



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 23, 2019 – 01:38 PM EST

PDB ID : 6T2V  
EMDB ID: : EMD-10370  
Title : Cryo-EM structure of the RecBCD in complex with Chi-plus2 substrate  
Authors : Cheng, K.; Wilkinson, M.; Wigley, D.B.  
Deposited on : 2019-10-09  
Resolution : 3.80 Å(reported)  
Based on PDB ID : 5LD2

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

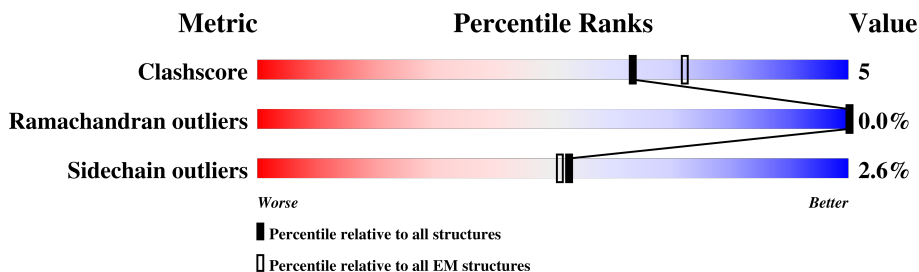
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	1181	82% 13% . .
2	C	1122	87% 13%
3	D	608	82% 15% . .
4	X	87	49% 13% 38%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23826 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RecBCD enzyme subunit RecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1129	Total	C	N	O	S	0	0
			9047	5713	1602	1694	38		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P08394
B	1080	ALA	ASP	engineered mutation	UNP P08394

- Molecule 2 is a protein called RecBCD enzyme subunit RecC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0
			9078	5783	1568	1684	43		

- Molecule 3 is a protein called RecBCD enzyme subunit RecD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	597	Total	C	N	O	S	0	0
			4603	2871	850	862	20		

- Molecule 4 is a DNA chain called DNA (Chi-plus2).

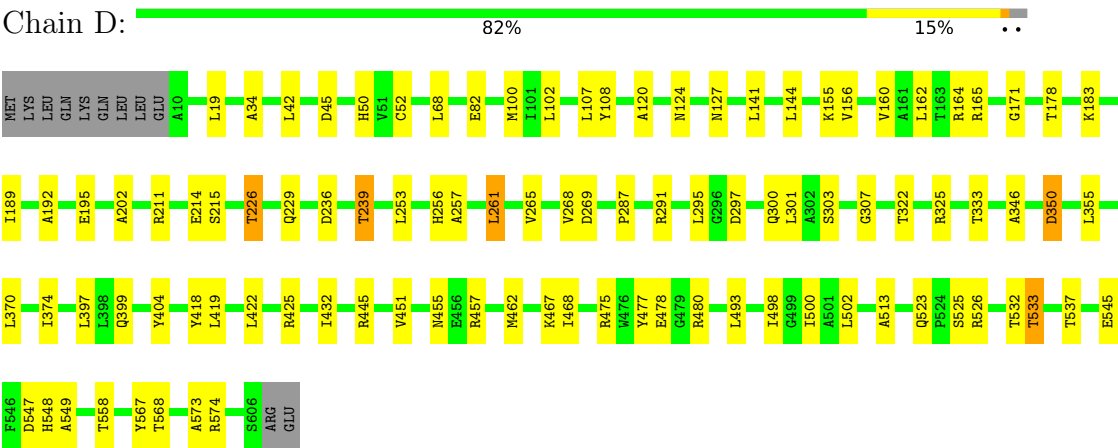
Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	54	Total	C	N	O	P	0	0
			1098	530	172	342	54		



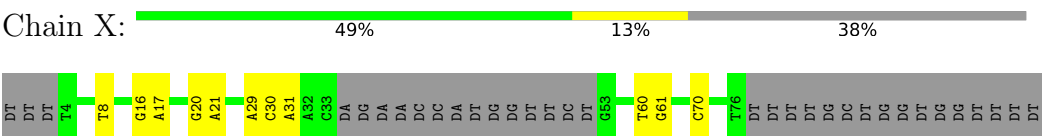
- Molecule 1: RecBCD enzyme subunit RecB



● Molecule 3: RecBCD enzyme subunit RecD



● Molecule 4: DNA (Chi-plus2)



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	380912	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	75.9	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality [i](#)

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	B	0.23	0/9242	0.38	0/12537
2	C	0.23	0/9305	0.37	0/12644
3	D	0.23	0/4683	0.39	0/6346
4	X	0.48	0/1222	1.01	0/1882
All	All	0.25	0/24452	0.44	0/33409

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 [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	B	9047	0	8906	87	0
2	C	9078	0	8877	80	0
3	D	4603	0	4622	53	0
4	X	1098	0	622	11	0
All	All	23826	0	23027	219	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 5.

The worst 5 of 219 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)
2:C:149:TRP:HE1	2:C:162:GLN:HE21	1.26	0.83
1:B:252:ILE:HG23	1:B:254:ARG:H	1.54	0.73
1:B:759:ASN:OD1	1:B:822:ARG:NH2	2.21	0.73
1:B:824:ARG:HG3	4:X:20:DG:H4'	1.70	0.72
3:D:100:MET:HB3	3:D:107:LEU:HD11	1.76	0.66

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 PDB entries followed by that with respect to all EM entries.

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	B	1123/1181 (95%)	1096 (98%)	26 (2%)	1 (0%)	53	87
2	C	1119/1122 (100%)	1106 (99%)	13 (1%)	0	100	100
3	D	595/608 (98%)	577 (97%)	18 (3%)	0	100	100
All	All	2837/2911 (98%)	2779 (98%)	57 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	877	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 PDB entries followed by that with respect to all EM entries.

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	B	958/998 (96%)	929 (97%)	29 (3%)	44	73
2	C	976/977 (100%)	961 (98%)	15 (2%)	67	85
3	D	481/492 (98%)	463 (96%)	18 (4%)	37	69
All	All	2415/2467 (98%)	2353 (97%)	62 (3%)	53	76

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1159	ARG
2	C	591	CYS
3	D	493	LEU
2	C	394	LEU
2	C	804	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1133	HIS
2	C	162	GLN
3	D	128	HIS
1	B	1134	HIS
1	B	1150	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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.