



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4QFK  
Title : Crystal structure of dipeptide binding protein from pseudoalteromonas sp. SM9913  
Authors : Li, C.Y.; Zhang, Y.Z.  
Deposited on : 2014-05-21  
Resolution : 2.29 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

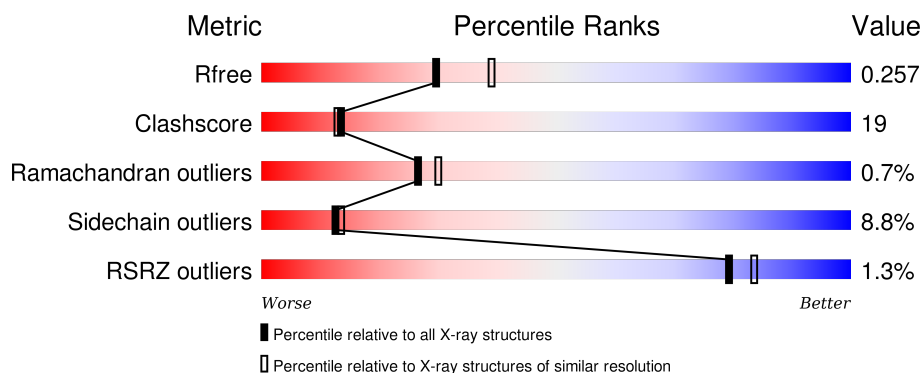
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	541	<div> <div>2%</div> <div>61% 29% 7%</div> </div>
1	B	541	<div> <div>2%</div> <div>63% 26% 5% 7%</div> </div>
1	C	541	<div> <div>2%</div> <div>60% 28% 5% 7%</div> </div>
1	D	541	<div> <div>2%</div> <div>64% 24% 5% 7%</div> </div>
1	E	541	<div> <div>2%</div> <div>59% 30% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	541	<div><div>%</div><div><div></div><div>60%</div><div>27%</div><div>6%</div><div>7%</div></div></div>
1	G	541	<div><div>3%</div><div><div></div><div>62%</div><div>26%</div><div>5%</div><div>7%</div></div></div>
1	H	541	<div><div></div><div><div></div><div>64%</div><div>24%</div><div>5%</div><div>7%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34170 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 ABC transporter periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	A	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	B	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	C	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	D	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	E	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	F	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0
1	G	505	Total 4061	C 2605	N 685	O 757	S 14	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
H	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
H	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
H	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
H	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
H	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
C	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
D	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
E	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
F	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
G	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	274	Total O 274 274	0	0
2	A	219	Total O 219 219	0	0

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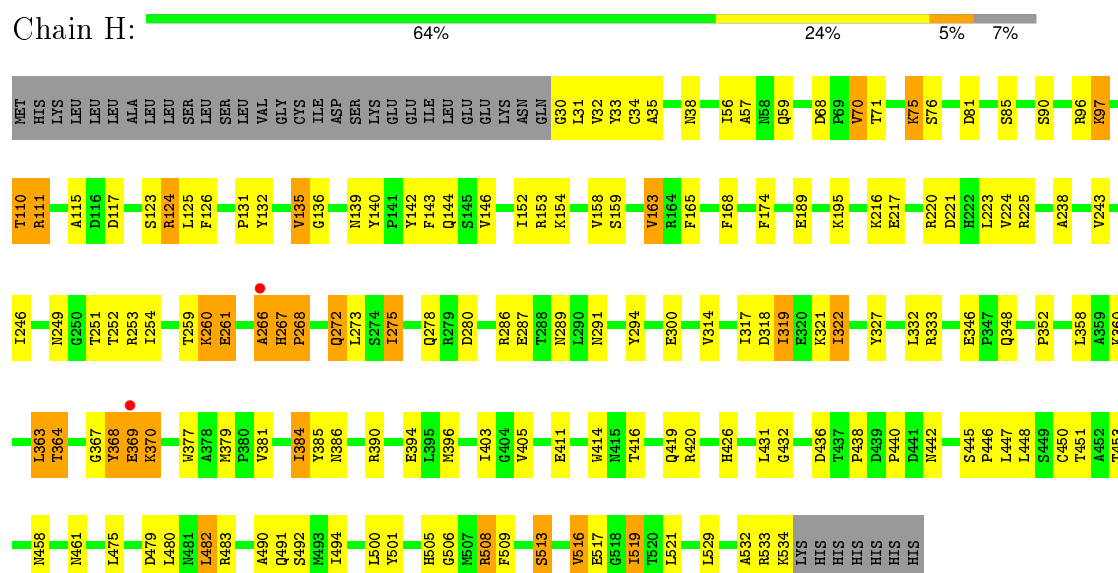
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	225	Total 225	O 225	0	0
2	C	227	Total 227	O 227	0	0
2	D	211	Total 211	O 211	0	0
2	E	159	Total 159	O 159	0	0
2	F	186	Total 186	O 186	0	0
2	G	181	Total 181	O 181	0	0

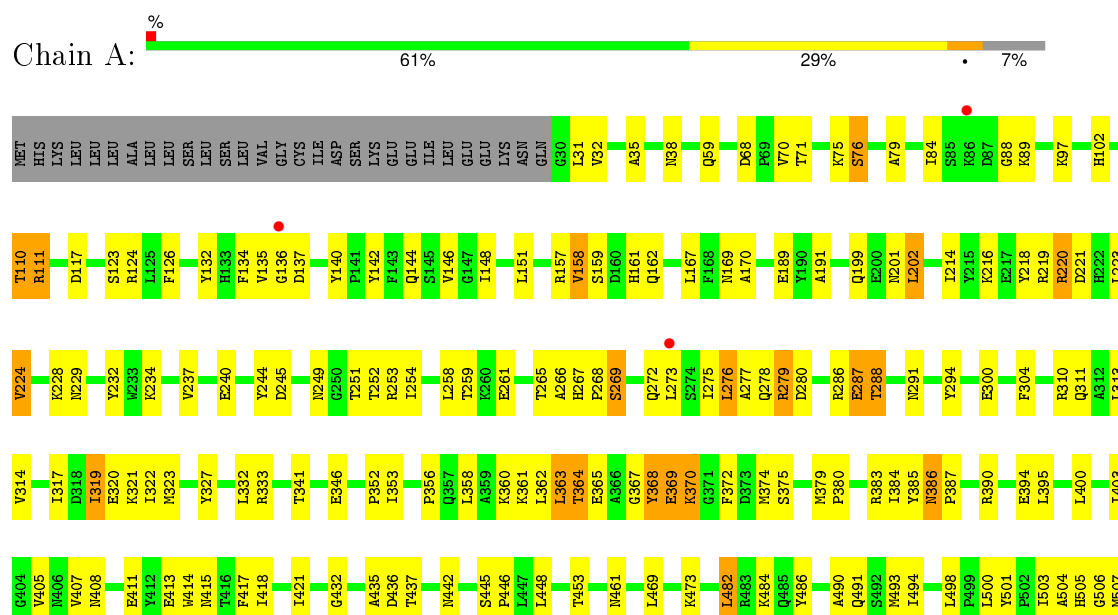
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: ABC transporter periplasmic peptide-binding protein

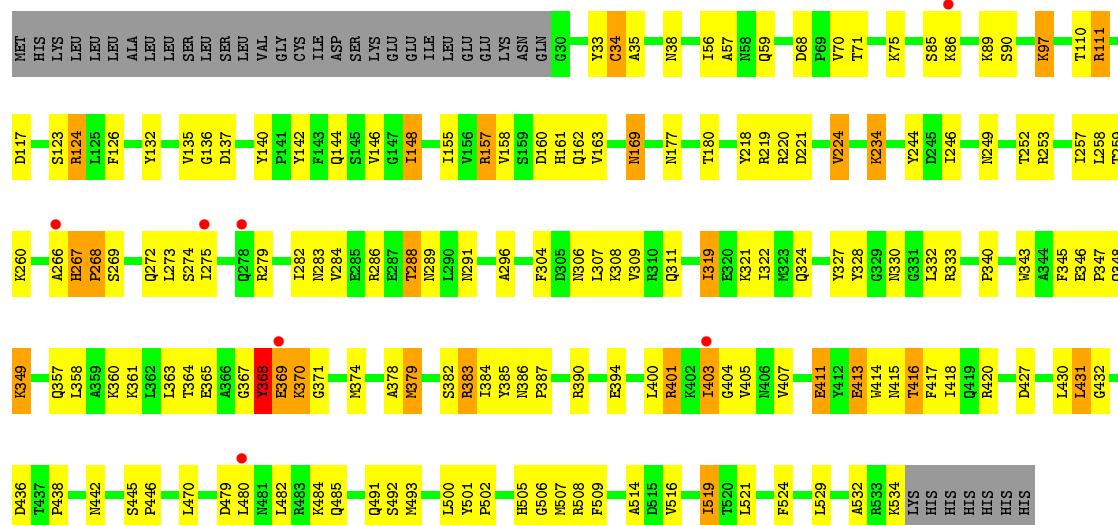


- Molecule 1: ABC transporter periplasmic peptide-binding protein

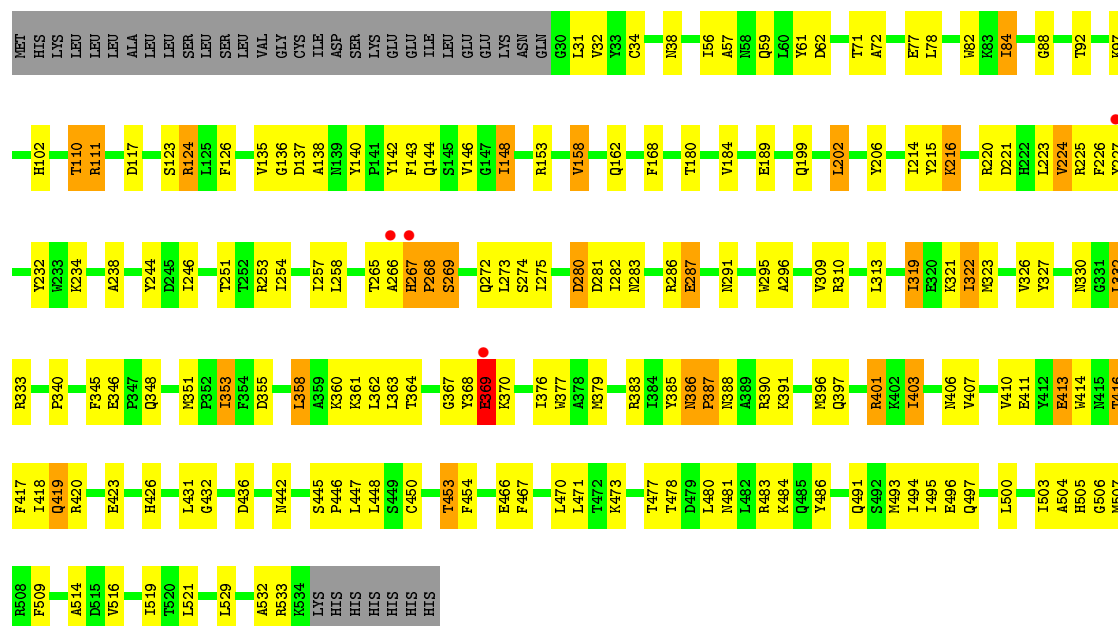




• Molecule 1: ABC transporter periplasmic peptide-binding protein



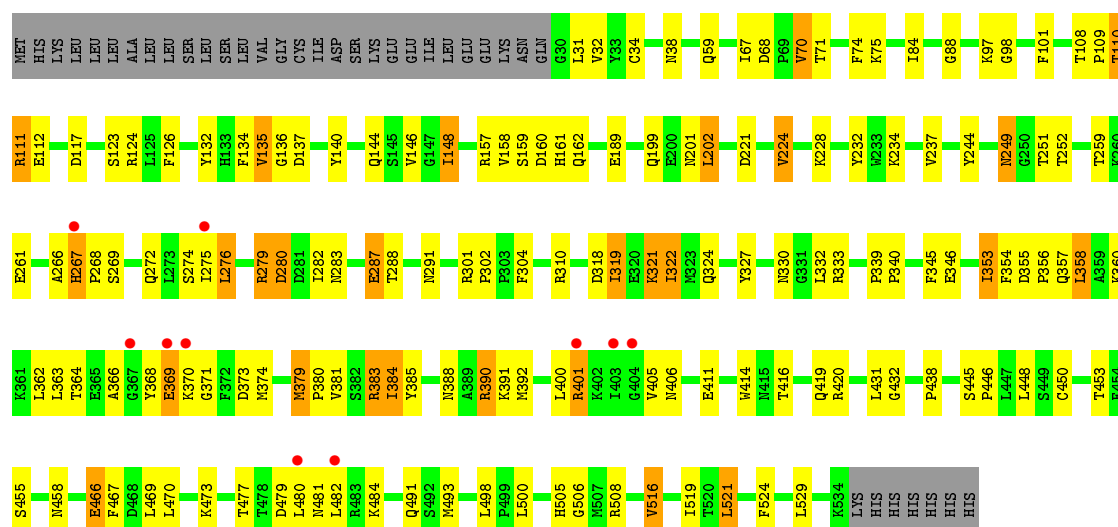
• Molecule 1: ABC transporter periplasmic peptide-binding protein



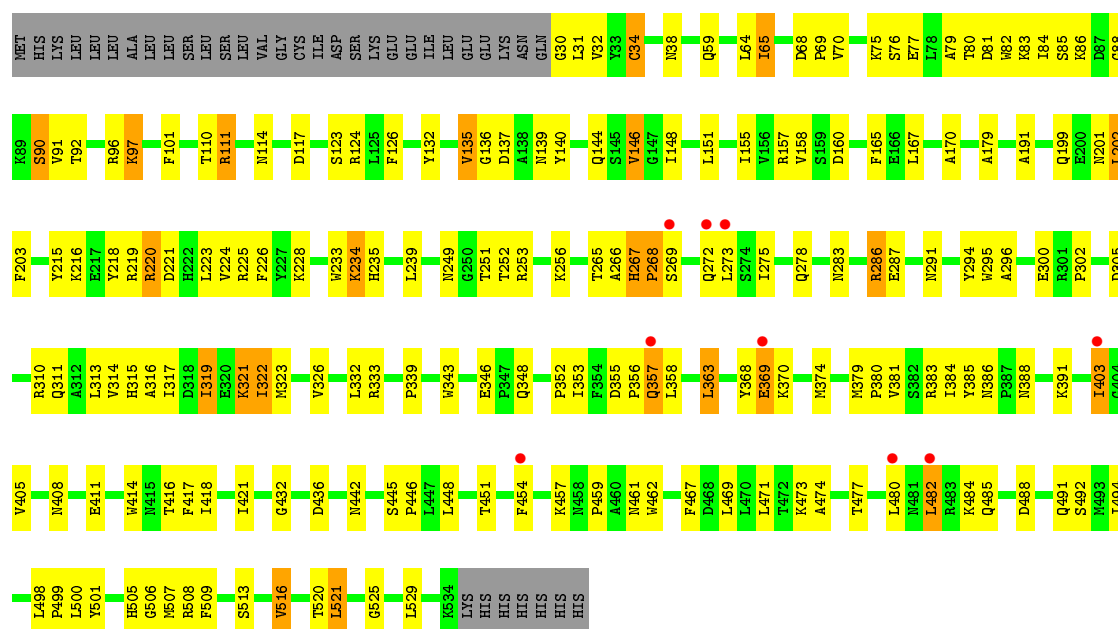
• Molecule 1: ABC transporter periplasmic peptide-binding protein



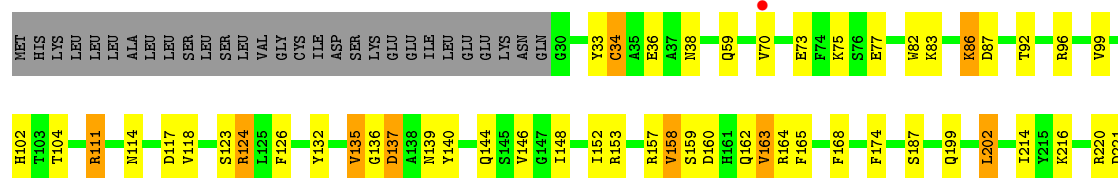


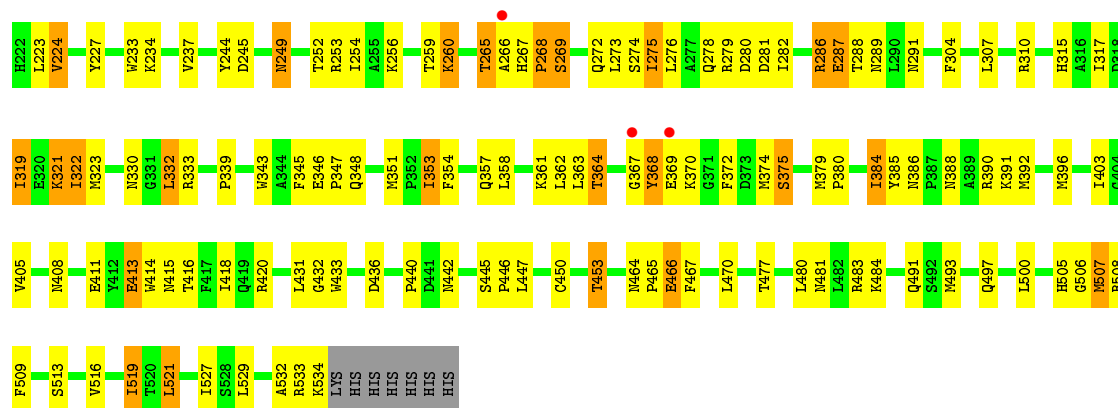


• Molecule 1: ABC transporter periplasmic peptide-binding protein

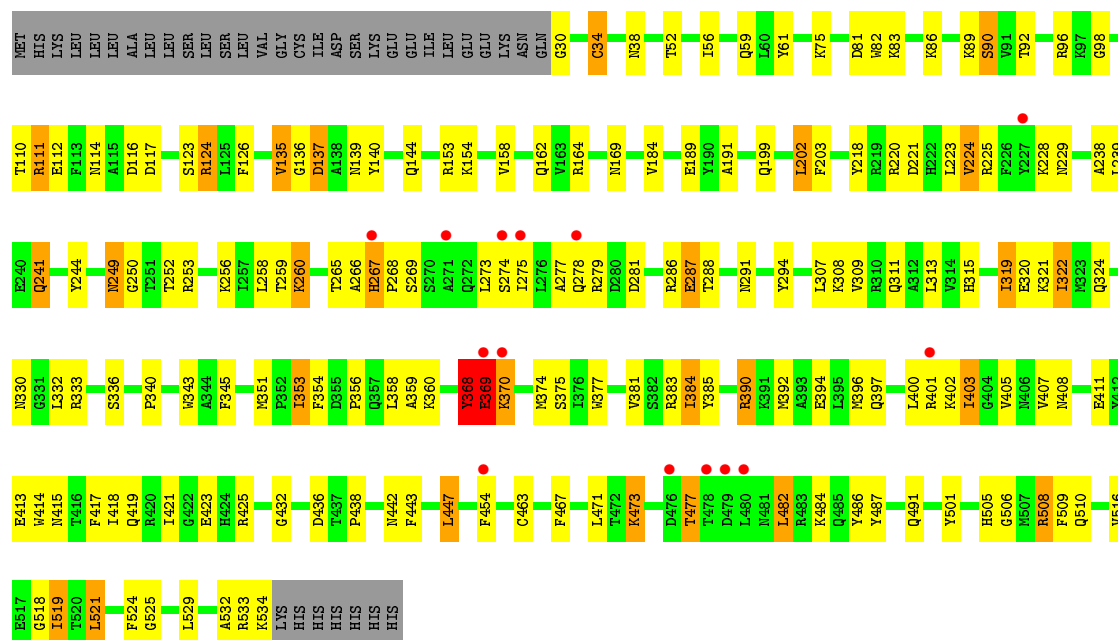


• Molecule 1: ABC transporter periplasmic peptide-binding protein





● Molecule 1: ABC transporter periplasmic peptide-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.39Å 93.97Å 140.55Å 80.03° 84.43° 69.84°	Depositor
Resolution (Å)	42.63 – 2.29 42.63 – 2.29	Depositor EDS
% Data completeness (in resolution range)	88.7 (42.63-2.29) 89.1 (42.63-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.191 , 0.257 0.196 , 0.257	Depositor DCC
$R_{free}$ test set	9376 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 185386 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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 ⓘ

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	0.45	1/4166 (0.0%)	0.61	1/5667 (0.0%)
1	B	0.45	1/4166 (0.0%)	0.62	2/5667 (0.0%)
1	C	0.45	1/4166 (0.0%)	0.62	1/5667 (0.0%)
1	D	0.41	0/4166	0.59	0/5667
1	E	0.40	1/4166 (0.0%)	0.58	1/5667 (0.0%)
1	F	0.39	0/4166	0.58	0/5667
1	G	0.39	0/4166	0.58	0/5667
1	H	0.45	0/4166	0.61	0/5667
All	All	0.42	4/33328 (0.0%)	0.60	5/45336 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	PRO	N-CD	5.35	1.55	1.47
1	C	387	PRO	N-CD	5.35	1.55	1.47
1	E	356	PRO	N-CD	5.28	1.55	1.47
1	B	387	PRO	N-CD	5.24	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ASN	C-N-CD	5.53	140.02	128.40
1	E	355	ASP	C-N-CD	5.53	140.01	128.40
1	B	386	ASN	C-N-CD	5.51	139.97	128.40
1	C	386	ASN	C-N-CD	5.50	139.96	128.40
1	B	157	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	4061	0	3968	164	0
1	B	4061	0	3968	151	0
1	C	4061	0	3968	177	0
1	D	4061	0	3968	145	0
1	E	4061	0	3968	139	0
1	F	4061	0	3968	169	0
1	G	4061	0	3968	136	0
1	H	4061	0	3968	138	0
2	A	219	0	0	10	0
2	B	225	0	0	9	0
2	C	227	0	0	3	0
2	D	211	0	0	5	0
2	E	159	0	0	4	0
2	F	186	0	0	7	0
2	G	181	0	0	3	0
2	H	274	0	0	7	0
All	All	34170	0	31744	1204	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 19.

The worst 5 of 1204 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:H:275:ILE:HD11	1:C:274:SER:HB2	1.30	1.12
1:D:279:ARG:HB2	1:D:280:ASP:CA	1.76	1.12
1:C:84:ILE:HD11	1:C:88:GLY:HA2	1.27	1.10
1:E:368:TYR:CA	1:E:369:GLU:HB2	1.82	1.09
1:H:384:ILE:H	1:H:384:ILE:HD13	1.12	1.08

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	503/541 (93%)	474 (94%)	25 (5%)	4 (1%)	24	26
1	B	503/541 (93%)	478 (95%)	21 (4%)	4 (1%)	24	26
1	C	503/541 (93%)	470 (93%)	29 (6%)	4 (1%)	24	26
1	D	503/541 (93%)	470 (93%)	30 (6%)	3 (1%)	30	34
1	E	503/541 (93%)	471 (94%)	29 (6%)	3 (1%)	30	34
1	F	503/541 (93%)	473 (94%)	28 (6%)	2 (0%)	39	47
1	G	503/541 (93%)	474 (94%)	24 (5%)	5 (1%)	19	20
1	H	503/541 (93%)	481 (96%)	18 (4%)	4 (1%)	24	26
All	All	4024/4328 (93%)	3791 (94%)	204 (5%)	29 (1%)	26	30

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	266	ALA
1	H	268	PRO
1	A	276	LEU
1	B	267	HIS
1	B	268	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	438/472 (93%)	405 (92%)	33 (8%)	17	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	438/472 (93%)	404 (92%)	34 (8%)	16	18
1	C	438/472 (93%)	405 (92%)	33 (8%)	17	19
1	D	438/472 (93%)	403 (92%)	35 (8%)	15	17
1	E	438/472 (93%)	397 (91%)	41 (9%)	11	11
1	F	438/472 (93%)	392 (90%)	46 (10%)	8	8
1	G	438/472 (93%)	394 (90%)	44 (10%)	9	10
1	H	438/472 (93%)	397 (91%)	41 (9%)	11	11
All	All	3504/3776 (93%)	3197 (91%)	307 (9%)	12	13

5 of 307 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	496	GLU
1	D	455	SER
1	G	322	ILE
1	D	70	VAL
1	D	280	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	497	GLN
1	D	491	GLN
1	G	205	GLN
1	D	38	ASN
1	D	267	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	505/541 (93%)	-0.29	3 (0%) 90 93	13, 25, 45, 63	0
1	B	505/541 (93%)	-0.18	7 (1%) 78 82	14, 24, 46, 71	0
1	C	505/541 (93%)	-0.22	4 (0%) 87 90	14, 25, 45, 66	0
1	D	505/541 (93%)	-0.21	10 (1%) 68 75	15, 27, 51, 72	0
1	E	505/541 (93%)	-0.06	9 (1%) 71 77	17, 31, 59, 78	0
1	F	505/541 (93%)	-0.15	4 (0%) 87 90	18, 30, 53, 72	0
1	G	505/541 (93%)	-0.13	14 (2%) 56 65	17, 30, 56, 82	0
1	H	505/541 (93%)	-0.35	2 (0%) 93 95	13, 22, 41, 55	0
All	All	4040/4328 (93%)	-0.20	53 (1%) 79 83	13, 27, 51, 82	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	266	ALA	6.1
1	G	275	ILE	5.7
1	G	369	GLU	5.4
1	C	369	GLU	5.0
1	H	369	GLU	3.9

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.