



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:21 PM GMT

PDB ID : 1D9Q  
Title : OXIDIZED PEA FRUCTOSE-1,6-BISPHOSPHATASEFORM 1  
Authors : Chiadmi, M.; Navaza, A.; Miginiac-Maslow, M.; Jacquot, J.-P.; Cherfils, J.  
Deposited on : 1999-10-29  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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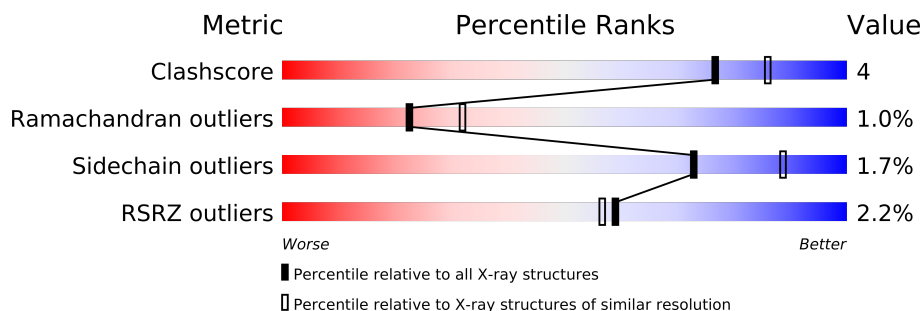
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	
1	C	357	
1	D	357	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10184 atoms, of which 0 are hydrogen and 0 are deuterium.

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 FRUCTOSE-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2457	1564	404	479	10			
1	B	333	Total	C	N	O	S	0	0	0
			2505	1590	408	497	10			
1	C	327	Total	C	N	O	S	0	0	0
			2464	1565	404	485	10			
1	D	325	Total	C	N	O	S	0	0	0
			2424	1542	393	479	10			

- Molecule 2 is water.

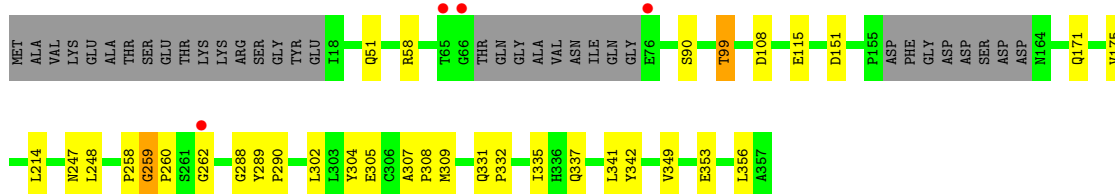
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	103	Total	O	0	0
			103	103		
2	C	83	Total	O	0	0
			83	83		
2	D	70	Total	O	0	0
			70	70		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

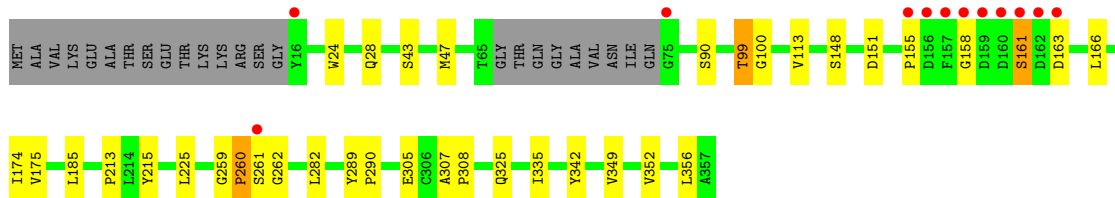
#### • Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

Chain A: 



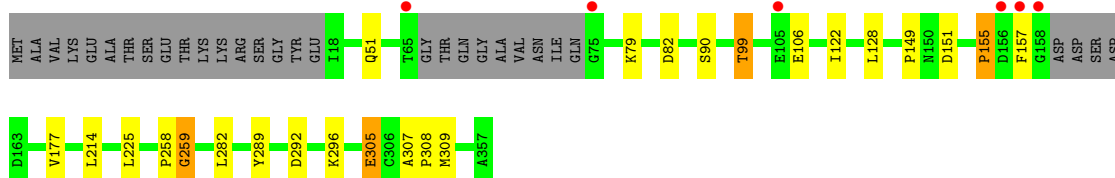
#### • Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

Chain B: 



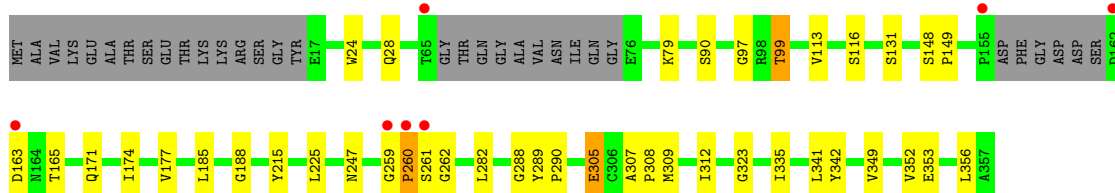
#### • Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

Chain C: 



#### • Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.94Å 113.99Å 94.81Å 90.00° 114.38° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 24.31 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.40) 89.1 (24.31-2.40)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.186 , 0.236 0.199 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 41.3	EDS
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53059 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.43	2/2500 (0.1%)	0.68	2/3385 (0.1%)
1	B	0.40	0/2551	0.66	0/3464
1	C	0.39	0/2507	0.64	1/3399 (0.0%)
1	D	0.38	0/2467	0.64	1/3352 (0.0%)
All	All	0.40	2/10025 (0.0%)	0.66	4/13600 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	GLU	CD-OE1	-5.77	1.19	1.25
1	A	115	GLU	CD-OE2	-5.45	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	A	260	PRO	N-CA-CB	6.00	110.50	103.30
1	D	260	PRO	N-CA-CB	5.70	110.14	103.30
1	C	155	PRO	N-CA-CB	5.62	110.04	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2457	0	2403	26	0
1	B	2505	0	2412	20	0
1	C	2464	0	2388	13	0
1	D	2424	0	2306	21	0
2	A	78	0	0	0	0
2	B	103	0	0	1	0
2	C	83	0	0	0	0
2	D	70	0	0	0	0
All	All	10184	0	9509	74	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:149:PRO:HB3	1:D:177:VAL:HG13	1.49	0.92
1:A:175:VAL:HG23	1:A:335:ILE:HG12	1.55	0.88
1:A:175:VAL:CG2	1:A:335:ILE:HG12	2.07	0.85
1:D:171:GLN:HB3	1:D:335:ILE:HG12	1.62	0.82
1:A:214:LEU:HD22	1:C:214:LEU:HD22	1.65	0.79
1:B:215:TYR:CE2	1:C:51:GLN:HG2	2.25	0.71
1:C:122:ILE:HG13	1:C:149:PRO:HG3	1.78	0.66
1:D:307:ALA:HB3	1:D:308:PRO:HD3	1.79	0.65
1:D:149:PRO:HB3	1:D:177:VAL:CG1	2.25	0.65
1:C:307:ALA:HB3	1:C:308:PRO:HD3	1.83	0.60
1:B:307:ALA:HB3	1:B:308:PRO:HD3	1.83	0.59
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.85	0.59
1:A:302:LEU:HD23	1:A:332:PRO:HG3	1.84	0.59
1:A:304:TYR:OH	1:A:335:ILE:CG2	2.51	0.58
1:B:113:VAL:HG11	1:B:174:ILE:HD13	1.85	0.58
1:B:90:SER:HA	1:B:99:THR:HG21	1.87	0.57
1:B:158:GLY:HA3	1:B:161:SER:HB2	1.87	0.56
1:D:79:LYS:HG2	1:D:131:SER:HB2	1.87	0.56
1:A:304:TYR:OH	1:A:335:ILE:HG21	2.06	0.56
1:A:171:GLN:HA	1:A:335:ILE:HD11	1.88	0.56
1:D:113:VAL:HG11	1:D:174:ILE:HD13	1.88	0.55
1:A:90:SER:HA	1:A:99:THR:HG21	1.90	0.54
1:B:43:SER:O	1:B:47:MET:HG3	2.09	0.53
1:C:149:PRO:HB3	1:C:177:VAL:CG1	2.40	0.52
1:D:163:ASP:C	1:D:165:THR:H	2.12	0.52
1:D:247:ASN:HB3	1:D:356:LEU:HD23	1.92	0.51
1:A:171:GLN:HB3	1:A:335:ILE:HG13	1.91	0.51
1:A:171:GLN:CA	1:A:335:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:290:PRO:HB3	1:D:342:TYR:OH	2.11	0.51
1:B:290:PRO:HB3	1:B:342:TYR:OH	2.11	0.51
1:D:90:SER:HA	1:D:99:THR:HG21	1.93	0.51
1:C:149:PRO:HB3	1:C:177:VAL:HG13	1.93	0.50
1:B:148:SER:HB2	1:B:185:LEU:HD11	1.94	0.49
1:A:51:GLN:HG2	1:D:215:TYR:CE2	2.47	0.49
1:A:51:GLN:HG2	1:D:215:TYR:CZ	2.47	0.49
1:A:171:GLN:O	1:A:335:ILE:HD11	2.13	0.48
1:B:215:TYR:CZ	1:C:51:GLN:HG2	2.49	0.48
1:B:260:PRO:C	1:B:262:GLY:H	2.17	0.47
1:C:79:LYS:O	1:C:82:ASP:HB2	2.14	0.47
1:A:332:PRO:HA	1:A:337:GLN:OE1	2.14	0.46
1:B:325:GLN:HB2	2:B:431:HOH:O	2.16	0.46
1:A:258:PRO:HB2	1:A:262:GLY:HA2	1.97	0.46
1:C:225:LEU:HD11	1:C:282:LEU:HD23	1.97	0.46
1:A:304:TYR:OH	1:A:335:ILE:HG22	2.16	0.46
1:A:290:PRO:HB3	1:A:342:TYR:OH	2.17	0.45
1:C:305:GLU:O	1:C:309:MET:HG2	2.17	0.45
1:A:349:VAL:O	1:A:353:GLU:HG3	2.17	0.45
1:B:175:VAL:HG21	1:B:335:ILE:HA	1.99	0.45
1:D:24:TRP:O	1:D:28:GLN:HG2	2.17	0.45
1:D:288:GLY:HA2	1:D:341:LEU:O	2.18	0.44
1:D:305:GLU:O	1:D:309:MET:HG2	2.17	0.44
1:B:260:PRO:HG2	1:B:261:SER:H	1.83	0.44
1:B:352:VAL:O	1:B:356:LEU:HG	2.18	0.44
1:A:305:GLU:O	1:A:309:MET:HG2	2.18	0.44
1:B:349:VAL:O	1:B:352:VAL:HG12	2.18	0.43
1:B:24:TRP:O	1:B:28:GLN:HG2	2.18	0.43
1:D:225:LEU:HD11	1:D:282:LEU:HD23	2.00	0.43
1:A:248:LEU:HD21	1:A:290:PRO:HG3	2.01	0.43
1:A:247:ASN:HB3	1:A:356:LEU:HD23	2.00	0.43
1:A:331:GLN:NE2	1:A:332:PRO:HD2	2.34	0.43
1:B:225:LEU:HD11	1:B:282:LEU:HD23	2.01	0.43
1:B:260:PRO:C	1:B:262:GLY:N	2.72	0.43
1:B:100:GLY:HA3	1:B:166:LEU:HD21	2.01	0.42
1:A:58:ARG:HG2	1:B:213:PRO:HD2	2.01	0.42
1:D:148:SER:HB2	1:D:185:LEU:HD11	2.02	0.42
1:D:188:GLY:HA2	1:D:312:ILE:HD11	2.01	0.42
1:C:82:ASP:OD2	1:C:128:LEU:HD12	2.19	0.41
1:D:97:GLY:HA3	1:D:116:SER:HA	2.02	0.41
1:A:258:PRO:O	1:A:259:GLY:O	2.38	0.41
1:D:323:GLY:O	1:D:353:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:90:SER:HA	1:C:99:THR:HG21	2.02	0.41
1:C:258:PRO:O	1:C:259:GLY:O	2.39	0.41
1:D:349:VAL:O	1:D:352:VAL:HG12	2.20	0.41
1:A:288:GLY:HA2	1:A:341:LEU:O	2.21	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	A	317/357 (89%)	304 (96%)	11 (4%)	2 (1%)	33	47
1	B	329/357 (92%)	311 (94%)	15 (5%)	3 (1%)	25	35
1	C	321/357 (90%)	302 (94%)	15 (5%)	4 (1%)	19	26
1	D	319/357 (89%)	306 (96%)	9 (3%)	4 (1%)	18	24
All	All	1286/1428 (90%)	1223 (95%)	50 (4%)	13 (1%)	22	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	259	GLY
1	B	260	PRO
1	B	155	PRO
1	C	155	PRO
1	C	259	GLY
1	D	260	PRO
1	D	261	SER
1	C	106	GLU
1	D	262	GLY
1	B	259	GLY
1	C	157	PHE
1	D	259	GLY

### 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	265/307 (86%)	262 (99%)	3 (1%)	84	94
1	B	269/307 (88%)	263 (98%)	6 (2%)	64	83
1	C	264/307 (86%)	258 (98%)	6 (2%)	63	82
1	D	255/307 (83%)	252 (99%)	3 (1%)	82	93
All	All	1053/1228 (86%)	1035 (98%)	18 (2%)	73	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	A	151	ASP
1	A	289	TYR
1	B	99	THR
1	B	151	ASP
1	B	161	SER
1	B	163	ASP
1	B	289	TYR
1	B	305	GLU
1	C	99	THR
1	C	151	ASP
1	C	289	TYR
1	C	292	ASP
1	C	296	LYS
1	C	305	GLU
1	D	99	THR
1	D	289	TYR
1	D	305	GLU

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

Mol	Chain	Res	Type
1	A	240	ASN
1	A	247	ASN
1	B	240	ASN

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Mol	Chain	Res	Type
1	C	240	ASN
1	C	325	GLN
1	D	240	ASN
1	D	325	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/357 (90%)	-0.60	4 (1%) 75 75	11, 28, 68, 100	0
1	B	333/357 (93%)	-0.65	12 (3%) 41 39	11, 24, 66, 100	0
1	C	327/357 (91%)	-0.64	6 (1%) 65 63	14, 29, 64, 100	0
1	D	325/357 (91%)	-0.54	7 (2%) 59 57	16, 34, 72, 100	0
All	All	1308/1428 (91%)	-0.61	29 (2%) 59 57	11, 29, 69, 100	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ASP	6.4
1	B	159	ASP	6.0
1	C	157	PHE	5.3
1	D	162	ASP	5.1
1	B	157	PHE	4.9
1	A	65	THR	4.4
1	A	66	GLY	4.0
1	D	260	PRO	3.9
1	C	156	ASP	3.8
1	B	156	ASP	3.7
1	B	158	GLY	3.6
1	B	162	ASP	3.3
1	B	161	SER	3.2
1	D	65	THR	3.2
1	D	259	GLY	3.1
1	C	158	GLY	3.1
1	C	65	THR	3.1
1	D	261	SER	3.0
1	B	155	PRO	3.0
1	B	261	SER	2.8
1	C	75	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	105	GLU	2.7
1	D	163	ASP	2.6
1	B	163	ASP	2.4
1	A	76	GLU	2.4
1	A	262	GLY	2.3
1	B	75	GLY	2.3
1	D	155	PRO	2.2
1	B	16	TYR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.