



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:44 pm GMT

PDB ID : 4B9M
Title : Structure of the high fidelity DNA polymerase I with an oxidative formamido pyrimidine-dA DNA lesion -thymine basepair in the post- insertion site.
Authors : Gehrke, T.H.; Lischke, U.; Arnold, S.; Schneider, S.; Carell, T.
Deposited on : 2012-09-05
Resolution : 2.05 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

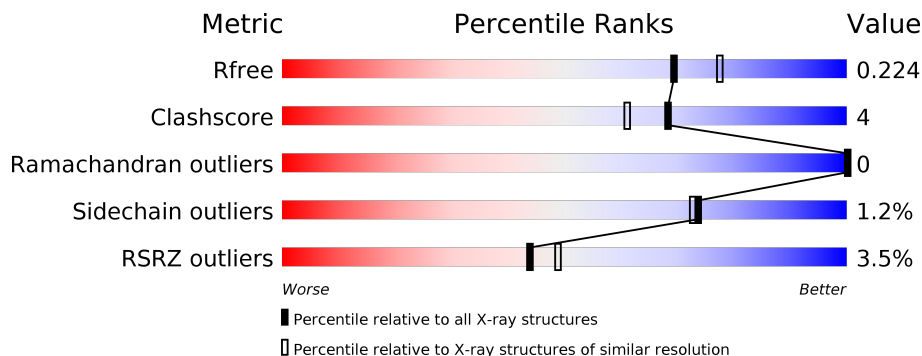
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	111664	1449 (2.04-2.04)
Clashscore	122126	1524 (2.04-2.04)
Ramachandran outliers	120053	1512 (2.04-2.04)
Sidechain outliers	120020	1512 (2.04-2.04)
RSRZ outliers	108989	1429 (2.04-2.04)

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. 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	619	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>6%</div> </div> </div>
2	B	11	<div> <div>36%</div> <div> <div></div> <div>45%</div> <div>27%</div> <div>27%</div> </div> </div>
3	C	15	<div> <div>20%</div> <div> <div></div> <div>27%</div> <div>40%</div> <div>13%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5383 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
1	A	580	Total	C	N	O	S	0	4	0
			4680	2975	817	871	17			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	MET	-	expression tag	UNP E1C9K5
A	259	ALA	-	expression tag	UNP E1C9K5
A	260	SER	-	expression tag	UNP E1C9K5
A	261	TRP	-	expression tag	UNP E1C9K5
A	262	SER	-	expression tag	UNP E1C9K5
A	263	HIS	-	expression tag	UNP E1C9K5
A	264	PRO	-	expression tag	UNP E1C9K5
A	265	GLN	-	expression tag	UNP E1C9K5
A	266	PHE	-	expression tag	UNP E1C9K5
A	267	GLU	-	expression tag	UNP E1C9K5
A	268	LYS	-	expression tag	UNP E1C9K5
A	269	GLY	-	expression tag	UNP E1C9K5
A	270	ALA	-	expression tag	UNP E1C9K5
A	271	SER	-	expression tag	UNP E1C9K5
A	272	THR	-	expression tag	UNP E1C9K5
A	273	SER	-	expression tag	UNP E1C9K5
A	274	LEU	-	expression tag	UNP E1C9K5
A	275	TYR	-	expression tag	UNP E1C9K5
A	276	LYS	-	expression tag	UNP E1C9K5
A	277	LYS	-	expression tag	UNP E1C9K5
A	278	ALA	-	expression tag	UNP E1C9K5
A	279	GLY	-	expression tag	UNP E1C9K5
A	280	SER	-	expression tag	UNP E1C9K5
A	281	ALA	-	expression tag	UNP E1C9K5
A	282	ALA	-	expression tag	UNP E1C9K5
A	283	ALA	-	expression tag	UNP E1C9K5
A	284	VAL	-	expression tag	UNP E1C9K5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	285	LEU	-	expression tag	UNP E1C9K5
A	286	GLU	-	expression tag	UNP E1C9K5
A	287	GLU	-	expression tag	UNP E1C9K5
A	288	ASN	-	expression tag	UNP E1C9K5
A	289	LEU	-	expression tag	UNP E1C9K5
A	290	TYR	-	expression tag	UNP E1C9K5
A	291	PHE	-	expression tag	UNP E1C9K5
A	292	GLN	-	expression tag	UNP E1C9K5
A	293	GLY	-	expression tag	UNP E1C9K5
A	294	SER	-	expression tag	UNP E1C9K5
A	295	PHE	-	expression tag	UNP E1C9K5
A	296	THR	-	expression tag	UNP E1C9K5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			221	106	35	69	11			

- Molecule 3 is a DNA chain called 5'-D(*DC*DA*DA*FAX*AP*GP*AP*GP*TP*CP*AP*GP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			251	119	50	70	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

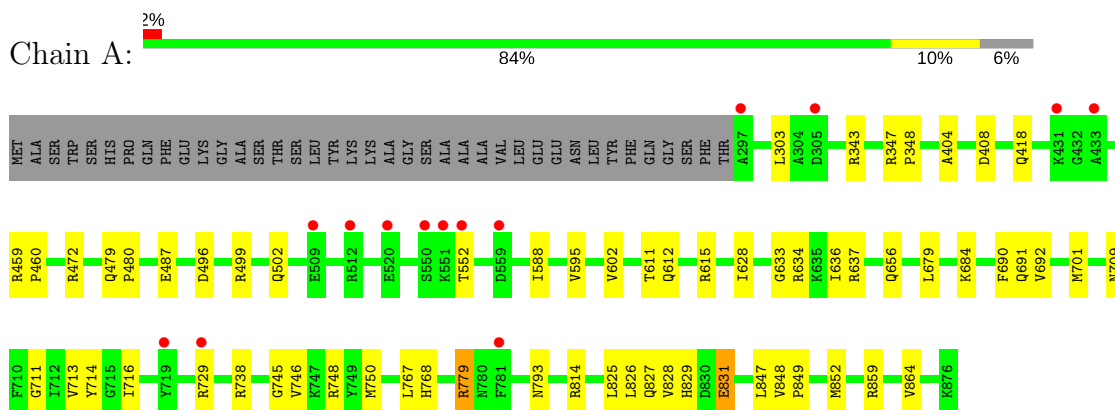
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	198	Total	O	0	0
			198	198		
6	B	2	Total	O	0	0
			2	2		

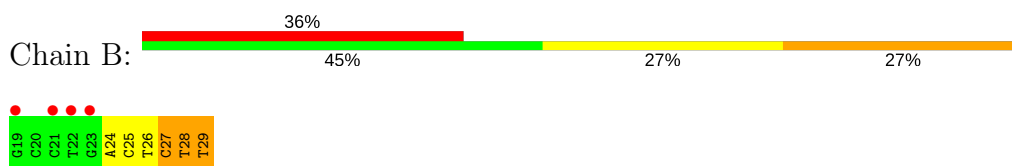
3 Residue-property plots [i](#)

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.

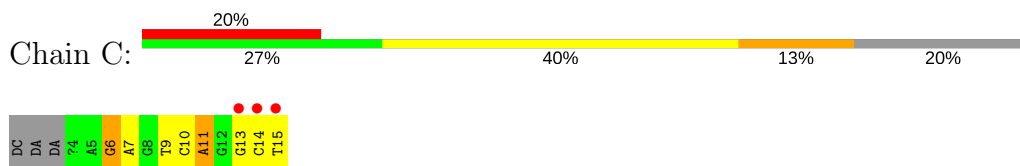
• Molecule 1: DNA POLYMERASE I



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



• Molecule 3: 5'-D(*DC*DA*DA*FAX*AP*GP*AP*GP*TP*CP*AP*GP*GP*CP*TP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.42Å 93.66Å 105.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.05 32.51 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.05) 98.0 (32.51-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.186 , 0.221 0.194 , 0.224	Depositor DCC
R_{free} test set	2918 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5383	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FAX, SO4

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	0.87	1/4775 (0.0%)	0.77	6/6451 (0.1%)
2	B	1.36	2/245 (0.8%)	1.92	8/375 (2.1%)
3	C	1.30	0/257	1.81	6/395 (1.5%)
All	All	0.93	3/5277 (0.1%)	0.95	20/7221 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	DT	C3'-O3'	-5.75	1.36	1.44
1	A	831	GLU	CB-CG	-5.55	1.41	1.52
2	B	28	DT	C5-C7	5.23	1.53	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	DT	C4-C5-C7	9.86	124.92	119.00
3	C	11	DA	O5'-P-OP1	-7.24	99.18	105.70
2	B	24	DA	O4'-C1'-N9	-6.95	103.13	108.00
2	B	29	DT	C5-C4-O4	-6.84	120.11	124.90
1	A	859	ARG	NE-CZ-NH1	6.83	123.72	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4680	0	4749	37	0
2	B	221	0	126	2	0
3	C	251	0	139	5	0
4	A	1	0	0	0	0
5	A	30	0	0	3	0
6	A	198	0	0	3	0
6	B	2	0	0	0	0
All	All	5383	0	5014	42	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.

The worst 5 of 42 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:748:ARG:NH1	5:A:1882:SO4:O4	2.15	0.78
3:C:10:DC:H2''	3:C:11:DA:H5'	1.69	0.73
1:A:746:VAL:O	1:A:750:MET:HG2	1.89	0.72
3:C:10:DC:H2''	3:C:11:DA:C5'	2.22	0.70
1:A:714:TYR:OH	2:B:29:DT:H2'	1.94	0.67

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	582/619 (94%)	567 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	499/526 (95%)	493 (99%)	6 (1%)	74	73

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	552	THR
1	A	831	GLU
1	A	779	ARG
1	A	472	ARG
1	A	827	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	A	612	GLN
1	A	709	ASN
1	A	829	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	FAX	C	4	3	18,23,24	1.58	3 (16%)	22,31,34	2.22	8 (36%)

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	FAX	C	4	3	-	0/10/24/25	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FAX	C6'-C1'	-4.43	1.44	1.53
3	C	4	FAX	C6'-C4'	-3.82	1.43	1.53
3	C	4	FAX	C5-N7	-2.34	1.38	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FAX	N3-C2-N1	-5.16	120.30	128.63
3	C	4	FAX	C6'-C4'-C5'	-2.52	107.84	112.57
3	C	4	FAX	C5'-C4'-C3'	-2.49	109.98	114.36
3	C	4	FAX	C2'-C1'-N9	-2.33	106.44	112.45
3	C	4	FAX	C5-C4-N3	2.01	120.32	117.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	SO4	A	1878	-	4,4,4	0.39	0	6,6,6	0.78	0
5	SO4	A	1879	-	4,4,4	0.23	0	6,6,6	0.28	0
5	SO4	A	1880	-	4,4,4	0.28	0	6,6,6	0.82	0
5	SO4	A	1881	-	4,4,4	0.25	0	6,6,6	0.79	0
5	SO4	A	1882	-	4,4,4	0.28	0	6,6,6	0.38	0
5	SO4	A	1883	-	4,4,4	0.19	0	6,6,6	0.15	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	SO4	A	1878	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1879	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1880	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1881	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1882	-	-	0/0/0/0	0/0/0/0
5	SO4	A	1883	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1878	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1882	SO4	1	0
5	A	1883	SO4	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	580/619 (93%)	-0.01	14 (2%) 59 64	17, 30, 50, 71	0
2	B	11/11 (100%)	0.95	4 (36%) 0 0	38, 48, 77, 77	0
3	C	11/15 (73%)	0.96	3 (27%) 0 0	40, 42, 80, 94	0
All	All	602/645 (93%)	0.03	21 (3%) 44 49	17, 30, 52, 94	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	15	DT	5.8
2	B	19	DG	4.1
1	A	433	ALA	3.7
1	A	520	GLU	3.5
3	C	13	DG	3.5

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
3	FAX	C	4	22/23	0.79	0.25	53,62,78,81	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
5	SO4	A	1878	5/5	0.79	0.21	41,42,49,50	5
5	SO4	A	1879	5/5	0.88	0.26	45,45,46,48	5
5	SO4	A	1882	5/5	0.92	0.27	41,41,43,44	5
4	MG	A	1877	1/1	0.92	0.13	38,38,38,38	0
5	SO4	A	1881	5/5	0.95	0.09	60,60,62,63	0
5	SO4	A	1883	5/5	0.95	0.23	89,90,90,91	0
5	SO4	A	1880	5/5	0.96	0.13	48,48,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.