



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 03:55 PM JST

PDB ID : 8IK4
Title : Structure of DNA binding domain of McrBC endonuclease bound to hemimethylated DNA: L68F mutant
Authors : Adhav, V.A.; Saikrishnan, K.
Deposited on : 2023-02-28
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

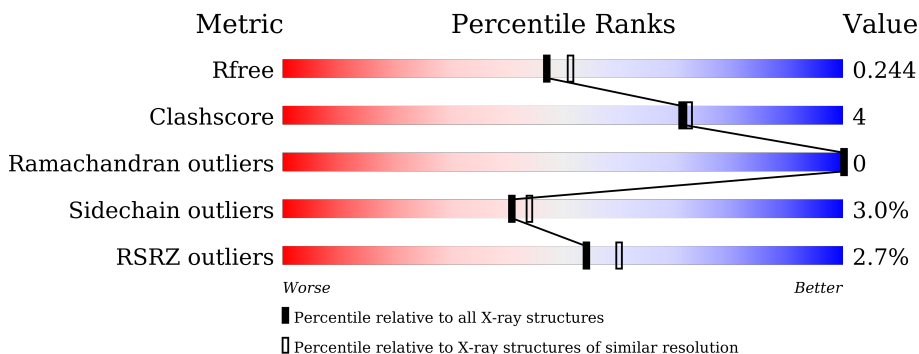
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	170	 2% (poor fit), 82% (0-1 outliers), 12% (2 outliers), 6% (3+ outliers)
1	B	170	 % (poor fit), 81% (0-1 outliers), 8% (2 outliers), 11% (3+ outliers)
2	C	13	 23% (poor fit), 54% (0-1 outliers), 15% (2 outliers), 8% (3+ outliers), 23% (not modelled)
3	D	13	 15% (poor fit), 69% (0-1 outliers), 8% (2 outliers), 23% (3+ outliers)

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3597 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 Type IV methyl-directed restriction enzyme EcoKMcrB subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1309	852	204	251	2	0	4	0
1	B	151	1227	800	188	236	3	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	PHE	LEU	engineered mutation	UNP P15005
A	162	LEU	-	expression tag	UNP P15005
A	163	GLU	-	expression tag	UNP P15005
A	164	GLY	-	expression tag	UNP P15005
A	165	HIS	-	expression tag	UNP P15005
A	166	HIS	-	expression tag	UNP P15005
A	167	HIS	-	expression tag	UNP P15005
A	168	HIS	-	expression tag	UNP P15005
A	169	HIS	-	expression tag	UNP P15005
A	170	HIS	-	expression tag	UNP P15005
B	68	PHE	LEU	engineered mutation	UNP P15005
B	162	LEU	-	expression tag	UNP P15005
B	163	GLU	-	expression tag	UNP P15005
B	164	GLY	-	expression tag	UNP P15005
B	165	HIS	-	expression tag	UNP P15005
B	166	HIS	-	expression tag	UNP P15005
B	167	HIS	-	expression tag	UNP P15005
B	168	HIS	-	expression tag	UNP P15005
B	169	HIS	-	expression tag	UNP P15005
B	170	HIS	-	expression tag	UNP P15005

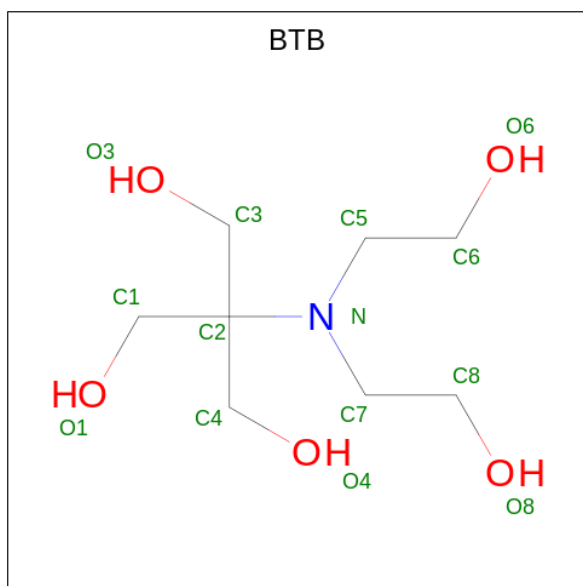
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*AP*(5CM)P*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	10	414	198	86	112	18	0	10	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	10	396	192	66	120	18	0	10	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	92	Total O 92 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	18	Total	O	0	0
			18	18		
5	D	21	Total	O	0	0
			21	21		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.10Å 70.28Å 144.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.32 – 2.10 50.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.32-2.10) 97.3 (50.32-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.246 0.196 , 0.244	Depositor DCC
R_{free} test set	1125 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtrriage
Anisotropy	0.714	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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: BTB, 5CM

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	0/1360	0.43	0/1846
1	B	0.25	0/1267	0.43	0/1721
2	C	0.49	0/420	0.77	0/642
3	D	0.50	0/440	0.91	0/674
All	All	0.33	0/3487	0.57	0/4883

There are no bond length outliers.

There are no bond angle outliers.

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	1309	0	1236	10	0
1	B	1227	0	1145	9	0
2	C	414	0	227	4	0
3	D	396	0	217	2	0
4	C	28	0	38	3	0
5	A	92	0	0	1	0
5	B	92	0	0	1	0
5	C	18	0	0	0	0
5	D	21	0	0	0	0
All	All	3597	0	2863	22	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 4.

All (22) 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:126:GLN:HE22	1:B:133:ASP:H	1.38	0.72
1:A:21:GLN:HB2	3:D:11[A]:DC:H5'	1.86	0.57
1:B:10:LYS:NZ	5:B:205:HOH:O	2.38	0.54
1:B:80:TYR:HB2	1:B:121:TYR:HB2	1.89	0.54
1:A:21:GLN:HB2	2:C:11[B]:DA:H5'	1.89	0.53
1:A:80:TYR:HB2	1:A:121:TYR:HB2	1.89	0.52
2:C:11[A]:DA:H2''	2:C:12[A]:DG:H5''	1.92	0.52
1:A:38:SER:HB2	4:C:101:BTB:H31	1.94	0.49
1:A:110:SER:HB2	1:A:112:VAL:HG22	1.95	0.48
1:A:116:LYS:HE2	1:A:117:TYR:CZ	2.49	0.48
1:A:12:ILE:HD11	1:A:76:LEU:HD22	1.97	0.47
1:A:78:LEU:HD21	1:A:144:ILE:HG13	1.97	0.46
1:B:126:GLN:NE2	1:B:133:ASP:H	2.09	0.46
1:A:136:ARG:NH2	5:A:207:HOH:O	2.50	0.45
1:B:31:ARG:HH22	1:B:146:ASN:ND2	2.14	0.45
4:C:101:BTB:H11	4:C:101:BTB:H52	1.83	0.44
1:B:12:ILE:HD11	1:B:76:LEU:HD22	1.99	0.44
4:C:102:BTB:H42	4:C:102:BTB:H52	1.73	0.43
1:A:2[A]:GLU:HG2	1:A:30:TYR:HD1	1.85	0.42
1:B:21:GLN:HB2	2:C:11[A]:DA:H5'	2.02	0.42
1:B:21:GLN:HB2	3:D:11[B]:DC:H5'	2.03	0.41
1:B:68:PHE:HE1	2:C:6[B]:5CM:H5A3	1.87	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	160/170 (94%)	155 (97%)	5 (3%)	0	100	100
1	B	150/170 (88%)	144 (96%)	6 (4%)	0	100	100
All	All	310/340 (91%)	299 (96%)	11 (4%)	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	140/150 (93%)	133 (95%)	7 (5%)	24	23
1	B	128/150 (85%)	125 (98%)	3 (2%)	50	55
All	All	268/300 (89%)	258 (96%)	10 (4%)	41	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	61	ASN
1	A	95	SER
1	A	119[A]	GLN
1	A	119[B]	GLN
1	A	143[A]	ASN
1	A	143[B]	ASN
1	B	24	LYS
1	B	37	LEU
1	B	110	SER

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	18	GLN
1	A	61	ASN

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Mol	Chain	Res	Type
1	A	89	HIS
1	B	16	GLN
1	B	32	ASN
1	B	91	GLN
1	B	119	GLN
1	B	126	GLN
1	B	130	GLN
1	B	143	ASN
1	B	146	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	5CM	C	6[A]	2	17,21,22	5.23	12 (70%)	24,30,33	1.23	1 (4%)
2	5CM	C	6[B]	2	17,21,22	5.21	12 (70%)	24,30,33	1.25	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
2	5CM	C	6[A]	2	-	5/7/21/22	0/2/2/2
2	5CM	C	6[B]	2	-	2/7/21/22	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6[A]	5CM	C6-C5	9.95	1.50	1.34
2	C	6[B]	5CM	C6-C5	9.85	1.50	1.34
2	C	6[B]	5CM	O4'-C1'	7.84	1.59	1.42
2	C	6[A]	5CM	O4'-C1'	7.82	1.59	1.42
2	C	6[A]	5CM	C2-N3	7.04	1.50	1.36
2	C	6[B]	5CM	C2-N3	7.02	1.50	1.36
2	C	6[A]	5CM	C2'-C1'	-6.88	1.33	1.52
2	C	6[B]	5CM	C2'-C1'	-6.84	1.33	1.52
2	C	6[B]	5CM	C4-N3	6.30	1.44	1.34
2	C	6[A]	5CM	C4-N3	6.29	1.44	1.34
2	C	6[B]	5CM	C3'-C4'	-6.20	1.36	1.53
2	C	6[A]	5CM	C3'-C4'	-6.19	1.36	1.53
2	C	6[A]	5CM	C4-N4	5.66	1.48	1.34
2	C	6[B]	5CM	C4-N4	5.65	1.48	1.34
2	C	6[A]	5CM	C6-N1	4.84	1.46	1.38
2	C	6[B]	5CM	C6-N1	4.78	1.46	1.38
2	C	6[B]	5CM	C2-N1	4.54	1.49	1.40
2	C	6[A]	5CM	C2-N1	4.52	1.49	1.40
2	C	6[A]	5CM	O2-C2	-4.45	1.15	1.23
2	C	6[B]	5CM	O2-C2	-4.42	1.15	1.23
2	C	6[A]	5CM	O4'-C4'	4.11	1.54	1.45
2	C	6[B]	5CM	O4'-C4'	4.10	1.54	1.45
2	C	6[B]	5CM	C2'-C3'	4.03	1.63	1.52
2	C	6[A]	5CM	C2'-C3'	4.00	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	6[B]	5CM	C5-C6-N1	-3.30	119.95	123.34
2	C	6[A]	5CM	C5-C6-N1	-3.28	119.96	123.34
2	C	6[B]	5CM	C4'-O4'-C1'	-2.15	104.26	109.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6[A]	5CM	C3'-C4'-C5'-O5'
2	C	6[B]	5CM	C3'-C4'-C5'-O5'
2	C	6[A]	5CM	O4'-C1'-N1-C6
2	C	6[A]	5CM	C2'-C1'-N1-C6
2	C	6[A]	5CM	O4'-C4'-C5'-O5'
2	C	6[A]	5CM	O4'-C1'-N1-C2
2	C	6[B]	5CM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6[B]	5CM	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	BTB	C	101	-	13,13,13	0.52	0	7,16,16	0.48	0
4	BTB	C	102	-	13,13,13	0.55	0	7,16,16	0.54	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
4	BTB	C	101	-	-	1/21/21/21	-
4	BTB	C	102	-	-	1/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	102	BTB	N-C7-C8-O8
4	C	101	BTB	N-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	101	BTB	2	0
4	C	102	BTB	1	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, 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	159/170 (93%)	-0.15	3 (1%) 66 71	13, 23, 51, 89	0
1	B	151/170 (88%)	-0.15	1 (0%) 87 89	14, 30, 55, 86	0
2	C	9/13 (69%)	0.80	3 (33%) 0 0	23, 31, 72, 85	0
3	D	10/13 (76%)	0.70	2 (20%) 1 1	26, 32, 79, 89	0
All	All	329/366 (89%)	-0.10	9 (2%) 54 60	13, 27, 61, 89	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	3[A]	DC	6.3
1	A	96	SER	4.4
2	C	3[A]	DA	4.0
1	A	159	ILE	3.3
1	A	160	PRO	3.1
1	B	95	SER	3.1
2	C	4[A]	DG	3.0
2	C	12[A]	DG	2.5
3	D	4[A]	DT	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
2	5CM	C	6[A]	20/21	0.94	0.11	19,28,30,30	20
2	5CM	C	6[B]	20/21	0.94	0.11	27,32,35,35	20

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	BTB	C	101	14/14	0.80	0.21	32,45,51,59	0
4	BTB	C	102	14/14	0.88	0.14	29,38,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.