



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

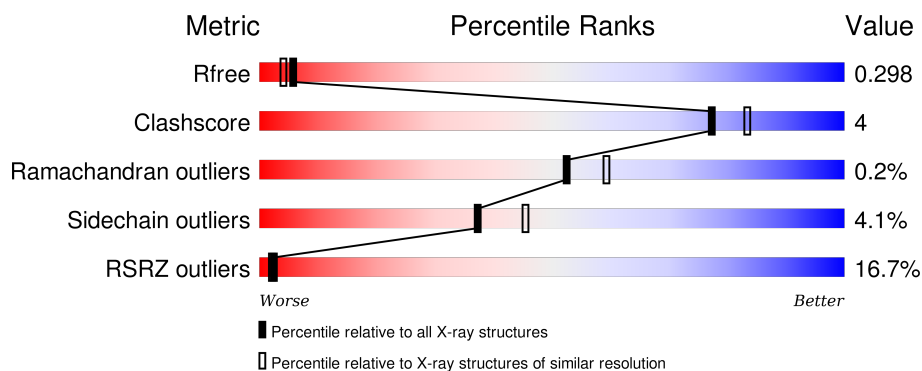
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 $\leq 5\%$. 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	456	<div> <div>14%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	456	<div> <div>13%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div></div> <div>14%</div> </div> </div>
1	C	456	<div> <div>14%</div> <div> <div></div> <div>62%</div> <div>5%</div> <div></div> <div>32%</div> </div> </div>

2 Entry composition [i](#)

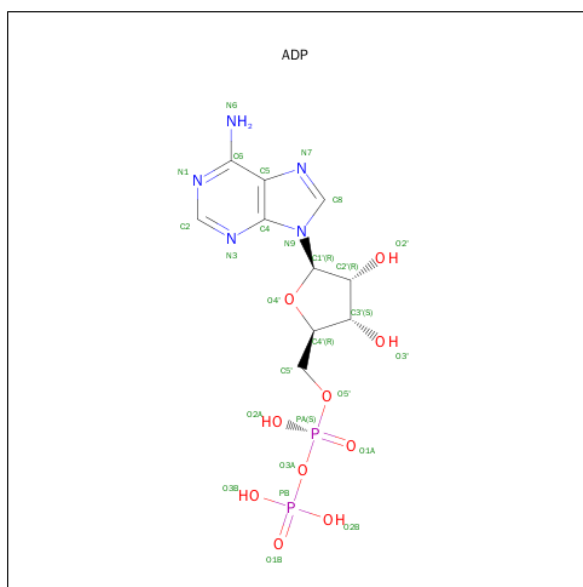
There are 3 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			

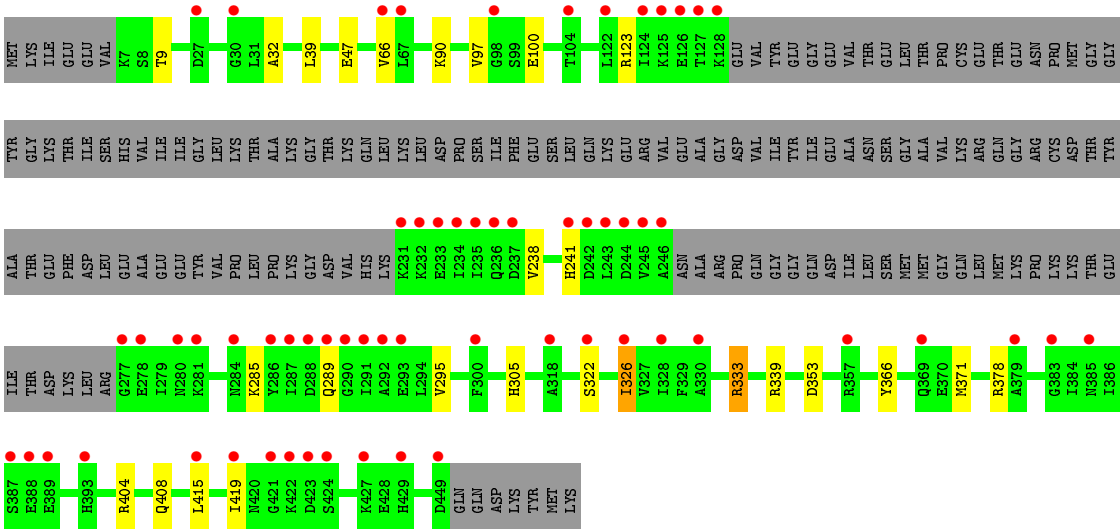
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	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	207.08 Å 207.08 Å 60.71 Å 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 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.257 0.265 , 0.298	Depositor DCC
R_{free} test set	3708 reflections (5.03%)	DCC
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 , 54.9	EDS
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 73733 reflections	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.*

¹ Intensities estimated from amplitudes.

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

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: 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 [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	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:C:9:THR:H	1:C:241:HIS:CE1	2.25	0.55
1:A:298:VAL:HG22	1:A:326:ILE:CG2	2.36	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:B:129:GLU:HG2	1:B:195:ALA:HB3	1.97	0.46
1:A:157:VAL:HG21	1:A:177:PHE:CG	2.51	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: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:173:ASP:HB2	1:B:174:PRO:HD2	2.01	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:39:LEU:HA	2:C:1450:ADP:N1	2.36	0.41
1:C:123:ARG:HG3	1:C:295:VAL:HG21	2.02	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%)	46	50
1	B	387/456 (85%)	380 (98%)	6 (2%)	1 (0%)	46	50
1	C	305/456 (67%)	301 (99%)	4 (1%)	0	100	100
All	All	1084/1368 (79%)	1063 (98%)	19 (2%)	2 (0%)	52	59

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%)	34	41
1	B	333/387 (86%)	318 (96%)	15 (4%)	34	41
1	C	262/387 (68%)	254 (97%)	8 (3%)	47	59
All	All	931/1161 (80%)	893 (96%)	38 (4%)	37	45

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	-	22,29,29	1.36	1 (4%)	27,45,45	2.36	5 (18%)
2	ADP	B	1449	-	22,29,29	0.95	1 (4%)	27,45,45	2.16	6 (22%)
2	ADP	C	1450	-	22,29,29	1.03	2 (9%)	27,45,45	2.04	7 (25%)

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 (4) 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	C	1450	ADP	O4'-C1'	2.14	1.43	1.41
2	C	1450	ADP	C5-C4	2.67	1.46	1.40
2	A	1450	ADP	O4'-C1'	5.11	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1450	ADP	N3-C2-N1	-9.36	121.73	128.89
2	B	1449	ADP	N3-C2-N1	-8.17	122.64	128.89
2	C	1450	ADP	N3-C2-N1	-7.48	123.17	128.89
2	A	1450	ADP	C1'-N9-C4	-3.76	121.27	126.94
2	C	1450	ADP	C1'-N9-C4	-3.27	122.01	126.94
2	B	1449	ADP	O4'-C1'-N9	-3.26	101.28	108.10
2	C	1450	ADP	O3A-PA-O5'	-3.02	94.93	102.94
2	C	1450	ADP	C4-C5-N7	-2.94	106.78	109.48
2	B	1449	ADP	C1'-N9-C4	-2.69	122.88	126.94
2	B	1449	ADP	C4-C5-N7	-2.66	107.04	109.48
2	A	1450	ADP	O3A-PA-O5'	-2.43	96.50	102.94
2	C	1450	ADP	PA-O3A-PB	-2.28	125.03	132.67
2	C	1450	ADP	O2B-PB-O1B	2.03	117.12	110.58
2	C	1450	ADP	C2-N1-C6	2.08	122.48	118.77
2	B	1449	ADP	O3B-PB-O1B	2.36	118.18	110.58
2	B	1449	ADP	C2-N1-C6	2.39	123.03	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1450	ADP	C2-N1-C6	2.56	123.35	118.77
2	A	1450	ADP	C2'-C1'-N9	3.29	119.33	114.29

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	398/456 (87%)	0.93	65 (16%) 2 2	38, 48, 59, 74	14 (3%)
1	B	393/456 (86%)	0.84	57 (14%) 3 3	39, 49, 59, 72	18 (4%)
1	C	311/456 (68%)	0.97	62 (19%) 1 1	27, 47, 56, 67	32 (10%)
All	All	1102/1368 (80%)	0.91	184 (16%) 2 2	27, 48, 59, 74	64 (5%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	9.6
1	B	291	ILE	8.2
1	C	127	THR	8.1
1	B	141	CYS	6.6
1	B	282	VAL	6.3
1	C	234	ILE	6.1
1	C	124	ILE	5.5
1	C	289	GLN	5.2
1	C	235	ILE	5.2
1	C	128	LYS	5.2
1	C	383	GLY	5.1
1	C	288	ASP	4.9
1	C	423	ASP	4.8
1	C	281	LYS	4.7
1	B	9	THR	4.6
1	C	126	GLU	4.5
1	B	421	GLY	4.5
1	C	421	GLY	4.4
1	C	449	ASP	4.3
1	A	217	ALA	4.1
1	B	290	GLY	4.1
1	A	419	ILE	4.0
1	C	290	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	4.0
1	C	291	ILE	4.0
1	C	286	TYR	3.9
1	B	322	SER	3.9
1	B	288	ASP	3.8
1	A	177	PHE	3.8
1	A	330	ALA	3.8
1	C	233	GLU	3.7
1	B	140	PRO	3.7
1	C	278	GLU	3.7
1	C	424	SER	3.6
1	A	9	THR	3.6
1	C	125	LYS	3.6
1	C	419	ILE	3.6
1	B	122	LEU	3.6
1	B	423	ASP	3.5
1	A	174	PRO	3.5
1	A	328	ILE	3.5
1	B	419	ILE	3.5
1	B	65	ALA	3.5
1	A	68	LEU	3.5
1	C	246	ALA	3.5
1	C	122	LEU	3.4
1	B	328	ILE	3.4
1	B	138	LEU	3.4
1	B	286	TYR	3.4
1	B	287	ILE	3.4
1	C	277	GLY	3.3
1	A	292	ALA	3.3
1	B	279	ILE	3.3
1	A	10	THR	3.2
1	C	67	LEU	3.2
1	B	361	ILE	3.2
1	A	77	THR	3.1
1	C	242	ASP	3.1
1	C	280	ASN	3.1
1	C	231	LYS	3.1
1	C	237	ASP	3.0
1	C	287	ILE	3.0
1	C	232	LYS	3.0
1	B	10	THR	3.0
1	C	244	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	389	GLU	3.0
1	C	328	ILE	3.0
1	A	278	GLU	3.0
1	A	301	VAL	2.9
1	C	385	ASN	2.9
1	C	241	HIS	2.9
1	A	80	ALA	2.9
1	B	417	ALA	2.9
1	A	291	ILE	2.9
1	C	27	ASP	2.9
1	B	293	GLU	2.9
1	A	327	VAL	2.8
1	B	156	HIS	2.8
1	B	294	LEU	2.8
1	A	66	VAL	2.7
1	B	177	PHE	2.7
1	A	300	PHE	2.7
1	A	67	LEU	2.7
1	C	236	GLN	2.7
1	A	70	GLY	2.7
1	B	236	GLN	2.7
1	A	69	ALA	2.7
1	A	358	VAL	2.7
1	A	235	ILE	2.7
1	C	422	LYS	2.7
1	A	351	PRO	2.6
1	A	312	PHE	2.6
1	A	74	THR	2.6
1	B	418	LYS	2.6
1	A	285	LYS	2.6
1	A	75	GLY	2.6
1	A	78	ALA	2.6
1	B	283	VAL	2.6
1	A	173	ASP	2.5
1	A	289	GLN	2.5
1	B	284	ASN	2.5
1	B	318	ALA	2.5
1	B	329	PHE	2.5
1	A	286	TYR	2.5
1	A	405	TYR	2.5
1	C	330	ALA	2.5
1	B	104	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	2.5
1	A	304	VAL	2.5
1	B	66	VAL	2.5
1	C	387	SER	2.5
1	B	106	ILE	2.5
1	C	393	HIS	2.5
1	A	355	LEU	2.5
1	C	104	THR	2.4
1	C	245	VAL	2.4
1	B	214	ASP	2.4
1	B	289	GLN	2.4
1	B	67	LEU	2.4
1	A	65	ALA	2.4
1	A	403	LEU	2.4
1	B	422	LYS	2.4
1	A	329	PHE	2.4
1	B	244	ASP	2.4
1	A	360	ILE	2.3
1	B	351	PRO	2.3
1	A	79	LEU	2.3
1	A	331	SER	2.3
1	A	375	ILE	2.3
1	B	157	VAL	2.3
1	C	66	VAL	2.3
1	C	292	ALA	2.3
1	C	357	ARG	2.3
1	B	393	HIS	2.3
1	A	287	ILE	2.3
1	A	361	ILE	2.3
1	B	360	ILE	2.3
1	C	429	HIS	2.3
1	C	98	GLY	2.3
1	B	350	ILE	2.2
1	A	156	HIS	2.2
1	A	226	GLY	2.2
1	C	300	PHE	2.2
1	B	281	LYS	2.2
1	B	68	LEU	2.2
1	C	326	ILE	2.2
1	A	404	ARG	2.2
1	C	415	LEU	2.2
1	A	313	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	2.2
1	A	354	LEU	2.2
1	B	126	GLU	2.2
1	C	322	SER	2.2
1	A	401	THR	2.2
1	A	82	ALA	2.2
1	A	245	VAL	2.1
1	C	388	GLU	2.1
1	A	49	CYS	2.1
1	B	52	ILE	2.1
1	C	293	GLU	2.1
1	A	81	LEU	2.1
1	B	82	ALA	2.1
1	C	427	LYS	2.1
1	A	96	MET	2.1
1	C	284	ASN	2.1
1	A	374	ILE	2.1
1	A	40	VAL	2.1
1	B	327	VAL	2.1
1	B	358	VAL	2.1
1	A	73	GLY	2.1
1	A	359	MET	2.1
1	B	354	LEU	2.1
1	B	392	ASN	2.1
1	C	379	ALA	2.1
1	C	369	GLN	2.1
1	A	122	LEU	2.0
1	A	236	GLN	2.0
1	C	30	GLY	2.0
1	B	315	LEU	2.0
1	C	243	LEU	2.0
1	C	318	ALA	2.0
1	A	233	GLU	2.0
1	B	292	ALA	2.0
1	B	184	ARG	2.0

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

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ADP	C	1450	27/27	0.96	0.16	0.19	33,44,51,52	0
2	ADP	B	1449	27/27	0.98	0.15	-1.45	30,35,38,38	0
2	ADP	A	1450	27/27	0.99	0.13	-2.68	18,27,29,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.