Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:04 AM GMT

PDB ID	:	3NRJ
Title	:	Crystal structure of probable yrbi family phosphatase from pseudomonas syringae pv.phaseolica 1448a complexed with magnesium
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	:	2010-06-30
Resolution	:	1.90 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:

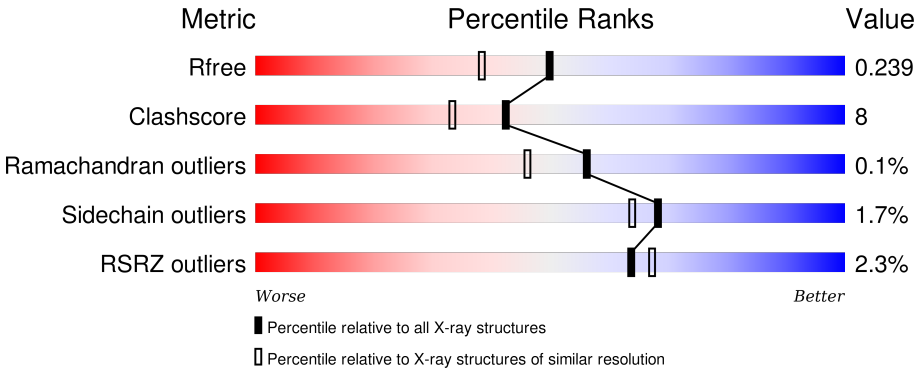
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	2% 75% 18% 7%
1	B	189	3% 79% 11% • 8%
1	C	189	2% 81% 10% 8%
1	D	189	% 80% 10% • 9%
1	E	189	% 82% 9% • 7%

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Mol	Chain	Length	Quality of chain
1	F	189	2% 79% 13% 8%
1	G	189	2% 79% 12% 8%
1	H	189	80% 11% 9%
1	I	189	2% 81% 12% 6%
1	J	189	2% 69% 21% 9%
1	K	189	6% 74% 16% 9%
1	L	189	3% 76% 15% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	F	191	-	-	-	X
4	PO4	D	190	-	-	X	-
4	PO4	H	189	-	-	X	-
4	PO4	I	189	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17050 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	176	Total	C	N	O	S	0	10	0
			1404	884	255	259	6			
1	B	173	Total	C	N	O	S	0	5	0
			1348	849	242	251	6			
1	C	173	Total	C	N	O	S	0	6	0
			1353	852	242	254	5			
1	D	172	Total	C	N	O	S	0	7	0
			1344	849	238	251	6			
1	E	175	Total	C	N	O	S	0	3	0
			1350	849	241	254	6			
1	F	174	Total	C	N	O	S	0	4	0
			1341	845	238	252	6			
1	G	173	Total	C	N	O	S	0	4	0
			1336	842	236	252	6			
1	H	172	Total	C	N	O	S	0	4	0
			1336	843	237	250	6			
1	I	177	Total	C	N	O	S	0	7	0
			1386	872	245	262	7			
1	J	172	Total	C	N	O	S	0	2	0
			1321	831	238	247	5			
1	K	172	Total	C	N	O	S	0	1	0
			1316	829	235	247	5			
1	L	172	Total	C	N	O	S	0	4	0
			1329	838	235	250	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	2	Total Cl 2 2	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	B	2	Total Cl 2 2	0	0
2	C	1	Total Cl 1 1	0	0
2	A	2	Total Cl 2 2	0	0
2	L	1	Total Cl 1 1	0	0
2	F	2	Total Cl 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0

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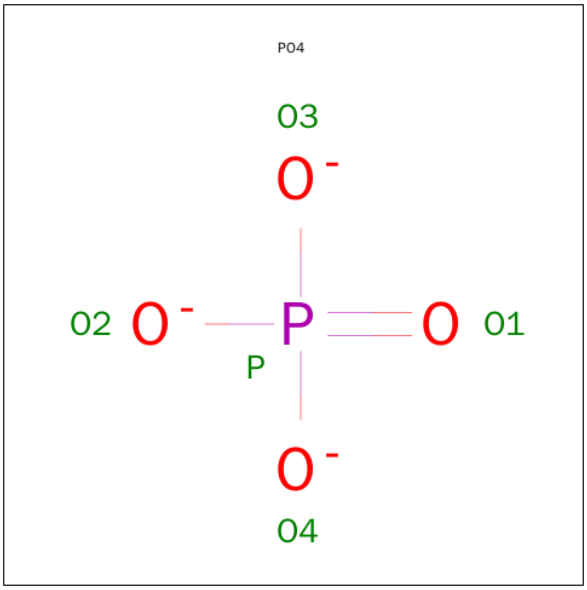
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0
4	K	1	Total O P 5 4 1	0	0
4	L	1	Total O P 5 4 1	0	0

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 4 1 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	92	Total O 92 92	0	0
6	B	52	Total O 52 52	0	0
6	C	82	Total O 82 82	0	0
6	D	85	Total O 86 86	0	1
6	E	65	Total O 65 65	0	0

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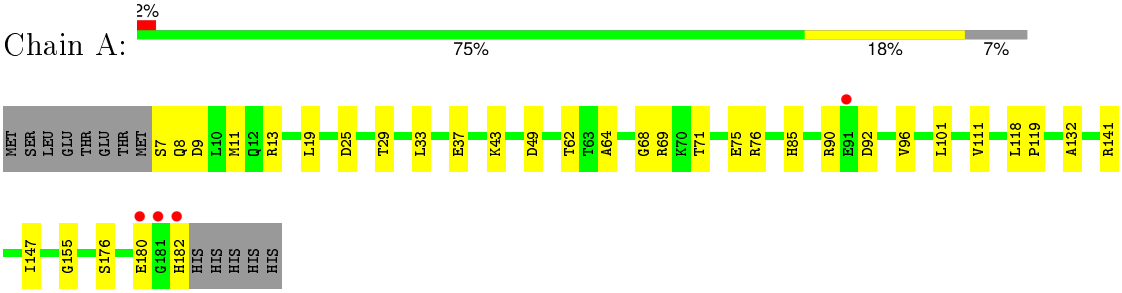
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	80	Total O 80 80	0	0
6	G	68	Total O 68 68	0	0
6	H	75	Total O 76 76	0	1
6	I	59	Total O 59 59	0	1
6	J	43	Total O 43 43	0	0
6	K	37	Total O 37 37	0	0
6	L	57	Total O 57 57	0	0

3 Residue-property plots (i)

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.

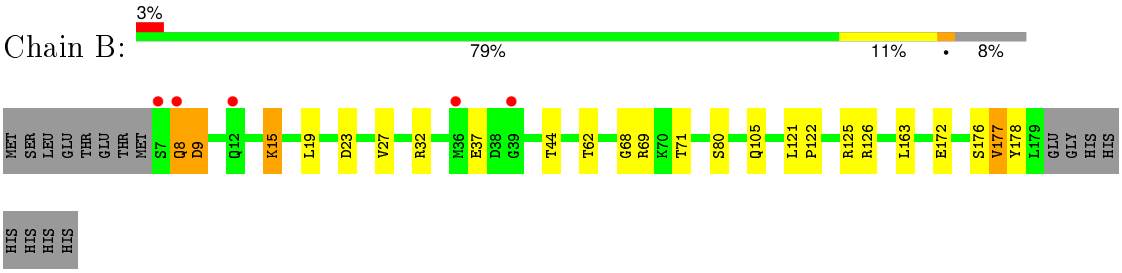
- Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain A:



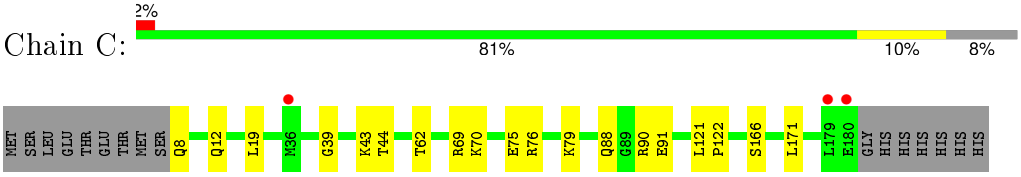
- Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain B:



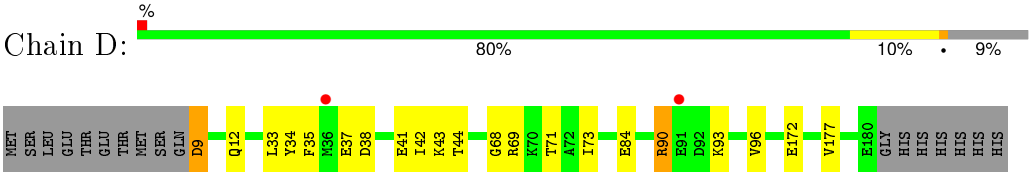
- Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain C:



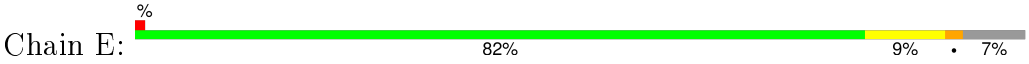
- Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

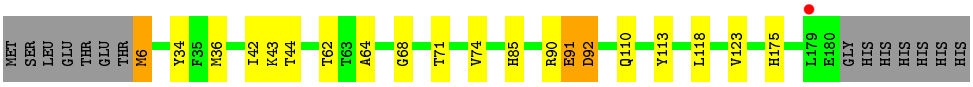
Chain D:



- Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

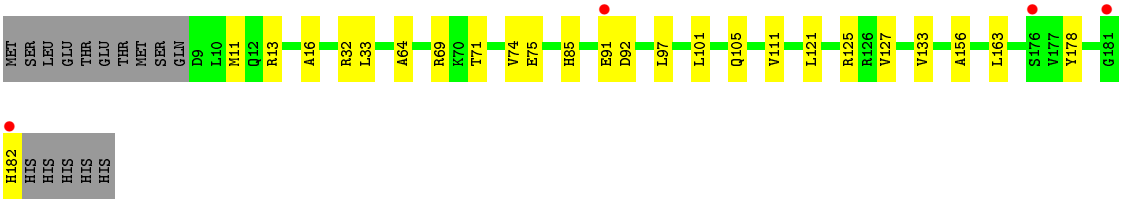
Chain E:





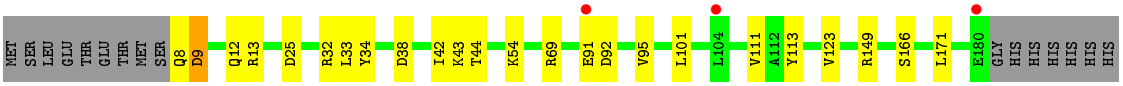
• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain F:



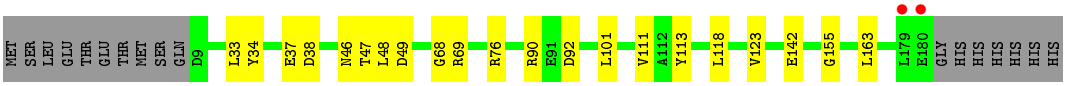
• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain G:



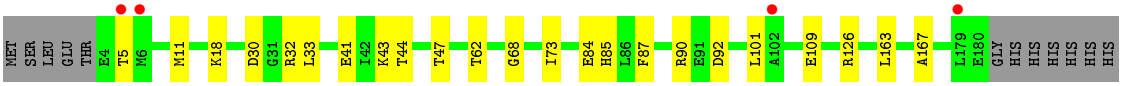
• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain H:



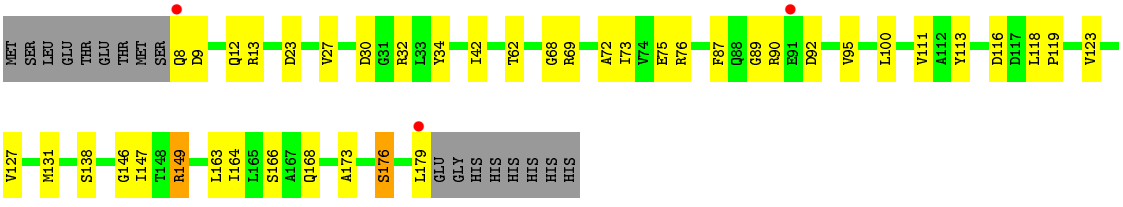
• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain I:



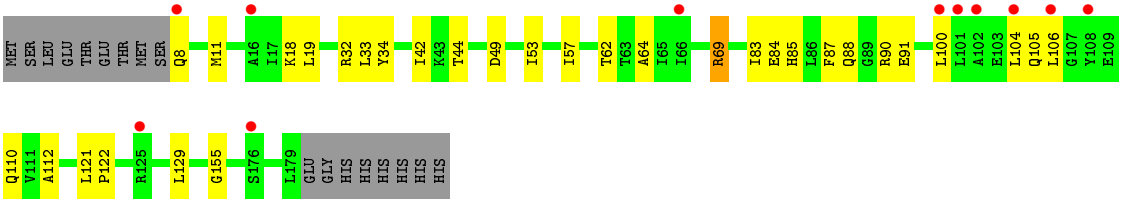
• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain J:

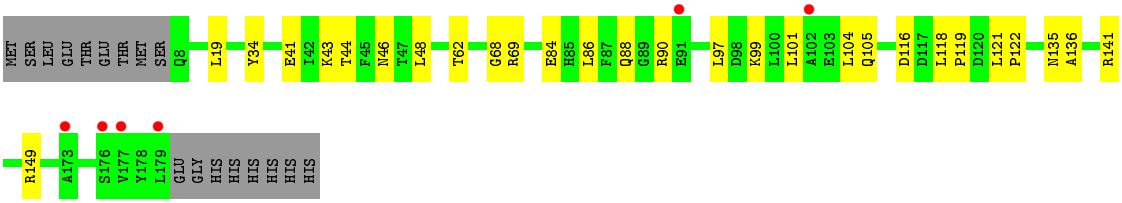


• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE

Chain K:



• Molecule 1: PROBABLE YRBI FAMILY PHOSPHATASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.30Å 126.73Å 106.53Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 43.21 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.00-1.90) 97.0 (43.21-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.179 , 0.240 0.180 , 0.239	Depositor DCC
R_{free} test set	4680 reflections (3.12%)	DCC
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.2	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 158908 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17050	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: PO4, UNL, MG, 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	0.53	0/1450	0.63	0/1945
1	B	0.49	0/1378	0.58	0/1851
1	C	0.56	0/1386	0.62	0/1862
1	D	0.57	0/1380	0.61	0/1853
1	E	0.43	0/1374	0.55	0/1846
1	F	0.48	0/1369	0.59	0/1840
1	G	0.43	0/1363	0.55	0/1832
1	H	0.56	0/1366	0.63	0/1836
1	I	0.42	0/1419	0.54	0/1905
1	J	0.47	0/1342	0.55	0/1804
1	K	0.41	0/1334	0.53	0/1794
1	L	0.41	0/1356	0.54	0/1823
All	All	0.49	0/16517	0.58	0/22191

There are no bond length outliers.

There are no bond angle outliers.

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	1404	0	1462	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1348	0	1390	25	0
1	C	1353	0	1394	19	0
1	D	1344	0	1394	23	0
1	E	1350	0	1384	19	0
1	F	1341	0	1373	20	0
1	G	1336	0	1371	24	0
1	H	1336	0	1378	22	0
1	I	1386	0	1428	30	0
1	J	1321	0	1350	37	0
1	K	1316	0	1346	34	0
1	L	1329	0	1364	23	0
2	A	2	0	0	0	0
2	B	2	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	1	0
2	G	2	0	0	1	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	1	0
4	D	5	0	0	4	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	2	0
4	I	5	0	0	2	0
4	J	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	5	0	0	0	0
4	L	5	0	0	1	0
5	I	4	0	0	0	0
6	A	92	0	0	6	0
6	B	52	0	0	4	0
6	C	82	0	0	0	0
6	D	86	0	0	3	0
6	E	65	0	0	5	0
6	F	80	0	0	3	0
6	G	68	0	0	6	0
6	H	76	0	0	2	0
6	I	59	0	0	8	0
6	J	43	0	0	2	0
6	K	37	0	0	0	0
6	L	57	0	0	3	0
All	All	17050	0	16634	272	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 8.

All (272) 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:E:6:MET:HE2	1:E:6:MET:HA	1.24	1.15
1:I:11[A]:MET:HE3	1:I:163:LEU:HD22	1.31	1.11
2:B:188:CL:CL	1:K:69[B]:ARG:NH1	2.23	1.07
1:E:6:MET:HA	1:E:6:MET:CE	1.85	1.02
1:E:36:MET:HE2	6:F:575:HOH:O	1.59	1.01
1:I:11[A]:MET:CE	1:I:163:LEU:HD22	1.92	1.00
1:F:91:GLU:N	1:F:91:GLU:OE1	1.95	0.98
1:L:19:LEU:CD1	1:L:62:THR:HG23	2.02	0.89
1:L:19:LEU:HD12	1:L:62:THR:HG23	1.53	0.89
1:B:125:ARG:NH1	1:J:179:LEU:HA	1.88	0.88
1:G:69[A]:ARG:HA	6:G:314:HOH:O	1.74	0.87
1:G:69[B]:ARG:HA	6:G:314:HOH:O	1.75	0.87
1:D:38:ASP:O	1:J:149[A]:ARG:HD2	1.78	0.84
1:K:8:GLN:CD	1:K:11:MET:HE3	1.98	0.84
1:B:8:GLN:H	1:B:8:GLN:HE21	1.23	0.82
1:K:19:LEU:HD13	1:K:62:THR:HG23	1.63	0.81
1:E:6:MET:CA	1:E:6:MET:CE	2.60	0.80
1:B:9:ASP:C	1:B:9:ASP:OD2	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:GLN:NE2	1:K:11:MET:HE3	1.97	0.79
1:A:8:GLN:OE1	1:A:8:GLN:HA	1.82	0.79
1:K:8:GLN:NE2	1:K:11:MET:CE	2.46	0.79
1:E:6:MET:HE2	1:E:6:MET:CA	2.11	0.76
1:J:89:GLY:C	1:J:90:ARG:HG2	2.05	0.75
1:D:68:GLY:HA3	4:D:190:PO4:O3	1.86	0.75
1:G:149:ARG:HH21	1:G:149:ARG:HB3	1.52	0.74
1:F:11[A]:MET:HE3	1:F:163:LEU:HD12	1.70	0.74
1:L:43:LYS:HE3	6:L:387:HOH:O	1.88	0.73
1:I:11[A]:MET:CE	1:I:163:LEU:CD2	2.68	0.72
1:E:92:ASP:N	1:E:92:ASP:OD1	2.23	0.72
1:A:29:THR:HG21	1:A:43[B]:LYS:HD3	1.72	0.72
1:J:8:GLN:HG3	1:J:12:GLN:CG	2.21	0.71
1:B:32[A]:ARG:NH1	1:K:32:ARG:HH12	1.88	0.70
1:A:68:GLY:HA3	4:A:191:PO4:O4	1.92	0.70
1:I:84:GLU:HG3	6:I:192:HOH:O	1.90	0.70
1:K:84:GLU:HA	1:K:84:GLU:OE2	1.91	0.70
1:I:11[A]:MET:HE1	1:I:167:ALA:HB2	1.72	0.70
1:K:8:GLN:HE22	1:K:11:MET:CE	2.03	0.70
1:K:8:GLN:HE22	1:K:11:MET:HE2	1.56	0.69
1:I:43[A]:LYS:HB2	1:I:73:ILE:HG21	1.75	0.69
1:A:75:GLU:OE2	1:L:141:ARG:NE	2.26	0.69
1:B:68:GLY:HA3	4:B:191:PO4:O4	1.94	0.67
1:C:70:LYS:HE3	1:J:138:SER:HB2	1.76	0.67
1:E:110:GLN:HG2	6:E:1365:HOH:O	1.93	0.67
1:J:89:GLY:O	1:J:90:ARG:HG2	1.95	0.66
1:J:8:GLN:HG3	1:J:12:GLN:HG2	1.77	0.66
1:H:68:GLY:HA3	4:H:189:PO4:O4	1.96	0.65
1:G:101:LEU:HD21	1:G:111:VAL:HG21	1.78	0.65
1:G:149:ARG:HB3	1:G:149:ARG:NH2	2.12	0.64
1:I:43[B]:LYS:HE2	6:I:1155:HOH:O	1.97	0.64
1:G:54:LYS:NZ	6:G:305:HOH:O	2.30	0.64
1:C:70:LYS:HE3	1:J:138:SER:CB	2.27	0.64
1:D:44:THR:HG22	1:H:34:TYR:CD1	2.33	0.64
1:G:92:ASP:OD1	1:G:95:VAL:HG23	2.00	0.62
1:A:141[A]:ARG:HG2	1:A:147:ILE:HD12	1.82	0.61
1:B:121:LEU:HB3	1:B:122:PRO:HD3	1.81	0.61
1:I:41:GLU:OE1	1:I:43[B]:LYS:NZ	2.31	0.61
1:L:19:LEU:HD13	1:L:62:THR:HG23	1.79	0.61
1:C:70:LYS:CE	1:J:138:SER:HB2	2.31	0.61
1:C:69[B]:ARG:NH2	4:C:190:PO4:O1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:O	1:A:11[A]:MET:HG3	2.02	0.60
1:L:68:GLY:HA3	4:L:190:PO4:O4	2.00	0.60
1:H:49:ASP:OD1	1:H:155:GLY:HA2	2.02	0.60
1:J:68:GLY:HA2	1:J:90:ARG:H	1.66	0.59
1:F:13:ARG:HH11	1:F:13:ARG:HG2	1.67	0.59
1:H:101:LEU:HD21	1:H:111:VAL:HG21	1.85	0.59
1:L:121:LEU:HB3	1:L:122:PRO:HD3	1.84	0.59
1:I:11[A]:MET:HE2	1:I:163:LEU:CD2	2.32	0.59
1:K:112:ALA:HB2	1:K:129:LEU:HB3	1.85	0.58
1:B:125:ARG:HH12	1:J:179:LEU:HA	1.68	0.58
1:C:76[B]:ARG:NH1	1:D:37:GLU:O	2.37	0.57
1:A:25:ASP:OD1	1:A:43[A]:LYS:HE3	2.04	0.57
1:L:19:LEU:HD13	1:L:62:THR:CG2	2.34	0.57
1:A:43[A]:LYS:HE2	6:A:325:HOH:O	2.05	0.57
1:K:49:ASP:OD1	1:K:155:GLY:HA2	2.04	0.57
1:K:8:GLN:CD	1:K:11:MET:CE	2.71	0.57
1:I:68:GLY:HA3	4:I:189:PO4:O4	2.05	0.57
1:A:76[A]:ARG:NH2	6:A:235:HOH:O	2.35	0.56
1:F:11[A]:MET:CE	1:F:163:LEU:HD12	2.35	0.56
1:K:112:ALA:CB	1:K:129:LEU:HB3	2.35	0.56
1:E:91:GLU:HA	6:E:1360:HOH:O	2.05	0.56
1:A:33:LEU:HD11	1:H:47:THR:HG22	1.86	0.56
1:K:8:GLN:OE1	1:K:11:MET:HE3	2.05	0.56
1:A:69[B]:ARG:NH2	6:A:226:HOH:O	2.38	0.56
1:I:43[A]:LYS:HE3	6:I:1155:HOH:O	2.05	0.56
1:G:92:ASP:OD1	1:G:95:VAL:CG2	2.54	0.56
1:C:79:LYS:HE3	1:J:147:ILE:HG13	1.88	0.56
1:J:87:PHE:HE2	1:J:100:LEU:HD22	1.71	0.56
1:K:19:LEU:CD1	1:K:62:THR:HG23	2.32	0.55
1:B:19:LEU:CD1	1:B:62:THR:HG23	2.36	0.55
1:K:8:GLN:OE1	1:K:11:MET:CE	2.55	0.54
1:F:32:ARG:NH1	6:F:589:HOH:O	2.40	0.54
1:L:19:LEU:CD1	1:L:62:THR:CG2	2.80	0.54
1:K:19:LEU:HD13	1:K:62:THR:CG2	2.33	0.54
1:H:163:LEU:C	1:H:163:LEU:HD23	2.28	0.54
1:G:101:LEU:HD21	1:G:111:VAL:CG2	2.37	0.54
1:F:75:GLU:OE1	1:H:142:GLU:HG3	2.07	0.54
1:B:37:GLU:HG3	1:J:73:ILE:CD1	2.38	0.53
1:H:69[C]:ARG:NH1	4:H:189:PO4:O3	2.39	0.53
1:G:113:TYR:CD1	1:G:123:VAL:HG11	2.44	0.53
1:J:164:ILE:O	1:J:168:GLN:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:LYS:O	1:I:62:THR:HG22	2.08	0.53
1:B:126[A]:ARG:NH1	6:B:212:HOH:O	2.41	0.53
1:A:76[A]:ARG:NE	6:A:235:HOH:O	2.41	0.53
1:D:43[B]:LYS:HD2	1:D:71:THR:HG21	1.91	0.53
1:J:9:ASP:HB3	1:J:12:GLN:H	1.74	0.52
1:J:92:ASP:HB2	1:J:95:VAL:CG2	2.39	0.52
1:A:25:ASP:OD1	1:A:43[A]:LYS:CE	2.58	0.52
2:F:191:CL:CL	1:G:32:ARG:NH1	2.75	0.52
1:K:87:PHE:CZ	1:K:100:LEU:HD13	2.45	0.51
1:I:84:GLU:HB2	1:I:85:HIS:CD2	2.46	0.51
1:H:113:TYR:CD1	1:H:123:VAL:HG11	2.46	0.51
1:B:176:SER:O	1:B:177:VAL:C	2.49	0.51
1:I:30:ASP:OD2	1:I:32:ARG:NH1	2.43	0.51
1:B:69[A]:ARG:NH1	6:B:195:HOH:O	2.40	0.51
1:J:173:ALA:O	1:J:176:SER:HB2	2.11	0.51
1:I:109:GLU:CD	1:I:109:GLU:H	2.13	0.51
1:L:41:GLU:OE1	1:L:69[A]:ARG:NH2	2.44	0.50
1:L:84:GLU:HG3	6:L:1171:HOH:O	2.10	0.50
1:L:86:LEU:HD21	1:L:88:GLN:HE21	1.76	0.50
1:I:43[B]:LYS:HG2	6:I:193:HOH:O	2.11	0.50
1:A:90[A]:ARG:HH21	1:A:92:ASP:CG	2.14	0.50
1:F:91:GLU:H	1:F:91:GLU:CD	2.03	0.50
1:E:175:HIS:CE1	6:E:1370:HOH:O	2.65	0.50
1:F:71:THR:HG23	1:F:74:VAL:H	1.76	0.50
1:K:64:ALA:HA	1:K:85:HIS:O	2.12	0.49
1:K:106:LEU:HD23	1:K:110:GLN:NE2	2.27	0.49
1:J:113:TYR:CD1	1:J:123:VAL:HG11	2.47	0.49
1:D:93:LYS:NZ	4:D:190:PO4:O4	2.33	0.49
1:D:44:THR:CG2	1:H:34:TYR:CD1	2.95	0.49
1:A:132:ALA:HB3	1:A:147:ILE:CD1	2.43	0.49
1:I:92:ASP:N	1:I:92:ASP:OD1	2.45	0.49
1:C:19:LEU:HD13	1:C:62:THR:HG23	1.95	0.49
1:K:84:GLU:CA	1:K:84:GLU:OE2	2.60	0.48
1:F:133:VAL:HG12	1:F:156:ALA:HB1	1.94	0.48
1:E:44:THR:HA	1:I:33:LEU:O	2.12	0.48
1:I:87:PHE:HB3	1:I:90[B]:ARG:HD3	1.95	0.48
1:K:121:LEU:HB3	1:K:122:PRO:HD3	1.96	0.48
1:D:38:ASP:OD1	1:D:38:ASP:C	2.50	0.48
1:J:111:VAL:O	1:J:127:VAL:HB	2.13	0.48
1:B:9:ASP:OD2	1:B:9:ASP:O	2.32	0.48
1:D:68:GLY:CA	4:D:190:PO4:O3	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:HIS:HE1	6:E:1370:HOH:O	1.97	0.48
1:C:166[B]:SER:OG	1:C:171:LEU:HD22	2.13	0.48
1:F:33:LEU:O	1:G:44:THR:HA	2.13	0.48
1:G:69[B]:ARG:NH2	6:G:300:HOH:O	2.47	0.48
1:F:13:ARG:HG2	1:F:13:ARG:NH1	2.28	0.48
1:D:69[B]:ARG:NH2	6:D:1489:HOH:O	2.47	0.48
1:B:32[A]:ARG:NH1	6:B:204:HOH:O	2.45	0.47
1:B:32[A]:ARG:HH12	1:K:32:ARG:HH12	1.58	0.47
1:A:90[B]:ARG:HG2	1:A:96:VAL:HG21	1.96	0.47
1:B:15:LYS:HD3	1:B:15:LYS:O	2.15	0.47
1:F:16:ALA:CB	6:F:203:HOH:O	2.62	0.47
1:A:180:GLU:HG2	6:A:595:HOH:O	2.15	0.47
1:K:88:GLN:O	1:K:90:ARG:HG2	2.15	0.47
1:J:92:ASP:N	1:J:92:ASP:OD1	2.45	0.47
1:L:90:ARG:HH22	1:L:99:LYS:NZ	2.13	0.47
1:H:46:ASN:OD1	1:H:48:LEU:HB2	2.15	0.47
1:J:72:ALA:O	1:J:76:ARG:HG3	2.15	0.47
1:D:90[A]:ARG:HG2	1:D:96:VAL:HG21	1.96	0.47
1:B:125:ARG:HH11	1:J:179:LEU:HA	1.75	0.47
1:J:89:GLY:C	1:J:90:ARG:CG	2.81	0.46
1:K:87:PHE:HZ	1:K:100:LEU:HD13	1.79	0.46
1:H:90:ARG:NH2	1:H:92:ASP:OD2	2.48	0.46
1:C:75:GLU:HG3	1:C:88:GLN:NE2	2.31	0.46
1:A:90[B]:ARG:HG2	1:A:96:VAL:CG2	2.45	0.46
1:H:38:ASP:OD1	1:H:38:ASP:C	2.52	0.46
1:K:53:ILE:O	1:K:57:ILE:HG13	2.16	0.46
1:K:104:LEU:C	1:K:105:GLN:HG2	2.36	0.46
1:J:72:ALA:HA	1:J:75:GLU:HG2	1.97	0.46
1:D:90[B]:ARG:HD2	1:D:90[B]:ARG:HA	1.60	0.46
1:C:75:GLU:HG3	1:C:88:GLN:HE22	1.79	0.46
1:A:9:ASP:O	1:A:13:ARG:HG3	2.16	0.46
1:B:19:LEU:HD12	1:B:62:THR:HG23	1.98	0.46
1:I:90[B]:ARG:NH1	6:I:1222:HOH:O	2.42	0.46
1:G:33:LEU:O	1:I:44:THR:HA	2.16	0.46
1:C:90[A]:ARG:HD2	1:C:90[A]:ARG:HA	1.69	0.46
1:G:25:ASP:OD2	1:G:69[B]:ARG:HD2	2.17	0.45
1:A:101:LEU:HD21	1:A:111:VAL:HG21	1.97	0.45
1:L:104:LEU:O	1:L:105:GLN:HB2	2.16	0.45
1:J:9:ASP:O	1:J:13:ARG:HG3	2.17	0.45
1:I:43[B]:LYS:CG	6:I:193:HOH:O	2.63	0.45
1:C:8:GLN:O	1:C:12:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:THR:HA	1:H:33:LEU:O	2.17	0.45
1:K:106:LEU:CD2	1:K:110:GLN:NE2	2.80	0.45
1:H:101:LEU:HD21	1:H:111:VAL:CG2	2.47	0.45
1:A:176[A]:SER:OG	1:A:182:HIS:HB3	2.17	0.45
1:B:19:LEU:HD13	1:B:62:THR:HG23	1.98	0.45
1:H:163:LEU:HD23	1:H:163:LEU:O	2.17	0.45
1:C:19:LEU:CD1	1:C:62:THR:HG23	2.47	0.45
1:D:90[A]:ARG:CG	1:D:96:VAL:HG21	2.46	0.45
1:D:73:ILE:HG13	1:H:37:GLU:HA	1.98	0.45
1:F:121:LEU:O	1:F:125:ARG:HG2	2.17	0.45
1:D:34:TYR:HB2	1:D:42:ILE:HB	1.99	0.45
1:C:44:THR:HA	1:D:33:LEU:O	2.18	0.44
1:J:69[B]:ARG:NH2	6:J:202:HOH:O	2.50	0.44
1:G:69[A]:ARG:HG2	6:G:314:HOH:O	2.18	0.44
1:C:39:GLY:O	1:L:149:ARG:NH1	2.50	0.44
1:E:118:LEU:HB3	1:F:178:TYR:CD2	2.53	0.44
1:A:118:LEU:N	1:A:119:PRO:CD	2.80	0.44
1:C:91:GLU:HG2	1:C:91:GLU:H	1.56	0.44
1:G:43:LYS:HE3	6:G:197:HOH:O	2.18	0.44
1:A:29:THR:HG21	1:A:43[B]:LYS:CD	2.44	0.43
1:J:92:ASP:HB2	1:J:95:VAL:HG21	1.99	0.43
1:D:90[A]:ARG:NH1	6:D:257:HOH:O	2.38	0.43
1:K:34:TYR:HB2	1:K:42:ILE:O	2.18	0.43
1:E:43:LYS:HB2	1:E:43:LYS:HE2	1.82	0.43
1:G:166[B]:SER:OG	1:G:171:LEU:HD22	2.18	0.43
1:E:68:GLY:HA3	4:E:190:PO4:O4	2.18	0.43
1:I:68:GLY:H	4:I:189:PO4:P	2.41	0.43
6:E:1364:HOH:O	1:I:32:ARG:HD3	2.18	0.43
1:L:116:ASP:HA	1:L:136:ALA:HB2	2.01	0.43
1:F:92:ASP:OD1	1:F:92:ASP:N	2.44	0.43
1:F:101:LEU:O	1:F:105:GLN:N	2.51	0.43
1:K:8:GLN:NE2	1:K:11:MET:HE2	2.22	0.43
1:G:34:TYR:HB2	1:G:42:ILE:HB	1.99	0.43
1:C:70:LYS:CE	1:J:138:SER:CB	2.92	0.43
1:D:84:GLU:HG2	6:D:194:HOH:O	2.18	0.43
1:L:118:LEU:HB2	1:L:119:PRO:HD3	2.01	0.43
1:C:43:LYS:HB2	1:C:43:LYS:HE2	1.68	0.43
1:J:30:ASP:OD2	1:J:32:ARG:NH1	2.52	0.42
1:J:34:TYR:HB2	1:J:42:ILE:HB	2.01	0.42
1:G:38:ASP:C	1:G:38:ASP:OD1	2.57	0.42
1:D:35:PHE:CE1	1:D:41:GLU:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:46:ASN:OD1	1:L:48:LEU:HB2	2.19	0.42
1:B:23:ASP:HB3	1:B:27:VAL:HG21	2.01	0.42
1:A:132:ALA:HB3	1:A:147:ILE:HD12	2.01	0.42
1:I:11[A]:MET:HE2	1:I:163:LEU:HD21	2.00	0.42
1:G:101:LEU:HD23	1:G:101:LEU:HA	1.89	0.42
1:A:76[A]:ARG:CZ	6:A:235:HOH:O	2.68	0.42
1:H:118:LEU:HD23	1:H:118:LEU:HA	1.89	0.42
1:B:163:LEU:HD23	1:B:163:LEU:C	2.40	0.42
1:A:37:GLU:O	1:H:76:ARG:NH2	2.50	0.42
1:F:111:VAL:O	1:F:127:VAL:HB	2.20	0.42
1:A:49:ASP:OD1	1:A:155:GLY:HA2	2.19	0.42
1:B:37:GLU:HG3	1:J:73:ILE:HD11	2.00	0.42
1:I:92:ASP:HB2	6:I:1157:HOH:O	2.19	0.42
1:E:34:TYR:HB2	1:E:42:ILE:HB	2.02	0.42
1:L:97:LEU:O	1:L:101:LEU:HG	2.19	0.42
1:I:62:THR:HG22	6:I:1156:HOH:O	2.19	0.42
1:J:118:LEU:N	1:J:119:PRO:CD	2.82	0.42
1:L:135:ASN:ND2	6:L:783:HOH:O	2.45	0.41
1:A:76[B]:ARG:NH2	1:L:149:ARG:HA	2.35	0.41
1:E:71:THR:HG23	1:E:74:VAL:H	1.85	0.41
1:A:19:LEU:HD13	1:A:62[A]:THR:HG23	2.02	0.41
1:I:101:LEU:HD23	1:I:101:LEU:HA	1.92	0.41
1:C:121:LEU:N	1:C:122:PRO:CD	2.84	0.41
1:D:68:GLY:H	4:D:190:PO4:P	2.43	0.41
1:H:38:ASP:HB2	6:H:299:HOH:O	2.20	0.41
1:K:112:ALA:HA	1:K:129:LEU:O	2.20	0.41
1:J:34:TYR:CD1	1:L:44:THR:HG22	2.55	0.41
1:G:9:ASP:OD1	1:G:12:GLN:N	2.52	0.41
1:K:44:THR:HG22	1:L:34:TYR:CD1	2.55	0.41
1:B:176:SER:C	1:B:178:TYR:N	2.72	0.41
1:E:64:ALA:HA	1:E:85:HIS:O	2.21	0.41
1:K:18:LYS:O	1:K:62:THR:HG22	2.21	0.41
1:F:97:LEU:O	1:F:101:LEU:HG	2.21	0.41
1:F:64:ALA:HA	1:F:85:HIS:O	2.20	0.41
1:J:23:ASP:HB3	1:J:27:VAL:HG21	2.03	0.41
1:F:69[B]:ARG:NH1	2:G:188:CL:CL	2.90	0.41
1:B:105:GLN:HG2	6:B:208:HOH:O	2.20	0.41
1:B:44:THR:HA	1:K:33:LEU:O	2.21	0.41
1:G:8:GLN:HA	1:G:13:ARG:HH21	1.85	0.41
1:H:76:ARG:NH1	6:H:200:HOH:O	2.51	0.40
1:A:64:ALA:HA	1:A:85:HIS:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:MET:HE3	1:J:146:GLY:HA3	2.02	0.40
1:J:69[B]:ARG:NH2	6:J:205:HOH:O	2.42	0.40
1:I:126:ARG:HH11	1:I:126:ARG:HG3	1.86	0.40
1:D:9:ASP:OD1	1:D:12:GLN:N	2.42	0.40
1:E:113:TYR:CD1	1:E:123:VAL:HG11	2.55	0.40
1:D:44:THR:HG21	1:H:34:TYR:CE1	2.56	0.40
1:G:33:LEU:HD11	1:I:47:THR:HG22	2.04	0.40
1:E:90[A]:ARG:HD2	1:E:90[A]:ARG:HA	1.81	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	185/189 (98%)	183 (99%)	2 (1%)	0	100	100
1	B	176/189 (93%)	171 (97%)	4 (2%)	1 (1%)	30	17
1	C	177/189 (94%)	172 (97%)	5 (3%)	0	100	100
1	D	177/189 (94%)	174 (98%)	2 (1%)	1 (1%)	30	17
1	E	176/189 (93%)	171 (97%)	5 (3%)	0	100	100
1	F	176/189 (93%)	173 (98%)	3 (2%)	0	100	100
1	G	175/189 (93%)	171 (98%)	4 (2%)	0	100	100
1	H	175/189 (93%)	174 (99%)	1 (1%)	0	100	100
1	I	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
1	J	172/189 (91%)	163 (95%)	9 (5%)	0	100	100
1	K	171/189 (90%)	166 (97%)	5 (3%)	0	100	100
1	L	174/189 (92%)	169 (97%)	5 (3%)	0	100	100
All	All	2116/2268 (93%)	2066 (98%)	48 (2%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	177	VAL
1	B	177	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	148/150 (99%)	147 (99%)	1 (1%)	88 88
1	B	140/150 (93%)	134 (96%)	6 (4%)	35 23
1	C	141/150 (94%)	141 (100%)	0	100 100
1	D	141/150 (94%)	137 (97%)	4 (3%)	51 41
1	E	140/150 (93%)	136 (97%)	4 (3%)	50 40
1	F	139/150 (93%)	138 (99%)	1 (1%)	88 88
1	G	139/150 (93%)	137 (99%)	2 (1%)	74 71
1	H	139/150 (93%)	139 (100%)	0	100 100
1	I	146/150 (97%)	145 (99%)	1 (1%)	88 88
1	J	135/150 (90%)	128 (95%)	7 (5%)	29 17
1	K	135/150 (90%)	131 (97%)	4 (3%)	48 38
1	L	138/150 (92%)	138 (100%)	0	100 100
All	All	1681/1800 (93%)	1651 (98%)	30 (2%)	68 61

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

Mol	Chain	Res	Type
1	A	71	THR
1	B	8	GLN
1	B	9	ASP
1	B	15	LYS
1	B	71	THR
1	B	80	SER
1	B	172	GLU

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Mol	Chain	Res	Type
1	D	9	ASP
1	D	90[A]	ARG
1	D	90[B]	ARG
1	D	172	GLU
1	E	6	MET
1	E	62	THR
1	E	91	GLU
1	E	92	ASP
1	F	182	HIS
1	G	9	ASP
1	G	91	GLU
1	I	5	THR
1	J	62	THR
1	J	116	ASP
1	J	149[A]	ARG
1	J	149[B]	ARG
1	J	163	LEU
1	J	166	SER
1	J	176	SER
1	K	69[A]	ARG
1	K	69[B]	ARG
1	K	83	ILE
1	K	91	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	8	GLN
1	C	105	GLN
1	E	105	GLN
1	G	151	GLN
1	I	85	HIS
1	J	51	GLN
1	K	8	GLN
1	K	151	GLN
1	L	8	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 1 is unknown and 25 are monoatomic - leaving 12 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	191	-	4,4,4	0.82	0	6,6,6	0.29	0
4	PO4	B	191	-	4,4,4	0.60	0	6,6,6	0.29	0
4	PO4	C	190	-	4,4,4	0.62	0	6,6,6	0.29	0
4	PO4	D	190	-	4,4,4	0.58	0	6,6,6	0.27	0
4	PO4	E	190	-	4,4,4	0.56	0	6,6,6	0.29	0
4	PO4	F	190	-	4,4,4	0.48	0	6,6,6	0.28	0
4	PO4	G	191	-	4,4,4	0.68	0	6,6,6	0.28	0
4	PO4	H	189	-	4,4,4	0.62	0	6,6,6	0.30	0
4	PO4	I	189	-	4,4,4	0.49	0	6,6,6	0.27	0
4	PO4	J	189	-	4,4,4	0.53	0	6,6,6	0.27	0
4	PO4	K	190	-	4,4,4	0.49	0	6,6,6	0.28	0
4	PO4	L	190	-	4,4,4	0.62	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	A	191	-	-	0/0/0/0	0/0/0/0
4	PO4	B	191	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	C	190	-	-	0/0/0/0	0/0/0/0
4	PO4	D	190	-	-	0/0/0/0	0/0/0/0
4	PO4	E	190	-	-	0/0/0/0	0/0/0/0
4	PO4	F	190	-	-	0/0/0/0	0/0/0/0
4	PO4	G	191	-	-	0/0/0/0	0/0/0/0
4	PO4	H	189	-	-	0/0/0/0	0/0/0/0
4	PO4	I	189	-	-	0/0/0/0	0/0/0/0
4	PO4	J	189	-	-	0/0/0/0	0/0/0/0
4	PO4	K	190	-	-	0/0/0/0	0/0/0/0
4	PO4	L	190	-	-	0/0/0/0	0/0/0/0

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.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	191	PO4	1	0
4	B	191	PO4	1	0
4	C	190	PO4	1	0
4	D	190	PO4	4	0
4	E	190	PO4	1	0
4	H	189	PO4	2	0
4	I	189	PO4	2	0
4	L	190	PO4	1	0

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	176/189 (93%)	0.04	4 (2%)	64	67	30, 41, 68, 128	0
1	B	173/189 (91%)	0.05	5 (2%)	55	59	37, 50, 77, 104	0
1	C	173/189 (91%)	-0.04	3 (1%)	73	76	30, 43, 68, 99	0
1	D	172/189 (91%)	-0.11	2 (1%)	81	83	31, 41, 65, 95	0
1	E	175/189 (92%)	-0.03	1 (0%)	90	91	35, 48, 81, 123	0
1	F	174/189 (92%)	-0.04	4 (2%)	64	67	31, 45, 72, 104	0
1	G	173/189 (91%)	-0.00	3 (1%)	73	76	35, 50, 75, 108	0
1	H	172/189 (91%)	-0.09	2 (1%)	81	83	25, 42, 65, 96	0
1	I	177/189 (93%)	0.05	4 (2%)	64	67	38, 50, 81, 120	0
1	J	172/189 (91%)	0.18	3 (1%)	73	76	39, 56, 86, 105	0
1	K	172/189 (91%)	0.33	11 (6%)	23	25	41, 61, 91, 112	0
1	L	172/189 (91%)	0.07	6 (3%)	48	51	35, 51, 78, 103	0
All	All	2081/2268 (91%)	0.03	48 (2%)	64	67	25, 48, 80, 128	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	HIS	9.2
1	E	179	LEU	4.7
1	H	179	LEU	4.3
1	I	102	ALA	4.2
1	I	179	LEU	4.1
1	K	102	ALA	4.1
1	L	179	LEU	3.7
1	J	91	GLU	3.7
1	F	181	GLY	3.7
1	D	91	GLU	3.5
1	J	8	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	L	176	SER	3.4
1	K	125	ARG	3.3
1	J	179	LEU	3.3
1	I	5	THR	3.1
1	B	12	GLN	3.0
1	K	8	GLN	3.0
1	C	180	GLU	2.9
1	L	102	ALA	2.9
1	G	104	LEU	2.9
1	H	180	GLU	2.8
1	C	179	LEU	2.7
1	F	182	HIS	2.6
1	L	173	ALA	2.6
1	L	91	GLU	2.6
1	C	36	MET	2.5
1	I	6	MET	2.5
1	G	180	GLU	2.5
1	K	101	LEU	2.4
1	K	100	LEU	2.4
1	A	181	GLY	2.4
1	B	39	GLY	2.4
1	B	36	MET	2.4
1	K	176	SER	2.3
1	K	16	ALA	2.3
1	L	177	VAL	2.3
1	B	8	GLN	2.2
1	K	106	LEU	2.2
1	A	180	GLU	2.2
1	B	7	SER	2.2
1	F	176[A]	SER	2.1
1	K	104	LEU	2.1
1	A	91	GLU	2.1
1	D	36	MET	2.1
1	K	108	TYR	2.1
1	F	91	GLU	2.0
1	K	66	ILE	2.0
1	G	91	GLU	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	F	191	1/1	0.91	0.23	4.52	89,89,89,89	0
5	UNL	I	190	4/-	0.92	0.12	1.33	72,78,80,82	0
4	PO4	D	190	5/5	0.97	0.14	0.84	46,54,63,66	5
4	PO4	G	191	5/5	0.96	0.12	0.61	38,45,59,64	5
3	MG	E	189	1/1	0.96	0.10	0.49	43,43,43,43	0
3	MG	I	188	1/1	0.91	0.09	0.40	55,55,55,55	0
2	CL	C	188	1/1	1.00	0.11	0.21	45,45,45,45	0
2	CL	A	188	1/1	0.99	0.15	0.21	46,46,46,46	0
4	PO4	B	191	5/5	0.98	0.13	0.05	39,42,55,67	5
4	PO4	I	189	5/5	0.96	0.13	0.02	43,44,60,66	5
4	PO4	A	191	5/5	0.99	0.13	-0.05	32,33,51,53	5
4	PO4	H	189	5/5	0.98	0.13	-0.10	38,41,49,53	5
2	CL	E	188	1/1	0.98	0.10	-0.20	55,55,55,55	0
2	CL	L	188	1/1	0.97	0.12	-0.24	57,57,57,57	0
4	PO4	C	190	5/5	0.96	0.12	-0.25	40,47,64,69	5
4	PO4	J	189	5/5	0.98	0.11	-0.30	55,56,60,61	5
4	PO4	K	190	5/5	0.98	0.11	-0.31	52,54,65,65	5
4	PO4	F	190	5/5	0.98	0.11	-0.36	43,49,59,60	5
4	PO4	L	190	5/5	0.98	0.10	-0.36	36,43,52,60	5
2	CL	B	188	1/1	0.99	0.10	-0.36	52,52,52,52	0
3	MG	C	189	1/1	0.98	0.09	-0.66	38,38,38,38	0
4	PO4	E	190	5/5	0.98	0.09	-0.71	33,46,57,61	5
2	CL	G	188	1/1	0.99	0.08	-0.81	48,48,48,48	0
3	MG	K	189	1/1	0.97	0.07	-0.88	49,49,49,49	0
3	MG	A	190	1/1	0.98	0.08	-0.91	36,36,36,36	0
2	CL	G	189	1/1	0.99	0.09	-0.97	48,48,48,48	0
2	CL	B	189	1/1	0.99	0.10	-1.10	51,51,51,51	0
2	CL	D	188	1/1	1.00	0.06	-1.15	43,43,43,43	0
2	CL	F	188	1/1	0.99	0.10	-1.18	44,44,44,44	0
2	CL	K	188	1/1	0.97	0.07	-1.29	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	A	189	1/1	1.00	0.05	-1.80	41,41,41,41	0
3	MG	B	190	1/1	0.98	0.06	-1.83	49,49,49,49	0
3	MG	L	189	1/1	0.97	0.07	-1.84	43,43,43,43	0
3	MG	G	190	1/1	0.96	0.04	-2.38	43,43,43,43	0
3	MG	H	188	1/1	0.99	0.06	-2.44	35,35,35,35	0
3	MG	J	188	1/1	0.98	0.04	-2.45	53,53,53,53	0
3	MG	D	189	1/1	0.97	0.04	-2.84	42,42,42,42	0
3	MG	F	189	1/1	0.98	0.04	-2.93	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.