



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:24 am GMT

PDB ID : 1WB9  
Title : CRYSTAL STRUCTURE OF E. COLI DNA MISMATCH REPAIR ENZYME MUTS, E38T MUTANT, IN COMPLEX WITH A G.T MISMATCH  
Authors : Natrajan, G.; Georgijevic, D.; Lebbink, J.H.G.; Winterwerp, H.H.K.; De Wind, N.; Sixma, T.K.  
Deposited on : 2004-10-31  
Resolution : 2.10 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](mailto: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.

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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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

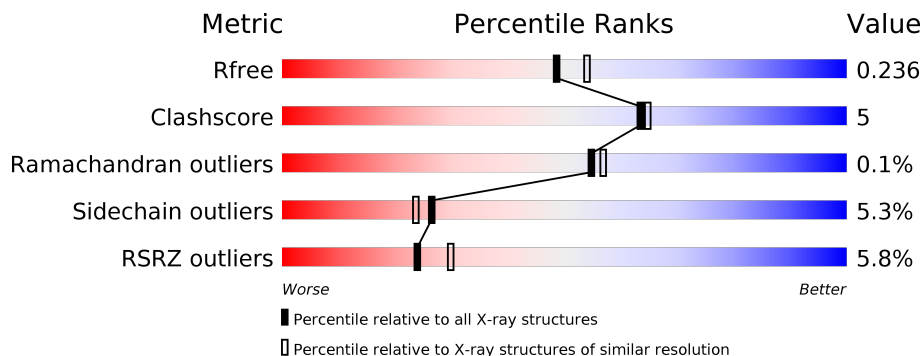
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	800	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>• •</div> </div> </div>
1	B	800	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
2	E	18	<div> <div>22%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
3	F	17	<div> <div>18%</div> <div> <div></div> <div>29%</div> <div>65%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13862 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	788	Total	C	N	O	S	0	0	0
			6204	3904	1103	1168	29			
1	B	754	Total	C	N	O	S	0	0	0
			5961	3755	1060	1118	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	THR	GLU	ENGINEERED MUTATION	UNP P23909
B	38	THR	GLU	ENGINEERED MUTATION	UNP P23909

- Molecule 2 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\*G)-3'.

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

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	492	Total O 492 492	0	0
6	B	423	Total O 423 423	0	0
6	E	23	Total O 23 23	0	0
6	F	17	Total O 17 17	0	0

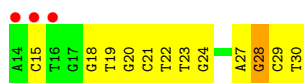




- Molecule 2: 5'-D(\*AP\*GP\*CP\*TP\*GP\*CP\*CP\*AP\*GP\*GP \*CP\*AP\*CP\*CP\*AP\*GP\*TP\*G)-3'



- Molecule 3: 5'-D(\*AP\*CP\*TP\*GP\*GP\*TP\*GP\*CP\*TP\*TP \*GP\*GP\*CP\*AP\*GP\*CP\*T)-3',



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.65Å 92.12Å 260.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.10) 91.5 (20.10-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.189 , 0.234 0.200 , 0.236	Depositor DCC
$R_{free}$ test set	2306 reflections (2.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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: 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	A	0.62	1/6310 (0.0%)	0.85	14/8542 (0.2%)
1	B	0.61	0/6059	0.81	15/8197 (0.2%)
2	E	1.05	0/412	1.65	7/634 (1.1%)
3	F	1.17	3/388 (0.8%)	1.98	15/598 (2.5%)
All	All	0.66	4/13169 (0.0%)	0.93	51/17971 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	MET	SD-CE	-9.15	1.26	1.77
3	F	30	DT	N1-C2	7.58	1.44	1.38
3	F	30	DT	C4-C5	6.03	1.50	1.45
3	F	30	DT	C1'-N1	5.11	1.55	1.49

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	17	DT	O4'-C1'-N1	12.04	116.43	108.00
3	F	23	DT	O4'-C1'-N1	-11.55	99.92	108.00
1	B	584	ARG	NE-CZ-NH2	-9.55	115.52	120.30
3	F	28	DG	O4'-C1'-N9	-8.39	102.13	108.00
2	E	4	DT	O4'-C1'-N1	-8.20	102.26	108.00
1	B	461	ASP	CB-CG-OD2	7.79	125.31	118.30
1	B	584	ARG	NE-CZ-NH1	7.42	124.01	120.30
3	F	27	DA	O4'-C1'-N9	-7.05	103.07	108.00
1	A	747	LEU	CA-CB-CG	-6.75	99.77	115.30
1	A	693	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	413	ASP	CB-CG-OD2	6.64	124.27	118.30
3	F	19	DT	O4'-C1'-N1	6.58	112.60	108.00
1	B	386	ASP	CB-CG-OD2	6.32	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ASP	CB-CG-OD2	6.30	123.97	118.30
3	F	21	DC	O4'-C1'-N1	-6.29	103.59	108.00
3	F	24	DG	N1-C6-O6	-6.26	116.15	119.90
3	F	22	DT	C4-C5-C7	6.24	122.74	119.00
3	F	24	DG	O4'-C1'-N9	-6.15	103.69	108.00
1	A	317	ASP	CB-CG-OD2	6.15	123.83	118.30
3	F	18	DG	O4'-C4'-C3'	-6.11	102.05	104.50
1	A	149	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	296	ASP	CB-CG-OD2	5.95	123.65	118.30
3	F	20	DG	O4'-C1'-N9	5.77	112.04	108.00
1	B	754	ASP	CB-CG-OD2	5.74	123.46	118.30
2	E	6	DC	O4'-C1'-N1	-5.58	104.09	108.00
1	A	748	ASP	CB-CG-OD2	5.58	123.32	118.30
3	F	22	DT	O4'-C1'-N1	-5.53	104.13	108.00
1	B	52	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	270	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	533	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	183	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	561	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	651	ASP	CB-CG-OD1	5.34	123.11	118.30
3	F	22	DT	C6-C5-C7	-5.31	119.72	122.90
1	B	347	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	364	ASP	CB-CG-OD2	5.28	123.05	118.30
3	F	24	DG	C5-C6-O6	5.28	131.77	128.60
1	B	221	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	421	ASP	CB-CG-OD2	5.28	123.05	118.30
2	E	16	DG	O4'-C1'-N9	5.26	111.68	108.00
3	F	15	DC	O4'-C1'-N1	5.26	111.68	108.00
1	B	413	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	265	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	754	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	35	ASP	CB-CG-OD2	5.12	122.91	118.30
2	E	16	DG	P-O3'-C3'	5.11	125.83	119.70
1	B	445	ASP	CB-CG-OD2	5.10	122.89	118.30
2	E	5	DG	O4'-C1'-N9	-5.06	104.46	108.00
2	E	11	DC	C1'-O4'-C4'	-5.05	105.05	110.10
3	F	18	DG	C4'-C3'-C2'	-5.03	98.57	103.10
1	A	358	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	6204	0	6252	65	0
1	B	5961	0	6019	67	0
2	E	367	0	202	0	0
3	F	347	0	194	1	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	492	0	0	11	0
6	B	423	0	0	13	0
6	E	23	0	0	0	0
6	F	17	0	0	0	0
All	All	13862	0	12679	125	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 5.

All (125) 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:674:MET:SD	6:B:2404:HOH:O	2.35	0.84
1:B:584:ARG:HD2	1:B:589:GLU:OE1	1.81	0.80
1:A:143:PHE:CB	1:A:166:MET:HE3	2.12	0.78
1:B:350:ARG:NH1	6:B:2198:HOH:O	2.21	0.73
1:A:707:LEU:HD23	1:B:773:LEU:CD2	2.20	0.71
1:B:108:ARG:N	6:B:2054:HOH:O	2.24	0.70
1:B:350:ARG:HH11	1:B:350:ARG:HG2	1.57	0.69
1:A:454:GLU:OE2	6:A:2299:HOH:O	2.11	0.69
1:B:350:ARG:HH11	1:B:350:ARG:CG	2.06	0.68
1:B:250:THR:HG22	1:B:251:THR:O	1.92	0.68
1:B:143:PHE:HB3	1:B:166:MET:CE	2.25	0.66
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.78	0.66
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.78	0.65
1:B:594:GLU:HG3	1:B:595:PRO:HD2	1.80	0.62
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.82	0.62
1:A:143:PHE:CG	1:A:166:MET:HE3	2.36	0.60
1:A:160:PRO:HB2	1:A:166:MET:HE2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLU:HG3	1:B:268:ILE:HD11	1.86	0.58
1:A:784:GLU:HG3	6:B:2363:HOH:O	2.05	0.55
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.87	0.55
1:B:151:SER:O	1:B:353:ALA:HB2	2.06	0.55
1:B:281:GLN:HE21	1:B:285:GLY:HA2	1.72	0.55
1:A:707:LEU:HD23	1:B:773:LEU:HD23	1.89	0.55
1:A:443:ALA:HB1	1:A:509:TYR:OH	2.08	0.54
1:A:709:TRP:CE3	1:A:732:LEU:HD23	2.42	0.54
1:B:584:ARG:CD	1:B:589:GLU:OE1	2.52	0.53
1:A:707:LEU:HD23	1:B:773:LEU:HD22	1.91	0.53
1:A:674:MET:CG	1:B:776:ALA:HA	2.39	0.53
1:A:199:ARG:HD3	1:A:203:GLU:OE1	2.08	0.53
1:B:139:ASP:HB3	1:B:141:LYS:H	1.74	0.52
1:B:315:VAL:HG23	6:B:2150:HOH:O	2.09	0.52
1:B:730:PHE:HD1	6:B:2399:HOH:O	1.93	0.52
1:A:171:GLN:OE1	1:A:274:ARG:HD2	2.10	0.52
1:A:143:PHE:HB3	1:A:166:MET:HE3	1.90	0.51
1:A:717:ASN:O	1:A:720:LYS:NZ	2.43	0.51
1:B:71:ILE:HD12	1:B:72:PRO:O	2.10	0.51
1:B:396:LYS:HD3	1:B:548:ALA:HB2	1.91	0.51
1:B:212:GLN:OE1	1:B:242:GLN:NE2	2.44	0.51
1:A:674:MET:HG2	1:B:776:ALA:HA	1.93	0.51
1:A:397:MET:HE1	1:A:549:LEU:HD21	1.92	0.50
1:B:154:ARG:HD2	6:B:2096:HOH:O	2.10	0.50
1:B:538:HIS:HE1	6:B:2267:HOH:O	1.93	0.50
1:B:692:MET:HE2	1:B:695:ILE:HD13	1.93	0.50
1:A:396:LYS:NZ	6:A:2271:HOH:O	2.44	0.50
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.94	0.50
1:B:427:SER:HB3	6:B:2243:HOH:O	2.12	0.50
3:F:28:DG:C5	3:F:29:DC:C4	3.00	0.50
1:B:397:MET:HG3	1:B:549:LEU:HD21	1.94	0.49
1:A:670:PHE:HD2	6:A:2400:HOH:O	1.95	0.49
1:B:179:LEU:HD23	1:B:197:ARG:HB2	1.94	0.49
1:B:332:GLN:NE2	1:B:333:ASP:OD1	2.42	0.49
1:B:143:PHE:HB3	1:B:166:MET:HE3	1.94	0.48
1:A:585:HIS:CD2	1:A:588:VAL:H	2.32	0.48
1:A:37:TYR:OH	1:A:94:GLU:OE2	2.23	0.48
1:B:143:PHE:CB	1:B:166:MET:CE	2.92	0.48
1:A:143:PHE:CB	1:A:166:MET:CE	2.88	0.47
1:A:436:TRP:CZ2	1:A:519:LYS:HD2	2.49	0.47
1:A:375:LEU:HD12	1:A:397:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:PRO:HD2	1:B:424:VAL:HG22	1.96	0.47
1:B:227:VAL:HG12	1:B:260:MET:HB2	1.97	0.47
1:B:27:ILE:HG12	1:B:89:SER:HB2	1.96	0.47
1:B:624:MET:HE1	1:B:692:MET:N	2.30	0.47
1:B:311:LEU:HD23	1:B:636:ILE:HD13	1.96	0.47
1:A:160:PRO:HG2	1:A:166:MET:HE2	1.98	0.46
1:A:585:HIS:HD2	1:A:588:VAL:H	1.64	0.46
1:A:585:HIS:CE1	6:A:2360:HOH:O	2.68	0.45
1:A:83:LEU:HD13	1:A:90:VAL:HG21	1.97	0.45
1:B:483:HIS:CE1	1:B:484:LEU:HG	2.51	0.45
1:A:463:LEU:HA	1:A:476:GLN:O	2.16	0.45
1:A:397:MET:CE	1:A:549:LEU:HD21	2.47	0.45
1:B:594:GLU:HG3	1:B:595:PRO:CD	2.46	0.45
1:A:160:PRO:HG2	1:A:166:MET:CE	2.47	0.45
1:A:83:LEU:HD13	1:A:90:VAL:CG2	2.47	0.45
1:B:268:ILE:HB	1:B:652:ARG:HG2	1.98	0.45
1:A:326:GLN:HB3	6:A:2266:HOH:O	2.16	0.45
1:B:350:ARG:CG	1:B:350:ARG:NH1	2.76	0.45
1:A:585:HIS:HE1	6:A:2360:HOH:O	2.00	0.45
1:A:781:VAL:HG21	1:B:674:MET:HE2	1.98	0.45
1:B:620:LYS:HG3	1:B:747:LEU:HD12	1.98	0.45
1:A:143:PHE:HB2	1:A:166:MET:CE	2.47	0.44
1:B:327:THR:HG22	1:B:331:LEU:HD12	1.99	0.44
1:A:585:HIS:CD2	1:A:588:VAL:HG23	2.52	0.44
1:A:686:GLU:HG2	1:A:720:LYS:HB2	1.98	0.44
1:B:677:THR:HG23	1:B:692:MET:HE3	1.98	0.44
1:B:718:LYS:HD2	6:B:2363:HOH:O	2.15	0.44
1:B:108:ARG:HA	6:B:2054:HOH:O	2.18	0.44
1:A:199:ARG:CD	1:A:203:GLU:OE1	2.66	0.44
1:A:345:VAL:HG11	1:A:549:LEU:HD13	2.00	0.43
1:B:692:MET:CE	1:B:695:ILE:HD13	2.48	0.43
1:A:388:ALA:HB3	1:A:389:PRO:HD3	2.00	0.43
1:B:183:ASP:OD1	1:B:201:LEU:HD11	2.19	0.43
1:A:488:ASN:ND2	6:A:2309:HOH:O	2.51	0.43
1:A:670:PHE:N	6:A:2400:HOH:O	2.51	0.43
1:A:755:THR:HG23	1:A:756:ILE:N	2.33	0.43
1:A:509:TYR:CZ	1:A:513:VAL:HG21	2.53	0.43
1:A:157:LEU:HD12	1:A:260:MET:HG3	2.01	0.43
1:B:582:GLU:HG3	6:B:2302:HOH:O	2.18	0.42
1:B:759:MET:CE	1:B:759:MET:HA	2.49	0.42
1:B:669:THR:CG2	1:B:672:VAL:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:ALA:HB3	1:B:771:TYR:CE1	2.54	0.42
1:A:160:PRO:CB	1:A:166:MET:HE2	2.48	0.42
1:A:143:PHE:HB2	1:A:166:MET:HE3	1.94	0.42
1:A:51:LEU:HD21	1:A:83:LEU:HG	2.01	0.42
1:A:579:ARG:HD3	6:A:2369:HOH:O	2.18	0.42
1:A:268:ILE:HB	1:A:652:ARG:HG2	2.02	0.42
1:B:41:TYR:HB3	1:B:42:ASP:H	1.78	0.42
1:B:30:PHE:HB2	1:B:92:ILE:HD13	2.02	0.41
1:A:652:ARG:HB3	1:A:652:ARG:HH11	1.86	0.41
1:A:674:MET:HG3	1:B:776:ALA:HA	2.02	0.41
1:A:492:ARG:HG2	6:A:2313:HOH:O	2.19	0.41
1:A:496:LYS:HE2	6:A:2314:HOH:O	2.19	0.41
1:A:311:LEU:HD23	1:A:636:ILE:HD13	2.02	0.41
1:B:388:ALA:HB3	1:B:389:PRO:HD3	2.03	0.41
1:A:781:VAL:HG21	1:B:674:MET:CE	2.51	0.41
1:B:718:LYS:CD	6:B:2363:HOH:O	2.68	0.41
1:B:669:THR:HG23	1:B:672:VAL:H	1.86	0.41
1:B:200:PRO:HG2	1:B:203:GLU:HG3	2.03	0.41
1:B:561:ARG:HA	1:B:561:ARG:HD2	1.72	0.41
1:A:624:MET:HE3	1:A:724:LEU:HB2	2.03	0.41
1:A:494:THR:OG1	1:A:499:GLU:OE2	2.20	0.40
1:A:447:LEU:HD21	1:A:509:TYR:CE2	2.55	0.40
1:B:71:ILE:HD11	1:B:76:VAL:HA	2.03	0.40
1:B:21:LYS:HE3	1:B:25:PRO:HA	2.04	0.40
1:A:23:GLN:HB3	1:A:24:HIS:CD2	2.56	0.40
1:A:561:ARG:HA	1:A:561:ARG:HD2	1.90	0.40

There are no symmetry-related clashes.

## 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	784/800 (98%)	762 (97%)	20 (3%)	2 (0%)	44	44
1	B	746/800 (93%)	733 (98%)	13 (2%)	0	100	100
All	All	1530/1600 (96%)	1495 (98%)	33 (2%)	2 (0%)	55	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	ALA
1	A	441	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	656/664 (99%)	622 (95%)	34 (5%)	27	24
1	B	631/664 (95%)	597 (95%)	34 (5%)	26	23
All	All	1287/1328 (97%)	1219 (95%)	68 (5%)	26	24

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	46	ARG
1	A	57	LYS
1	A	58	ARG
1	A	126	GLN
1	A	155	PHE
1	A	190	ILE
1	A	275	ARG
1	A	332	GLN
1	A	375	LEU
1	A	386	ASP
1	A	420	ARG
1	A	441	ASP
1	A	479	ARG

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	492	ARG
1	A	495	LEU
1	A	512	LYS
1	A	516	SER
1	A	584	ARG
1	A	591	VAL
1	A	594	GLU
1	A	652	ARG
1	A	656	ARG
1	A	670	PHE
1	A	673	GLU
1	A	674	MET
1	A	697	ARG
1	A	705	LEU
1	A	707	LEU
1	A	735	LEU
1	A	747	LEU
1	A	755	THR
1	A	790	ARG
1	B	16	GLN
1	B	18	LEU
1	B	19	ARG
1	B	32	ARG
1	B	41	TYR
1	B	46	ARG
1	B	49	GLN
1	B	55	LEU
1	B	71	ILE
1	B	78	ASN
1	B	93	CYS
1	B	109	LYS
1	B	115	THR
1	B	126	GLN
1	B	137	TRP
1	B	140	SER
1	B	155	PHE
1	B	211	GLN
1	B	313	MET
1	B	315	VAL
1	B	403	LEU
1	B	404	ARG

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Mol	Chain	Res	Type
1	B	456	GLU
1	B	464	LYS
1	B	479	ARG
1	B	491	ARG
1	B	561	ARG
1	B	584	ARG
1	B	617	MET
1	B	656	ARG
1	B	669	THR
1	B	735	LEU
1	B	737	GLU
1	B	759	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	131	ASN
1	A	248	GLN
1	A	585	HIS
1	A	616	ASN
1	A	679	ASN
1	A	734	GLN
1	A	760	HIS
1	B	211	GLN
1	B	242	GLN
1	B	248	GLN
1	B	281	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
4	ADP	A	1801	5	25,29,29	1.22	2 (8%)	24,45,45	2.21	1 (4%)

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
4	ADP	A	1801	5	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N1	2.19	1.38	1.33
4	A	1801	ADP	C2-N3	4.26	1.39	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ADP	N3-C2-N1	-9.97	120.18	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	788/800 (98%)	0.10	37 (4%) 32 38	4, 18, 27, 38	0
1	B	754/800 (94%)	0.21	47 (6%) 21 27	9, 18, 26, 38	0
2	E	18/18 (100%)	0.65	4 (22%) 1 1	10, 17, 37, 45	0
3	F	17/17 (100%)	0.51	3 (17%) 2 2	12, 20, 39, 40	0
All	All	1577/1635 (96%)	0.16	91 (5%) 24 30	4, 18, 27, 45	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	8.0
1	B	41	TYR	6.8
1	A	62	ALA	6.7
2	E	18	DG	6.6
1	A	61	SER	6.4
1	B	74	HIS	6.2
1	B	658	GLY	5.4
1	A	593	ASN	5.3
1	A	441	ASP	5.1
3	F	14	DA	5.0
1	A	63	GLY	4.6
1	B	25	PRO	4.6
1	B	52	ASP	4.6
1	A	658	GLY	4.3
1	A	103	LYS	4.3
1	B	56	THR	4.3
1	A	752	HIS	4.2
1	B	55	LEU	4.2
1	A	192	GLY	4.1
1	B	39	LEU	3.9
1	B	445	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	286	GLY	3.9
1	B	140	SER	3.7
2	E	16	DG	3.7
2	E	17	DT	3.6
1	B	29	LEU	3.6
1	B	15	GLN	3.6
1	A	60	ALA	3.5
1	B	28	LEU	3.5
1	B	592	LEU	3.5
1	A	100	ALA	3.5
2	E	1	DA	3.5
1	B	73	TYR	3.5
1	B	475	ILE	3.5
1	B	30	PHE	3.4
1	B	24	HIS	3.4
1	A	800	SER	3.2
3	F	15	DC	3.2
1	A	475	ILE	3.2
1	B	457	ARG	3.2
1	A	549	LEU	3.2
1	A	753	GLY	3.0
1	A	284	ALA	3.0
1	A	220	ARG	3.0
1	B	456	GLU	3.0
1	A	443	ALA	2.9
1	B	506	LEU	2.9
1	B	90	VAL	2.9
1	B	284	ALA	2.8
1	B	19	ARG	2.8
1	A	386	ASP	2.7
1	A	445	ASP	2.7
3	F	16	DT	2.6
1	A	440	ALA	2.6
1	A	672	VAL	2.6
1	B	26	GLU	2.6
1	A	768	SER	2.6
1	A	365	LEU	2.6
1	B	22	ALA	2.5
1	B	136	ILE	2.5
1	B	54	SER	2.5
1	B	593	ASN	2.5
1	A	555	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	35	ASP	2.4
1	B	386	ASP	2.4
1	A	670	PHE	2.4
1	A	97	GLY	2.4
1	B	49	GLN	2.4
1	B	78	ASN	2.3
1	B	431	GLU	2.3
1	A	563	TYR	2.3
1	A	448	GLU	2.3
1	B	161	ALA	2.3
1	B	414	THR	2.3
1	A	402	GLU	2.3
1	A	556	VAL	2.3
1	A	64	GLU	2.3
1	B	402	GLU	2.2
1	A	750	LEU	2.2
1	B	552	LEU	2.2
1	A	754	ASP	2.2
1	A	595	PRO	2.2
1	B	141	LYS	2.2
1	B	18	LEU	2.1
1	B	192	GLY	2.1
1	B	36	PHE	2.1
1	A	442	GLY	2.1
1	B	737	GLU	2.0
1	B	450	LEU	2.0
1	B	413	ASP	2.0
1	B	574	ASP	2.0

## 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 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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	A	1801	27/27	0.98	0.08	-1.02	13,19,21,26	0
5	MG	A	1802	1/1	0.95	0.07	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.