

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 16, 2020 – 12:08 pm GMT

PDB ID	:	6YMG
$\operatorname{Title}$	:	VcaM4I restriction endonuclease in complex with $5mC$ -modified dsDNA
Authors	:	Pastor, M.; Czapinska, H.; Lutz, T.; Helbrecht, I.; Xu, S.; Bochtler, M.
Deposited on		
Resolution	:	3.14 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 (i) symbol.

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

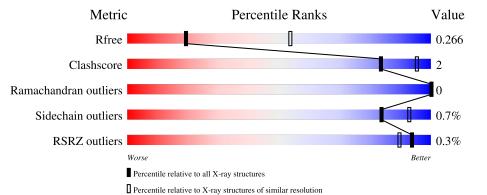
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.15.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

# 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 3.14 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677(3.18-3.10)
Sidechain outliers	138945	1677(3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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 <=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	А	309	93% 7%
1	В	309	94% 6%
2	С	11	9%
2	Е	11	100%
3	D	11	45% 55%



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Mol	Chain	Length	Quality of chair	1
3	F	11	64%	36%



# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6063 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 HNH endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	309	Total 2514	m C 1597	± 1	0 475	S 10	0	4	0
1	В	309	Total 2525	C 1601			S 8	0	3	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	C	11	Total	С	Ν	Ο	Р	0	0	0
	U	11	222	107	41	64	10	0	0	0
9	Е	11	Total	С	Ν	Ο	Р	0	0	0
			222	107	41	64	10		U	

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

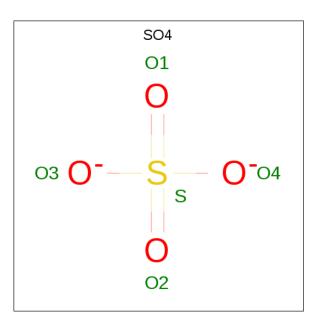
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	п	11	Total	С	Ν	Ο	Р	0	0	0
0	D	11	224	107	43	64	10	0	0	0
2	Б	11	Total	С	Ν	Ο	Р	0	0	0
0	Г	11	224	107	43	64	10	0	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Cl 1 1	0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	0	0
6	В	37	$\begin{array}{cc} {\rm Total} & {\rm O} \\ 37 & 37 \end{array}$	0	0
6	С	2	Total O 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	2	Total O 2 2	0	0
6	Ε	2	Total O 2 2	0	0
6	F	1	Total O 1 1	0	0



#### 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:	93	%	7%
M1 W5 V6 P24 N27 N28 N28 N28 N28 N28 N28 N28	F51 F51 F51 F52 F52 F33 F33 F33 F110 F111 F111 F111	1154 F157 F157 N218 N263 6264 E265 F300 Y300	
• Molecule 1: HNH	I endonuclease		
Chain B:	94	1%	6%
MI WE VG SSO FE1 F51 S58 S58 V69 F75	1.01 1.01 1.03 1.03 1.03 1.03 1.157 1.160 1.163 1.163	11263 11263 11265 12265 12668 1268 1272	
	$\Lambda (5'-D(*CP*CP*AP*$	TP*GP*(5CM)P*GP	*CP*TP*GP*A)-3')
Chain C:		100%	
<b>11</b>			
• Molecule 2: $DNA$	$\Lambda (5'-D(*CP*CP*AP*$	TP*GP*(5CM)P*GP	*CP*TP*GP*A)-3`)
Chain E:		100%	
There are no outlie	er residues recorded fo	or this chain.	
• Molecule 3: DNA	(5'-D(P*CP*AP*GP))	P*CP*GP*CP*AP*TI	D*GP*G)-3')
Chain D:	45%	55%	
11 88 61 10 61 11 61			
• Molecule 3: DNA	(5'-D(P*CP*AP*GP))	P*CP*GP*CP*AP*TI	D*GP*G)-3')
Chain F:	64%	3	6%

• Molecule 1: HNH endonuclease







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	81.11Å 81.11Å 617.31Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	49.10 - 3.14	Depositor
	49.07 - 3.14	EDS
% Data completeness	92.8 (49.10-3.14)	Depositor
(in resolution range)	$92.8 \ (49.07 - 3.14)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.21	Depositor
$< I/\sigma(I) > 1$	$1.07 (at 3.12 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.241 , $0.266$	Depositor
$R, R_{free}$	0.244 , $0.266$	DCC
$R_{free}$ test set	1031 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	69.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $41.7$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.37, \langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6063	wwPDB-VP
Average B, all atoms $(Å^2)$	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: 5CM, SO4, CL

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		
	Cham	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.64	0/2594	0.73	0/3508	
1	В	0.65	0/2589	0.74	0/3501	
2	С	0.25	0/225	0.62	0/343	
2	Ε	0.31	0/225	0.67	0/343	
3	D	0.37	0/251	0.74	0/386	
3	F	0.35	0/251	0.76	0/386	
All	All	0.61	0/6135	0.73	0/8467	

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	А	2514	0	2412	14	0
1	В	2525	0	2420	10	0
2	С	222	0	127	0	0
2	Е	222	0	127	0	0
3	D	224	0	125	3	0
3	F	224	0	125	2	0
4	А	1	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	25	0	0	0	0
5	В	20	0	0	0	0
6	А	42	0	0	1	0
6	В	37	0	0	0	0
6	С	2	0	0	0	0
6	D	2	0	0	0	0
6	Е	2	0	0	0	0
6	F	1	0	0	0	0
All	All	6063	0	5336	27	0

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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 2.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom D	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
3:D:2:DC:H2"	3:D:3:DA:OP2	2.03	0.58
1:A:152:GLU:O	1:B:218:ASN:HB3	2.07	0.55
1:A:218:ASN:HB3	1:B:152:GLU:O	2.07	0.54
3:D:10:DG:H2"	3:D:11:DG:OP2	2.07	0.54
3:D:6:DG:H2'	3:D:7:DC:C6	2.43	0.53
3:F:10:DG:H2"	3:F:11:DG:OP2	2.09	0.52
1:B:268:VAL:HG13	1:B:272:LEU:HD23	1.94	0.50
3:F:6:DG:H2'	3:F:7:DC:C6	2.46	0.50
1:A:263:ASN:OD1	1:A:265:GLU:HB2	2.15	0.47
1:B:263:ASN:OD1	1:B:265:GLU:HB2	2.15	0.47
1:A:5:TRP:CZ2	1:A:51:PHE:CD1	3.04	0.46
1:A:110:ARG:HB3	1:A:111:PRO:HD3	1.97	0.45
1:B:5:TRP:CZ2	1:B:51:PHE:CD1	3.05	0.45
1:A:24:PRO:HG3	1:A:82:TRP:HB3	2.00	0.44
1:A:230:VAL:HG11	1:A:300:TYR:OH	2.17	0.44
1:B:160:THR:HA	1:B:163:ILE:HD12	2.01	0.43
1:B:6:VAL:O	1:B:6:VAL:HG13	2.17	0.43
1:A:6:VAL:O	1:A:6:VAL:HG13	2.19	0.43
1:A:29:ASN:N	6:A:505:HOH:O	2.51	0.42
1:B:50:SER:HB2	1:B:58:SER:HB3	1.99	0.42
1:A:27:ASN:HD21	1:A:33:SER:HB2	1.84	0.42
1:B:91:LEU:HD23	1:B:93:TYR:CZ	2.54	0.42
1:A:230:VAL:O	1:A:230:VAL:HG22	2.19	0.42
1:A:91:LEU:HD23	1:A:93:TYR:CZ	2.55	0.41
1:B:57:LEU:CD2	1:B:99:LYS:HD2	2.51	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
1:A:5:TRP:HZ2	1:A:51:PHE:CD1	2.39	0.40	
1:A:47:VAL:HG21	1:A:154:ILE:HG12	2.04	0.40	

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There are no symmetry-related clashes.

### 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	А	311/309~(101%)	296~(95%)	15~(5%)	0	100	100	
1	В	310/309~(100%)	295~(95%)	15~(5%)	0	100	100	
All	All	621/618~(100%)	$591 \ (95\%)$	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	Analysed Rotameric Outliers		Percentiles		
1	А	273/269~(102%)	271~(99%)	2 (1%)	84	93	
1	В	272/269~(101%)	270~(99%)	2 (1%)	84	93	
All	All	545/538~(101%)	541~(99%)	4 (1%)	84	93	

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	69	TYR
1	А	157	PHE
1	В	69	TYR
1	В	157	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	105	HIS
1	А	304	ASN
1	В	34	HIS
1	В	176	ASN
1	В	304	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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).

	Mal	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
Mol	Type		nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	#  Z  > 2	
	2	$5\mathrm{CM}$	С	6	2	15,21,22	0.75	0	$19,\!30,\!33$	0.71	0
	2	$5\mathrm{CM}$	Е	6	2	15,21,22	0.78	0	$19,\!30,\!33$	0.74	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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
2	5CM	С	6	2	-	1/4/21/22	0/2/2/2



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5CM	Ε	6	2	-	1/4/21/22	0/2/2/2

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
2	С	6	5CM	O4'-C1'-N1-C6
2	Е	6	5CM	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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).

Mal	Mol Type		Res	Link	B	Bond lengths			Bond angles		
	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
5	SO4	А	403	-	4,4,4	0.39	0	$^{6,6,6}$	0.06	0	
5	SO4	В	403	-	4,4,4	0.38	0	$^{6,6,6}$	0.05	0	
5	SO4	А	406	-	4,4,4	0.36	0	$^{6,6,6}$	0.05	0	
5	SO4	В	404	-	4,4,4	0.38	0	$^{6,6,6}$	0.06	0	
5	SO4	А	405	-	4,4,4	0.39	0	$^{6,6,6}$	0.05	0	
5	SO4	А	402	-	4,4,4	0.38	0	$^{6,6,6}$	0.04	0	
5	SO4	В	402	-	4,4,4	0.36	0	$^{6,6,6}$	0.04	0	
5	SO4	В	401	-	4,4,4	0.37	0	$^{6,6,6}$	0.04	0	



Mol Type	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Tink	B	ond leng	$\mathbf{gths}$	В	ond ang	gles
	туре		nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2					
5	SO4	А	404	-	4,4,4	0.38	0	$^{6,6,6}$	0.05	0					

There are no bond length outliers.

There are no bond angle outliers.

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 (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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$\mathbf{Q}{<}0.9$
1	А	309/309~(100%)	-0.27	0 100 100	48, 70, 100, 117	0
1	В	309/309~(100%)	-0.17	1 (0%) 94 89	54, 76, 102, 112	0
2	С	10/11~(90%)	0.29	1 (10%) 7 2	61, 93, 145, 178	0
2	Е	$10/11 \ (90\%)$	-0.30	0 100 100	75, 90, 121, 123	0
3	D	11/11~(100%)	-0.23	0 100 100	66, 90, 141, 141	0
3	F	11/11~(100%)	-0.21	0 100 100	80, 94, 105, 106	0
All	All	660/662~(99%)	-0.22	2 (0%) 94 89	48, 75, 105, 178	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	С	11	DA	5.8
1	В	75	PHE	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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
2	5CM	Ε	6	20/21	0.96	0.19	$70,\!72,\!76,\!76$	0
2	5CM	С	6	20/21	0.98	0.17	$50,\!52,\!54,\!55$	0

# 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$Q{<}0.9$
5	SO4	В	402	5/5	0.61	0.28	$161,\!162,\!168,\!169$	0
5	SO4	В	401	5/5	0.68	0.30	$145,\!147,\!151,\!155$	0
5	SO4	А	403	5/5	0.85	0.24	$124,\!128,\!129,\!130$	0
5	SO4	В	403	5/5	0.86	0.20	$132,\!136,\!138,\!140$	0
5	SO4	А	406	5/5	0.86	0.29	82,83,84,86	5
5	SO4	А	405	5/5	0.87	0.23	$136,\!138,\!139,\!139$	0
5	SO4	В	404	5/5	0.90	0.52	$90,\!91,\!92,\!93$	5
4	CL	А	401	1/1	0.95	0.13	80,80,80,80	0
5	SO4	А	404	5/5	0.97	0.15	75, 75, 76, 76	5
5	SO4	А	402	5/5	0.98	0.11	71,71,73,74	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

