



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2016 – 04:37 PM EDT

PDB ID : 4NH0  
Title : Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC  
Authors : Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.  
Deposited on : 2013-11-03  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

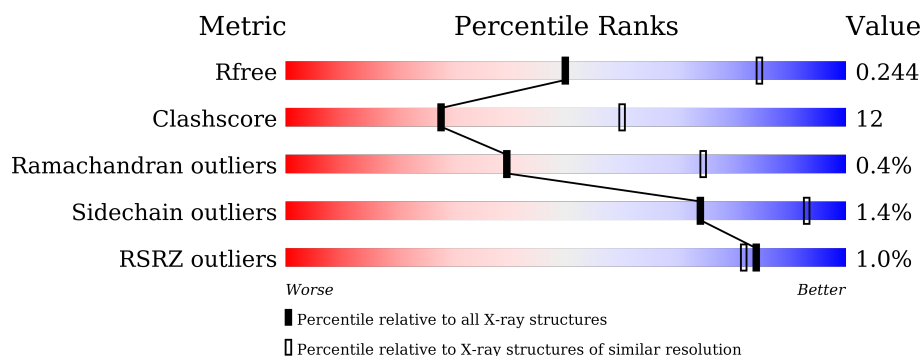
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	1147	
1	B	1147	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	0	0
			6663	4212	1181	1249	21			
1	B	859	Total	C	N	O	S	0	0	0
			6626	4186	1175	1244	21			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	EXPRESSION TAG	UNP D1A4G7
A	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
A	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	180	SER	-	EXPRESSION TAG	UNP D1A4G7
A	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
A	183	SER	-	EXPRESSION TAG	UNP D1A4G7
A	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
A	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
A	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	188	SER	-	EXPRESSION TAG	UNP D1A4G7
A	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
A	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
A	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
A	193	PHE	-	EXPRESSION TAG	UNP D1A4G7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
A	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
A	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
A	197	SER	-	EXPRESSION TAG	UNP D1A4G7
A	198	SER	-	EXPRESSION TAG	UNP D1A4G7
A	199	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	169	MET	-	EXPRESSION TAG	UNP D1A4G7
B	170	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	171	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	172	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	173	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	174	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	175	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	176	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	177	HIS	-	EXPRESSION TAG	UNP D1A4G7
B	178	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	179	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	180	SER	-	EXPRESSION TAG	UNP D1A4G7
B	181	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	182	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	183	SER	-	EXPRESSION TAG	UNP D1A4G7
B	184	ILE	-	EXPRESSION TAG	UNP D1A4G7
B	185	ASP	-	EXPRESSION TAG	UNP D1A4G7
B	186	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	187	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	188	SER	-	EXPRESSION TAG	UNP D1A4G7
B	189	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	190	GLU	-	EXPRESSION TAG	UNP D1A4G7
B	191	VAL	-	EXPRESSION TAG	UNP D1A4G7
B	192	LEU	-	EXPRESSION TAG	UNP D1A4G7
B	193	PHE	-	EXPRESSION TAG	UNP D1A4G7
B	194	GLN	-	EXPRESSION TAG	UNP D1A4G7
B	195	GLY	-	EXPRESSION TAG	UNP D1A4G7
B	196	PRO	-	EXPRESSION TAG	UNP D1A4G7
B	197	SER	-	EXPRESSION TAG	UNP D1A4G7
B	198	SER	-	EXPRESSION TAG	UNP D1A4G7
B	199	PRO	-	EXPRESSION TAG	UNP D1A4G7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

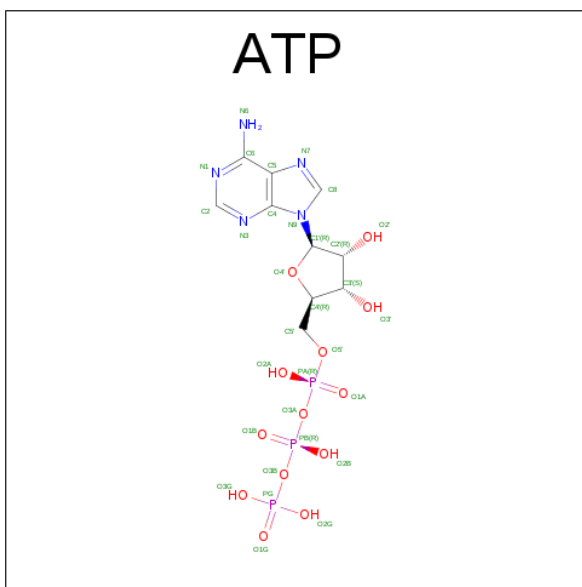


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- 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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	4	Total O 4 4	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: Cell divisionFtsK/SpoIIIE



- Molecule 1: Cell divisionFtsK/SpoIIIE



W1176	Y1001	L850	ARG	S655	L589	GLU	ASN	GLU	MET
R1177	E1002	L851	ALA	R656	R601	GLU	GLU	ASP	HIS
K1180	D1006	R852	GLU	V657	R660	VAL	THR	ASP	HIS
M1183	K1009	T853	ASN	V658	S662	LEU	MET	GLY	HIS
L1187	Y1013	P854	LYS	G660	Y665	S414	LEU	PRO	HIS
P1188	R1020	F859	SER	V661	Y668	A415	ARG	GLU	HIS
P1189	G1021	D863	SER	Y665	Y671	A416	LEU	ILE	HIS
L1192	F1029	S742	THR	B666	B572	L419	VAL	LYS	HIS
R1200	L1030	L743	THR	L667	B575	L422	THR	ARG	GLY
S1201	L1033	D744	THR	P668	B576	Y429	PRO	GLY	SER
P1227	R1034	D745	THR	Y675	B577	P432	ARG	PHE	PHE
R1236	I1036	V746	THR	R685	G578	D432	VAL	GLY	SER
D1237	D1037	V747	THR	Y690	A579	P433	TYR	ALA	ILE
I1238	G1038	P756	THR	V691	P580	A434	VAL	ALA	GLY
L1242	T1040	P757	THR	V697	L581	V435	VAL	ALA	GLY
I1243	T1044	P758	THR	D696	P585	Q442	LYS	CYS	SER
I1244	E905	P764	THR	B698	D592	R445	ARG	ALA	LEU
M1248	Q906	L765	THR	P694	P594	L446	ALA	GLU	VAL
G1275	E910	L766	THR	D696	S595	P449	LYS	ARG	LEU
G1294	R920	P769	THR	B697	R601	D453	GLU	MET	GLN
F1298	R923	L772	THR	GLU	L607	R457	VAL	PRO	GLY
I1308	F933	S782	THR	PRO	R613	D462	SER	GLN	PRO
Q1309	G934	A783	THR	GLN	L614	I463	ILE	GLN	ASP
T1310	D835	G796	THR	ILE	A625	K464	VAL	ALA	LEU
S1315	D941	R797	THR	ARG	S626	Q468	GLN	TYR	VAL
	N942	R798	THR	VAL	R628	M471	ALA	ASP	ILE
	Y950	R805	THR	ARG	L629	G475	SER	SER	SER
	L953	D806	THR	GLN	B630	L476	ILE	GLN	LEU
	S956	R807	THR	VAL	P831	S483	ALA	HIS	LEU
	R963	P808	THR	LEU	G632	E487	ALA	ASP	ALA
	S975	F809	THR	TYR	K633	T491	GLY	GLY	ALA
	E980	D810	THR	ILE	L634	E503	VAL	GLN	PRO
	L989	Q811	THR	ARG	G636	L524	ILE	VAL	ASP
	S1152	R812	THR	THR	L637	L534	ALA	ARG	GLY
	L1153	D819	THR	GLN	D638	V541	ALA	LEU	LYS
	A1166	G822	THR	VAL	T639	D542	THR	HIS	VAL
	L1175	G823	THR	VAL	L641	D642	SER	TYR	TYR
		A824	THR	VAL	S642	Y645	ALA	GLY	GLY
		G828	THR	VAL	R644	M653	ASP	VAL	MET
		P832	THR	GLN	L647	D654	GLU	GLU	VAL
		P833	THR	GLN	P650		PRO	THR	ARG
		Q834	THR	PRO			GLN	THR	
		K837	THR	GLN			GLN	THR	



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.226 , 0.246 0.225 , 0.244	Depositor DCC
$R_{free}$ test set	1330 reflections (1.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.6	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 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	0.25	0/6813	0.41	1/9264 (0.0%)
1	B	0.27	0/6774	0.47	2/9215 (0.0%)
All	All	0.26	0/13587	0.44	3/18479 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	807	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	579	ALA	C-N-CD	6.66	142.39	128.40
1	A	563	GLY	N-CA-C	-5.68	98.91	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	Peptide

## 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	6663	0	6636	118	0
1	B	6626	0	6588	196	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	314	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 12.

The worst 5 of 314 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:B:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93

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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	52	84
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	34	71
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	39	74

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO

### 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	709/953 (74%)	704 (99%)	5 (1%)	88	97
1	B	703/953 (74%)	688 (98%)	15 (2%)	61	88
All	All	1412/1906 (74%)	1392 (99%)	20 (1%)	74	93

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	577	GLU
1	B	629	LEU
1	B	742	SER
1	B	575	ARG
1	B	576	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS
1	B	640	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SO4	A	1401	-	4,4,4	0.30	0	6,6,6	0.07	0
4	ATP	A	1404	3	26,33,33	0.96	1 (3%)	26,52,52	1.63	1 (3%)
4	ATP	A	1405	3	26,33,33	0.96	1 (3%)	26,52,52	1.62	1 (3%)
2	SO4	B	1401	-	4,4,4	0.29	0	6,6,6	0.08	0
4	ATP	B	1404	3	26,33,33	0.96	1 (3%)	26,52,52	1.61	1 (3%)
4	ATP	B	1405	3	26,33,33	0.97	1 (3%)	26,52,52	1.66	1 (3%)

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	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	A	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/18/38/38	0/3/3/3
2	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
4	ATP	B	1404	3	-	0/18/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1404	ATP	C5-C4	3.04	1.47	1.40
4	B	1404	ATP	C5-C4	3.06	1.47	1.40
4	A	1405	ATP	C5-C4	3.09	1.47	1.40
4	B	1405	ATP	C5-C4	3.12	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	ATP	N3-C2-N1	-6.58	123.70	128.87
4	A	1405	ATP	N3-C2-N1	-6.54	123.73	128.87
4	A	1404	ATP	N3-C2-N1	-6.46	123.80	128.87
4	B	1404	ATP	N3-C2-N1	-6.44	123.81	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	SO4	1	0
4	A	1405	ATP	1	0
4	B	1404	ATP	2	0
4	B	1405	ATP	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	861/1147 (75%)	-0.19	4 (0%) 91 90	44, 80, 113, 151	0
1	B	859/1147 (74%)	-0.10	13 (1%) 76 74	35, 84, 128, 161	0
All	All	1720/2294 (74%)	-0.15	17 (0%) 84 82	35, 82, 125, 161	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	578	GLY	3.8
1	B	580	PRO	3.5
1	B	634	LEU	3.2
1	B	565	TYR	2.5
1	B	560	ARG	2.2

### 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	ATP	B	1404	31/31	0.97	0.16	0.19	34,63,78,97	0
4	ATP	A	1404	31/31	0.97	0.14	0.05	61,73,96,101	0
4	ATP	A	1405	31/31	0.97	0.14	-0.69	65,92,108,113	0
4	ATP	B	1405	31/31	0.96	0.14	-0.80	69,117,135,141	0
2	SO4	B	1401	5/5	0.92	0.11	-1.04	97,105,124,150	0
2	SO4	A	1401	5/5	0.96	0.11	-1.48	72,86,91,93	0
3	MG	A	1403	1/1	0.96	0.11	-	77,77,77,77	0
3	MG	A	1402	1/1	0.97	0.05	-	82,82,82,82	0
3	MG	B	1403	1/1	0.97	0.06	-	86,86,86,86	0
3	MG	B	1402	1/1	0.97	0.11	-	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.