



Full wwPDB X-ray Structure Validation Report i

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PDB ID : 1WUD
Title : E. coli RecQ HRDC domain
Authors : Bernstein, D.A.; Keck, J.L.
Deposited on : 2004-12-04
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

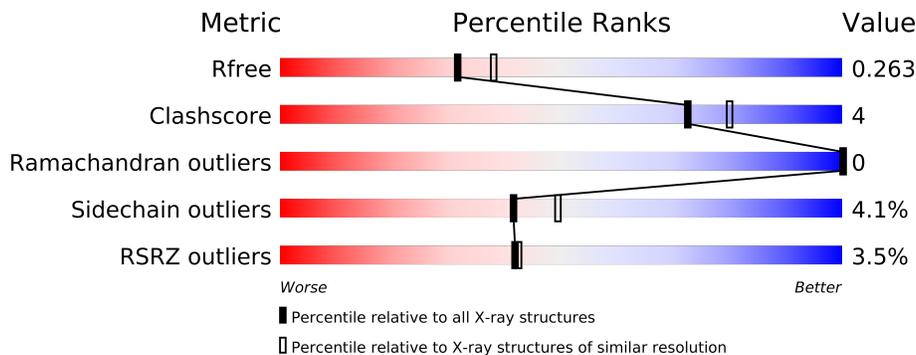
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	89	
1	B	89	
1	D	89	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1901 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP-dependent DNA helicase recQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	77	611	388	108	110	5	0	0	0
1	B	76	603	384	106	108	5	0	0	0
1	D	76	603	384	106	108	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	GLY	-	CLONING ARTIFACT	UNP P15043
A	522	SER	-	CLONING ARTIFACT	UNP P15043
A	523	HIS	-	CLONING ARTIFACT	UNP P15043
A	566	MSE	MET	MODIFIED RESIDUE	UNP P15043
A	570	MSE	MET	MODIFIED RESIDUE	UNP P15043
A	577	MSE	MET	MODIFIED RESIDUE	UNP P15043
A	585	MSE	MET	MODIFIED RESIDUE	UNP P15043
A	596	MSE	MET	MODIFIED RESIDUE	UNP P15043
B	521	GLY	-	CLONING ARTIFACT	UNP P15043
B	522	SER	-	CLONING ARTIFACT	UNP P15043
B	523	HIS	-	CLONING ARTIFACT	UNP P15043
B	566	MSE	MET	MODIFIED RESIDUE	UNP P15043
B	570	MSE	MET	MODIFIED RESIDUE	UNP P15043
B	577	MSE	MET	MODIFIED RESIDUE	UNP P15043
B	585	MSE	MET	MODIFIED RESIDUE	UNP P15043
B	596	MSE	MET	MODIFIED RESIDUE	UNP P15043
D	521	GLY	-	CLONING ARTIFACT	UNP P15043
D	522	SER	-	CLONING ARTIFACT	UNP P15043
D	523	HIS	-	CLONING ARTIFACT	UNP P15043
D	566	MSE	MET	MODIFIED RESIDUE	UNP P15043
D	570	MSE	MET	MODIFIED RESIDUE	UNP P15043
D	577	MSE	MET	MODIFIED RESIDUE	UNP P15043
D	585	MSE	MET	MODIFIED RESIDUE	UNP P15043

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Chain	Residue	Modelled	Actual	Comment	Reference
D	596	MSE	MET	MODIFIED RESIDUE	UNP P15043

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	38	Total O 38 38	0	0
2	D	24	Total O 24 24	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.30Å 64.61Å 98.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.20) 99.6 (19.72-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.225 , 0.263 0.225 , 0.263	Depositor DCC
R_{free} test set	628 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	25.2	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.0	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Outliers	0 of 12879 reflections	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	1901	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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 >5	RMSZ	# Z >5
1	A	0.43	0/616	0.64	2/818 (0.2%)
1	B	0.44	0/608	0.62	0/807
1	D	0.42	0/608	0.60	1/807 (0.1%)
All	All	0.43	0/1832	0.62	3/2432 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	606	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	560	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	611	0	627	5	0
1	B	603	0	621	7	0
1	D	603	0	621	6	0
2	A	22	0	0	0	0
2	B	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	24	0	0	0	0
All	All	1901	0	1869	16	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:531:TYR:HB3	1:B:568:GLU:HG3	1.82	0.61
1:B:533:ARG:HE	1:D:600:ARG:HE	1.47	0.61
1:A:531:TYR:HB3	1:A:568:GLU:HG3	1.85	0.58
1:D:531:TYR:HD1	1:D:568:GLU:HG3	1.68	0.58
1:B:572:ILE:HD11	1:B:603:VAL:HG21	1.89	0.55
1:A:572:ILE:HG12	1:A:600:ARG:HG2	1.91	0.53
1:B:593:LYS:HA	1:B:596:MSE:HE3	1.93	0.51
1:A:571:PRO:HD2	1:A:599:ILE:HD13	1.97	0.47
1:A:593:LYS:HB3	1:A:594:PRO:HD3	1.98	0.44
1:B:533:ARG:NE	1:D:600:ARG:HE	2.15	0.44
1:B:592:GLY:O	1:B:596:MSE:HG3	2.18	0.42
1:D:531:TYR:CD1	1:D:568:GLU:HG3	2.51	0.42
1:D:593:LYS:HB2	1:D:594:PRO:HD3	2.01	0.42
1:B:606:ASP:OD1	1:B:606:ASP:N	2.53	0.41
1:D:571:PRO:HB2	1:D:577:MSE:HG2	2.03	0.40
1:A:539:LEU:HD23	1:A:598:LEU:HD23	2.04	0.40

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 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	75/89 (84%)	74 (99%)	1 (1%)	0	100	100
1	B	74/89 (83%)	73 (99%)	1 (1%)	0	100	100
1	D	74/89 (83%)	73 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	223/267 (84%)	220 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 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	66/70 (94%)	65 (98%)	1 (2%)	76	86
1	B	65/70 (93%)	63 (97%)	2 (3%)	52	63
1	D	65/70 (93%)	60 (92%)	5 (8%)	18	18
All	All	196/210 (93%)	188 (96%)	8 (4%)	41	49

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	ARG
1	B	590	ARG
1	B	606	ASP
1	D	534	LYS
1	D	572	ILE
1	D	575	SER
1	D	581	ASN
1	D	590	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	530	ASN
1	A	551	ASN
1	B	602	HIS
1	D	602	HIS

5.3.3 RNA

There are no RNA chains 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.

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, 95th 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 ²)	Q<0.9
1	A	77/89 (86%)	0.16	1 (1%) 74 74	13, 26, 42, 47	0
1	B	76/89 (85%)	-0.12	1 (1%) 74 74	13, 22, 40, 50	0
1	D	76/89 (85%)	0.29	6 (7%) 13 12	13, 28, 49, 56	0
All	All	229/267 (85%)	0.11	8 (3%) 42 42	13, 24, 45, 56	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	606	ASP	3.4
1	D	585	MSE	3.1
1	D	572	ILE	3.0
1	D	555	TYR	2.4
1	B	606	ASP	2.3
1	A	530	ASN	2.2
1	D	581	ASN	2.0
1	D	571	PRO	2.0

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)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.