Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:40 AM GMT

PDB ID	:	3MN1
Title	:	Crystal structure of probable yrbi family phosphatase from pseudomonas syringae pv.phaseolica 1448a
Authors	:	Patskovsky, Y.; Ramagopal, U.; Toro, R.; Freeman, J.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-04-20
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

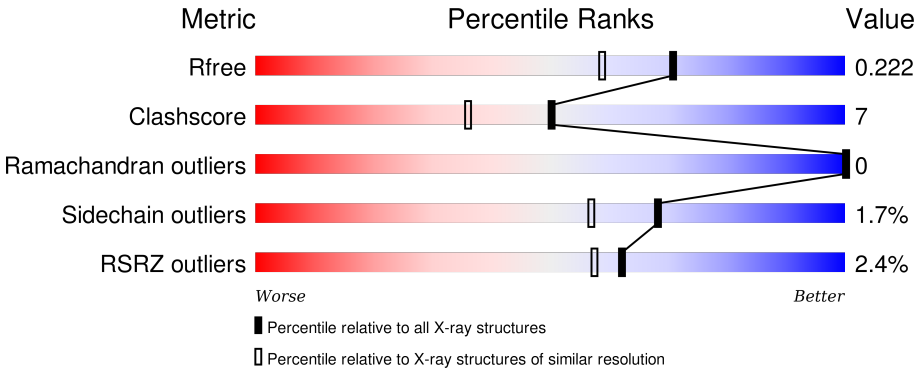
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	189	4% 85% 12% •
1	B	189	3% 78% 13% • 8%
1	C	189	2% 85% 7% 8%
1	D	189	2% 86% 7% 7%
1	E	189	2% 81% 11% • 8%

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Mol	Chain	Length	Quality of chain
1	F	189	2% 81% 11% • 7%
1	G	189	3% 82% 9% • 8%
1	H	189	83% 8% • 8%
1	I	189	% 80% 11% • 8%
1	J	189	3% 81% 12% 7%
1	K	189	4% 78% 13% • 7%
1	L	189	3% 79% 12% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17767 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 probable yrbi family phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	7	0
			1421	896	247	272	6			
1	B	174	Total	C	N	O	S	0	6	0
			1355	854	238	257	6			
1	C	174	Total	C	N	O	S	0	6	0
			1350	851	237	256	6			
1	D	176	Total	C	N	O	S	0	6	0
			1360	858	238	258	6			
1	E	174	Total	C	N	O	S	0	2	0
			1330	837	234	254	5			
1	F	176	Total	C	N	O	S	0	4	0
			1352	851	238	257	6			
1	G	173	Total	C	N	O	S	0	8	0
			1356	856	237	257	6			
1	H	173	Total	C	N	O	S	0	6	0
			1347	849	236	256	6			
1	I	174	Total	C	N	O	S	0	5	0
			1345	848	235	257	5			
1	J	176	Total	C	N	O	S	0	4	0
			1368	861	246	255	6			
1	K	176	Total	C	N	O	S	0	3	0
			1353	852	239	257	5			
1	L	173	Total	C	N	O	S	0	8	0
			1361	858	239	258	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q48EB9
A	0	SER	-	expression tag	UNP Q48EB9
A	1	LEU	-	expression tag	UNP Q48EB9
A	151	GLN	ARG	engineered	UNP Q48EB9
A	180	GLU	-	expression tag	UNP Q48EB9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLY	-	expression tag	UNP Q48EB9
A	182	HIS	-	expression tag	UNP Q48EB9
A	183	HIS	-	expression tag	UNP Q48EB9
A	184	HIS	-	expression tag	UNP Q48EB9
A	185	HIS	-	expression tag	UNP Q48EB9
A	186	HIS	-	expression tag	UNP Q48EB9
A	187	HIS	-	expression tag	UNP Q48EB9
B	-1	MET	-	expression tag	UNP Q48EB9
B	0	SER	-	expression tag	UNP Q48EB9
B	1	LEU	-	expression tag	UNP Q48EB9
B	151	GLN	ARG	engineered	UNP Q48EB9
B	180	GLU	-	expression tag	UNP Q48EB9
B	181	GLY	-	expression tag	UNP Q48EB9
B	182	HIS	-	expression tag	UNP Q48EB9
B	183	HIS	-	expression tag	UNP Q48EB9
B	184	HIS	-	expression tag	UNP Q48EB9
B	185	HIS	-	expression tag	UNP Q48EB9
B	186	HIS	-	expression tag	UNP Q48EB9
B	187	HIS	-	expression tag	UNP Q48EB9
C	-1	MET	-	expression tag	UNP Q48EB9
C	0	SER	-	expression tag	UNP Q48EB9
C	1	LEU	-	expression tag	UNP Q48EB9
C	151	GLN	ARG	engineered	UNP Q48EB9
C	180	GLU	-	expression tag	UNP Q48EB9
C	181	GLY	-	expression tag	UNP Q48EB9
C	182	HIS	-	expression tag	UNP Q48EB9
C	183	HIS	-	expression tag	UNP Q48EB9
C	184	HIS	-	expression tag	UNP Q48EB9
C	185	HIS	-	expression tag	UNP Q48EB9
C	186	HIS	-	expression tag	UNP Q48EB9
C	187	HIS	-	expression tag	UNP Q48EB9
D	-1	MET	-	expression tag	UNP Q48EB9
D	0	SER	-	expression tag	UNP Q48EB9
D	1	LEU	-	expression tag	UNP Q48EB9
D	151	GLN	ARG	engineered	UNP Q48EB9
D	180	GLU	-	expression tag	UNP Q48EB9
D	181	GLY	-	expression tag	UNP Q48EB9
D	182	HIS	-	expression tag	UNP Q48EB9
D	183	HIS	-	expression tag	UNP Q48EB9
D	184	HIS	-	expression tag	UNP Q48EB9
D	185	HIS	-	expression tag	UNP Q48EB9
D	186	HIS	-	expression tag	UNP Q48EB9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	187	HIS	-	expression tag	UNP Q48EB9
E	-1	MET	-	expression tag	UNP Q48EB9
E	0	SER	-	expression tag	UNP Q48EB9
E	1	LEU	-	expression tag	UNP Q48EB9
E	151	GLN	ARG	engineered	UNP Q48EB9
E	180	GLU	-	expression tag	UNP Q48EB9
E	181	GLY	-	expression tag	UNP Q48EB9
E	182	HIS	-	expression tag	UNP Q48EB9
E	183	HIS	-	expression tag	UNP Q48EB9
E	184	HIS	-	expression tag	UNP Q48EB9
E	185	HIS	-	expression tag	UNP Q48EB9
E	186	HIS	-	expression tag	UNP Q48EB9
E	187	HIS	-	expression tag	UNP Q48EB9
F	-1	MET	-	expression tag	UNP Q48EB9
F	0	SER	-	expression tag	UNP Q48EB9
F	1	LEU	-	expression tag	UNP Q48EB9
F	151	GLN	ARG	engineered	UNP Q48EB9
F	180	GLU	-	expression tag	UNP Q48EB9
F	181	GLY	-	expression tag	UNP Q48EB9
F	182	HIS	-	expression tag	UNP Q48EB9
F	183	HIS	-	expression tag	UNP Q48EB9
F	184	HIS	-	expression tag	UNP Q48EB9
F	185	HIS	-	expression tag	UNP Q48EB9
F	186	HIS	-	expression tag	UNP Q48EB9
F	187	HIS	-	expression tag	UNP Q48EB9
G	-1	MET	-	expression tag	UNP Q48EB9
G	0	SER	-	expression tag	UNP Q48EB9
G	1	LEU	-	expression tag	UNP Q48EB9
G	151	GLN	ARG	engineered	UNP Q48EB9
G	180	GLU	-	expression tag	UNP Q48EB9
G	181	GLY	-	expression tag	UNP Q48EB9
G	182	HIS	-	expression tag	UNP Q48EB9
G	183	HIS	-	expression tag	UNP Q48EB9
G	184	HIS	-	expression tag	UNP Q48EB9
G	185	HIS	-	expression tag	UNP Q48EB9
G	186	HIS	-	expression tag	UNP Q48EB9
G	187	HIS	-	expression tag	UNP Q48EB9
H	-1	MET	-	expression tag	UNP Q48EB9
H	0	SER	-	expression tag	UNP Q48EB9
H	1	LEU	-	expression tag	UNP Q48EB9
H	151	GLN	ARG	engineered	UNP Q48EB9
H	180	GLU	-	expression tag	UNP Q48EB9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	181	GLY	-	expression tag	UNP Q48EB9
H	182	HIS	-	expression tag	UNP Q48EB9
H	183	HIS	-	expression tag	UNP Q48EB9
H	184	HIS	-	expression tag	UNP Q48EB9
H	185	HIS	-	expression tag	UNP Q48EB9
H	186	HIS	-	expression tag	UNP Q48EB9
H	187	HIS	-	expression tag	UNP Q48EB9
I	-1	MET	-	expression tag	UNP Q48EB9
I	0	SER	-	expression tag	UNP Q48EB9
I	1	LEU	-	expression tag	UNP Q48EB9
I	151	GLN	ARG	engineered	UNP Q48EB9
I	180	GLU	-	expression tag	UNP Q48EB9
I	181	GLY	-	expression tag	UNP Q48EB9
I	182	HIS	-	expression tag	UNP Q48EB9
I	183	HIS	-	expression tag	UNP Q48EB9
I	184	HIS	-	expression tag	UNP Q48EB9
I	185	HIS	-	expression tag	UNP Q48EB9
I	186	HIS	-	expression tag	UNP Q48EB9
I	187	HIS	-	expression tag	UNP Q48EB9
J	-1	MET	-	expression tag	UNP Q48EB9
J	0	SER	-	expression tag	UNP Q48EB9
J	1	LEU	-	expression tag	UNP Q48EB9
J	151	GLN	ARG	engineered	UNP Q48EB9
J	180	GLU	-	expression tag	UNP Q48EB9
J	181	GLY	-	expression tag	UNP Q48EB9
J	182	HIS	-	expression tag	UNP Q48EB9
J	183	HIS	-	expression tag	UNP Q48EB9
J	184	HIS	-	expression tag	UNP Q48EB9
J	185	HIS	-	expression tag	UNP Q48EB9
J	186	HIS	-	expression tag	UNP Q48EB9
J	187	HIS	-	expression tag	UNP Q48EB9
K	-1	MET	-	expression tag	UNP Q48EB9
K	0	SER	-	expression tag	UNP Q48EB9
K	1	LEU	-	expression tag	UNP Q48EB9
K	151	GLN	ARG	engineered	UNP Q48EB9
K	180	GLU	-	expression tag	UNP Q48EB9
K	181	GLY	-	expression tag	UNP Q48EB9
K	182	HIS	-	expression tag	UNP Q48EB9
K	183	HIS	-	expression tag	UNP Q48EB9
K	184	HIS	-	expression tag	UNP Q48EB9
K	185	HIS	-	expression tag	UNP Q48EB9
K	186	HIS	-	expression tag	UNP Q48EB9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	187	HIS	-	expression tag	UNP Q48EB9
L	-1	MET	-	expression tag	UNP Q48EB9
L	0	SER	-	expression tag	UNP Q48EB9
L	1	LEU	-	expression tag	UNP Q48EB9
L	151	GLN	ARG	engineered	UNP Q48EB9
L	180	GLU	-	expression tag	UNP Q48EB9
L	181	GLY	-	expression tag	UNP Q48EB9
L	182	HIS	-	expression tag	UNP Q48EB9
L	183	HIS	-	expression tag	UNP Q48EB9
L	184	HIS	-	expression tag	UNP Q48EB9
L	185	HIS	-	expression tag	UNP Q48EB9
L	186	HIS	-	expression tag	UNP Q48EB9
L	187	HIS	-	expression tag	UNP Q48EB9

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	K	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is water.

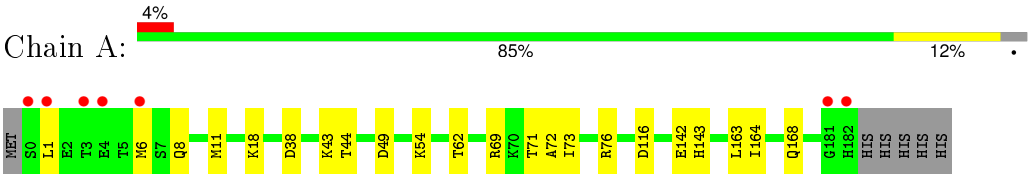
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	163	Total O 166 166	0	3
3	B	112	Total O 113 113	0	1
3	C	132	Total O 134 134	0	2
3	D	150	Total O 152 152	0	2
3	E	107	Total O 108 108	0	1
3	F	121	Total O 122 122	0	1
3	G	121	Total O 121 121	0	0
3	H	140	Total O 140 140	0	0
3	I	116	Total O 116 116	0	0
3	J	96	Total O 96 96	0	0
3	K	75	Total O 75 75	0	0
3	L	114	Total O 114 114	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

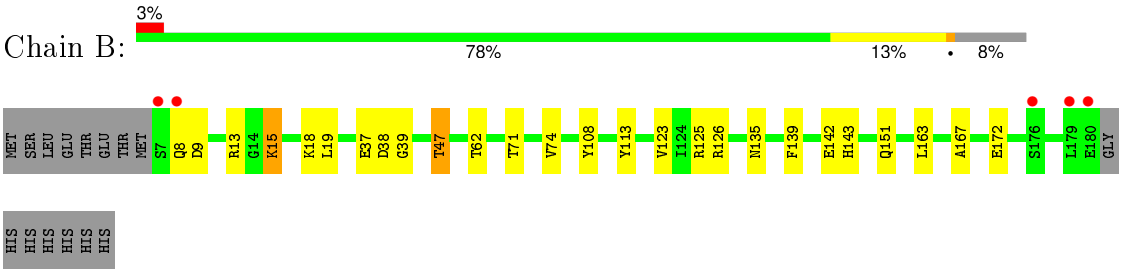
- Molecule 1: probable yrbi family phosphatase

Chain A:



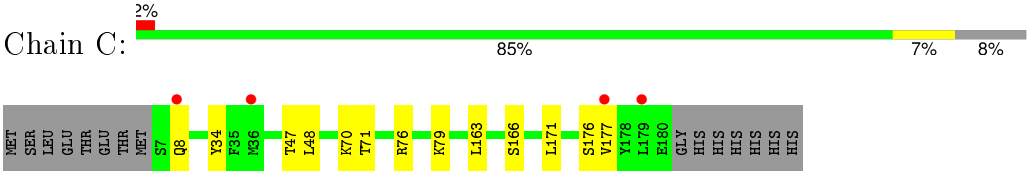
- Molecule 1: probable yrbi family phosphatase

Chain B:



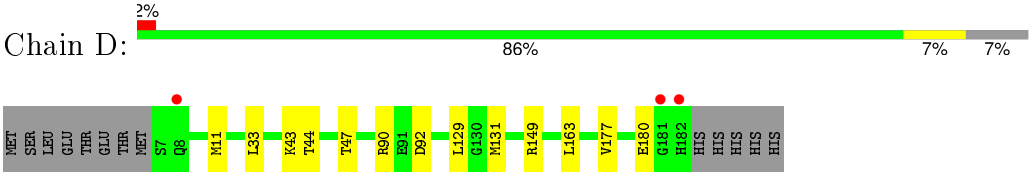
- Molecule 1: probable yrbi family phosphatase

Chain C:



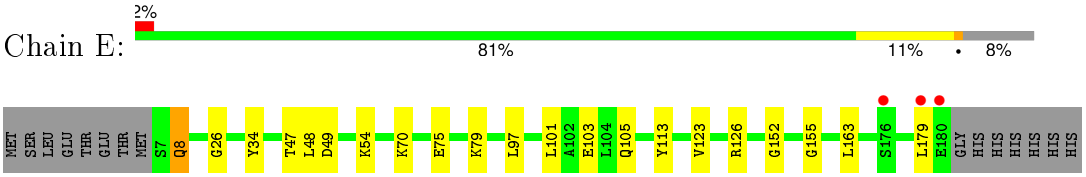
- Molecule 1: probable yrbi family phosphatase

Chain D:



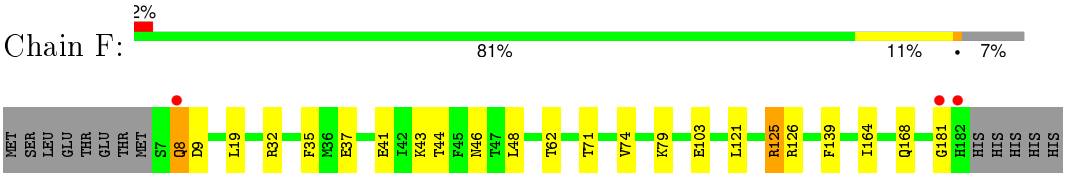
- Molecule 1: probable yrbi family phosphatase

Chain E:



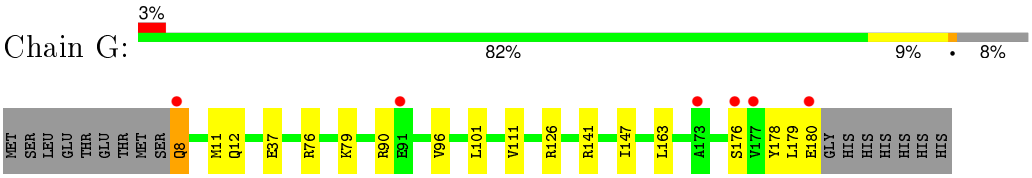
- Molecule 1: probable yrbi family phosphatase

Chain F:



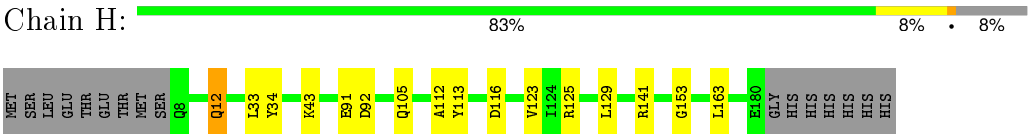
- Molecule 1: probable yrbi family phosphatase

Chain G:



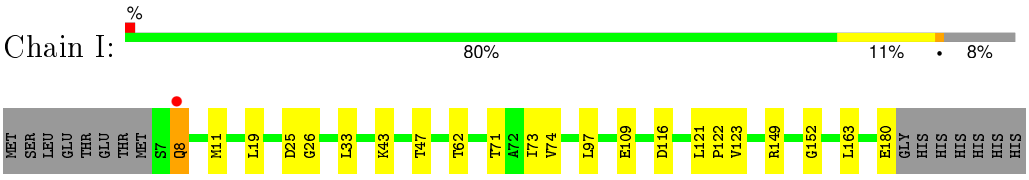
- Molecule 1: probable yrbi family phosphatase

Chain H:



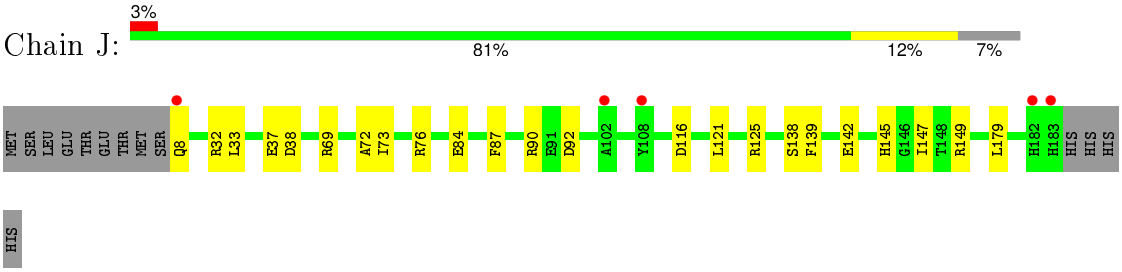
- Molecule 1: probable yrbi family phosphatase

Chain I:



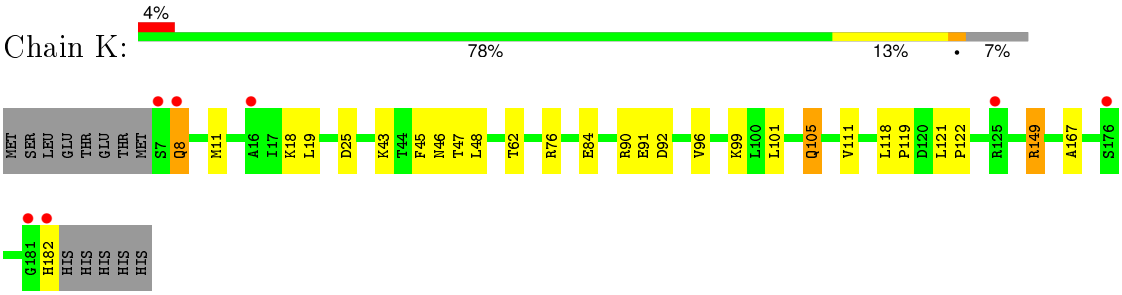
- Molecule 1: probable yrbi family phosphatase

Chain J:



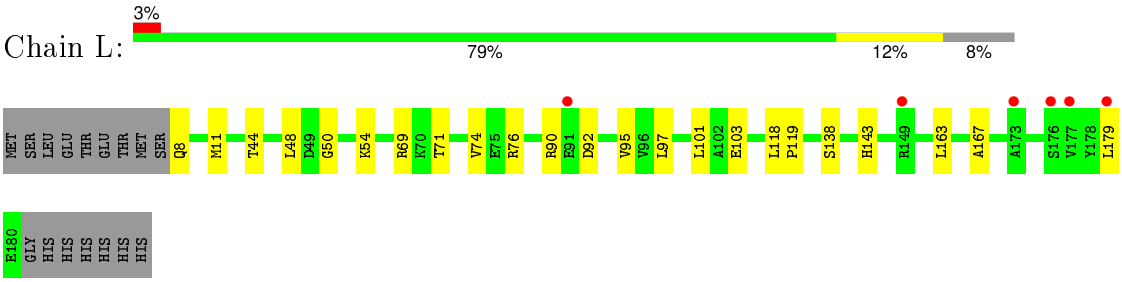
- Molecule 1: probable yrbi family phosphatase

Chain K:



- Molecule 1: probable yrbi family phosphatase

Chain L:


3%
79%
12%
8%
MET SER LEU GLU THR GLU THR MET SER Q8 M11 T44 L48 D49 G50 K54 R69 K70 T71 V74 E75 R76 R90 E91 D92 V95 V96 L97 L101 A102 E103 L118 P119 S138 H143 R149 L163 A167 A173 S176 V177 Y178 L179
E180 GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.97Å 127.02Å 107.42Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 39.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.80) 99.5 (39.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.222 0.177 , 0.222	Depositor DCC
R_{free} test set	5717 reflections (3.12%)	DCC
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 189188 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17767	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/1458	0.58	1/1960 (0.1%)
1	B	0.39	0/1388	0.53	0/1866
1	C	0.53	0/1383	0.57	0/1860
1	D	0.47	0/1394	0.55	0/1875
1	E	0.42	0/1351	0.53	0/1818
1	F	0.47	0/1380	0.55	0/1856
1	G	0.38	0/1395	0.51	0/1874
1	H	0.51	0/1380	0.58	0/1856
1	I	0.39	0/1375	0.51	0/1849
1	J	0.37	0/1397	0.50	0/1877
1	K	0.34	0/1378	0.46	0/1853
1	L	0.39	0/1400	0.52	0/1882
All	All	0.43	0/16679	0.53	1/22426 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	ASP	CB-CG-OD1	5.34	123.11	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1421	0	1467	22	0
1	B	1355	0	1392	23	0
1	C	1350	0	1390	11	0
1	D	1360	0	1396	19	0
1	E	1330	0	1356	16	0
1	F	1352	0	1380	28	0
1	G	1356	0	1399	25	0
1	H	1347	0	1381	11	0
1	I	1345	0	1380	27	0
1	J	1368	0	1397	24	0
1	K	1353	0	1380	31	0
1	L	1361	0	1400	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	166	0	0	3	0
3	B	113	0	0	3	0
3	C	134	0	0	3	0
3	D	152	0	0	6	0
3	E	108	0	0	3	0
3	F	122	0	0	2	0
3	G	121	0	0	3	0
3	H	140	0	0	1	0
3	I	116	0	0	6	0
3	J	96	0	0	5	0
3	K	75	0	0	5	0
3	L	114	0	0	9	0
All	All	17767	0	16718	230	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 7.

All (230) 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:125:ARG:HH11	1:F:125:ARG:HG3	1.08	1.13
1:F:126:ARG:HH22	1:G:180:GLU:HG3	1.18	1.08
1:I:11:MET:CE	1:I:163:LEU:HD22	1.85	1.05
1:I:47[B]:THR:HG22	3:I:922:HOH:O	1.52	1.05
1:K:105:GLN:HA	1:K:105:GLN:HE21	1.23	1.02
1:F:125:ARG:HH11	1:F:125:ARG:CG	1.72	1.01
1:I:11:MET:HE1	1:I:163:LEU:HD22	1.44	0.98
1:G:37:GLU:HG3	3:G:531:HOH:O	1.65	0.97
1:A:6:MET:CE	1:A:11:MET:HG2	1.96	0.93
1:A:6:MET:HE3	1:A:11:MET:HG2	1.48	0.92
1:L:11[A]:MET:CE	1:L:163:LEU:HD12	2.03	0.88
1:L:11[A]:MET:HE3	1:L:163:LEU:HD12	1.55	0.88
1:L:143:HIS:HD2	3:L:826:HOH:O	1.56	0.88
1:F:125:ARG:HG3	1:F:125:ARG:NH1	1.86	0.87
1:F:126:ARG:NH2	1:G:180:GLU:HG3	1.92	0.84
3:D:426:HOH:O	1:H:125:ARG:HD3	1.77	0.82
1:I:11:MET:CE	1:I:163:LEU:CD2	2.58	0.81
1:E:8:GLN:OE1	1:E:8:GLN:O	1.99	0.79
1:K:84[A]:GLU:HG3	3:K:978:HOH:O	1.83	0.79
1:K:105:GLN:CA	1:K:105:GLN:HE21	1.96	0.78
1:G:180:GLU:HG2	3:G:1169:HOH:O	1.84	0.78
1:J:121:LEU:O	1:J:125[B]:ARG:HG3	1.83	0.78
1:G:11[A]:MET:HA	1:G:11[A]:MET:HE2	1.67	0.77
1:K:47[B]:THR:CG2	3:L:1460:HOH:O	2.33	0.77
1:I:11:MET:HE3	1:I:163:LEU:CD2	2.15	0.76
1:E:126:ARG:HH22	1:F:181:GLY:HA2	1.49	0.76
1:A:43[A]:LYS:HB2	1:A:73:ILE:HG21	1.69	0.74
1:E:126:ARG:NH2	1:F:181:GLY:HA2	2.03	0.74
1:D:11[A]:MET:CE	1:D:163[A]:LEU:HD12	2.17	0.74
1:I:43[A]:LYS:HE3	3:I:451:HOH:O	1.89	0.72
1:A:72:ALA:O	1:A:76:ARG:HG3	1.90	0.72
1:J:87:PHE:HB3	1:J:90[B]:ARG:HD2	1.72	0.71
1:F:126:ARG:HH22	1:G:180:GLU:CG	2.02	0.71
1:F:8:GLN:HG2	1:F:9:ASP:N	2.06	0.69
1:K:47[B]:THR:HG23	3:L:1460:HOH:O	1.92	0.68
1:F:125:ARG:NH1	1:F:125:ARG:CG	2.44	0.67
1:G:11[A]:MET:HE1	1:G:163:LEU:HD12	1.74	0.67
1:B:142[A]:GLU:HG3	1:B:143:HIS:ND1	2.10	0.66
1:L:138:SER:HB2	3:L:585:HOH:O	1.95	0.66
1:A:6:MET:HE2	1:A:11:MET:HG2	1.77	0.66
1:G:180:GLU:OE1	1:G:180:GLU:HA	1.97	0.65
1:I:11:MET:HE3	1:I:163:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:HG2	3:D:1392:HOH:O	1.95	0.65
1:K:99:LYS:HB2	1:K:99:LYS:NZ	2.12	0.64
1:I:47[B]:THR:HG21	3:I:929:HOH:O	1.98	0.64
1:J:87:PHE:HB3	1:J:90[B]:ARG:CD	2.28	0.64
1:A:54[B]:LYS:HB2	1:A:54[B]:LYS:HZ2	1.62	0.63
1:A:54[B]:LYS:HB2	1:A:54[B]:LYS:NZ	2.13	0.63
1:D:11[A]:MET:HE1	1:D:163[A]:LEU:HD12	1.81	0.62
1:A:54[B]:LYS:CB	1:A:54[B]:LYS:NZ	2.62	0.62
1:J:32:ARG:NH2	3:J:1536:HOH:O	2.32	0.62
1:G:126:ARG:HH22	1:I:180:GLU:C	2.03	0.62
1:L:8:GLN:OE1	1:L:8:GLN:N	2.34	0.61
1:F:125:ARG:HH11	1:F:125:ARG:CB	2.14	0.61
1:F:139:PHE:HZ	1:G:179:LEU:HD11	1.65	0.61
1:B:47[B]:THR:HG21	3:B:1101:HOH:O	2.00	0.60
1:B:163:LEU:HD23	1:B:163:LEU:C	2.22	0.60
1:A:38:ASP:O	1:K:149:ARG:NH2	2.35	0.60
1:J:69:ARG:HD2	3:J:1542:HOH:O	2.02	0.60
1:J:139:PHE:O	1:J:142[A]:GLU:HG2	2.03	0.59
1:K:47[B]:THR:HG21	3:L:1460:HOH:O	1.98	0.59
1:B:139:PHE:O	1:B:142[A]:GLU:HG2	2.03	0.59
1:D:43:LYS:HG3	3:D:286[B]:HOH:O	2.01	0.59
1:I:109:GLU:CD	1:I:109:GLU:H	2.06	0.58
1:D:11[A]:MET:HE3	1:D:163[A]:LEU:HD12	1.86	0.58
1:I:47[B]:THR:CG2	3:I:929:HOH:O	2.51	0.58
1:B:142[A]:GLU:HG3	1:B:143:HIS:CE1	2.39	0.57
1:J:37:GLU:O	1:L:76:ARG:NH2	2.37	0.57
1:D:149:ARG:NH1	3:E:1614:HOH:O	2.37	0.57
3:A:1426:HOH:O	1:E:70:LYS:HE2	2.04	0.57
1:K:43[B]:LYS:HE3	3:K:665:HOH:O	2.06	0.56
1:A:8:GLN:OE1	1:A:8:GLN:HA	2.05	0.56
1:B:108:TYR:CE2	1:B:126[A]:ARG:HD2	2.41	0.56
1:D:177:VAL:O	1:D:180:GLU:HG2	2.04	0.56
1:K:105:GLN:NE2	1:K:105:GLN:HA	2.07	0.55
1:B:19:LEU:CD1	1:B:62:THR:HG23	2.36	0.55
1:H:163:LEU:C	1:H:163:LEU:HD23	2.26	0.55
1:E:79:LYS:CE	3:E:342:HOH:O	2.54	0.55
1:G:11[A]:MET:CE	1:G:11[A]:MET:HA	2.35	0.55
1:K:46:ASN:OD1	1:K:48:LEU:HB2	2.06	0.55
1:F:121:LEU:O	1:F:125:ARG:HG2	2.07	0.55
1:J:84:GLU:HG3	3:J:407:HOH:O	2.06	0.55
1:F:32:ARG:NH1	3:F:1517:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47[B]:THR:CG2	3:B:1101:HOH:O	2.54	0.54
1:K:90:ARG:CZ	1:K:96:VAL:CG2	2.85	0.54
1:G:11[A]:MET:CE	1:G:163:LEU:CD1	2.86	0.54
1:J:142[B]:GLU:HG3	3:J:402:HOH:O	2.08	0.54
1:L:69:ARG:HD2	3:L:1446:HOH:O	2.07	0.54
1:I:163:LEU:HD13	1:I:163:LEU:C	2.28	0.54
1:D:92:ASP:OD1	1:D:92:ASP:N	2.35	0.54
1:B:19:LEU:HD13	1:B:62:THR:HG23	1.89	0.53
1:I:71:THR:HG23	1:I:74:VAL:H	1.73	0.53
1:I:47[B]:THR:CG2	3:I:922:HOH:O	2.30	0.53
1:G:11[A]:MET:CE	1:G:163:LEU:HD12	2.39	0.53
1:F:125:ARG:CB	1:F:125:ARG:NH1	2.72	0.53
1:A:69:ARG:HD2	3:A:988:HOH:O	2.08	0.53
1:E:47[A]:THR:HG23	1:E:48:LEU:N	2.24	0.52
1:E:54:LYS:HB3	1:E:54:LYS:NZ	2.25	0.52
1:J:125[B]:ARG:NE	1:L:179:LEU:HD12	2.25	0.52
1:D:11[B]:MET:HG2	3:D:1477:HOH:O	2.09	0.52
1:G:141:ARG:HG2	1:G:147:ILE:HD12	1.91	0.52
1:F:37:GLU:O	1:G:76:ARG:NH2	2.40	0.52
1:K:90:ARG:NH1	1:K:96:VAL:HG22	2.26	0.51
1:K:25:ASP:OD1	1:K:43[A]:LYS:NZ	2.41	0.51
1:F:71:THR:HG23	1:F:74:VAL:H	1.76	0.51
1:F:19:LEU:HD13	1:F:62[B]:THR:HG23	1.92	0.50
1:K:43[B]:LYS:CE	3:K:671:HOH:O	2.60	0.50
1:B:37:GLU:HG3	1:J:73:ILE:HG13	1.93	0.50
1:K:18:LYS:O	1:K:62:THR:HG22	2.11	0.50
1:L:143:HIS:CD2	3:L:826:HOH:O	2.42	0.50
1:G:11[A]:MET:HE1	1:G:163:LEU:CD1	2.38	0.50
1:L:8:GLN:NE2	3:L:1054:HOH:O	2.45	0.50
1:K:76:ARG:NH1	3:K:714:HOH:O	2.37	0.50
1:K:11:MET:HE1	1:K:167:ALA:HB2	1.95	0.49
1:B:9:ASP:O	1:B:13:ARG:HG3	2.12	0.49
1:L:11[A]:MET:CE	1:L:163:LEU:CD1	2.83	0.49
1:E:8:GLN:C	1:E:8:GLN:OE1	2.50	0.49
1:C:76[B]:ARG:HH21	1:J:149:ARG:HA	1.78	0.49
1:K:105:GLN:NE2	1:K:105:GLN:CA	2.70	0.49
1:E:75:GLU:O	1:E:79:LYS:HG2	2.13	0.49
1:B:39:GLY:HA2	3:B:877:HOH:O	2.12	0.49
1:K:43[A]:LYS:HD2	1:K:45:PHE:CZ	2.48	0.48
1:D:11[A]:MET:HE3	1:D:163[A]:LEU:CD1	2.43	0.48
1:F:79:LYS:HE3	1:H:141:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:HE2	1:J:145:HIS:O	2.14	0.48
1:J:92:ASP:N	1:J:92:ASP:OD1	2.47	0.48
1:A:6:MET:HE2	1:A:11:MET:CG	2.42	0.48
1:D:131:MET:SD	1:D:163[A]:LEU:CD2	3.01	0.48
1:B:135:ASN:ND2	1:B:151:GLN:OE1	2.47	0.48
1:F:37:GLU:O	1:G:76:ARG:NH1	2.46	0.48
1:I:71:THR:CG2	1:I:74:VAL:HG23	2.43	0.47
1:K:91:GLU:OE1	1:K:91:GLU:HA	2.15	0.47
1:D:149:ARG:HD3	3:D:1611:HOH:O	2.14	0.47
1:F:19:LEU:CD1	1:F:62[B]:THR:HG23	2.44	0.47
1:I:25:ASP:OD1	1:I:43[A]:LYS:NZ	2.47	0.47
1:G:8:GLN:OE1	1:G:12:GLN:HB2	2.15	0.47
1:C:163:LEU:C	1:C:163:LEU:HD23	2.35	0.47
3:C:1540:HOH:O	1:J:147:ILE:CD1	2.62	0.47
1:J:121:LEU:HG	1:J:125[B]:ARG:HD2	1.97	0.46
1:G:11[A]:MET:HE3	1:G:163:LEU:HD11	1.97	0.46
3:C:1540:HOH:O	1:J:147:ILE:HD13	2.15	0.46
1:D:90:ARG:NH2	1:D:92:ASP:OD2	2.37	0.46
1:F:35:PHE:CE1	1:F:41:GLU:HG2	2.50	0.46
1:K:90:ARG:NH2	1:K:92:ASP:OD2	2.38	0.46
1:A:164:ILE:O	1:A:168:GLN:HG3	2.16	0.46
1:C:47[A]:THR:HG23	1:C:48:LEU:N	2.31	0.46
3:J:1500:HOH:O	1:L:48:LEU:HD13	2.16	0.45
1:I:149:ARG:HD2	3:I:1244:HOH:O	2.16	0.45
1:L:71:THR:HG23	1:L:74:VAL:HG23	1.97	0.45
1:E:113:TYR:CD1	1:E:123:VAL:HG11	2.51	0.45
1:A:6:MET:HE2	1:A:6:MET:HB3	1.68	0.45
1:E:47[B]:THR:HG22	1:I:33:LEU:HD11	1.97	0.45
1:A:6:MET:CE	1:A:11:MET:CG	2.82	0.45
1:C:70:LYS:HE3	1:J:138:SER:HB2	1.98	0.45
1:F:43:LYS:HG3	3:F:746[B]:HOH:O	2.16	0.45
1:C:166[B]:SER:OG	1:C:171:LEU:HD22	2.16	0.45
1:K:43[B]:LYS:HG2	3:K:193:HOH:O	2.17	0.45
1:D:47[B]:THR:HG21	3:D:808:HOH:O	2.16	0.45
1:B:113:TYR:CD1	1:B:123:VAL:HG11	2.52	0.45
1:C:47[A]:THR:HG21	3:C:1057:HOH:O	2.16	0.45
1:B:37:GLU:HA	1:J:73:ILE:HG12	1.99	0.45
1:K:182:HIS:HD2	1:L:95:VAL:HG23	1.82	0.45
1:K:101:LEU:HD21	1:K:111:VAL:HG21	1.99	0.45
1:B:15:LYS:HD3	1:B:167:ALA:O	2.16	0.44
1:E:26:GLY:O	1:E:152:GLY:HA3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90[A]:ARG:HD2	1:L:90[A]:ARG:HA	1.76	0.44
1:F:46:ASN:OD1	1:F:48:LEU:HB2	2.17	0.44
1:G:79:LYS:HG2	3:G:1192:HOH:O	2.15	0.44
1:I:97:LEU:HD22	1:I:123:VAL:HG13	1.99	0.44
1:G:176:SER:C	1:G:178:TYR:N	2.71	0.44
1:L:97:LEU:O	1:L:101:LEU:HG	2.18	0.44
1:K:99:LYS:HB2	1:K:99:LYS:HZ3	1.82	0.44
1:A:76:ARG:NH1	3:A:1575:HOH:O	2.51	0.43
1:H:12:GLN:HE21	1:H:12:GLN:HA	1.83	0.43
1:A:1:LEU:N	1:A:1:LEU:HD23	2.33	0.43
1:A:6:MET:SD	1:A:163:LEU:HD23	2.59	0.43
1:E:97:LEU:O	1:E:101:LEU:HG	2.19	0.43
1:G:8:GLN:HB2	1:G:11[B]:MET:HE3	2.01	0.43
1:I:26:GLY:O	1:I:152:GLY:HA3	2.18	0.43
1:A:18:LYS:O	1:A:62[A]:THR:HG22	2.19	0.43
1:H:153:GLY:HA2	3:H:459:HOH:O	2.18	0.43
1:J:33:LEU:O	1:L:44:THR:HA	2.19	0.43
1:L:118:LEU:N	1:L:119:PRO:CD	2.82	0.43
1:G:90:ARG:HG3	1:G:96:VAL:HG21	2.00	0.43
1:A:54[A]:LYS:HG2	1:L:8:GLN:NE2	2.33	0.42
1:K:8:GLN:C	1:K:8:GLN:NE2	2.73	0.42
1:I:19:LEU:CD1	1:I:62:THR:HG23	2.49	0.42
1:B:18:LYS:O	1:B:62:THR:HG22	2.19	0.42
1:D:44:THR:HG22	1:H:34:TYR:CD1	2.55	0.42
1:B:163:LEU:HD23	1:B:163:LEU:O	2.19	0.42
1:K:25:ASP:OD1	1:K:43[B]:LYS:NZ	2.51	0.42
1:C:176:SER:O	1:C:177:VAL:C	2.56	0.42
1:H:112:ALA:HA	1:H:129:LEU:O	2.20	0.42
1:F:164:ILE:O	1:F:168:GLN:HG3	2.20	0.42
1:K:118:LEU:N	1:K:119:PRO:CD	2.81	0.42
1:I:43[B]:LYS:HB2	1:I:43[B]:LYS:HE2	1.85	0.42
1:B:71:THR:HG23	1:B:74:VAL:H	1.83	0.42
1:B:38:ASP:OD2	1:B:39:GLY:N	2.53	0.42
1:D:44:THR:HA	1:H:33:LEU:O	2.20	0.42
1:H:113:TYR:CD1	1:H:123:VAL:HG11	2.55	0.42
1:B:139:PHE:HA	1:B:142[A]:GLU:OE1	2.20	0.42
1:E:34:TYR:CD1	1:F:44:THR:HG22	2.54	0.42
1:K:121:LEU:N	1:K:122:PRO:CD	2.83	0.42
1:D:129:LEU:HD21	1:D:163[B]:LEU:HD12	2.01	0.41
1:F:35:PHE:CD1	1:F:41:GLU:HG2	2.55	0.41
1:I:163:LEU:HD13	1:I:163:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47[B]:THR:CG2	1:D:33:LEU:HD11	2.50	0.41
1:C:47[B]:THR:HG22	1:D:33:LEU:HD11	2.02	0.41
1:I:19:LEU:HD12	1:I:62:THR:HG23	2.01	0.41
1:B:125:ARG:HD2	1:J:179:LEU:CD1	2.50	0.41
1:J:72:ALA:O	1:J:76:ARG:HG3	2.21	0.41
1:I:8:GLN:HE21	1:I:8:GLN:HB2	1.63	0.41
1:G:11[A]:MET:HE3	1:G:163:LEU:CD1	2.50	0.41
1:L:11[A]:MET:HE1	1:L:167:ALA:HB2	2.01	0.41
1:K:19:LEU:CD1	1:K:62:THR:HG23	2.50	0.41
1:A:142:GLU:HG3	1:A:143:HIS:ND1	2.36	0.41
1:B:37:GLU:HA	1:J:73:ILE:CG1	2.51	0.41
1:L:50:GLY:O	1:L:54:LYS:HE2	2.21	0.41
1:F:71:THR:CG2	1:F:74:VAL:HG23	2.50	0.41
1:L:54:LYS:HE3	3:L:1525:HOH:O	2.21	0.41
1:A:44:THR:HG22	1:C:34:TYR:CD1	2.55	0.41
1:H:43:LYS:HE2	1:H:43:LYS:HB2	1.84	0.40
1:E:49:ASP:OD1	1:E:155:GLY:HA2	2.21	0.40
1:J:38:ASP:OD1	1:J:38:ASP:C	2.60	0.40
1:I:121:LEU:N	1:I:122:PRO:CD	2.84	0.40
1:I:43[A]:LYS:HB2	1:I:73:ILE:HG21	2.02	0.40
1:G:101:LEU:HD21	1:G:111:VAL:HG21	2.04	0.40
1:E:103:GLU:HG3	3:E:972:HOH:O	2.21	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	A	188/189 (100%)	185 (98%)	3 (2%)	0	100	100
1	B	178/189 (94%)	174 (98%)	4 (2%)	0	100	100
1	C	178/189 (94%)	175 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	180/189 (95%)	176 (98%)	4 (2%)	0	100	100
1	E	174/189 (92%)	170 (98%)	4 (2%)	0	100	100
1	F	178/189 (94%)	175 (98%)	3 (2%)	0	100	100
1	G	179/189 (95%)	174 (97%)	5 (3%)	0	100	100
1	H	177/189 (94%)	174 (98%)	3 (2%)	0	100	100
1	I	177/189 (94%)	172 (97%)	5 (3%)	0	100	100
1	J	178/189 (94%)	176 (99%)	2 (1%)	0	100	100
1	K	177/189 (94%)	172 (97%)	5 (3%)	0	100	100
1	L	179/189 (95%)	175 (98%)	4 (2%)	0	100	100
All	All	2143/2268 (94%)	2098 (98%)	45 (2%)	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	A	151/150 (101%)	149 (99%)	2 (1%)	76	68
1	B	142/150 (95%)	137 (96%)	5 (4%)	43	25
1	C	142/150 (95%)	140 (99%)	2 (1%)	74	65
1	D	143/150 (95%)	143 (100%)	0	100	100
1	E	138/150 (92%)	134 (97%)	4 (3%)	50	34
1	F	141/150 (94%)	138 (98%)	3 (2%)	61	47
1	G	143/150 (95%)	142 (99%)	1 (1%)	88	86
1	H	141/150 (94%)	137 (97%)	4 (3%)	51	35
1	I	141/150 (94%)	139 (99%)	2 (1%)	74	65
1	J	141/150 (94%)	139 (99%)	2 (1%)	74	65
1	K	140/150 (93%)	137 (98%)	3 (2%)	61	47
1	L	143/150 (95%)	141 (99%)	2 (1%)	74	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1706/1800 (95%)	1676 (98%)	30 (2%)	68 54

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

Mol	Chain	Res	Type
1	A	71	THR
1	A	116	ASP
1	B	8	GLN
1	B	15	LYS
1	B	47[A]	THR
1	B	47[B]	THR
1	B	172	GLU
1	C	8	GLN
1	C	71	THR
1	E	8	GLN
1	E	105	GLN
1	E	163	LEU
1	E	179	LEU
1	F	8	GLN
1	F	103	GLU
1	F	125	ARG
1	G	8	GLN
1	H	12	GLN
1	H	91	GLU
1	H	105	GLN
1	H	116	ASP
1	I	8	GLN
1	I	116	ASP
1	J	8	GLN
1	J	116	ASP
1	K	8	GLN
1	K	105	GLN
1	K	149	ARG
1	L	103[A]	GLU
1	L	103[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	8	GLN

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Mol	Chain	Res	Type
1	B	135	ASN
1	B	151	GLN
1	B	170	ASN
1	C	8	GLN
1	C	151	GLN
1	D	105	GLN
1	E	105	GLN
1	G	143	HIS
1	H	12	GLN
1	H	143	HIS
1	I	8	GLN
1	J	51	GLN
1	K	8	GLN
1	K	105	GLN
1	K	151	GLN
1	K	182	HIS
1	L	8	GLN
1	L	12	GLN
1	L	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	183/189 (96%)	-0.27	7 (3%)	44	38	16, 26, 52, 71	0
1	B	174/189 (92%)	-0.20	5 (2%)	55	49	22, 30, 55, 78	0
1	C	174/189 (92%)	-0.37	4 (2%)	64	59	15, 26, 49, 71	0
1	D	176/189 (93%)	-0.34	3 (1%)	73	69	16, 25, 47, 72	0
1	E	174/189 (92%)	-0.30	3 (1%)	73	69	21, 30, 54, 85	0
1	F	176/189 (93%)	-0.32	3 (1%)	73	69	18, 28, 51, 81	0
1	G	173/189 (91%)	-0.28	6 (3%)	48	42	21, 31, 54, 85	0
1	H	173/189 (91%)	-0.46	0	100	100	15, 25, 41, 67	0
1	I	174/189 (92%)	-0.35	1 (0%)	90	88	20, 30, 51, 75	0
1	J	176/189 (93%)	-0.06	5 (2%)	56	51	22, 36, 62, 91	0
1	K	176/189 (93%)	0.10	7 (3%)	42	36	26, 41, 69, 87	0
1	L	173/189 (91%)	-0.21	6 (3%)	48	42	21, 31, 53, 81	0
All	All	2102/2268 (92%)	-0.25	50 (2%)	62	57	15, 30, 56, 91	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	GLN	4.7
1	L	179	LEU	4.1
1	J	108	TYR	3.9
1	A	182	HIS	3.9
1	J	183	HIS	3.8
1	D	8	GLN	3.7
1	K	7	SER	3.7
1	E	179	LEU	3.5
1	L	176	SER	3.4
1	A	0	SER	3.3
1	A	3	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	8	GLN	3.2
1	F	182	HIS	3.2
1	G	177	VAL	3.1
1	L	177	VAL	3.1
1	B	179	LEU	3.1
1	D	181	GLY	3.1
1	J	182	HIS	3.1
1	C	179	LEU	3.0
1	E	180	GLU	2.9
1	B	180	GLU	2.8
1	K	182	HIS	2.8
1	F	8	GLN	2.8
1	C	36	MET	2.7
1	G	176	SER	2.7
1	B	7	SER	2.6
1	A	181	GLY	2.5
1	F	181	GLY	2.5
1	K	181	GLY	2.5
1	C	177	VAL	2.5
1	J	8	GLN	2.4
1	G	180	GLU	2.4
1	K	176	SER	2.4
1	D	182	HIS	2.4
1	A	4	GLU	2.4
1	A	6	MET	2.3
1	K	125	ARG	2.3
1	B	176	SER	2.2
1	K	16	ALA	2.2
1	L	149[A]	ARG	2.2
1	J	102	ALA	2.1
1	A	1	LEU	2.1
1	G	91	GLU	2.1
1	E	176	SER	2.1
1	I	8	GLN	2.1
1	L	91	GLU	2.1
1	L	173	ALA	2.1
1	B	8	GLN	2.0
1	C	8	GLN	2.0
1	G	173	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	G	188	1/1	1.00	0.08	0.06	37,37,37,37	0
2	CL	L	188	1/1	0.99	0.08	-0.26	41,41,41,41	0
2	CL	K	188	1/1	0.99	0.07	-0.64	46,46,46,46	0
2	CL	C	188	1/1	0.96	0.07	-1.20	47,47,47,47	0
2	CL	F	188	1/1	0.98	0.06	-1.80	46,46,46,46	0
2	CL	B	188	1/1	0.97	0.07	-1.83	48,48,48,48	0
2	CL	D	188	1/1	0.99	0.04	-2.15	34,34,34,34	0
2	CL	E	188	1/1	0.97	0.05	-2.36	47,47,47,47	0
2	CL	A	188	1/1	0.98	0.04	-3.01	46,46,46,46	0
2	CL	I	188	1/1	1.00	0.04	-3.16	38,38,38,38	0
2	CL	H	188	1/1	0.99	0.03	-3.57	36,36,36,36	0
2	CL	J	188	1/1	0.98	0.05	-4.83	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.