

Full wwPDB X-ray Structure Validation Report (i)

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 Title : Crystal structure of YrbI phosphatase from Escherichia coli in complex wit phosphate and a calcium ion Authors : Tsodikov, O.V.; Aggarwal, P.; Rubin, J.R.; Stuckey, J.A.; Woodard, R.V Biswas, T. Deposited on : 2007-09-11 Resolution : 2.10 Å(reported) 	PDB ID	:	2R8Z
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	Resolution	:	2.10 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.10 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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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%

Mol	Chain	Length	Quality of chain	
1	А	188	92%	• •
1	В	188	91%	5%••
1	С	188	91%	
1	D	188	86%	10% • •
1	Е	188	84%	10% • 5%
1	F	188	86%	10% • •
1	G	188	87%	9% • •



Mol	Chain	Length	Quality of chain	
1	Н	188	88%	7% • •
1	Ι	188	89%	7% •
1	J	188	85%	11% •
1	K	188	92%	
1	L	188	93%	• •
1	М	188	91%	5%••
1	Ν	188	89%	7% • •
1	Ο	188	90%	••5%
1	Р	188	78%	18% ••



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24342 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace	
1	Δ	101	Total	С	Ν	0	S	0	0	0	
	A	101	1356	856	232	261	7	0	0	0	
1	P	101	Total	С	Ν	0	S	0	0	0	
	D	101	1356	856	232	261	7	0	0	0	
1	С	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	U	101	1356	856	232	261	7	0	0	0	
1	П	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	D	101	1356	856	232	261	7	0	0	0	
1	E	178	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1		110	1332	842	228	255	7	0	0	0	
1	F	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	Ľ	101	1356	856	232	261	7	0	0	0	
1	G	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	G	101	1356	856	232	261	7		0	0	
1	н	181	181 Total C N O S		0	0	0				
1	11	181	1356	856	232	261	7	0	0	0	
1	т	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	T	181	1356	856	232	261	7	0		0	
1	Т	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	0	101	1356	856	232	261	7	0	0		
1	K	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	11	101	1356	856	232	261	7	0	0	0	
1	L	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	Ľ	101	1356	856	232	261	7	0	0	0	
1	М	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	111	101	1356	856	232	261	7	0	0	0	
1	N	181	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
1	11	101	1356	856	232	261	7	0	0	0	
1	0	178	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
		110	1332	842	228	255	7	0		0	
1	P	181	Total	С	Ν	Ο	S	0	0	0	
	1	101	1356	856	232	261	7	U	U	U	

• Molecule 1 is a protein called 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0
2	С	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	Ε	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	Н	1	Total Ca 1 1	0	0
2	Ι	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	Κ	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0
2	М	1	Total Ca 1 1	0	0
2	Ν	1	Total Ca 1 1	0	0
2	0	1	Total Ca 1 1	0	0
2	Р	1	Total Ca 1 1	0	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Ι	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	J	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	К	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Ν	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	О	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
3	Р	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	211	Total O 211 211	0	0
4	В	188	Total O 188 188	0	0
4	С	210	Total O 210 210	0	0
4	D	221	Total O 221 221	0	0
4	Е	227	Total O 227 227	0	0
4	F	192	Total O 192 192	0	0
4	G	190	Total O 190 190	0	0
4	Н	192	Total O 192 192	0	0
4	Ι	110	Total O 110 110	0	0
4	J	124	Total O 124 124	0	0
4	K	105	Total O 105 105	0	0
4	L	114	Total O 114 114	0	0
4	М	118	Total O 118 118	0	0
4	Ν	140	Total O 140 140	0	0
4	О	122	Total O 122 122	0	0
4	Р	134	Total O 134 134	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. 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. 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: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase





7%

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain G:			87%	9% • •
MET SER LYS ALA GLY ALA SER SER	D32 V33 D34 G35 V36 Y43	E50 L51 V56 Y60 R63	T67 A73 A73 S100 N101 L109 S187 L188	

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain H:						88	8%					7%	••			
MET SER LYS ALA GLY ALA SER SER	L28	D34	G45	N55 V56	N5/ D58	T67 S68	H94	N101	11 <mark>15</mark>	1150 P151	R163	K179	<mark>S187</mark> I188			

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain I:				89%			
					La La	ood oo	l
MET SER LYS ALA GLY ALA ALA SER SER	N25	D34 Y43	E49 E50 L51 K52	V56 S68	L82 T89 L17	K17 L18 D18 T18	

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain J:			85%			11%	·
MET SER LYS ALA GLY GLY SER SER	L28 D32 V33 D34	Y43 L51 K52 V56	R63 T67 S68 L82 Y96	K102 L109 D125 M133 V136	1150 V156 K179 S187	1188	

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

 Chain K:
 92%
 .

 • Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain L: 93% · ·

• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase

Chain M: 91% 5%..



• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



• Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	85.37Å 156.91Å 114.05Å	Depositor
a, b, c, α , β , γ	90.00° 96.54° 90.00°	Depositor
Bosolution (Å)	30.00 - 2.10	Depositor
Resolution (A)	38.43 - 1.95	EDS
% Data completeness	98.4 (30.00-2.10)	Depositor
(in resolution range)	88.5 (38.43-1.95)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 1.95 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D .	0.184 , 0.231	Depositor
n, n_{free}	0.185 , 0.231	DCC
R_{free} test set	9662 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	26.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 36.1	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24342	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, PO4

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		Bo	nd lengths	Bond angles		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.38	0/1372	0.53	0/1858	
1	В	0.36	0/1372	0.52	0/1858	
1	С	0.38	0/1372	0.51	0/1858	
1	D	0.39	0/1372	0.53	0/1858	
1	Е	0.39	0/1348	0.52	0/1827	
1	F	0.38	0/1372	0.52	0/1858	
1	G	0.38	0/1372	0.54	0/1858	
1	Н	0.38	0/1372	0.54	0/1858	
1	Ι	0.33	0/1372	0.48	0/1858	
1	J	0.33	0/1372	0.48	0/1858	
1	Κ	0.32	0/1372	0.47	0/1858	
1	L	0.32	0/1372	0.47	0/1858	
1	М	0.33	0/1372	0.49	0/1858	
1	Ν	0.34	0/1372	0.50	0/1858	
1	0	0.34	0/1348	0.49	0/1827	
1	Р	0.86	$5/\overline{1372}~(0.4\%)$	0.73	4/1858~(0.2%)	
All	All	0.41	5/21904~(0.0%)	0.52	4/29666~(0.0%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Р	134	GLU	C-O	8.66	1.39	1.23
1	Р	86	ARG	CZ-NH1	8.13	1.43	1.33
1	Р	106	PHE	CG-CD1	5.92	1.47	1.38
1	Р	136	VAL	C-O	-5.89	1.12	1.23
1	Р	111	GLU	CD-OE1	5.62	1.31	1.25

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	Р	106	PHE	CB-CG-CD2	-8.77	114.66	120.80
1	Р	106	PHE	CG-CD2-CE2	-7.97	112.03	120.80
1	Р	86	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Р	106	PHE	CD1-CG-CD2	6.11	126.25	118.30

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	А	1356	0	1385	5	0
1	В	1356	0	1385	7	0
1	С	1356	0	1385	6	0
1	D	1356	0	1385	14	0
1	Е	1332	0	1361	17	0
1	F	1356	0	1385	14	0
1	G	1356	0	1385	13	0
1	Н	1356	0	1385	10	0
1	Ι	1356	0	1385	7	0
1	J	1356	0	1385	12	0
1	Κ	1356	0	1385	6	0
1	L	1356	0	1385	4	0
1	М	1356	0	1385	6	0
1	Ν	1356	0	1385	9	0
1	0	1332	0	1361	4	0
1	Р	1356	0	1385	24	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0



2F	28	Ζ
	00	_

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	М	1	0	0	0	0
2	N	1	0	0	0	0
2	0	1	0	0	0	0
2	Р	1	0	0	0	0
3	А	5	0	0	1	0
3	В	5	0	0	0	0
3	С	5	0	0	0	0
3	D	5	0	0	1	0
3	Е	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	1	0
3	Н	5	0	0	1	0
3	Ι	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	М	5	0	0	0	0
3	N	5	0	0	0	0
3	0	5	0	0	0	0
3	Р	5	0	0	0	0
4	А	211	0	0	7	0
4	В	188	0	0	1	0
4	С	210	0	0	2	0
4	D	221	0	0	3	0
4	Е	227	0	0	6	0
4	F	192	0	0	3	0
4	G	190	0	0	4	0
4	Н	192	0	0	4	0
4	Ι	110	0	0	1	0
4	J	124	0	0	0	0
4	K	105	0	0	1	0
4	L	114	0	0	0	0
4	М	118	0	0	0	0
4	Ν	140	0	0	2	0
4	0	122	0	0	0	0
4	Р	134	0	0	11	0
All	All	24342	0	22112	147	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 3.



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:P:87:CYS:SG	4:P:336:HOH:O	2.26	0.93	
3:H:209:PO4:O2	4:H:212:HOH:O	1.91	0.88	
1:E:105:ALA:HB2	4:E:379:HOH:O	1.73	0.87	
1:P:82:LEU:HG	4:P:331:HOH:O	1.74	0.86	
1:F:89:THR:HB	4:F:367:HOH:O	1.74	0.86	
1:P:130:TRP:HZ3	4:P:346:HOH:O	1.61	0.82	
1:E:99:GLN:HG2	4:E:214:HOH:O	1.78	0.82	
1:P:27:ARG:HB2	1:P:115:ILE:CD1	2.10	0.81	
1:P:27:ARG:HB2	1:P:115:ILE:HD11	1.64	0.79	
3:D:205:PO4:O2	4:D:210:HOH:O	2.01	0.78	
1:E:99:GLN:HB2	4:E:210:HOH:O	1.86	0.76	
1:D:63:ARG:HE	1:D:186:GLN:HE22	1.31	0.75	
3:A:202:PO4:O2	4:A:205:HOH:O	2.11	0.69	
1:P:120:VAL:HG13	4:P:312:HOH:O	1.94	0.68	
1:P:80:ALA:HB3	4:P:331:HOH:O	1.94	0.67	
4:A:376:HOH:O	1:D:187:SER:HB3	1.96	0.66	
1:E:99:GLN:HB3	4:E:356:HOH:O	1.95	0.66	
1:G:67:THR:HG23	4:G:258:HOH:O	1.95	0.65	
1:J:56:VAL:HG21	1:K:34:ASP:HB3	1.78	0.65	
1:P:30:ILE:HG21	1:P:75:ILE:HD12	1.79	0.63	
1:F:42:ILE:HD12	1:F:52:LYS:HZ3	1.64	0.63	
1:G:76:THR:HG21	4:G:248:HOH:O	1.98	0.63	
1:G:63:ARG:O	1:G:67:THR:HG22	1.99	0.62	
1:E:99:GLN:CB	4:E:356:HOH:O	2.48	0.61	
1:M:56:VAL:HG12	1:N:42:ILE:HG12	1.82	0.61	
1:D:39:ASP:OD1	4:D:254:HOH:O	2.16	0.60	
1:N:99:GLN:HG3	4:N:289:HOH:O	2.00	0.60	
1:P:99:GLN:NE2	4:P:253:HOH:O	2.33	0.60	
1:D:63:ARG:HE	1:D:186:GLN:NE2	2.00	0.60	
1:P:133:MET:SD	4:P:335:HOH:O	2.56	0.59	
1:I:89:THR:HG21	4:I:292:HOH:O	2.01	0.59	
1:G:8:LEU:N	4:G:360:HOH:O	2.35	0.58	
1:P:27:ARG:HB2	1:P:115:ILE:HD12	1.83	0.58	
1:E:55:ASN:HD22	1:E:58:ASP:H	1.50	0.58	
1:P:149:LEU:HD11	4:P:335:HOH:O	2.04	0.58	
1:P:132:VAL:HB	4:P:338:HOH:O	2.05	0.56	
1:E:110:LEU:HD22	1:E:115:ILE:HG23	1.88	0.56	
1:F:28:LEU:HD21	1:F:109:LEU:HD13	1.86	0.56	
1:I:43:TYR:HB2	1:I:51:LEU:HB2	1.88	0.56	
1:D:63:ARG:O	1:D:67:THR:HB	2.06	0.55	

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



	lo uo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:63:ARG:O	1:E:67:THR:HB	2.06	0.55	
1:K:56:VAL:HG21	1:L:34:ASP:HB3	1.88	0.55	
1:G:56:VAL:HG21	1:H:34:ASP:HB3	1.89	0.55	
1:F:67:THR:HG23	4:F:345:HOH:O	2.07	0.54	
1:E:68:SER:HB3	1:E:179:LYS:HD3	1.89	0.54	
1:K:55:ASN:HD22	1:K:58:ASP:H	1.56	0.53	
1:F:56:VAL:HG21	1:G:34:ASP:HB3	1.89	0.53	
1:I:56:VAL:HG21	1:J:34:ASP:HB3	1.90	0.53	
1:B:13:GLY:HA2	4:H:347:HOH:O	2.09	0.53	
1:E:111:GLU:HG3	1:N:103:LEU:HD13	1.90	0.52	
1:0:63:ARG:0	1:O:67:THR:HG22	2.10	0.52	
1:C:67:THR:HG23	4:C:378:HOH:O	2.09	0.51	
1:F:42:ILE:CD1	1:F:52:LYS:NZ	2.73	0.51	
1:J:68:SER:HB3	1:J:179:LYS:HD3	1.91	0.51	
1:I:34:ASP:HB3	1:L:56:VAL:HG21	1.93	0.51	
1:M:43:TYR:HB2	1:M:51:LEU:HB2	1.91	0.51	
1:N:110:LEU:HD22	1:N:115:ILE:HG23	1.91	0.51	
1:N:94:HIS:HD2	4:N:258:HOH:O	1.94	0.50	
1:E:101:ASN:HD22	1:E:101:ASN:C	2.14	0.50	
1:G:73:ALA:CB	1:G:109:LEU:HD11	2.41	0.50	
1:P:106:PHE:HE2	1:P:120:VAL:HG11	1.77	0.50	
1:A:56:VAL:HG21	1:B:34:ASP:HB3	1.94	0.49	
1:P:83:VAL:CG1	4:P:336:HOH:O	2.60	0.49	
1:D:94:HIS:HD2	4:D:259:HOH:O	1.96	0.49	
1:B:57:ARG:HD2	4:B:335:HOH:O	2.12	0.49	
1:J:150:ILE:HG23	1:J:156:VAL:HG21	1.95	0.48	
1:A:94:HIS:HD2	4:A:261:HOH:O	1.95	0.48	
1:C:68:SER:HB3	1:C:179:LYS:HD3	1.96	0.48	
1:J:32:ASP:OD2	1:J:102:LYS:NZ	2.46	0.48	
1:F:42:ILE:CD1	1:F:52:LYS:HZ3	2.25	0.48	
1:C:8:LEU:N	4:C:394:HOH:O	2.45	0.48	
1:F:32:ASP:HB2	1:F:36:VAL:HG21	1.97	0.47	
1:I:68:SER:HB3	1:I:179:LYS:HD3	1.97	0.47	
1:K:43:TYR:HB2	1:K:51:LEU:HB2	1.95	0.47	
1:A:43:TYR:HB2	1:A:51:LEU:HB2	1.96	0.47	
1:J:133:MET:O	1:J:136:VAL:HG22	2.15	0.47	
1:G:76:THR:HG23	3:G:208:PO4:O3	2.15	0.47	
1:N:43:TYR:HB2	1:N:51:LEU:HB2	1.96	0.47	
1:P:71:GLU:HG2	1:P:113:LEU:HD11	1.97	0.46	
1:P:83:VAL:HG12	4:P:336:HOH:O	2.14	0.46	
1:B:32:ASP:HB2	1:B:36:VAL:HG21	1.97	0.46	



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:63:ARG:O	1:A:67:THR:HG22	2.15	0.46	
1:I:52:LYS:HE2	1:I:82:LEU:HD11	1.98	0.46	
1:J:43:TYR:HB2	1:J:51:LEU:HB2	1.98	0.46	
1:H:163:ARG:HD3	4:H:350:HOH:O	2.15	0.46	
1:P:28:LEU:HB3	1:P:115:ILE:HD13	1.98	0.45	
1:C:55:ASN:HD22	1:C:58:ASP:H	1.65	0.45	
1:D:27:ARG:HB2	1:D:115:ILE:HD12	1.98	0.45	
1:E:74:ILE:HD12	1:E:87:CYS:SG	2.56	0.45	
4:A:402:HOH:O	1:D:163:ARG:NH1	2.49	0.45	
1:F:8:LEU:N	4:F:352:HOH:O	2.50	0.45	
1:I:175:LEU:HB2	1:I:180:LEU:HD22	1.99	0.45	
1:B:43:TYR:HB2	1:B:51:LEU:HB2	1.99	0.45	
1:J:63:ARG:O	1:J:67:THR:HG22	2.16	0.45	
1:G:60:TYR:HB2	1:G:187:SER:HA	1.99	0.44	
1:P:43:TYR:HB2	1:P:51:LEU:HB2	1.99	0.44	
1:E:101:ASN:ND2	4:E:327:HOH:O	2.49	0.44	
1:M:52:LYS:HE2	1:M:82:LEU:HD11	1.99	0.44	
1:H:68:SER:HB3	1:H:179:LYS:HD2	2.00	0.44	
1:F:68:SER:HB3	1:F:179:LYS:HD3	1.99	0.44	
1:E:43:TYR:HB2	1:E:51:LEU:HB2	2.00	0.44	
1:D:32:ASP:OD1	1:D:102:LYS:NZ	2.51	0.43	
1:H:55:ASN:HD22	1:H:58:ASP:H	1.65	0.43	
1:G:50:GLU:O	1:H:45:GLY:HA2	2.19	0.43	
1:D:101:ASN:C	1:D:101:ASN:HD22	2.22	0.43	
1:F:27:ARG:HB2	1:F:115:ILE:HD12	2.00	0.43	
1:L:43:TYR:HB2	1:L:51:LEU:HB2	2.00	0.43	
1:E:42:ILE:HG12	1:H:56:VAL:HG12	2.01	0.43	
1:D:74:ILE:HD12	1:D:87:CYS:SG	2.58	0.43	
1:N:52:LYS:HE2	1:N:82:LEU:HD11	2.00	0.43	
1:H:28:LEU:HB3	1:H:115:ILE:HD13	2.00	0.43	
1:M:60:TYR:HB2	1:M:187:SER:HA	2.01	0.43	
1:M:55:ASN:O	1:M:58:ASP:HB2	2.19	0.42	
1:D:58:ASP:OD1	1:D:164:GLY:HA2	2.19	0.42	
1:E:99:GLN:HG3	1:E:101:ASN:H	1.84	0.42	
1:F:42:ILE:HD12	1:F:52:LYS:NZ	2.29	0.42	
1:O:101:ASN:HD21	1:O:103:LEU:HD12	1.84	0.42	
1:G:43:TYR:HB2	1:G:51:LEU:HB2	2.00	0.42	
1:P:68:SER:HB3	1:P:179:LYS:HD3	2.01	0.42	
1:A:94:HIS:HE1	4:A:285:HOH:O	2.02	0.42	
1:O:43:TYR:HB2	1:O:51:LEU:HB2	2.02	0.42	
1:K:8:LEU:N	4:K:286:HOH:O	2.52	0.42	



A 4 amo 1	A.t.a.m. D	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:58:ASP:OD1	1:B:164:GLY:HA2	2.19	0.42	
1:E:50:GLU:O	1:F:45:GLY:HA2	2.20	0.42	
1:J:52:LYS:HE2	1:J:82:LEU:HD11	2.02	0.42	
1:P:32:ASP:HB3	1:P:36:VAL:HG21	2.01	0.42	
1:G:32:ASP:HB3	1:G:36:VAL:HG21	2.01	0.41	
1:J:56:VAL:HG22	1:K:40:GLY:O	2.21	0.41	
1:J:96:TYR:CE1	1:J:109:LEU:HG	2.55	0.41	
1:P:118:GLU:O	1:P:137:GLY:HA3	2.19	0.41	
1:D:43:TYR:HB2	1:D:51:LEU:HB2	2.01	0.41	
1:H:94:HIS:HD2	4:H:233:HOH:O	2.02	0.41	
1:J:28:LEU:HD21	1:J:109:LEU:HD13	2.03	0.41	
1:N:27:ARG:HB2	1:N:115:ILE:HD12	2.03	0.41	
1:C:30:ILE:HG21	1:C:75:ILE:HD12	2.02	0.41	
1:H:101:ASN:C	1:H:101:ASN:HD22	2.24	0.41	
1:N:42:ILE:HG22	1:N:44:MET:HG3	2.02	0.41	
1:F:55:ASN:HD22	1:F:58:ASP:H	1.68	0.41	
1:G:100:SER:HA	4:G:374:HOH:O	2.20	0.41	
1:M:55:ASN:HD22	1:M:58:ASP:H	1.68	0.41	
1:P:67:THR:HG21	1:P:184:LYS:O	2.20	0.41	
1:P:28:LEU:HD22	1:P:113:LEU:HD12	2.02	0.40	
1:H:150:ILE:HB	1:H:151:PRO:HD3	2.04	0.40	
4:A:376:HOH:O	1:D:187:SER:CB	2.61	0.40	
4:A:391:HOH:O	1:O:182:GLU:HG3	2.21	0.40	
1:B:53:ALA:HA	1:C:42:ILE:O	2.22	0.40	
1:L:142:VAL:HA	1:L:157:THR:OG1	2.22	0.40	

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles
1	А	179/188~(95%)	176 (98%)	3 (2%)	0	100 100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	В	179/188~(95%)	178~(99%)	1 (1%)	0	100 100
1	С	179/188~(95%)	177~(99%)	2(1%)	0	100 100
1	D	179/188~(95%)	178~(99%)	1 (1%)	0	100 100
1	Е	176/188~(94%)	174 (99%)	2(1%)	0	100 100
1	F	179/188~(95%)	177~(99%)	2(1%)	0	100 100
1	G	179/188~(95%)	176~(98%)	3~(2%)	0	100 100
1	Н	179/188~(95%)	178 (99%)	1 (1%)	0	100 100
1	Ι	179/188~(95%)	176~(98%)	3~(2%)	0	100 100
1	J	179/188~(95%)	177~(99%)	2(1%)	0	100 100
1	K	179/188~(95%)	176~(98%)	3~(2%)	0	100 100
1	L	179/188~(95%)	177~(99%)	2(1%)	0	100 100
1	М	179/188~(95%)	177~(99%)	2(1%)	0	100 100
1	Ν	179/188~(95%)	177 (99%)	2(1%)	0	100 100
1	Ο	176/188 (94%)	172 (98%)	4 (2%)	0	100 100
1	Р	179/188~(95%)	176 (98%)	3(2%)	0	100 100
All	All	$285\overline{8/3008}~(95\%)$	2822 (99%)	36 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	А	142/147~(97%)	140 (99%)	2(1%)	67 73
1	В	142/147~(97%)	141 (99%)	1 (1%)	84 88
1	С	142/147~(97%)	141 (99%)	1 (1%)	84 88
1	D	142/147~(97%)	138~(97%)	4 (3%)	43 47
1	Ε	139/147~(95%)	135~(97%)	4 (3%)	42 46
1	F	142/147~(97%)	138~(97%)	4 (3%)	43 47



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	G	142/147~(97%)	140 (99%)	2 (1%)	67	73
1	Н	142/147~(97%)	138~(97%)	4 (3%)	43	47
1	Ι	142/147~(97%)	139~(98%)	3 (2%)	53	59
1	J	142/147~(97%)	140 (99%)	2 (1%)	67	73
1	К	142/147~(97%)	142 (100%)	0	100	100
1	L	142/147~(97%)	141 (99%)	1 (1%)	84	88
1	М	142/147~(97%)	140 (99%)	2 (1%)	67	73
1	Ν	142/147~(97%)	139 (98%)	3 (2%)	53	59
1	Ο	139/147~(95%)	136 (98%)	3 (2%)	52	57
1	Р	142/147~(97%)	138 (97%)	4 (3%)	43	47
All	All	2266/2352~(96%)	2226 (98%)	40 (2%)	59	65

All (40) residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	69	ASP
1	А	187	SER
1	В	32	ASP
1	С	67	THR
1	D	67	THR
1	D	100	SER
1	D	101	ASN
1	D	109	LEU
1	Ε	24	GLU
1	Ε	67	THR
1	Е	100	SER
1	Ε	101	ASN
1	F	76	THR
1	F	78	ARG
1	F	109	LEU
1	F	187	SER
1	G	76	THR
1	G	101	ASN
1	Н	56	VAL
1	Н	67	THR
1	Н	101	ASN
1	Н	187	SER
1	Ι	25	ASN



Mol	Chain	Res	Type
1	Ι	49	GLU
1	Ι	181	ASP
1	J	125	ASP
1	J	187	SER
1	L	76	THR
1	М	101	ASN
1	М	187	SER
1	N	99	GLN
1	N	101	ASN
1	N	187	SER
1	0	76	THR
1	0	125	ASP
1	0	182	GLU
1	Р	18	ASP
1	Р	99	GLN
1	Р	125	ASP
1	Р	187	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	25	ASN
1	А	47	ASN
1	А	55	ASN
1	А	94	HIS
1	А	101	ASN
1	В	25	ASN
1	В	55	ASN
1	В	94	HIS
1	С	25	ASN
1	С	55	ASN
1	С	101	ASN
1	С	119	ASN
1	D	55	ASN
1	D	94	HIS
1	D	101	ASN
1	D	186	GLN
1	Е	25	ASN
1	Е	55	ASN
1	Е	94	HIS
1	Е	101	ASN
1	Е	119	ASN



Mol	Chain	Res	Type
1	F	25	ASN
1	F	47	ASN
1	F	55	ASN
1	F	101	ASN
1	F	119	ASN
1	G	25	ASN
1	G	55	ASN
1	G	99	GLN
1	G	101	ASN
1	G	119	ASN
1	Н	25	ASN
1	Н	55	ASN
1	Н	94	HIS
1	Н	101	ASN
1	Ι	55	ASN
1	Ι	101	ASN
1	J	55	ASN
1	J	101	ASN
1	K	55	ASN
1	Κ	99	GLN
1	Κ	101	ASN
1	L	55	ASN
1	L	94	HIS
1	L	101	ASN
1	М	25	ASN
1	М	55	ASN
1	М	101	ASN
1	Ν	55	ASN
1	Ν	94	HIS
1	Ν	101	ASN
1	N	119	ASN
1	0	55	ASN
1	0	101	ASN
1	Р	25	ASN
1	Р	47	ASN
1	Р	101	ASN
1	Р	119	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Tuno	Chain	Dog	Link	B	ond leng	gths	E	Bond ang	gles
	Type	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	Ν	215	2	4,4,4	0.93	0	6,6,6	2.23	2 (33%)
3	PO4	Р	217	2	4,4,4	0.90	0	6,6,6	1.87	3 (50%)
3	PO4	М	214	2	4,4,4	0.89	0	6,6,6	1.13	0
3	PO4	С	204	2	4,4,4	0.88	0	6,6,6	1.14	1 (16%)
3	PO4	Ι	210	2	4,4,4	0.89	0	6,6,6	1.34	1 (16%)
3	PO4	J	211	2	4,4,4	0.93	0	6,6,6	1.00	0
3	PO4	L	213	2	4,4,4	0.93	0	6,6,6	1.31	1 (16%)
3	PO4	G	208	2	4,4,4	0.95	0	6,6,6	1.55	2 (33%)
3	PO4	Н	209	2	4,4,4	0.98	0	6,6,6	1.49	2 (33%)
3	PO4	0	216	2	4,4,4	0.91	0	6,6,6	1.02	0
3	PO4	D	205	2	4,4,4	1.07	0	6,6,6	1.96	3 (50%)
3	PO4	Е	206	2	4,4,4	0.97	0	6,6,6	1.60	2 (33%)
3	PO4	Κ	212	2	4,4,4	0.95	0	6,6,6	0.86	0
3	PO4	A	202	2	4,4,4	1.01	0	6,6,6	1.30	1 (16%)
3	PO4	F	207	2	4,4,4	0.92	0	6,6,6	2.11	2 (33%)
3	PO4	В	203	2	4,4,4	0.96	0	6,6,6	1.57	2 (33%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
3	F	207	PO4	02-P-01	-4.05	96.06	110.89
3	Ν	215	PO4	04-P-01	-4.05	96.07	110.89
3	D	205	PO4	O4-P-O2	-2.93	98.58	107.97
3	Ι	210	PO4	O3-P-O2	2.71	116.66	107.97
3	Н	209	PO4	O4-P-O2	-2.61	99.60	107.97
3	Е	206	PO4	O4-P-O2	-2.58	99.70	107.97
3	F	207	PO4	03-P-01	2.48	119.97	110.89
3	В	203	PO4	04-P-O3	-2.43	100.16	107.97
3	Р	217	PO4	O3-P-O2	2.40	115.67	107.97
3	L	213	PO4	03-P-01	2.40	119.67	110.89
3	Е	206	PO4	O3-P-O2	2.35	115.50	107.97
3	Н	209	PO4	O3-P-O2	2.33	115.44	107.97
3	Р	217	PO4	04-P-02	-2.22	100.85	107.97
3	D	205	PO4	O3-P-O2	2.21	115.05	107.97
3	G	208	PO4	O3-P-O2	-2.20	100.90	107.97
3	А	202	PO4	O3-P-O2	2.16	114.90	107.97
3	Ν	215	PO4	04-P-O3	2.15	114.87	107.97
3	Р	217	PO4	03-P-01	-2.11	103.19	110.89
3	В	203	PO4	03-P-01	2.10	118.57	110.89
3	D	205	PO4	03-P-01	2.08	118.49	110.89
3	С	204	PO4	O4-P-O2	-2.06	101.35	107.97
3	G	208	PO4	03-P-01	2.06	118.42	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	208	PO4	1	0
3	Н	209	PO4	1	0
3	D	205	PO4	1	0
3	А	202	PO4	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

