



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2023 – 04:59 am GMT

PDB ID : 2XUR
Title : The G157C mutation in the Escherichia coli sliding clamp specifically affects initiation of replication
Authors : Johnsen, L.; Morigen; Dalhus, B.; Bjoras, M.; Flaatten, I.; Waldminghaus, T.; Skarstad, K.
Deposited on : 2010-10-20
Resolution : 1.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (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) : 2.36

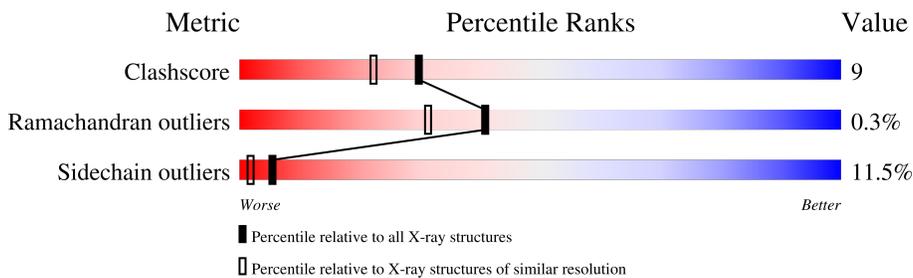
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6224 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
			Total	C	N	O	S			
1	A	366	2846	1787	498	541	20	0	0	0
1	B	364	2826	1775	493	538	20	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P0A988
A	-5	HIS	-	expression tag	UNP P0A988
A	-4	HIS	-	expression tag	UNP P0A988
A	-3	HIS	-	expression tag	UNP P0A988
A	-2	HIS	-	expression tag	UNP P0A988
A	-1	HIS	-	expression tag	UNP P0A988
A	0	HIS	-	expression tag	UNP P0A988
A	157	CYS	GLY	engineered mutation	UNP P0A988
B	-6	MET	-	expression tag	UNP P0A988
B	-5	HIS	-	expression tag	UNP P0A988
B	-4	HIS	-	expression tag	UNP P0A988
B	-3	HIS	-	expression tag	UNP P0A988
B	-2	HIS	-	expression tag	UNP P0A988
B	-1	HIS	-	expression tag	UNP P0A988
B	0	HIS	-	expression tag	UNP P0A988
B	157	CYS	GLY	engineered mutation	UNP P0A988

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	295	Total	O	0	0
			295	295		
2	B	257	Total	O	0	0
			257	257		

SEQUENCE-PLOTS INFOmissingINFO

3 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 a, b, c, α , β , γ	79.98Å 66.49Å 81.70Å 90.00° 113.75° 90.00°	Depositor
Resolution (Å)	36.61 – 1.90	Depositor
% Data completeness (in resolution range)	99.9 (36.61-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.252	Depositor
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.067	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.019 for l,-k,h	Xtrriage
Total number of atoms	6224	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 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 >5	RMSZ	# Z >5
1	A	0.91	0/2895	0.91	7/3918 (0.2%)
1	B	0.86	1/2875 (0.0%)	0.94	7/3893 (0.2%)
All	All	0.88	1/5770 (0.0%)	0.92	14/7811 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	GLU	CB-CG	-5.23	1.42	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	VAL	CB-CA-C	-6.91	98.27	111.40
1	B	168	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	17	VAL	CG1-CB-CG2	6.37	121.09	110.90
1	B	168	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	245	ARG	NE-CZ-NH2	-6.33	117.14	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2846	0	2863	44	1
1	B	2826	0	2839	64	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	295	0	0	18	1
2	B	257	0	0	12	1
All	All	6224	0	5702	107	2

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 9.

The worst 5 of 107 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:A:12:LYS:HE2	2:A:2013:HOH:O	1.60	1.00
1:A:24:ARG:CZ	2:A:2020:HOH:O	2.18	0.90
1:A:8:GLU:HB2	2:A:2009:HOH:O	1.70	0.89
1:A:12:LYS:HD2	2:A:2167:HOH:O	1.75	0.84
1:B:69:THR:HB	1:B:111:LEU:O	1.79	0.82

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH2	1:B:39:ASP:OD2[1_455]	2.15	0.05
2:A:2116:HOH:O	2:B:2176:HOH:O[1_556]	2.19	0.01

4.3 Torsion angles [i](#)

4.3.1 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	364/373 (98%)	359 (99%)	5 (1%)	0	100 100
1	B	362/373 (97%)	348 (96%)	12 (3%)	2 (1%)	25 15
All	All	726/746 (97%)	707 (97%)	17 (2%)	2 (0%)	41 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ARG
1	B	22	GLY

4.3.2 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	314/321 (98%)	288 (92%)	26 (8%)	11 4
1	B	312/321 (97%)	266 (85%)	46 (15%)	3 1
All	All	626/642 (98%)	554 (88%)	72 (12%)	5 2

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	240	ARG
1	B	361	VAL
1	B	262	LEU
1	B	308	VAL
1	A	340	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	ASN
1	B	212	ASN
1	B	32	ASN
1	B	15	GLN
1	B	143	GLN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

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

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5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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