



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 01:31 AM JST

PDB ID : 7EF8
Title : Crystal structure of mouse MUTYH in complex with DNA containing AP site analogue:8-oxoG (Form I)
Authors : Nakamura, T.; Nakabeppu, Y.; Yamagata, Y.
Deposited on : 2021-03-21
Resolution : 2.45 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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

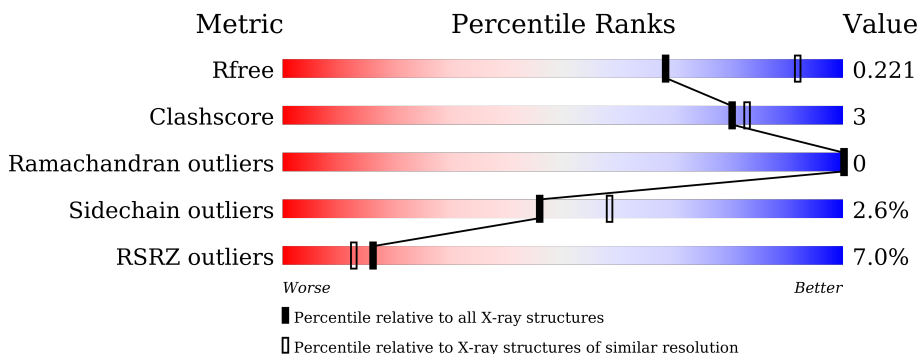
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 $\leq 5\%$. 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	458	 7% 80% 7% 7%
2	B	14	 71% 21% 7%
3	C	14	 86% 7% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3807 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 Adenine DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3193	2014	578	583	18	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP Q99P21
A	31	PRO	-	expression tag	UNP Q99P21
A	32	GLY	-	expression tag	UNP Q99P21
A	33	TYR	-	expression tag	UNP Q99P21
A	34	GLN	-	expression tag	UNP Q99P21

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*AP*GP*AP*CP*(8OG)P*GP*GP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	271	128	55	76	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	233	111	35	75	12	0	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

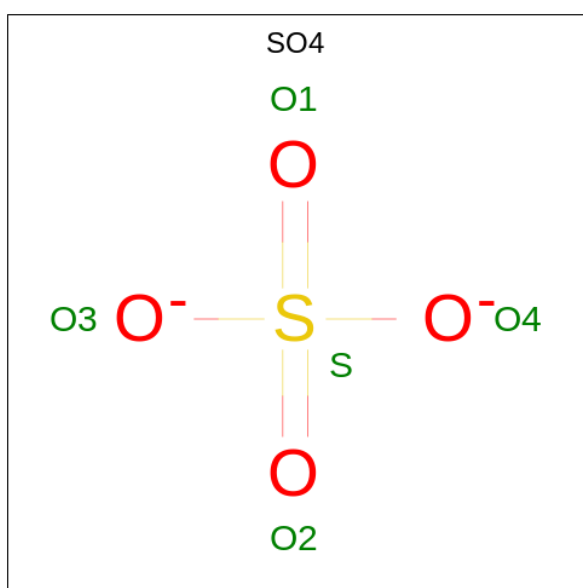


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

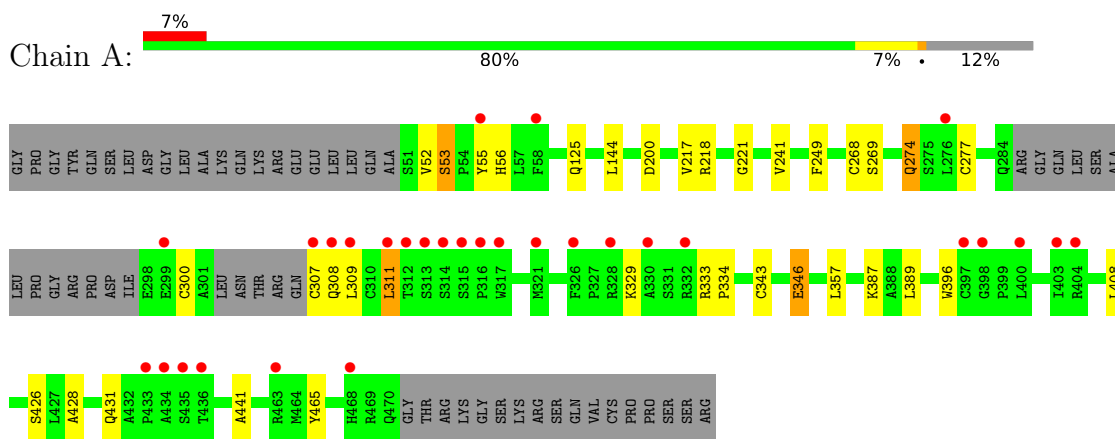
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	3	Total	O	0	0
			3	3		
7	C	3	Total	O	0	0
			3	3		

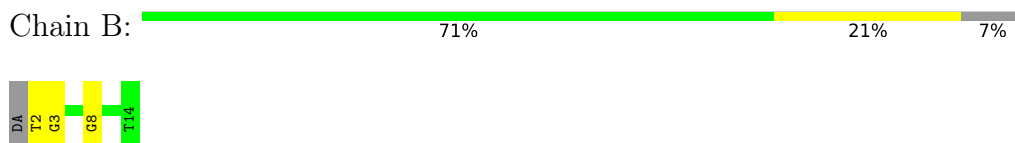
3 Residue-property plots [i](#)

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.

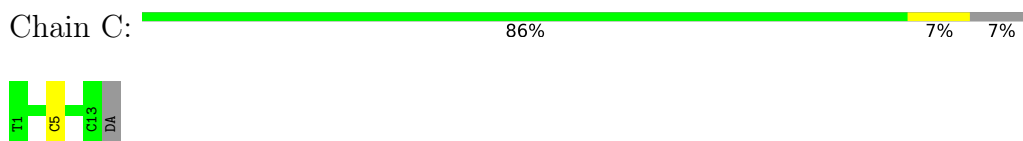
- Molecule 1: Adenine DNA glycosylase



- Molecule 2: DNA (5'-D(*TP*GP*AP*GP*AP*CP*(8OG)P*GP*GP*GP*AP*CP*T)-3')



- Molecule 3: DNA (5'-D(*TP*AP*GP*TP*CP*CP*CP*(3DR)P*GP*TP*CP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.27Å 107.24Å 156.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.89 – 2.45 46.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.89-2.45) 99.7 (46.89-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.198 , 0.221 0.198 , 0.221	Depositor DCC
R_{free} test set	1186 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtrriage
Anisotropy	0.305	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3807	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: 3DR, SF4, SOG, SO4, ZN

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	0.24	0/3274	0.41	0/4459
2	B	0.49	0/278	0.88	0/426
3	C	0.50	0/245	0.97	0/374
All	All	0.29	0/3797	0.52	0/5259

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

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	3193	0	3127	18	0
2	B	271	0	147	1	0
3	C	233	0	134	1	0
4	A	8	0	0	0	0
5	A	1	0	0	0	0
6	A	35	0	0	0	0
7	A	60	0	0	0	0
7	B	3	0	0	0	0
7	C	3	0	0	0	0
All	All	3807	0	3408	19	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.

All (19) 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:268:CYS:O	1:A:274:GLN:NE2	2.34	0.61
1:A:333:ARG:HD3	1:A:334:PRO:HD2	1.86	0.56
1:A:408:LEU:HD11	1:A:426:SER:HB2	1.88	0.55
1:A:218:ARG:HE	1:A:218:ARG:HA	1.74	0.53
1:A:307:CYS:SG	1:A:308:GLN:N	2.83	0.49
1:A:357:LEU:HD11	1:A:441:ALA:HB1	1.94	0.49
1:A:431:GLN:N	1:A:431:GLN:OE1	2.48	0.46
1:A:56:HIS:CD2	1:A:309:LEU:HB2	2.50	0.46
1:A:241:VAL:HA	1:A:249:PHE:CD1	2.52	0.45
1:A:55:TYR:CD1	1:A:300:CYS:HB2	2.53	0.44
1:A:217:VAL:HA	1:A:277:CYS:SG	2.58	0.44
1:A:52:VAL:HG12	1:A:53:SER:N	2.33	0.43
1:A:343:CYS:HB2	1:A:389:LEU:HD21	2.00	0.43
1:A:221:GLY:HA3	1:A:311:LEU:HG	2.01	0.42
2:B:2:DT:H2''	2:B:3:DG:H5'	2.02	0.42
1:A:329:LYS:HE3	3:C:5:DC:H5''	2.02	0.41
1:A:387:LYS:HE2	1:A:387:LYS:HB2	1.92	0.41
1:A:396:TRP:CE3	1:A:441:ALA:HB2	2.56	0.40
1:A:346:GLU:HG2	1:A:428:ALA:HA	2.02	0.40

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	398/458 (87%)	386 (97%)	12 (3%)	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	Rotameric	Outliers	Percentiles
1	A	342/386 (89%)	333 (97%)	9 (3%)	46 58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	125	GLN
1	A	144	LEU
1	A	200	ASP
1	A	269	SER
1	A	274	GLN
1	A	311	LEU
1	A	346	GLU
1	A	465	TYR

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

Mol	Chain	Res	Type
1	A	112	GLN
1	A	125	GLN
1	A	274	GLN
1	A	308	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
3	3DR	C	8	3	8,11,12	0.55	0	9,14,17	0.73	0
2	8OG	B	8	2	22,25,26	1.54	3 (13%)	30,37,40	2.12	6 (20%)

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	3DR	C	8	3	-	1/3/15/16	0/1/1/1
2	8OG	B	8	2	-	2/7/21/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	8	8OG	C8-N9	4.88	1.49	1.40
2	B	8	8OG	C6-N1	-2.92	1.33	1.38
2	B	8	8OG	C5-N7	2.36	1.41	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	8OG	C5-C4-N3	-6.88	120.69	127.80
2	B	8	8OG	N9-C4-N3	4.80	131.29	125.81
2	B	8	8OG	C2-N1-C6	-4.59	116.73	125.10
2	B	8	8OG	O6-C6-C5	-3.39	119.46	127.24
2	B	8	8OG	C5-C6-N1	2.98	121.17	112.31
2	B	8	8OG	C2-N3-C4	2.55	116.84	112.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	8OG	C4'-C5'-O5'-P
2	B	8	8OG	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	C	8	3DR	C4'-C5'-O5'-P

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
6	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	507	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SF4	A	501	1	0,12,12	-	-	-		
6	SO4	A	506	-	4,4,4	0.13	0	6,6,6	0.05	0
6	SO4	A	509	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	A	508	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.07	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	501	1	-	-	0/6/5/5

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

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	402/458 (87%)	0.25	30 (7%) 14 11	39, 63, 136, 171	0
2	B	12/14 (85%)	-0.11	0 100 100	52, 90, 127, 156	0
3	C	12/14 (85%)	-0.13	0 100 100	56, 88, 145, 147	0
All	All	426/486 (87%)	0.23	30 (7%) 16 13	39, 64, 136, 171	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	ALA	5.3
1	A	311	LEU	4.6
1	A	313	SER	4.5
1	A	314	SER	4.1
1	A	328	ARG	4.1
1	A	315	SER	4.0
1	A	299	GLU	3.9
1	A	312	THR	3.9
1	A	435	SER	3.8
1	A	400	LEU	3.7
1	A	307	CYS	3.4
1	A	317	TRP	3.3
1	A	55	TYR	3.1
1	A	326	PHE	3.0
1	A	308	GLN	2.9
1	A	433	PRO	2.8
1	A	468	HIS	2.8
1	A	316	PRO	2.8
1	A	403	ILE	2.8
1	A	321	MET	2.7
1	A	463	ARG	2.6
1	A	436	THR	2.6
1	A	276	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	404	ARG	2.6
1	A	309	LEU	2.4
1	A	330	ALA	2.3
1	A	332	ARG	2.3
1	A	397	CYS	2.2
1	A	58	PHE	2.2
1	A	398	GLY	2.1

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, 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	3DR	C	8	11/12	0.97	0.17	52,60,64,65	0
2	8OG	B	8	23/24	0.98	0.15	44,52,55,59	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, 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
6	SO4	A	509	5/5	0.69	0.25	127,127,129,130	5
6	SO4	A	504	5/5	0.76	0.29	129,131,132,133	5
6	SO4	A	505	5/5	0.83	0.17	104,112,113,116	0
6	SO4	A	507	5/5	0.84	0.27	119,121,121,122	5
6	SO4	A	506	5/5	0.87	0.13	111,114,115,116	0
6	SO4	A	508	5/5	0.92	0.22	97,98,100,100	5
5	ZN	A	502	1/1	0.93	0.09	126,126,126,126	0
6	SO4	A	503	5/5	0.98	0.14	69,73,76,79	0
4	SF4	A	501	8/8	0.99	0.16	63,71,77,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.