1:D:77:ASP:C	2.51	0.54
1:C:53:HIS:NE2	1:C:222:ASP:OD2	2.41	0.54
1:A:5:ILE:O	1:A:17:ARG:NH1	2.41	0.53
1:A:38:ILE:HD13	1:A:63:ALA:HB3	1.90	0.53
1:D:214:ASP:OD1	1:D:215:LYS:N	2.42	0.53
1:D:8:LYS:HE2	1:D:10:ASP:HB3	1.89	0.53
1:C:255:ARG:HG3	1:C:255:ARG:NH2	2.21	0.52
1:A:68:HIS:NE2	1:A:71:HIS:CE1	2.77	0.52
1:C:2:LYS:HA	1:C:30:GLU:O	2.10	0.52
1:A:214:ASP:OD1	1:A:215:LYS:N	2.42	0.52
1:D:16:LEU:HD11	1:D:80:PRO:HB3	1.92	0.52
1:D:75:TYR:O	2:D:312:HOH:O	2.18	0.52
1:A:187:ILE:HG12	2:C:390:HOH:O	2.09	0.52
1:B:77:ASP:OD1	1:B:251:PHE:CD2	2.62	0.52
1:C:125:THR:HB	1:C:184:MET:HE1	1.92	0.52
1:A:68:HIS:HD2	1:A:70:GLY:H	1.58	0.51
1:C:34:VAL:N	2:C:311:HOH:O	2.43	0.51
1:C:32:ASP:HB3	2:C:306:HOH:O	2.10	0.51
1:D:153:CYS:HB2	1:D:184:MET:HE3	1.92	0.51
1:A:53:HIS:ND1	1:A:56:GLU:OE2	2.38	0.51
1:B:53:HIS:NE2	1:B:222:ASP:OD2	2.44	0.50
1:D:15:LEU:N	2:D:303:HOH:O	2.40	0.50
1:C:68:HIS:HB3	1:C:76:ALA:HB3	1.94	0.50
1:A:99:SER:HB3	1:A:242:LYS:HD3	1.93	0.50
1:D:77:ASP:OD1	1:D:78:TRP:CD1	2.65	0.50
1:C:163:TYR:HE2	1:C:184:MET:HE2	1.76	0.50
1:D:163:TYR:CE2	1:D:184:MET:HE2	2.44	0.50
1:C:173:HIS:CD2	1:D:205:HIS:HE1	2.29	0.50
1:A:26:GLU:HG3	1:A:27:TYR:CD2	2.48	0.49
1:A:228:HIS:HA	2:A:320:HOH:O	2.12	0.49
1:B:53:HIS:HE1	1:B:119:LEU:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLU:HB3	1:C:203:LYS:NZ	2.28	0.49
1:C:142:ILE:HG21	1:D:255:ARG:NE	2.27	0.49
1:C:235:ARG:NE	2:C:324:HOH:O	2.38	0.49
1:C:142:ILE:HG21	1:D:255:ARG:HE	1.78	0.48
1:C:84:ASP:O	1:C:87:VAL:HB	2.14	0.48
1:D:211:PRO:HB3	1:D:217:PHE:HZ	1.78	0.48
1:D:262:ILE:O	1:D:263:GLU:HB2	2.13	0.48
1:A:2:LYS:NZ	2:A:322:HOH:O	2.45	0.48
1:D:78:TRP:HZ2	1:D:248:PHE:HB2	1.79	0.48
1:C:231:VAL:HA	2:C:301:HOH:O	2.12	0.48
1:D:4:MET:HG2	1:D:36:PRO:HG3	1.96	0.48
1:B:215:LYS:CB	1:B:230:ASP:HA	2.44	0.48
1:C:251:PHE:O	1:C:256:ARG:NH1	2.47	0.48
1:A:23:GLY:O	1:A:26:GLU:HG2	2.14	0.48
1:A:26:GLU:HG2	1:A:26:GLU:H	1.51	0.47
1:C:147:PHE:CD1	1:C:194:THR:HG21	2.50	0.47
1:B:220:SER:HA	1:B:225:SER:HA	1.96	0.47
1:C:77:ASP:OD1	1:C:77:ASP:C	2.57	0.47
1:C:147:PHE:HD1	1:C:194:THR:HG21	1.80	0.47
1:A:202:PRO:HG2	1:A:205:HIS:CD2	2.50	0.47
1:D:1:MET:SD	1:D:3:TYR:CB	2.97	0.47
1:B:96:GLN:HA	1:B:96:GLN:OE1	2.14	0.46
1:D:41:SER:O	1:D:67:ILE:N	2.43	0.46
1:B:212:VAL:O	2:B:310:HOH:O	2.21	0.46
1:C:65:ILE:HD11	1:C:78:TRP:HE1	1.80	0.46
1:B:214:ASP:OD1	1:B:215:LYS:N	2.49	0.46
1:D:29:MET:HB3	1:D:29:MET:HE3	1.56	0.46
1:B:127:LYS:NZ	2:B:325:HOH:O	2.48	0.46
1:A:60:ASP:OD1	1:A:60:ASP:N	2.48	0.45
1:B:84:ASP:O	1:B:87:VAL:HG22	2.15	0.45
1:B:85:LYS:O	1:B:89:LEU:HG	2.16	0.45
1:A:16:LEU:HD22	1:A:80:PRO:HB3	1.98	0.45
1:B:77:ASP:CG	1:B:251:PHE:HD2	2.24	0.45
1:B:133:PHE:HB3	1:B:149:GLY:O	2.17	0.45
1:A:5:ILE:HB	1:A:17:ARG:NH1	2.27	0.45
1:C:65:ILE:HD11	1:C:78:TRP:CD1	2.51	0.45
1:A:148:ARG:HG2	1:A:187:ILE:HD12	1.98	0.44
1:A:220:SER:HA	1:A:225:SER:HA	1.98	0.44
1:D:20:MET:HE3	1:D:87:VAL:HG23	1.99	0.44
1:D:35:GLU:HA	1:D:58:ARG:CZ	2.47	0.44
1:D:153:CYS:HB2	1:D:184:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:THR:N	2:C:302:HOH:O	2.51	0.44
1:D:81:ALA:N	2:D:316:HOH:O	2.29	0.44
1:A:99:SER:OG	1:A:244:HIS:ND1	2.49	0.44
1:B:99:SER:HA	1:B:243:ILE:O	2.18	0.44
1:A:92:LYS:HD2	1:A:92:LYS:C	2.41	0.44
1:C:225:SER:O	1:C:226:ILE:HD13	2.18	0.44
1:D:258:HIS:HD2	1:D:259:ASP:OD1	2.00	0.44
1:C:17:ARG:HD3	2:C:315:HOH:O	2.18	0.44
1:A:35:GLU:HG2	2:A:321:HOH:O	2.17	0.43
1:B:147:PHE:HD1	1:B:194:THR:HG21	1.84	0.43
1:C:17:ARG:O	1:C:21:ILE:HG23	2.18	0.43
1:B:40:ILE:HG23	1:B:65:ILE:HG23	2.00	0.43
1:B:120:ALA:HB2	1:B:221:VAL:HG13	2.01	0.43
1:D:79:ARG:HG3	1:D:80:PRO:CD	2.48	0.43
1:D:97:LYS:HE2	1:D:97:LYS:HB2	1.84	0.43
1:A:4:MET:HE2	1:A:5:ILE:C	2.44	0.43
1:D:36:PRO:O	1:D:58:ARG:NH2	2.49	0.43
1:C:173:HIS:CD2	1:D:205:HIS:CE1	3.07	0.43
1:A:219:ILE:O	1:A:225:SER:HA	2.19	0.42
1:B:172:MET:HB3	1:B:172:MET:HE2	1.67	0.42
1:C:28:ASP:O	1:C:29:MET:HG2	2.18	0.42
1:C:124:SER:HA	1:C:220:SER:O	2.19	0.42
1:C:247:ARG:NE	2:C:322:HOH:O	2.51	0.42
1:D:2:LYS:HA	1:D:30:GLU:O	2.18	0.42
1:D:172:MET:HE1	1:D:178:ALA:HB3	2.00	0.42
1:B:5:ILE:HG12	1:B:40:ILE:HB	2.01	0.42
1:C:95:TYR:C	1:C:95:TYR:CD2	2.98	0.42
1:C:172:MET:HE2	1:C:172:MET:HB3	1.83	0.42
1:D:50:SER:N	2:D:302:HOH:O	2.07	0.42
1:B:165:LYS:NZ	2:B:312:HOH:O	2.25	0.42
1:D:22:ALA:C	2:D:329:HOH:O	2.63	0.42
1:D:78:TRP:HE1	1:D:86:LEU:HD13	1.85	0.42
1:B:148:ARG:HD3	1:B:192:TYR:CE2	2.55	0.42
1:D:63:ALA:HA	1:D:244:HIS:O	2.19	0.42
1:A:125:THR:OG1	1:A:220:SER:HB2	2.20	0.41
1:A:219:ILE:HG23	2:A:318:HOH:O	2.19	0.41
1:B:85:LYS:H	1:B:85:LYS:HG3	1.61	0.41
1:C:32:ASP:C	2:C:311:HOH:O	2.63	0.41
1:C:53:HIS:HA	1:C:56:GLU:HG3	2.01	0.41
1:D:23:GLY:N	2:D:329:HOH:O	2.52	0.41
1:A:251:PHE:HA	1:A:252:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:O	1:A:20:MET:HG3	2.20	0.41
1:D:66:GLY:N	2:D:312:HOH:O	2.50	0.41
1:C:17:ARG:NH1	2:C:315:HOH:O	2.26	0.41
1:C:163:TYR:CE2	1:C:184:MET:HE2	2.54	0.41
1:A:23:GLY:O	1:A:26:GLU:CG	2.69	0.41
1:B:86:LEU:O	1:B:86:LEU:HD12	2.21	0.41
1:B:258:HIS:HD2	1:B:259:ASP:OD1	2.03	0.41
1:D:12:LYS:HA	1:D:15:LEU:HD23	2.03	0.41
1:D:157:PRO:HG2	1:D:176:ILE:O	2.21	0.41
1:C:32:ASP:O	2:C:311:HOH:O	2.21	0.41
1:A:1:MET:HE1	1:A:95:TYR:OH	2.21	0.40
1:B:33:ASP:CG	2:B:314:HOH:O	2.64	0.40
1:C:104:LYS:CE	2:C:308:HOH:O	2.64	0.40
1:C:210:GLN:HA	1:C:211:PRO:HD3	1.97	0.40
1:C:218:GLN:HE21	1:C:227:LEU:HB2	1.87	0.40
1:D:218:GLN:OE1	1:D:227:LEU:HB2	2.21	0.40
1:D:150:ASP:HB2	1:D:184:MET:O	2.21	0.40
1:A:4:MET:SD	1:A:55:TYR:OH	2.69	0.40
1:A:94:GLU:O	1:A:95:TYR:O	2.39	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:366:HOH:O	2:A:418:HOH:O[2_544]	2.11	0.09
1:C:230:ASP:OD2	1:D:17:ARG:NH1[1_455]	2.13	0.07

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	249/272 (92%)	236 (95%)	11 (4%)	2 (1%)	16 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	245/272 (90%)	235 (96%)	10 (4%)	0	100	100
1	C	241/272 (89%)	231 (96%)	9 (4%)	1 (0%)	30	28
1	D	240/272 (88%)	229 (95%)	10 (4%)	1 (0%)	30	28
All	All	975/1088 (90%)	931 (96%)	40 (4%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	95	TYR
1	D	130	GLY
1	C	191	VAL

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	215/236 (91%)	209 (97%)	6 (3%)	38	42
1	B	208/236 (88%)	204 (98%)	4 (2%)	50	57
1	C	204/236 (86%)	195 (96%)	9 (4%)	25	25
1	D	205/236 (87%)	197 (96%)	8 (4%)	28	29
All	All	832/944 (88%)	805 (97%)	27 (3%)	34	37

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LYS
1	A	88	LYS
1	A	203	LYS
1	A	212	VAL
1	A	232	GLN
1	A	260	SER
1	B	8	LYS

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Mol	Chain	Res	Type
1	B	85	LYS
1	B	90	LEU
1	B	97	LYS
1	C	1	MET
1	C	21	ILE
1	C	34	VAL
1	C	77	ASP
1	C	85	LYS
1	C	127	LYS
1	C	206	VAL
1	C	220	SER
1	C	255	ARG
1	D	1	MET
1	D	7	SER
1	D	34	VAL
1	D	61	GLU
1	D	79	ARG
1	D	85	LYS
1	D	90	LEU
1	D	263	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	ASN
1	B	258	HIS
1	B	267	HIS
1	C	68	HIS
1	C	164	ASN
1	C	218	GLN
1	C	232	GLN
1	D	205	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 [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	254/272 (93%)	0.37	12 (4%) 36 39	15, 37, 65, 78	16 (6%)
1	B	253/272 (93%)	0.54	24 (9%) 14 15	16, 42, 75, 103	16 (6%)
1	C	251/272 (92%)	0.74	20 (7%) 18 20	19, 47, 83, 107	16 (6%)
1	D	250/272 (91%)	0.66	18 (7%) 21 23	20, 43, 83, 107	9 (3%)
All	All	1008/1088 (92%)	0.58	74 (7%) 21 23	15, 42, 77, 107	57 (5%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	6.9
1	D	248	PHE	6.5
1	C	251	PHE	5.5
1	A	250	SER	5.2
1	A	249	ARG	4.3
1	A	71	HIS	4.2
1	C	95	TYR	4.1
1	D	13	SER	4.1
1	C	34	VAL	4.0
1	B	86	LEU	3.9
1	D	78	TRP	3.7
1	B	249	ARG	3.5
1	B	87	VAL	3.5
1	C	248	PHE	3.3
1	D	34	VAL	3.3
1	D	187	ILE	3.3
1	B	85	LYS	3.2
1	B	223	HIS	3.1
1	B	212	VAL	3.1
1	C	55	TYR	3.0
1	B	18	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	249	ARG	3.0
1	C	26	GLU	3.0
1	C	77	ASP	2.9
1	D	32	ASP	2.9
1	C	25	GLY	2.9
1	C	223	HIS	2.9
1	C	191	VAL	2.9
1	B	248	PHE	2.9
1	D	33	ASP	2.8
1	D	214	ASP	2.8
1	B	246	ALA	2.8
1	C	70	GLY	2.8
1	C	78	TRP	2.8
1	A	223	HIS	2.7
1	C	60	ASP	2.7
1	B	15	LEU	2.7
1	C	190	ARG	2.6
1	A	93	GLY	2.6
1	B	72	LEU	2.6
1	D	256	ARG	2.6
1	C	246	ALA	2.6
1	D	15	LEU	2.6
1	A	1	MET	2.5
1	B	91	ALA	2.5
1	B	135	VAL	2.5
1	A	69	THR	2.5
1	D	49	LEU	2.5
1	A	251	PHE	2.5
1	B	31	TYR	2.4
1	B	128	SER	2.4
1	A	132	PRO	2.4
1	D	223	HIS	2.4
1	A	213	ASN	2.3
1	B	23	GLY	2.3
1	C	250	SER	2.3
1	D	87	VAL	2.3
1	B	1	MET	2.3
1	B	19	ASN	2.2
1	C	97	LYS	2.2
1	D	44	GLY	2.2
1	D	132	PRO	2.1
1	C	24	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	2.1
1	D	224	LEU	2.1
1	B	71	HIS	2.1
1	B	79	ARG	2.1
1	B	34	VAL	2.1
1	C	27	TYR	2.1
1	B	231	VAL	2.1
1	B	78	TRP	2.1
1	B	76	ALA	2.1
1	A	187	ILE	2.0
1	D	74	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.