



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:39 AM GMT

PDB ID : 4B9T
Title : Structure of the high fidelity DNA polymerase I with an oxidative formamido pyrimidine-dGDNA lesion -dC basepair in the post-insertion site.
Authors : Gehrke, T.H.; Lischke, U.; Arnold, S.; Schneider, S.; Carell, T.
Deposited on : 2012-09-06
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

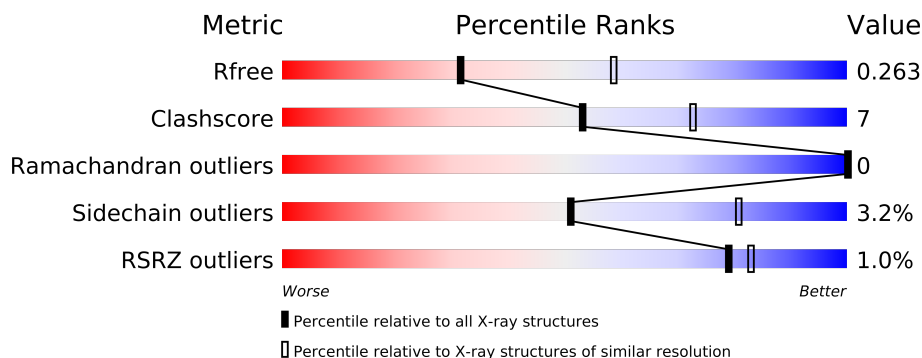
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	619	
2	B	11	
3	C	15	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	SO4	A	1878	-	X
5	SO4	A	1879	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5201 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	580	Total	C	N	O	S	0	1	0
			4658	2959	810	872	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(*AP*CP*CP*TP*GP*AP*CP*TP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			222	105	39	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			251	118	51	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		

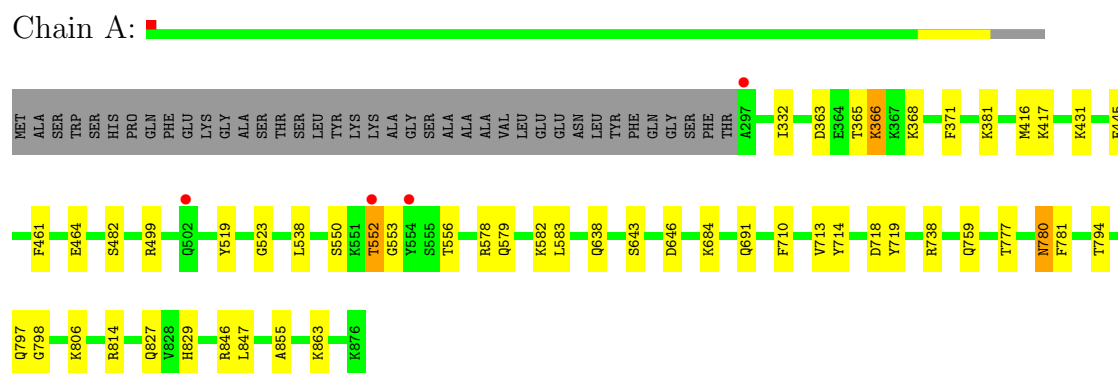
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total	O	0	0
			59	59		

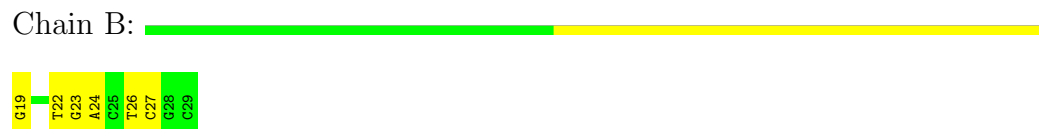
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

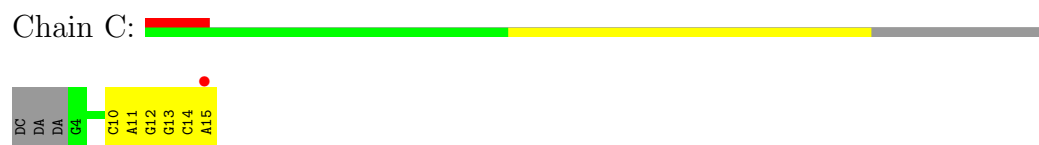
• Molecule 1: DNA POLYMERASE



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



• Molecule 3: 5'-D(*CP*AP*TP*FOXP*AP*GP*AP*GP*TP*CP*AP*GP*GP*TP*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	88.38Å 93.78Å 105.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.65 45.33 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.00-2.65) 94.4 (45.33-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.221 , 0.273 0.220 , 0.263	Depositor DCC
R_{free} test set	1240 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 24704 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5201	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FOX, 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	0.51	0/4744	0.60	0/6411
2	B	0.74	0/247	1.14	1/378 (0.3%)
3	C	0.72	0/256	1.06	0/393
All	All	0.54	0/5247	0.67	1/7182 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	27	DC	O4'-C4'-C3'	-5.09	102.47	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4658	0	0	24	0
2	B	222	0	0	5	0
3	C	251	0	0	7	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	59	0	0	3	1
All	All	5201	0	0	32	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:552:THR:OG1	2:B:24:DA:OP1	1.59	1.17
3:C:15:DA:C8	3:C:15:DA:OP2	2.30	0.84
3:C:14:DC:C2'	3:C:15:DA:O5'	2.30	0.80
3:C:13:DG:C2'	3:C:14:DC:O5'	2.30	0.79
1:A:691:GLN:OE1	1:A:738:ARG:NH2	2.23	0.72
1:A:366:LYS:O	1:A:368:LYS:NZ	2.27	0.68
1:A:552:THR:OG1	2:B:24:DA:P	2.55	0.62
1:A:582:LYS:NZ	2:B:26:DT:O2	2.32	0.61
1:A:371:PHE:O	6:A:2012:HOH:O	2.16	0.59
3:C:10:DC:C2'	3:C:11:DA:C5'	2.81	0.58
1:A:827:GLN:NE2	1:A:829:HIS:N	2.52	0.57
1:A:780:ASN:ND2	1:A:781:PHE:N	2.53	0.57
1:A:718:ASP:OD1	1:A:719:TYR:N	2.39	0.55
1:A:780:ASN:C	1:A:780:ASN:ND2	2.58	0.55
1:A:684:LYS:NZ	6:A:2052:HOH:O	2.39	0.55
1:A:646:ASP:N	6:A:2045:HOH:O	2.43	0.51
1:A:417:LYS:NZ	1:A:464:GLU:OE1	2.43	0.51
1:A:713:VAL:O	1:A:797:GLN:NE2	2.44	0.51
3:C:12:DG:C2'	3:C:13:DG:OP2	2.59	0.50
1:A:806:LYS:NZ	1:A:855:ALA:O	2.46	0.49
2:B:22:DT:C2'	2:B:23:DG:C8	2.98	0.47
1:A:794:THR:O	1:A:798:GLY:N	2.47	0.47
2:B:19:DG:N2	3:C:14:DC:C2	2.82	0.47
1:A:710:PHE:CE2	1:A:714:TYR:CE2	3.03	0.47
1:A:416:MET:CE	1:A:461:PHE:CE2	2.98	0.46
1:A:519:TYR:O	1:A:523:GLY:N	2.50	0.45
1:A:556:THR:O	1:A:578:ARG:NH1	2.51	0.44
1:A:814:ARG:NH2	1:A:847:LEU:CD1	2.80	0.44
1:A:499:ARG:NH2	1:A:638:GLN:OE1	2.53	0.42
1:A:363:ASP:OD1	1:A:365:THR:OG1	2.38	0.42
1:A:550:SER:N	1:A:553:GLY:O	2.53	0.41
3:C:15:DA:P	3:C:15:DA:C8	3.13	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:2056:HOH:O	6:A:2058:HOH:O[3_554]	2.01	0.19

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	579/619 (94%)	563 (97%)	16 (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	496/526 (94%)	480 (97%)	16 (3%)	51	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	332	ILE
1	A	366	LYS
1	A	381	LYS
1	A	431	LYS
1	A	445	GLU
1	A	482	SER
1	A	538	LEU
1	A	552	THR
1	A	579	GLN
1	A	583	LEU

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Mol	Chain	Res	Type
1	A	643	SER
1	A	759	GLN
1	A	777	THR
1	A	780	ASN
1	A	846	ARG
1	A	863	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	FOX	C	4	3,2	22,24,25	2.18	6 (27%)	28,33,36	2.54	10 (35%)

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	FOX	C	4	3,2	-	0/11/24/25	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FOX	C6'-C1'	-6.77	1.43	1.53
3	C	4	FOX	P-O1P	4.16	1.51	1.46
3	C	4	FOX	C6'-C4'	-3.85	1.43	1.53
3	C	4	FOX	C5-N7	-3.10	1.37	1.43
3	C	4	FOX	C2-N2	2.35	1.36	1.32
3	C	4	FOX	C4-N9	2.21	1.36	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	FOX	O8-C8-N7	-8.67	115.58	125.86
3	C	4	FOX	C4'-C6'-C1'	4.56	111.39	103.88
3	C	4	FOX	C6-N1-C2	3.62	120.83	116.91
3	C	4	FOX	C2'-C1'-N9	-3.39	106.51	112.57
3	C	4	FOX	C6'-C4'-C3'	3.04	108.26	102.47
3	C	4	FOX	C6-C5-N7	2.75	123.54	118.07
3	C	4	FOX	C5-N7-C8	2.67	126.78	123.69
3	C	4	FOX	C6-C5-C4	2.65	117.02	114.56
3	C	4	FOX	N2-C2-N3	2.35	120.43	117.85
3	C	4	FOX	C3'-C2'-C1'	2.34	107.03	104.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is 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	SO4	A	1878	-	4,4,4	0.29	0	6,6,6	0.22	0
5	SO4	A	1879	-	4,4,4	0.78	0	6,6,6	0.98	1 (16%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1879	SO4	O4-S-O3	2.27	118.68	109.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.15	4 (0%) 84 88	44, 57, 88, 104	0
2	B	11/11 (100%)	0.48	0 100 100	83, 108, 122, 130	0
3	C	12/15 (80%)	0.80	1 (8%) 11 11	94, 111, 197, 225	0
All	All	603/645 (93%)	-0.12	5 (0%) 79 86	44, 58, 94, 225	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	15	DA	3.6
1	A	552	THR	2.9
1	A	554	TYR	2.6
1	A	297	ALA	2.6
1	A	502	GLN	2.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FOX	C	4	23/24	0.26	1.45	138,144,166,173	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	1878	5/5	0.41	8.89	133,134,135,136	0
5	SO4	A	1879	5/5	0.30	2.88	124,124,124,124	0
4	MG	A	1877	1/1	0.15	-0.23	48,48,48,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.