



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:38 PM UTC

PDB ID : 2R6D / pdb_00002r6d
Title : Crystal Form B1
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.
Deposited on : 2007-09-05
Resolution : 3.70 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

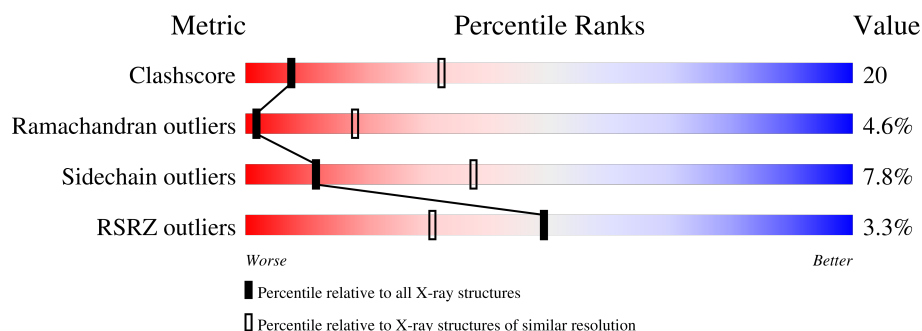
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	454	4% 52% 30% 5% • 11%
1	B	454	2% 53% 23% 6% • 17%
1	C	454	3% 56% 25% 5% • 12%
1	D	454	4% 52% 24% 5% • 17%
1	E	454	3% 58% 22% 6% • 14%
1	F	454	2% 57% 23% 5% • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18085 atoms, of which 0 are hydrogens and 0 are deuteriums.

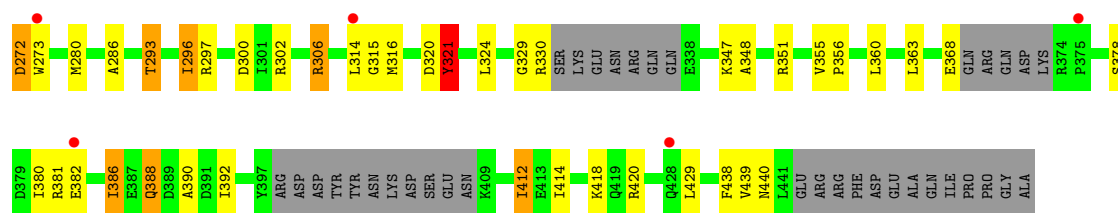
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Replicative helicase.

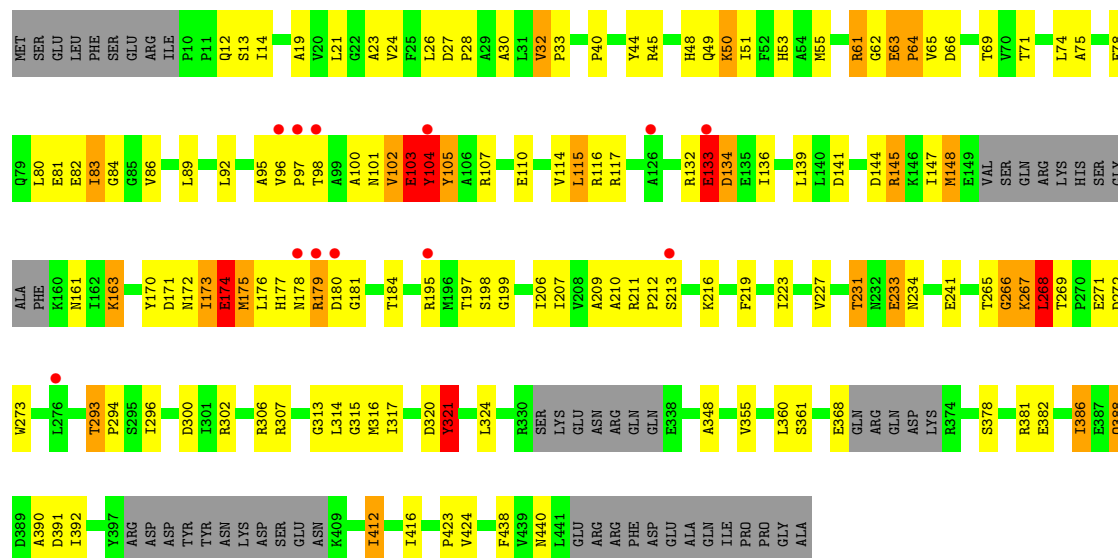
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3138	1969	544	611	14			
1	B	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	C	399	Total	C	N	O	S	0	0	0
			3089	1938	534	603	14			
1	D	376	Total	C	N	O	S	0	0	0
			2897	1820	500	564	13			
1	E	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			
1	F	392	Total	C	N	O	S	0	0	0
			3032	1905	521	593	13			

- Molecule 1: Replicative helicase

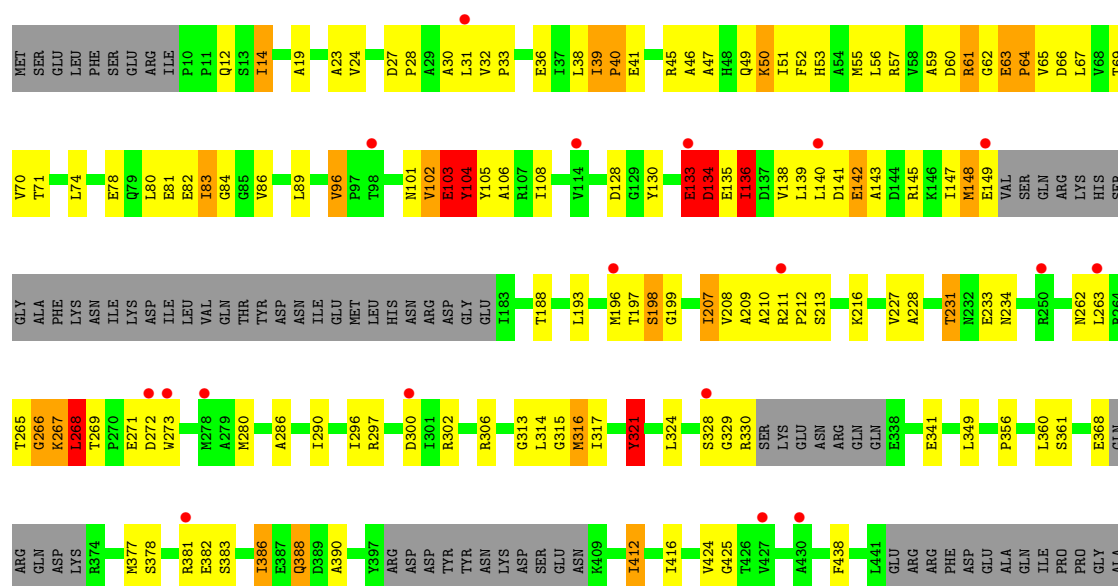




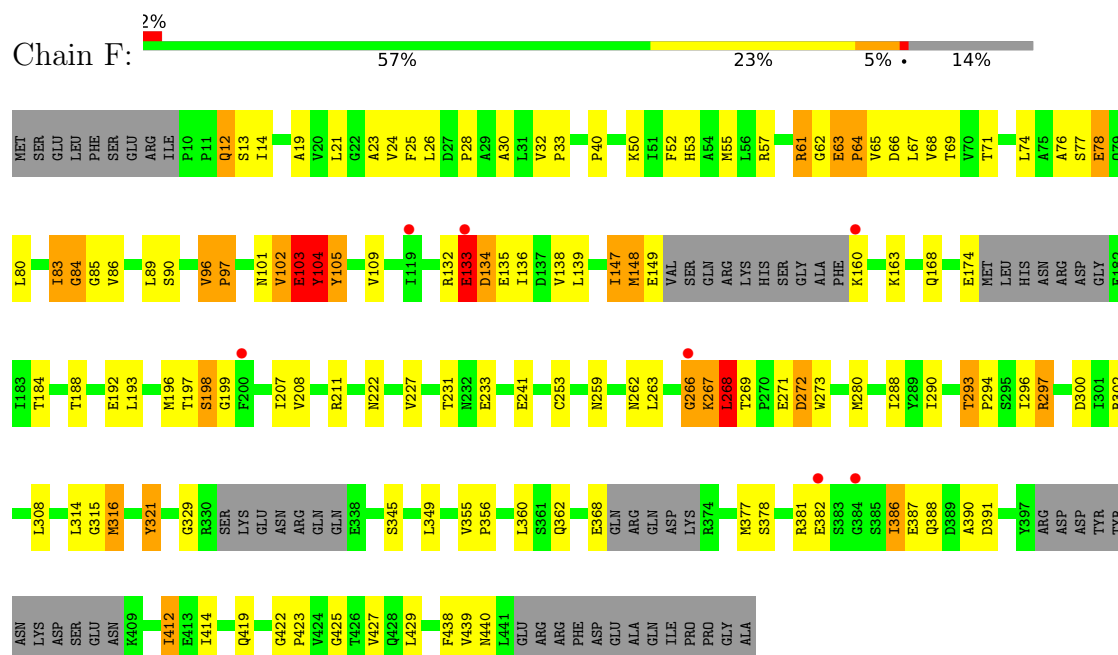
• Molecule 1: Replicative helicase



• Molecule 1: Replicative helicase



• Molecule 1: Replicative helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	371.26Å 110.30Å 112.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.70) 97.3 (20.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.71Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.309 , 0.322 0.289 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	145.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 199.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.077 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18085	wwPDB-VP
Average B, all atoms (Å ²)	177.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

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	0.57	0/3173	0.98	10/4285 (0.2%)
1	B	0.58	0/2929	1.04	19/3957 (0.5%)
1	C	0.58	3/3123 (0.1%)	1.05	14/4218 (0.3%)
1	D	0.52	0/2929	1.02	16/3957 (0.4%)
1	E	0.50	0/3064	1.00	15/4138 (0.4%)
1	F	0.54	0/3064	1.03	19/4138 (0.5%)
All	All	0.55	3/18282 (0.0%)	1.02	93/24693 (0.4%)

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	1	0
1	C	1	2
1	D	1	1
1	E	1	0
1	F	1	1
All	All	5	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	GLU	C-N	7.41	1.44	1.33
1	C	32	VAL	CA-CB	6.02	1.57	1.54
1	C	61	ARG	CA-C	5.65	1.55	1.52

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	GLU	N-CA-C	11.37	125.42	112.57
1	E	10	PRO	CA-C-N	9.76	132.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	PRO	C-N-CA	9.76	132.04	119.84
1	C	293	THR	CA-C-N	9.60	131.83	119.84
1	C	293	THR	C-N-CA	9.60	131.83	119.84

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	104	TYR	CA
1	C	104	TYR	CA
1	D	104	TYR	CA
1	E	104	TYR	CA
1	F	104	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	103	GLU	Peptide
1	C	174	GLU	Mainchain
1	D	104	TYR	Peptide
1	F	104	TYR	Peptide

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	A	3138	0	3190	148	0
1	B	2897	0	2953	135	0
1	C	3089	0	3141	152	2
1	D	2897	0	2953	162	0
1	E	3032	0	3087	117	0
1	F	3032	0	3087	114	2
All	All	18085	0	18411	742	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 20.

The worst 5 of 742 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:133:GLU:N	1:A:134:ASP:HB2	1.33	1.43
1:E:133:GLU:N	1:E:134:ASP:HB2	1.36	1.40
1:F:133:GLU:N	1:F:134:ASP:HB2	1.39	1.38
1:C:133:GLU:N	1:C:134:ASP:HB2	1.32	1.35
1:E:330:ARG:NH1	1:F:148:MET:O	1.63	1.32

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:C:178:ASN:ND2	1:F:97:PRO:CB[1_565]	2.12	0.08
1:C:178:ASN:CG	1:F:97:PRO:CB[1_565]	2.13	0.07

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	Allowed	Outliers	Percentiles	
1	A	395/454 (87%)	334 (85%)	43 (11%)	18 (5%)	2	18
1	B	366/454 (81%)	308 (84%)	46 (13%)	12 (3%)	3	25
1	C	389/454 (86%)	327 (84%)	37 (10%)	25 (6%)	1	14
1	D	366/454 (81%)	308 (84%)	42 (12%)	16 (4%)	2	19
1	E	380/454 (84%)	325 (86%)	38 (10%)	17 (4%)	2	18
1	F	380/454 (84%)	331 (87%)	33 (9%)	16 (4%)	2	20
All	All	2276/2724 (84%)	1933 (85%)	239 (10%)	104 (5%)	2	18

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	134	ASP
1	A	162	ILE

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Mol	Chain	Res	Type
1	A	179	ARG
1	A	180	ASP

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	341/386 (88%)	309 (91%)	32 (9%)	8	32
1	B	314/386 (81%)	288 (92%)	26 (8%)	10	35
1	C	336/386 (87%)	314 (94%)	22 (6%)	15	43
1	D	314/386 (81%)	289 (92%)	25 (8%)	11	37
1	E	330/386 (86%)	308 (93%)	22 (7%)	15	42
1	F	330/386 (86%)	303 (92%)	27 (8%)	10	36
All	All	1965/2316 (85%)	1811 (92%)	154 (8%)	11	37

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	148	MET
1	F	268	LEU
1	E	231	THR
1	F	65	VAL
1	F	362	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	GLN
1	E	53	HIS
1	D	53	HIS
1	D	226	ASN
1	E	226	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

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	405/454 (89%)	0.40	18 (4%) 39 25	153, 178, 179, 207	0
1	B	376/454 (82%)	0.27	8 (2%) 63 40	175, 178, 179, 186	0
1	C	399/454 (87%)	0.26	12 (3%) 52 32	145, 178, 179, 209	0
1	D	376/454 (82%)	0.25	18 (4%) 35 23	165, 178, 179, 184	0
1	E	392/454 (86%)	0.21	15 (3%) 44 28	169, 178, 179, 198	0
1	F	392/454 (86%)	0.21	7 (1%) 67 42	176, 178, 180, 189	0
All	All	2340/2724 (85%)	0.27	78 (3%) 49 31	145, 178, 179, 209	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	VAL	6.1
1	A	265	THR	4.9
1	F	133	GLU	4.7
1	C	179	ARG	4.6
1	C	178	ASN	4.5

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.