

Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 11:33 AM EDT

PDB ID	:	2F6M
Title	:	Structure of a Vps23-C:Vps28-N subcomplex
Authors	:	Kostelansky, M.S.; Lee, S.; Kim, J.; Hurley, J.H.
Deposited on	:	2005-11-29
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) 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	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647(2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	А	65	20%	1.4%
		00	15%	
1	С	65	82%	12% • •
2	В	109	87%	10% ••
2	D	109	43%	12% • 6%

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-fi	t crite-
ria:														

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DDQ	С	105	-	-	-	Х
4	DDQ	С	108	-	-	-	Х



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2913 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 Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	65	Total	С	Ν	0	S	0	0	0
1	A		531	335	97	97	2	0		
1	C	62	Total	С	Ν	0	S	0	0	0
	U	03	516	326	95	93	2	0		0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	321	MET	-	cloning artifact	UNP P25604
А	344	ALA	CYS	engineered mutation	UNP P25604
С	321	MET	-	cloning artifact	UNP P25604
С	344	ALA	CYS	engineered mutation	UNP P25604

• Molecule 2 is a protein called Vacuolar protein sorting-associated protein VPS28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	107	Total C N O S 874 552 140 181 1	0	0	0
2	D	102	Total C N O 839 532 135 172	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	10	GLY	-	cloning artifact	UNP Q02767
В	11	ALA	-	cloning artifact	UNP Q02767
В	12	MET	-	cloning artifact	UNP Q02767
В	101	ALA	CYS	engineered mutation	UNP Q02767
D	10	GLY	-	cloning artifact	UNP Q02767
D	11	ALA	-	cloning artifact	UNP Q02767
D	12	MET	-	cloning artifact	UNP Q02767



Chain	Residue	Modelled	Actual	Comment	Reference
D	101	ALA	CYS	engineered mutation	UNP Q02767

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0

• Molecule 4 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: C₁₂H₂₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	Δ	1	Total	С	Ν	Ο	0	0
4	A	1	14	12	1	1	0	0
4	Λ	1	Total	С	Ν	Ο	0	0
4	Л	1	14	12	1	1	0	0
4	Δ	1	Total	С	Ν	Ο	0	0
4	Л	T	14	12	1	1	0	0
4	В	1	Total	С	Ν	Ο	0	0
4	D	T	14	12	1	1	0	0
4	В	1	Total	С	Ν	Ο	0	0
T	D	1	14	12	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
4	U	I	14	12	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
4			14	12	1	1	U	



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C 19	N 1	0	0	0
			14	12	T	1		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	11	Total O 11 11	0	0
5	В	9	Total O 9 9	0	0
5	С	16	Total O 16 16	0	0
5	D	4	Total O 4 4	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.

 \bullet Molecule 1: Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease



• Molecule 1: Suppressor protein STP22 of temperature-sensitive alpha-factor receptor and arginine permease



• Molecule 2: Vacuolar protein sorting-associated protein VPS28



• Molecule 2: Vacuolar protein sorting-associated protein VPS28





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants	61.24Å 119.25Å 125.39Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	19.51 - 2.10	Depositor
Resolution (A)	19.51 - 2.10	EDS
% Data completeness	100.0 (19.51-2.10)	Depositor
(in resolution range)	97.5(19.51-2.10)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	4.67 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.241 , 0.261	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.241 , 0.227	DCC
R_{free} test set	1318 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	46.1	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.34, 77.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2913	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	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 22.40 % 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 5.7495e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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: MG, DDQ

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).

Mal	Chain	Bond	lengths	Bond angles	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/540	0.50	0/730
1	С	0.38	0/525	0.55	0/711
2	В	0.35	0/887	0.45	0/1198
2	D	0.38	0/852	0.45	0/1153
All	All	0.38	0/2804	0.48	0/3792

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	А	531	0	537	7	0
1	С	516	0	521	12	0
2	В	874	0	855	7	0
2	D	839	0	823	10	0
3	А	1	0	0	0	0
4	А	42	0	81	3	0
4	В	28	0	54	1	0
4	С	28	0	54	0	0
4	D	14	0	27	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	А	11	0	0	0	0
5	В	9	0	0	0	0
5	С	16	0	0	0	0
5	D	4	0	0	0	0
All	All	2913	0	2952	30	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 (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:327:GLN:HE22	2:D:22:VAL:H	1.22	0.87
1:A:341:THR:HG21	4:A:101:DDQ:CM2	2.06	0.86
1:C:379:ARG:NH1	2:D:23:PRO:O	2.19	0.76
1:C:349:LEU:HD11	2:D:62:ILE:HD11	1.72	0.71
2:B:112:ILE:O	2:B:116:GLU:HG2	1.95	0.67
1:A:378:GLN:HG2	4:B:119:DDQ:H42	1.78	0.66
1:A:341:THR:HG21	4:A:101:DDQ:HM22	1.78	0.65
1:C:356:LEU:HD22	2:D:62:ILE:HG12	1.79	0.64
2:D:86:ASN:HB3	2:D:89:GLU:HB2	1.82	0.61
1:C:348:MET:HE2	1:C:353:THR:HG22	1.84	0.58
1:C:323:ASP:HB3	2:D:21:GLU:HG3	1.87	0.55
1:C:348:MET:HE3	1:C:353:THR:HG21	1.90	0.54
1:A:341:THR:HG21	4:A:101:DDQ:HM23	1.92	0.51
1:A:346:SER:O	1:A:350:HIS:CD2	2.64	0.50
2:D:108:ALA:O	2:D:112:ILE:HG12	2.13	0.49
1:C:348:MET:CE	1:C:353:THR:CG2	2.91	0.49
1:C:343:GLU:O	1:C:347:ARG:HG2	2.12	0.48
2:B:36:VAL:HG22	2:B:85:GLN:HB3	1.96	0.48
1:A:346:SER:O	1:A:350:HIS:HD2	1.96	0.47
1:C:348:MET:HE3	1:C:353:THR:CG2	2.45	0.46
1:C:348:MET:CE	1:C:353:THR:HG22	2.46	0.46
1:A:356:LEU:HD22	2:B:62:ILE:HG21	1.99	0.44
2:D:94:PHE:HE1	2:D:104:TYR:HE1	1.66	0.43
2:B:108:ALA:O	2:B:112:ILE:HG12	2.19	0.43
1:C:343:GLU:OE2	1:C:347:ARG:HD3	2.20	0.42
2:D:36:VAL:HG13	2:D:90:ILE:HG22	2.02	0.41
2:D:113:THR:O	2:D:116:GLU:HG2	2.19	0.41
2:B:25:PHE:CE1	2:B:34:LYS:HE3	2.55	0.41
2:B:50:LEU:HD22	2:B:54:GLU:HG2	2.02	0.41



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:C	2:B:87:LYS:H	2.23	0.41

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	А	63/65~(97%)	61 (97%)	0	2(3%)	4 1
1	С	61/65~(94%)	61~(100%)	0	0	100 100
2	В	105/109~(96%)	100 (95%)	5 (5%)	0	100 100
2	D	100/109~(92%)	91~(91%)	9~(9%)	0	100 100
All	All	329/348~(94%)	313~(95%)	14 (4%)	2(1%)	25 21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	384	LEU
1	А	383	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	58/58~(100%)	56~(97%)	2(3%)	37 39



Mol	Chain	Analysed	Rotameric	Outliers	Percent	tiles
1	С	56/58~(97%)	53~(95%)	3~(5%)	22	20
2	В	101/101~(100%)	99~(98%)	2(2%)	55	60
2	D	97/101~(96%)	94~(97%)	3(3%)	40	43
All	All	312/318~(98%)	302~(97%)	10 (3%)	39	41

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All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	357	ASP
1	А	372	LEU
2	В	16	GLN
2	В	50	LEU
1	С	347	ARG
1	С	353	THR
1	С	372	LEU
2	D	54	GLU
2	D	62	ILE
2	D	94	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	326	ASN
1	А	350	HIS
2	В	19	HIS
2	В	105	ASN
1	С	326	ASN
1	С	327	GLN
1	С	330	ASN

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 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).

Mal	Turne	Chain	Dec	Tink	Bo	Bond lengths		B	ond ang	les
	туре	Unain	nes		Counts	RMSZ	$RMSZ \mid \# Z > 2 \mid$		RMSZ	# Z > 2
4	DDQ	А	101	-	10, 13, 13	0.63	0	$12,\!15,\!15$	0.65	0
4	DDQ	С	105	-	10,13,13	0.68	1 (10%)	12,15,15	0.71	0
4	DDQ	А	102	-	10,13,13	0.60	0	12,15,15	0.60	0
4	DDQ	D	119	-	10,13,13	0.67	0	12,15,15	0.61	0
4	DDQ	А	104	-	10,13,13	0.71	1 (10%)	12,15,15	0.60	0
4	DDQ	В	120	-	10,13,13	0.69	1 (10%)	12,15,15	0.55	0
4	DDQ	С	108	-	10,13,13	0.78	1 (10%)	12,15,15	0.69	0
4	DDQ	В	119	-	10,13,13	0.68	1 (10%)	12,15,15	0.69	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DDQ	А	101	-	-	4/11/11/11	-
4	DDQ	С	105	-	-	6/11/11/11	-
4	DDQ	А	102	-	-	4/11/11/11	-
4	DDQ	D	119	-	-	3/11/11/11	-
4	DDQ	А	104	-	-	5/11/11/11	-
4	DDQ	В	120	-	-	8/11/11/11	-
4	DDQ	С	108	-	-	9/11/11/11	-
4	DDQ	В	119	-	-	2/11/11/11	-



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	С	108	DDQ	01-N1	2.22	1.47	1.42
4	А	104	DDQ	01-N1	2.11	1.47	1.42
4	В	119	DDQ	O1-N1	2.07	1.47	1.42
4	В	120	DDQ	01-N1	2.06	1.46	1.42
4	С	105	DDQ	01-N1	2.04	1.46	1.42

All (5) bond length outliers are listed below:

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	101	DDQ	C2-C1-N1-CM1
4	А	102	DDQ	N1-C1-C2-C3
4	А	104	DDQ	C2-C1-N1-CM1
4	А	104	DDQ	C2-C1-N1-CM2
4	В	120	DDQ	C2-C1-N1-CM2
4	С	108	DDQ	C2-C1-N1-CM2
4	С	108	DDQ	C5-C6-C7-C8
4	А	101	DDQ	C2-C3-C4-C5
4	С	105	DDQ	C5-C6-C7-C8
4	D	119	DDQ	C3-C4-C5-C6
4	С	108	DDQ	C3-C4-C5-C6
4	D	119	DDQ	C4-C5-C6-C7
4	D	119	DDQ	C5-C6-C7-C8
4	С	108	DDQ	C2-C3-C4-C5
4	А	102	DDQ	C4-C5-C6-C7
4	С	105	DDQ	C1-C2-C3-C4
4	С	105	DDQ	C2-C3-C4-C5
4	А	102	DDQ	C7-C8-C9-C10
4	А	104	DDQ	C7-C8-C9-C10
4	С	105	DDQ	C4-C5-C6-C7
4	А	104	DDQ	C3-C4-C5-C6
4	А	101	DDQ	C3-C4-C5-C6
4	В	120	DDQ	C3-C4-C5-C6
4	A	101	DDQ	C2-C1-N1-CM2
4	В	120	DDQ	C2-C1-N1-CM1
4	С	108	DDQ	C2-C1-N1-CM1
4	С	108	DDQ	C2-C1-N1-O1
4	В	120	DDQ	C6-C7-C8-C9
4	С	108	DDQ	C4-C5-C6-C7
4	С	105	DDQ	C6-C7-C8-C9



Mol	Chain	Res	Type	Atoms
4	В	120	DDQ	C2-C3-C4-C5
4	С	108	DDQ	C1-C2-C3-C4
4	В	119	DDQ	C7-C8-C9-C10
4	С	105	DDQ	C7-C8-C9-C10
4	С	108	DDQ	C7-C8-C9-C10
4	А	102	DDQ	C2-C1-N1-CM2
4	В	120	DDQ	C7-C8-C9-C10
4	В	120	DDQ	C1-C2-C3-C4
4	В	120	DDQ	C4-C5-C6-C7
4	В	119	DDQ	C3-C4-C5-C6
4	А	104	DDQ	C2-C1-N1-O1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	101	DDQ	3	0
4	В	119	DDQ	1	0

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, 95^{th} 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	2	$OWAB(Å^2)$	Q<0.9
1	А	65/65~(100%)	1.22	13 (20%) 1	1	53, 57, 64, 75	0
1	С	63/65~(96%)	1.07	10 (15%) 1	2	54, 57, 64, 68	0
2	В	107/109~(98%)	1.67	33 (30%) 0	0	53, 58, 61, 69	0
2	D	102/109~(93%)	2.27	47 (46%) 0	0	52, 58, 62, 63	0
All	All	337/348~(96%)	1.65	103 (30%) 0	0	52, 58, 63, 75	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	384	LEU	11.0
2	В	86	ASN	8.7
2	В	12	MET	8.3
2	D	83	ASN	7.7
2	D	97	ILE	7.6
2	D	95	GLN	7.5
2	D	88	GLU	7.2
2	D	85	GLN	7.2
1	А	385	SER	6.9
2	D	92	LYS	6.7
2	D	94	PHE	6.6
2	D	84	SER	5.8
2	D	102	ASP	5.6
2	В	85	GLN	5.4
2	D	27	ASN	5.1
2	В	13	ASP	5.1
2	D	89	GLU	5.0
2	В	118	GLY	4.8
1	С	383	PRO	4.7
1	А	377	ILE	4.6
2	В	53	VAL	4.6



Mol	Chain	Res	Type	RSRZ	
2	В	95	GLN	4.6	
2	В	91	ASN	4.4	
2	D	60	ASP	4.4	
2	D	117	ARG	4.4	
2	D	96	SER	4.3	
2	D	53	VAL	4.2	
2	D	90	ILE	4.0	
2	D	40	LEU	3.9	
2	D	82	LEU	3.9	
2	D	93	HIS	3.9	
1	С	331	LEU	3.9	
2	В	57	TYR	3.9	
2	В	88	GLU	3.8	
2	D	107	THR	3.7	
2	D	113	THR	3.7	
2	В	102	ASP	3.6	
2	В	50	LEU	3.5	
2	В	65	THR	3.4	
2	D	116	GLU	3.4	
1	А	383	PRO	3.3	
1	С	377	ILE	3.3	
2	D	16	GLN	3.3	
2	D	79	LYS	3.2	
1	А	336	TYR	3.2	
2	D	98	GLU	3.2	
2	D	109	SER	3.2	
1	С	328	LEU	3.2	
2	D	44	TYR	3.0	
2	В	66	GLN	3.0	
1	А	371	PHE	3.0	
2	B	46	ILE	3.0	
2	D	100	PHE	3.0	
2	В	60	ASP	2.9	
2	В	71	VAL	2.9	
2	D	36	VAL	2.9	
2	D	87	LYS	2.9	
2	D	17	LEU	2.9	
2	В	18	PHE	2.8	
2	B	99	ALA	2.8	
2	D	72	ASP	2.8	
2	В	76	LYS	2.8	
2	В	94	PHE	2.8	



Mol	Chain	Res	Type	RSRZ	
2	D	99 ALA		2.7	
1	А	380	ILE	2.7	
2	В	43	ILE	2.7	
2	D	58 LEU		2.6	
2	D	101	ALA	2.6	
2	В	83	ASN	2.6	
1	А	375	TRP	2.6	
2	В	28	SER	2.5	
2	D	91	ASN	2.5	
1	С	321	MET	2.5	
2	В	82	LEU	2.5	
2	В	27	ASN	2.5	
2	D	37	ILE	2.4	
2	D	49	THR	2.4	
1	С	373	VAL	2.4	
2	В	49	THR	2.4	
2	D	46	ILE	2.4	
2	D	64	ASP	2.4	
2	В	69	ASN	2.4	
2	D	112	ILE	2.4	
2	D	20	ASP	2.4	
1	С	371	PHE	2.3	
2	D	56	ALA	2.3	
2	В	74	LEU	2.3	
1	С	323	ASP	2.3	
2	D	50	LEU	2.3	
1	А	331	LEU	2.2	
2	В	47	VAL	2.2	
2	D	48	ILE	2.2	
2	В	108	ALA	2.2	
1	А	372	LEU	2.2	
1	А	373	VAL	2.2	
2	D	47	VAL	2.1	
1	А	322	THR	2.1	
2	В	98	GLU	2.1	
2	В	87	LYS	2.1	
2	D	32	LYS	2.1	
1	А	349	LEU	2.0	
1	С	332	VAL	2.0	
1	С	368	ARG	2.0	

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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, 95^{th} 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
4	DDQ	С	105	14/14	-0.14	0.53	75,81,87,87	0
4	DDQ	С	108	14/14	0.11	0.49	100,103,106,106	0
4	DDQ	В	119	14/14	0.51	0.36	64,71,80,80	0
4	DDQ	В	120	14/14	0.53	0.30	74,75,79,79	0
4	DDQ	D	119	14/14	0.54	0.29	71,73,76,76	0
4	DDQ	А	102	14/14	0.57	0.27	$57,\!60,\!72,\!73$	0
4	DDQ	А	104	14/14	0.62	0.30	83,86,91,91	0
4	DDQ	А	101	14/14	0.80	0.23	70,73,79,79	0
3	MG	A	109	1/1	0.94	0.40	62,62,62,62	1

6.5 Other polymers (i)

There are no such residues in this entry.

