



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:27 am BST

PDB ID : 5YW1
Title : Crystal structure of full length NS3 protein (eD4NS2BNS3) in complex with
Bovine Pancreatic Trypsin Inhibitor
Authors : Phoo, W.W.; El Sahili, A.
Deposited on : 2017-11-28
Resolution : 2.60 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	:	2.11
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)	:	2.11

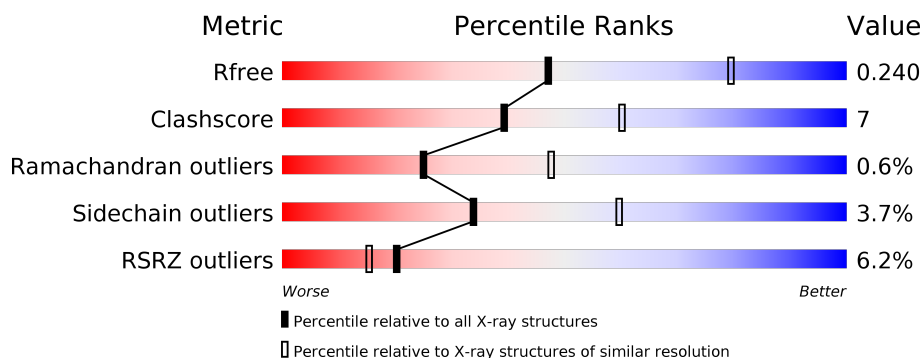
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	B	618	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>
2	A	54	<div> <div>9%</div> <div> <div></div> <div>41%</div> <div>22%</div> <div>6%</div> <div>31%</div> </div> </div>
3	I	55	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>•</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5277 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 Peptidase S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	601	Total	C	N	O	S	0	0	0
			4597	2902	809	866	20			

- Molecule 2 is a protein called FLAVIVIRUS_NS2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	37	Total	C	N	O	S	0	0	0
			250	156	41	52	1			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP W0LLP9
A	96	GLY	-	expression tag	UNP W0LLP9
A	97	VAL	-	expression tag	UNP W0LLP9
A	98	LYS	-	expression tag	UNP W0LLP9
A	99	THR	-	expression tag	UNP W0LLP9
A	100	GLN	-	expression tag	UNP W0LLP9
A	101	ARG	-	expression tag	UNP W0LLP9

- Molecule 3 is a protein called PTI protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	55	Total	C	N	O	S	0	0	0
			428	267	79	74	8			

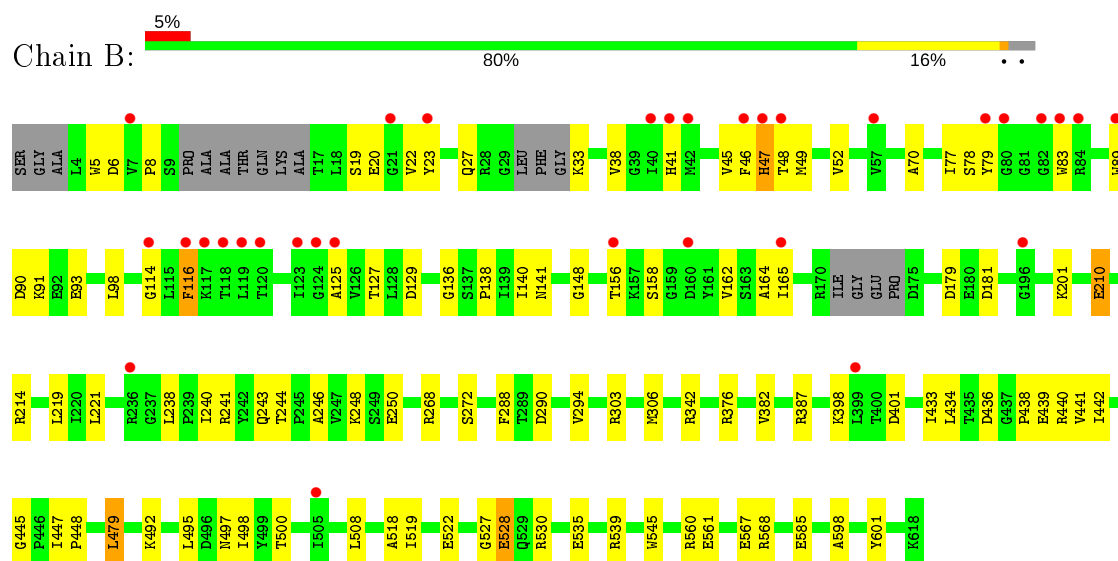
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	O	0	0
			2	2		

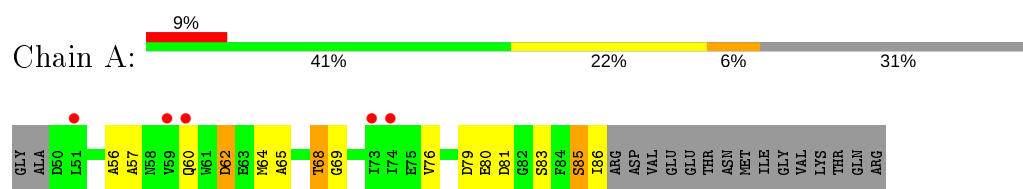
3 Residue-property plots [i](#)

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.

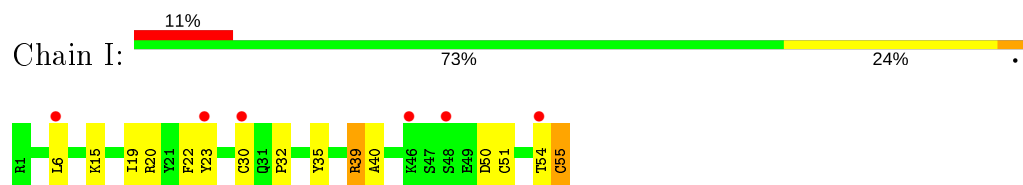
• Molecule 1: Peptidase S7



• Molecule 2: FLAVIVIRUS_NS2B



• Molecule 3: PTI protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.02Å 87.49Å 86.45Å 90.00° 98.25° 90.00°	Depositor
Resolution (Å)	45.00 – 2.60 45.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.00-2.60) 92.1 (45.00-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.221 , 0.240 0.221 , 0.240	Depositor DCC
R_{free} test set	1177 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.4	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	5277	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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](#)

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	B	0.26	0/4699	0.48	0/6381
2	A	0.32	0/253	0.56	0/346
3	I	0.33	0/439	0.54	1/590 (0.2%)
All	All	0.27	0/5391	0.49	1/7317 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	I	6	LEU	CA-CB-CG	5.21	127.29	115.30

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	B	4597	0	4419	61	0
2	A	250	0	214	11	0
3	I	428	0	403	11	0
4	B	2	0	0	0	0
All	All	5277	0	5036	76	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 7.

All (76) 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:497:ASN:O	1:B:530:ARG:NH1	2.08	0.86
1:B:78:SER:HB3	1:B:83:TRP:CD1	2.22	0.74
1:B:156:THR:HG22	1:B:158:SER:H	1.57	0.70
1:B:89:TRP:NE1	1:B:93:GLU:O	2.19	0.69
1:B:495:LEU:HA	1:B:498:ILE:HD12	1.77	0.65
1:B:19:SER:O	1:B:41:HIS:ND1	2.29	0.64
1:B:210:GLU:HG2	1:B:214:ARG:HH12	1.62	0.64
3:I:19:ILE:HD11	3:I:32:PRO:HB2	1.79	0.64
1:B:445:GLY:HA2	1:B:447:ILE:HG23	1.82	0.62
1:B:90:ASP:OD1	1:B:93:GLU:N	2.34	0.61
1:B:22:VAL:HG23	2:A:56:ALA:HB3	1.83	0.61
1:B:114:GLY:O	1:B:125:ALA:N	2.33	0.59
1:B:248:LYS:HB3	1:B:272:SER:HB2	1.85	0.59
3:I:23:TYR:HD1	3:I:30:CYS:SG	2.26	0.58
2:A:79:ASP:O	2:A:81:ASP:N	2.37	0.57
1:B:116:PHE:CD2	1:B:164:ALA:HB2	2.39	0.57
1:B:27:GLN:O	1:B:33:LYS:HA	2.04	0.56
1:B:19:SER:OG	1:B:20:GLU:N	2.39	0.55
1:B:5:TRP:O	1:B:201:LYS:NZ	2.32	0.54
2:A:83:SER:HB3	3:I:39:ARG:HE	1.71	0.54
1:B:23:TYR:HE2	1:B:41:HIS:HB2	1.71	0.54
1:B:535:GLU:HG3	1:B:539:ARG:HH11	1.72	0.54
3:I:20:ARG:O	3:I:32:PRO:HA	2.07	0.53
1:B:519:ILE:N	1:B:522:GLU:OE2	2.39	0.53
1:B:45:VAL:HB	1:B:47:HIS:HE1	1.75	0.52
1:B:303:ARG:HA	1:B:306:MET:HE2	1.92	0.51
1:B:48:THR:HG22	1:B:49:MET:H	1.75	0.51
3:I:22:PHE:O	3:I:30:CYS:HA	2.10	0.51
1:B:448:PRO:HB2	1:B:479:LEU:HB2	1.92	0.50
1:B:241:ARG:NH1	1:B:250:GLU:OE2	2.44	0.50
1:B:22:VAL:HG11	1:B:138:PRO:HG3	1.92	0.50
1:B:238:LEU:HB2	1:B:240:ILE:HD11	1.94	0.50
1:B:23:TYR:CE2	1:B:41:HIS:HB2	2.47	0.50
3:I:50:ASP:O	3:I:54:THR:OG1	2.17	0.50
1:B:98:LEU:HD12	1:B:140:ILE:HD11	1.95	0.49
1:B:70:ALA:HB2	1:B:77:ILE:HG13	1.94	0.49
1:B:398:LYS:N	1:B:398:LYS:HD2	2.28	0.48
1:B:376:ARG:NH1	1:B:382:VAL:O	2.42	0.48
1:B:439:GLU:HG2	1:B:545:TRP:HZ2	1.79	0.48
1:B:129:ASP:OD1	3:I:15:LYS:NZ	2.42	0.47
1:B:434:LEU:HD11	1:B:442:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:GLU:OE1	1:B:585:GLU:N	2.47	0.47
1:B:492:LYS:HD3	1:B:518:ALA:HB3	1.97	0.46
3:I:51:CYS:O	3:I:55:CYS:N	2.48	0.46
2:A:83:SER:CB	3:I:39:ARG:HE	2.28	0.46
1:B:41:HIS:HD2	1:B:46:PHE:HD2	1.62	0.46
1:B:294:VAL:HG12	1:B:508:LEU:HD22	1.97	0.45
1:B:290:ASP:OD1	1:B:387:ARG:NH2	2.49	0.45
2:A:76:VAL:HG23	2:A:85:SER:C	2.36	0.45
1:B:179:ASP:OD1	1:B:181:ASP:HB2	2.17	0.45
1:B:210:GLU:HG2	1:B:214:ARG:NH1	2.31	0.45
1:B:433:ILE:HG12	1:B:441:VAL:HG22	1.98	0.45
2:A:62:ASP:HB3	2:A:65:ALA:HB2	1.98	0.45
1:B:48:THR:HG22	1:B:49:MET:N	2.32	0.45
1:B:116:PHE:O	2:A:76:VAL:HG12	2.17	0.44
1:B:49:MET:HB2	1:B:52:VAL:HG23	2.00	0.44
1:B:89:TRP:CZ3	1:B:91:LYS:HA	2.53	0.44
2:A:83:SER:HB3	3:I:39:ARG:NE	2.32	0.43
1:B:38:VAL:O	1:B:48:THR:HG23	2.19	0.43
2:A:76:VAL:HA	2:A:86:ILE:C	2.39	0.43
1:B:244:THR:HG22	1:B:246:ALA:H	1.83	0.43
1:B:148:GLY:HA3	1:B:165:ILE:HG23	2.00	0.43
1:B:219:LEU:HD21	1:B:221:LEU:HD21	2.00	0.43
1:B:243:GLN:HB3	1:B:268:ARG:NH2	2.33	0.43
3:I:35:TYR:CZ	3:I:40:ALA:HB2	2.54	0.43
1:B:439:GLU:HG2	1:B:545:TRP:CZ2	2.54	0.43
1:B:560:ARG:HA	1:B:560:ARG:HD3	1.91	0.42
1:B:598:ALA:HA	1:B:601:TYR:CE2	2.53	0.42
1:B:528:GLU:CD	1:B:528:GLU:H	2.23	0.42
1:B:127:THR:HG22	1:B:162:VAL:HG13	2.01	0.42
1:B:140:ILE:HG22	1:B:141:ASN:H	1.85	0.42
1:B:77:ILE:HD13	1:B:79:TYR:HE1	1.86	0.41
2:A:68:THR:HG22	2:A:69:GLY:H	1.84	0.41
1:B:22:VAL:HG22	2:A:57:ALA:O	2.20	0.41
1:B:438:PRO:O	1:B:440:ARG:NH1	2.54	0.40
1:B:38:VAL:O	1:B:136:GLY:HA3	2.22	0.40

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	B	593/618 (96%)	562 (95%)	28 (5%)	3 (0%)	29	52
2	A	35/54 (65%)	32 (91%)	2 (6%)	1 (3%)	4	7
3	I	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	681/727 (94%)	644 (95%)	33 (5%)	4 (1%)	25	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	80	GLU
1	B	527	GLY
1	B	8	PRO
1	B	436	ASP

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	B	470/524 (90%)	457 (97%)	13 (3%)	43	69
2	A	23/46 (50%)	18 (78%)	5 (22%)	1	1
3	I	44/47 (94%)	42 (96%)	2 (4%)	27	52
All	All	537/617 (87%)	517 (96%)	20 (4%)	34	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	ASP
1	B	47	HIS
1	B	116	PHE
1	B	210	GLU
1	B	288	PHE
1	B	342	ARG
1	B	401	ASP
1	B	479	LEU
1	B	500	THR
1	B	528	GLU
1	B	561	GLU
1	B	567	GLU
1	B	568	ARG
2	A	60	GLN
2	A	62	ASP
2	A	64	MET
2	A	68	THR
2	A	85	SER
3	I	39	ARG
3	I	55	CYS

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

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 ⓘ

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 ⓘ

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	B	601/618 (97%)	0.20	32 (5%)	26 20	30, 64, 127, 176	0
2	A	37/54 (68%)	0.94	5 (13%)	3 1	78, 102, 121, 127	0
3	I	55/55 (100%)	0.57	6 (10%)	5 3	63, 92, 134, 141	0
All	All	693/727 (95%)	0.27	43 (6%)	20 15	30, 69, 129, 176	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	59	VAL	5.2
1	B	118	THR	4.7
3	I	6	LEU	4.5
1	B	116	PHE	4.3
1	B	46	PHE	4.3
1	B	114	GLY	4.2
2	A	51	LEU	3.9
3	I	48	SER	3.7
2	A	74	ILE	3.7
1	B	83	TRP	3.6
1	B	84	ARG	3.5
1	B	41	HIS	3.4
1	B	165	ILE	3.4
1	B	42	MET	3.1
1	B	40	ILE	3.1
2	A	60	GLN	3.1
1	B	48	THR	3.0
1	B	160	ASP	3.0
1	B	196	GLY	2.9
2	A	73	ILE	2.9
1	B	21	GLY	2.9
1	B	125	ALA	2.8
1	B	80	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	79	TYR	2.7
1	B	156	THR	2.7
1	B	82	GLY	2.6
1	B	89	TRP	2.6
1	B	399	LEU	2.6
1	B	23	TYR	2.5
1	B	123	ILE	2.5
1	B	119	LEU	2.5
1	B	47	HIS	2.5
3	I	30	CYS	2.4
1	B	236	ARG	2.3
3	I	46	LYS	2.3
1	B	117	LYS	2.3
1	B	7	VAL	2.3
3	I	54	THR	2.2
1	B	57	VAL	2.1
3	I	23	TYR	2.1
1	B	124	GLY	2.1
1	B	120	THR	2.1
1	B	505	ILE	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 carbohydrates 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.