



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2023 – 06:37 pm GMT

PDB ID : 2XY6  
Title : Crystal structure of a salicylic aldehyde basepair in complex with fragment DNA polymerase I from *Bacillus stearothermophilus*  
Authors : Kaul, C.; Mueller, M.; Wagner, M.; Schneider, S.; Carell, T.  
Deposited on : 2010-11-15  
Resolution : 2.30 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 : 1.8.4, 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

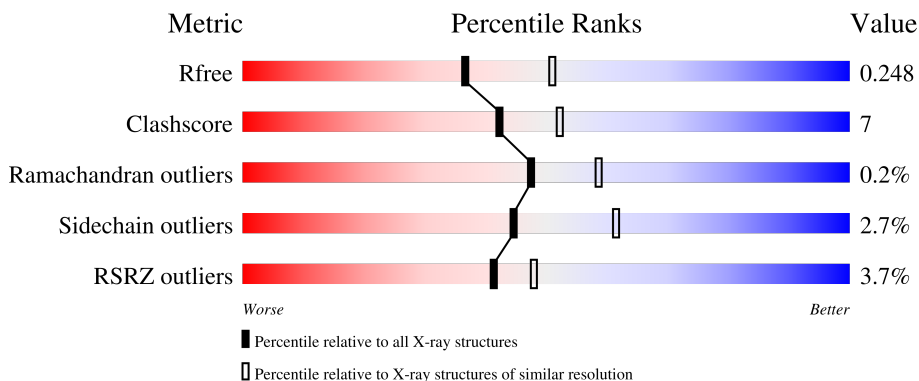
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	581	 3% 87% 12%
2	B	10	 40% 20% 60% 20%
3	C	10	 10% 30% 30% 40%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5168 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 DNA POLYMERASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4577	2911	785	864	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	THR	-	expression tag	UNP E1C9K5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	10	195	97	29	60	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	10	208	101	40	58	9	0	0	0

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



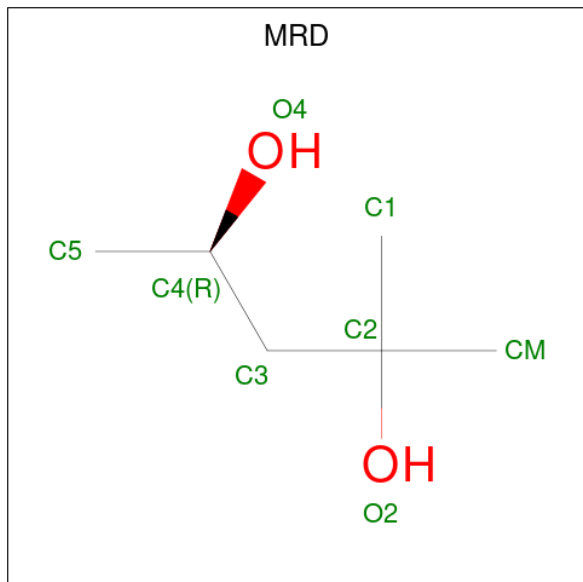
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- 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
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

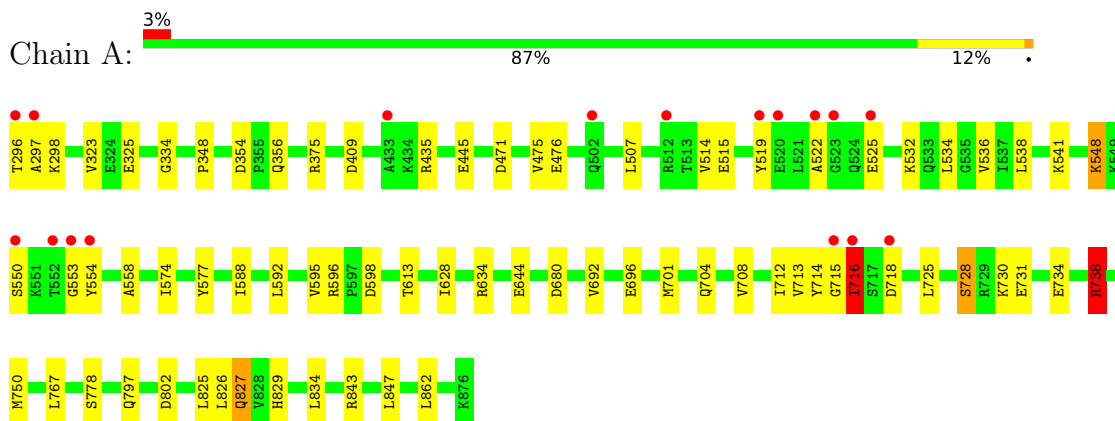
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total	O	0	0
			157	157		
7	C	1	Total	O	0	0
			1	1		

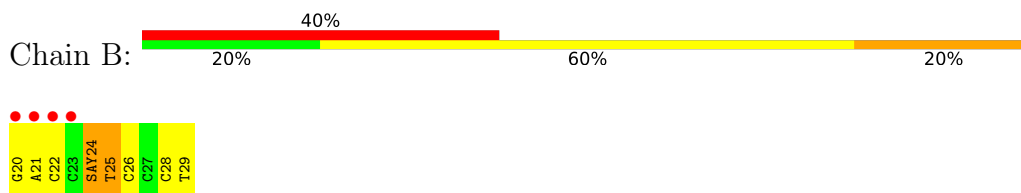
### 3 Residue-property plots [i](#)

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.

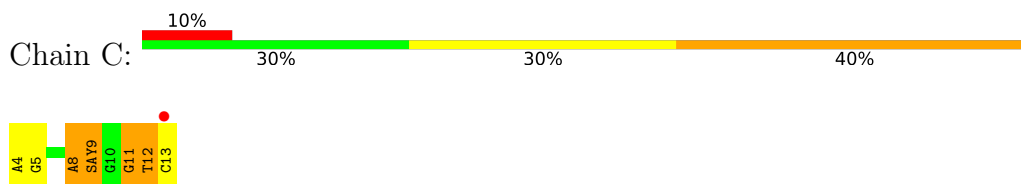
- Molecule 1: DNA POLYMERASE I



- Molecule 2: 5'-D(\*GP\*AP\*CP\*CP\*SAYP\*TP\*CP\*CP\*CP\*TP)-3'



- Molecule 3: 5'-D(\*AP\*GP\*GP\*GP\*AP\*SAYP\*GP\*GP\*TP\*CP)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.23Å 93.13Å 105.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.28 – 2.30 42.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.28-2.30) 99.9 (42.60-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.213 , 0.254 0.210 , 0.248	Depositor DCC
$R_{free}$ test set	1963 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: MRD, SO4, MES, SAY

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	0.62	0/4659	0.69	2/6313 (0.0%)
2	B	1.11	0/193	1.51	1/292 (0.3%)
3	C	1.05	0/211	1.60	4/323 (1.2%)
All	All	0.67	0/5063	0.80	7/6928 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	11	DG	O4'-C1'-N9	-9.79	101.15	108.00
2	B	25	DT	O4'-C1'-N1	7.47	113.23	108.00
1	A	738	ARG	NE-CZ-NH1	7.10	123.85	120.30
3	C	12	DT	N3-C4-O4	6.13	123.58	119.90
3	C	8	DA	O4'-C1'-N9	5.72	112.01	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	4577	0	4548	54	0
2	B	195	0	114	8	0
3	C	208	0	113	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
5	A	12	0	12	3	0
6	A	8	0	14	2	0
7	A	157	0	0	1	0
7	C	1	0	0	0	0
All	All	5168	0	4801	68	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 7.

The worst 5 of 68 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)
6:A:1880:MRD:H1C3	6:A:1880:MRD:O4	1.60	0.97
1:A:375:ARG:NH2	5:A:1879:MES:H52	1.83	0.92
1:A:738:ARG:HH11	1:A:738:ARG:HG3	1.35	0.90
1:A:323:VAL:O	1:A:435:ARG:NH2	2.07	0.88
3:C:12:DT:H2''	3:C:13:DC:H5'	1.66	0.77

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	579/581 (100%)	560 (97%)	18 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	716	ILE

### 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	477/497 (96%)	464 (97%)	13 (3%)	44 61

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	718	ASP
1	A	728	SER
1	A	827	GLN
1	A	750	MET
1	A	778	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	726	ASN
1	A	797	GLN
1	A	827	GLN
1	A	510	GLN
1	A	502	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](#)

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	SAY	B	24	2	18,21,22	0.98	1 (5%)	25,29,32	0.87	1 (4%)
3	SAY	C	9	3	18,21,22	1.13	2 (11%)	25,29,32	0.96	1 (4%)

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	SAY	B	24	2	-	1/9/23/24	0/2/2/2
3	SAY	C	9	3	-	2/9/23/24	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	24	SAY	CAD-CAG	3.29	1.54	1.47
3	C	9	SAY	CAD-CAG	2.97	1.53	1.47
3	C	9	SAY	CAA-C1'	2.47	1.55	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	24	SAY	C4'-O4'-C1'	-2.48	103.69	108.83
3	C	9	SAY	C3'-C2'-C1'	2.38	105.00	102.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	9	SAY	CAC-CAD-CAG-OAH
2	B	24	SAY	CAC-CAD-CAG-OAH
3	C	9	SAY	CAE-CAD-CAG-OAH

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	24	SAY	1	0
3	C	9	SAY	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	SO4	A	1877	-	4,4,4	0.23	0	6,6,6	0.42	0
4	SO4	A	1878	-	4,4,4	0.17	0	6,6,6	0.29	0
5	MES	A	1879	-	12,12,12	2.18	1 (8%)	14,16,16	2.63	6 (42%)
6	MRD	A	1880	-	7,7,7	0.39	0	9,10,10	0.50	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
5	MES	A	1879	-	-	2/6/14/14	0/1/1/1
6	MRD	A	1880	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1879	MES	C8-S	-7.18	1.67	1.77

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1879	MES	C5-N4-C3	5.82	121.94	108.83
5	A	1879	MES	O1S-S-C8	5.08	113.03	106.92
5	A	1879	MES	C7-N4-C3	3.35	119.81	111.23
5	A	1879	MES	C7-N4-C5	2.74	118.25	111.23
5	A	1879	MES	C6-C5-N4	2.45	113.82	110.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1879	MES	C8-C7-N4-C5
6	A	1880	MRD	C1-C2-C3-C4
5	A	1879	MES	C8-C7-N4-C3
6	A	1880	MRD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1879	MES	3	0
6	A	1880	MRD	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	24:SAY	C3'	25:DT	P	2.68
1	C	9:SAY	C3'	10:DG	P	2.62

## 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	581/581 (100%)	-0.05	17 (2%) 51 58	14, 25, 41, 47	4 (0%)
2	B	9/10 (90%)	1.51	4 (44%) 0 0	35, 43, 68, 72	0
3	C	9/10 (90%)	0.59	1 (11%) 5 7	32, 44, 57, 68	0
All	All	599/601 (99%)	-0.02	22 (3%) 41 48	14, 25, 43, 72	4 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	553	GLY	5.3
1	A	296	THR	4.9
2	B	20	DG	4.5
1	A	433	ALA	4.3
1	A	552	THR	4.1

### 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
2	SAY	B	24	20/21	0.83	0.20	56,61,64,64	0
3	SAY	C	9	20/21	0.88	0.18	51,52,54,55	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<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( $\text{\AA}^2$ )	Q<0.9
6	MRD	A	1880	8/8	0.75	0.26	33,34,36,38	0
5	MES	A	1879	12/12	0.85	0.37	22,26,26,27	12
4	SO4	A	1877	5/5	0.96	0.13	35,35,37,37	0
4	SO4	A	1878	5/5	0.96	0.11	47,48,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.