

Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 03:43 PM EDT

PDB ID : 4PNV

Title : E. coli sliding clamp apo-crystal in P21 space group with larger cell dimensions

Authors : Yin, Z.; Oakley, A.J.

Deposited on : 2014-02-21

Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

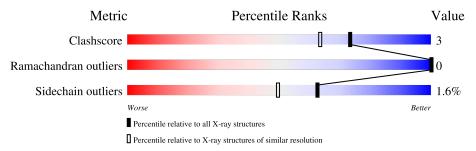
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.86 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain				
1	A	366	94%	5%			
1	В	366	93%	7%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6743 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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	366	Total 2900	C 1834	N 496	O 550	S 20	0	13	0
1	В	366	Total 2894	C 1828	N 493	O 553	S 20	0	17	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

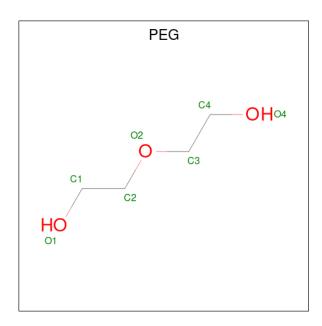
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Ca 5 5	0	0
2	В	3	Total Ca 3 3	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	В	3	Total Cl 3 3	0	0

• Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	В	1	Total C O 7 4 3	0	0
4	В	1	Total C O 7 4 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	445	Total O 445 445	0	0
5	В	471	Total O 471 471	0	0

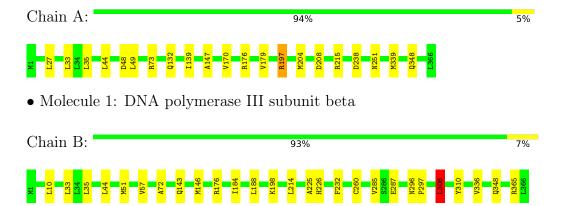


3 Residue-property plots (i)

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. 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.

Note EDS failed to run properly.

• Molecule 1: DNA polymerase III subunit beta





4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	80.14Å 70.26Å 84.47Å	Depositor
a, b, c, α , β , γ	90.00° 114.67° 90.00°	Depositor
Resolution (Å)	27.55 - 1.86	Depositor
% Data completeness	90.2 (27.55-1.86)	Depositor
(in resolution range)	, , ,	•
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.87 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.183 , 0.234	Depositor
Wilson B-factor (\mathring{A}^2)	18.5	Xtriage
Anisotropy	0.084	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6743	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 15.07% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: PEG, CL, CA

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.36	0/2989	0.60	1/4048 (0.0%)	
1	В	0.38	0/2995	0.63	1/4063 (0.0%)	
All	All	0.37	0/5984	0.62	2/8111 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms Z		$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	197	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	В	306	LEU	CA-CB-CG	5.03	126.86	115.30

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	2900	0	2937	20	0
1	В	2894	0	2914	18	0
2	A	5	0	0	0	0
2	В	3	0	0	0	0
3	A	1	0	0	0	0
3	В	3	0	0	2	0
4	A	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	14	0	20	0	0
5	A	445	0	0	2	0
5	В	471	0	0	3	0
All	All	6743	0	5881	39	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 3.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		${\rm distance} (\rm \AA)$	overlap (Å)
1:B:260[B]:CYS:SG	1:B:336[B]:VAL:HG13	1.44	1.54
1:B:260[B]:CYS:SG	1:B:336[B]:VAL:CG1	2.35	1.13
1:A:35[B]:LEU:CD2	1:A:44[B]:LEU:HD23	2.05	0.85
1:A:35[B]:LEU:HD22	1:A:44[B]:LEU:CD2	2.08	0.83
1:A:35[B]:LEU:CD2	1:A:44[B]:LEU:CD2	2.57	0.82
1:A:147:ALA:O	1:A:197:ARG:NH2	2.17	0.77
1:A:35[B]:LEU:HD22	1:A:44[B]:LEU:HD23	1.65	0.75
1:A:139:ILE:HB	1:A:204:MET:HE1	1.76	0.66
1:A:35[B]:LEU:HD23	1:A:44[B]:LEU:HD23	1.80	0.62
1:A:139:ILE:HB	1:A:204:MET:CE	2.31	0.60
1:A:73:ARG:NH1	5:A:920:HOH:O	2.38	0.55
1:A:33[B]:LEU:HD11	1:A:44[B]:LEU:HB3	1.91	0.52
1:A:132:GLN:HE22	1:A:208:ASP:H	1.57	0.52
1:B:285[B]:VAL:HG22	1:B:310:TYR:CD2	2.45	0.52
1:A:33[B]:LEU:CD2	1:A:35[B]:LEU:HD21	2.39	0.52
1:A:33[B]:LEU:HD21	1:A:35[B]:LEU:HD21	1.94	0.49
1:B:33[B]:LEU:HG	1:B:72:ALA:CB	2.43	0.49
3:B:408:CL:CL	5:B:958:HOH:O	2.56	0.49
1:A:339[A]:MET:HE1	1:A:348:GLN:HG2	1.96	0.47
1:B:35[A]:LEU:HD22	1:B:44:LEU:CD2	2.44	0.46
1:B:184:ILE:HD11	1:B:188:LEU:HD11	1.98	0.45
1:A:170:VAL:HG22	1:A:179:VAL:HG23	1.97	0.45
1:A:48:ASP:O	1:A:49:LEU:HB2	2.16	0.45
1:B:33[A]:LEU:CD2	1:B:35[A]:LEU:HD21	2.47	0.45
1:A:139:ILE:HD12	1:A:204:MET:HE2	1.99	0.44
1:B:306:LEU:HD12	1:B:306:LEU:N	2.33	0.44
1:B:51:MET:HE1	1:B:198:LYS:C	2.38	0.43
1:B:287:GLU:O	3:B:407:CL:CL	2.73	0.43
1:A:251:ASN:HB2	5:A:653:HOH:O	2.17	0.43
1:B:348:GLN:NE2	5:B:684:HOH:O	2.46	0.43
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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ ({\rm \AA})$	overlap (Å)
1:B:51:MET:CE	1:B:198:LYS:HG3	2.48	0.42
1:A:35[B]:LEU:CD2	1:A:44[B]:LEU:HD22	2.43	0.42
1:A:73:ARG:HG2	5:B:670:HOH:O	2.19	0.42
1:B:51:MET:HE2	1:B:232:PHE:HZ	1.85	0.41
1:B:33[A]:LEU:HD23	1:B:35[A]:LEU:HD21	2.01	0.41
1:B:296:ASN:HB2	1:B:297:PRO:CD	2.51	0.41
1:B:51:MET:HE3	1:B:198:LYS:HG3	2.03	0.41
1:B:214:LEU:HD11	1:B:225:ALA:HB1	2.02	0.41
1:B:143:GLN:HG3	1:B:146:MET:CE	2.52	0.40

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 Al		Allowed	Outliers	Perce	entiles
1	A	377/366 (103%)	372 (99%)	5 (1%)	0	100	100
1	В	381/366 (104%)	377 (99%)	4 (1%)	0	100	100
All	All	758/732 (104%)	749 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	322/313 (103%)	318 (99%)	4 (1%)	71 62
1	В	323/313 (103%)	316 (98%)	7 (2%)	52 36
All	All	645/626 (103%)	634 (98%)	11 (2%)	62 47

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	176	ARG
1	A	215	ARG
1	A	238	ASP
1	В	10	LEU
1	В	57	VAL
1	В	176	ARG
1	В	226[A]	HIS
1	В	226[B]	HIS
1	В	306	LEU
1	В	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	132	GLN
1	A	143	GLN
1	A	191	HIS
1	A	289	GLN
1	A	299	GLN
1	В	36	GLN
1	В	212	ASN
1	В	217	GLN
1	В	348	GLN

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)

Of 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	B	ond leng	gths	В	ond ang	gles
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	PEG	В	402	-	6,6,6	0.56	0	5,5,5	0.49	0
4	PEG	В	403	-	6,6,6	0.32	0	5,5,5	0.74	0
4	PEG	A	404	-	6,6,6	0.51	0	5,5,5	0.40	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	PEG	В	402	-	-	1/4/4/4	-
4	PEG	В	403	-	-	1/4/4/4	-
4	PEG	A	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	PEG	O1-C1-C2-O2
4	В	403	PEG	O1-C1-C2-O2
4	A	404	PEG	C4-C3-O2-C2
4	В	402	PEG	C1-C2-O2-C3



There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

