



## wwPDB EM Map/Model Validation Report ⓘ

Sep 29, 2016 – 11:14 AM EDT

PDB ID : 5LD2  
EMDB ID: : EMD-4038  
Title : Cryo-EM structure of RecBCD+DNA complex revealing activated nuclease domain  
Authors : Wilkinson, M.; Chaban, Y.; Wigley, D.B.  
Deposited on : 2016-06-23  
Resolution : 3.83 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

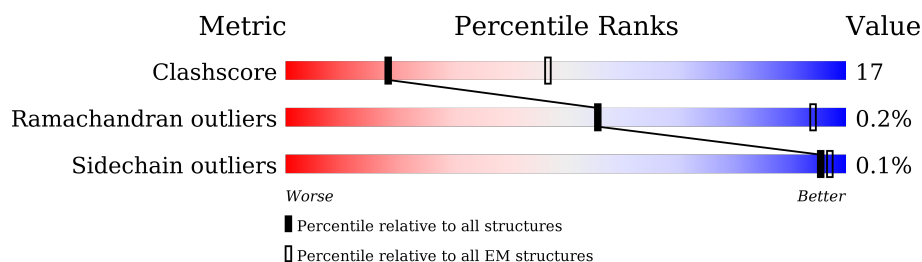
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.83 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	<div> <div>63%</div> <div>34%</div> <div>• •</div> </div>
2	C	1122	<div> <div>65%</div> <div>34%</div> </div>
3	D	609	<div> <div>67%</div> <div>32%</div> <div>•</div> </div>
4	X	70	<div> <div>24%</div> <div>47%</div> <div>•</div> <div>27%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23981 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, RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1151	Total	C	N	O	S	0	0
			9164	5781	1628	1717	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	605	Total	C	N	O	S	0	0
			4672	2916	862	874	20		

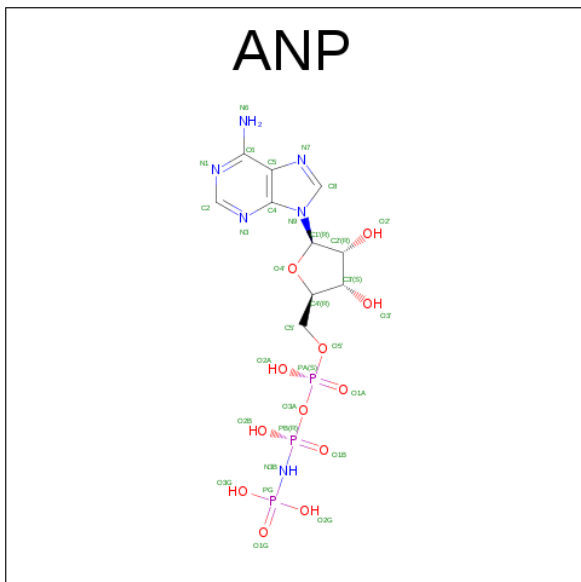
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P04993
D	1	GLY	-	expression tag	UNP P04993

- Molecule 4 is a DNA chain called Fork-Hairpin DNA (70-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	51	Total	C	N	O	P	0	0
			1035	501	165	319	50		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

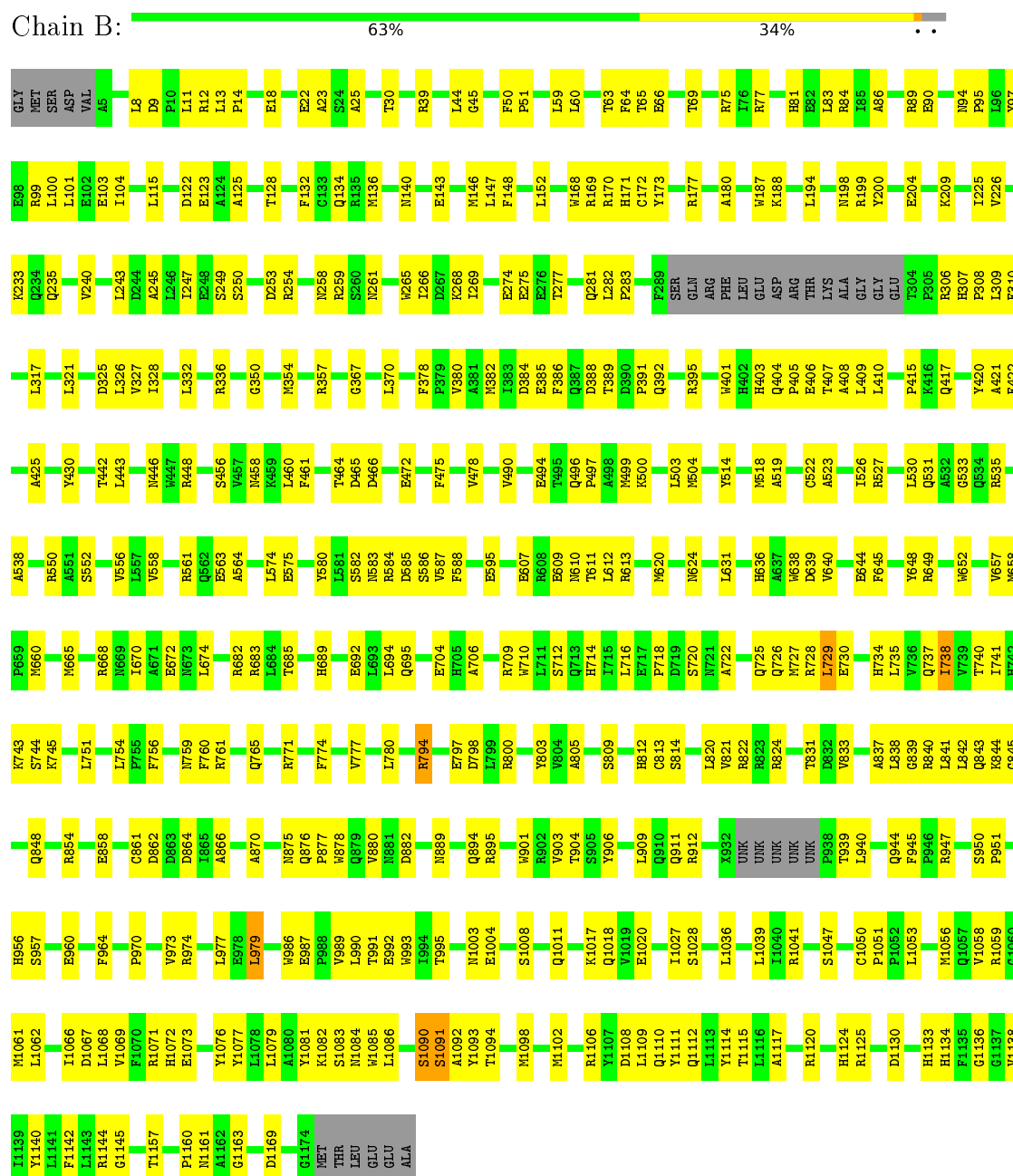
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	

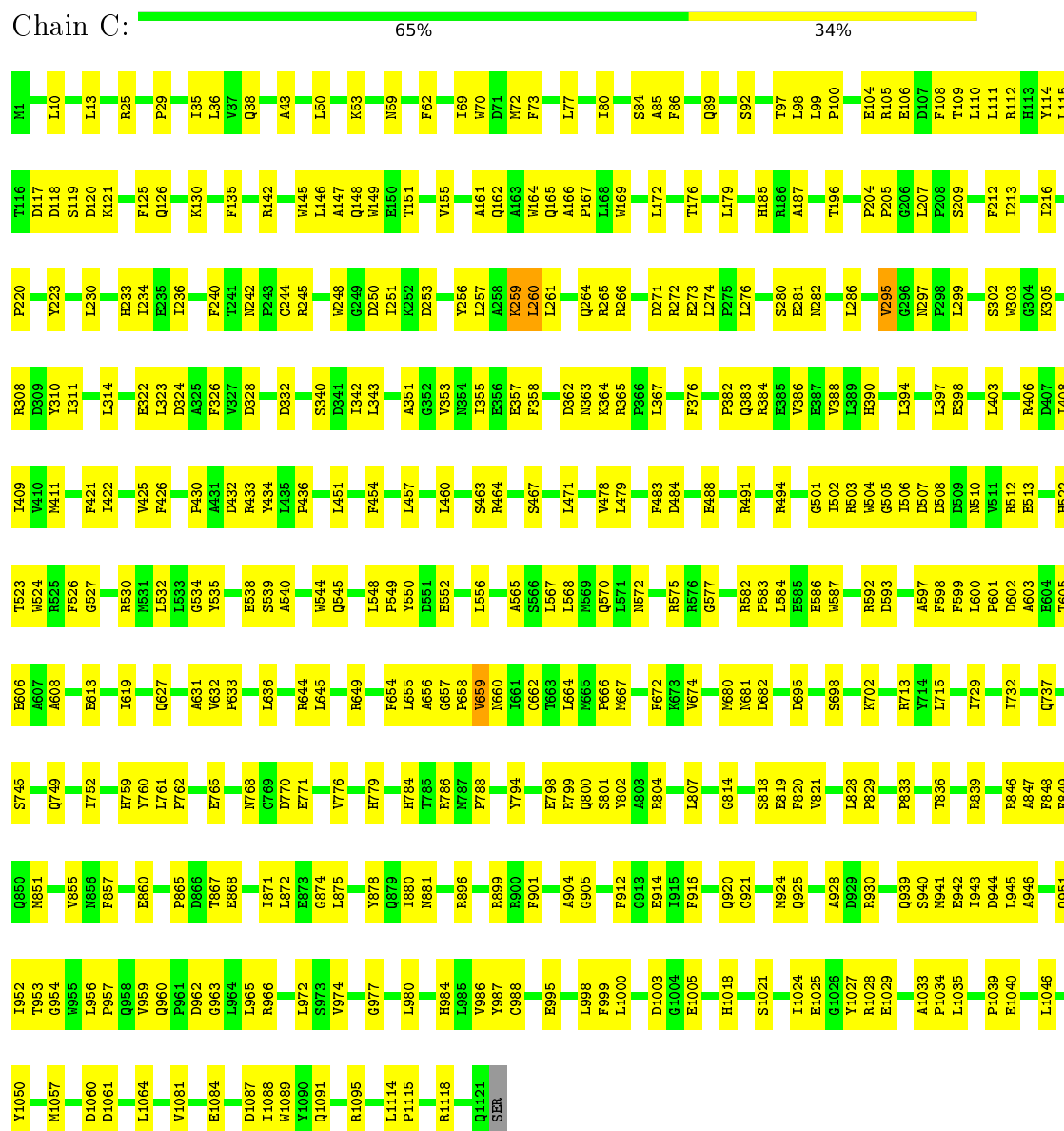
### 3 Residue-property plots

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. 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. 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.

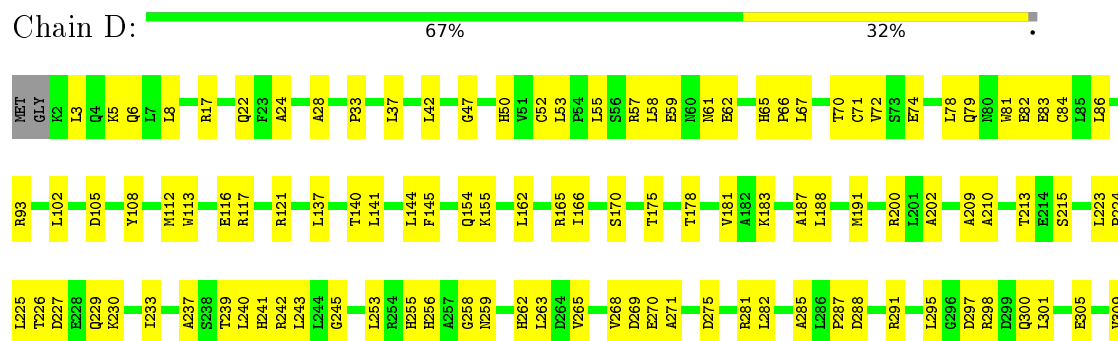
- Molecule 1: RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB

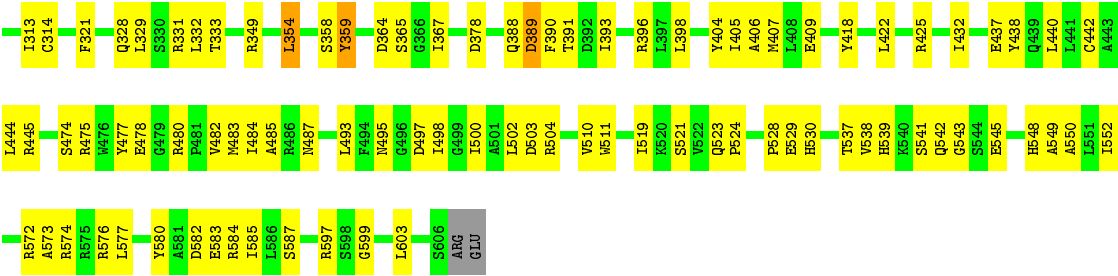


• Molecule 2: RecBCD enzyme subunit RecC

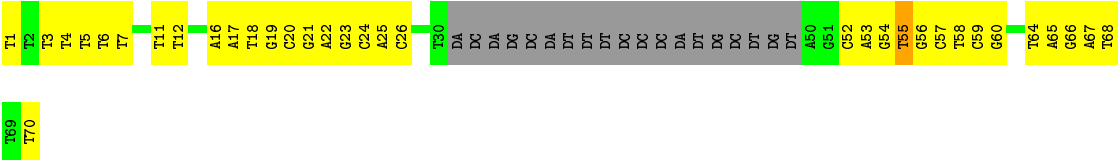
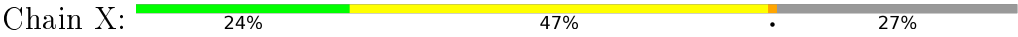


• Molecule 3: RecBCD enzyme subunit RecD





● Molecule 4: Fork-Hairpin DNA (70-MER)



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	74656	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor



## 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: MG, ANP

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	0.46	0/9262	0.57	3/12563 (0.0%)
2	C	0.51	2/9305 (0.0%)	0.55	0/12644
3	D	0.39	2/4752 (0.0%)	0.52	0/6437
4	X	0.88	1/1153 (0.1%)	1.12	1/1776 (0.1%)
All	All	0.49	5/24472 (0.0%)	0.60	4/33420 (0.0%)

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	B	0	1
2	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	259	LYS	C-N	8.76	1.54	1.34
2	C	260	LEU	C-N	6.70	1.49	1.34
4	X	66	DG	C4'-O4'	6.09	1.51	1.45
3	D	359	TYR	C-N	5.40	1.46	1.34
3	D	285	ALA	C-N	-5.25	1.22	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	ILE	N-CA-C	-7.28	91.35	111.00
1	B	737	GLN	N-CA-C	-6.09	94.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	729	LEU	CA-CB-CG	5.64	128.26	115.30
4	X	55	DT	O4'-C1'-N1	5.01	111.51	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	720	SER	Peptide
2	C	259	LYS	Mainchain

## 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	B	9164	0	8943	327	0
2	C	9078	0	8877	316	0
3	D	4672	0	4703	166	0
4	X	1035	0	588	44	0
5	B	31	0	13	1	0
6	B	1	0	0	0	0
All	All	23981	0	23124	808	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 17.

The worst 5 of 808 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:251:ILE:HG22	2:C:286:LEU:HD22	1.28	1.08
2:C:251:ILE:CG2	2:C:286:LEU:HD22	1.85	1.06
2:C:941:MET:HE3	2:C:956:LEU:HD12	1.41	1.03
1:B:460:LEU:HD23	1:B:841:LEU:HD13	1.41	1.02
2:C:245:ARG:HH21	2:C:266:ARG:HH22	1.00	0.98

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1126/1181 (95%)	1054 (94%)	70 (6%)	2 (0%)	52	86
2	C	1119/1122 (100%)	1058 (94%)	58 (5%)	3 (0%)	46	83
3	D	603/609 (99%)	566 (94%)	35 (6%)	2 (0%)	46	83
All	All	2848/2912 (98%)	2678 (94%)	163 (6%)	7 (0%)	56	86

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1091	SER
2	C	282	ASN
1	B	1090	SER
3	D	389	ASP
2	C	295	VAL

### 5.3.2 Protein sidechains

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	960/980 (98%)	958 (100%)	2 (0%)	95	98
2	C	976/977 (100%)	976 (100%)	0	100	100
3	D	489/492 (99%)	488 (100%)	1 (0%)	95	98
All	All	2425/2449 (99%)	2422 (100%)	3 (0%)	95	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	794	ARG
1	B	979	LEU
3	D	354	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	185	HIS
2	C	510	ASN
3	D	473	HIS
2	C	233	HIS
2	C	237	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
5	ANP	B	1501	6	29,33,33	2.43	9 (31%)	26,52,52	2.01	7 (26%)

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
5	ANP	B	1501	6	-	0/13/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1501	ANP	PB-O1B	-7.32	1.38	1.46
5	B	1501	ANP	PB-O3A	-3.27	1.55	1.59
5	B	1501	ANP	PG-O3G	-2.05	1.51	1.56
5	B	1501	ANP	O4'-C1'	2.01	1.44	1.41
5	B	1501	ANP	C2-N3	2.63	1.36	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1501	ANP	N3-C2-N1	-4.97	124.97	128.87
5	B	1501	ANP	PA-O3A-PB	-3.70	119.29	132.71
5	B	1501	ANP	O3'-C3'-C4'	-2.38	103.90	111.01
5	B	1501	ANP	O2'-C2'-C3'	2.23	119.06	111.86
5	B	1501	ANP	O3'-C3'-C2'	2.43	119.70	111.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1501	ANP	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.