



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:00 pm GMT

PDB ID : 4CGZ
Title : Crystal structure of the Bloom's syndrome helicase BLM in complex with DNA
Authors : Newman, J.A.; Savitsky, P.; Krojer, T.; von Delft, F.; Arrowsmith, C.H.;
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Deposited on : 2013-11-27
Resolution : 3.20 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

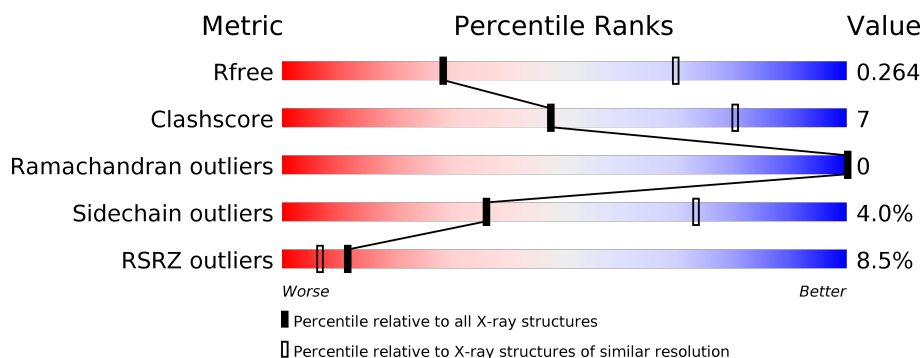
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 ≥ 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	665	<div> <div>8%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
2	B	12	<div> <div>75%</div> <div>25%</div> </div>
3	C	17	<div> <div>47%</div> <div>53%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5591 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 BLOOM'S SYNDROME HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	629	Total	C	N	O	S	0	0	0
			4981	3158	863	925	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	634	SER	-	EXPRESSION TAG	UNP P54132
A	635	MET	-	EXPRESSION TAG	UNP P54132

- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*GP*TP*CP*GP*AP*GP*AP*TP*C P)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			245	117	48	69	11			

- Molecule 3 is a DNA chain called 5'-D(*GP*AP*TP*CP*TP*CP*GP*AP*CP*GP*CP*TP*CP*DT *CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	17	Total	C	N	O	P	0	0	0
			337	162	57	102	16			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	149.53Å 149.53Å 64.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 3.20 48.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.65-3.20) 99.4 (48.65-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.229 , 0.259 0.232 , 0.264	Depositor DCC
R_{free} test set	1176 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	147.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 93.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5591	wwPDB-VP
Average B, all atoms (Å ²)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.31	0/5078	0.59	1/6855 (0.0%)
2	B	0.67	0/275	0.91	0/423
3	C	0.61	0/375	0.96	0/575
All	All	0.37	0/5728	0.64	1/7853 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1161	ILE	N-CA-C	-5.20	96.95	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4981	0	4940	65	1
2	B	245	0	136	3	0
3	C	337	0	193	12	0
4	A	1	0	0	0	0
5	A	27	0	12	0	0
All	All	5591	0	5281	74	1

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 7.

All (74) 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:1033:ILE:HD11	1:A:1192:THR:HG21	1.58	0.85
1:A:641:HIS:HB3	1:A:644:PHE:HD2	1.42	0.84
1:A:1028:HIS:CE1	1:A:1151:LEU:HG	2.16	0.80
1:A:858:ASN:HB2	1:A:1042:LEU:HD11	1.64	0.79
1:A:676:ILE:HD13	1:A:701:LEU:HD23	1.73	0.70
1:A:671:ASN:ND2	1:A:854:SER:O	2.26	0.69
1:A:733:PRO:HB2	1:A:760:ILE:HA	1.75	0.68
1:A:1153:LYS:HE2	1:A:1176:LYS:HE3	1.77	0.66
1:A:870:LYS:HD3	1:A:873:LYS:HD3	1.77	0.65
1:A:1116:ASP:OD1	1:A:1139:ARG:NH2	2.26	0.65
1:A:1028:HIS:HE1	1:A:1151:LEU:HG	1.63	0.63
1:A:1211:ARG:NH1	1:A:1288:TRP:O	2.31	0.63
1:A:641:HIS:HB3	1:A:644:PHE:CD2	2.29	0.62
1:A:1180:VAL:HG22	1:A:1185:LEU:HD23	1.82	0.62
1:A:1121:SER:OG	1:A:1122:LYS:N	2.37	0.58
3:C:4:DC:H5'	3:C:4:DC:H6	1.69	0.58
1:A:1149:LEU:O	1:A:1155:LEU:N	2.34	0.57
1:A:1168:ILE:HD13	2:B:2:DG:H4'	1.86	0.57
1:A:859:ARG:NH1	1:A:978:GLY:O	2.38	0.56
1:A:954:ASP:HB2	1:A:979:ARG:NH2	2.21	0.56
1:A:1158:ASP:O	1:A:1169:ALA:HA	2.07	0.53
3:C:9:DC:H2''	3:C:10:DG:C8	2.43	0.53
1:A:756:LYS:NZ	1:A:782:ASN:HB3	2.24	0.53
1:A:1002:LYS:HB3	1:A:1159:LEU:HD11	1.91	0.52
1:A:1161:ILE:HD13	1:A:1167:ALA:HB2	1.91	0.51
3:C:7:DG:H1'	3:C:8:DA:C8	2.45	0.51
1:A:1015:THR:O	1:A:1018:THR:OG1	2.18	0.51
1:A:1003:ARG:HH12	3:C:14:DT:H5''	1.75	0.50
1:A:919:HIS:HB2	3:C:17:DC:OP1	2.11	0.50
1:A:735:THR:HG21	1:A:749:ILE:HD12	1.92	0.50
1:A:1158:ASP:HB3	1:A:1170:TYR:HB2	1.93	0.50
1:A:1017:GLU:O	1:A:1020:PHE:HB2	2.12	0.49
1:A:1175:ASN:OD1	1:A:1176:LYS:N	2.46	0.49
1:A:875:ALA:HA	1:A:904:MET:HE1	1.93	0.49
1:A:756:LYS:HG2	1:A:786:ARG:HG2	1.95	0.48
3:C:16:DC:N4	3:C:17:DC:H42	2.12	0.48
1:A:679:ALA:O	1:A:791:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:ASP:HA	1:A:1067:CYS:HB2	1.98	0.46
1:A:1162:ASN:OD1	1:A:1163:ALA:N	2.48	0.46
1:A:998:VAL:HG12	1:A:1002:LYS:HE3	1.97	0.46
1:A:1064:ASP:OD1	1:A:1065:ASN:N	2.48	0.46
3:C:4:DC:H5'	3:C:4:DC:C6	2.50	0.45
1:A:1179:THR:O	1:A:1184:ASN:HB2	2.15	0.45
1:A:1081:VAL:HG21	1:A:1187:VAL:HG21	1.98	0.45
1:A:1178:GLN:HA	1:A:1181:LEU:HB2	1.98	0.45
1:A:1162:ASN:C	1:A:1164:ASN:H	2.18	0.45
1:A:1002:LYS:HG2	1:A:1020:PHE:CE1	2.52	0.44
1:A:1014:HIS:HB3	1:A:1017:GLU:OE2	2.17	0.44
1:A:654:GLU:O	1:A:658:ILE:HG13	2.17	0.44
1:A:701:LEU:HB3	1:A:702:PRO:HD3	2.00	0.44
3:C:13:DC:H6	3:C:13:DC:O5'	2.01	0.43
1:A:1178:GLN:O	1:A:1182:ASN:N	2.52	0.43
1:A:747:THR:HA	1:A:750:TYR:HD2	1.83	0.43
1:A:1003:ARG:NH1	3:C:14:DT:OP1	2.52	0.42
1:A:1211:ARG:HH12	1:A:1289:THR:HA	1.84	0.42
1:A:1140:HIS:HD2	1:A:1144:ARG:HD2	1.85	0.42
1:A:658:ILE:HD12	1:A:705:VAL:HB	2.01	0.42
1:A:1154:ILE:O	1:A:1174:GLY:N	2.50	0.42
1:A:1161:ILE:HD13	1:A:1161:ILE:HA	1.97	0.42
1:A:871:PRO:O	2:B:5:DT:OP1	2.38	0.41
2:B:4:DG:H2'	2:B:5:DT:H72	2.03	0.41
3:C:9:DC:H2''	3:C:10:DG:H8	1.84	0.41
1:A:971:GLU:HG2	1:A:972:GLY:H	1.85	0.41
1:A:1033:ILE:HB	1:A:1068:LYS:HE3	2.02	0.41
1:A:735:THR:OG1	1:A:736:TYR:N	2.54	0.41
3:C:17:DC:H6	3:C:17:DC:H2'	1.64	0.41
1:A:1004:LEU:HD13	1:A:1004:LEU:HA	1.90	0.41
1:A:1014:HIS:C	1:A:1017:GLU:HG2	2.41	0.40
1:A:784:TYR:OH	1:A:823:SER:HB3	2.21	0.40
1:A:1162:ASN:CG	1:A:1163:ALA:H	2.22	0.40
1:A:1081:VAL:O	1:A:1085:VAL:HG23	2.22	0.40
1:A:657:LYS:HG3	1:A:661:LYS:NZ	2.37	0.40
1:A:1178:GLN:HG3	1:A:1182:ASN:OD1	2.22	0.40
1:A:1166:GLN:NE2	3:C:13:DC:OP2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:SER:OG	1:A:1162:ASN:O[3_554]	1.91	0.29

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	623/665 (94%)	593 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	548/593 (92%)	526 (96%)	22 (4%)	36	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	LYS
1	A	688	LEU
1	A	709	VAL
1	A	714	SER
1	A	722	ASP
1	A	756	LYS
1	A	786	ARG
1	A	789	LEU

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Mol	Chain	Res	Type
1	A	818	ARG
1	A	819	GLN
1	A	872	LYS
1	A	874	VAL
1	A	910	ARG
1	A	949	PHE
1	A	955	LYS
1	A	994	THR
1	A	1010	ASP
1	A	1012	ASN
1	A	1056	LYS
1	A	1133	LYS
1	A	1156	ASP
1	A	1181	LEU

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	660	HIS
1	A	819	GLN
1	A	1022	ASN
1	A	1028	HIS
1	A	1089	GLN
1	A	1140	HIS
1	A	1166	GLN
1	A	1210	GLN

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 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
5	ADP	A	2292	-	25,29,29	0.94	1 (4%)	24,45,45	1.68	2 (8%)

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	2292	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2292	ADP	C5-C4	2.82	1.46	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2292	ADP	N3-C2-N1	-6.31	123.36	128.86
5	A	2292	ADP	C4-C5-N7	-2.28	107.21	109.41

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 [i](#)

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, 95th 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 ²)	Q<0.9
1	A	629/665 (94%)	0.31	56 (8%) 10 6	129, 176, 221, 240	0
2	B	12/12 (100%)	-0.49	0 100 100	160, 183, 205, 205	0
3	C	17/17 (100%)	-0.42	0 100 100	182, 192, 206, 218	0
All	All	658/694 (94%)	0.27	56 (8%) 11 7	129, 178, 220, 240	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	792	PHE	7.6
1	A	1126	ILE	6.7
1	A	828	ALA	5.2
1	A	1222	LEU	5.0
1	A	709	VAL	4.8
1	A	1249	LEU	4.5
1	A	1125	LYS	4.4
1	A	789	LEU	4.4
1	A	1214	MET	4.4
1	A	1131	PHE	4.4
1	A	1146	PHE	4.2
1	A	663	PHE	3.7
1	A	1130	ILE	3.6
1	A	960	PHE	3.6
1	A	826	VAL	3.5
1	A	1278	VAL	3.3
1	A	711	VAL	3.2
1	A	1282	LEU	3.1
1	A	762	LEU	3.1
1	A	1087	PHE	3.0
1	A	827	MET	3.0
1	A	686	PHE	3.0
1	A	1128	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1145	LEU	3.0
1	A	953	ILE	2.9
1	A	698	CYS	2.9
1	A	780	LEU	2.8
1	A	1192	THR	2.8
1	A	763	LEU	2.8
1	A	1253	LEU	2.8
1	A	1118	PHE	2.8
1	A	1127	GLN	2.7
1	A	1084	ILE	2.7
1	A	772	ALA	2.6
1	A	1114	LEU	2.6
1	A	1139	ARG	2.6
1	A	1218	CYS	2.6
1	A	753	LEU	2.6
1	A	1106	SER	2.6
1	A	1117	ILE	2.5
1	A	1129	GLY	2.5
1	A	1149	LEU	2.5
1	A	1241	PHE	2.5
1	A	918	TYR	2.5
1	A	710	THR	2.5
1	A	1285	TYR	2.5
1	A	685	CYS	2.5
1	A	1210	GLN	2.4
1	A	1070	LYS	2.3
1	A	1093	SER	2.2
1	A	794	ILE	2.2
1	A	1121	SER	2.2
1	A	1191	GLU	2.2
1	A	1111	MET	2.1
1	A	992	PHE	2.1
1	A	1279	ILE	2.1

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 [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, 95th 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(Å ²)	Q<0.9
5	ADP	A	2292	27/27	0.90	0.30	0.98	136,163,170,173	0
4	ZN	A	2291	1/1	0.98	0.24	0.46	155,155,155,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.