



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2022 – 12:11 AM JST

PDB ID : 7EGT
Title : The crystal structure of the C-terminal domain of T. thermophilus UvrD complexed with the N-terminal domain of UvrB
Authors : Zheng, F.; Shen, L.; Li, L.; Zhang, Y.
Deposited on : 2021-03-26
Resolution : 2.58 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	:	2.27
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)	:	2.27

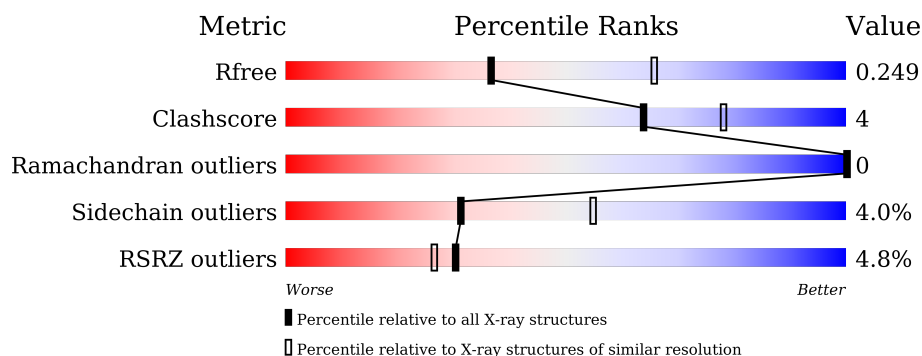
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	411	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	C	411	<div> <div>6%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	B	59	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
2	D	59	<div> <div>2%</div> <div>75%</div> <div>5%</div> <div>20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7297 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 UvrABC system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3258	2097	558	598	5			
1	C	409	Total	C	N	O	S	0	0	0
			3280	2109	564	601	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q56243
A	-1	MET	-	expression tag	UNP Q56243
A	0	ASP	-	expression tag	UNP Q56243
C	-2	ALA	-	expression tag	UNP Q56243
C	-1	MET	-	expression tag	UNP Q56243
C	0	ASP	-	expression tag	UNP Q56243

- Molecule 2 is a protein called DNA helicase UvrD.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	47	Total	C	N	O	0	0	0
			346	226	62	58			
2	D	47	Total	C	N	O	0	0	0
			350	228	62	60			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	634	ALA	-	expression tag	UNP O24736
B	635	MET	-	expression tag	UNP O24736
B	636	ASP	-	expression tag	UNP O24736
D	634	ALA	-	expression tag	UNP O24736
D	635	MET	-	expression tag	UNP O24736
D	636	ASP	-	expression tag	UNP O24736

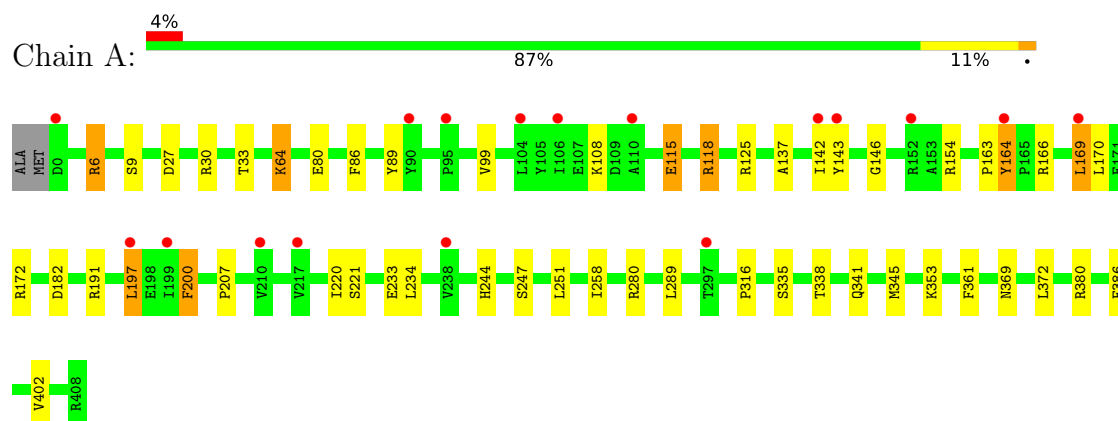
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	1	Total 1	O 1	0	0
3	C	30	Total 30	O 30	0	0
3	D	4	Total 4	O 4	0	0

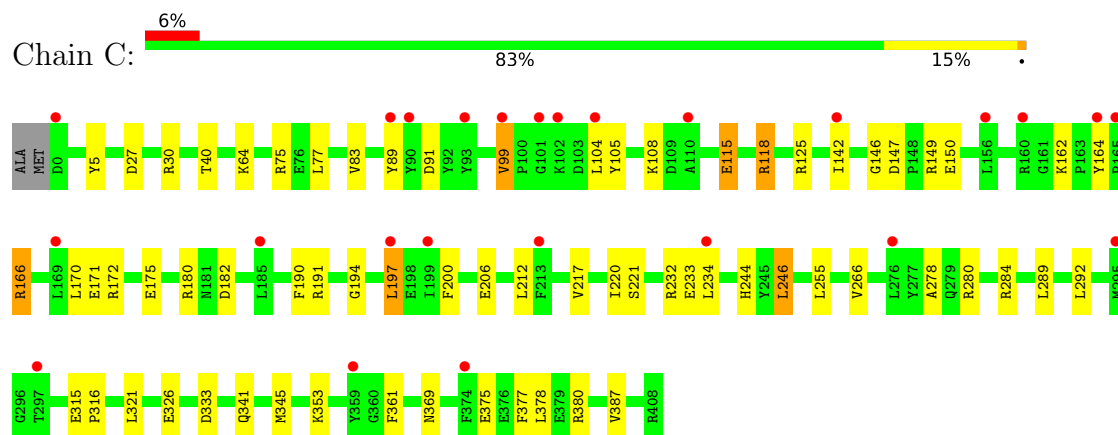
3 Residue-property plots

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.

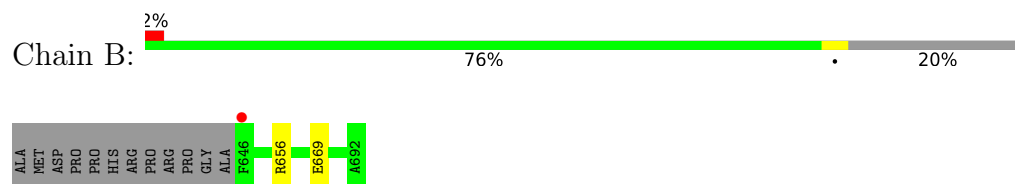
- Molecule 1: UvrABC system protein B



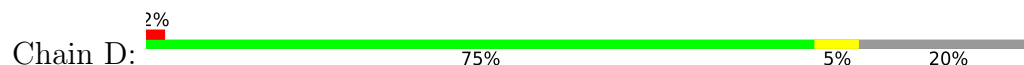
- Molecule 1: UvrABC system protein B



- Molecule 2: DNA helicase UvrD



- Molecule 2: DNA helicase UvrD



ALA	NEI	ASP	PRO	PRO	HIS	ARG	ARG	ARG	PRO	GLY	ALA	E646	E647	E650	E656	E692

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.33Å 114.61Å 125.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 2.58 46.17 – 2.58	Depositor EDS
% Data completeness (in resolution range)	97.5 (46.17-2.58) 97.9 (46.17-2.58)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.215 , 0.249 0.215 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7297	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1352e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.30	0/3336	0.51	2/4532 (0.0%)
1	C	0.31	0/3358	0.52	0/4558
2	B	0.32	0/355	0.52	0/479
2	D	0.31	0/359	0.48	0/484
All	All	0.30	0/7408	0.51	2/10053 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	TYR	N-CA-C	6.15	127.60	111.00
1	A	163	PRO	C-N-CA	5.04	134.29	121.70

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	3258	0	3212	25	0
1	C	3280	0	3246	35	0
2	B	346	0	340	2	0
2	D	350	0	344	2	0
3	A	28	0	0	0	0
3	B	1	0	0	0	0
3	C	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	0	0	0
All	All	7297	0	7142	61	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 4.

All (61) 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:154:ARG:NH2	1:A:247:SER:O	2.25	0.70
1:C:166:ARG:NH1	1:C:194:GLY:O	2.28	0.67
1:A:353:LYS:NZ	1:A:369:ASN:O	2.31	0.64
1:C:353:LYS:NZ	1:C:369:ASN:O	2.30	0.64
1:C:284:ARG:NH2	1:C:361:PHE:O	2.35	0.60
1:C:105:TYR:OH	1:C:284:ARG:NH1	2.35	0.59
1:A:143:TYR:OH	1:A:353:LYS:NZ	2.18	0.57
2:B:656:ARG:NH2	1:C:27:ASP:OD2	2.37	0.56
1:A:280:ARG:HD3	1:A:361:PHE:CE1	2.41	0.55
1:A:146:GLY:HA3	1:A:244:HIS:O	2.07	0.54
2:B:669:GLU:HG3	1:C:30:ARG:HD3	1.89	0.54
1:A:64:LYS:HD3	1:A:64:LYS:H	1.73	0.54
1:A:316:PRO:HG3	1:A:380:ARG:HH12	1.74	0.52
1:C:115:GLU:OE1	1:C:118:ARG:HD3	2.10	0.52
1:C:75:ARG:HG3	1:C:83:VAL:HB	1.92	0.52
1:A:86:PHE:HB3	1:A:137:ALA:HB2	1.92	0.51
1:C:170:LEU:HD21	1:C:197:LEU:HD11	1.93	0.51
1:A:341:GLN:O	1:A:345:MET:HG2	2.11	0.51
1:A:115:GLU:OE1	1:A:118:ARG:HD3	2.12	0.50
1:A:316:PRO:CG	1:A:380:ARG:HH12	2.24	0.50
2:D:647:ARG:N	2:D:650:GLU:OE1	2.36	0.50
1:C:220:ILE:HG22	1:C:234:LEU:HB2	1.92	0.49
1:A:164:TYR:CD1	1:A:169:LEU:HG	2.47	0.49
1:C:341:GLN:O	1:C:345:MET:HG2	2.12	0.49
1:C:280:ARG:HD3	1:C:361:PHE:CE1	2.47	0.49
1:C:182:ASP:HA	1:C:191:ARG:HD3	1.95	0.48
1:A:27:ASP:OD2	2:D:656:ARG:NH2	2.45	0.48
1:C:315:GLU:HG2	1:C:316:PRO:HD2	1.95	0.48
1:A:182:ASP:HA	1:A:191:ARG:HD3	1.95	0.48
1:C:30:ARG:NH1	1:C:378:LEU:O	2.37	0.48
1:A:6:ARG:NH1	1:A:80:GLU:OE2	2.47	0.47
1:C:316:PRO:HG3	1:C:380:ARG:HH12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:LEU:HD22	1:C:289:LEU:HB3	1.96	0.47
1:A:169:LEU:HD13	1:A:197:LEU:HD22	1.96	0.46
1:C:171:GLU:O	1:C:175:GLU:HG3	2.15	0.46
1:C:221:SER:HB3	1:C:233:GLU:OE2	2.15	0.46
1:C:99:VAL:HG13	1:C:104:LEU:HB3	1.98	0.46
1:A:166:ARG:O	1:A:170:LEU:HD12	2.16	0.45
1:A:221:SER:OG	1:A:233:GLU:OE2	2.25	0.45
1:C:89:TYR:CZ	1:C:108:LYS:HG3	2.52	0.45
1:A:258:ILE:HG21	1:A:289:LEU:HD21	1.99	0.44
1:C:180:ARG:HB2	1:C:190:PHE:CZ	2.52	0.44
1:A:335:SER:OG	1:A:386:PHE:HB3	2.17	0.44
1:A:33:THR:HB	1:A:402:VAL:HG22	2.00	0.44
1:C:266:VAL:HG13	1:C:278:ALA:HB1	2.00	0.44
1:C:99:VAL:CG1	1:C:104:LEU:HB3	2.47	0.43
1:C:147:ASP:OD1	1:C:149:ARG:HD3	2.18	0.43
1:C:5:TYR:CE1	1:C:77:LEU:HD22	2.54	0.43
1:A:220:ILE:HG22	1:A:234:LEU:HB2	1.99	0.43
1:C:146:GLY:HA3	1:C:244:HIS:O	2.18	0.42
1:C:150:GLU:HB3	1:C:246:LEU:HB3	2.01	0.42
1:C:64:LYS:HD3	1:C:91:ASP:HB3	2.00	0.42
1:C:206:GLU:OE2	1:C:232:ARG:NH1	2.52	0.42
1:A:89:TYR:CZ	1:A:108:LYS:HG2	2.55	0.42
1:A:142:ILE:HG23	1:A:372:LEU:HD12	2.02	0.41
1:C:142:ILE:HG12	1:C:377:PHE:CD2	2.55	0.41
1:C:375:GLU:OE1	1:C:375:GLU:N	2.47	0.41
1:C:375:GLU:H	1:C:375:GLU:CD	2.24	0.41
1:C:321:LEU:HD13	1:C:380:ARG:HB2	2.02	0.41
1:C:333:ASP:HA	1:C:387:VAL:HB	2.02	0.41
1:A:200:PHE:CZ	1:A:207:PRO:HD3	2.56	0.41

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	407/411 (99%)	400 (98%)	7 (2%)	0	100	100
1	C	407/411 (99%)	401 (98%)	6 (2%)	0	100	100
2	B	45/59 (76%)	45 (100%)	0	0	100	100
2	D	45/59 (76%)	45 (100%)	0	0	100	100
All	All	904/940 (96%)	891 (99%)	13 (1%)	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	337/353 (96%)	323 (96%)	14 (4%)	30	53
1	C	341/353 (97%)	325 (95%)	16 (5%)	26	48
2	B	32/45 (71%)	32 (100%)	0	100	100
2	D	33/45 (73%)	33 (100%)	0	100	100
All	All	743/796 (93%)	713 (96%)	30 (4%)	31	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	9	SER
1	A	30	ARG
1	A	64	LYS
1	A	99	VAL
1	A	115	GLU
1	A	118	ARG
1	A	125	ARG
1	A	169	LEU
1	A	172	ARG
1	A	197	LEU
1	A	200	PHE
1	A	251	LEU

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Mol	Chain	Res	Type
1	A	338	THR
1	C	40	THR
1	C	99	VAL
1	C	115	GLU
1	C	118	ARG
1	C	125	ARG
1	C	162	LYS
1	C	164	TYR
1	C	166	ARG
1	C	172	ARG
1	C	197	LEU
1	C	200	PHE
1	C	212	LEU
1	C	217	VAL
1	C	246	LEU
1	C	292	LEU
1	C	326	GLU

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	409/411 (99%)	0.32	17 (4%) 36 32	45, 59, 87, 98	0
1	C	409/411 (99%)	0.33	25 (6%) 21 17	43, 60, 92, 110	0
2	B	47/59 (79%)	0.10	1 (2%) 63 60	47, 56, 72, 78	0
2	D	47/59 (79%)	0.24	1 (2%) 63 60	48, 58, 76, 79	0
All	All	912/940 (97%)	0.31	44 (4%) 30 26	43, 59, 88, 110	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	4.5
1	C	164	TYR	4.2
1	C	104	LEU	3.9
1	C	297	THR	3.3
2	D	692	ALA	3.3
1	A	297	THR	3.3
1	C	213	PHE	3.3
2	B	646	PHE	3.1
1	A	169	LEU	2.9
1	A	104	LEU	2.9
1	C	374	PHE	2.8
1	C	0	ASP	2.8
1	C	185	LEU	2.8
1	C	110	ALA	2.7
1	C	359	TYR	2.7
1	C	101	GLY	2.6
1	C	99	VAL	2.6
1	C	160	ARG	2.6
1	A	95	PRO	2.5
1	A	238	VAL	2.5
1	C	169	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	164	TYR	2.5
1	A	197	LEU	2.4
1	A	143	TYR	2.4
1	C	142	ILE	2.4
1	A	110	ALA	2.4
1	A	90	TYR	2.3
1	C	199	ILE	2.3
1	A	106	ILE	2.2
1	C	165	PRO	2.2
1	C	89	TYR	2.2
1	A	0	ASP	2.2
1	C	234	LEU	2.1
1	A	210	VAL	2.1
1	C	102	LYS	2.1
1	C	197	LEU	2.1
1	A	152	ARG	2.1
1	A	217	VAL	2.1
1	A	199	ILE	2.1
1	C	295	MET	2.0
1	C	90	TYR	2.0
1	C	156	LEU	2.0
1	C	276	LEU	2.0
1	C	93	TYR	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.