



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:35 PM GMT

PDB ID : 3DNT  
Title : structures of MDT proteins  
Authors : Schumacher, M.A.  
Deposited on : 2008-07-02  
Resolution : 1.66 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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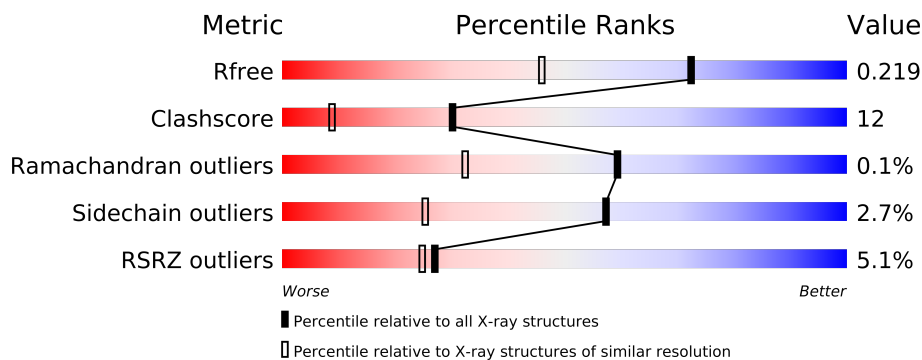
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.66 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	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	440	
1	B	440	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7499 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.

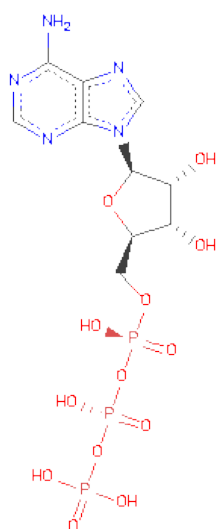
- Molecule 1 is a protein called Protein hipA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	Se	0	0	0
			3284	2107	573	591	3	10			
1	B	419	Total	C	N	O	S	Se	0	0	0
			3312	2120	579	600	3	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLN	ASP	ENGINEERED	UNP P23874
B	309	GLN	ASP	ENGINEERED	UNP P23874

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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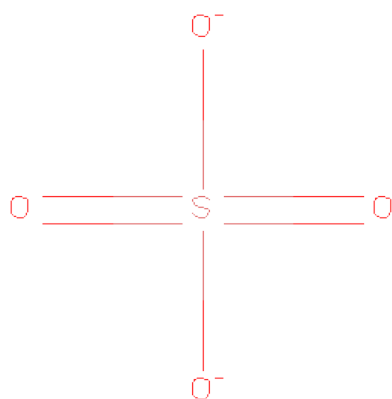
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

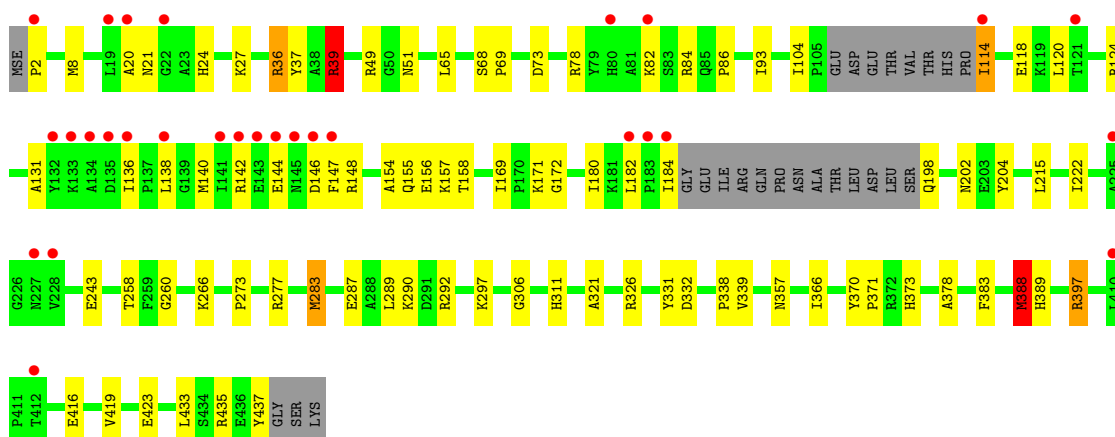
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	401	Total	O	0	0
			401	401		
5	B	426	Total	O	0	0
			426	426		

### 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.

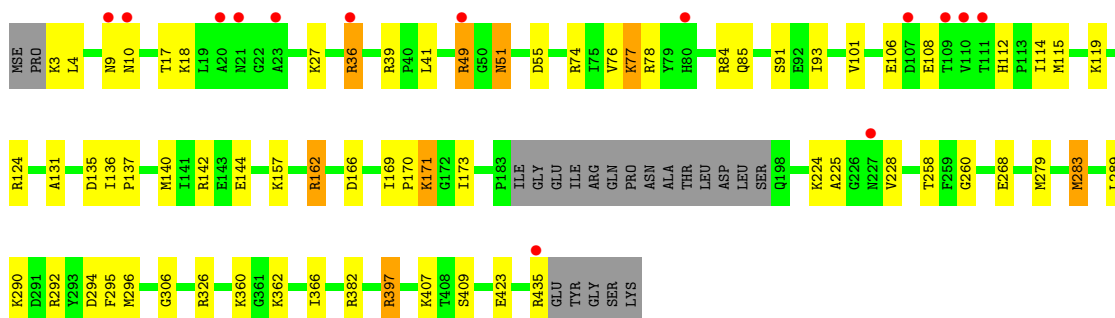
#### • Molecule 1: Protein hipA

Chain A: 



#### • Molecule 1: Protein hipA

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.54Å 84.09Å 69.25Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	42.58 – 1.66 42.58 – 1.66	Depositor EDS
% Data completeness (in resolution range)	94.7 (42.58-1.66) 96.0 (42.58-1.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 1.66Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.184 , 0.217 0.186 , 0.219	Depositor DCC
$R_{free}$ test set	8591 reflections (9.65%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.1	EDS
Estimated twinning fraction	0.001 for l,k,-h 0.019 for h,-k,-l 0.021 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 173306 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 32.37 % 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 9.4989e-04. 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: MG, SO4, ATP

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	0.47	0/3346	0.69	4/4514 (0.1%)
1	B	0.49	0/3375	0.68	1/4557 (0.0%)
All	All	0.48	0/6721	0.68	5/9071 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	MSE	CG-SE-CE	6.45	113.08	98.90
1	A	39	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	397	ARG	CG-CD-NE	-5.83	99.56	111.80
1	A	397	ARG	CG-CD-NE	-5.69	99.85	111.80
1	A	39	ARG	NE-CZ-NH1	5.56	123.08	120.30

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	A	3284	0	3335	87	0
1	B	3312	0	3355	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	12	6	0
2	B	31	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
5	A	401	0	0	13	0
5	B	426	0	0	18	0
All	All	7499	0	6714	161	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 12.

All (161) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279:MSE:HE2	1:B:295:PHE:CD2	1.64	1.32
1:B:279:MSE:HE3	1:B:296:MSE:SE	1.97	1.14
1:A:36:ARG:HD3	1:A:36:ARG:H	1.05	1.09
1:B:279:MSE:CE	1:B:295:PHE:HD2	1.71	1.02
1:A:370:TYR:H	1:A:373:HIS:HD2	1.17	0.89
1:A:36:ARG:HD3	1:A:36:ARG:N	1.90	0.87
1:B:101:VAL:HG22	5:B:1012:HOH:O	1.77	0.83
1:B:326:ARG:HG2	5:B:971:HOH:O	1.79	0.83
1:B:36:ARG:HD3	1:B:36:ARG:H	1.43	0.82
1:B:3:LYS:HD2	1:B:17:THR:HG22	1.61	0.82
1:B:409:SER:HB2	5:B:1170:HOH:O	1.79	0.81
1:B:279:MSE:HE2	1:B:295:PHE:HD2	0.76	0.79
1:B:225:ALA:O	1:B:228:VAL:HG12	1.82	0.79
1:B:114:ILE:HG22	1:B:173:ILE:HD11	1.64	0.78
1:B:283:MSE:HE3	1:B:292:ARG:CD	2.16	0.76
1:A:36:ARG:H	1:A:36:ARG:CD	1.91	0.75
1:A:283:MSE:CE	1:A:283:MSE:HA	2.19	0.73
1:B:435:ARG:HB2	5:B:1034:HOH:O	1.88	0.72
1:A:326:ARG:HG2	5:A:843:HOH:O	1.89	0.72
1:A:378:ALA:CB	1:A:388:MSE:HG3	2.20	0.72
1:A:378:ALA:HB2	1:A:388:MSE:HG3	1.72	0.72
1:B:76:VAL:HG21	1:B:84:ARG:HG2	1.73	0.70
1:A:306:GLY:HA2	1:A:366:ILE:HD13	1.74	0.70
1:A:21:ASN:HA	1:B:289:LEU:CD1	2.22	0.69
1:A:39:ARG:HD2	5:A:893:HOH:O	1.91	0.69
1:A:156:GLU:H	1:A:184:ILE:HD11	1.58	0.67
1:B:77:LYS:HD2	1:B:78:ARG:N	2.09	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:ARG:CD	1:B:36:ARG:H	2.07	0.66
1:B:36:ARG:HD3	1:B:36:ARG:N	2.10	0.66
1:A:156:GLU:H	1:A:184:ILE:CD1	2.09	0.65
1:A:21:ASN:HA	1:B:289:LEU:HD12	1.80	0.64
1:A:370:TYR:H	1:A:373:HIS:CD2	2.09	0.64
1:B:106:GLU:HG3	5:B:1204:HOH:O	1.99	0.63
1:A:383:PHE:CE2	1:A:388:MSE:HG2	2.33	0.63
1:A:20:ALA:O	1:B:289:LEU:HD12	1.98	0.63
1:A:155:GLN:HG3	1:A:184:ILE:HD11	1.81	0.62
1:A:283:MSE:HA	1:A:283:MSE:HE2	1.81	0.62
1:A:435:ARG:NH2	5:A:1122:HOH:O	2.33	0.62
1:B:162:ARG:HH11	1:B:162:ARG:CG	2.11	0.62
1:B:326:ARG:CG	5:B:971:HOH:O	2.43	0.61
1:B:77:LYS:HD2	1:B:77:LYS:C	2.20	0.61
1:B:283:MSE:HE3	1:B:292:ARG:HD2	1.80	0.61
1:B:74:ARG:O	1:B:77:LYS:HE3	2.00	0.61
1:A:383:PHE:CD2	1:A:388:MSE:HG2	2.35	0.61
1:B:9:ASN:HA	5:B:1208:HOH:O	2.01	0.60
1:A:332:ASP:HB2	2:A:500:ATP:PA	2.41	0.60
1:B:279:MSE:CE	1:B:296:MSE:HG2	2.31	0.60
1:A:419:VAL:O	1:A:423:GLU:HG2	2.01	0.60
1:A:114:ILE:HD13	1:A:114:ILE:N	2.16	0.60
1:A:243:GLU:OE2	5:A:965:HOH:O	2.16	0.60
1:B:77:LYS:HE2	1:B:135:ASP:O	2.02	0.59
1:B:407:LYS:HE3	1:B:423:GLU:OE1	2.02	0.59
1:B:283:MSE:HE2	1:B:283:MSE:HA	1.84	0.59
1:A:332:ASP:HB2	2:A:500:ATP:O1A	2.03	0.59
1:A:37:TYR:HB3	1:A:321:ALA:HB1	1.84	0.58
1:A:8:MSE:SE	5:A:1066:HOH:O	2.70	0.58
1:A:326:ARG:CG	5:A:843:HOH:O	2.50	0.57
1:A:118:GLU:CD	1:A:124:ARG:HH12	2.06	0.57
1:B:397:ARG:NH1	1:B:397:ARG:HG2	2.19	0.57
1:A:373:HIS:HE1	4:A:833:SO4:O4	1.88	0.57
1:A:297:LYS:HD3	5:A:944:HOH:O	2.05	0.56
1:B:283:MSE:CE	1:B:283:MSE:HA	2.35	0.56
1:B:279:MSE:HE3	1:B:296:MSE:CG	2.35	0.56
1:B:36:ARG:HH11	1:B:36:ARG:H	1.54	0.55
1:B:41:LEU:HD11	1:B:101:VAL:HG11	1.89	0.55
1:B:279:MSE:CE	1:B:295:PHE:HB3	2.36	0.55
1:B:4:LEU:HD21	1:B:91:SER:HA	1.90	0.54
1:B:124:ARG:HD3	5:B:1210:HOH:O	2.08	0.54
1:B:77:LYS:NZ	1:B:136:ILE:HD13	2.23	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:ARG:CD	5:A:893:HOH:O	2.51	0.54
1:A:389:HIS:HD2	1:A:437:TYR:OH	1.90	0.54
1:A:78:ARG:NH2	1:A:142:ARG:HA	2.22	0.54
1:A:289:LEU:H	1:A:289:LEU:HD22	1.73	0.54
1:B:170:PRO:C	1:B:171:LYS:HD2	2.29	0.53
1:B:224:LYS:HB3	5:B:1157:HOH:O	2.08	0.53
1:A:154:ALA:N	2:A:500:ATP:O2G	2.34	0.53
1:A:289:LEU:N	1:A:289:LEU:HD22	2.24	0.53
1:A:144:GLU:HG2	1:A:147:PHE:HB2	1.91	0.53
1:A:146:ASP:CG	1:A:172:GLY:H	2.12	0.52
1:B:279:MSE:HE1	1:B:295:PHE:HB3	1.92	0.52
1:A:155:GLN:CG	1:A:184:ILE:HD11	2.38	0.52
1:B:17:THR:HG23	5:B:1008:HOH:O	2.10	0.52
1:A:202:ASN:ND2	1:A:338:PRO:HG3	2.25	0.51
1:B:49:ARG:HH11	1:B:49:ARG:CB	2.24	0.51
1:A:198:GLN:N	5:A:1131:HOH:O	2.44	0.51
1:B:162:ARG:HD3	5:B:886:HOH:O	2.11	0.50
1:B:131:ALA:HB1	1:B:136:ILE:HB	1.93	0.50
1:A:157:LYS:HA	1:A:182:LEU:CD2	2.41	0.50
1:B:41:LEU:HD11	1:B:101:VAL:CG1	2.41	0.50
1:B:124:ARG:NH2	1:B:144:GLU:OE1	2.45	0.50
1:A:146:ASP:HB3	1:A:171:LYS:HD2	1.93	0.50
1:A:339:VAL:O	1:A:339:VAL:HG12	2.13	0.49
1:B:397:ARG:HG2	1:B:397:ARG:HH11	1.76	0.49
1:A:332:ASP:HB2	2:A:500:ATP:O2A	2.13	0.49
1:A:2:PRO:HD2	1:A:82:LYS:NZ	2.28	0.49
1:B:435:ARG:HD2	5:B:1239:HOH:O	2.12	0.48
1:B:77:LYS:HZ1	1:B:136:ILE:HD13	1.78	0.48
1:A:78:ARG:O	1:A:78:ARG:HD3	2.14	0.48
1:B:279:MSE:CE	1:B:295:PHE:CD2	2.61	0.48
1:B:18:LYS:NZ	5:B:1198:HOH:O	2.39	0.48
1:A:24:HIS:NE2	1:A:86:PRO:HG2	2.28	0.48
1:A:397:ARG:NH1	1:A:397:ARG:HG2	2.29	0.47
1:A:78:ARG:CZ	1:A:142:ARG:HA	2.45	0.47
1:B:74:ARG:O	1:B:77:LYS:HG3	2.15	0.47
1:A:260:GLY:HA2	5:A:865:HOH:O	2.15	0.47
1:A:120:LEU:HD21	1:A:169:ILE:HG13	1.97	0.46
1:A:273:PRO:HB3	1:A:277:ARG:HD3	1.95	0.46
1:A:93:ILE:HG21	1:A:140:MSE:HE1	1.98	0.46
1:A:357:ASN:ND2	5:A:918:HOH:O	2.47	0.46
1:B:162:ARG:NH1	1:B:162:ARG:CG	2.74	0.46
1:A:27:LYS:HD3	1:A:51:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.81	0.46
1:B:283:MSE:HE3	1:B:292:ARG:HD3	1.93	0.46
1:A:204:TYR:HB2	1:A:222:ILE:HD11	1.97	0.46
1:A:283:MSE:HE3	1:A:292:ARG:CD	2.46	0.46
1:B:18:LYS:HE3	1:B:85:GLN:NE2	2.32	0.46
1:B:137:PRO:HG2	1:B:140:MSE:HE3	1.97	0.46
1:A:144:GLU:OE2	1:A:171:LYS:HE3	2.16	0.45
1:B:144:GLU:HG3	1:B:169:ILE:HD13	1.98	0.45
1:B:108:GLU:OE2	1:B:112:HIS:NE2	2.41	0.45
1:A:157:LYS:HA	1:A:182:LEU:HD22	1.98	0.45
1:B:142:ARG:NH2	5:B:1100:HOH:O	2.50	0.45
1:A:131:ALA:O	1:A:136:ILE:HB	2.17	0.44
1:B:49:ARG:HH11	1:B:49:ARG:HB2	1.82	0.44
1:A:65:LEU:HD11	1:A:86:PRO:HA	1.99	0.44
1:B:162:ARG:HH11	1:B:162:ARG:HG2	1.83	0.44
1:B:27:LYS:HB2	1:B:51:ASN:ND2	2.33	0.44
1:A:8:MSE:HE1	1:A:39:ARG:CD	2.47	0.44
1:A:331:TYR:CE1	2:A:500:ATP:H2'	2.53	0.43
1:B:306:GLY:HA2	1:B:366:ILE:HD13	2.01	0.43
1:A:68:SER:HA	1:A:69:PRO:HD3	1.94	0.43
1:B:171:LYS:N	1:B:171:LYS:HD2	2.32	0.43
1:A:156:GLU:N	1:A:184:ILE:HD11	2.31	0.43
1:B:260:GLY:HA2	5:B:871:HOH:O	2.18	0.43
1:B:382:ARG:HD3	5:B:1085:HOH:O	2.19	0.43
1:A:93:ILE:HA	1:A:148:ARG:HB3	2.00	0.43
1:A:8:MSE:HE1	1:A:39:ARG:HD3	2.00	0.43
1:B:115:MSE:SE	5:B:1154:HOH:O	2.87	0.42
1:B:119:LYS:HE3	1:B:166:ASP:OD1	2.18	0.42
1:A:118:GLU:OE1	1:A:124:ARG:NH1	2.50	0.42
1:A:158:THR:HG22	1:A:180:ILE:HB	2.00	0.42
1:A:73:ASP:OD1	1:A:84:ARG:NH1	2.52	0.42
1:B:279:MSE:HE1	1:B:296:MSE:HG2	2.00	0.42
1:A:158:THR:CG2	1:A:180:ILE:HB	2.49	0.42
1:B:268:GLU:OE2	1:B:362:LYS:NZ	2.50	0.42
1:A:371:PRO:HG3	1:A:433:LEU:HD23	2.02	0.42
1:A:157:LYS:HB2	1:A:180:ILE:O	2.19	0.42
1:A:215:LEU:HD21	1:A:297:LYS:HE2	2.02	0.42
1:A:8:MSE:HE2	5:A:1223:HOH:O	2.19	0.42
1:A:416:GLU:HG2	5:A:1028:HOH:O	2.19	0.42
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.84	0.41
1:B:93:ILE:HG21	1:B:140:MSE:HE1	2.02	0.41
1:B:142:ARG:NH2	5:B:1153:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:LYS:HD2	1:A:311:HIS:CE1	2.55	0.41
1:A:138:LEU:HB2	1:A:140:MSE:HE2	2.02	0.41
1:A:287:GLU:HG3	1:A:290:LYS:HB3	2.03	0.41
1:A:283:MSE:HA	1:A:283:MSE:HE3	2.00	0.41
1:A:331:TYR:CE1	2:A:500:ATP:H3'	2.54	0.41
1:A:202:ASN:ND2	1:A:338:PRO:CG	2.83	0.41
1:B:290:LYS:HD2	1:B:294:ASP:OD2	2.21	0.40
1:B:290:LYS:HB3	1:B:290:LYS:HE2	1.90	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	409/440 (93%)	404 (99%)	5 (1%)	0	100	100
1	B	415/440 (94%)	407 (98%)	7 (2%)	1 (0%)	56	29
All	All	824/880 (94%)	811 (98%)	12 (2%)	1 (0%)	59	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	ASN

### 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	352/363 (97%)	345 (98%)	7 (2%)	68	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	356/363 (98%)	344 (97%)	12 (3%)	49	17
All	All	708/726 (98%)	689 (97%)	19 (3%)	57	25

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	39	ARG
1	A	104	ILE
1	A	114	ILE
1	A	258	THR
1	A	283	MSE
1	A	388	MSE
1	B	36	ARG
1	B	39	ARG
1	B	49	ARG
1	B	51	ASN
1	B	55	ASP
1	B	77	LYS
1	B	157	LYS
1	B	162	ARG
1	B	171	LYS
1	B	258	THR
1	B	283	MSE
1	B	360	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	216	ASN
1	A	357	ASN
1	A	373	HIS
1	A	389	HIS
1	B	51	ASN
1	B	216	ASN
1	B	389	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
2	ATP	A	500	3	33,33,33	1.96	9 (27%)	52,52,52	1.80	13 (25%)
4	SO4	A	833	-	4,4,4	0.19	0	6,6,6	0.20	0
2	ATP	B	501	3	33,33,33	1.99	9 (27%)	52,52,52	1.65	14 (26%)
4	SO4	B	834	-	4,4,4	0.36	0	6,6,6	0.16	0

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	ATP	A	500	3	-	0/22/38/38	0/1/3/3
4	SO4	A	833	-	-	0/0/0/0	0/0/0/0
2	ATP	B	501	3	-	0/22/38/38	0/1/3/3
4	SO4	B	834	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ATP	PG-O3B	6.97	1.72	1.60
2	A	500	ATP	PA-O3A	5.20	1.69	1.59
2	A	500	ATP	PG-O3B	4.51	1.68	1.60
2	A	500	ATP	C4-N3	4.49	1.42	1.35
2	B	501	ATP	C4-N3	3.80	1.41	1.35
2	B	501	ATP	PB-O3B	3.45	1.66	1.59
2	A	500	ATP	C2-N3	3.39	1.38	1.32
2	A	500	ATP	PB-O3B	2.90	1.65	1.59
2	B	501	ATP	PA-O3A	2.74	1.64	1.59
2	B	501	ATP	C2-N3	2.71	1.37	1.32
2	A	500	ATP	O4'-C1'	2.42	1.45	1.41
2	B	501	ATP	PG-O2G	-2.40	1.45	1.54
2	B	501	ATP	C2'-C1'	-2.34	1.50	1.53
2	A	500	ATP	PG-O2G	-2.21	1.46	1.54
2	B	501	ATP	PB-O2B	-2.11	1.45	1.55
2	B	501	ATP	O4'-C1'	2.10	1.44	1.41
2	A	500	ATP	PA-O2A	-2.09	1.45	1.55
2	A	500	ATP	C8-N7	-2.04	1.30	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ATP	O3A-PB-O3B	-5.09	91.32	101.66
2	A	500	ATP	PA-O3A-PB	3.98	143.36	131.68
2	A	500	ATP	O2B-PB-O1B	3.93	134.15	112.21
2	B	501	ATP	O2B-PB-O1B	3.92	134.12	112.21
2	A	500	ATP	O3A-PB-O1B	-3.88	83.46	111.28
2	B	501	ATP	O3A-PB-O1B	-3.77	84.22	111.28
2	A	500	ATP	C3'-C2'-C1'	3.50	106.38	100.91
2	B	501	ATP	PB-O3B-PG	-3.36	121.83	131.68
2	B	501	ATP	O3A-PB-O3B	-3.31	94.93	101.66
2	A	500	ATP	PB-O3B-PG	-3.16	122.43	131.68
2	A	500	ATP	N3-C2-N1	-3.05	126.15	128.71
2	B	501	ATP	C3'-C2'-C1'	3.04	105.67	100.91
2	A	500	ATP	C4'-O4'-C1'	3.00	113.00	109.75
2	B	501	ATP	N3-C2-N1	-2.93	126.25	128.71
2	B	501	ATP	PA-O3A-PB	2.76	139.77	131.68
2	B	501	ATP	C8-N9-C1'	2.61	131.53	126.38
2	A	500	ATP	C4-C5-N7	2.60	111.75	109.52
2	B	501	ATP	C4-C5-N7	2.56	111.72	109.52
2	B	501	ATP	O2B-PB-O3A	-2.56	93.01	105.14
2	B	501	ATP	O4'-C1'-C2'	-2.42	103.06	106.77
2	B	501	ATP	C1'-N9-C4	-2.40	122.49	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ATP	O4'-C1'-C2'	-2.36	103.15	106.77
2	B	501	ATP	C2'-C1'-N9	2.33	119.24	113.27
2	A	500	ATP	O2B-PB-O3A	-2.26	94.41	105.14
2	A	500	ATP	C8-N9-C1'	2.24	130.79	126.38
2	B	501	ATP	C4'-O4'-C1'	2.05	111.97	109.75
2	A	500	ATP	C2'-C1'-N9	2.01	118.43	113.27

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	415/440 (94%)	0.19	29 (6%) 16 15	10, 21, 48, 63	0
1	B	419/440 (95%)	-0.03	14 (3%) 44 44	10, 18, 41, 53	0
All	All	834/880 (94%)	0.08	43 (5%) 27 24	10, 20, 45, 63	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	THR	8.3
1	A	184	ILE	7.9
1	A	142	ARG	6.2
1	A	141	ILE	5.7
1	A	132	TYR	4.7
1	A	143	GLU	4.5
1	B	20	ALA	4.4
1	A	145	ASN	4.4
1	A	227	ASN	4.2
1	A	183	PRO	3.8
1	A	80	HIS	3.8
1	A	114	ILE	3.6
1	B	110	VAL	3.6
1	A	2	PRO	3.5
1	A	135	ASP	3.5
1	B	9	ASN	3.5
1	A	146	ASP	3.4
1	A	20	ALA	3.4
1	A	134	ALA	3.3
1	B	23	ALA	3.3
1	A	136	ILE	3.2
1	B	227	ASN	3.1
1	B	49	ARG	2.9
1	A	133	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	107	ASP	2.9
1	B	111	THR	2.8
1	A	82	LYS	2.6
1	A	225	ALA	2.6
1	A	121	THR	2.5
1	B	10	ASN	2.5
1	A	144	GLU	2.5
1	A	410	LEU	2.4
1	A	182	LEU	2.4
1	A	412	THR	2.3
1	A	19	LEU	2.2
1	A	147	PHE	2.2
1	B	36	ARG	2.2
1	B	435	ARG	2.1
1	B	80	HIS	2.1
1	A	22	GLY	2.0
1	A	228	VAL	2.0
1	B	21	ASN	2.0
1	A	138	LEU	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
2	ATP	B	501	31/31	0.11	1.81	10,14,40,47	0
2	ATP	A	500	31/31	0.15	1.80	16,26,44,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	833	5/5	0.09	0.48	31,32,38,42	0
3	MG	A	442	1/1	0.12	0.19	41,41,41,41	0
3	MG	A	441	1/1	0.10	-0.37	30,30,30,30	0
4	SO4	B	834	5/5	0.08	-0.70	34,39,41,42	0
3	MG	B	442	1/1	0.04	-1.97	15,15,15,15	0
3	MG	B	441	1/1	0.04	-2.84	17,17,17,17	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.