



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2022 – 04:39 PM EDT

PDB ID : 7N5V
Title : ZBTB7A Zinc Finger Domain Bound to DNA Duplex Containing GGACCC
(Oligo 20)
Authors : Horton, J.R.; Ren, R.; Cheng, X.
Deposited on : 2021-06-06
Resolution : 3.08 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

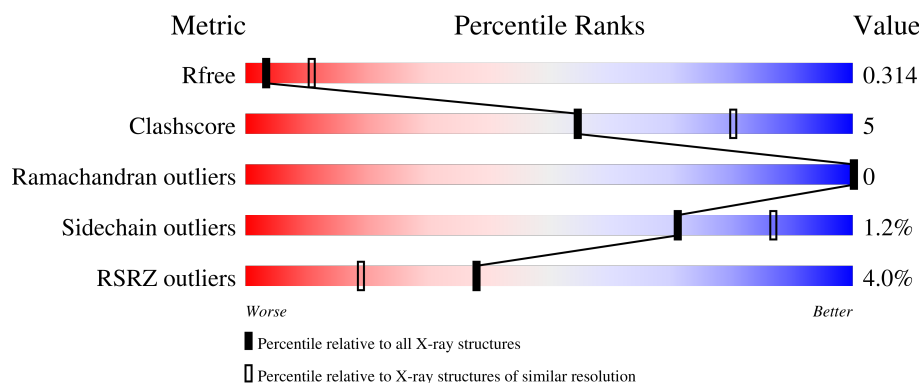
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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.




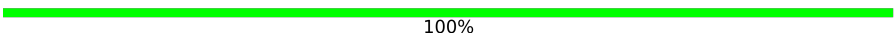
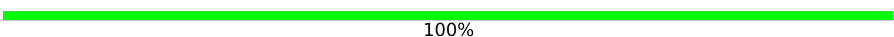
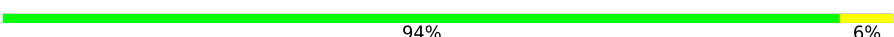
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	143	<div> <div>6%</div> <div>33%</div> <div>6%</div> <div>61%</div> </div>
1	B	143	<div> <div>64%</div> <div>15%</div> <div>21%</div> </div>
1	F	143	<div> <div>2%</div> <div>32%</div> <div>7%</div> <div>61%</div> </div>
2	D	16	<div> <div>6%</div> <div>50%</div> <div>50%</div> </div>
2	H	16	<div> <div>75%</div> <div>25%</div> </div>

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Mol	Chain	Length	Quality of chain
2	X	16	 6% 81% 19%
3	E	16	 100%
3	I	16	 100%
3	Y	16	 94% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3661 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 Zinc finger and BTB domain-containing protein 7A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	0	0
			430	268	89	68	5			
1	B	113	Total	C	N	O	S	0	0	0
			844	517	173	142	12			
1	F	56	Total	C	N	O	S	0	0	0
			431	271	86	69	5			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	GLY	-	expression tag	UNP O95365
A	366	PRO	-	expression tag	UNP O95365
A	367	LEU	-	expression tag	UNP O95365
A	368	GLY	-	expression tag	UNP O95365
A	501	LEU	-	expression tag	UNP O95365
A	502	GLU	-	expression tag	UNP O95365
A	503	ARG	-	expression tag	UNP O95365
A	504	PRO	-	expression tag	UNP O95365
A	505	HIS	-	expression tag	UNP O95365
A	506	ARG	-	expression tag	UNP O95365
A	507	ASP	-	expression tag	UNP O95365
B	365	GLY	-	expression tag	UNP O95365
B	366	PRO	-	expression tag	UNP O95365
B	367	LEU	-	expression tag	UNP O95365
B	368	GLY	-	expression tag	UNP O95365
B	501	LEU	-	expression tag	UNP O95365
B	502	GLU	-	expression tag	UNP O95365
B	503	ARG	-	expression tag	UNP O95365
B	504	PRO	-	expression tag	UNP O95365
B	505	HIS	-	expression tag	UNP O95365
B	506	ARG	-	expression tag	UNP O95365
B	507	ASP	-	expression tag	UNP O95365
F	365	GLY	-	expression tag	UNP O95365

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Chain	Residue	Modelled	Actual	Comment	Reference
F	366	PRO	-	expression tag	UNP O95365
F	367	LEU	-	expression tag	UNP O95365
F	368	GLY	-	expression tag	UNP O95365
F	501	LEU	-	expression tag	UNP O95365
F	502	GLU	-	expression tag	UNP O95365
F	503	ARG	-	expression tag	UNP O95365
F	504	PRO	-	expression tag	UNP O95365
F	505	HIS	-	expression tag	UNP O95365
F	506	ARG	-	expression tag	UNP O95365
F	507	ASP	-	expression tag	UNP O95365

- Molecule 2 is a DNA chain called DNA Strand I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	16	Total	C	N	O	P	0	0	0
			324	155	64	90	15			
2	H	16	Total	C	N	O	P	0	0	0
			324	155	64	90	15			
2	D	16	Total	C	N	O	P	0	0	0
			323	154	64	90	15			

- Molecule 3 is a DNA chain called DNA Strand II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	16	Total	C	N	O	P	0	0	0
			325	156	56	98	15			
3	I	16	Total	C	N	O	P	0	0	0
			325	157	56	97	15			
3	E	16	Total	C	N	O	P	0	0	0
			326	157	56	98	15			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	4	Total	Zn	0	0
			4	4		
4	F	2	Total	Zn	0	0
			2	2		

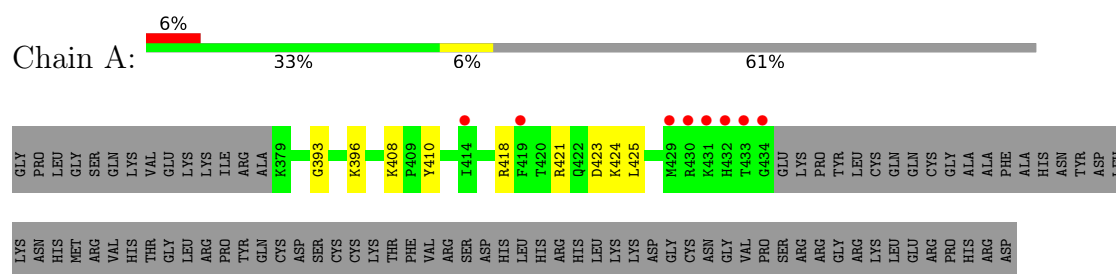
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		

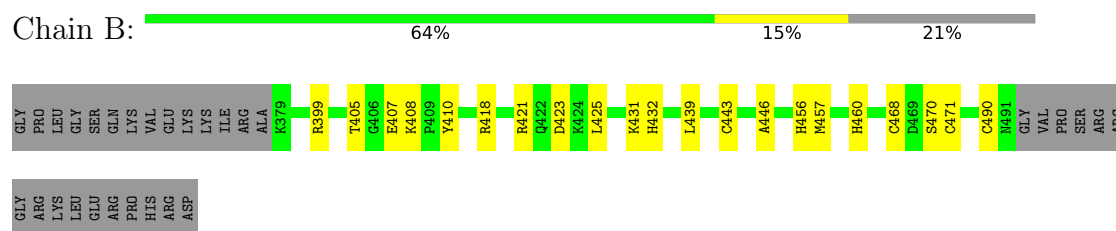
3 Residue-property plots

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.

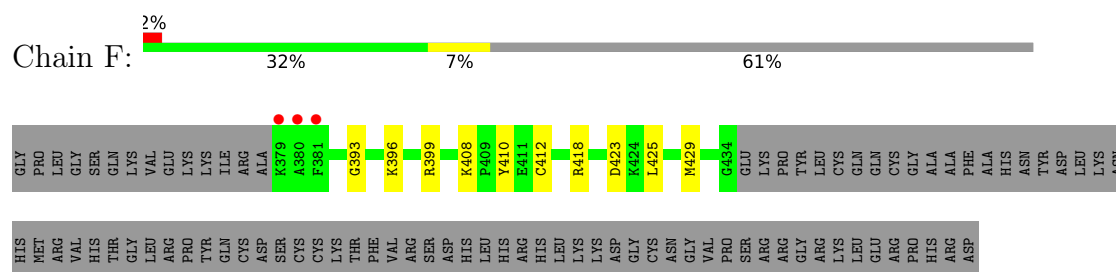
- Molecule 1: Zinc finger and BTB domain-containing protein 7A



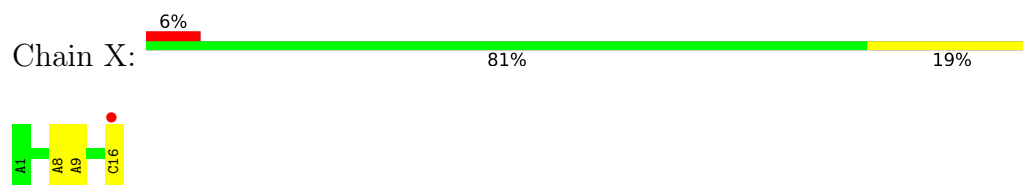
- Molecule 1: Zinc finger and BTB domain-containing protein 7A




- Molecule 1: Zinc finger and BTB domain-containing protein 7A

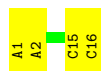


- Molecule 2: DNA Strand I



- Molecule 2: DNA Strand I

Chain H:  75% 25%



- Molecule 2: DNA Strand I

Chain D:  6% 50% 50%



- Molecule 3: DNA Strand II

Chain Y:  94% 6%



- Molecule 3: DNA Strand II

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA Strand II

Chain E:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.29Å 60.07Å 133.73Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	43.47 – 3.08 43.47 – 3.08	Depositor EDS
% Data completeness (in resolution range)	94.3 (43.47-3.08) 75.2 (43.47-3.08)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.260 , 0.314 0.260 , 0.314	Depositor DCC
R_{free} test set	723 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	1.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3661	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.88% 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	0.23	0/438	0.48	0/584
1	B	0.24	0/864	0.48	0/1162
1	F	0.24	0/440	0.47	0/588
2	D	0.56	0/362	0.86	0/554
2	H	0.56	0/364	0.84	0/559
2	X	0.54	0/364	0.86	0/559
3	E	0.54	0/364	0.95	0/561
3	I	0.55	0/363	0.96	0/559
3	Y	0.51	0/362	0.96	0/556
All	All	0.43	0/3921	0.76	0/5682

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	430	0	428	5	0
1	B	844	0	759	14	0
1	F	431	0	424	7	0
2	D	323	0	176	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	324	0	180	2	0
2	X	324	0	180	2	0
3	E	326	0	184	0	0
3	I	325	0	182	0	0
3	Y	325	0	180	2	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
4	F	2	0	0	0	0
5	B	1	0	0	0	0
All	All	3661	0	2693	32	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 5.

All (32) 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:B:399:ARG:NH2	2:D:12:DG:N7	2.29	0.79
1:B:471:CYS:HB3	1:B:490:CYS:SG	2.25	0.76
1:B:408:LYS:NZ	2:D:9:DA:OP1	2.35	0.60
2:H:1:DA:H2''	2:H:2:DA:H5''	1.85	0.59
1:B:431:LYS:NZ	2:D:7:DC:OP1	2.37	0.58
1:F:396:LYS:O	1:F:399:ARG:HG2	2.05	0.56
1:B:468:CYS:SG	1:B:470:SER:OG	2.64	0.53
1:B:408:LYS:HB2	1:B:418:ARG:HB3	1.92	0.52
1:F:393:GLY:HA3	1:F:396:LYS:HB2	1.90	0.52
1:B:410:TYR:HB3	1:B:425:LEU:HD22	1.90	0.52
1:A:423:ASP:OD1	1:A:423:ASP:N	2.43	0.51
1:F:408:LYS:HB3	1:F:418:ARG:HB3	1.93	0.50
1:B:423:ASP:N	1:B:423:ASP:OD1	2.45	0.50
1:F:410:TYR:HB3	1:F:425:LEU:HD22	1.94	0.49
1:F:412:CYS:HA	1:F:429:MET:HE1	1.92	0.49
2:H:15:DC:H4'	2:H:16:DC:OP1	2.12	0.49
1:A:410:TYR:HB3	1:A:425:LEU:HD22	1.94	0.49
2:D:4:DC:H2''	2:D:5:DA:C8	2.48	0.49
1:A:421:ARG:HB2	1:A:424:LYS:HG2	1.95	0.48
1:B:439:LEU:HA	1:B:446:ALA:HA	1.96	0.48
1:B:421:ARG:NH1	2:D:11:DG:N7	2.62	0.47
1:F:423:ASP:OD1	1:F:423:ASP:N	2.43	0.45
2:D:1:DA:H2''	2:D:2:DA:C8	2.52	0.45
1:A:408:LYS:HB3	1:A:418:ARG:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:NH2	1:B:423:ASP:OD2	2.49	0.44
1:B:443:CYS:HB3	1:B:460:HIS:CE1	2.53	0.44
1:B:443:CYS:SG	1:B:456:HIS:HE1	2.26	0.44
1:A:393:GLY:HA3	1:A:396:LYS:HB2	2.00	0.43
1:B:405:THR:HG23	1:B:407:GLU:H	1.86	0.41
2:X:8:DA:H2''	2:X:9:DA:C8	2.56	0.41
1:F:418:ARG:NH2	3:Y:2:DG:O3'	2.54	0.40
2:X:16:DC:O2	3:Y:2:DG:N2	2.54	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	54/143 (38%)	53 (98%)	1 (2%)	0	100	100
1	B	111/143 (78%)	102 (92%)	9 (8%)	0	100	100
1	F	54/143 (38%)	54 (100%)	0	0	100	100
All	All	219/429 (51%)	209 (95%)	10 (5%)	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	43/126 (34%)	43 (100%)	0	100	100
1	B	80/126 (64%)	78 (98%)	2 (2%)	47	74
1	F	43/126 (34%)	43 (100%)	0	100	100
All	All	166/378 (44%)	164 (99%)	2 (1%)	71	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	432	HIS
1	B	457	MET

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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

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	56/143 (39%)	0.43	8 (14%) 2 1	95, 138, 217, 245	0
1	B	113/143 (79%)	-0.10	0 100 100	90, 116, 163, 192	0
1	F	56/143 (39%)	0.28	3 (5%) 25 11	98, 132, 190, 217	0
2	D	16/16 (100%)	0.21	1 (6%) 20 8	108, 139, 176, 211	0
2	H	16/16 (100%)	0.18	0 100 100	113, 130, 164, 190	0
2	X	16/16 (100%)	0.59	1 (6%) 20 8	143, 173, 209, 217	0
3	E	16/16 (100%)	-0.00	0 100 100	96, 143, 160, 160	0
3	I	16/16 (100%)	0.21	0 100 100	104, 133, 162, 183	0
3	Y	16/16 (100%)	0.48	0 100 100	133, 161, 213, 216	0
All	All	321/525 (61%)	0.17	13 (4%) 38 19	90, 133, 195, 245	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	380	ALA	5.1
1	A	433	THR	4.5
1	A	434	GLY	3.9
1	A	429	MET	3.5
1	A	432	HIS	3.2
2	X	16	DC	3.0
1	F	381	PHE	2.7
2	D	1	DA	2.6
1	F	379	LYS	2.5
1	A	431	LYS	2.5
1	A	430	ARG	2.3
1	A	414	ILE	2.2
1	A	419	PHE	2.2

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 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(\AA^2)	Q<0.9
4	ZN	A	602	1/1	0.82	0.17	142,142,142,142	0
4	ZN	B	601	1/1	0.82	0.09	174,174,174,174	0
4	ZN	F	602	1/1	0.83	0.17	112,112,112,112	0
4	ZN	B	602	1/1	0.86	0.13	128,128,128,128	0
4	ZN	B	604	1/1	0.92	0.14	132,132,132,132	0
4	ZN	A	601	1/1	0.93	0.04	197,197,197,197	0
4	ZN	F	601	1/1	0.97	0.10	174,174,174,174	0
4	ZN	B	603	1/1	0.98	0.13	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.