Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:22 AM EDT

PDB ID	:	5EJF
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:

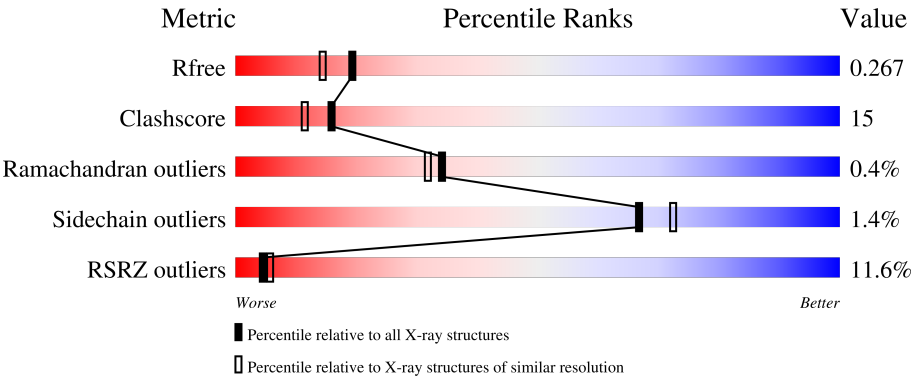
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.12 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}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 <=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% 71% 21% · 7%
1	B	272	11% 76% 17% 7%
1	C	272	15% 68% 22% · 8%
1	D	272	13% 64% 25% · 8%

2 Entry composition (i)

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.

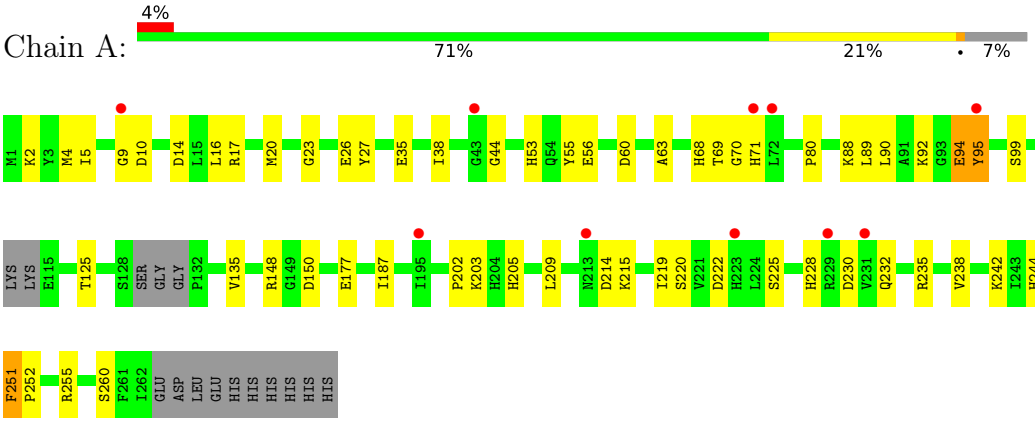
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	147	Total O 147 147	0	0
2	B	131	Total O 131 131	0	0
2	C	118	Total O 118 118	0	0
2	D	112	Total O 112 112	0	0

3 Residue-property plots

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.

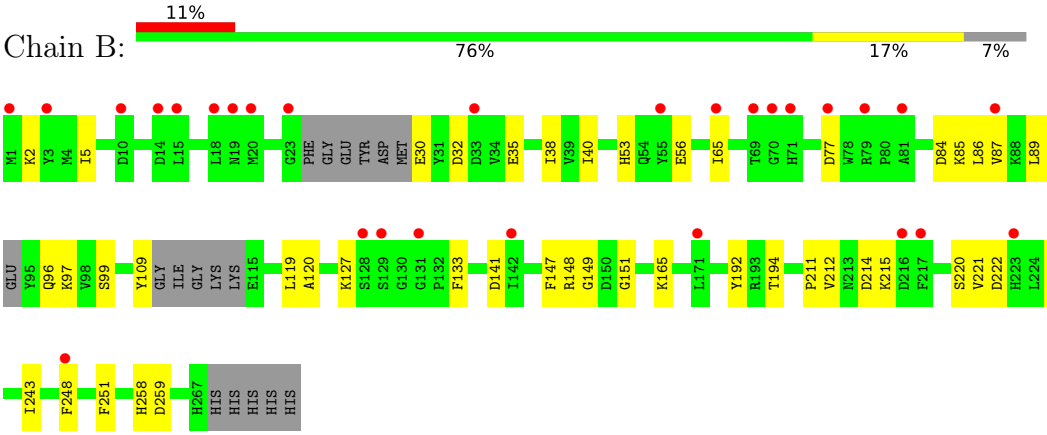
• Molecule 1: NAD kinase 1

Chain A:



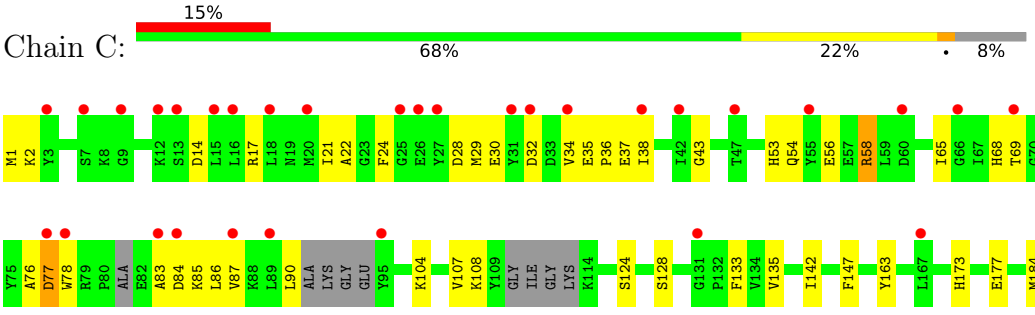
• Molecule 1: NAD kinase 1

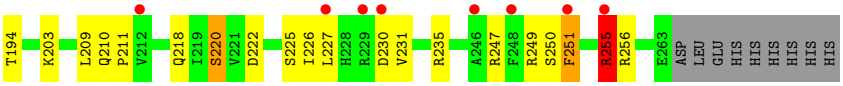
Chain B:



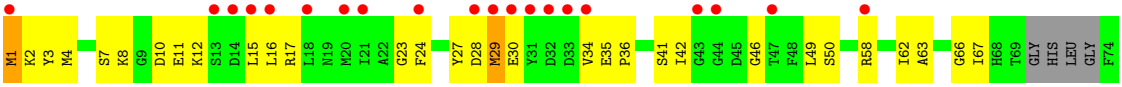
• Molecule 1: NAD kinase 1

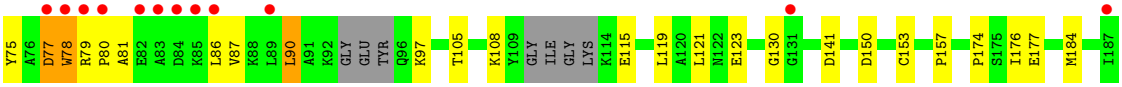
Chain C:

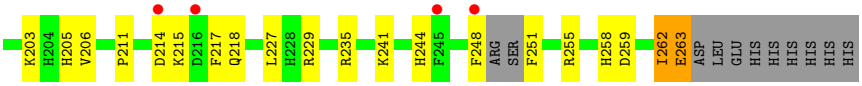




• Molecule 1: NAD kinase 1







4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.25 (at 2.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.269 0.213 , 0.267	Depositor DCC
R_{free} test set	2981 reflections (5.07%)	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)	0.33 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[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	0.66	1/2063 (0.0%)	0.73	0/2789
1	B	0.53	0/2012	0.71	0/2725
1	C	0.54	0/1990	0.73	2/2696 (0.1%)
1	D	0.55	1/1987 (0.1%)	0.80	4/2685 (0.1%)
All	All	0.57	2/8052 (0.0%)	0.74	6/10895 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	PHE	C-N	5.90	1.45	1.34
1	D	78	TRP	C-N	-5.74	1.20	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	29	MET	CG-SD-CE	-13.72	78.25	100.20
1	D	1	MET	CG-SD-CE	-8.18	87.11	100.20
1	D	29	MET	CA-CB-CG	-6.48	102.28	113.30
1	C	255	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	D	77	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	58	ARG	NE-CZ-NH1	-5.84	117.38	120.30

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 (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	2012	0	1944	56	0
1	B	1967	0	1903	38	0
1	C	1946	0	1845	67	1
1	D	1945	0	1876	70	1
2	A	147	0	0	14	1
2	B	131	0	0	10	0
2	C	118	0	0	26	0
2	D	112	0	0	15	0
All	All	8378	0	7568	226	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 15.

All (226) 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	0.98
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	1.52	0.88
1:D:1:MET:SD	1:D:3:TYR:HB3	2.14	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:NZ	2:C:308:HOH:O	2.09	0.86
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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ASP:HA	1:B:87:VAL:HG22	1.79	0.65
1:C:54:GLN:OE1	2:C:309:HOH:O	2.13	0.65
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: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:177:GLU:HB3	1:C:203:LYS:HZ3	1.63	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:D:1:MET:HE1	1:D:90:LEU:CD2	2.31	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:HD3	2:C:311:HOH:O	2.06	0.55
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: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: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:D:153:CYS:HB2	1:D:184:MET:HE2	1.91	0.52
1:C:1:MET:H2	1:C:29:MET:HA	1.73	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: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: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: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
1:D:77:ASP:OD1	1:D:77:ASP:C	2.51	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:28:ASP:C	1:D:29:MET:CG	2.68	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: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:D:24:PHE:CD1	1:D:29:MET:HE3	2.50	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: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: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:35:GLU:HA	1:D:58:ARG:CZ	2.47	0.44
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:C:225:SER:O	1:C:226:ILE:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:CYS:HB2	1:D:184:MET:CE	2.47	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: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: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:C:77:ASP:OD1	1:C:77:ASP:C	2.57	0.42
1:B:5:ILE:HG12	1:B:40:ILE:HB	2.01	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: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: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:4:MET:HE3	1:A:4:MET:HB2	1.95	0.41
1:A:251:PHE:HA	1:A:252:PRO:HD3	1.89	0.41
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:A:23:GLY:O	1:A:26:GLU:CG	2.69	0.41
1:B:86:LEU:HD12	1:B:86:LEU:O	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:B:77:ASP:CG	1:B:251:PHE:HD2	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:150:ASP:OD2	1:C:163:TYR:OH	2.31	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 (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	249/272 (92%)	236 (95%)	11 (4%)	2 (1%)	19 14
1	B	245/272 (90%)	235 (96%)	10 (4%)	0	100 100
1	C	241/272 (89%)	231 (96%)	9 (4%)	1 (0%)	34 32
1	D	240/272 (88%)	229 (95%)	10 (4%)	1 (0%)	34 32
All	All	975/1088 (90%)	931 (96%)	40 (4%)	4 (0%)	34 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLU

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

5.3.2 Protein sidechains (i)

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%)	212 (99%)	3 (1%)	67	72
1	B	208/236 (88%)	207 (100%)	1 (0%)	88	92
1	C	204/236 (86%)	200 (98%)	4 (2%)	55	59
1	D	205/236 (87%)	201 (98%)	4 (2%)	55	59
All	All	832/944 (88%)	820 (99%)	12 (1%)	67	72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	232	GLN
1	A	260	SER
1	B	97	LYS
1	C	77	ASP
1	C	220	SER
1	C	251	PHE
1	C	255	ARG
1	D	7	SER
1	D	34	VAL
1	D	90	LEU
1	D	263	GLU

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

Mol	Chain	Res	Type
1	A	143	HIS

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Mol	Chain	Res	Type
1	B	267	HIS
1	C	68	HIS
1	D	143	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides 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	254/272 (93%)	0.53	11 (4%) 35 41	15, 37, 68, 83	15 (5%)
1	B	253/272 (93%)	0.80	29 (11%) 4 6	16, 42, 77, 103	16 (6%)
1	C	251/272 (92%)	0.93	41 (16%) 1 2	19, 47, 83, 107	16 (6%)
1	D	250/272 (91%)	0.95	36 (14%) 2 3	20, 43, 85, 107	10 (4%)
All	All	1008/1088 (92%)	0.80	117 (11%) 4 6	15, 42, 79, 107	57 (5%)

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	9.6
1	D	78	TRP	6.5
1	D	34	VAL	6.1
1	D	13	SER	5.5
1	D	84	ASP	5.4
1	C	34	VAL	5.2
1	D	15	LEU	5.1
1	A	9	GLY	5.0
1	C	25	GLY	4.9
1	C	84	ASP	4.9
1	C	78	TRP	4.7
1	D	131	GLY	4.3
1	C	191	VAL	4.3
1	D	43	GLY	4.2
1	D	20	MET	4.2
1	D	28	ASP	4.2
1	B	15	LEU	4.1
1	C	27	TYR	4.0
1	B	19	ASN	4.0
1	B	217	PHE	3.9
1	C	55	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	16	LEU	3.8
1	B	216	ASP	3.7
1	D	32	ASP	3.7
1	C	9	GLY	3.7
1	C	42	ILE	3.5
1	C	77	ASP	3.5
1	D	77	ASP	3.4
1	B	87	VAL	3.3
1	B	18	LEU	3.2
1	A	71	HIS	3.2
1	B	3	TYR	3.2
1	B	77	ASP	3.2
1	A	95	TYR	3.1
1	B	20	MET	3.1
1	B	129	SER	3.1
1	C	31	TYR	3.1
1	B	10	ASP	3.1
1	D	29	MET	3.0
1	C	15	LEU	3.0
1	C	131	GLY	3.0
1	D	83	ALA	3.0
1	D	47	THR	2.9
1	B	33	ASP	2.9
1	D	33	ASP	2.9
1	D	89	LEU	2.9
1	D	21	ILE	2.8
1	B	1	MET	2.8
1	D	248	PHE	2.8
1	C	3	TYR	2.8
1	D	14	ASP	2.7
1	C	230	ASP	2.7
1	B	231	VAL	2.6
1	D	187	ILE	2.6
1	D	214	ASP	2.6
1	B	55	TYR	2.6
1	D	80	PRO	2.6
1	D	85	LYS	2.6
1	C	69	THR	2.6
1	C	18	LEU	2.6
1	C	60	ASP	2.5
1	C	89	LEU	2.5
1	C	190	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	81	ALA	2.5
1	A	223	HIS	2.5
1	C	38	ILE	2.5
1	D	82	GLU	2.5
1	A	72	LEU	2.4
1	A	229	ARG	2.4
1	D	31	TYR	2.4
1	B	14	ASP	2.4
1	D	24	PHE	2.4
1	C	227	LEU	2.4
1	B	69	THR	2.4
1	B	128	SER	2.4
1	A	231	VAL	2.3
1	C	95	TYR	2.3
1	C	26	GLU	2.3
1	C	12	LYS	2.3
1	C	251	PHE	2.3
1	B	223	HIS	2.3
1	C	212	VAL	2.3
1	C	87	VAL	2.2
1	C	83	ALA	2.2
1	D	18	LEU	2.2
1	D	58	ARG	2.2
1	B	131	GLY	2.2
1	C	20	MET	2.2
1	C	248	PHE	2.2
1	B	71	HIS	2.2
1	A	195	ILE	2.2
1	B	171	LEU	2.2
1	D	30	GLU	2.2
1	A	43	GLY	2.2
1	D	44	GLY	2.2
1	B	142	ILE	2.1
1	B	248	PHE	2.1
1	C	66	GLY	2.1
1	D	79	ARG	2.1
1	B	70	GLY	2.1
1	C	7	SER	2.1
1	D	216	ASP	2.1
1	D	16	LEU	2.1
1	A	250	SER	2.1
1	B	65	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	246	ALA	2.1
1	C	229	ARG	2.1
1	A	213	ASN	2.1
1	B	79	ARG	2.1
1	D	245	PHE	2.1
1	C	167	LEU	2.0
1	C	255	ARG	2.0
1	D	86	LEU	2.0
1	C	47	THR	2.0
1	C	13	SER	2.0
1	C	32	ASP	2.0
1	B	23	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 monosaccharides 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.