



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2023 – 07:40 PM EDT

PDB ID : 5DEU  
Title : Crystal structure of TET2-5hmC complex  
Authors : Hu, L.; Cheng, J.; Rao, Q.; Li, Z.; Li, J.; Xu, Y.  
Deposited on : 2015-08-26  
Resolution : 1.80 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

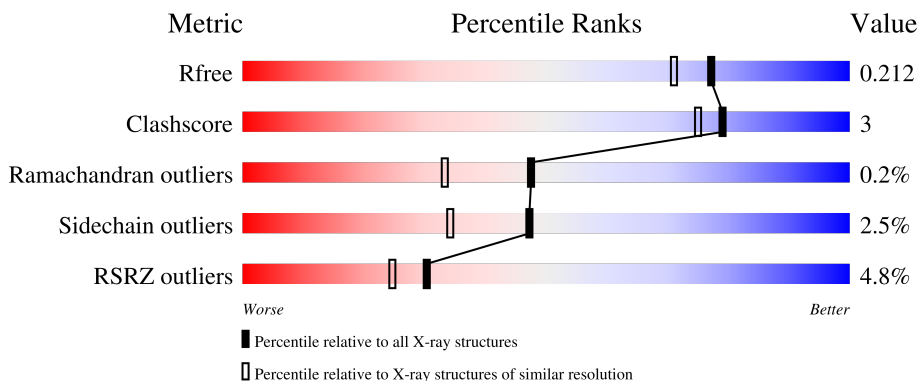
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	462	 4% 82% 6% • 11%
2	B	12	 8% 83% 17%
3	C	11	 36% 64%

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 4067 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 Methylcytosine dioxygenase TET2, chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3259	2036	584	615	24	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1127	GLY	-	expression tag	UNP Q6N021
A	1128	SER	-	expression tag	UNP Q6N021
A	1829	GLY	-	linker	UNP Q6N021
A	1830	GLY	-	linker	UNP Q6N021
A	1831	GLY	-	linker	UNP Q6N021
A	1832	GLY	-	linker	UNP Q6N021
A	1833	SER	-	linker	UNP Q6N021
A	1834	GLY	-	linker	UNP Q6N021
A	1835	GLY	-	linker	UNP Q6N021
A	1836	GLY	-	linker	UNP Q6N021
A	1837	GLY	-	linker	UNP Q6N021
A	1838	SER	-	linker	UNP Q6N021
A	1839	GLY	-	linker	UNP Q6N021
A	1840	GLY	-	linker	UNP Q6N021
A	1841	GLY	-	linker	UNP Q6N021
A	1842	GLY	-	linker	UNP Q6N021
A	1843	SER	-	linker	UNP Q6N021
A	1936	GLY	-	expression tag	UNP Q6N021

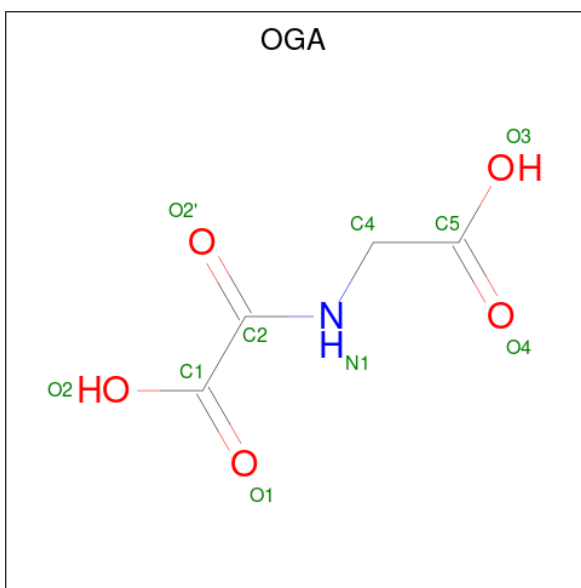
- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*CP\*CP\*AP\*CP\*(5HC)P\*GP\*GP\*TP\*GP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	12	245	117	46	71	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	11	227	107	41	68	11	0	0	0

- Molecule 4 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: C<sub>4</sub>H<sub>5</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	4	1	5	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	12	6	1	4	1	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
6	A	1	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	A	3	3	3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	280	280	280	0	0

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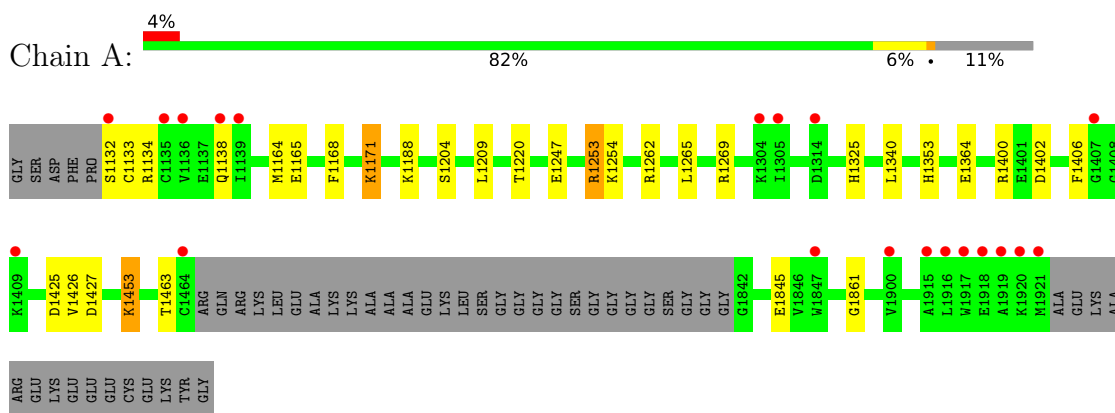
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
9	B	21	Total O 21 21	0	0
9	C	8	Total O 8 8	0	0

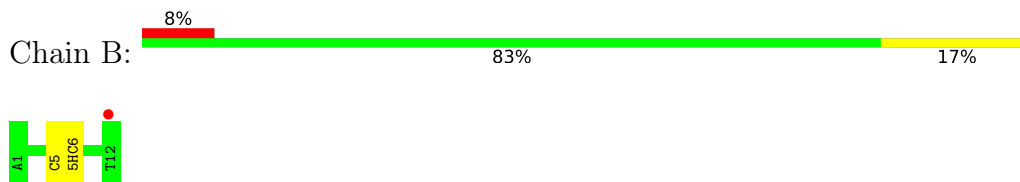
### 3 Residue-property plots [i](#)

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.

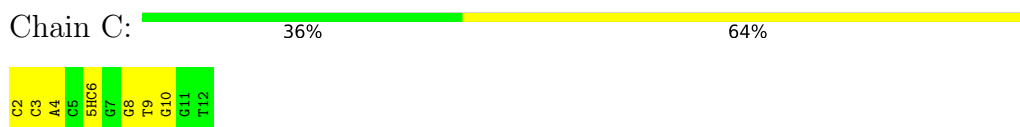
- Molecule 1: Methylcytosine dioxygenase TET2, chimeric construct



- Molecule 2: DNA (5'-D(\*AP\*CP\*CP\*AP\*CP\*(5HC)P\*GP\*GP\*TP\*GP\*GP\*T)-3')



- Molecule 3: DNA (5'-D(P\*CP\*CP\*AP\*CP\*(5HC)P\*GP\*GP\*TP\*GP\*GP\*T)-3')



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.26Å 87.52Å 260.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.26 – 1.80 42.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.26-1.80) 93.6 (42.26-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 1.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.177 , 0.212 0.177 , 0.212	Depositor DCC
$R_{free}$ test set	1995 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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, 0.333 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: FE, ZN, CL, 5HC, MES, OGA

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	0.35	0/3324	0.52	0/4481
2	B	0.63	0/250	1.24	0/382
3	C	0.58	0/229	1.35	1/349 (0.3%)
All	All	0.39	0/3803	0.69	1/5212 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	DG	O4'-C1'-N9	-7.76	102.56	108.00

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	3259	0	3224	16	0
2	B	245	0	137	2	0
3	C	227	0	126	4	0
4	A	10	0	3	0	0
5	A	12	0	12	0	0
6	A	1	0	0	0	0
7	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
9	A	280	0	0	1	0
9	B	21	0	0	0	0
9	C	8	0	0	0	0
All	All	4067	0	3502	20	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 3.

The worst 5 of 20 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:1262:ARG:HB2	2:B:5:DC:H5'	1.79	0.64
1:A:1253:ARG:HD2	1:A:1254:LYS:HZ2	1.70	0.56
1:A:1463:THR:HG23	2:B:5:DC:OP2	2.07	0.54
1:A:1262:ARG:NE	9:A:2109:HOH:O	2.37	0.53
3:C:2:DC:H2'	3:C:3:DC:C6	2.43	0.53

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	A	410/462 (89%)	403 (98%)	6 (2%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1861	GLY

### 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	356/385 (92%)	347 (98%)	9 (2%)	47 34

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1427	ASP
1	A	1453	LYS
1	A	1188	LYS
1	A	1220	THR
1	A	1253	ARG

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

Mol	Chain	Res	Type
1	A	1346	ASN
1	A	1353	HIS

### 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	5HC	C	6	3,2	18,22,23	3.89	11 (61%)	23,31,34	2.46	7 (30%)
2	5HC	B	6	2	18,22,23	3.58	9 (50%)	23,31,34	2.60	8 (34%)

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	5HC	C	6	3,2	-	2/9/23/24	0/2/2/2
2	5HC	B	6	2	-	4/9/23/24	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	5HC	C2'-C1'	-7.30	1.32	1.52
3	C	6	5HC	C2'-C3'	-7.07	1.34	1.52
2	B	6	5HC	C2'-C1'	-6.84	1.33	1.52
2	B	6	5HC	C2'-C3'	-6.54	1.35	1.52
3	C	6	5HC	C6-N1	5.85	1.48	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	5HC	C3'-C2'-C1'	6.27	118.25	102.54
2	B	6	5HC	C3'-C2'-C1'	6.03	117.64	102.54
3	C	6	5HC	N1-C2-N3	5.06	128.03	118.81
2	B	6	5HC	C6-N1-C2	-4.86	114.14	120.87
2	B	6	5HC	N1-C2-N3	4.53	127.06	118.81

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	6	5HC	C3'-C4'-C5'-O5'
2	B	6	5HC	C2'-C1'-N1-C2
3	C	6	5HC	O4'-C4'-C5'-O5'
2	B	6	5HC	C2'-C1'-N1-C6
2	B	6	5HC	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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	MES	A	2002	-	12,12,12	2.13	1 (8%)	14,16,16	2.25	5 (35%)
4	OGA	A	2001	6	9,9,9	2.60	2 (22%)	10,11,11	1.74	3 (30%)

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	MES	A	2002	-	-	2/6/14/14	0/1/1/1
4	OGA	A	2001	6	-	0/8/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2002	MES	C8-S	-6.93	1.67	1.77
4	A	2001	OGA	C2-N1	6.56	1.44	1.33
4	A	2001	OGA	C2-C1	-2.79	1.50	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2002	MES	O2S-S-C8	4.93	112.85	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2002	MES	C5-N4-C3	4.85	119.76	108.83
4	A	2001	OGA	C4-N1-C2	-3.18	116.28	121.25
5	A	2002	MES	C7-N4-C5	2.50	117.64	111.23
4	A	2001	OGA	O2'-C2-N1	-2.46	118.79	123.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	MES	C7-C8-S-O2S
5	A	2002	MES	C8-C7-N4-C5

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	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	413/462 (89%)	0.16	20 (4%) 30 25	24, 38, 73, 107	0
2	B	11/12 (91%)	0.17	1 (9%) 9 7	43, 61, 85, 103	0
3	C	10/11 (90%)	0.12	0 100 100	48, 64, 86, 89	0
All	All	434/485 (89%)	0.16	21 (4%) 30 25	24, 39, 74, 107	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1305	ILE	5.9
1	A	1921	MET	5.2
1	A	1920	LYS	4.6
1	A	1132	SER	4.4
1	A	1917	TRP	4.2

### 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<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	B-factors(Å <sup>2</sup> )	Q<0.9
3	5HC	C	6	21/22	0.91	0.14	42,53,75,88	0
2	5HC	B	6	21/22	0.98	0.12	27,30,35,40	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<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	B-factors(Å <sup>2</sup> )	Q<0.9
4	OGA	A	2001	10/10	0.93	0.10	29,32,35,36	0
5	MES	A	2002	12/12	0.95	0.13	34,57,73,74	0
8	CL	A	2007	1/1	0.97	0.10	30,30,30,30	0
7	ZN	A	2006	1/1	0.98	0.08	33,33,33,33	0
7	ZN	A	2004	1/1	0.98	0.04	46,46,46,46	0
6	FE	A	2003	1/1	0.99	0.09	27,27,27,27	0
7	ZN	A	2005	1/1	0.99	0.06	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.