



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2019 – 04:20 AM EDT

PDB ID : 2C9O
Title : 3D Structure of the human RuvB-like helicase RuvBL1
Authors : Matias, P.M.; Gorynia, S.; Donner, P.; Carrondo, M.A.
Deposited on : 2005-12-14
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

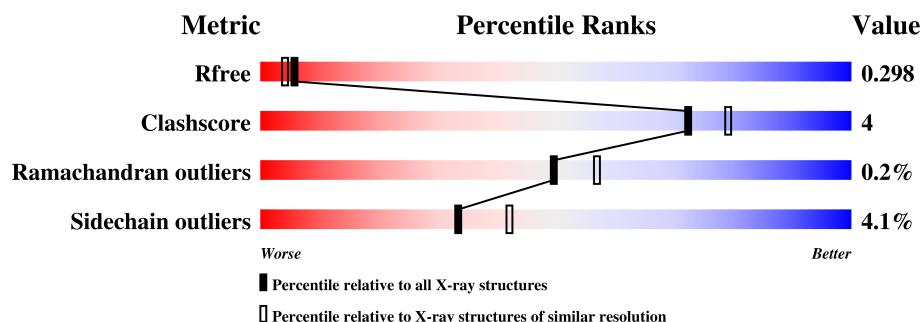
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (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. 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	A	456	 76% 9% 13%
1	B	456	 76% 10% 14%
1	C	456	 62% 5% 32%

2 Entry composition [i](#)

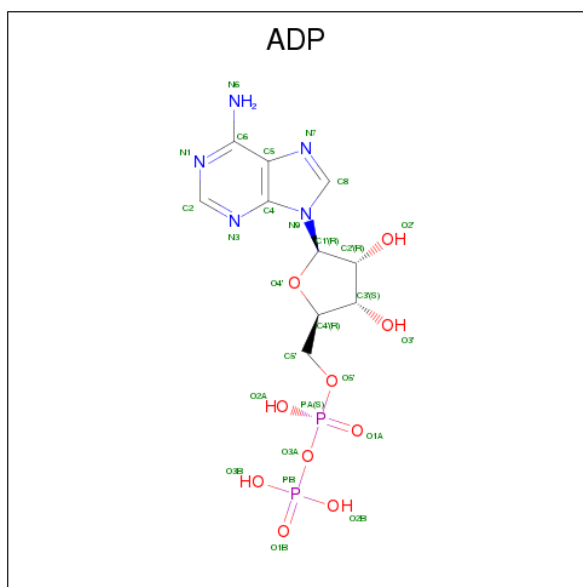
There are 3 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RUVB-LIKE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3061	1932	523	593	13			
1	B	393	Total	C	N	O	S	0	0	0
			3026	1912	517	584	13			
1	C	311	Total	C	N	O	S	0	0	0
			2380	1503	411	455	11			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total 91	O 91	0	0
3	B	45	Total 45	O 45	0	0
3	C	22	Total 22	O 22	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	207.08Å 207.08Å 60.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	179.61 – 2.20 39.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (179.61-2.20) 97.1 (39.39-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.257 0.267 , 0.298	Depositor DCC
R_{free} test set	3705 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8706	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1589e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.78	0/3100	0.79	3/4182 (0.1%)
1	B	0.64	0/3065	0.71	1/4134 (0.0%)
1	C	0.57	0/2407	0.64	0/3243
All	All	0.68	0/8572	0.72	4/11559 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	LEU	CA-CB-CG	5.89	128.86	115.30
1	A	404	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	339	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	377	ILE	CB-CA-C	-5.19	101.22	111.60

There are no chirality outliers.

There are no planarity outliers.

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	3061	0	3151	29	0
1	B	3026	0	3123	22	0
1	C	2380	0	2480	14	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	0	0
2	C	27	0	12	1	0
3	A	91	0	0	1	0
3	B	45	0	0	0	0
3	C	22	0	0	0	0
All	All	8706	0	8790	63	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 4.

All (63) 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:C:97:VAL:O	1:C:100:GLU:HG2	1.84	0.76
1:C:285:LYS:O	1:C:289:GLN:HG2	1.95	0.67
1:B:372:LYS:NZ	1:B:392:ASN:OD1	2.27	0.65
1:B:117:ARG:HH12	1:B:280:ASN:HD21	1.46	0.63
1:A:238:VAL:HG22	1:A:242:ASP:HB2	1.82	0.60
1:A:426:GLU:H	1:A:429:HIS:HD2	1.51	0.59
1:A:203:GLN:HE21	1:A:203:GLN:HA	1.68	0.59
1:C:238:VAL:HG22	1:C:241:HIS:CG	2.38	0.58
1:C:238:VAL:HG22	1:C:241:HIS:ND1	2.21	0.56
1:B:366:TYR:HB2	1:B:371:MET:HE3	1.87	0.56
1:B:309:ILE:HD11	1:B:341:THR:CG2	2.36	0.56
1:A:298:VAL:HG22	1:A:326:ILE:CG2	2.36	0.55
1:C:9:THR:H	1:C:241:HIS:CE1	2.25	0.55
1:B:68:LEU:HD23	1:B:361:ILE:HB	1.89	0.55
1:A:285:LYS:HE2	1:A:289:GLN:HE22	1.72	0.55
1:B:122:LEU:HD23	1:B:124:ILE:HD11	1.91	0.53
1:C:66:VAL:HG23	1:C:326:ILE:HD11	1.89	0.53
1:B:366:TYR:HB2	1:B:371:MET:CE	2.41	0.50
1:A:20:HIS:CD2	1:A:377:ILE:HG21	2.47	0.50
1:A:90:LYS:CD	1:A:90:LYS:H	2.24	0.49
1:A:238:VAL:CG2	1:A:242:ASP:HB2	2.43	0.49
1:A:61:MET:CE	1:A:326:ILE:HD11	2.43	0.49
1:B:127:THR:HA	1:B:232:LYS:O	2.13	0.49
1:A:210:ALA:HB2	1:A:220:TYR:CD2	2.49	0.48
1:A:101:VAL:HB	1:A:108:LYS:HB2	1.96	0.48
1:A:319:LEU:C	1:A:319:LEU:HD12	2.36	0.47
1:A:341:THR:O	1:A:342:GLU:HB2	2.15	0.47
1:B:215:LEU:HD23	1:B:215:LEU:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HD3	1:A:90:LYS:H	1.80	0.46
1:C:305:HIS:CE1	1:C:333:ARG:HD3	2.50	0.46
1:A:308:ASP:HB3	1:A:339:ARG:HG2	1.97	0.46
1:A:97:VAL:HG13	1:A:303:GLU:HB2	1.96	0.46
1:A:157:VAL:HG21	1:A:177:PHE:CG	2.51	0.46
1:B:129:GLU:HG2	1:B:195:ALA:HB3	1.97	0.46
1:B:417:ALA:HA	1:B:429:HIS:CE1	2.52	0.45
1:C:32:ALA:HB2	1:C:47:GLU:HG3	1.98	0.45
1:A:285:LYS:HG2	1:A:289:GLN:HE22	1.81	0.44
1:C:238:VAL:HG23	1:C:241:HIS:H	1.82	0.44
1:A:426:GLU:H	1:A:429:HIS:CD2	2.32	0.44
1:A:183:GLU:O	1:A:184:ARG:HG3	2.17	0.44
1:A:305:HIS:CD2	1:A:333:ARG:HD2	2.53	0.43
1:A:415:LEU:O	1:A:419:ILE:HG12	2.19	0.43
1:C:366:TYR:HB2	1:C:371:MET:HG3	2.00	0.43
1:B:173:ASP:HB2	1:B:174:PRO:HD2	2.01	0.42
1:B:426:GLU:H	1:B:429:HIS:CD2	2.37	0.42
1:C:404:ARG:O	1:C:408:GLN:HG2	2.19	0.42
1:B:343:ASP:OD1	1:C:339:ARG:NH2	2.52	0.42
1:A:61:MET:HE3	1:A:326:ILE:HD11	2.01	0.42
1:B:98:GLY:O	1:B:101:VAL:HG22	2.20	0.42
1:B:157:VAL:HG11	1:B:177:PHE:CD1	2.55	0.42
1:A:285:LYS:HG2	1:A:289:GLN:NE2	2.34	0.42
1:B:129:GLU:HG2	1:B:195:ALA:CB	2.50	0.42
1:B:312:PHE:CD1	1:B:354:LEU:HD12	2.54	0.42
1:A:298:VAL:HG22	1:A:326:ILE:HG22	2.02	0.41
1:B:113:MET:CE	1:B:117:ARG:HG3	2.51	0.41
1:B:346:SER:HB2	1:B:347:PRO:HD2	2.01	0.41
1:C:123:ARG:HG3	1:C:295:VAL:HG21	2.02	0.41
1:C:39:LEU:HA	2:C:1450:ADP:N1	2.36	0.41
1:A:180:LEU:HA	1:A:200:VAL:HG11	2.03	0.41
1:A:59:LYS:HA	3:A:2013:HOH:O	2.21	0.41
1:A:287:ILE:HA	1:A:292:ALA:O	2.22	0.40
1:A:176:ILE:HD12	1:B:214:ASP:O	2.21	0.40
1:B:401:THR:OG1	1:B:402:THR:N	2.53	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	392/456 (86%)	382 (97%)	9 (2%)	1 (0%)	43	48
1	B	387/456 (85%)	380 (98%)	6 (2%)	1 (0%)	43	48
1	C	305/456 (67%)	301 (99%)	4 (1%)	0	100	100
All	All	1084/1368 (79%)	1063 (98%)	19 (2%)	2 (0%)	49	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	34	GLN

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	336/387 (87%)	321 (96%)	15 (4%)	30	37
1	B	333/387 (86%)	318 (96%)	15 (4%)	30	37
1	C	262/387 (68%)	254 (97%)	8 (3%)	43	55
All	All	931/1161 (80%)	893 (96%)	38 (4%)	33	42

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL

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Mol	Chain	Res	Type
1	A	90	LYS
1	A	123	ARG
1	A	184	ARG
1	A	230	LYS
1	A	233	GLU
1	A	236	GLN
1	A	295	VAL
1	A	303	GLU
1	A	353	ASP
1	A	354	LEU
1	A	382	GLU
1	A	399	THR
1	A	404	ARG
1	A	426	GLU
1	B	104	THR
1	B	175	SER
1	B	215	LEU
1	B	216	GLU
1	B	225	LYS
1	B	236	GLN
1	B	284	ASN
1	B	316	HIS
1	B	333	ARG
1	B	353	ASP
1	B	354	LEU
1	B	371	MET
1	B	380	GLN
1	B	428	GLU
1	B	445	LYS
1	C	90	LYS
1	C	322	SER
1	C	326	ILE
1	C	333	ARG
1	C	353	ASP
1	C	378	ARG
1	C	415	LEU
1	C	419	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	305	HIS
1	A	335	ASN
1	A	393	HIS
1	A	429	HIS
1	B	156	HIS
1	B	169	GLN
1	B	236	GLN
1	B	280	ASN
1	B	369	GLN
1	B	429	HIS
1	C	280	ASN
1	C	289	GLN
1	C	380	GLN
1	C	408	GLN
1	C	420	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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
2	ADP	A	1450	-	24,29,29	1.42	2 (8%)	25,45,45	1.55	4 (16%)
2	ADP	B	1449	-	24,29,29	1.10	2 (8%)	25,45,45	1.43	4 (16%)
2	ADP	C	1450	-	24,29,29	1.27	2 (8%)	25,45,45	1.46	5 (20%)

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
2	ADP	A	1450	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1449	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1450	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1449	ADP	C5-C4	2.09	1.45	1.40
2	B	1449	ADP	PB-O3A	2.66	1.64	1.60
2	C	1450	ADP	C5-C4	2.67	1.46	1.40
2	A	1450	ADP	PB-O3A	3.34	1.65	1.60
2	C	1450	ADP	PB-O3A	3.81	1.65	1.60
2	A	1450	ADP	O4'-C1'	4.60	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1450	ADP	N3-C2-N1	-4.31	121.73	128.68
2	B	1449	ADP	N3-C2-N1	-3.75	122.64	128.68
2	C	1450	ADP	N3-C2-N1	-3.42	123.17	128.68
2	A	1450	ADP	C1'-N9-C4	-3.10	121.27	126.64
2	C	1450	ADP	C1'-N9-C4	-2.68	122.01	126.64
2	C	1450	ADP	C4-C5-N7	-2.52	106.78	109.40
2	C	1450	ADP	PA-O3A-PB	-2.37	125.03	132.57
2	B	1449	ADP	C4-C5-N7	-2.27	107.04	109.40
2	B	1449	ADP	C1'-N9-C4	-2.17	122.88	126.64
2	C	1450	ADP	C2-N1-C6	2.14	122.48	118.77
2	A	1450	ADP	N6-C6-N1	2.24	123.22	118.57
2	B	1449	ADP	C2-N1-C6	2.46	123.03	118.77
2	A	1450	ADP	C2-N1-C6	2.64	123.35	118.77

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
2	C	1450	ADP	1	0

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.