



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 11:34 am BST

PDB ID : 6RT6 / pdb_00006rt6
Title : The YTH domain of YTHDC1 protein in complex with GGm6AC oligonucleotide
Authors : Bedi, R.; Sledz, P.; Caffisch, A.
Deposited on : 2019-05-22
Resolution : 1.46 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

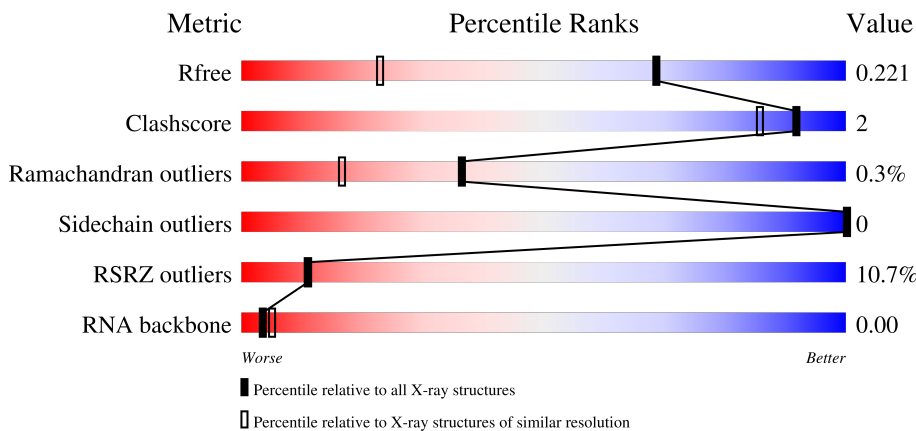
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)
RNA backbone	3983	1019 (2.10-0.86)

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	4	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 25%, orange 25%, yellow 50%, green 90%, grey 100%);"></div> <div style="text-align: center;">25%</div> <div style="text-align: center;">50%</div> </div>
1	E	4	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">25%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 25%, orange 25%, yellow 50%, green 90%, grey 100%);"></div> <div style="text-align: center;">50%</div> <div style="text-align: center;">50%</div> </div>
2	B	166	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">11%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 11%, orange 11%, yellow 90%, green 96%, grey 100%);"></div> <div style="text-align: center;">90%</div> <div style="text-align: center;">6%</div> </div>
2	C	166	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">9%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 9%, orange 9%, yellow 96%, green 96%, grey 100%);"></div> <div style="text-align: center;">96%</div> <div style="text-align: center;">..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2903 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 RNA chain called RNA (5'-R*(6MZ)P*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2	Total 24	C 11	N 5	O 7	P 1	0	0	0
1	E	2	Total 40	C 20	N 8	O 11	P 1	0	0	0

- Molecule 2 is a protein called YTH domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	160	Total 1233	C 799	N 212	O 217	S 5	0	0	0
2	C	164	Total 1264	C 816	N 219	O 224	S 5	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	344	GLY	-	expression tag	UNP Q96MU7
C	344	GLY	-	expression tag	UNP Q96MU7

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

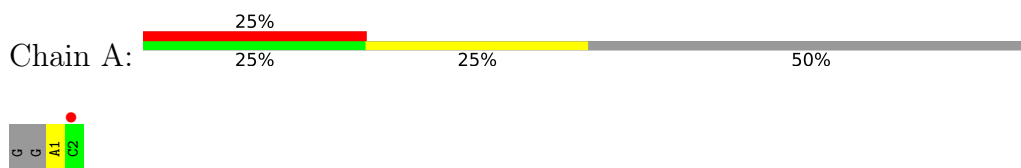
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	131	Total O 131 131	0	0
4	C	187	Total O 187 187	0	0

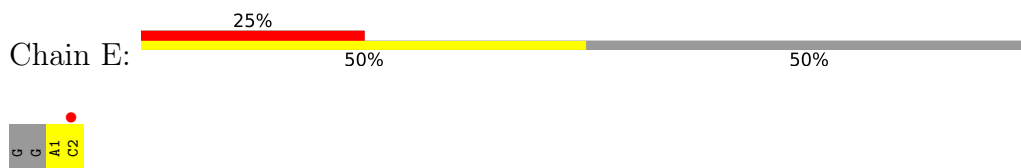
3 Residue-property plots [i](#)

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.

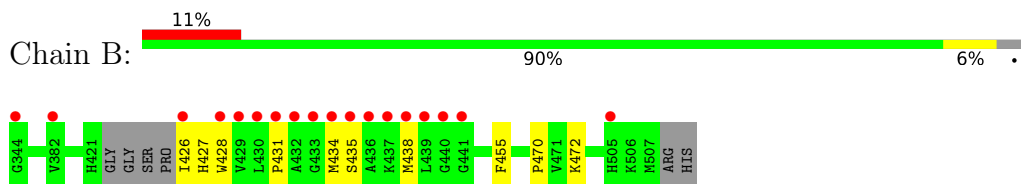
- Molecule 1: RNA (5'-R*(6MZ)P*C)-3')



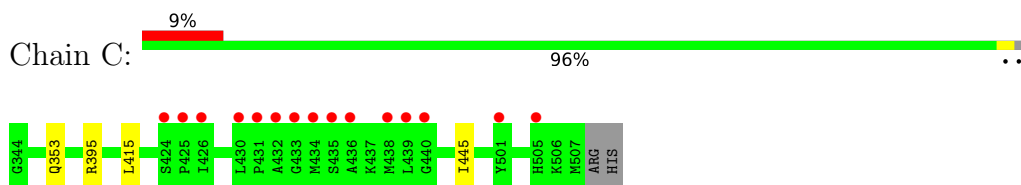
- Molecule 1: RNA (5'-R*(6MZ)P*C)-3')



- Molecule 2: YTH domain-containing protein 1



- Molecule 2: YTH domain-containing protein 1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.91Å 103.74Å 41.98Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	40.65 – 1.46 40.65 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.65-1.46) 99.5 (40.65-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.46Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.206 , 0.220 0.206 , 0.221	Depositor DCC
R_{free} test set	2004 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.042 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2903	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 6MZ

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	0.20	0/3	0.57	0/3
1	E	0.26	0/21	0.43	0/30
2	B	0.27	0/1263	0.48	0/1711
2	C	0.27	0/1302	0.50	0/1765
All	All	0.27	0/2589	0.49	0/3509

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 [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	24	0	13	0	0
1	E	40	0	25	0	0
2	B	1233	0	1207	6	0
2	C	1264	0	1238	2	0
3	B	5	0	0	0	0
3	C	15	0	0	0	0
4	A	4	0	0	0	0
4	B	131	0	0	1	2
4	C	187	0	0	0	3
All	All	2903	0	2483	8	3

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 2.

All (8) 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)
2:B:435:SER:HB2	2:B:438:MET:HG3	1.86	0.58
2:C:415:LEU:HD23	2:C:445:ILE:HG22	1.96	0.48
2:B:470:PRO:HD3	4:B:780:HOH:O	2.14	0.47
2:B:455:PHE:HB3	2:B:472:LYS:HD3	1.97	0.46
2:B:431:PRO:HD2	2:B:434:MET:CB	2.47	0.44
2:B:438:MET:HE2	2:B:438:MET:HB3	1.91	0.43
2:C:353:GLN:O	2:C:395:ARG:NH2	2.51	0.43
2:B:426:ILE:HD12	2:B:428:TRP:CZ2	2.56	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:709:HOH:O	4:C:823:HOH:O[1_655]	2.16	0.04
4:B:790:HOH:O	4:C:795:HOH:O[2_545]	2.17	0.03
4:B:724:HOH:O	4:C:733:HOH:O[2_645]	2.19	0.01

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	
2	B	156/166 (94%)	152 (97%)	3 (2%)	1 (1%)	21	6
2	C	163/166 (98%)	162 (99%)	1 (1%)	0	100	100
All	All	319/332 (96%)	314 (98%)	4 (1%)	1 (0%)	36	16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	427	HIS

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	
2	B	128/145 (88%)	128 (100%)	0	100	100
2	C	133/145 (92%)	133 (100%)	0	100	100
All	All	261/290 (90%)	261 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/4	-	-
1	E	1/4 (25%)	1 (100%)	0
All	All	1/8 (12%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	2	C

There are no RNA pucker outliers to report.

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
1	6MZ	A	1	1	22,22,26	4.07	5 (22%)	30,32,39	2.39	10 (33%)
1	6MZ	E	1	1	22,22,26	4.02	5 (22%)	30,32,39	2.30	10 (33%)

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
1	6MZ	A	1	1	-	2/8/24/28	0/3/3/3
1	6MZ	E	1	1	-	4/8/24/28	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	6MZ	C6-N6	17.94	1.53	1.34
1	E	1	6MZ	C6-N6	17.69	1.53	1.34
1	A	1	6MZ	C8-N7	3.33	1.37	1.31
1	E	1	6MZ	C8-N7	3.12	1.37	1.31
1	A	1	6MZ	C9-N6	3.00	1.50	1.45
1	E	1	6MZ	C9-N6	2.95	1.50	1.45
1	A	1	6MZ	C2-N3	2.46	1.38	1.33
1	E	1	6MZ	C5-N7	-2.42	1.34	1.39
1	E	1	6MZ	C2-N3	2.38	1.38	1.33
1	A	1	6MZ	C5-N7	-2.38	1.34	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	6MZ	C5-C4-N3	-5.57	119.48	126.75
1	A	1	6MZ	N1-C2-N3	-5.45	120.07	128.60
1	E	1	6MZ	N1-C2-N3	-5.34	120.24	128.60
1	E	1	6MZ	C5-C4-N3	-4.76	120.54	126.75
1	A	1	6MZ	N9-C8-N7	-4.54	107.71	113.91
1	E	1	6MZ	C9-N6-C6	-4.37	119.11	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	6MZ	N9-C8-N7	-4.33	107.99	113.91
1	A	1	6MZ	C4-C5-C6	4.15	120.03	116.81
1	A	1	6MZ	C2-N3-C4	3.68	120.44	111.75
1	A	1	6MZ	N3-C4-N9	3.63	133.06	127.08
1	E	1	6MZ	C4-C5-C6	3.59	119.59	116.81
1	E	1	6MZ	C2-N3-C4	3.20	119.32	111.75
1	A	1	6MZ	C9-N6-C6	-3.18	120.13	122.87
1	A	1	6MZ	C5-N7-C8	3.04	107.83	103.51
1	E	1	6MZ	N3-C4-N9	2.90	131.87	127.08
1	E	1	6MZ	C5-N7-C8	2.73	107.39	103.51
1	E	1	6MZ	C4-N9-C1'	-2.67	120.24	126.59
1	E	1	6MZ	C4-N9-C8	2.44	108.37	105.73
1	A	1	6MZ	C4-N9-C8	2.43	108.36	105.73
1	A	1	6MZ	C4-N9-C1'	-2.00	121.82	126.59

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	6MZ	O4'-C4'-C5'-O5'
1	E	1	6MZ	N1-C6-N6-C9
1	E	1	6MZ	O4'-C4'-C5'-O5'
1	A	1	6MZ	C3'-C4'-C5'-O5'
1	E	1	6MZ	C3'-C4'-C5'-O5'
1	E	1	6MZ	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	SO4	B	601	-	4,4,4	0.20	0	6,6,6	0.50	0
3	SO4	C	602	-	4,4,4	0.11	0	6,6,6	0.10	0
3	SO4	C	603	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	C	601	-	4,4,4	0.17	0	6,6,6	0.10	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.

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

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	1/4 (25%)	2.19	1 (100%) 0 0	50, 50, 50, 50	0
1	E	1/4 (25%)	2.16	1 (100%) 0 0	49, 49, 49, 49	0
2	B	160/166 (96%)	0.51	18 (11%) 10 10	18, 27, 55, 63	0
2	C	164/166 (98%)	0.35	15 (9%) 15 14	15, 24, 47, 57	1 (0%)
All	All	326/340 (95%)	0.44	35 (10%) 11 11	15, 26, 49, 63	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	432	ALA	4.8
2	C	436	ALA	4.8
2	B	426	ILE	4.4
2	C	433	GLY	4.2
2	C	439	LEU	4.1
2	B	433	GLY	3.9
2	B	435	SER	3.6
2	B	434	MET	3.5
2	B	344	GLY	3.4
2	B	430	LEU	3.3
2	B	431	PRO	3.2
2	C	440	GLY	3.1
2	B	439	LEU	2.9
2	B	505	HIS	2.9
2	C	435	SER	2.9
2	C	432	ALA	2.7
2	C	505	HIS	2.7
2	C	424	SER	2.6
2	C	438	MET	2.6
2	B	437	LYS	2.5
2	B	436	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	429	VAL	2.5
2	B	382	VAL	2.4
2	B	440	GLY	2.4
2	B	438	MET	2.3
2	C	431	PRO	2.2
1	A	2	C	2.2
2	C	425	PRO	2.2
2	C	434	MET	2.2
1	E	2	C	2.2
2	B	428	TRP	2.1
2	C	501	TYR	2.1
2	B	441	GLY	2.1
2	C	430	LEU	2.1
2	C	426	ILE	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
1	6MZ	A	1	20/24	0.72	0.14	29,40,54,55	0
1	6MZ	E	1	20/24	0.76	0.13	34,43,53,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
3	SO4	B	601	5/5	0.89	0.12	33,35,40,42	0
3	SO4	C	603	5/5	0.90	0.08	43,48,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	C	602	5/5	0.91	0.09	33,38,42,45	0
3	SO4	C	601	5/5	0.98	0.05	26,26,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.