



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:59 AM UTC

PDB ID : 2C0F / pdb_00002c0f
Title : Structure of Wind Y53F mutant
Authors : Sevvana, M.; Ma, Q.; Barnewitz, K.; Guo, C.; Soling, H.-D.; Ferrari, D.M.;
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Deposited on : 2005-09-02
Resolution : 2.28 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
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

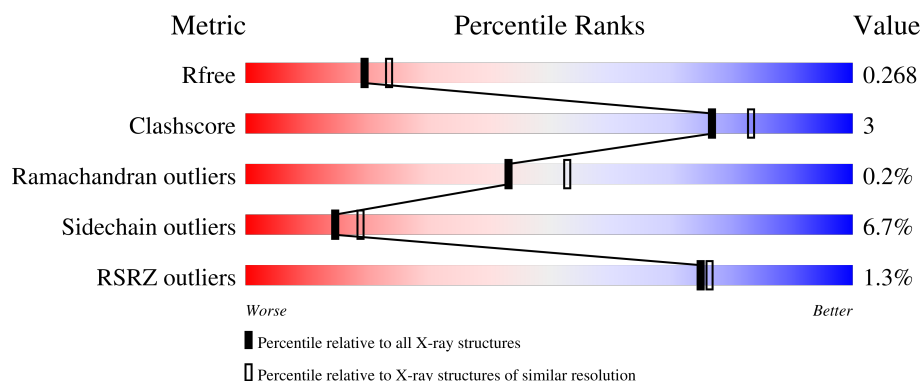
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	248	67% 21% 8%
1	B	248	2% 70% 17% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3353 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 WINDBEUTEL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1677	1083	279	311	4			
1	B	223	Total	C	N	O	S	0	0	0
			1578	1013	264	297	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	PHE	TYR	engineered mutation	UNP O44342
B	53	PHE	TYR	engineered mutation	UNP O44342

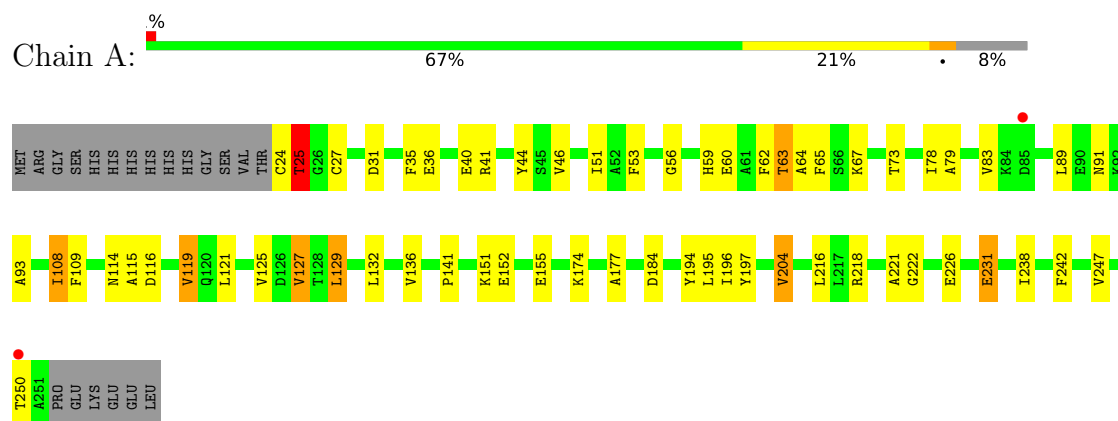
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total	O	0	0
			73	73		
2	B	25	Total	O	0	0
			25	25		

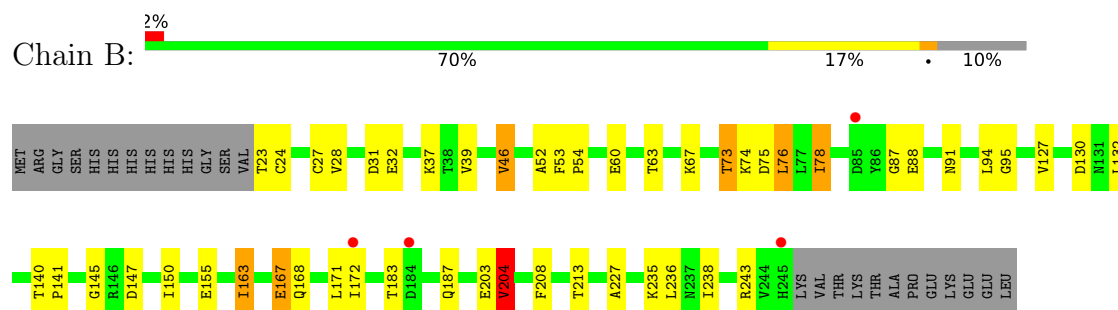
3 Residue-property plots

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: WINDBEUTEL PROTEIN



• Molecule 1: WINDBEUTEL PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.44Å 51.72Å 100.66Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	20.24 – 2.28 20.24 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.24-2.28) 91.9 (20.24-2.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.281 0.216 , 0.268	Depositor DCC
R_{free} test set	4284 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3353	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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

5.1 Standard geometry

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	1.92	35/1708 (2.0%)	1.61	26/2314 (1.1%)
1	B	1.69	18/1609 (1.1%)	1.56	17/2180 (0.8%)
All	All	1.81	53/3317 (1.6%)	1.59	43/4494 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	ALA	CA-CB	7.44	1.65	1.53
1	A	238	ILE	CA-CB	7.28	1.62	1.54
1	B	204	VAL	CA-CB	7.27	1.63	1.54
1	A	196	ILE	CA-CB	7.04	1.63	1.54
1	A	226	GLU	CA-C	6.88	1.61	1.52
1	B	235	LYS	N-CA	6.77	1.54	1.46
1	A	125	VAL	CA-CB	6.60	1.61	1.53
1	A	109	PHE	N-CA	6.41	1.53	1.46
1	B	39	VAL	CA-CB	6.33	1.63	1.54
1	A	136	VAL	CA-CB	6.26	1.61	1.54
1	A	79	ALA	CA-CB	6.22	1.65	1.54
1	A	194	TYR	C-O	-6.17	1.17	1.24
1	B	150	ILE	CA-CB	6.06	1.61	1.54
1	A	247	VAL	N-CA	5.99	1.52	1.46
1	B	127	VAL	CA-CB	5.90	1.62	1.54
1	A	108	ILE	N-CA	5.89	1.53	1.46
1	A	204	VAL	CA-CB	5.88	1.61	1.54
1	A	64	ALA	C-O	-5.87	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ILE	CA-CB	5.78	1.62	1.54
1	A	67	LYS	N-CA	5.76	1.53	1.46
1	A	83	VAL	CA-CB	5.75	1.60	1.54
1	A	56	GLY	C-O	-5.73	1.18	1.23
1	B	172	ILE	CA-CB	5.60	1.61	1.54
1	A	46	VAL	CA-CB	5.59	1.61	1.54
1	A	93	ALA	CA-CB	5.58	1.62	1.53
1	A	247	VAL	CA-CB	5.51	1.60	1.54
1	A	197	TYR	N-CA	5.49	1.53	1.46
1	B	76	LEU	N-CA	5.47	1.52	1.46
1	A	125	VAL	CA-C	5.44	1.58	1.52
1	A	221	ALA	CA-C	5.44	1.60	1.52
1	B	145	GLY	N-CA	5.39	1.50	1.44
1	A	222	GLY	C-O	5.37	1.29	1.23
1	B	243	ARG	N-CA	5.35	1.52	1.46
1	A	141	PRO	CA-C	5.32	1.57	1.52
1	A	152	GLU	CB-CG	5.32	1.68	1.52
1	B	213	THR	CA-C	5.30	1.59	1.52
1	A	127	VAL	CA-CB	5.25	1.59	1.53
1	A	174	LYS	CA-C	5.24	1.59	1.52
1	A	218	ARG	CZ-NH1	5.23	1.40	1.32
1	A	250	THR	CA-CB	5.22	1.61	1.53
1	A	63	THR	CA-CB	5.21	1.61	1.53
1	B	28	VAL	CA-C	5.21	1.59	1.52
1	B	163	ILE	CA-CB	5.18	1.60	1.54
1	B	78	ILE	CB-CG2	5.16	1.69	1.52
1	B	172	ILE	CA-C	5.13	1.59	1.52
1	B	37	LYS	CA-CB	5.12	1.61	1.53
1	A	44	TYR	N-CA	5.10	1.52	1.45
1	A	119	VAL	CA-C	5.07	1.58	1.52
1	A	31	ASP	C-O	5.07	1.30	1.24
1	B	31	ASP	C-O	5.04	1.30	1.23
1	B	147	ASP	N-CA	5.04	1.52	1.46
1	B	95	GLY	N-CA	5.03	1.52	1.45
1	A	242	PHE	CB-CG	5.01	1.62	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	THR	N-CA-C	10.02	121.91	108.38
1	B	88	GLU	N-CA-C	-9.81	92.62	108.41
1	A	119	VAL	CB-CA-C	7.66	121.52	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	THR	CB-CA-C	7.66	121.21	109.34
1	A	53	PHE	CA-C-N	-7.64	112.95	120.52
1	A	53	PHE	C-N-CA	-7.64	112.95	120.52
1	A	127	VAL	N-CA-CB	6.70	119.30	111.66
1	B	130	ASP	N-CA-C	6.43	117.95	111.07
1	A	25	THR	N-CA-CB	-6.41	101.11	110.40
1	B	155	GLU	N-CA-C	5.98	118.58	111.71
1	A	174	LYS	N-CA-C	5.93	118.23	111.11
1	A	136	VAL	N-CA-C	5.79	115.91	110.30
1	A	125	VAL	N-CA-C	5.75	116.43	108.84
1	B	236	LEU	N-CA-C	5.75	117.54	111.28
1	B	27	CYS	CB-CA-C	-5.72	100.52	109.84
1	A	59	HIS	CA-C-N	5.71	128.72	120.38
1	A	59	HIS	C-N-CA	5.71	128.72	120.38
1	A	231	GLU	N-CA-C	5.50	117.36	111.36
1	B	183	THR	N-CA-C	5.50	120.00	113.12
1	B	187	GLN	N-CA-C	5.50	117.36	111.36
1	A	91	ASN	N-CA-C	5.47	122.46	110.80
1	B	150	ILE	N-CA-C	-5.36	100.60	108.11
1	B	203	GLU	N-CA-C	5.34	117.18	111.36
1	B	227	ALA	N-CA-C	5.33	117.84	111.71
1	A	115	ALA	N-CA-C	-5.33	106.81	113.15
1	B	52	ALA	CA-C-N	-5.32	116.62	123.16
1	B	52	ALA	C-N-CA	-5.32	116.62	123.16
1	A	60	GLU	N-CA-C	5.29	118.53	111.75
1	A	184	ASP	CA-C-N	5.28	125.34	119.32
1	A	184	ASP	C-N-CA	5.28	125.34	119.32
1	A	216	LEU	N-CA-C	5.28	117.03	111.28
1	A	56	GLY	CA-C-N	5.25	127.57	120.38
1	A	56	GLY	C-N-CA	5.25	127.57	120.38
1	A	25	THR	CA-CB-CG2	5.24	119.41	110.50
1	A	35	PHE	N-CA-C	5.21	117.38	111.02
1	B	67	LYS	N-CA-C	5.20	116.63	111.07
1	B	53	PHE	CA-C-N	-5.16	115.25	120.31
1	B	53	PHE	C-N-CA	-5.16	115.25	120.31
1	A	73	THR	N-CA-C	5.10	116.83	109.07
1	A	62	PHE	N-CA-C	5.07	116.81	111.28
1	B	238	ILE	N-CA-C	5.00	115.22	110.42
1	A	121	LEU	CA-C-N	-5.00	114.61	119.76
1	A	121	LEU	C-N-CA	-5.00	114.61	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	87	GLY	Peptide

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	1677	0	1560	7	0
1	B	1578	0	1375	13	0
2	A	73	0	0	0	0
2	B	25	0	0	1	0
All	All	3353	0	2935	18	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 3.

All (18) 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:204:VAL:CG1	1:B:208:PHE:HB2	2.14	0.77
1:B:73:THR:OG1	1:B:74:LYS:N	2.17	0.74
1:B:23:THR:O	1:B:24:CYS:HB2	1.87	0.74
1:B:46:VAL:HG12	1:B:76:LEU:HD11	1.75	0.68
1:A:41:ARG:NH2	1:B:75:ASP:OD1	2.38	0.56
1:B:204:VAL:HG11	1:B:208:PHE:HB2	1.86	0.55
1:A:36:GLU:O	1:A:40:GLU:HG2	2.06	0.55
1:B:54:PRO:HG3	2:B:2011:HOH:O	2.10	0.52
1:A:25:THR:HG23	1:A:27:CYS:H	1.74	0.51
1:A:114:ASN:C	1:A:116:ASP:H	2.17	0.51
1:A:151:LYS:O	1:A:155:GLU:HG3	2.12	0.50
1:B:163:ILE:HD12	1:B:167:GLU:HB3	1.96	0.48
1:B:204:VAL:HG12	1:B:208:PHE:HB2	1.94	0.48
1:B:140:THR:HB	1:B:141:PRO:CD	2.47	0.44
1:B:163:ILE:HG13	1:B:168:GLN:HG3	2.01	0.43
1:A:24:CYS:SG	1:B:32:GLU:HB2	2.59	0.43
1:B:91:ASN:O	1:B:94:LEU:HB2	2.19	0.42
1:A:65:PHE:HA	1:A:129:LEU:HD23	2.02	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	A	226/248 (91%)	218 (96%)	7 (3%)	1 (0%)	30	36
1	B	221/248 (89%)	209 (95%)	12 (5%)	0	100	100
All	All	447/496 (90%)	427 (96%)	19 (4%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	LEU

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	154/218 (71%)	143 (93%)	11 (7%)	13	17
1	B	131/218 (60%)	123 (94%)	8 (6%)	17	22
All	All	285/436 (65%)	266 (93%)	19 (7%)	15	19

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	63	THR

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Mol	Chain	Res	Type
1	A	78	ILE
1	A	108	ILE
1	A	119	VAL
1	A	127	VAL
1	A	129	LEU
1	A	132	LEU
1	A	195	LEU
1	A	204	VAL
1	A	231	GLU
1	B	46	VAL
1	B	60	GLU
1	B	63	THR
1	B	78	ILE
1	B	132	LEU
1	B	167	GLU
1	B	171	LEU
1	B	204	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	228/248 (91%)	-0.27	2 (0%) 81 82	18, 30, 46, 61	0
1	B	223/248 (89%)	0.12	4 (1%) 67 69	23, 39, 65, 78	0
All	All	451/496 (90%)	-0.08	6 (1%) 75 76	18, 34, 60, 78	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	250	THR	3.2
1	B	172	ILE	3.0
1	B	85	ASP	2.3
1	B	184	ASP	2.3
1	A	85	ASP	2.2
1	B	245	HIS	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 oligosaccharides 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.