



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:44 am GMT

PDB ID : 3QYN
Title : Structure of p63 DNA Binding Domain in Complex with a 22 Base Pair A/T Rich Response Element Containing 2 Base Pair Spacer Between Half Sites
Authors : Chen, C.; Herzberg, O.
Deposited on : 2011-03-03
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

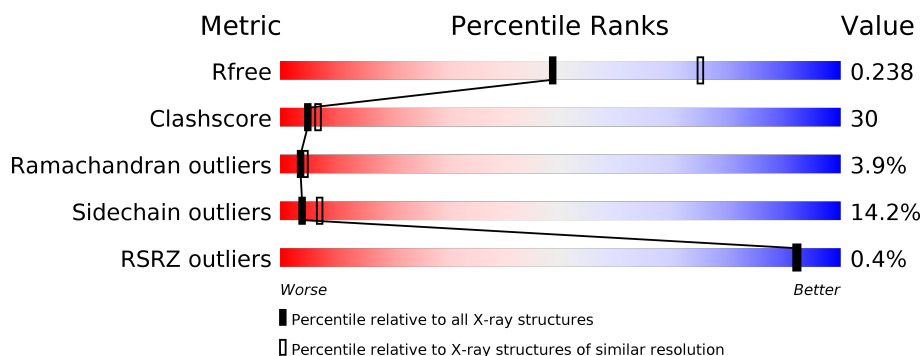
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	203	<div> <div>42%</div> <div>38%</div> <div>15%</div> <div>.</div> </div>
1	B	203	<div> <div>59%</div> <div>30%</div> <div>6%</div> <div>5%</div> </div>
1	C	203	<div> <div>%</div> <div>52%</div> <div>37%</div> <div>6%</div> <div>.</div> </div>
1	D	203	<div> <div>61%</div> <div>28%</div> <div>.</div> <div>6%</div> </div>
2	E	22	<div> <div>5%</div> <div>55%</div> <div>41%</div> </div>
2	F	22	<div> <div>14%</div> <div>55%</div> <div>32%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	901	-	-	-	X
3	ZN	B	901	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7333 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 Tumor protein 63.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1501	938	266	285	12			
1	B	193	Total	C	N	O	S	0	0	0
			1490	934	262	281	13			
1	C	196	Total	C	N	O	S	0	0	0
			1508	945	263	288	12			
1	D	190	Total	C	N	O	S	0	0	0
			1467	921	255	278	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	EXPRESSION TAG	UNP Q9H3D4
A	122	SER	-	EXPRESSION TAG	UNP Q9H3D4
A	123	HIS	-	EXPRESSION TAG	UNP Q9H3D4
A	124	MET	-	EXPRESSION TAG	UNP Q9H3D4
A	125	ALA	-	EXPRESSION TAG	UNP Q9H3D4
A	126	SER	-	EXPRESSION TAG	UNP Q9H3D4
B	121	GLY	-	EXPRESSION TAG	UNP Q9H3D4
B	122	SER	-	EXPRESSION TAG	UNP Q9H3D4
B	123	HIS	-	EXPRESSION TAG	UNP Q9H3D4
B	124	MET	-	EXPRESSION TAG	UNP Q9H3D4
B	125	ALA	-	EXPRESSION TAG	UNP Q9H3D4
B	126	SER	-	EXPRESSION TAG	UNP Q9H3D4
C	121	GLY	-	EXPRESSION TAG	UNP Q9H3D4
C	122	SER	-	EXPRESSION TAG	UNP Q9H3D4
C	123	HIS	-	EXPRESSION TAG	UNP Q9H3D4
C	124	MET	-	EXPRESSION TAG	UNP Q9H3D4
C	125	ALA	-	EXPRESSION TAG	UNP Q9H3D4
C	126	SER	-	EXPRESSION TAG	UNP Q9H3D4
D	121	GLY	-	EXPRESSION TAG	UNP Q9H3D4
D	122	SER	-	EXPRESSION TAG	UNP Q9H3D4
D	123	HIS	-	EXPRESSION TAG	UNP Q9H3D4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	124	MET	-	EXPRESSION TAG	UNP Q9H3D4
D	125	ALA	-	EXPRESSION TAG	UNP Q9H3D4
D	126	SER	-	EXPRESSION TAG	UNP Q9H3D4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	22	Total	C	N	O	P	0	0	0
			448	218	79	130	21			
2	F	22	Total	C	N	O	P	0	0	0
			448	218	79	130	21			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

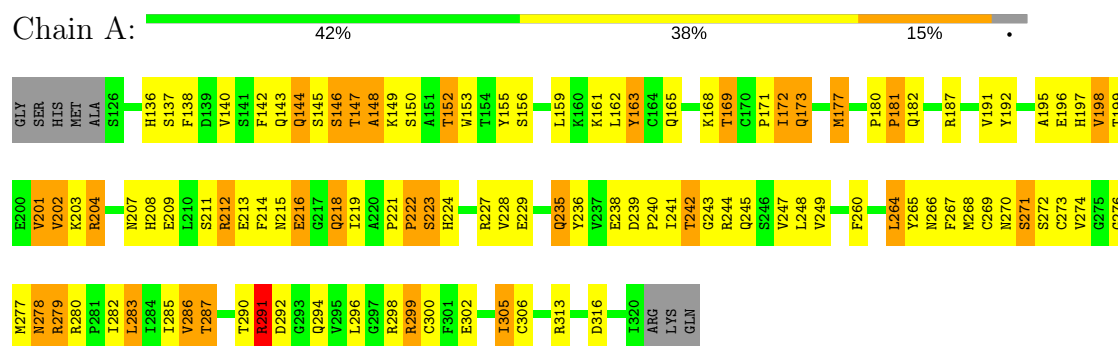
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	115	Total	O	0	0
			115	115		
4	C	72	Total	O	0	0
			72	72		
4	D	127	Total	O	0	0
			127	127		
4	E	30	Total	O	0	0
			30	30		
4	F	36	Total	O	0	0
			36	36		

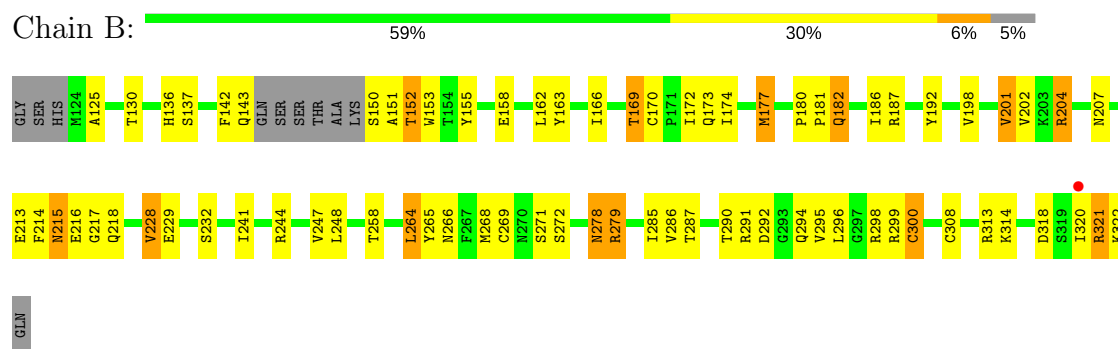
3 Residue-property plots

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

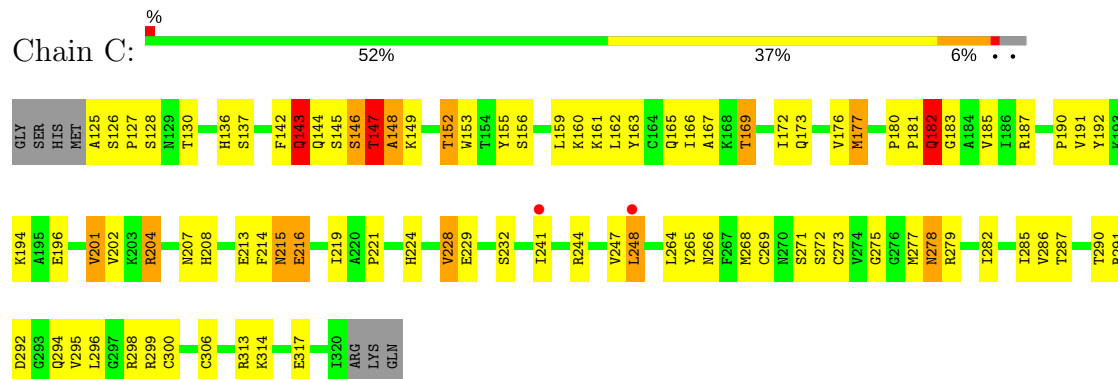
• Molecule 1: Tumor protein 63



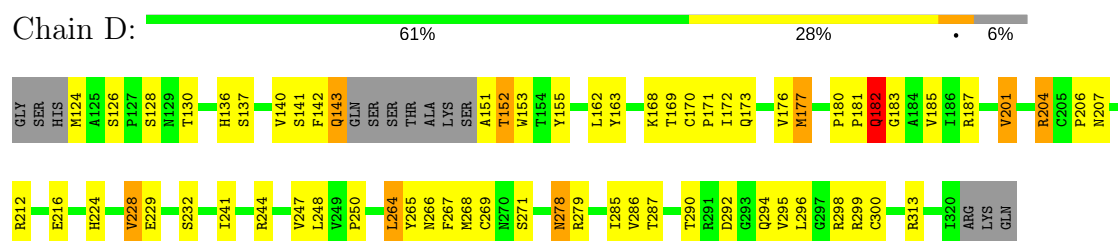
• Molecule 1: Tumor protein 63



• Molecule 1: Tumor protein 63



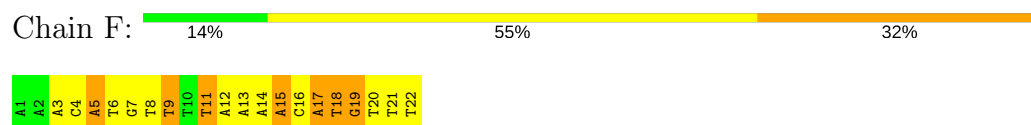
- Molecule 1: Tumor protein 63



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	140.98Å 140.98Å 119.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.05 – 2.50 85.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.05-2.50) 99.9 (85.35-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.210 , 0.245 0.203 , 0.238	Depositor DCC
R_{free} test set	2385 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7333	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: 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	0.60	1/1537 (0.1%)	0.78	0/2092
1	B	0.54	1/1525 (0.1%)	0.73	0/2072
1	C	0.56	1/1544 (0.1%)	0.73	0/2103
1	D	0.53	0/1502	0.72	0/2045
2	E	1.03	0/502	1.82	16/773 (2.1%)
2	F	0.99	0/502	1.83	18/773 (2.3%)
All	All	0.64	3/7112 (0.0%)	0.99	34/9858 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	CYS	CB-SG	-6.50	1.71	1.82
1	C	273	CYS	CB-SG	-5.79	1.72	1.81
1	B	300	CYS	CB-SG	-5.48	1.72	1.81

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	DA	O4'-C1'-N9	-10.04	100.97	108.00
2	E	5	DA	O4'-C1'-N9	-8.49	102.06	108.00
2	E	8	DT	O4'-C1'-N1	-7.86	102.50	108.00
2	F	15	DA	O4'-C1'-C2'	-7.82	99.65	105.90
2	E	9	DT	C4'-C3'-C2'	-7.71	96.16	103.10

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	1501	0	1453	126	0
1	B	1490	0	1448	71	0
1	C	1508	0	1466	84	0
1	D	1467	0	1416	60	0
2	E	448	0	253	35	0
2	F	448	0	253	26	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	87	0	0	13	0
4	B	115	0	0	15	0
4	C	72	0	0	15	0
4	D	127	0	0	14	0
4	E	30	0	0	8	0
4	F	36	0	0	4	0
All	All	7333	0	6289	396	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 30.

The worst 5 of 396 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:C:287:THR:HG22	4:C:462:HOH:O	1.34	1.24
2:E:13:DA:H1'	4:E:436:HOH:O	1.05	1.22
1:C:161:LYS:HB3	4:C:459:HOH:O	1.44	1.16
1:D:290:THR:HG22	1:D:294:GLN:H	1.12	1.15
1:B:290:THR:HG22	1:B:294:GLN:H	1.14	1.13

There are no symmetry-related clashes.

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	193/203 (95%)	161 (83%)	19 (10%)	13 (7%)	1	1
1	B	189/203 (93%)	176 (93%)	7 (4%)	6 (3%)	5	6
1	C	194/203 (96%)	177 (91%)	9 (5%)	8 (4%)	3	4
1	D	186/203 (92%)	176 (95%)	7 (4%)	3 (2%)	11	19
All	All	762/812 (94%)	690 (91%)	42 (6%)	30 (4%)	3	4

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	149	LYS
1	A	181	PRO
1	A	216	GLU
1	B	125	ALA

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	166/179 (93%)	136 (82%)	30 (18%)	2	3
1	B	165/179 (92%)	145 (88%)	20 (12%)	6	11
1	C	168/179 (94%)	143 (85%)	25 (15%)	3	6
1	D	162/179 (90%)	143 (88%)	19 (12%)	6	12
All	All	661/716 (92%)	567 (86%)	94 (14%)	4	7

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	241	ILE
1	C	143	GLN
1	D	232	SER
1	B	248	LEU
1	B	286	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	266	ASN
1	C	182	GLN
1	D	218	GLN
1	B	215	ASN
1	D	224	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	195/203 (96%)	-0.47	0 100 100	28, 55, 96, 120	0
1	B	193/203 (95%)	-0.40	1 (0%) 90 91	31, 50, 94, 122	0
1	C	196/203 (96%)	-0.08	2 (1%) 82 83	36, 61, 107, 120	0
1	D	190/203 (93%)	-0.43	0 100 100	31, 59, 95, 114	0
2	E	22/22 (100%)	-0.71	0 100 100	34, 57, 67, 72	0
2	F	22/22 (100%)	-0.73	0 100 100	41, 54, 64, 70	0
All	All	818/856 (95%)	-0.36	3 (0%) 92 92	28, 56, 97, 122	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ILE	3.3
1	C	248	LEU	3.1
1	C	241	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	A	901	1/1	0.99	0.17	2.69	49,49,49,49	0
3	ZN	B	901	1/1	1.00	0.16	2.40	41,41,41,41	0
3	ZN	D	901	1/1	0.99	0.14	1.21	53,53,53,53	0
3	ZN	C	901	1/1	0.99	0.15	0.21	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.