



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:46 PM GMT

PDB ID : 4DBL  
Title : Crystal structure of E159Q mutant of BtuCDF  
Authors : Korkhov, V.M.; Mireku, S.M.; Hvorup, R.N.; Locher, K.P.  
Deposited on : 2012-01-16  
Resolution : 3.49 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

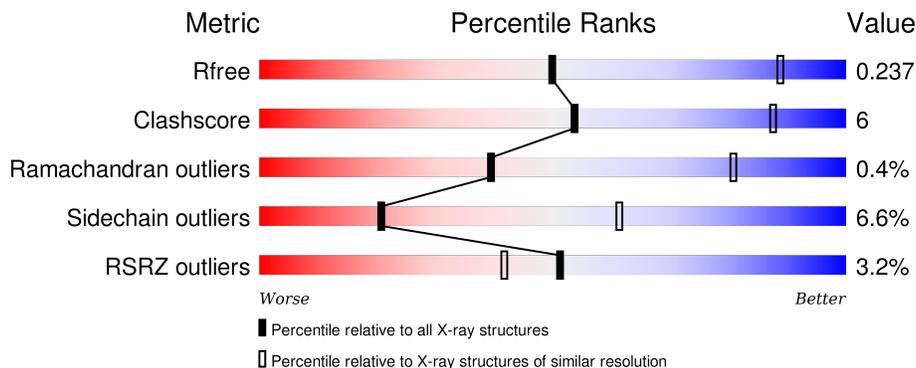
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	349	 6% 71% 19% • 7%
1	B	349	 % 72% 18% • 7%
1	F	349	 5% 73% 17% • 7%
1	G	349	 % 73% 17% • 7%
2	C	249	 % 85% 12% •

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Mol	Chain	Length	Quality of chain
2	D	249	 84% 13% .
2	H	249	 84% 12% .
2	I	249	 85% 12% .
3	E	255	 78% 18% . .
3	J	255	 78% 18% . .

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
4	PO4	C	301	-	-	X	-
4	PO4	H	301	-	-	X	-
5	SO4	I	303	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21230 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 Vitamin B12 import system permease protein BtuC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2441	1611	418	400	12	0	0	0
1	B	324	2441	1611	418	400	12	0	0	0
1	F	324	2441	1611	418	400	12	0	0	0
1	G	324	2441	1611	418	400	12	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP P06609
A	-21	GLY	-	EXPRESSION TAG	UNP P06609
A	-20	HIS	-	EXPRESSION TAG	UNP P06609
A	-19	HIS	-	EXPRESSION TAG	UNP P06609
A	-18	HIS	-	EXPRESSION TAG	UNP P06609
A	-17	HIS	-	EXPRESSION TAG	UNP P06609
A	-16	HIS	-	EXPRESSION TAG	UNP P06609
A	-15	HIS	-	EXPRESSION TAG	UNP P06609
A	-14	HIS	-	EXPRESSION TAG	UNP P06609
A	-13	HIS	-	EXPRESSION TAG	UNP P06609
A	-12	HIS	-	EXPRESSION TAG	UNP P06609
A	-11	HIS	-	EXPRESSION TAG	UNP P06609
A	-10	SER	-	EXPRESSION TAG	UNP P06609
A	-9	SER	-	EXPRESSION TAG	UNP P06609
A	-8	GLY	-	EXPRESSION TAG	UNP P06609
A	-7	GLU	-	EXPRESSION TAG	UNP P06609
A	-6	ASN	-	EXPRESSION TAG	UNP P06609
A	-5	LEU	-	EXPRESSION TAG	UNP P06609
A	-4	TYR	-	EXPRESSION TAG	UNP P06609
A	-3	PHE	-	EXPRESSION TAG	UNP P06609
A	-2	GLN	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P06609
A	0	HIS	-	EXPRESSION TAG	UNP P06609
A	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
A	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	-22	MET	-	EXPRESSION TAG	UNP P06609
B	-21	GLY	-	EXPRESSION TAG	UNP P06609
B	-20	HIS	-	EXPRESSION TAG	UNP P06609
B	-19	HIS	-	EXPRESSION TAG	UNP P06609
B	-18	HIS	-	EXPRESSION TAG	UNP P06609
B	-17	HIS	-	EXPRESSION TAG	UNP P06609
B	-16	HIS	-	EXPRESSION TAG	UNP P06609
B	-15	HIS	-	EXPRESSION TAG	UNP P06609
B	-14	HIS	-	EXPRESSION TAG	UNP P06609
B	-13	HIS	-	EXPRESSION TAG	UNP P06609
B	-12	HIS	-	EXPRESSION TAG	UNP P06609
B	-11	HIS	-	EXPRESSION TAG	UNP P06609
B	-10	SER	-	EXPRESSION TAG	UNP P06609
B	-9	SER	-	EXPRESSION TAG	UNP P06609
B	-8	GLY	-	EXPRESSION TAG	UNP P06609
B	-7	GLU	-	EXPRESSION TAG	UNP P06609
B	-6	ASN	-	EXPRESSION TAG	UNP P06609
B	-5	LEU	-	EXPRESSION TAG	UNP P06609
B	-4	TYR	-	EXPRESSION TAG	UNP P06609
B	-3	PHE	-	EXPRESSION TAG	UNP P06609
B	-2	GLN	-	EXPRESSION TAG	UNP P06609
B	-1	GLY	-	EXPRESSION TAG	UNP P06609
B	0	HIS	-	EXPRESSION TAG	UNP P06609
B	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
B	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	-22	MET	-	EXPRESSION TAG	UNP P06609
F	-21	GLY	-	EXPRESSION TAG	UNP P06609
F	-20	HIS	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	HIS	-	EXPRESSION TAG	UNP P06609
F	-18	HIS	-	EXPRESSION TAG	UNP P06609
F	-17	HIS	-	EXPRESSION TAG	UNP P06609
F	-16	HIS	-	EXPRESSION TAG	UNP P06609
F	-15	HIS	-	EXPRESSION TAG	UNP P06609
F	-14	HIS	-	EXPRESSION TAG	UNP P06609
F	-13	HIS	-	EXPRESSION TAG	UNP P06609
F	-12	HIS	-	EXPRESSION TAG	UNP P06609
F	-11	HIS	-	EXPRESSION TAG	UNP P06609
F	-10	SER	-	EXPRESSION TAG	UNP P06609
F	-9	SER	-	EXPRESSION TAG	UNP P06609
F	-8	GLY	-	EXPRESSION TAG	UNP P06609
F	-7	GLU	-	EXPRESSION TAG	UNP P06609
F	-6	ASN	-	EXPRESSION TAG	UNP P06609
F	-5	LEU	-	EXPRESSION TAG	UNP P06609
F	-4	TYR	-	EXPRESSION TAG	UNP P06609
F	-3	PHE	-	EXPRESSION TAG	UNP P06609
F	-2	GLN	-	EXPRESSION TAG	UNP P06609
F	-1	GLY	-	EXPRESSION TAG	UNP P06609
F	0	HIS	-	EXPRESSION TAG	UNP P06609
F	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
F	267	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	-22	MET	-	EXPRESSION TAG	UNP P06609
G	-21	GLY	-	EXPRESSION TAG	UNP P06609
G	-20	HIS	-	EXPRESSION TAG	UNP P06609
G	-19	HIS	-	EXPRESSION TAG	UNP P06609
G	-18	HIS	-	EXPRESSION TAG	UNP P06609
G	-17	HIS	-	EXPRESSION TAG	UNP P06609
G	-16	HIS	-	EXPRESSION TAG	UNP P06609
G	-15	HIS	-	EXPRESSION TAG	UNP P06609
G	-14	HIS	-	EXPRESSION TAG	UNP P06609
G	-13	HIS	-	EXPRESSION TAG	UNP P06609
G	-12	HIS	-	EXPRESSION TAG	UNP P06609
G	-11	HIS	-	EXPRESSION TAG	UNP P06609
G	-10	SER	-	EXPRESSION TAG	UNP P06609
G	-9	SER	-	EXPRESSION TAG	UNP P06609
G	-8	GLY	-	EXPRESSION TAG	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	GLU	-	EXPRESSION TAG	UNP P06609
G	-6	ASN	-	EXPRESSION TAG	UNP P06609
G	-5	LEU	-	EXPRESSION TAG	UNP P06609
G	-4	TYR	-	EXPRESSION TAG	UNP P06609
G	-3	PHE	-	EXPRESSION TAG	UNP P06609
G	-2	GLN	-	EXPRESSION TAG	UNP P06609
G	-1	GLY	-	EXPRESSION TAG	UNP P06609
G	0	HIS	-	EXPRESSION TAG	UNP P06609
G	18	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	32	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	120	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	156	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	205	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	206	SER	CYS	ENGINEERED MUTATION	UNP P06609
G	267	SER	CYS	ENGINEERED MUTATION	UNP P06609

- Molecule 2 is a protein called Vitamin B12 import ATP-binding protein BtuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	248	1893	1184	352	349	8	0	0	0
2	D	248	1893	1184	352	349	8	0	0	0
2	H	248	1893	1184	352	349	8	0	0	0
2	I	248	1893	1184	352	349	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
C	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
D	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
D	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
H	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
H	180	SER	CYS	ENGINEERED MUTATION	UNP P06611
I	159	GLN	GLU	ENGINEERED MUTATION	UNP P06611
I	180	SER	CYS	ENGINEERED MUTATION	UNP P06611

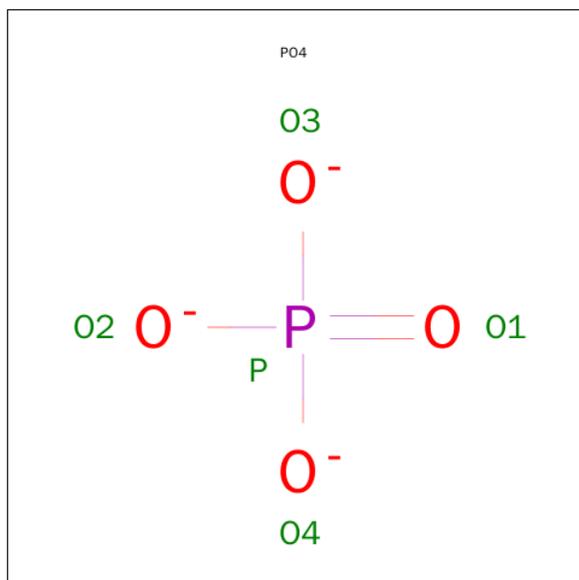
- Molecule 3 is a protein called Vitamin B12-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	245	Total	C	N	O	S	0	0	0
			1907	1216	332	355	4			
3	J	245	Total	C	N	O	S	0	0	0
			1907	1216	332	355	4			

There are 20 discrepancies between the modelled and reference sequences:

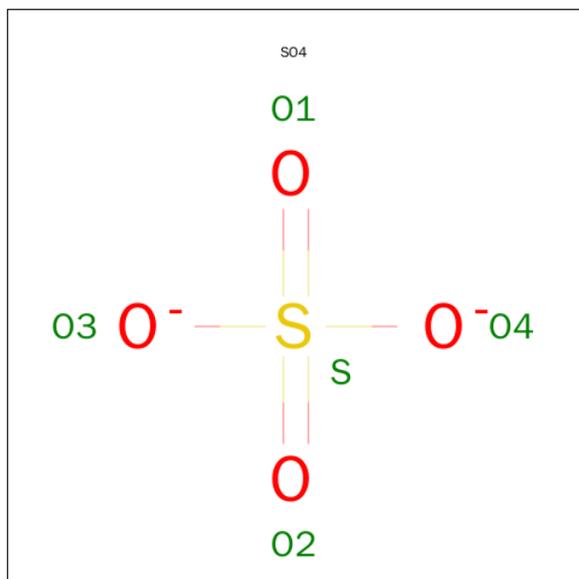
Chain	Residue	Modelled	Actual	Comment	Reference
E	21	MET	-	INITIATING METHIONINE	UNP P37028
E	267	SER	-	EXPRESSION TAG	UNP P37028
E	268	GLY	-	EXPRESSION TAG	UNP P37028
E	269	SER	-	EXPRESSION TAG	UNP P37028
E	270	HIS	-	EXPRESSION TAG	UNP P37028
E	271	HIS	-	EXPRESSION TAG	UNP P37028
E	272	HIS	-	EXPRESSION TAG	UNP P37028
E	273	HIS	-	EXPRESSION TAG	UNP P37028
E	274	HIS	-	EXPRESSION TAG	UNP P37028
E	275	HIS	-	EXPRESSION TAG	UNP P37028
J	21	MET	-	INITIATING METHIONINE	UNP P37028
J	267	SER	-	EXPRESSION TAG	UNP P37028
J	268	GLY	-	EXPRESSION TAG	UNP P37028
J	269	SER	-	EXPRESSION TAG	UNP P37028
J	270	HIS	-	EXPRESSION TAG	UNP P37028
J	271	HIS	-	EXPRESSION TAG	UNP P37028
J	272	HIS	-	EXPRESSION TAG	UNP P37028
J	273	HIS	-	EXPRESSION TAG	UNP P37028
J	274	HIS	-	EXPRESSION TAG	UNP P37028
J	275	HIS	-	EXPRESSION TAG	UNP P37028

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0
4	D	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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

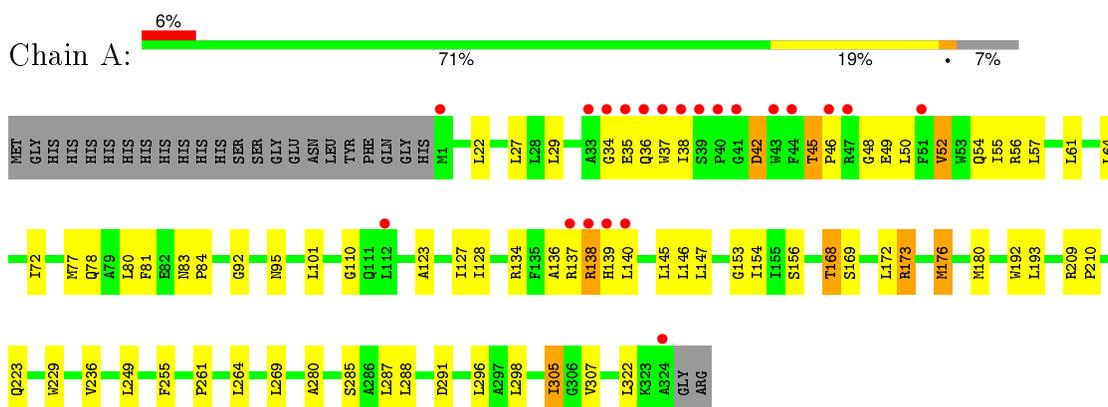


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total 5 4 1	0	0
5	C	1	Total 5 4 1	0	0
5	C	1	Total 5 4 1	0	0
5	D	1	Total 5 4 1	0	0
5	D	1	Total 5 4 1	0	0
5	D	1	Total 5 4 1	0	0
5	H	1	Total 5 4 1	0	0
5	H	1	Total 5 4 1	0	0
5	H	1	Total 5 4 1	0	0
5	I	1	Total 5 4 1	0	0
5	I	1	Total 5 4 1	0	0
5	I	1	Total 5 4 1	0	0

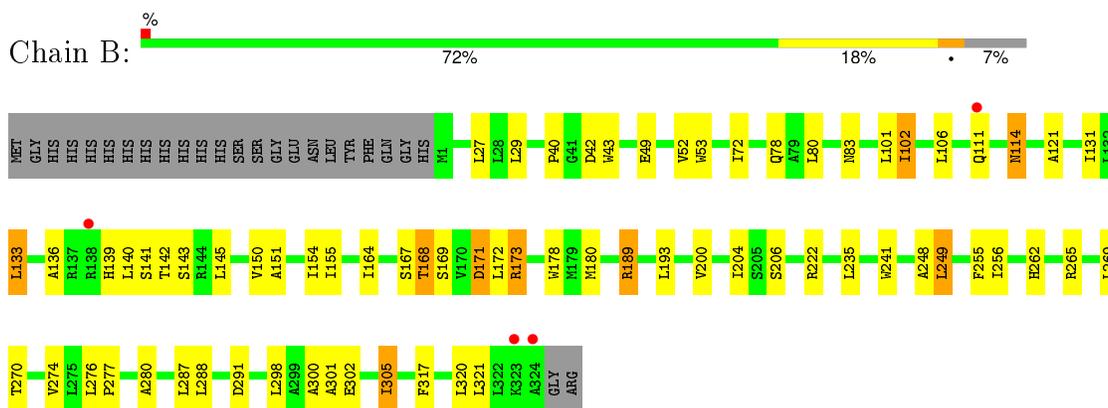
### 3 Residue-property plots [i](#)

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.

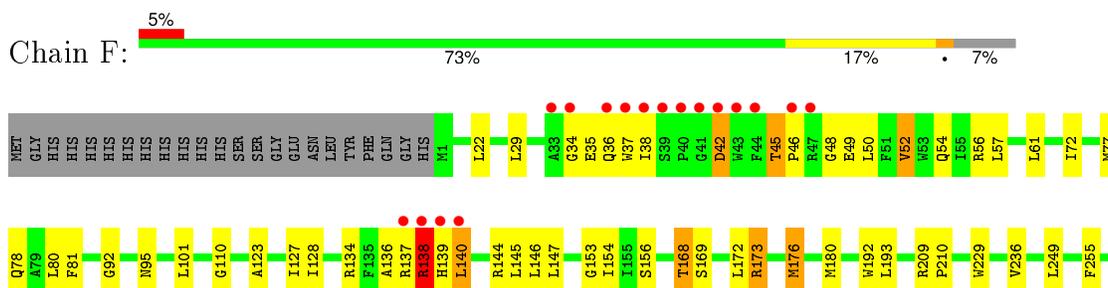
- Molecule 1: Vitamin B12 import system permease protein BtuC



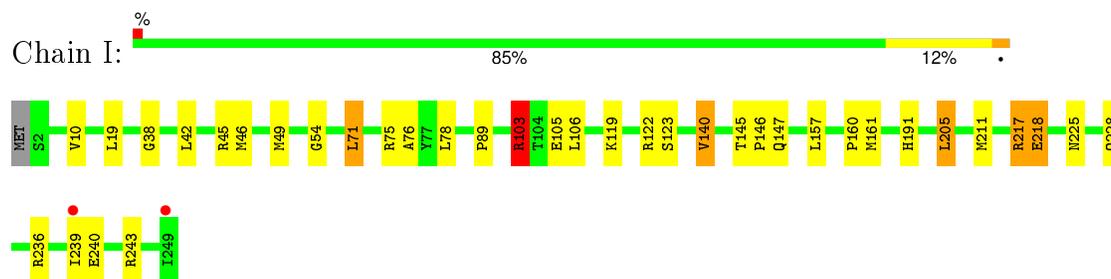
- Molecule 1: Vitamin B12 import system permease protein BtuC



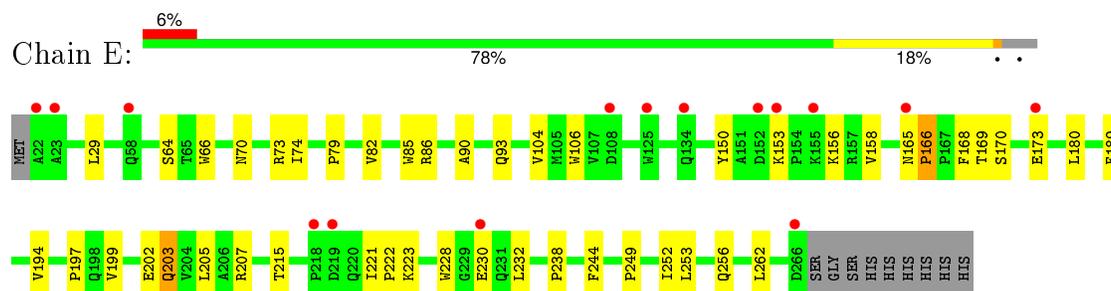
- Molecule 1: Vitamin B12 import system permease protein BtuC



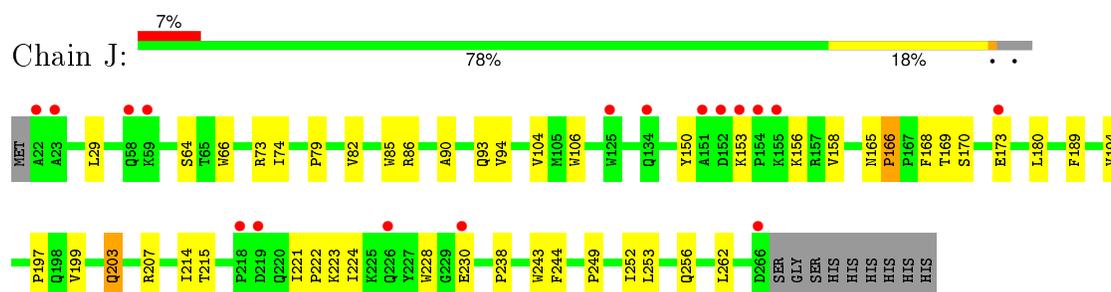




- Molecule 3: Vitamin B12-binding protein



- Molecule 3: Vitamin B12-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.65Å 166.93Å 132.82Å 90.00° 119.76° 90.00°	Depositor
Resolution (Å)	30.02 – 3.49 30.02 – 3.49	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.02-3.49) 92.6 (30.02-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.47Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.214 , 0.251 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	2016 reflections (3.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.2	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.7	EDS
Estimated twinning fraction	0.005 for l,k,-h-l 0.005 for -h-l,k,h 0.418 for -h-l,-k,l 0.015 for h,-k,-h-l 0.012 for l,-k,h	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 59355 reflections	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	21230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SO4

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	0.27	0/2495	0.59	3/3408 (0.1%)
1	B	0.24	0/2495	0.41	0/3408
1	F	0.27	0/2495	0.52	3/3408 (0.1%)
1	G	0.24	0/2495	0.41	0/3408
2	C	0.24	0/1927	0.65	6/2611 (0.2%)
2	D	0.25	0/1927	0.65	6/2611 (0.2%)
2	H	0.24	0/1927	0.65	6/2611 (0.2%)
2	I	0.24	0/1927	0.64	6/2611 (0.2%)
3	E	0.22	0/1951	0.41	0/2661
3	J	0.22	0/1951	0.41	0/2661
All	All	0.25	0/21590	0.54	30/29398 (0.1%)

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	NE-CZ-NH2	15.78	128.19	120.30
1	A	138	ARG	NE-CZ-NH1	-15.16	112.72	120.30
2	H	45	ARG	NE-CZ-NH2	-13.07	113.77	120.30
2	C	45	ARG	NE-CZ-NH2	-12.95	113.83	120.30
2	D	45	ARG	NE-CZ-NH1	-12.68	113.96	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2441	0	2606	41	0
1	B	2441	0	2606	42	0
1	F	2441	0	2606	39	0
1	G	2441	0	2606	41	0
2	C	1893	0	1927	22	0
2	D	1893	0	1927	24	0
2	H	1893	0	1927	22	0
2	I	1893	0	1927	25	0
3	E	1907	0	1924	28	0
3	J	1907	0	1924	27	0
4	C	5	0	0	2	0
4	D	5	0	0	1	0
4	H	5	0	0	2	0
4	I	5	0	0	1	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	H	15	0	0	0	0
5	I	15	0	0	2	0
All	All	21230	0	21980	280	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 6.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:GLY:O	3:J:223:LYS:NZ	2.12	0.83
1:G:173:ARG:NH2	3:J:66:TRP:O	2.15	0.79
1:A:110:GLY:O	3:E:223:LYS:NZ	2.16	0.77
1:B:173:ARG:NH2	3:E:66:TRP:O	2.18	0.77
1:A:38:ILE:HD13	1:A:48:GLY:HA2	1.71	0.72

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	322/349 (92%)	309 (96%)	13 (4%)	0	100	100
1	B	322/349 (92%)	306 (95%)	14 (4%)	2 (1%)	30	75
1	F	322/349 (92%)	309 (96%)	13 (4%)	0	100	100
1	G	322/349 (92%)	306 (95%)	14 (4%)	2 (1%)	30	75
2	C	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	39	81
2	D	246/249 (99%)	243 (99%)	2 (1%)	1 (0%)	39	81
2	H	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	39	81
2	I	246/249 (99%)	242 (98%)	3 (1%)	1 (0%)	39	81
3	E	243/255 (95%)	225 (93%)	16 (7%)	2 (1%)	24	70
3	J	243/255 (95%)	225 (93%)	16 (7%)	2 (1%)	24	70
All	All	2758/2902 (95%)	2649 (96%)	97 (4%)	12 (0%)	39	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	103	ARG
2	H	103	ARG
1	B	139	HIS
1	B	142	THR
2	D	103	ARG

### 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	249/270 (92%)	227 (91%)	22 (9%)	12	48
1	B	249/270 (92%)	227 (91%)	22 (9%)	12	48
1	F	249/270 (92%)	227 (91%)	22 (9%)	12	48
1	G	249/270 (92%)	227 (91%)	22 (9%)	12	48
2	C	200/201 (100%)	189 (94%)	11 (6%)	27	67
2	D	200/201 (100%)	190 (95%)	10 (5%)	30	69
2	H	200/201 (100%)	189 (94%)	11 (6%)	27	67
2	I	200/201 (100%)	191 (96%)	9 (4%)	34	73
3	E	205/214 (96%)	197 (96%)	8 (4%)	39	76
3	J	205/214 (96%)	197 (96%)	8 (4%)	39	76
All	All	2206/2312 (95%)	2061 (93%)	145 (7%)	21	61

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	73	ARG
1	F	61	LEU
2	I	217	ARG
3	E	173	GLU
1	F	29	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	62	GLN
1	F	272	HIS
2	I	195	HIS
2	D	199	HIS
2	I	97	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](#)

16 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	$\# Z  > 2$
4	PO4	C	301	-	4,4,4	0.60	0	6,6,6	0.29	0
5	SO4	C	302	-	4,4,4	0.19	0	6,6,6	0.08	0
5	SO4	C	303	-	4,4,4	0.19	0	6,6,6	0.08	0
5	SO4	C	304	-	4,4,4	0.17	0	6,6,6	0.07	0
4	PO4	D	301	-	4,4,4	0.57	0	6,6,6	0.28	0
5	SO4	D	302	-	4,4,4	0.19	0	6,6,6	0.07	0
5	SO4	D	303	-	4,4,4	0.18	0	6,6,6	0.09	0
5	SO4	D	304	-	4,4,4	0.18	0	6,6,6	0.08	0
4	PO4	H	301	-	4,4,4	0.51	0	6,6,6	0.27	0
5	SO4	H	302	-	4,4,4	0.17	0	6,6,6	0.09	0
5	SO4	H	303	-	4,4,4	0.17	0	6,6,6	0.08	0
5	SO4	H	304	-	4,4,4	0.18	0	6,6,6	0.08	0
4	PO4	I	301	-	4,4,4	0.43	0	6,6,6	0.28	0
5	SO4	I	302	-	4,4,4	0.17	0	6,6,6	0.07	0
5	SO4	I	303	-	4,4,4	0.19	0	6,6,6	0.08	0
5	SO4	I	304	-	4,4,4	0.19	0	6,6,6	0.09	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	C	301	-	-	0/0/0/0	0/0/0/0
5	SO4	C	302	-	-	0/0/0/0	0/0/0/0
5	SO4	C	303	-	-	0/0/0/0	0/0/0/0
5	SO4	C	304	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	D	301	-	-	0/0/0/0	0/0/0/0
5	SO4	D	302	-	-	0/0/0/0	0/0/0/0
5	SO4	D	303	-	-	0/0/0/0	0/0/0/0
5	SO4	D	304	-	-	0/0/0/0	0/0/0/0
4	PO4	H	301	-	-	0/0/0/0	0/0/0/0
5	SO4	H	302	-	-	0/0/0/0	0/0/0/0
5	SO4	H	303	-	-	0/0/0/0	0/0/0/0
5	SO4	H	304	-	-	0/0/0/0	0/0/0/0
4	PO4	I	301	-	-	0/0/0/0	0/0/0/0
5	SO4	I	302	-	-	0/0/0/0	0/0/0/0
5	SO4	I	303	-	-	0/0/0/0	0/0/0/0
5	SO4	I	304	-	-	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.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	PO4	2	0
4	D	301	PO4	1	0
4	H	301	PO4	2	0
4	I	301	PO4	1	0
5	I	303	SO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	324/349 (92%)	-0.21	21 (6%) 22 17	16, 52, 148, 268	0
1	B	324/349 (92%)	-0.42	4 (1%) 81 72	15, 46, 114, 241	0
1	F	324/349 (92%)	-0.20	18 (5%) 28 22	15, 50, 144, 254	0
1	G	324/349 (92%)	-0.39	4 (1%) 81 72	16, 45, 117, 237	0
2	C	248/249 (99%)	-0.25	2 (0%) 87 80	17, 52, 115, 165	0
2	D	248/249 (99%)	-0.34	1 (0%) 93 90	12, 35, 96, 159	0
2	H	248/249 (99%)	-0.21	4 (1%) 74 65	16, 53, 113, 202	0
2	I	248/249 (99%)	-0.36	2 (0%) 87 80	12, 36, 93, 183	0
3	E	245/255 (96%)	0.10	15 (6%) 25 19	42, 98, 160, 208	0
3	J	245/255 (96%)	0.12	17 (6%) 20 16	46, 95, 165, 224	0
All	All	2778/2902 (95%)	-0.23	88 (3%) 51 42	12, 53, 138, 268	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	36	GLN	10.1
1	A	36	GLN	8.5
1	G	324	ALA	7.9
1	B	323	LYS	7.9
1	B	324	ALA	7.8

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PO4	C	301	5/5	0.96	0.11	-1.69	39,40,40,41	0
4	PO4	I	301	5/5	0.97	0.10	-1.96	34,35,36,36	0
4	PO4	H	301	5/5	0.98	0.09	-2.09	41,42,42,43	0
4	PO4	D	301	5/5	0.98	0.09	-2.12	28,29,30,30	0
5	SO4	C	303	5/5	0.86	0.59	-	139,139,140,140	0
5	SO4	I	302	5/5	0.77	0.31	-	152,153,153,155	0
5	SO4	H	304	5/5	0.84	0.40	-	153,153,153,155	0
5	SO4	D	303	5/5	0.91	0.29	-	144,144,144,145	0
5	SO4	D	304	5/5	0.78	0.48	-	142,142,143,143	0
5	SO4	H	302	5/5	0.92	0.43	-	146,146,147,148	0
5	SO4	I	304	5/5	0.93	0.40	-	159,159,160,162	0
5	SO4	D	302	5/5	0.81	0.37	-	145,145,146,146	0
5	SO4	C	302	5/5	0.94	0.35	-	142,142,143,143	0
5	SO4	H	303	5/5	0.85	0.51	-	143,143,143,145	0
5	SO4	C	304	5/5	0.81	0.33	-	145,145,146,146	0
5	SO4	I	303	5/5	0.89	0.31	-	157,157,158,159	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.