wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:04 AM EDT

PDB ID	:	6GEB
Title	:	X-ray structure of the Legionella pneumophila ATPase DotB
Authors	:	Prevost, M.S.; Waksman, G.
Deposited on	:	2018-04-26
Resolution	:	3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

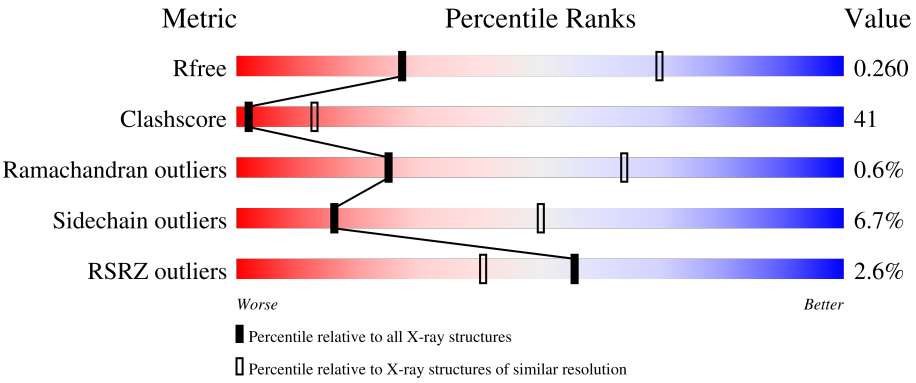
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	4% 50% 42% · 6%
1	B	391	% 56% 36% · 5%
1	C	391	% 50% 39% 5% 6%
1	D	391	2% 48% 44% · 6%
1	E	391	2% 49% 40% · 6%

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Mol	Chain	Length	Quality of chain
1	F	391	2% 44% 46% 6%
1	G	391	3% 38% 49% 6% 6%
1	H	391	2% 51% 38% 5% 5%
1	I	391	3% 39% 49% 6% 6%
1	J	391	% 38% 50% 6% 6%
1	K	391	5% 42% 45% 6% 6%
1	L	391	4% 42% 48% 6%

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	PO4	J	401	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34658 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 DotB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2907	1826	512	558	11			
1	B	371	Total	C	N	O	S	0	0	0
			2906	1826	510	559	11			
1	C	369	Total	C	N	O	S	0	0	0
			2886	1814	503	558	11			
1	D	368	Total	C	N	O	S	0	0	0
			2874	1806	503	554	11			
1	E	367	Total	C	N	O	S	0	0	0
			2867	1805	498	553	11			
1	F	366	Total	C	N	O	S	0	0	0
			2859	1800	495	553	11			
1	G	369	Total	C	N	O	S	0	0	0
			2907	1826	512	558	11			
1	H	371	Total	C	N	O	S	0	0	0
			2906	1826	510	559	11			
1	I	369	Total	C	N	O	S	0	0	0
			2886	1814	503	558	11			
1	J	368	Total	C	N	O	S	0	0	0
			2874	1806	503	554	11			
1	K	367	Total	C	N	O	S	0	0	0
			2867	1805	498	553	11			
1	L	366	Total	C	N	O	S	0	0	0
			2859	1800	495	553	11			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP O52185
A	-12	ALA	-	expression tag	UNP O52185
A	-11	SER	-	expression tag	UNP O52185
A	-10	TRP	-	expression tag	UNP O52185
A	-9	SER	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP O52185
A	-7	PRO	-	expression tag	UNP O52185
A	-6	GLN	-	expression tag	UNP O52185
A	-5	PHE	-	expression tag	UNP O52185
A	-4	GLU	-	expression tag	UNP O52185
A	-3	LYS	-	expression tag	UNP O52185
A	-2	ILE	-	expression tag	UNP O52185
A	-1	GLU	-	expression tag	UNP O52185
A	0	GLY	-	expression tag	UNP O52185
A	1	ARG	-	expression tag	UNP O52185
B	-13	MET	-	initiating methionine	UNP O52185
B	-12	ALA	-	expression tag	UNP O52185
B	-11	SER	-	expression tag	UNP O52185
B	-10	TRP	-	expression tag	UNP O52185
B	-9	SER	-	expression tag	UNP O52185
B	-8	HIS	-	expression tag	UNP O52185
B	-7	PRO	-	expression tag	UNP O52185
B	-6	GLN	-	expression tag	UNP O52185
B	-5	PHE	-	expression tag	UNP O52185
B	-4	GLU	-	expression tag	UNP O52185
B	-3	LYS	-	expression tag	UNP O52185
B	-2	ILE	-	expression tag	UNP O52185
B	-1	GLU	-	expression tag	UNP O52185
B	0	GLY	-	expression tag	UNP O52185
B	1	ARG	-	expression tag	UNP O52185
C	-13	MET	-	initiating methionine	UNP O52185
C	-12	ALA	-	expression tag	UNP O52185
C	-11	SER	-	expression tag	UNP O52185
C	-10	TRP	-	expression tag	UNP O52185
C	-9	SER	-	expression tag	UNP O52185
C	-8	HIS	-	expression tag	UNP O52185
C	-7	PRO	-	expression tag	UNP O52185
C	-6	GLN	-	expression tag	UNP O52185
C	-5	PHE	-	expression tag	UNP O52185
C	-4	GLU	-	expression tag	UNP O52185
C	-3	LYS	-	expression tag	UNP O52185
C	-2	ILE	-	expression tag	UNP O52185
C	-1	GLU	-	expression tag	UNP O52185
C	0	GLY	-	expression tag	UNP O52185
C	1	ARG	-	expression tag	UNP O52185
D	-13	MET	-	initiating methionine	UNP O52185
D	-12	ALA	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	SER	-	expression tag	UNP O52185
D	-10	TRP	-	expression tag	UNP O52185
D	-9	SER	-	expression tag	UNP O52185
D	-8	HIS	-	expression tag	UNP O52185
D	-7	PRO	-	expression tag	UNP O52185
D	-6	GLN	-	expression tag	UNP O52185
D	-5	PHE	-	expression tag	UNP O52185
D	-4	GLU	-	expression tag	UNP O52185
D	-3	LYS	-	expression tag	UNP O52185
D	-2	ILE	-	expression tag	UNP O52185
D	-1	GLU	-	expression tag	UNP O52185
D	0	GLY	-	expression tag	UNP O52185
D	1	ARG	-	expression tag	UNP O52185
E	-13	MET	-	initiating methionine	UNP O52185
E	-12	ALA	-	expression tag	UNP O52185
E	-11	SER	-	expression tag	UNP O52185
E	-10	TRP	-	expression tag	UNP O52185
E	-9	SER	-	expression tag	UNP O52185
E	-8	HIS	-	expression tag	UNP O52185
E	-7	PRO	-	expression tag	UNP O52185
E	-6	GLN	-	expression tag	UNP O52185
E	-5	PHE	-	expression tag	UNP O52185
E	-4	GLU	-	expression tag	UNP O52185
E	-3	LYS	-	expression tag	UNP O52185
E	-2	ILE	-	expression tag	UNP O52185
E	-1	GLU	-	expression tag	UNP O52185
E	0	GLY	-	expression tag	UNP O52185
E	1	ARG	-	expression tag	UNP O52185
F	-13	MET	-	initiating methionine	UNP O52185
F	-12	ALA	-	expression tag	UNP O52185
F	-11	SER	-	expression tag	UNP O52185
F	-10	TRP	-	expression tag	UNP O52185
F	-9	SER	-	expression tag	UNP O52185
F	-8	HIS	-	expression tag	UNP O52185
F	-7	PRO	-	expression tag	UNP O52185
F	-6	GLN	-	expression tag	UNP O52185
F	-5	PHE	-	expression tag	UNP O52185
F	-4	GLU	-	expression tag	UNP O52185
F	-3	LYS	-	expression tag	UNP O52185
F	-2	ILE	-	expression tag	UNP O52185
F	-1	GLU	-	expression tag	UNP O52185
F	0	GLY	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ARG	-	expression tag	UNP O52185
G	-13	MET	-	initiating methionine	UNP O52185
G	-12	ALA	-	expression tag	UNP O52185
G	-11	SER	-	expression tag	UNP O52185
G	-10	TRP	-	expression tag	UNP O52185
G	-9	SER	-	expression tag	UNP O52185
G	-8	HIS	-	expression tag	UNP O52185
G	-7	PRO	-	expression tag	UNP O52185
G	-6	GLN	-	expression tag	UNP O52185
G	-5	PHE	-	expression tag	UNP O52185
G	-4	GLU	-	expression tag	UNP O52185
G	-3	LYS	-	expression tag	UNP O52185
G	-2	ILE	-	expression tag	UNP O52185
G	-1	GLU	-	expression tag	UNP O52185
G	0	GLY	-	expression tag	UNP O52185
G	1	ARG	-	expression tag	UNP O52185
H	-13	MET	-	initiating methionine	UNP O52185
H	-12	ALA	-	expression tag	UNP O52185
H	-11	SER	-	expression tag	UNP O52185
H	-10	TRP	-	expression tag	UNP O52185
H	-9	SER	-	expression tag	UNP O52185
H	-8	HIS	-	expression tag	UNP O52185
H	-7	PRO	-	expression tag	UNP O52185
H	-6	GLN	-	expression tag	UNP O52185
H	-5	PHE	-	expression tag	UNP O52185
H	-4	GLU	-	expression tag	UNP O52185
H	-3	LYS	-	expression tag	UNP O52185
H	-2	ILE	-	expression tag	UNP O52185
H	-1	GLU	-	expression tag	UNP O52185
H	0	GLY	-	expression tag	UNP O52185
H	1	ARG	-	expression tag	UNP O52185
I	-13	MET	-	initiating methionine	UNP O52185
I	-12	ALA	-	expression tag	UNP O52185
I	-11	SER	-	expression tag	UNP O52185
I	-10	TRP	-	expression tag	UNP O52185
I	-9	SER	-	expression tag	UNP O52185
I	-8	HIS	-	expression tag	UNP O52185
I	-7	PRO	-	expression tag	UNP O52185
I	-6	GLN	-	expression tag	UNP O52185
I	-5	PHE	-	expression tag	UNP O52185
I	-4	GLU	-	expression tag	UNP O52185
I	-3	LYS	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	ILE	-	expression tag	UNP O52185
I	-1	GLU	-	expression tag	UNP O52185
I	0	GLY	-	expression tag	UNP O52185
I	1	ARG	-	expression tag	UNP O52185
J	-13	MET	-	initiating methionine	UNP O52185
J	-12	ALA	-	expression tag	UNP O52185
J	-11	SER	-	expression tag	UNP O52185
J	-10	TRP	-	expression tag	UNP O52185
J	-9	SER	-	expression tag	UNP O52185
J	-8	HIS	-	expression tag	UNP O52185
J	-7	PRO	-	expression tag	UNP O52185
J	-6	GLN	-	expression tag	UNP O52185
J	-5	PHE	-	expression tag	UNP O52185
J	-4	GLU	-	expression tag	UNP O52185
J	-3	LYS	-	expression tag	UNP O52185
J	-2	ILE	-	expression tag	UNP O52185
J	-1	GLU	-	expression tag	UNP O52185
J	0	GLY	-	expression tag	UNP O52185
J	1	ARG	-	expression tag	UNP O52185
K	-13	MET	-	initiating methionine	UNP O52185
K	-12	ALA	-	expression tag	UNP O52185
K	-11	SER	-	expression tag	UNP O52185
K	-10	TRP	-	expression tag	UNP O52185
K	-9	SER	-	expression tag	UNP O52185
K	-8	HIS	-	expression tag	UNP O52185
K	-7	PRO	-	expression tag	UNP O52185
K	-6	GLN	-	expression tag	UNP O52185
K	-5	PHE	-	expression tag	UNP O52185
K	-4	GLU	-	expression tag	UNP O52185
K	-3	LYS	-	expression tag	UNP O52185
K	-2	ILE	-	expression tag	UNP O52185
K	-1	GLU	-	expression tag	UNP O52185
K	0	GLY	-	expression tag	UNP O52185
K	1	ARG	-	expression tag	UNP O52185
L	-13	MET	-	initiating methionine	UNP O52185
L	-12	ALA	-	expression tag	UNP O52185
L	-11	SER	-	expression tag	UNP O52185
L	-10	TRP	-	expression tag	UNP O52185
L	-9	SER	-	expression tag	UNP O52185
L	-8	HIS	-	expression tag	UNP O52185
L	-7	PRO	-	expression tag	UNP O52185
L	-6	GLN	-	expression tag	UNP O52185

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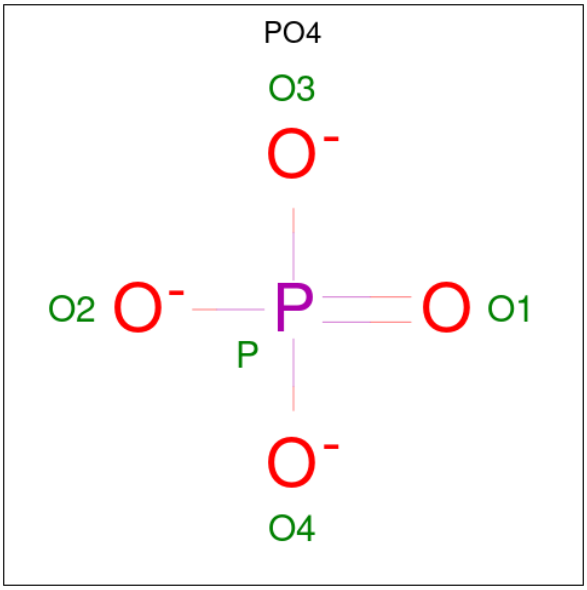
Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	PHE	-	expression tag	UNP O52185
L	-4	GLU	-	expression tag	UNP O52185
L	-3	LYS	-	expression tag	UNP O52185
L	-2	ILE	-	expression tag	UNP O52185
L	-1	GLU	-	expression tag	UNP O52185
L	0	GLY	-	expression tag	UNP O52185
L	1	ARG	-	expression tag	UNP O52185

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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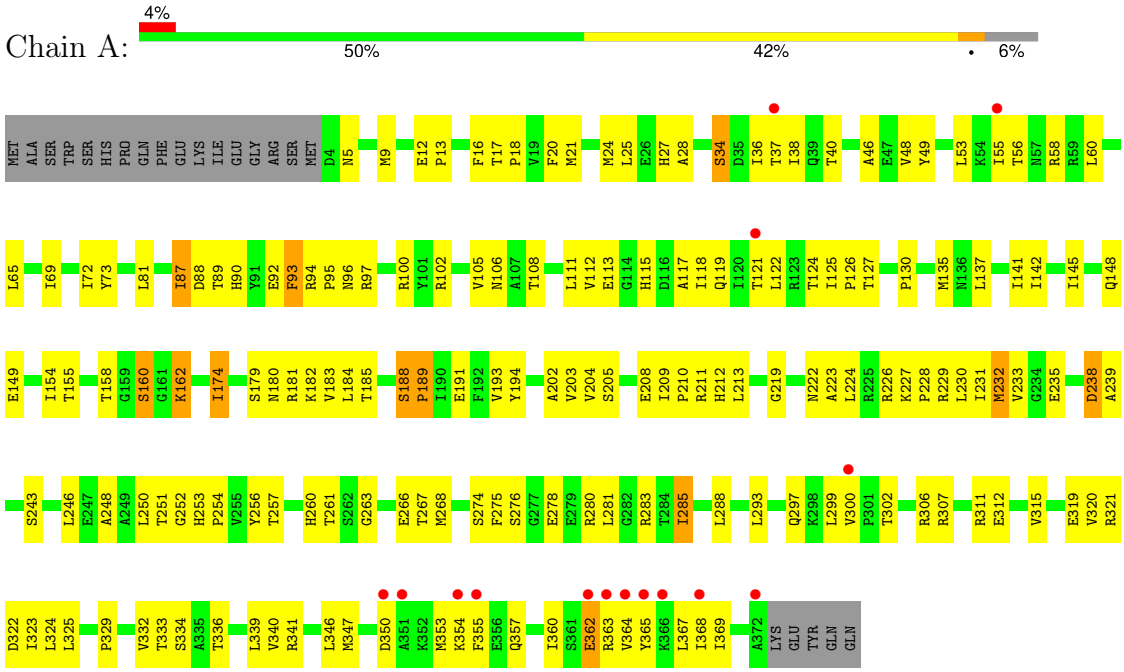
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

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 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: DotB

Chain A:

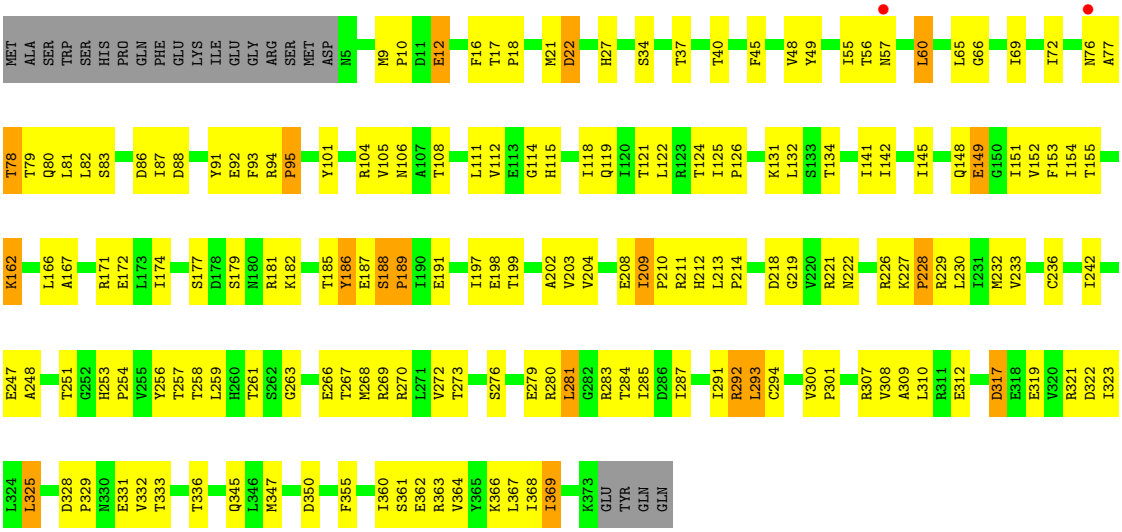


• Molecule 1: DotB

Chain B:

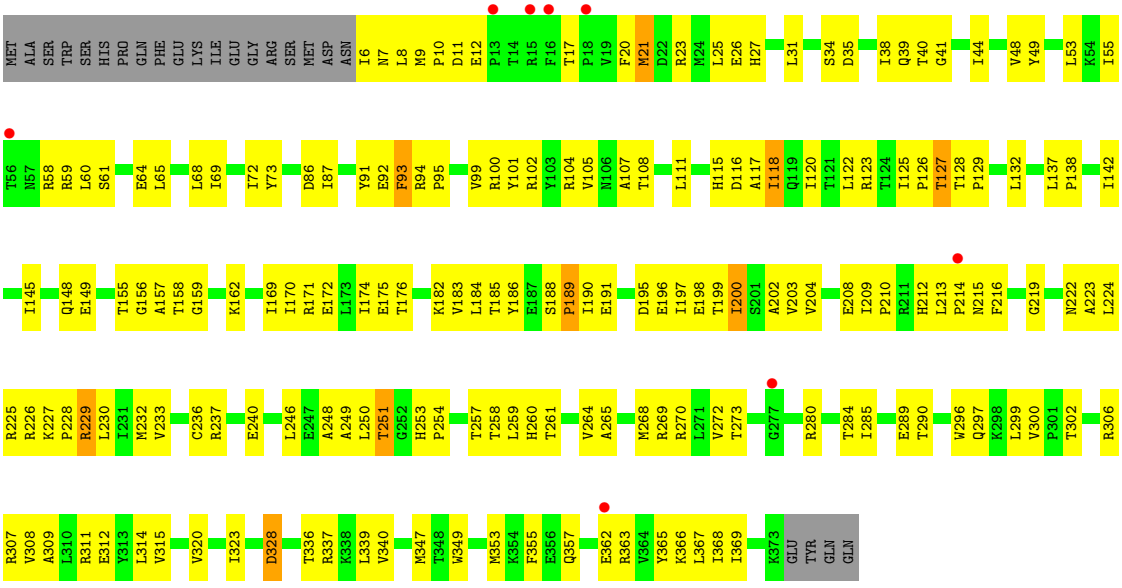
• Molecule 1: DotB

Chain C:



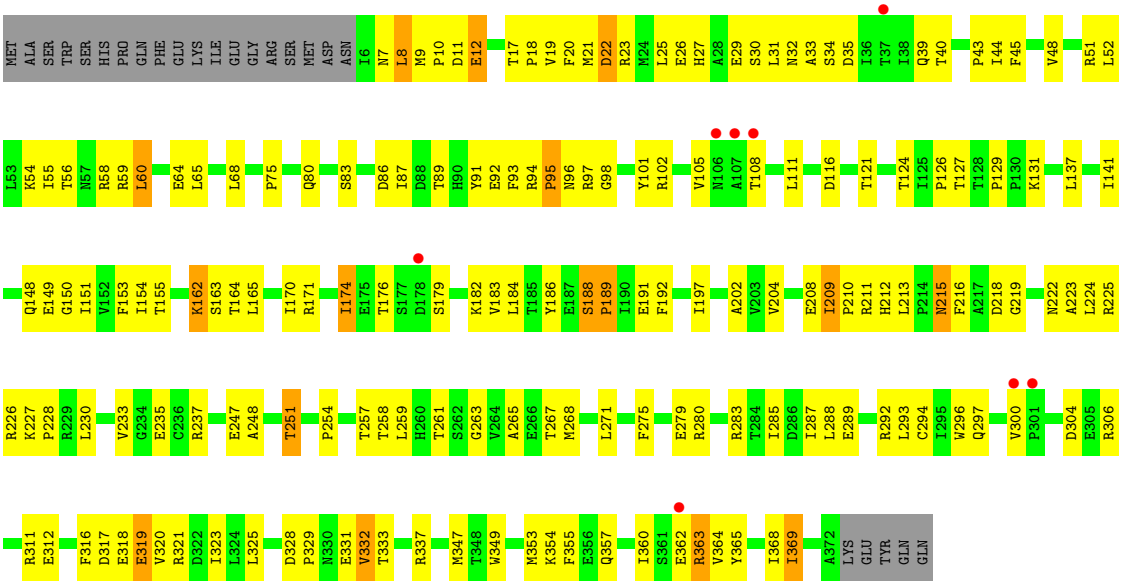
• Molecule 1: DotB

Chain D:



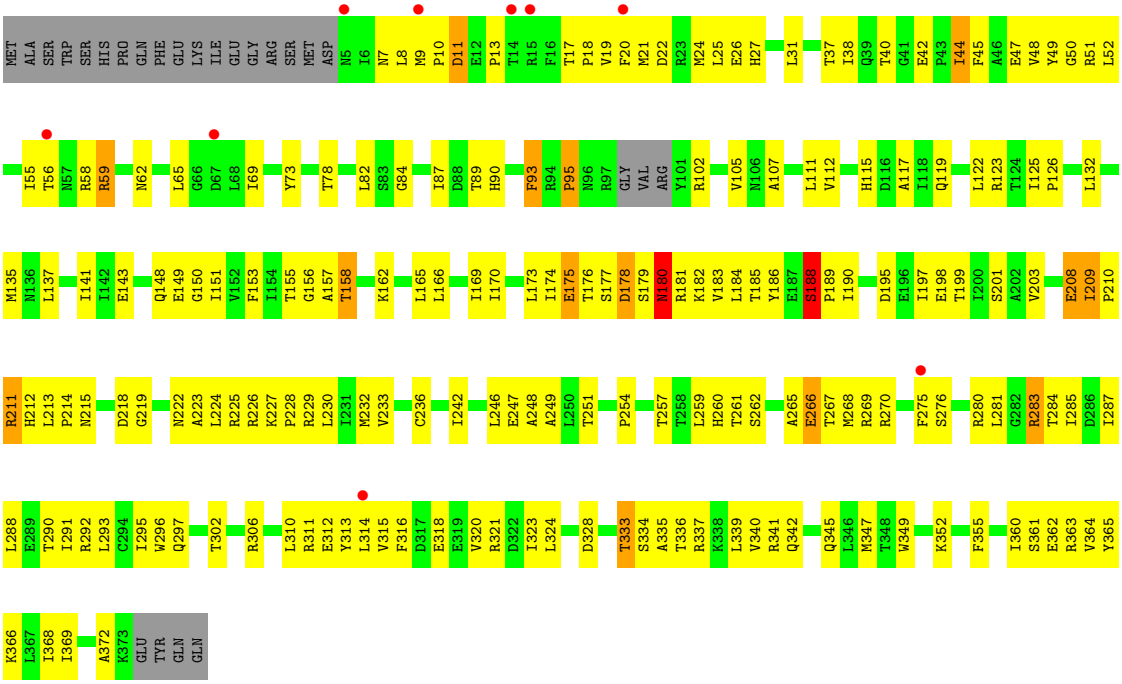
• Molecule 1: DotB

Chain E:



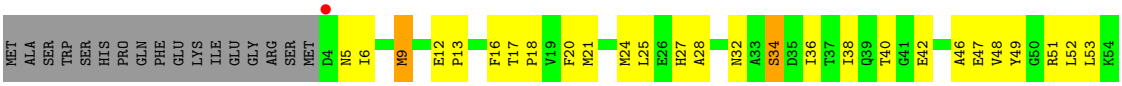
• Molecule 1: DotB

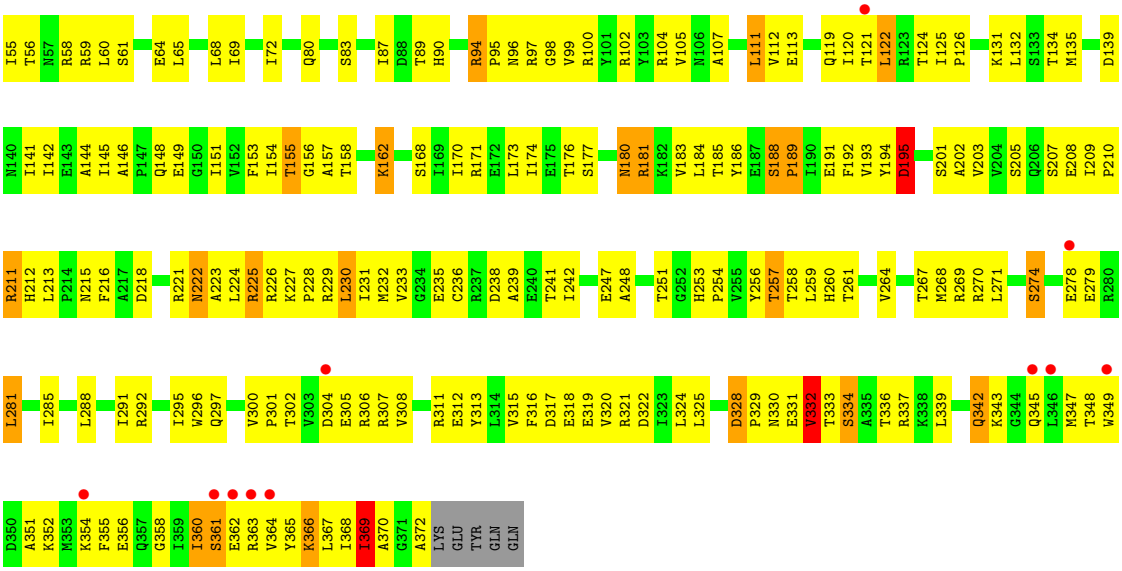
Chain F:



• Molecule 1: DotB

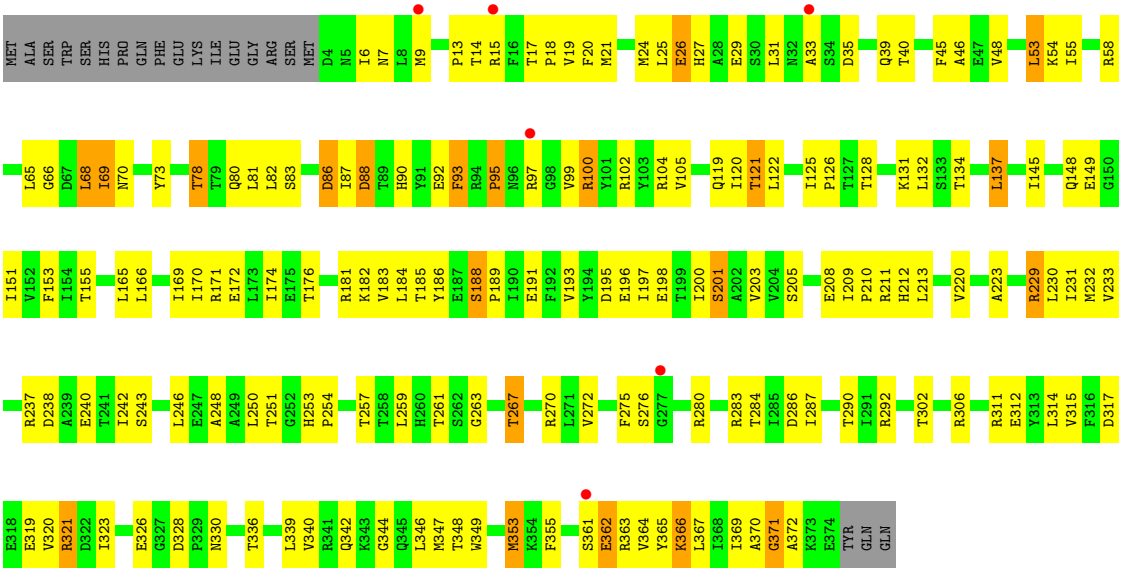
Chain G:





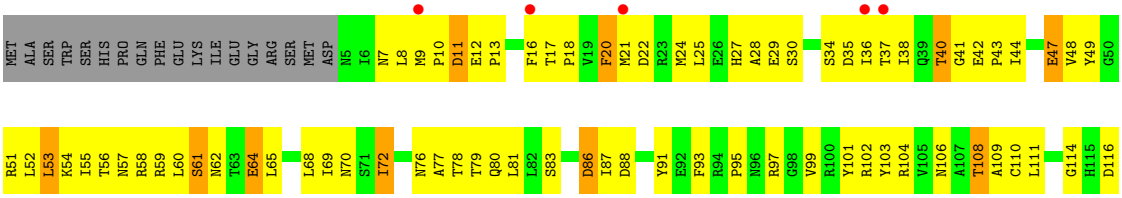
• Molecule 1: DotB

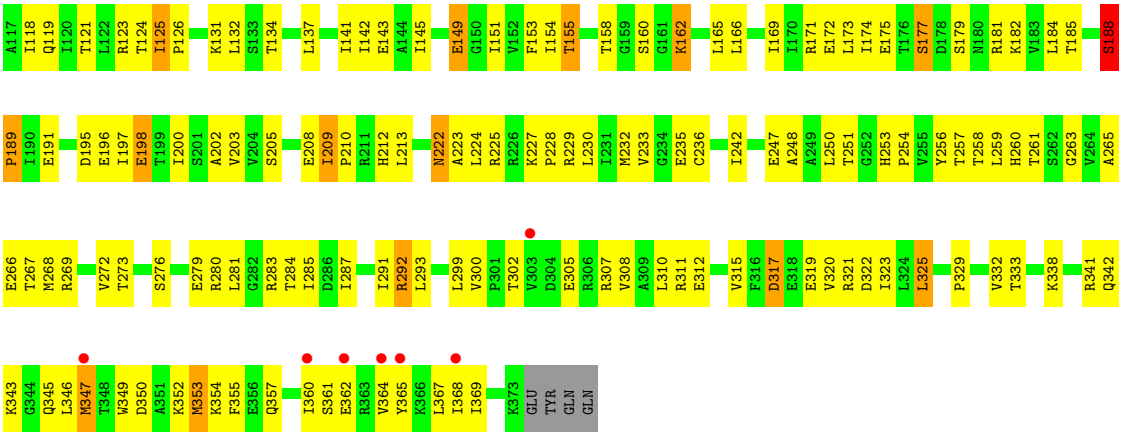
Chain H:



• Molecule 1: DotB

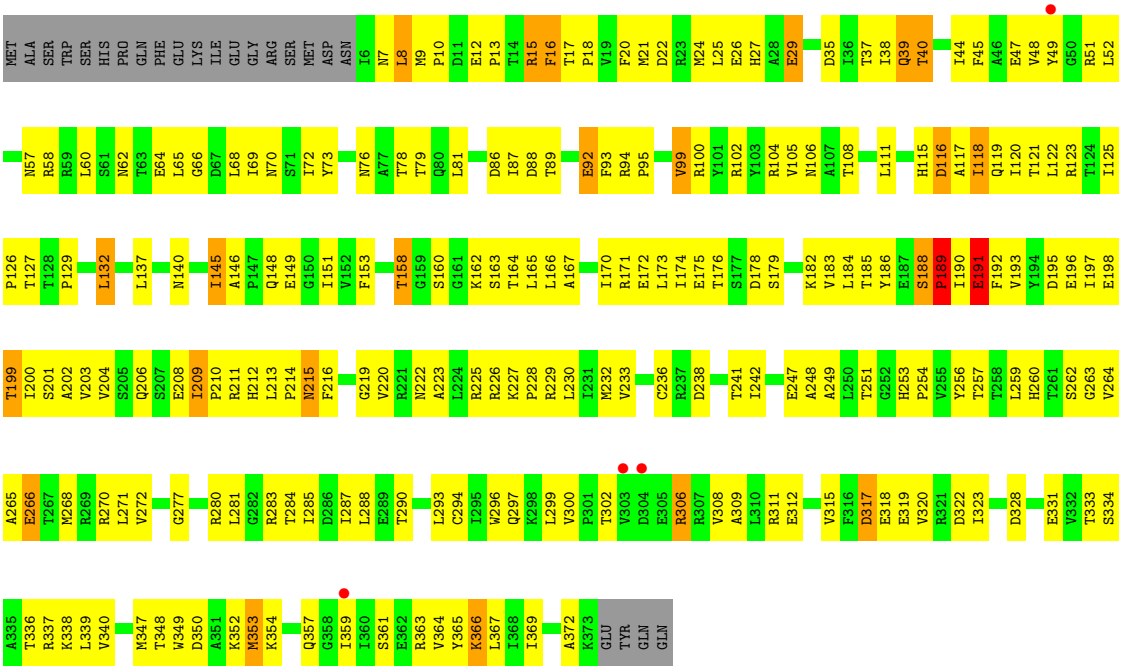
Chain I:





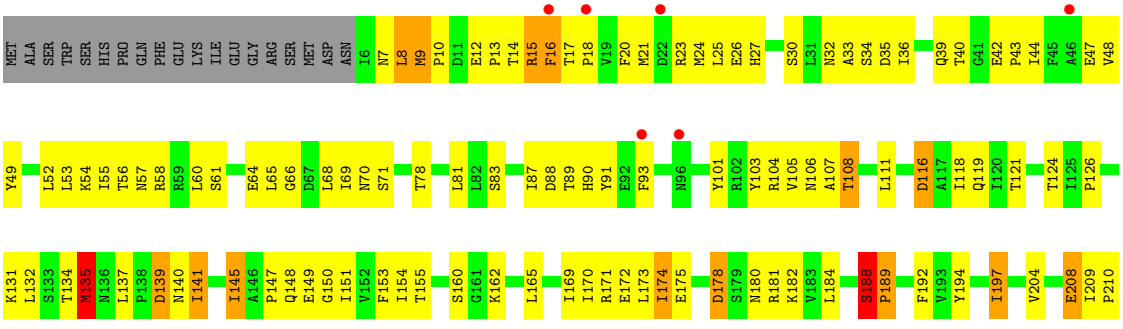
• Molecule 1: DotB

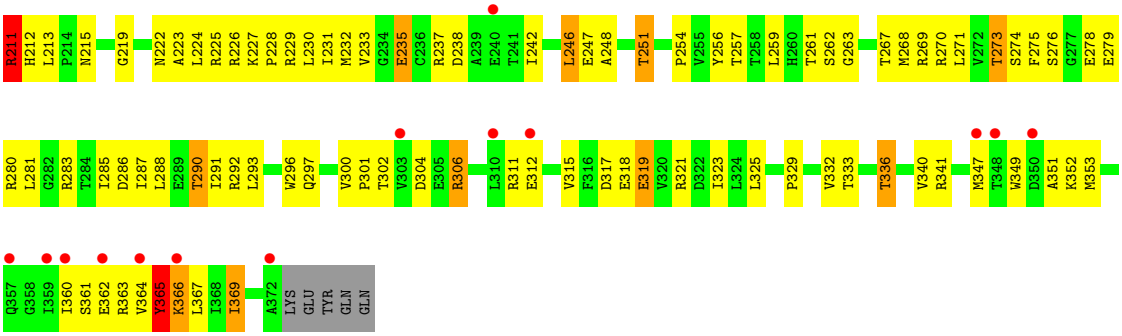
Chain J:



• Molecule 1: DotB

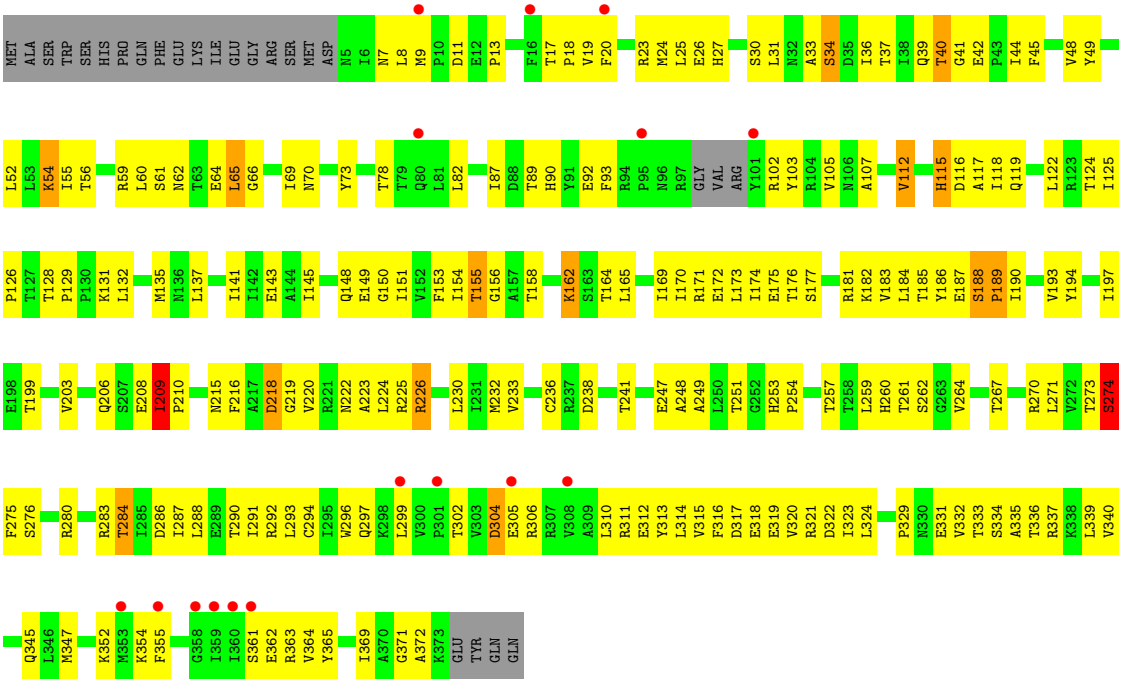
Chain K:





- Molecule 1: DotB

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	109.20Å 109.30Å 119.80Å 83.70° 86.60° 60.70°	Depositor
Resolution (Å)	36.04 – 3.19 49.10 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.04-3.19) 98.1 (49.10-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.233 , 0.261 0.234 , 0.260	Depositor DCC
R_{free} test set	3841 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	103.3	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for h-k,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	34658	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.73	0/2954	0.78	4/4009 (0.1%)
1	B	0.78	0/2953	0.77	6/4009 (0.1%)
1	C	0.73	0/2933	0.77	5/3984 (0.1%)
1	D	0.79	0/2920	0.78	4/3965 (0.1%)
1	E	0.78	1/2914 (0.0%)	0.79	4/3958 (0.1%)
1	F	0.81	2/2904 (0.1%)	0.80	5/3943 (0.1%)
1	G	0.91	1/2954 (0.0%)	0.90	5/4009 (0.1%)
1	H	0.82	0/2953	0.77	4/4009 (0.1%)
1	I	0.84	1/2933 (0.0%)	0.81	4/3984 (0.1%)
1	J	0.82	0/2920	0.84	6/3965 (0.2%)
1	K	0.84	0/2914	0.86	6/3958 (0.2%)
1	L	0.84	0/2904	0.82	2/3943 (0.1%)
All	All	0.81	5/35156 (0.0%)	0.81	55/47736 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	K	0	1
1	L	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	312	GLU	CD-OE1	5.61	1.31	1.25
1	F	175	GLU	CD-OE2	-5.35	1.19	1.25
1	E	12	GLU	CG-CD	5.23	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	369	ILE	N-CA	-5.10	1.36	1.46
1	I	61	SER	CB-OG	-5.08	1.35	1.42

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ASP	CB-CG-OD2	10.49	127.74	118.30
1	F	211	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	C	317	ASP	CB-CG-OD2	7.73	125.26	118.30
1	B	304	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	G	195	ASP	CB-CG-OD1	-7.33	111.70	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	180	ASN	Mainchain
1	K	246	LEU	Mainchain
1	L	372	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2907	0	2949	206	0
1	B	2906	0	2929	199	0
1	C	2886	0	2907	195	1
1	D	2874	0	2901	193	0
1	E	2867	0	2891	214	0
1	F	2859	0	2876	241	1
1	G	2907	0	2949	359	0
1	H	2906	0	2929	230	0
1	I	2886	0	2907	332	0
1	J	2874	0	2901	341	0
1	K	2867	0	2891	273	0
1	L	2859	0	2876	245	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	2	0
2	K	5	0	0	1	0
2	L	5	0	0	0	0
All	All	34658	0	34906	2849	1

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 41.

The worst 5 of 2849 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:J:9:MET:CE	1:J:24:MET:HA	1.29	1.53
1:J:9:MET:HE3	1:J:24:MET:CA	1.57	1.35
1:G:291:ILE:HD13	1:G:316:PHE:CE2	1.64	1.31
1:G:355:PHE:CZ	1:G:365:TYR:CD2	2.23	1.25
1:D:236:CYS:SG	1:D:259:LEU:HD21	1.79	1.23

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLU:OE1	1:F:7:ASN:ND2[1_565]	2.18	0.02

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	367/391 (94%)	352 (96%)	14 (4%)	1 (0%)	41	74
1	B	369/391 (94%)	351 (95%)	16 (4%)	2 (0%)	29	67
1	C	367/391 (94%)	349 (95%)	15 (4%)	3 (1%)	19	58
1	D	366/391 (94%)	352 (96%)	13 (4%)	1 (0%)	41	74
1	E	365/391 (93%)	346 (95%)	15 (4%)	4 (1%)	14	51
1	F	362/391 (93%)	344 (95%)	16 (4%)	2 (1%)	25	64
1	G	367/391 (94%)	351 (96%)	13 (4%)	3 (1%)	19	58
1	H	369/391 (94%)	346 (94%)	19 (5%)	4 (1%)	14	51
1	I	367/391 (94%)	347 (95%)	19 (5%)	1 (0%)	41	74
1	J	366/391 (94%)	347 (95%)	18 (5%)	1 (0%)	41	74
1	K	365/391 (93%)	346 (95%)	18 (5%)	1 (0%)	41	74
1	L	362/391 (93%)	345 (95%)	14 (4%)	3 (1%)	19	58
All	All	4392/4692 (94%)	4176 (95%)	190 (4%)	26 (1%)	25	64

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	SER
1	E	332	VAL
1	G	332	VAL
1	H	188	SER
1	C	95	PRO

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	322/343 (94%)	304 (94%)	18 (6%)	21	57
1	B	319/343 (93%)	304 (95%)	15 (5%)	26	62
1	C	318/343 (93%)	301 (95%)	17 (5%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	316/343 (92%)	301 (95%)	15 (5%)	26 62
1	E	315/343 (92%)	301 (96%)	14 (4%)	28 64
1	F	314/343 (92%)	296 (94%)	18 (6%)	20 56
1	G	322/343 (94%)	289 (90%)	33 (10%)	7 29
1	H	319/343 (93%)	301 (94%)	18 (6%)	21 57
1	I	318/343 (93%)	293 (92%)	25 (8%)	12 43
1	J	316/343 (92%)	288 (91%)	28 (9%)	9 35
1	K	315/343 (92%)	283 (90%)	32 (10%)	7 29
1	L	314/343 (92%)	292 (93%)	22 (7%)	15 48
All	All	3808/4116 (92%)	3553 (93%)	255 (7%)	16 50

5 of 255 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	225	ARG
1	K	232	MET
1	H	267	THR
1	K	211	ARG
1	L	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	253	HIS
1	L	39	GLN
1	I	357	GLN
1	K	27	HIS
1	L	222	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)

12 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	PO4	C	401	-	4,4,4	0.82	0	6,6,6	0.81	0
2	PO4	I	401	-	4,4,4	0.82	0	6,6,6	1.40	0
2	PO4	L	401	-	4,4,4	0.87	0	6,6,6	0.67	0
2	PO4	H	401	-	4,4,4	0.85	0	6,6,6	1.37	1 (16%)
2	PO4	E	401	-	4,4,4	1.08	0	6,6,6	0.95	0
2	PO4	K	401	-	4,4,4	0.90	0	6,6,6	1.18	0
2	PO4	A	401	-	4,4,4	0.66	0	6,6,6	0.93	0
2	PO4	B	401	-	4,4,4	0.88	0	6,6,6	1.32	1 (16%)
2	PO4	F	401	-	4,4,4	0.94	0	6,6,6	1.41	0
2	PO4	G	401	-	4,4,4	0.85	0	6,6,6	1.29	1 (16%)
2	PO4	J	401	-	4,4,4	0.71	0	6,6,6	1.37	0
2	PO4	D	401	-	4,4,4	0.94	0	6,6,6	1.41	2 (33%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	PO4	O4-P-O3	2.65	116.15	107.91
2	H	401	PO4	O4-P-O1	-2.54	101.98	110.95
2	G	401	PO4	O3-P-O1	-2.51	102.08	110.95
2	D	401	PO4	O4-P-O1	-2.14	103.37	110.95
2	B	401	PO4	O2-P-O1	-2.08	103.58	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	401	PO4	1	0
2	J	401	PO4	2	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

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	369/391 (94%)	0.12	15 (4%)	37	24	60, 96, 130, 172	0
1	B	371/391 (94%)	-0.07	3 (0%)	86	78	62, 86, 119, 162	0
1	C	369/391 (94%)	-0.06	2 (0%)	91	86	57, 85, 115, 161	0
1	D	368/391 (94%)	-0.01	8 (2%)	62	48	57, 90, 121, 160	0
1	E	367/391 (93%)	0.08	8 (2%)	62	48	66, 96, 139, 164	0
1	F	366/391 (93%)	0.04	9 (2%)	57	43	64, 93, 122, 140	0
1	G	369/391 (94%)	0.08	12 (3%)	46	30	69, 101, 142, 165	0
1	H	371/391 (94%)	-0.02	6 (1%)	72	59	58, 89, 118, 169	0
1	I	369/391 (94%)	0.20	12 (3%)	46	30	71, 111, 151, 170	0
1	J	368/391 (94%)	0.08	4 (1%)	80	69	75, 102, 125, 141	0
1	K	367/391 (93%)	0.20	20 (5%)	25	14	74, 112, 150, 168	0
1	L	366/391 (93%)	0.31	16 (4%)	34	21	79, 110, 138, 162	0
All	All	4420/4692 (94%)	0.08	115 (2%)	56	40	57, 98, 136, 172	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	ASP	5.3
1	J	49	TYR	5.3
1	F	56	THR	4.4
1	J	304	ASP	4.3
1	G	362	GLU	4.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. 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	B-factors(Å^2)	Q<0.9
2	PO4	E	401	5/5	0.89	0.21	82,82,85,88	0
2	PO4	A	401	5/5	0.90	0.24	65,68,71,73	0
2	PO4	H	401	5/5	0.90	0.34	72,73,74,75	0
2	PO4	L	401	5/5	0.91	0.22	100,104,115,124	0
2	PO4	F	401	5/5	0.93	0.29	73,74,78,84	0
2	PO4	J	401	5/5	0.94	0.23	86,89,99,104	0
2	PO4	G	401	5/5	0.95	0.29	65,71,78,82	0
2	PO4	K	401	5/5	0.95	0.27	93,97,98,101	0
2	PO4	I	401	5/5	0.95	0.26	88,91,104,105	0
2	PO4	B	401	5/5	0.96	0.27	66,67,72,74	0
2	PO4	D	401	5/5	0.96	0.18	75,77,83,88	0
2	PO4	C	401	5/5	0.98	0.27	69,71,73,77	0

6.5 Other polymers (i)

There are no such residues in this entry.