



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:07 PM UTC

PDB ID : 3ND5 / pdb_00003nd5
Title : Crystal structure of phosphopantetheine adenylyltransferase (PPAT) from *Enterococcus faecalis*
Authors : Yoon, H.J.; Lee, H.H.; Suh, S.W.
Deposited on : 2010-06-07
Resolution : 2.30 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

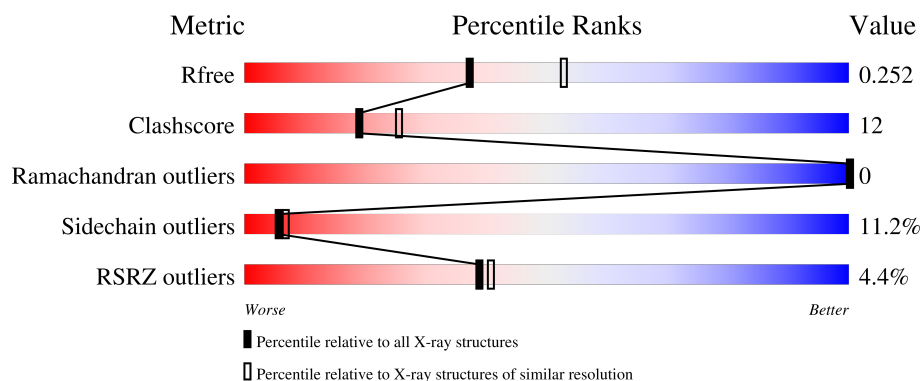
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	171	 3% 70% 17% 11%
1	B	171	 2% 67% 19% 11%
1	C	171	 5% 57% 25% 6% 11%
1	D	171	 6% 59% 26% 11%
1	E	171	 2% 67% 16% 6% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	171	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7878 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 Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	B	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	C	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	D	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	E	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			
1	F	152	Total	C	N	O	S	0	0	0
			1224	791	201	227	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	LEU	-	expression tag	UNP Q831P9
A	165	GLU	-	expression tag	UNP Q831P9
A	166	HIS	-	expression tag	UNP Q831P9
A	167	HIS	-	expression tag	UNP Q831P9
A	168	HIS	-	expression tag	UNP Q831P9
A	169	HIS	-	expression tag	UNP Q831P9
A	170	HIS	-	expression tag	UNP Q831P9
A	171	HIS	-	expression tag	UNP Q831P9
B	164	LEU	-	expression tag	UNP Q831P9
B	165	GLU	-	expression tag	UNP Q831P9
B	166	HIS	-	expression tag	UNP Q831P9
B	167	HIS	-	expression tag	UNP Q831P9
B	168	HIS	-	expression tag	UNP Q831P9
B	169	HIS	-	expression tag	UNP Q831P9
B	170	HIS	-	expression tag	UNP Q831P9
B	171	HIS	-	expression tag	UNP Q831P9
C	164	LEU	-	expression tag	UNP Q831P9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	165	GLU	-	expression tag	UNP Q831P9
C	166	HIS	-	expression tag	UNP Q831P9
C	167	HIS	-	expression tag	UNP Q831P9
C	168	HIS	-	expression tag	UNP Q831P9
C	169	HIS	-	expression tag	UNP Q831P9
C	170	HIS	-	expression tag	UNP Q831P9
C	171	HIS	-	expression tag	UNP Q831P9
D	164	LEU	-	expression tag	UNP Q831P9
D	165	GLU	-	expression tag	UNP Q831P9
D	166	HIS	-	expression tag	UNP Q831P9
D	167	HIS	-	expression tag	UNP Q831P9
D	168	HIS	-	expression tag	UNP Q831P9
D	169	HIS	-	expression tag	UNP Q831P9
D	170	HIS	-	expression tag	UNP Q831P9
D	171	HIS	-	expression tag	UNP Q831P9
E	164	LEU	-	expression tag	UNP Q831P9
E	165	GLU	-	expression tag	UNP Q831P9
E	166	HIS	-	expression tag	UNP Q831P9
E	167	HIS	-	expression tag	UNP Q831P9
E	168	HIS	-	expression tag	UNP Q831P9
E	169	HIS	-	expression tag	UNP Q831P9
E	170	HIS	-	expression tag	UNP Q831P9
E	171	HIS	-	expression tag	UNP Q831P9
F	164	LEU	-	expression tag	UNP Q831P9
F	165	GLU	-	expression tag	UNP Q831P9
F	166	HIS	-	expression tag	UNP Q831P9
F	167	HIS	-	expression tag	UNP Q831P9
F	168	HIS	-	expression tag	UNP Q831P9
F	169	HIS	-	expression tag	UNP Q831P9
F	170	HIS	-	expression tag	UNP Q831P9
F	171	HIS	-	expression tag	UNP Q831P9

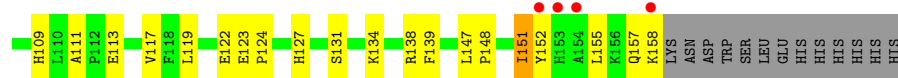
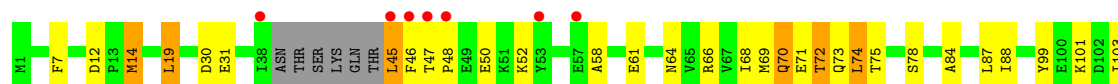
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	102	Total O 102 102	0	0
2	B	82	Total O 82 82	0	0
2	C	74	Total O 74 74	0	0
2	D	82	Total O 82 82	0	0

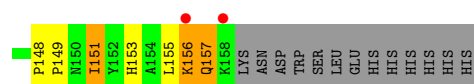
Continued on next page...

Continued from previous page...

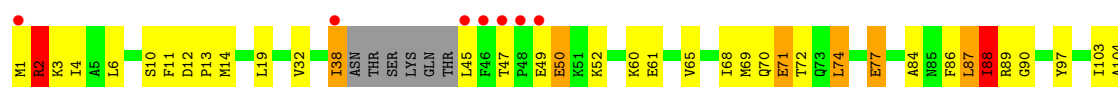
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	100	Total 100	O 100	0	0
2	F	94	Total 94	O 94	0	0



● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.20Å 125.68Å 125.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.3 (20.00-2.30) 97.9 (20.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.249 0.202 , 0.252	Depositor DCC
R_{free} test set	3845 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7878	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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	1.43	3/1248 (0.2%)	1.25	3/1683 (0.2%)
1	B	1.40	4/1248 (0.3%)	1.28	3/1683 (0.2%)
1	C	1.50	10/1248 (0.8%)	1.33	8/1683 (0.5%)
1	D	1.41	4/1248 (0.3%)	1.24	5/1683 (0.3%)
1	E	1.45	5/1248 (0.4%)	1.28	5/1683 (0.3%)
1	F	1.33	9/1248 (0.7%)	1.28	5/1683 (0.3%)
All	All	1.42	35/7488 (0.5%)	1.28	29/10098 (0.3%)

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

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	117	VAL	CA-CB	8.13	1.65	1.54
1	E	88	ILE	CA-CB	7.91	1.64	1.54
1	D	7	PHE	N-CA	-7.63	1.38	1.46
1	F	32	VAL	CA-CB	7.45	1.64	1.54
1	C	55	ILE	CA-CB	7.30	1.62	1.54
1	C	4	ILE	CA-CB	6.96	1.63	1.54
1	F	88	ILE	CB-CG2	6.76	1.74	1.52
1	F	65	VAL	CA-CB	6.58	1.62	1.54
1	C	99	TYR	CA-C	6.40	1.60	1.52
1	F	88	ILE	CA-CB	5.95	1.61	1.54
1	B	47	THR	CA-CB	5.94	1.62	1.53
1	B	6	LEU	CA-C	5.81	1.59	1.52
1	E	4	ILE	CA-CB	5.79	1.61	1.54
1	C	148	PRO	CA-C	5.74	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	VAL	CA-CB	5.72	1.62	1.54
1	E	77	GLU	CB-CG	-5.70	1.35	1.52
1	C	4	ILE	CA-C	5.50	1.59	1.52
1	C	119	LEU	CA-C	5.43	1.59	1.52
1	C	19	LEU	CG-CD2	5.40	1.70	1.52
1	E	117	VAL	CA-CB	5.34	1.62	1.54
1	A	117	VAL	CA-CB	5.31	1.61	1.54
1	B	129	SER	N-CA	5.28	1.52	1.45
1	C	87	LEU	C-O	-5.21	1.17	1.24
1	D	84	ALA	N-CA	5.18	1.52	1.46
1	F	97	TYR	CA-C	5.18	1.59	1.52
1	F	103	ILE	CA-CB	-5.15	1.48	1.54
1	C	65	VAL	CA-CB	5.14	1.60	1.54
1	F	84	ALA	CA-CB	5.13	1.60	1.53
1	F	117	VAL	CA-CB	5.12	1.61	1.54
1	F	2	ARG	C-O	5.09	1.29	1.23
1	C	32	VAL	CA-CB	5.08	1.60	1.54
1	D	78	SER	N-CA	-5.05	1.40	1.46
1	A	114	ILE	CA-C	5.02	1.58	1.52
1	A	91	ILE	CA-CB	5.01	1.60	1.54
1	E	27	LYS	N-CA	5.01	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	PRO	N-CA-C	-6.94	103.88	113.53
1	D	72	THR	CB-CA-C	6.85	120.59	109.90
1	F	71	GLU	N-CA-C	-6.62	100.63	110.23
1	B	2	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	D	113	GLU	N-CA-C	-6.35	105.57	113.38
1	B	2	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	D	71	GLU	N-CA-C	-6.15	101.31	110.23
1	C	4	ILE	CB-CA-C	5.90	119.78	110.81
1	A	26	ALA	N-CA-C	-5.84	105.65	112.89
1	F	50	GLU	N-CA-C	5.84	117.64	111.28
1	C	87	LEU	CA-C-N	-5.84	115.49	123.14
1	C	87	LEU	C-N-CA	-5.84	115.49	123.14
1	D	111	ALA	CA-C-N	5.82	125.52	119.82
1	D	111	ALA	C-N-CA	5.82	125.52	119.82
1	A	88	ILE	CB-CA-C	-5.75	102.26	110.83
1	F	88	ILE	N-CA-CB	5.72	117.85	110.99
1	E	89	ARG	CG-CD-NE	-5.61	99.66	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	THR	N-CA-CB	5.53	116.15	109.74
1	C	147	LEU	CA-C-N	-5.48	114.73	120.38
1	C	147	LEU	C-N-CA	-5.48	114.73	120.38
1	F	118	PHE	N-CA-C	5.47	118.40	109.59
1	C	47	THR	N-CA-C	-5.41	102.18	110.07
1	C	118	PHE	N-CA-C	5.39	118.18	109.40
1	C	72	THR	CB-CA-C	5.37	117.52	110.06
1	E	66	ARG	CB-CG-CD	-5.21	99.33	111.30
1	E	118	PHE	N-CA-C	5.13	117.85	109.59
1	F	104	ALA	N-CA-C	5.12	116.54	111.07
1	E	111	ALA	CA-C-N	5.08	124.80	119.82
1	E	111	ALA	C-N-CA	5.08	124.80	119.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MET	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	1224	0	1245	22	0
1	B	1224	0	1246	23	0
1	C	1224	0	1246	38	0
1	D	1224	0	1246	33	0
1	E	1224	0	1246	21	0
1	F	1224	0	1246	53	0
2	A	102	0	0	7	0
2	B	82	0	0	2	0
2	C	74	0	0	3	0
2	D	82	0	0	5	0
2	E	100	0	0	7	0
2	F	94	0	0	10	0
All	All	7878	0	7475	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 12.

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:F:88:ILE:CB	1:F:88:ILE:CG2	1.74	1.61
1:F:68:ILE:CD1	1:F:70:GLN:HG2	1.99	0.91
1:A:66:ARG:CZ	2:A:244:HOH:O	2.18	0.90
1:E:105:LYS:HE3	1:F:123:GLU:OE2	1.72	0.90
1:A:77:GLU:HG2	2:A:298:HOH:O	1.76	0.84
1:F:3:LYS:HG3	2:F:306:HOH:O	1.79	0.83
1:C:38:ILE:HD11	1:C:69:MET:HE3	1.64	0.79
1:A:123:GLU:HG3	1:F:123:GLU:HG2	1.63	0.79
1:C:38:ILE:HD11	1:C:69:MET:CE	2.13	0.78
1:D:123:GLU:HG3	1:D:124:PRO:HD3	1.66	0.78
1:F:2:ARG:HH11	1:F:2:ARG:CG	1.96	0.77
1:F:68:ILE:HD12	1:F:68:ILE:O	1.86	0.76
1:F:130:SER:HB3	2:F:238:HOH:O	1.86	0.76
1:C:123:GLU:HA	2:C:229:HOH:O	1.84	0.76
1:D:147:LEU:HD12	1:D:152:TYR:HD1	1.52	0.75
1:F:47:THR:HG21	1:F:49:GLU:OE1	1.89	0.72
1:F:12:ASP:HB3	2:F:266:HOH:O	1.88	0.72
1:F:2:ARG:HH11	1:F:2:ARG:HG3	1.53	0.72
1:B:14:MET:HE3	1:B:148:PRO:HG2	1.74	0.70
1:E:57:GLU:HG2	2:E:223:HOH:O	1.92	0.69
1:A:123:GLU:CG	1:F:123:GLU:HG2	2.23	0.69
1:D:68:ILE:HD12	1:D:68:ILE:O	1.92	0.68
1:F:123:GLU:N	1:F:124:PRO:HD2	2.08	0.68
1:F:68:ILE:HD13	1:F:70:GLN:HG2	1.73	0.68
1:C:153:HIS:HB3	2:C:349:HOH:O	1.93	0.68
1:F:74:LEU:HB2	1:F:77:GLU:HG3	1.75	0.67
1:D:147:LEU:HD12	1:D:152:TYR:CD1	2.29	0.67
1:E:89:ARG:HD3	2:E:227:HOH:O	1.93	0.67
1:F:52:LYS:HD2	1:F:69:MET:HG2	1.76	0.67
1:B:19:LEU:O	1:B:23:GLU:HG3	1.94	0.66
1:D:109:HIS:ND1	2:D:569:HOH:O	2.29	0.66
1:C:4:ILE:HD11	1:C:33:ILE:HD11	1.76	0.65
1:F:153:HIS:HB3	2:F:438:HOH:O	1.96	0.65
1:B:89:ARG:HD3	1:B:100:GLU:OE1	1.97	0.65
1:C:123:GLU:N	1:C:124:PRO:HD2	2.12	0.64
1:D:14:MET:HE3	1:D:148:PRO:HG2	1.80	0.64
1:F:88:ILE:CG2	1:F:88:ILE:HB	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:HB2	1:C:69:MET:SD	2.38	0.64
1:B:123:GLU:OE1	2:B:296:HOH:O	2.15	0.63
1:E:148:PRO:HB2	1:E:151:ILE:HG13	1.79	0.63
1:C:1:MET:HB3	1:C:85:ASN:HD21	1.64	0.63
1:C:4:ILE:HG13	1:C:84:ALA:HA	1.81	0.63
1:D:139:PHE:HB2	1:F:74:LEU:HD13	1.79	0.63
1:A:123:GLU:N	1:A:124:PRO:HD2	2.13	0.62
1:C:31:GLU:OE2	1:C:66:ARG:HD3	1.99	0.62
1:D:12:ASP:OD1	1:D:45:LEU:HD11	2.00	0.62
1:C:31:GLU:OE2	1:C:66:ARG:NH1	2.28	0.62
1:B:14:MET:HE1	1:B:58:ALA:HB3	1.82	0.62
1:A:66:ARG:NH1	2:A:244:HOH:O	2.28	0.61
1:F:1:MET:O	1:F:3:LYS:HD3	2.00	0.61
1:D:12:ASP:O	1:D:134:LYS:HE2	2.00	0.61
1:A:120:LEU:HD22	1:B:118:PHE:CE2	2.35	0.60
1:D:69:MET:N	1:D:69:MET:HE2	2.17	0.60
1:B:69:MET:HE2	1:B:69:MET:CA	2.31	0.60
1:F:47:THR:CG2	1:F:49:GLU:OE1	2.51	0.59
1:E:2:ARG:NH1	2:E:245:HOH:O	2.35	0.58
1:F:88:ILE:CG2	1:F:88:ILE:CG1	2.77	0.57
1:A:66:ARG:NE	2:A:244:HOH:O	2.30	0.57
1:B:139:PHE:HB2	1:D:74:LEU:HD13	1.87	0.56
1:D:73:GLN:HG3	1:D:74:LEU:N	2.20	0.55
1:C:74:LEU:HD13	1:E:139:PHE:HB2	1.87	0.55
1:D:14:MET:HE1	1:D:58:ALA:CB	2.36	0.55
1:F:12:ASP:CB	2:F:266:HOH:O	2.48	0.55
1:B:145:ASP:OD1	1:B:145:ASP:N	2.37	0.55
1:B:14:MET:HE2	1:B:151:ILE:CD1	2.37	0.54
1:C:4:ILE:HD11	1:C:33:ILE:CD1	2.36	0.54
1:E:3:LYS:HG3	2:F:306:HOH:O	2.06	0.54
1:A:57:GLU:O	1:A:57:GLU:HG3	2.08	0.54
1:F:105:LYS:NZ	2:F:277:HOH:O	2.41	0.54
1:C:4:ILE:CD1	1:C:33:ILE:HD11	2.39	0.53
1:F:38:ILE:O	1:F:72:THR:HG23	2.08	0.53
1:D:73:GLN:CG	1:D:74:LEU:N	2.72	0.53
1:E:123:GLU:N	1:E:124:PRO:HD2	2.24	0.53
1:F:88:ILE:CG2	1:F:88:ILE:CA	2.82	0.53
1:D:122:GLU:HG3	2:D:371:HOH:O	2.09	0.52
1:D:52:LYS:HB2	1:D:69:MET:HE3	1.91	0.52
1:F:68:ILE:HD12	1:F:68:ILE:C	2.34	0.52
1:B:14:MET:HE1	1:B:58:ALA:CB	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:GLU:H	1:C:71:GLU:CD	2.18	0.51
1:B:123:GLU:N	1:B:124:PRO:HD2	2.24	0.51
1:E:149:PRO:HD2	2:E:394:HOH:O	2.10	0.51
1:C:138:ARG:O	1:C:138:ARG:HG2	2.09	0.51
1:C:31:GLU:CD	1:C:66:ARG:HH11	2.16	0.50
1:C:14:MET:HB3	1:C:151:ILE:HD13	1.94	0.50
1:C:46:PHE:HB3	1:C:50:GLU:HB3	1.93	0.50
1:A:57:GLU:HB2	2:A:316:HOH:O	2.10	0.50
1:A:138:ARG:CZ	1:A:138:ARG:HB3	2.42	0.50
1:C:136:VAL:HG11	1:C:143:VAL:HG13	1.94	0.50
1:D:127:HIS:HB3	2:D:291:HOH:O	2.11	0.50
1:F:71:GLU:H	1:F:71:GLU:CD	2.20	0.50
1:C:123:GLU:N	1:C:124:PRO:CD	2.75	0.49
1:F:74:LEU:HB2	1:F:77:GLU:CG	2.41	0.49
1:E:89:ARG:CD	2:E:227:HOH:O	2.58	0.49
1:A:3:LYS:HE3	1:B:28:LEU:O	2.12	0.49
1:D:101:LYS:NZ	2:D:788:HOH:O	2.42	0.49
1:F:10:SER:O	1:F:11:PHE:C	2.55	0.49
1:E:113:GLU:HB2	2:E:201:HOH:O	2.13	0.48
1:C:31:GLU:CD	1:C:66:ARG:NH1	2.71	0.48
1:A:66:ARG:HD3	2:A:807:HOH:O	2.12	0.48
1:B:152:TYR:CE2	1:B:156:LYS:HD2	2.49	0.48
1:C:66:ARG:HE	1:C:68:ILE:HD11	1.79	0.48
1:E:153:HIS:CE1	1:E:157:GLN:OE1	2.67	0.48
1:C:2:ARG:HG3	1:C:3:LYS:N	2.29	0.47
1:D:151:ILE:O	1:D:155:LEU:HB2	2.13	0.47
1:F:68:ILE:HD13	1:F:70:GLN:CG	2.43	0.47
1:F:90:GLY:HA2	1:F:119:LEU:O	2.14	0.47
1:E:2:ARG:HB2	2:E:321:HOH:O	2.15	0.47
1:F:89:ARG:HB2	1:F:118:PHE:CD1	2.50	0.47
1:D:30:ASP:O	1:D:64:ASN:HB2	2.15	0.47
1:F:127:HIS:HB3	2:F:264:HOH:O	2.15	0.47
1:D:47:THR:O	1:D:48:PRO:C	2.57	0.46
1:D:73:GLN:CD	1:D:74:LEU:H	2.24	0.46
1:E:2:ARG:HH11	1:E:2:ARG:HG2	1.80	0.46
1:C:129:SER:O	1:C:133:LEU:HB2	2.16	0.46
1:F:52:LYS:HB2	1:F:69:MET:SD	2.56	0.46
1:D:139:PHE:CB	1:F:74:LEU:HD13	2.45	0.46
1:C:88:ILE:C	1:C:88:ILE:HD13	2.41	0.46
1:A:30:ASP:O	1:A:64:ASN:HB2	2.16	0.45
1:B:157:GLN:HG3	1:B:157:GLN:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:SER:O	1:F:131:SER:C	2.57	0.45
1:C:1:MET:HB3	1:C:85:ASN:ND2	2.31	0.45
1:E:122:GLU:C	1:E:124:PRO:HD2	2.42	0.45
1:F:49:GLU:HG2	1:F:50:GLU:N	2.29	0.45
1:E:156:LYS:HB2	1:E:156:LYS:HE3	1.61	0.45
1:F:2:ARG:HG3	1:F:2:ARG:NH1	2.26	0.45
1:C:123:GLU:HB3	1:C:124:PRO:HD3	1.98	0.45
1:A:90:GLY:HA2	1:A:119:LEU:O	2.16	0.45
1:E:24:ARG:NE	1:F:115:GLU:OE1	2.33	0.45
1:F:74:LEU:HB3	1:F:77:GLU:HG2	1.99	0.45
1:A:3:LYS:HE3	1:B:28:LEU:C	2.41	0.45
1:F:12:ASP:HA	1:F:13:PRO:HA	1.78	0.45
1:F:6:LEU:HB3	1:F:87:LEU:HD12	1.99	0.44
1:E:135:GLU:O	1:E:138:ARG:HG2	2.18	0.44
1:D:14:MET:HE2	1:D:14:MET:HB3	1.75	0.44
1:F:108:GLN:HG3	2:F:208:HOH:O	2.18	0.44
1:B:25:SER:OG	1:B:88:ILE:HD12	2.19	0.43
1:B:122:GLU:HG3	2:B:287:HOH:O	2.18	0.43
1:A:123:GLU:CG	1:F:123:GLU:CG	2.94	0.43
1:D:68:ILE:C	1:D:69:MET:HE2	2.43	0.43
1:C:104:ALA:O	1:C:108:GLN:HB3	2.17	0.43
1:D:68:ILE:HD13	1:D:70:GLN:NE2	2.33	0.43
1:E:123:GLU:N	1:E:124:PRO:CD	2.81	0.43
1:F:1:MET:HE3	1:F:86:PHE:CZ	2.53	0.43
1:B:14:MET:HE2	1:B:151:ILE:HD11	2.01	0.43
1:C:36:VAL:CG1	1:C:51:LYS:HE3	2.48	0.43
1:C:62:MET:HA	1:C:63:PRO:HD2	1.92	0.42
1:D:19:LEU:HD12	1:D:148:PRO:HG3	2.01	0.42
1:C:46:PHE:HB3	1:C:50:GLU:CB	2.48	0.42
1:A:66:ARG:CD	2:A:244:HOH:O	2.65	0.42
1:B:10:SER:HB3	1:B:12:ASP:OD2	2.18	0.42
1:C:38:ILE:HD12	1:C:48:PRO:HB3	2.02	0.42
1:D:46:PHE:HB3	1:D:50:GLU:HB2	2.01	0.42
1:F:77:GLU:HG2	1:F:77:GLU:H	1.59	0.42
1:F:61:GLU:HB2	2:F:271:HOH:O	2.20	0.42
1:B:151:ILE:O	1:B:155:LEU:HB2	2.20	0.42
1:D:99:TYR:CZ	1:D:103:ILE:HD11	2.55	0.42
1:A:123:GLU:HG2	1:F:123:GLU:CG	2.50	0.42
1:D:68:ILE:HD12	1:D:68:ILE:C	2.44	0.42
1:A:139:PHE:HB2	1:E:74:LEU:HD13	2.02	0.42
1:B:62:MET:HA	1:B:63:PRO:HD3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LYS:O	2:C:172:HOH:O	2.22	0.41
1:F:45:LEU:HG	1:F:158:LYS:HD2	2.02	0.41
1:D:147:LEU:CD1	1:D:152:TYR:HD1	2.29	0.41
1:D:88:ILE:HD11	1:D:119:LEU:HG	2.02	0.41
1:F:14:MET:CE	1:F:148:PRO:HG2	2.51	0.41
1:C:4:ILE:CD1	1:C:33:ILE:HG13	2.51	0.41
1:C:74:LEU:HD13	1:E:139:PHE:CB	2.51	0.41
1:C:136:VAL:HG11	1:C:143:VAL:CG1	2.51	0.41
1:D:72:THR:HG23	2:D:294:HOH:O	2.20	0.41
1:A:47:THR:HB	1:A:50:GLU:H	1.86	0.41
1:A:11:PHE:O	1:A:51:LYS:HE2	2.21	0.40
1:C:38:ILE:HD12	1:C:48:PRO:HG3	2.03	0.40
1:F:38:ILE:H	1:F:38:ILE:HG12	1.61	0.40
1:F:138:ARG:HG3	1:F:139:PHE:N	2.37	0.40
1:B:80:LYS:HG3	1:B:114:ILE:HD11	2.04	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	148/171 (86%)	144 (97%)	4 (3%)	0	100	100
1	B	148/171 (86%)	146 (99%)	2 (1%)	0	100	100
1	C	148/171 (86%)	144 (97%)	4 (3%)	0	100	100
1	D	148/171 (86%)	146 (99%)	2 (1%)	0	100	100
1	E	148/171 (86%)	144 (97%)	4 (3%)	0	100	100
1	F	148/171 (86%)	145 (98%)	3 (2%)	0	100	100
All	All	888/1026 (86%)	869 (98%)	19 (2%)	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	135/154 (88%)	123 (91%)	12 (9%)	9	12
1	B	135/154 (88%)	124 (92%)	11 (8%)	11	14
1	C	135/154 (88%)	118 (87%)	17 (13%)	4	5
1	D	135/154 (88%)	120 (89%)	15 (11%)	6	7
1	E	135/154 (88%)	116 (86%)	19 (14%)	3	3
1	F	135/154 (88%)	118 (87%)	17 (13%)	4	5
All	All	810/924 (88%)	719 (89%)	91 (11%)	6	7

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ILE
1	A	45	LEU
1	A	47	THR
1	A	57	GLU
1	A	74	LEU
1	A	80	LYS
1	A	87	LEU
1	A	108	GLN
1	A	120	LEU
1	A	122	GLU
1	A	131	SER
1	A	155	LEU
1	B	10	SER
1	B	19	LEU
1	B	51	LYS
1	B	74	LEU
1	B	87	LEU
1	B	88	ILE
1	B	108	GLN
1	B	129	SER
1	B	131	SER
1	B	145	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	155	LEU
1	C	2	ARG
1	C	4	ILE
1	C	19	LEU
1	C	27	LYS
1	C	33	ILE
1	C	38	ILE
1	C	49	GLU
1	C	50	GLU
1	C	74	LEU
1	C	87	LEU
1	C	88	ILE
1	C	108	GLN
1	C	129	SER
1	C	131	SER
1	C	155	LEU
1	C	157	GLN
1	C	158	LYS
1	D	14	MET
1	D	19	LEU
1	D	31	GLU
1	D	45	LEU
1	D	61	GLU
1	D	66	ARG
1	D	70	GLN
1	D	74	LEU
1	D	75	THR
1	D	87	LEU
1	D	131	SER
1	D	138	ARG
1	D	151	ILE
1	D	157	GLN
1	D	158	LYS
1	E	2	ARG
1	E	19	LEU
1	E	45	LEU
1	E	61	GLU
1	E	74	LEU
1	E	77	GLU
1	E	80	LYS
1	E	87	LEU
1	E	88	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	105	LYS
1	E	120	LEU
1	E	122	GLU
1	E	130	SER
1	E	131	SER
1	E	133	LEU
1	E	151	ILE
1	E	155	LEU
1	E	156	LYS
1	E	157	GLN
1	F	2	ARG
1	F	4	ILE
1	F	19	LEU
1	F	38	ILE
1	F	60	LYS
1	F	74	LEU
1	F	77	GLU
1	F	87	LEU
1	F	88	ILE
1	F	105	LYS
1	F	122	GLU
1	F	123	GLU
1	F	133	LEU
1	F	135	GLU
1	F	138	ARG
1	F	145	ASP
1	F	157	GLN

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

Mol	Chain	Res	Type
1	A	153	HIS
1	B	70	GLN
1	B	108	GLN
1	D	70	GLN
1	F	16	ASN
1	F	70	GLN
1	F	108	GLN
1	F	109	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	152/171 (88%)	-0.23	5 (3%)	49	51	18, 34, 67, 81	0
1	B	152/171 (88%)	-0.07	3 (1%)	65	66	18, 37, 75, 90	0
1	C	152/171 (88%)	0.19	8 (5%)	32	34	18, 42, 83, 98	0
1	D	152/171 (88%)	0.20	11 (7%)	21	23	18, 42, 90, 101	0
1	E	152/171 (88%)	-0.18	3 (1%)	65	66	18, 34, 68, 84	0
1	F	152/171 (88%)	0.13	10 (6%)	24	26	20, 41, 84, 95	0
All	All	912/1026 (88%)	0.01	40 (4%)	39	41	18, 39, 79, 101	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	LEU	6.8
1	C	45	LEU	5.2
1	A	45	LEU	5.2
1	D	45	LEU	4.4
1	A	153	HIS	3.6
1	E	156	LYS	3.2
1	C	158	LYS	3.1
1	C	48	PRO	3.0
1	F	46	PHE	2.9
1	D	38	ILE	2.9
1	D	153	HIS	2.8
1	F	153	HIS	2.8
1	F	48	PRO	2.8
1	F	158	LYS	2.7
1	C	46	PHE	2.7
1	F	49	GLU	2.6
1	C	152	TYR	2.6
1	A	158	LYS	2.6
1	B	46	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	158	LYS	2.5
1	D	53	TYR	2.5
1	C	1	MET	2.5
1	D	47	THR	2.4
1	F	47	THR	2.4
1	F	38	ILE	2.4
1	D	158	LYS	2.4
1	F	45	LEU	2.4
1	D	152	TYR	2.4
1	B	153	HIS	2.3
1	D	154	ALA	2.2
1	E	45	LEU	2.2
1	C	155	LEU	2.2
1	F	1	MET	2.2
1	C	47	THR	2.2
1	D	46	PHE	2.1
1	A	47	THR	2.1
1	D	57	GLU	2.1
1	D	48	PRO	2.1
1	A	49	GLU	2.0
1	F	154	ALA	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.