



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:21 PM 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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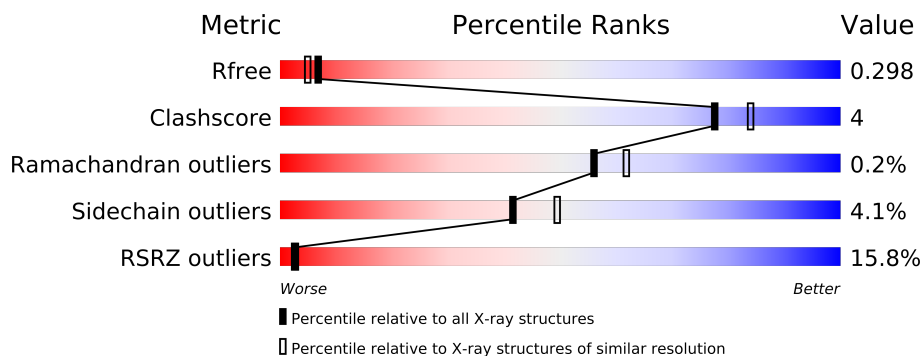
The following versions of software and data (see [references](#)) were used in the production of this report:

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  $\geq 3$ , 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	456	
1	B	456	
1	C	456	

## 2 Entry composition i

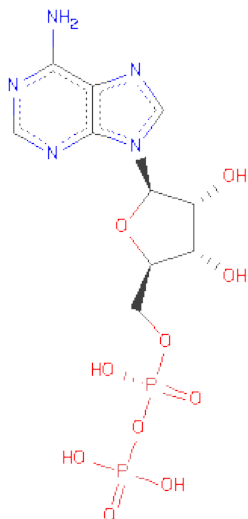
There are 3 unique types of molecules in this entry. The entry contains 8706 atoms, of which 0 are hydrogen and 0 are deuterium.

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 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.

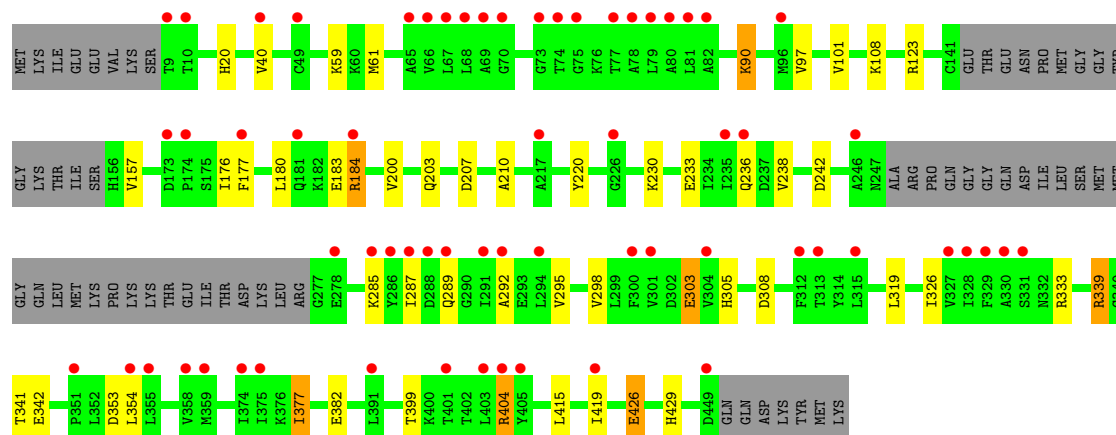
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total 91	O 91	0	0
3	B	45	Total 45	O 45	0	0
3	C	22	Total 22	O 22	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

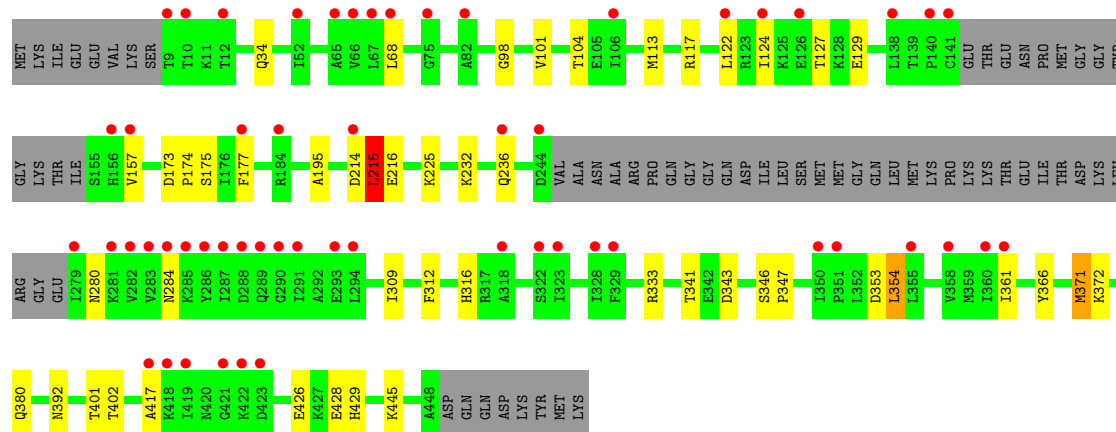
#### • Molecule 1: RUVB-LIKE 1

Chain A: 



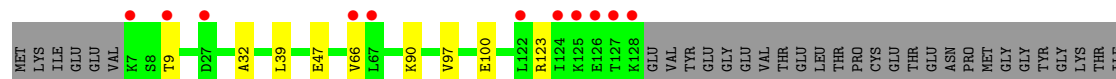
#### • Molecule 1: RUVB-LIKE 1

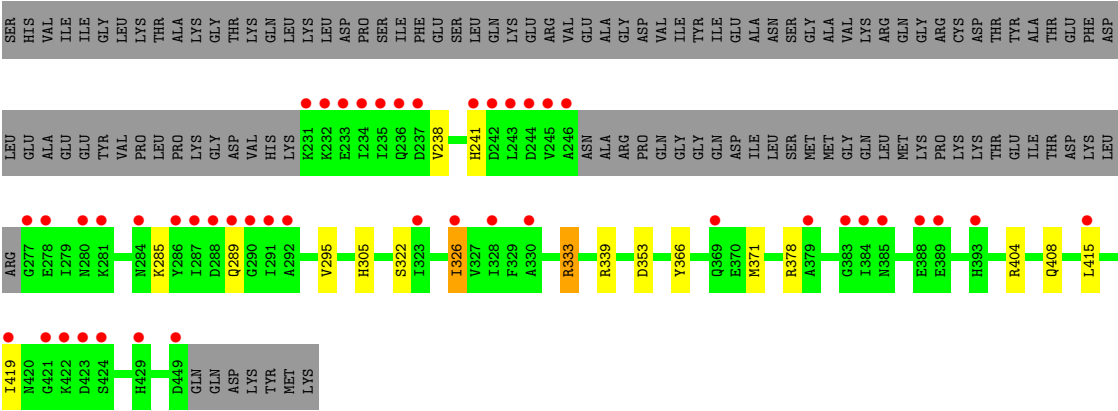
Chain B: 



#### • Molecule 1: RUVB-LIKE 1

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	3708 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.4	EDS
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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 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 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	3061	0	3151	29	0
1	B	3026	0	3123	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2380	0	2480	14	0
2	A	27	0	12	0	0
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

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

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	50	53
1	B	387/456 (85%)	380 (98%)	6 (2%)	1 (0%)	50	53
1	C	305/456 (67%)	301 (99%)	4 (1%)	0	100	100
All	All	1084/1368 (79%)	1063 (98%)	19 (2%)	2 (0%)	56	62

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%)	38	44
1	B	333/387 (86%)	318 (96%)	15 (4%)	38	44
1	C	262/387 (68%)	254 (97%)	8 (3%)	52	63
All	All	931/1161 (80%)	893 (96%)	38 (4%)	41	49

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

Mol	Chain	Res	Type
1	A	40	VAL
1	A	90	LYS
1	A	123	ARG
1	A	184	ARG

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Mol	Chain	Res	Type
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
1	A	289	GLN
1	A	305	HIS
1	A	335	ASN

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Mol	Chain	Res	Type
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 ⓘ

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 ⓘ

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	-	29,29,29	1.62	5 (17%)	45,45,45	2.12	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	B	1449	-	29,29,29	1.18	4 (13%)	45,45,45	2.31	10 (22%)
2	ADP	C	1450	-	29,29,29	1.35	4 (13%)	45,45,45	1.89	11 (24%)

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	-	-	0/16/32/32	0/1/3/3
2	ADP	B	1449	-	-	0/16/32/32	0/1/3/3
2	ADP	C	1450	-	-	0/16/32/32	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	ADP	C2'-C1'	-4.53	1.47	1.53
2	A	1450	ADP	O4'-C1'	4.11	1.47	1.41
2	C	1450	ADP	C4-N9	-3.31	1.32	1.37
2	C	1450	ADP	PB-O3A	3.24	1.65	1.60
2	A	1450	ADP	PB-O3A	2.83	1.65	1.60
2	B	1449	ADP	C4-N9	-2.71	1.33	1.37
2	C	1450	ADP	C5-C4	2.67	1.46	1.40
2	A	1450	ADP	C4-N9	-2.45	1.34	1.37
2	C	1450	ADP	C2'-C1'	-2.27	1.50	1.53
2	A	1450	ADP	C8-N9	-2.27	1.33	1.36
2	B	1449	ADP	PB-O3A	2.25	1.64	1.60
2	B	1449	ADP	C2'-C1'	-2.10	1.50	1.53
2	B	1449	ADP	C5-C4	2.09	1.45	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1450	ADP	N3-C2-N1	-8.35	121.73	128.71
2	B	1449	ADP	O4'-C1'-N9	-7.70	101.28	108.44
2	B	1449	ADP	N3-C2-N1	-7.26	122.64	128.71
2	C	1450	ADP	N3-C2-N1	-6.63	123.17	128.71
2	B	1449	ADP	N3-C4-N9	5.58	135.50	125.43
2	A	1450	ADP	N3-C4-N9	5.21	134.83	125.43
2	B	1449	ADP	C8-N9-C4	4.99	110.71	106.90
2	C	1450	ADP	N3-C4-N9	4.61	133.75	125.43
2	A	1450	ADP	O4'-C1'-N9	-4.60	104.16	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1450	ADP	C8-N9-C4	3.90	109.88	106.90
2	C	1450	ADP	O4'-C1'-N9	-3.58	105.11	108.44
2	A	1450	ADP	C8-N9-C4	3.54	109.60	106.90
2	C	1450	ADP	C4-C5-N7	-3.21	106.78	109.52
2	A	1450	ADP	C1'-N9-C4	-3.10	121.27	126.64
2	B	1449	ADP	C4-C5-N7	-2.90	107.04	109.52
2	B	1449	ADP	C5-C4-N3	-2.71	119.79	125.70
2	C	1450	ADP	C1'-N9-C4	-2.68	122.01	126.64
2	A	1450	ADP	C2-N1-C6	2.53	123.35	118.77
2	C	1450	ADP	C5-C4-N3	-2.37	120.54	125.70
2	B	1449	ADP	O3B-PB-O1B	2.37	118.18	110.44
2	B	1449	ADP	C2-N1-C6	2.36	123.03	118.77
2	A	1450	ADP	C2'-C1'-N9	2.36	119.33	113.27
2	A	1450	ADP	C2-N3-C4	2.31	120.58	114.01
2	C	1450	ADP	PA-O3A-PB	-2.27	125.03	131.68
2	A	1450	ADP	C5-C4-N3	-2.26	120.79	125.70
2	B	1449	ADP	C2-N3-C4	2.24	120.40	114.01
2	B	1449	ADP	C1'-N9-C4	-2.17	122.88	126.64
2	C	1450	ADP	C2-N3-C4	2.09	119.97	114.01
2	C	1450	ADP	C2-N1-C6	2.06	122.48	118.77
2	C	1450	ADP	O2B-PB-O1B	2.04	117.12	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	398/456 (87%)	0.91	64 (16%) 2 2	38, 48, 59, 74	14 (3%)
1	B	393/456 (86%)	0.85	55 (13%) 3 3	39, 49, 59, 72	18 (4%)
1	C	311/456 (68%)	0.98	56 (18%) 2 2	27, 47, 56, 67	32 (10%)
All	All	1102/1368 (80%)	0.91	175 (15%) 3 2	27, 48, 59, 74	64 (5%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	8.9
1	B	291	ILE	8.6
1	C	127	THR	8.1
1	C	234	ILE	6.6
1	B	9	THR	6.1
1	B	141	CYS	5.7
1	B	282	VAL	5.6
1	C	423	ASP	5.5
1	C	289	GLN	5.4
1	C	124	ILE	5.3
1	C	288	ASP	5.0
1	C	383	GLY	4.9
1	C	128	LYS	4.8
1	C	235	ILE	4.7
1	C	246	ALA	4.4
1	C	126	GLU	4.4
1	A	9	THR	4.3
1	C	122	LEU	4.3
1	C	233	GLU	4.3
1	B	421	GLY	4.2
1	B	419	ILE	4.2
1	C	281	LYS	4.0
1	C	286	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	122	LEU	3.9
1	C	291	ILE	3.9
1	A	288	ASP	3.8
1	C	290	GLY	3.8
1	B	10	THR	3.8
1	A	330	ALA	3.8
1	B	288	ASP	3.8
1	C	125	LYS	3.7
1	C	421	GLY	3.7
1	C	419	ILE	3.7
1	A	177	PHE	3.7
1	A	328	ILE	3.6
1	B	290	GLY	3.6
1	A	419	ILE	3.6
1	B	138	LEU	3.6
1	C	278	GLU	3.6
1	C	424	SER	3.5
1	B	140	PRO	3.5
1	B	287	ILE	3.4
1	B	322	SER	3.4
1	A	278	GLU	3.4
1	A	174	PRO	3.4
1	B	423	ASP	3.3
1	C	449	ASP	3.3
1	A	292	ALA	3.3
1	C	277	GLY	3.3
1	B	323	ILE	3.2
1	A	77	THR	3.2
1	A	68	LEU	3.2
1	C	67	LEU	3.2
1	A	80	ALA	3.2
1	B	361	ILE	3.2
1	B	286	TYR	3.2
1	B	328	ILE	3.1
1	B	279	ILE	3.1
1	C	244	ASP	3.1
1	A	301	VAL	3.1
1	C	231	LYS	3.1
1	C	232	LYS	3.1
1	C	242	ASP	3.1
1	A	327	VAL	3.0
1	C	280	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	417	ALA	2.9
1	C	287	ILE	2.9
1	B	418	LYS	2.9
1	A	300	PHE	2.9
1	A	289	GLN	2.8
1	C	389	GLU	2.8
1	C	415	LEU	2.8
1	A	217	ALA	2.8
1	C	245	VAL	2.8
1	B	65	ALA	2.7
1	C	243	LEU	2.7
1	A	351	PRO	2.7
1	B	284	ASN	2.7
1	C	237	ASP	2.7
1	C	241	HIS	2.7
1	B	294	LEU	2.7
1	C	328	ILE	2.7
1	C	385	ASN	2.7
1	A	312	PHE	2.7
1	C	323	ILE	2.6
1	A	66	VAL	2.6
1	A	78	ALA	2.6
1	B	293	GLU	2.6
1	A	75	GLY	2.6
1	C	330	ALA	2.6
1	A	67	LEU	2.6
1	C	27	ASP	2.5
1	B	281	LYS	2.5
1	C	422	LYS	2.5
1	B	177	PHE	2.5
1	B	289	GLN	2.5
1	C	236	GLN	2.5
1	B	67	LEU	2.5
1	A	74	THR	2.5
1	A	235	ILE	2.5
1	A	449	ASP	2.5
1	A	79	LEU	2.5
1	A	354	LEU	2.5
1	B	244	ASP	2.5
1	B	360	ILE	2.5
1	A	358	VAL	2.4
1	A	184	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	ALA	2.4
1	B	318	ALA	2.4
1	A	285	LYS	2.4
1	A	304	VAL	2.4
1	A	329	PHE	2.4
1	A	286	TYR	2.4
1	B	66	VAL	2.4
1	A	313	THR	2.3
1	B	106	ILE	2.3
1	A	331	SER	2.3
1	A	287	ILE	2.3
1	B	124	ILE	2.3
1	A	81	LEU	2.3
1	A	294	LEU	2.3
1	C	292	ALA	2.3
1	A	10	THR	2.3
1	A	374	ILE	2.3
1	B	184	ARG	2.3
1	B	68	LEU	2.3
1	B	156	HIS	2.3
1	B	350	ILE	2.3
1	C	393	HIS	2.3
1	A	65	ALA	2.3
1	A	82	ALA	2.3
1	C	384	ILE	2.2
1	C	429	HIS	2.2
1	A	405	TYR	2.2
1	A	236	GLN	2.2
1	B	329	PHE	2.2
1	A	226	GLY	2.2
1	A	355	LEU	2.2
1	B	12	THR	2.2
1	C	7	LYS	2.2
1	C	379	ALA	2.2
1	A	315	LEU	2.2
1	B	285	LYS	2.2
1	C	9	THR	2.2
1	A	70	GLY	2.2
1	A	375	ILE	2.1
1	A	404	ARG	2.1
1	C	326	ILE	2.1
1	B	82	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	284	ASN	2.1
1	B	283	VAL	2.1
1	C	66	VAL	2.1
1	B	236	GLN	2.1
1	C	369	GLN	2.1
1	C	388	GLU	2.1
1	A	49	CYS	2.1
1	A	173	ASP	2.1
1	A	291	ILE	2.1
1	B	351	PRO	2.1
1	A	403	LEU	2.1
1	B	75	GLY	2.1
1	B	157	VAL	2.1
1	B	422	LYS	2.1
1	B	214	ASP	2.1
1	A	96	MET	2.1
1	A	359	MET	2.1
1	A	181	GLN	2.1
1	B	126	GLU	2.1
1	A	401	THR	2.0
1	B	355	LEU	2.0
1	A	40	VAL	2.0
1	B	52	ILE	2.0
1	A	73	GLY	2.0
1	A	391	LEU	2.0
1	B	358	VAL	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	C	1450	27/27	0.16	0.27	33,44,51,52	0
2	ADP	B	1449	27/27	0.15	-1.31	30,35,38,38	0
2	ADP	A	1450	27/27	0.13	-2.34	18,27,29,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.