



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:36 PM GMT

PDB ID : 1NG9  
Title : E.coli MutS R697A: an ATPase-asymmetry mutant  
Authors : Lamers, M.H.; Winterwerp, H.H.K.; Sixma, T.K.  
Deposited on : 2002-12-17  
Resolution : 2.60 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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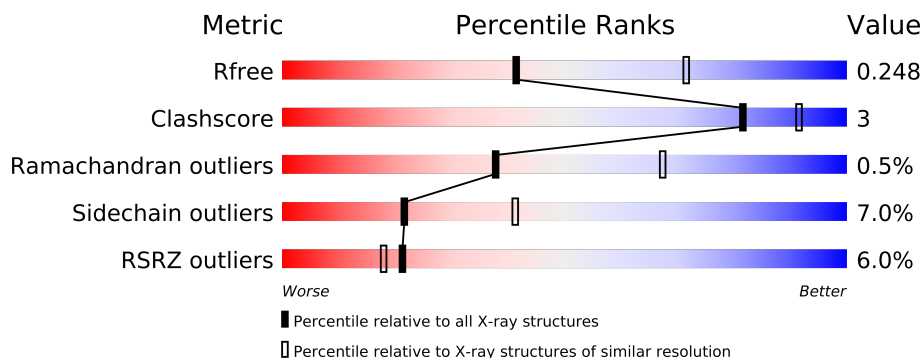
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 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	E	30	
2	F	30	
3	A	800	
3	B	800	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	1001	-	X
4	MG	B	1002	-	X
5	ADP	A	2001	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13420 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 DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*GP\*GP\*CP\*A P\*CP\*CP\*AP\*GP\*TP\*GP\*TP\*CP\*AP\*GP\*CP\*GP\*TP\*CP\*CP\*TP\*AP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			

- Molecule 2 is a DNA chain called 5'-D(\*AP\*TP\*AP\*GP\*GP\*AP\*CP\*GP\*CP\*TP\*GP\*A P\*CP\*AP\*CP\*TP\*GP\*GP\*TP\*GP\*CP\*TP\*TP\*GP\*GP\*CP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	17	Total	C	N	O	P	0	0	0
			347	166	62	103	16			

- Molecule 3 is a protein called DNA mismatch repair protein MutS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	794	Total	C	N	O	S	0	0	0
			6241	3925	1109	1177	30			
3	B	766	Total	C	N	O	S	0	0	0
			6045	3808	1072	1136	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	ALA	ARG	ENGINEERED	UNP P23909
B	697	ALA	ARG	ENGINEERED	UNP P23909

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

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

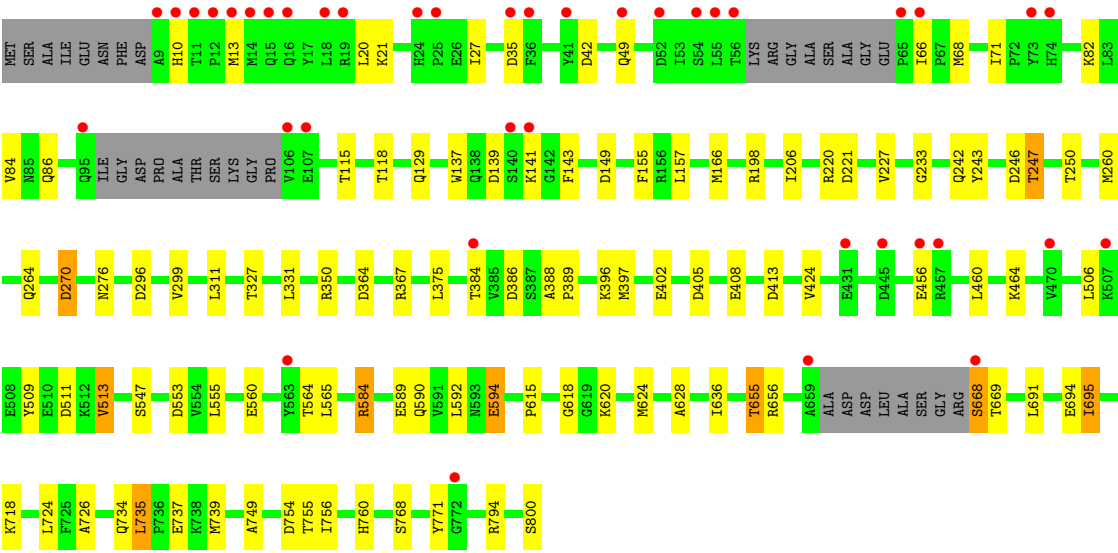


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	165	Total	O	0	0
			165	165		
6	B	192	Total	O	0	0
			192	192		
6	E	3	Total	O	0	0
			3	3		
6	F	4	Total	O	0	0
			4	4		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.90Å 92.40Å 261.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-2.60) 98.2 (20.00-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.215 , 0.249 0.213 , 0.248	Depositor DCC
$R_{free}$ test set	1283 reflections (1.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , -3.5	EDS
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 66556 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	13420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MG, 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	E	0.75	0/412	1.40	4/634 (0.6%)
2	F	0.71	0/388	1.50	4/598 (0.7%)
3	A	0.40	0/6347	0.73	12/8591 (0.1%)
3	B	0.42	0/6146	0.71	13/8318 (0.2%)
All	All	0.44	0/13293	0.79	33/18141 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	14	DA	O4'-C1'-N9	9.82	114.87	108.00
2	F	23	DT	O4'-C1'-N1	-7.59	102.69	108.00
1	E	1	DA	O4'-C1'-N9	7.51	113.26	108.00
2	F	18	DG	O4'-C4'-C3'	-7.22	101.61	104.50
3	B	270	ASP	CB-CG-OD2	6.55	124.20	118.30
3	B	754	ASP	CB-CG-OD2	6.36	124.02	118.30
3	B	149	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	17	DT	O4'-C1'-N1	5.83	112.08	108.00
3	B	364	ASP	CB-CG-OD2	5.82	123.54	118.30
3	A	441	ASP	CB-CG-OD2	5.79	123.51	118.30
3	B	246	ASP	CB-CG-OD2	5.75	123.48	118.30
3	B	221	ASP	CB-CG-OD2	5.68	123.42	118.30
3	A	754	ASP	CB-CG-OD2	5.65	123.39	118.30
3	A	445	ASP	CB-CG-OD2	5.58	123.32	118.30
3	B	35	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	7	DC	C1'-O4'-C4'	-5.45	104.65	110.10
3	A	149	ASP	CB-CG-OD2	5.42	123.18	118.30
3	B	296	ASP	CB-CG-OD2	5.38	123.14	118.30
3	B	42	ASP	CB-CG-OD2	5.37	123.13	118.30
3	B	511	ASP	CB-CG-OD2	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	121	ASP	CB-CG-OD2	5.33	123.09	118.30
3	A	139	ASP	CB-CG-OD2	5.28	123.05	118.30
3	A	8	ASP	CB-CG-OD2	5.28	123.05	118.30
1	E	11	DC	O4'-C4'-C3'	5.28	109.17	106.00
3	B	413	ASP	CB-CG-OD2	5.26	123.03	118.30
3	B	405	ASP	CB-CG-OD2	5.22	123.00	118.30
3	A	364	ASP	CB-CG-OD2	5.18	122.96	118.30
3	A	405	ASP	CB-CG-OD2	5.14	122.92	118.30
3	B	386	ASP	CB-CG-OD2	5.13	122.92	118.30
3	A	52	ASP	CB-CG-OD2	5.12	122.91	118.30
3	A	533	ASP	CB-CG-OD2	5.09	122.89	118.30
2	F	23	DT	C4-C5-C7	5.04	122.02	119.00
3	A	461	ASP	CB-CG-OD2	5.01	122.81	118.30

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	E	367	0	202	1	0
2	F	347	0	194	1	0
3	A	6241	0	6288	43	0
3	B	6045	0	6095	38	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	1	0
6	A	165	0	0	9	0
6	B	192	0	0	5	0
6	E	3	0	0	1	0
6	F	4	0	0	0	0
All	All	13420	0	12803	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:E:358:HOH:O	3:A:58:ARG:HD3	1.85	0.76
3:B:327:THR:HG21	3:B:555:LEU:HD13	1.71	0.73
3:A:74:HIS:ND1	6:A:2120:HOH:O	2.20	0.72
3:A:74:HIS:CE1	6:A:2120:HOH:O	2.47	0.68
3:A:133:LEU:HG	3:A:240:LEU:HD11	1.78	0.64
3:B:276:ASN:HD22	3:B:655:THR:HG22	1.64	0.63
3:A:73:TYR:O	3:A:76:VAL:HG22	1.99	0.62
3:A:190:ILE:HG23	3:A:196:LEU:HD11	1.82	0.61
3:A:396:LYS:NZ	6:A:2108:HOH:O	2.28	0.60
3:A:616:ASN:ND2	3:B:668:SER:OG	2.31	0.59
3:A:593:ASN:O	3:A:594:GLU:HB3	2.02	0.59
3:B:157:LEU:HD13	3:B:233:GLY:HA3	1.87	0.56
3:A:141:LYS:HE3	6:A:2154:HOH:O	2.05	0.55
3:A:458:THR:HG22	3:A:460:LEU:HG	1.89	0.55
3:B:242:GLN:NE2	6:B:2124:HOH:O	2.39	0.55
3:A:609:MET:HE3	3:A:712:ALA:HB1	1.90	0.54
3:A:199:ARG:HD3	3:A:203:GLU:OE1	2.06	0.54
3:B:618:GLY:O	3:B:760:HIS:HD2	1.91	0.54
3:A:640:VAL:HG11	3:A:645:VAL:HG21	1.87	0.54
3:B:143:PHE:HB3	3:B:166:MET:CE	2.38	0.54
3:B:227:VAL:HG12	3:B:260:MET:HB2	1.89	0.53
3:A:454:GLU:O	3:A:458:THR:HB	2.09	0.53
3:B:82:LYS:O	3:B:86:GLN:HG3	2.08	0.52
3:B:327:THR:HG22	3:B:331:LEU:HD12	1.90	0.52
3:B:276:ASN:HB2	3:B:655:THR:HG21	1.92	0.52
3:B:276:ASN:HD22	3:B:655:THR:CG2	2.23	0.51
3:A:328:ILE:HG23	3:A:559:ALA:HA	1.92	0.51
3:B:624:MET:CE	3:B:724:LEU:O	2.58	0.51
3:B:565:LEU:HD22	3:B:590:GLN:NE2	2.26	0.51
3:A:345:VAL:HG11	3:A:549:LEU:HD13	1.92	0.51
3:A:281:GLN:HE21	3:A:285:GLY:HA2	1.76	0.50
3:B:749:ALA:HB3	3:B:771:TYR:CE1	2.47	0.49
3:B:584:ARG:HD2	3:B:589:GLU:OE1	2.12	0.49
3:A:560:GLU:OE1	3:A:561:ARG:HD2	2.13	0.49
3:A:116:PRO:O	3:A:131:ASN:ND2	2.45	0.49
3:B:509:TYR:O	3:B:513:VAL:HG13	2.13	0.49
3:B:311:LEU:HD23	3:B:636:ILE:HD13	1.95	0.48
3:A:403:LEU:HD22	3:A:535:LEU:HD23	1.95	0.48
3:A:621:SER:OG	3:A:693:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:412:ILE:HD13	3:A:426:ALA:HB2	1.95	0.47
3:A:245:LYS:NZ	6:A:2116:HOH:O	2.44	0.47
3:A:656:ARG:CZ	3:A:695:ILE:HG21	2.45	0.47
3:B:118:THR:CB	3:B:247:THR:HG21	2.45	0.47
3:A:536:LEU:N	3:A:537:PRO:HD2	2.30	0.46
3:A:133:LEU:HG	3:A:240:LEU:CD1	2.45	0.46
3:B:755:THR:OG1	3:B:756:ILE:N	2.49	0.46
3:A:588:VAL:O	3:A:592:LEU:HB2	2.15	0.46
3:A:375:LEU:O	3:A:379:ARG:HG3	2.16	0.45
3:B:656:ARG:O	3:B:656:ARG:HG3	2.16	0.45
3:A:458:THR:CG2	3:A:460:LEU:HD12	2.47	0.45
3:A:388:ALA:HB3	3:A:389:PRO:HD3	1.99	0.45
3:B:615:PRO:O	6:B:2179:HOH:O	2.21	0.45
3:A:468:ASN:ND2	6:A:2008:HOH:O	2.49	0.45
3:A:171:GLN:HG2	3:A:274:ARG:HD2	1.99	0.44
3:A:5:GLU:HB3	3:A:10:HIS:HE1	1.83	0.44
3:B:760:HIS:HB3	5:B:2002:ADP:C6	2.53	0.44
3:B:620:LYS:HD3	3:B:726:ALA:HB1	1.98	0.44
3:B:735:LEU:HD12	3:B:739:MET:SD	2.57	0.44
3:B:143:PHE:HB3	3:B:166:MET:HE3	1.99	0.43
3:B:375:LEU:HD22	3:B:397:MET:HG2	1.99	0.43
3:B:594:GLU:HG3	6:B:2018:HOH:O	2.18	0.43
3:A:157:LEU:C	3:A:157:LEU:HD23	2.39	0.43
3:A:727:THR:HG21	3:A:732:LEU:HD12	2.00	0.42
3:B:21:LYS:NZ	3:B:27:ILE:O	2.51	0.42
3:A:397:MET:HA	3:A:545:SER:HA	2.01	0.42
3:A:794:ARG:HD2	6:A:2104:HOH:O	2.19	0.42
3:B:628:ALA:HB2	3:B:691:LEU:HD11	2.00	0.42
3:B:695:ILE:O	3:B:695:ILE:HG13	2.19	0.42
3:B:243:TYR:O	3:B:247:THR:HB	2.19	0.42
3:A:722:LEU:HG	6:A:2159:HOH:O	2.19	0.42
1:E:11:DC:H2''	1:E:12:DA:H5'	2.01	0.42
3:A:276:ASN:ND2	6:A:2160:HOH:O	2.52	0.41
3:A:139:ASP:O	3:A:140:SER:C	2.59	0.41
3:A:609:MET:HE2	3:A:742:VAL:HG13	2.02	0.41
3:B:384:THR:HB	6:B:2073:HOH:O	2.20	0.41
3:A:375:LEU:HD22	3:A:397:MET:HE3	2.03	0.41
3:B:367:ARG:HD3	6:B:2186:HOH:O	2.19	0.41
3:B:157:LEU:C	3:B:157:LEU:HD12	2.41	0.41
3:B:299:VAL:HG22	3:B:553:ASP:OD1	2.20	0.41
3:B:560:GLU:OE2	3:B:564:THR:OG1	2.37	0.41
3:B:388:ALA:N	3:B:389:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:17:DG:H1'	2:F:18:DG:C8	2.56	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	
3	A	790/800 (99%)	765 (97%)	18 (2%)	7 (1%)	25	49
3	B	758/800 (95%)	733 (97%)	25 (3%)	0	100	100
All	All	1548/1600 (97%)	1498 (97%)	43 (3%)	7 (0%)	38	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	2	SER
3	A	594	GLU
3	A	439	LEU
3	A	3	ALA
3	A	140	SER
3	A	152	SER
3	A	438	ALA

### 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	
3	A	659/663 (99%)	615 (93%)	44 (7%)	23	44
3	B	640/663 (96%)	593 (93%)	47 (7%)	20	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1299/1326 (98%)	1208 (93%)	91 (7%)	21	41

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1	MET
3	A	35	ASP
3	A	42	ASP
3	A	54	SER
3	A	58	ARG
3	A	65	PRO
3	A	76	VAL
3	A	84	VAL
3	A	108	ARG
3	A	109	LYS
3	A	112	ARG
3	A	137	TRP
3	A	150	ILE
3	A	154	ARG
3	A	155	PHE
3	A	157	LEU
3	A	194	ARG
3	A	199	ARG
3	A	254	HIS
3	A	260	MET
3	A	264	GLN
3	A	300	THR
3	A	335	THR
3	A	431	GLU
3	A	437	ARG
3	A	439	LEU
3	A	445	ASP
3	A	464	LYS
3	A	479	ARG
3	A	492	ARG
3	A	507	LYS
3	A	552	LEU
3	A	575	LYS
3	A	584	ARG
3	A	593	ASN
3	A	656	ARG
3	A	667	ARG

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Mol	Chain	Res	Type
3	A	695	ILE
3	A	700	SER
3	A	739	MET
3	A	752	HIS
3	A	761	SER
3	A	768	SER
3	A	784	GLU
3	B	10	HIS
3	B	13	MET
3	B	20	LEU
3	B	49	GLN
3	B	66	ILE
3	B	68	MET
3	B	71	ILE
3	B	84	VAL
3	B	115	THR
3	B	129	GLN
3	B	137	TRP
3	B	139	ASP
3	B	141	LYS
3	B	155	PHE
3	B	198	ARG
3	B	206	ILE
3	B	220	ARG
3	B	247	THR
3	B	250	THR
3	B	264	GLN
3	B	270	ASP
3	B	350	ARG
3	B	396	LYS
3	B	402	GLU
3	B	408	GLU
3	B	424	VAL
3	B	456	GLU
3	B	460	LEU
3	B	464	LYS
3	B	506	LEU
3	B	513	VAL
3	B	547	SER
3	B	584	ARG
3	B	592	LEU
3	B	594	GLU

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Mol	Chain	Res	Type
3	B	655	THR
3	B	668	SER
3	B	669	THR
3	B	694	GLU
3	B	695	ILE
3	B	718	LYS
3	B	734	GLN
3	B	735	LEU
3	B	737	GLU
3	B	768	SER
3	B	794	ARG
3	B	800	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	281	GLN
3	A	430	ASN
3	A	471	HIS
3	A	538	HIS
3	A	593	ASN
3	A	616	ASN
3	B	49	GLN
3	B	214	ASN
3	B	276	ASN
3	B	289	ASN
3	B	332	GLN
3	B	344	GLN
3	B	370	HIS
3	B	590	GLN
3	B	760	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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
5	ADP	A	2001	4	29,29,29	1.06	2 (6%)	45,45,45	2.10	5 (11%)
5	ADP	B	2002	4	29,29,29	1.04	2 (6%)	45,45,45	1.97	6 (13%)

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
5	ADP	A	2001	4	-	0/16/32/32	0/1/3/3
5	ADP	B	2002	4	-	0/16/32/32	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	ADP	C2-N3	3.37	1.38	1.32
5	B	2002	ADP	C2-N3	3.27	1.38	1.32
5	A	2001	ADP	C2-N1	2.77	1.39	1.33
5	B	2002	ADP	C2-N1	2.25	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	ADP	N3-C2-N1	-11.44	119.14	128.71
5	B	2002	ADP	N3-C2-N1	-10.19	120.19	128.71
5	B	2002	ADP	N3-C4-N9	3.93	132.54	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	ADP	N3-C4-N9	3.44	131.64	125.43
5	A	2001	ADP	PA-O3A-PB	-3.28	122.07	131.68
5	A	2001	ADP	C3'-C2'-C1'	2.77	105.25	100.91
5	A	2001	ADP	O3B-PB-O3A	2.41	116.56	105.14
5	B	2002	ADP	C5-C4-N3	-2.35	120.58	125.70
5	B	2002	ADP	C3'-C2'-C1'	2.21	104.36	100.91
5	B	2002	ADP	N7-C8-N9	-2.13	108.35	114.36
5	B	2002	ADP	C2-N3-C4	2.12	120.06	114.01

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	E	18/30 (60%)	1.23	3 (16%) <b>2</b> <b>1</b>	4, 10, 16, 19	0
2	F	17/30 (56%)	4.45	17 (100%) <b>0</b> <b>0</b>	5, 10, 15, 18	0
3	A	794/800 (99%)	0.19	36 (4%) 32 28	4, 10, 14, 20	0
3	B	766/800 (95%)	0.27	40 (5%) 26 22	4, 10, 14, 23	0
All	All	1595/1660 (96%)	0.28	96 (6%) 21 18	4, 10, 14, 23	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	22	DT	7.3
2	F	18	DG	6.9
3	A	441	ASP	6.9
2	F	28	DG	6.6
3	B	659	ALA	6.2
3	A	754	ASP	5.4
3	A	659	ALA	5.2
3	B	12	PRO	5.1
2	F	29	DC	5.0
2	F	27	DA	5.0
2	F	17	DG	5.0
3	A	442	GLY	4.9
3	B	65	PRO	4.9
2	F	21	DC	4.7
2	F	19	DT	4.7
3	B	9	ALA	4.6
2	F	16	DT	4.6
3	B	41	TYR	4.5
3	B	95	GLN	4.5
3	A	445	ASP	4.3
2	F	20	DG	4.2

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Mol	Chain	Res	Type	RSRZ
3	B	106	VAL	4.2
3	B	49	GLN	4.2
3	B	56	THR	4.2
3	A	666	GLY	4.1
3	A	444	THR	3.9
3	A	593	ASN	3.8
3	B	73	TYR	3.8
2	F	23	DT	3.6
2	F	15	DC	3.6
3	A	386	ASP	3.6
3	B	13	MET	3.6
3	B	668	SER	3.6
3	A	667	ARG	3.4
3	B	66	ILE	3.4
3	A	100	ALA	3.3
1	E	18	DG	3.3
3	A	63	GLY	3.2
3	A	1	MET	3.2
3	B	55	LEU	3.2
3	B	74	HIS	3.2
3	A	440	ALA	3.1
3	A	62	ALA	3.0
3	A	443	ALA	3.0
3	B	35	ASP	3.0
2	F	26	DC	3.0
2	F	14	DA	2.9
3	B	52	ASP	2.9
3	B	16	GLN	2.9
2	F	30	DT	2.9
3	A	669	THR	2.8
2	F	24	DG	2.8
3	B	10	HIS	2.8
3	B	15	GLN	2.8
3	A	437	ARG	2.8
3	B	140	SER	2.8
3	A	658	GLY	2.8
3	A	475	ILE	2.8
2	F	25	DG	2.7
3	A	439	LEU	2.7
3	A	449	ARG	2.6
3	B	470	VAL	2.6
3	B	19	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	64	GLU	2.6
3	A	752	HIS	2.5
3	A	420	ARG	2.5
3	B	456	GLU	2.5
1	E	1	DA	2.5
3	A	52	ASP	2.4
3	A	220	ARG	2.4
3	A	140	SER	2.4
3	B	36	PHE	2.4
3	A	141	LYS	2.4
3	A	103	LYS	2.4
3	B	54	SER	2.4
3	B	384	THR	2.4
3	A	431	GLU	2.4
3	B	14	MET	2.3
3	A	768	SER	2.3
3	B	25	PRO	2.2
3	B	107	GLU	2.2
3	B	507	LYS	2.2
3	B	24	HIS	2.2
3	B	772	GLY	2.2
3	B	11	THR	2.1
3	B	18	LEU	2.1
1	E	17	DT	2.1
3	B	431	GLU	2.1
3	B	141	LYS	2.1
3	A	98	ASP	2.1
3	B	563	TYR	2.1
3	B	445	ASP	2.0
3	A	421	ASP	2.0
3	A	283	LEU	2.0
3	B	457	ARG	2.0
3	A	668	SER	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(Å <sup>2</sup> )	Q<0.9
4	MG	B	1002	1/1	0.19	31.00	54,54,54,54	0
4	MG	A	1001	1/1	0.19	2.86	41,41,41,41	0
5	ADP	A	2001	27/27	0.29	2.67	50,56,58,58	0
5	ADP	B	2002	27/27	0.24	0.71	64,71,73,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.