



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:07 AM GMT

PDB ID : 1ZTH  
Title : Crystal Structure of A.fulgidus Rio1 serine protein kinase bound to ADP and Manganese ion  
Authors : Wlodawer, A.; LaRonde-LeBlanc, N.  
Deposited on : 2005-05-27  
Resolution : 1.89 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

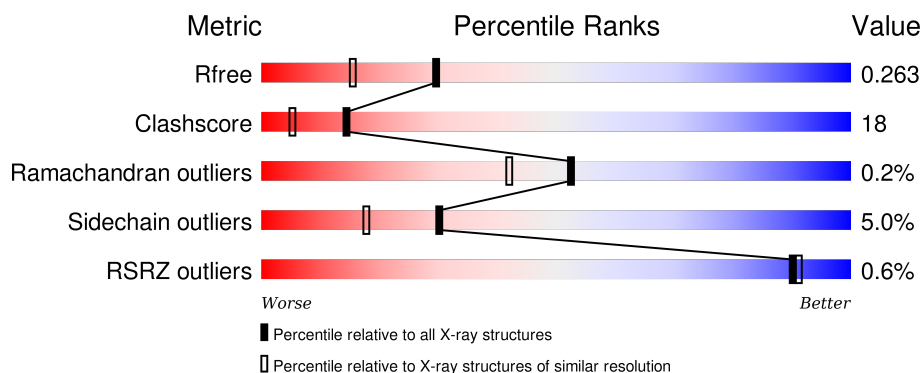
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	258	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	B	258	<div> <div></div> <div>75%</div> <div>16%</div> <div>• 7%</div> </div>
1	C	258	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	D	258	<div> <div></div> <div>65%</div> <div>26%</div> <div>• 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8764 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 Rio1 serine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	Se	0	0	0
			1974	1270	321	373	10			
1	B	241	Total	C	N	O	Se	0	0	0
			1951	1259	316	368	8			
1	C	241	Total	C	N	O	Se	0	0	0
			1930	1243	313	365	9			
1	D	244	Total	C	N	O	Se	0	0	0
			1975	1276	319	371	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	51	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	77	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	92	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	104	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	141	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	147	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	203	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	213	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	223	MSE	MET	MODIFIED RESIDUE	GB 11499392
A	251	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	1	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	51	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	77	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	92	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	104	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	141	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	147	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	203	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	213	MSE	MET	MODIFIED RESIDUE	GB 11499392
B	223	MSE	MET	MODIFIED RESIDUE	GB 11499392

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Chain	Residue	Modelled	Actual	Comment	Reference
B	251	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	1	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	51	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	77	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	92	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	104	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	141	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	147	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	203	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	213	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	223	MSE	MET	MODIFIED RESIDUE	GB 11499392
C	251	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	1	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	51	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	77	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	92	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	104	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	141	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	147	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	203	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	213	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	223	MSE	MET	MODIFIED RESIDUE	GB 11499392
D	251	MSE	MET	MODIFIED RESIDUE	GB 11499392

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 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
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

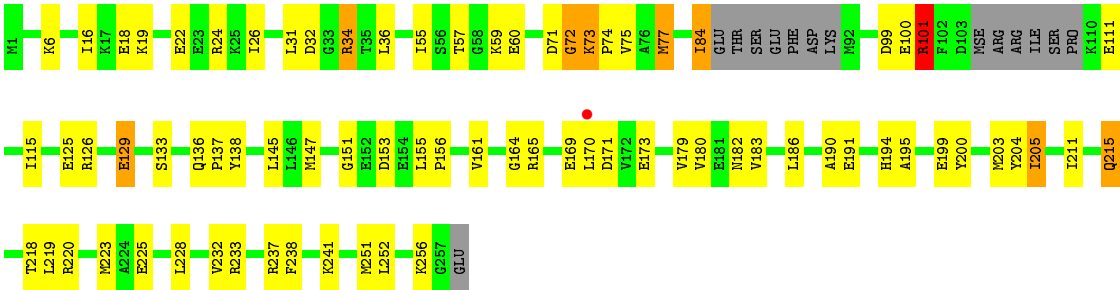
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0
4	B	240	Total O 240 240	0	0
4	C	199	Total O 199 199	0	0
4	D	179	Total O 179 179	0	0



- Molecule 1: Rio1 serine protein kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.41Å 80.08Å 121.06Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	30.00 – 1.89 28.30 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-1.89) 95.2 (28.30-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.262 0.190 , 0.263	Depositor DCC
$R_{free}$ test set	3935 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.2	EDS
Estimated twinning fraction	0.266 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 78499 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, 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	0.75	1/1998 (0.1%)	0.80	0/2668
1	B	0.73	0/1977	0.80	2/2644 (0.1%)
1	C	0.68	0/1954	0.77	0/2614
1	D	0.69	0/2001	0.77	1/2673 (0.0%)
All	All	0.71	1/7930 (0.0%)	0.78	3/10599 (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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	SER	C-O	7.22	1.37	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	D	101	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	B	126	ARG	NE-CZ-NH2	-5.82	117.39	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	204	TYR	Mainchain
1	D	72	GLY	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	1974	0	1957	71	0
1	B	1951	0	1938	52	0
1	C	1930	0	1917	69	0
1	D	1975	0	1976	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	2	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	204	0	0	26	0
4	B	240	0	0	25	0
4	C	199	0	0	28	0
4	D	179	0	0	29	0
All	All	8764	0	7836	284	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 18.

The worst 5 of 284 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:213:MSE:SE	1:B:213:MSE:CE	2.14	1.44
1:D:223:MSE:HG3	4:D:939:HOH:O	1.45	1.14
1:C:237:ARG:HD3	4:C:999:HOH:O	1.50	1.12
1:C:1:MSE:HA	4:C:1021:HOH:O	1.49	1.12
1:D:225:GLU:HG3	4:D:1040:HOH:O	1.51	1.10

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	239/258 (93%)	229 (96%)	10 (4%)	0	100	100
1	B	235/258 (91%)	229 (97%)	5 (2%)	1 (0%)	39	27
1	C	235/258 (91%)	226 (96%)	8 (3%)	1 (0%)	39	27
1	D	238/258 (92%)	228 (96%)	10 (4%)	0	100	100
All	All	947/1032 (92%)	912 (96%)	33 (4%)	2 (0%)	52	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	TYR
1	B	205	ILE

### 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	206/216 (95%)	199 (97%)	7 (3%)	44	33
1	B	204/216 (94%)	195 (96%)	9 (4%)	35	22
1	C	201/216 (93%)	191 (95%)	10 (5%)	30	18
1	D	207/216 (96%)	192 (93%)	15 (7%)	18	7
All	All	818/864 (95%)	777 (95%)	41 (5%)	30	18

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	73	LYS
1	C	165	ARG
1	D	205	ILE
1	C	99	ASP
1	C	142	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	GLN
1	B	215	GLN
1	D	182	ASN
1	B	136	GLN
1	B	177	ASN

### 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 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
3	ADP	A	901	2	22,29,29	1.11	1 (4%)	27,45,45	2.34	7 (25%)
3	ADP	B	903	2	22,29,29	1.24	2 (9%)	27,45,45	1.89	4 (14%)
3	ADP	C	905	2	22,29,29	0.88	1 (4%)	27,45,45	2.25	5 (18%)
3	ADP	D	907	2	22,29,29	1.09	2 (9%)	27,45,45	2.19	5 (18%)

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
3	ADP	A	901	2	-	0/12/32/32	0/3/3/3
3	ADP	B	903	2	-	0/12/32/32	0/3/3/3
3	ADP	C	905	2	-	0/12/32/32	0/3/3/3
3	ADP	D	907	2	-	0/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	ADP	C2-N3	2.24	1.36	1.32
3	C	905	ADP	C5-C4	2.35	1.45	1.40
3	D	907	ADP	O4'-C1'	2.51	1.44	1.41
3	D	907	ADP	C5-C4	3.08	1.47	1.40
3	A	901	ADP	C5-C4	3.49	1.48	1.40

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	ADP	N3-C2-N1	-8.29	122.55	128.89
3	D	907	ADP	N3-C2-N1	-7.39	123.23	128.89
3	C	905	ADP	N3-C2-N1	-7.23	123.36	128.89
3	C	905	ADP	C2'-C1'-N9	-6.47	104.40	114.29
3	D	907	ADP	C2'-C1'-N9	-5.95	105.20	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	ADP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	235/258 (91%)	-0.18	2 (0%) 85 87	17, 25, 46, 54	0
1	B	233/258 (90%)	-0.16	1 (0%) 93 93	16, 25, 44, 55	0
1	C	231/258 (89%)	-0.11	2 (0%) 85 87	17, 27, 48, 56	0
1	D	234/258 (90%)	-0.09	1 (0%) 93 93	19, 30, 47, 56	0
All	All	933/1032 (90%)	-0.14	6 (0%) 90 91	16, 27, 47, 56	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	GLY	3.0
1	D	170	LEU	2.8
1	A	98	GLY	2.3
1	B	97	TYR	2.3
1	A	96	LEU	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
3	ADP	C	905	27/27	0.98	0.11	0.21	14,19,25,28	0
3	ADP	D	907	27/27	0.99	0.09	-0.18	18,22,25,30	0
3	ADP	A	901	27/27	0.98	0.09	-0.34	14,19,26,33	0
3	ADP	B	903	27/27	0.99	0.08	-1.07	15,19,25,30	0
2	MN	C	906	1/1	0.99	0.09	-	21,21,21,21	0
2	MN	D	908	1/1	1.00	0.08	-	22,22,22,22	0
2	MN	B	904	1/1	1.00	0.09	-	22,22,22,22	0
2	MN	A	902	1/1	1.00	0.06	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.