

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 11:50 pm BST

PDB ID : 5LTY

> Title : Homeobox transcription factor CDX2 bound to methylated DNA

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2016-09-07 Deposited on

2.66 Å(reported) Resolution

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

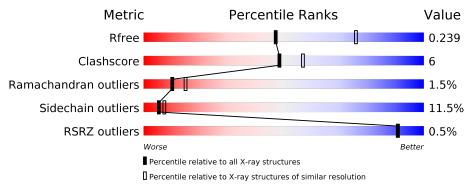
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.66 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 >=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 <=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	18	50%	44%	6%					
1	В	18	6%	339	%					
2	K	71	80%		15% • •					
2	M	71	70%	23%						
3	Е	18	50%	44%	6%					
3	F	18	67%	28%	6%					



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2757 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 DNA chain called DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*AP *(5CM)P*GP*AP*CP*CP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	18	Total 364				P 18	0	0	0
1	В	18	Total	С	N		Р	0	0	0

• Molecule 2 is a protein called Homeobox protein CDX-2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	К	71	Total 625	_	N 124	O 108	0	0	0
2	М	70	Total 618	C 389	N 123	O 106	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2 E	1.0	Total	С	N	Ο	Р	0	0	0
Э Г	18	376	178	78	102	18	U	U		
2	F	18	Total	С	N	О	Р	0	0	0
3	3 E		376	178	78	102	18	U	U	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total O 5 5	0	0
4	В	2	Total O 2 2	0	0
4	К	9	Total O 9 9	0	0

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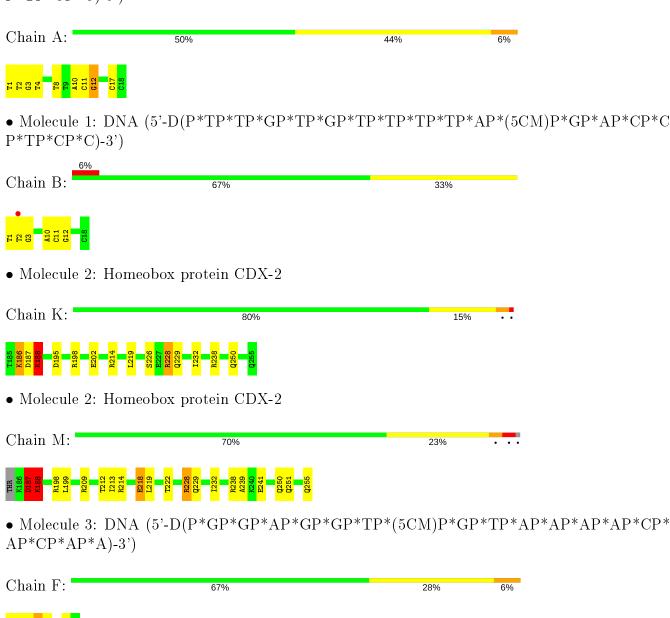
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	12	Total O 12 12	0	0
4	F	1	Total O 1 1	0	0
4	E	5	Total O 5 5	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: DNA (5'-D(P*TP*TP*GP*TP*GP*TP*TP*TP*TP*AP*(5CM)P*GP*AP*CP*C P*TP*CP*C)-3')





 \bullet Molecule 3: DNA (5'-D(P*GP*GP*AP*GP*GP*TP*(5CM)P*GP*TP*AP*AP*AP*AP*CP* AP*CP*AP*A)-3')

Chain E: 50% 44% 6%





4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 1 2 1	Depositor	
Cell constants	68.88Å 46.61Å 120.43Å	Depositor	
a, b, c, α , β , γ	90.00° 98.46° 90.00°	Depositor	
Resolution (Å)	63.29 - 2.66	Depositor	
resolution (A)	55.71 - 2.66	EDS	
% Data completeness	98.5 (63.29-2.66)	Depositor	
(in resolution range)	98.5 (55.71-2.66)	EDS	
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.60 \; ({\rm at} \; 2.65 {\rm \AA})$	Xtriage	
Refinement program	REFMAC 5.8.0135	Depositor	
P. P.	0.202 , 0.242	Depositor	
R, R_{free}	0.205 , 0.239	DCC	
R_{free} test set	519 reflections $(4.73%)$	wwPDB-VP	
Wilson B-factor (\mathring{A}^2)	71.9	Xtriage	
Anisotropy	0.353	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 47.7	EDS	
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	2757	wwPDB-VP	
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.73% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: $5\mathrm{CM}$

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	Boı	nd lengths	Bond angles		
MIOI		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.85	1/381~(0.3%)	1.25	3/583~(0.5%)	
1	В	0.81	0/381	1.14	$2/583 \ (0.3\%)$	
2	K	1.16	1/634~(0.2%)	1.23	6/843 (0.7%)	
2	M	1.18	3/627~(0.5%)	1.24	$6/833 \; (0.7\%)$	
3	E	0.82	1/401~(0.2%)	1.14	3/615~(0.5%)	
3	F	0.82	2/401~(0.5%)	1.19	4/615 (0.7%)	
All	All	0.99	$8/2825 \ (0.3\%)$	1.20	$24/4072 \ (0.6\%)$	

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
2	M	218	GLU	CG-CD	7.77	1.63	1.51
3	F	22	DG	O3'-P	-7.22	1.52	1.61
3	Е	22	DG	O3'-P	-6.01	1.53	1.61
3	F	23	DG	O3'-P	-6.01	1.53	1.61
2	M	218	GLU	CB-CG	5.97	1.63	1.52
2	M	239	ALA	C-O	5.96	1.34	1.23
1	A	8	DT	O3'-P	-5.41	1.54	1.61
2	K	202	GLU	CD-OE2	5.15	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	K	195	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	12	DG	O5'-P-OP2	-7.78	98.69	105.70
3	Е	22	DG	O5'-P-OP1	-7.53	98.93	105.70
2	M	218	GLU	OE1-CD-OE2	-7.45	114.36	123.30
3	Е	30	DA	O5'-P-OP1	-7.20	99.22	105.70
2	K	238	ARG	NE-CZ-NH1	6.45	123.53	120.30
2	K	195	ASP	CB-CG-OD1	6.26	123.93	118.30

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Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
2	M	188	LYS	CB-CA-C	6.01	122.42	110.40
2	M	198	ARG	NE-CZ-NH1	5.71	123.16	120.30
3	F	22	DG	O5'-P-OP2	5.69	117.53	110.70
3	F	19	DG	O5'-P-OP1	5.68	117.52	110.70
2	Μ	214	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	Μ	238	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	K	214	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	Μ	187	ASP	CB-CG-OD2	5.36	123.12	118.30
2	K	198	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	В	1	DT	C1'-O4'-C4'	-5.34	104.76	110.10
1	В	1	DT	N1-C1'-C2'	5.30	122.68	112.60
1	A	1	DT	C1'-O4'-C4'	-5.14	104.96	110.10
2	K	202	GLU	CG-CD-OE2	5.13	128.57	118.30
3	F	20	DG	O5'-P-OP1	5.07	116.78	110.70
1	A	1	DT	N1-C1'-C2'	5.07	122.22	112.60
3	Ε	22	DG	C1'-O4'-C4'	-5.04	105.06	110.10
3	F	35	DA	O5'-P-OP1	-5.03	101.17	105.70

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	364	0	209	5	2
1	В	364	0	209	6	0
2	K	625	0	650	5	0
2	M	618	0	643	9	0
3	E	376	0	203	6	2
3	F	376	0	203	2	0
4	A	5	0	0	0	0
4	В	2	0	0	0	0
4	E	5	0	0	3	0
4	F	1	0	0	0	0
4	K	9	0	0	0	0
4	M	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2757	0	2117	29	2

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 6.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
3:E:35:DA:N1	4:E:101:HOH:O	1.85	1.08
1:B:11:5CM:OP2	2:M:228:ARG:NH2	2.00	0.94
1:A:11:5CM:OP2	2:K:228:ARG:NH2	2.12	0.81
1:B:2:DT:H4'	1:B:3:DG:OP1	1.90	0.72
1:A:10:DA:OP2	2:K:229:GLN:NE2	2.30	0.65
3:F:21:DA:H2"	3:F:22:DG:O5'	1.96	0.64
2:M:187:ASP:O	2:M:188:LYS:HG3	1.98	0.63
1:A:11:5CM:H2'	1:A:12:DG:C8	2.34	0.63
1:B:11:5CM:H2'	1:B:12:DG:C8	2.34	0.63
1:A:2:DT:H2"	1:A:3:DG:C8	2.35	0.61
3:E:21:DA:H2"	3:E:22:DG:O5'	2.00	0.60
1:B:2:DT:H2"	1:B:3:DG:C8	2.38	0.58
1:B:10:DA:OP2	2:M:229:GLN:NE2	2.35	0.58
3:E:33:DA:H2'	4:E:102:HOH:O	2.03	0.58
2:M:209:ARG:NH1	2:M:241:GLU:OE1	2.35	0.57
2:M:228:ARG:O	2:M:232:ILE:HG12	2.05	0.57
2:M:188:LYS:NZ	2:M:188:LYS:HB3	2.21	0.56
2:K:228:ARG:O	2:K:232:ILE:HG12	2.06	0.55
3:E:36:DA:N6	4:E:103:HOH:O	2.40	0.54
3:F:21:DA:H2'	3:F:22:DG:C8	2.44	0.53
3:E:21:DA:H2'	3:E:22:DG:C8	2.45	0.52
1:B:10:DA:H2"	1:B:11:5CM:O5'	2.11	0.50
2:M:212:THR:HG23	4:M:311:HOH:O	2.11	0.49
2:M:251:GLN:HB3	2:M:255:GLN:OE1	2.13	0.48
2:M:187:ASP:O	2:M:188:LYS:CG	2.63	0.47
2:K:186:LYS:HE2	2:K:226:SER:OG	2.14	0.46
1:A:3:DG:H4'	1:A:4:DT:OP1	2.19	0.42
2:K:188:LYS:NZ	2:K:188:LYS:HB2	2.35	0.42
3:E:24:DT:H2"	3:E:25:5CM:O5'	2.20	0.41

All (2) 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	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:A:17:DC:OP2	3:E:19:DG:P[2_465]	2.05	0.15
1:A:17:DC:OP2	3:E:19:DG:O5'[2_465]	2.08	0.12

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		
2	K	$69/71 \; (97\%)$	67 (97%)	1 (1%)	1 (1%)	11	16	
2	М	$68/71 \ (96\%)$	66 (97%)	1 (2%)	1 (2%)	10	15	
All	All	$137/142 \ (96\%)$	133 (97%)	2 (2%)	2 (2%)	10	15	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	188	LYS
2	M	188	LYS

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	Analysed Rotameric Outliers			
2	K	66/66 (100%)	60 (91%)	6 (9%)	9 13	
2	М	65/66 (98%)	56 (86%)	9 (14%)	3 4	
All	All	131/132 (99%)	116 (88%)	15 (12%)	5 7	

All (15) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	K	186	LYS
2	K	187	ASP
2	K	188	LYS
2	K	219	LEU
2	K	228	ARG
2	K	250	GLN
2	M	187	ASP
2	M	188	LYS
2	M	199	LEU
2	M	213	ILE
2	M	218	GLU
2	M	219	LEU
2	M	222	THR
2	M	228	ARG
2	M	250	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
2	K	250	GLN
2	M	250	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)

4 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 C	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	Во	nd leng	$ ag{ths}$	В	ond ang	les
MIOI	Туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2														
1	5CM	В	11	1,3	15,21,22	1.52	3 (20%)	19,30,33	1.66	3 (15%)														
3	5CM	F	25	1,3	15,21,22	1.60	1 (6%)	19,30,33	1.50	3 (15%)														



Mol Type Cha		Chain Res		Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5CM	Е	25	1,3	15,21,22	1.60	1 (6%)	19,30,33	1.38	2 (10%)
1	5CM	A	11	1,3	15,21,22	1.48	3 (20%)	19,30,33	1.76	2 (10%)

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
1	5CM	В	11	1,3	-	0/4/21/22	0/2/2/2
3	5CM	F	25	1,3	-	1/4/21/22	0/2/2/2
3	5CM	E	25	1,3	-	1/4/21/22	0/2/2/2
1	5CM	A	11	1,3	-	0/4/21/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
3	Ε	25	5CM	C5-C4	5.23	1.49	1.41
3	F	25	5CM	C5-C4	5.19	1.49	1.41
1	В	11	5CM	C5-C4	3.82	1.47	1.41
1	A	11	5CM	C5-C4	3.34	1.46	1.41
1	В	11	5CM	O5'-C5'	-2.70	1.38	1.44
1	A	11	5CM	O4'-C1'	2.62	1.48	1.42
1	В	11	5CM	C2-N3	-2.19	1.33	1.38
1	A	11	5CM	C2-N3	-2.09	1.34	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
1	A	11	5CM	C2-N3-C4	5.53	122.69	116.02
1	В	11	5CM	C2-N3-C4	5.00	122.05	116.02
3	F	25	5CM	C5-C6-N1	-3.12	118.84	122.19
3	E	25	5CM	C5-C6-N1	-3.01	118.95	122.19
1	A	11	5CM	C5-C4-N3	-2.94	116.61	121.26
3	E	25	5CM	C2'-C3'-C4'	2.78	108.54	102.76
3	F	25	5CM	C2'-C3'-C4'	2.77	108.53	102.76
1	В	11	5CM	C5-C4-N3	-2.71	116.98	121.26
3	F	25	5CM	C2-N3-C4	2.20	118.68	116.02
1	В	11	5CM	O3'-C3'-C2'	2.15	118.58	110.90

There are no chirality outliers.



All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	25	5CM	O4'-C1'-N1-C6
3	Е	25	5CM	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	11	5CM	3	0
3	E	25	5CM	1	0
1	A	11	5CM	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	17/18 (94%)	-0.43	0 100 100	53, 78, 132, 143	0
1	В	17/18 (94%)	-0.28	1 (5%) 22 19	60, 81, 155, 171	0
2	K	71/71 (100%)	-0.17	0 100 100	46, 64, 95, 113	0
2	M	70/71 (98%)	-0.15	0 100 100	48, 68, 96, 116	0
3	E	17/18 (94%)	-0.33	0 100 100	61, 78, 141, 169	0
3	F	17/18 (94%)	-0.63	0 100 100	59, 72, 94, 105	0
All	All	209/214 (97%)	-0.24	1 (0%) 91 91	46, 69, 113, 171	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	2	DT	2.8

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, 95^{th} 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	${f B-factors}({f \AA}^2)$	Q < 0.9
3	5CM	F	25	20/21	0.96	0.13	56,67,76,78	0
3	5CM	E	25	20/21	0.96	0.14	62,75,81,91	0
1	5CM	В	11	20/21	0.98	0.14	54,63,66,70	0
1	5CM	A	11	20/21	0.98	0.12	50,55,59,63	0



6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

