



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 02:40 PM EDT

PDB ID : 9OU6 / pdb\_00009ou6  
Title : Crystal Structure of Salmonella FraB Deglycase, Crystal Form 1  
Authors : Bell, C.E.; Zakharova, K.  
Deposited on : 2025-05-28  
Resolution : 1.48 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

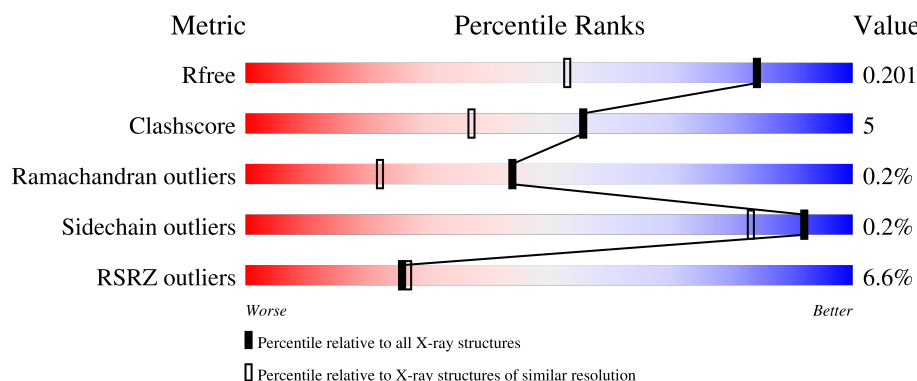
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.48 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))
$R_{free}$	164625	6131 (1.50-1.46)
Clashscore	180529	6623 (1.50-1.46)
Ramachandran outliers	177936	6521 (1.50-1.46)
Sidechain outliers	177891	6518 (1.50-1.46)
RSRZ outliers	164620	6132 (1.50-1.46)

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  $\geq 3$ , 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	345	<div> <div>5%</div> <div>81%</div> <div>8%</div> <div>10%</div> </div>
1	B	345	<div> <div>7%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5294 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 SIS domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2405	1536	401	458	10			
1	B	313	Total	C	N	O	S	0	0	0
			2413	1539	407	456	11			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP V7IWJ0
A	-18	ASP	-	expression tag	UNP V7IWJ0
A	-17	HIS	-	expression tag	UNP V7IWJ0
A	-16	HIS	-	expression tag	UNP V7IWJ0
A	-15	HIS	-	expression tag	UNP V7IWJ0
A	-14	HIS	-	expression tag	UNP V7IWJ0
A	-13	HIS	-	expression tag	UNP V7IWJ0
A	-12	HIS	-	expression tag	UNP V7IWJ0
A	-11	GLU	-	expression tag	UNP V7IWJ0
A	-10	ASN	-	expression tag	UNP V7IWJ0
A	-9	LEU	-	expression tag	UNP V7IWJ0
A	-8	TYR	-	expression tag	UNP V7IWJ0
A	-7	PHE	-	expression tag	UNP V7IWJ0
A	-6	GLN	-	expression tag	UNP V7IWJ0
A	232	ALA	PRO	engineered mutation	UNP V7IWJ0
A	275	ALA	LYS	engineered mutation	UNP V7IWJ0
A	276	ALA	GLU	engineered mutation	UNP V7IWJ0
B	-19	MET	-	expression tag	UNP V7IWJ0
B	-18	ASP	-	expression tag	UNP V7IWJ0
B	-17	HIS	-	expression tag	UNP V7IWJ0
B	-16	HIS	-	expression tag	UNP V7IWJ0
B	-15	HIS	-	expression tag	UNP V7IWJ0
B	-14	HIS	-	expression tag	UNP V7IWJ0
B	-13	HIS	-	expression tag	UNP V7IWJ0
B	-12	HIS	-	expression tag	UNP V7IWJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	GLU	-	expression tag	UNP V7IWJ0
B	-10	ASN	-	expression tag	UNP V7IWJ0
B	-9	LEU	-	expression tag	UNP V7IWJ0
B	-8	TYR	-	expression tag	UNP V7IWJ0
B	-7	PHE	-	expression tag	UNP V7IWJ0
B	-6	GLN	-	expression tag	UNP V7IWJ0
B	232	ALA	PRO	engineered mutation	UNP V7IWJ0
B	275	ALA	LYS	engineered mutation	UNP V7IWJ0
B	276	ALA	GLU	engineered mutation	UNP V7IWJ0

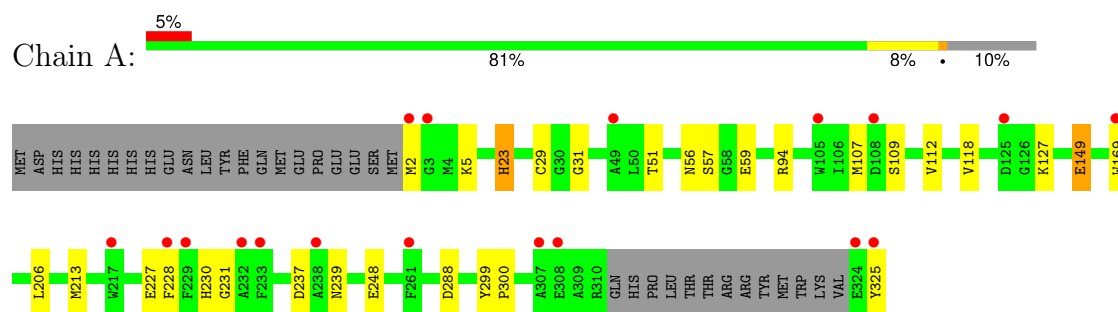
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	213	Total O 213 213	0	0
2	B	263	Total O 263 263	0	0

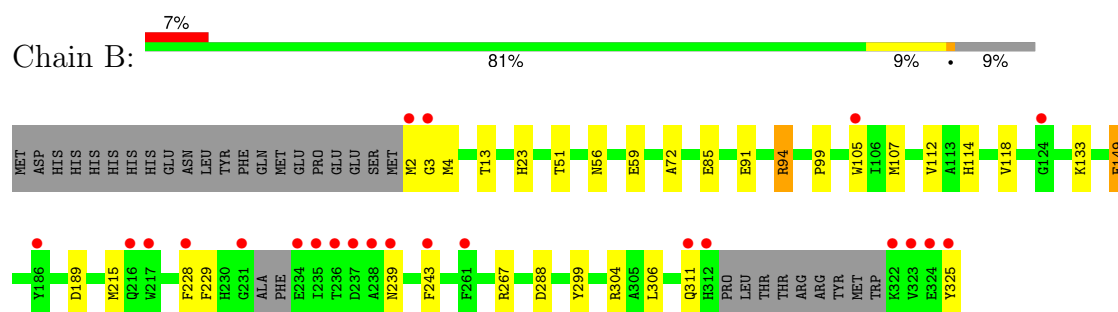
### 3 Residue-property plots [i](#)

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.

#### • Molecule 1: SIS domain protein



#### • Molecule 1: SIS domain protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.71Å 109.33Å 114.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.08 – 1.48 79.08 – 1.48	Depositor EDS
% Data completeness (in resolution range)	77.3 (79.08-1.48) 77.3 (79.08-1.48)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.169 , 0.201 0.168 , 0.201	Depositor DCC
$R_{free}$ test set	4610 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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	0.68	0/2460	1.05	5/3334 (0.1%)
1	B	0.68	0/2467	1.10	6/3343 (0.2%)
All	All	0.68	0/4927	1.07	11/6677 (0.2%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	PHE	N-CA-CB	-9.33	96.68	110.49
1	B	229	PHE	CB-CA-C	7.97	123.41	110.09
1	B	149	GLU	CB-CA-C	-7.10	96.37	109.29
1	B	288	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	237	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	228	PHE	CB-CA-C	-5.95	97.55	109.99
1	B	13	THR	CA-CB-OG1	-5.83	100.85	109.60
1	A	228	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	149	GLU	CB-CA-C	-5.42	99.96	109.07
1	A	288	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	23	HIS	CB-CG-CD2	-5.01	124.68	131.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ARG	Sidechain
1	B	94	ARG	Sidechain

## 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	2405	0	2312	20	0
1	B	2413	0	2316	25	0
2	A	213	0	0	8	1
2	B	263	0	0	7	1
All	All	5294	0	4628	43	1

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 (43) 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:239:ASN:O	2:A:401:HOH:O	1.74	1.03
1:B:133:LYS:NZ	1:B:325:TYR:OXT	2.11	0.78
1:B:243:PHE:HE1	1:B:299:TYR:CE1	2.02	0.78
1:A:213:MET:HA	1:A:213:MET:HE2	1.70	0.73
2:A:595:HOH:O	1:B:23:HIS:HE1	1.72	0.73
1:A:51:THR:HG22	1:B:51:THR:HG22	1.71	0.73
1:B:325:TYR:CB	2:B:593:HOH:O	2.39	0.71
1:B:133:LYS:HZ1	1:B:325:TYR:C	1.98	0.70
1:A:231:GLY:HA3	2:A:431:HOH:O	1.94	0.68
1:A:227:GLU:OE2	2:A:402:HOH:O	2.11	0.68
1:A:2:MET:N	2:A:403:HOH:O	2.25	0.67
1:A:149:GLU:HG3	2:A:414:HOH:O	1.94	0.67
1:A:23:HIS:HE1	2:B:634:HOH:O	1.79	0.65
1:A:23:HIS:HD2	1:A:51:THR:OG1	1.85	0.57
1:B:56:ASN:HD22	1:B:59:GLU:H	1.52	0.57
1:B:107:MET:HE1	1:B:118:VAL:HG12	1.86	0.57
1:B:133:LYS:NZ	1:B:325:TYR:C	2.61	0.56
1:A:109:SER:O	1:A:112:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TRP:CZ3	2:B:511:HOH:O	2.53	0.56
1:A:56:ASN:HD22	1:A:59:GLU:H	1.54	0.56
1:B:105:TRP:HZ3	2:B:511:HOH:O	1.89	0.52
1:B:3:GLY:O	1:B:4:MET:HB2	2.11	0.51
1:A:325:TYR:CB	2:A:576:HOH:O	2.58	0.50
1:A:5:LYS:NZ	2:A:411:HOH:O	2.46	0.49
1:A:127:LYS:O	1:A:169:TRP:HZ2	1.95	0.48
1:B:215:MET:HE2	1:B:306:LEU:HD21	1.96	0.48
1:B:149:GLU:CG	2:B:438:HOH:O	2.62	0.47
1:B:91:GLU:OE1	1:B:114:HIS:ND1	2.45	0.47
1:A:107:MET:HE1	1:A:118:VAL:HG12	1.96	0.46
1:B:239:ASN:HD22	1:B:267:ARG:NH2	2.14	0.46
1:B:304:ARG:NH2	2:B:408:HOH:O	2.49	0.46
1:A:230:HIS:HE1	1:B:85:GLU:OE1	1.98	0.45
1:B:189:ASP:O	1:B:215:MET:HE3	2.16	0.45
1:B:23:HIS:HD2	1:B:51:THR:OG1	2.00	0.44
1:B:112:VAL:HG13	1:B:118:VAL:HG21	1.99	0.43
1:B:72:ALA:O	1:B:99:PRO:HD2	2.18	0.43
1:B:2:MET:O	1:B:3:GLY:C	2.63	0.41
1:A:29:CYS:SG	1:A:57:SER:HB2	2.61	0.41
1:A:31:GLY:HA2	1:A:206:LEU:HD21	2.03	0.41
1:A:23:HIS:CD2	1:A:51:THR:OG1	2.71	0.41
1:B:94:ARG:HH11	1:B:94:ARG:HD2	1.73	0.41
1:B:149:GLU:HG2	2:B:438:HOH:O	2.19	0.41
1:A:299:TYR:N	1:A:300:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:542:HOH:O	2:B:650:HOH:O[2_455]	2.15	0.05

## 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	307/345 (89%)	303 (99%)	4 (1%)	0	100	100
1	B	307/345 (89%)	300 (98%)	6 (2%)	1 (0%)	37	17
All	All	614/690 (89%)	603 (98%)	10 (2%)	1 (0%)	44	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	GLN

### 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	244/281 (87%)	243 (100%)	1 (0%)	89	79
1	B	244/281 (87%)	244 (100%)	0	100	100
All	All	488/562 (87%)	487 (100%)	1 (0%)	92	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	GLN
1	A	23	HIS
1	A	56	ASN
1	A	95	GLN
1	A	153	HIS

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Mol	Chain	Res	Type
1	A	230	HIS
1	B	10	ASN
1	B	15	GLN
1	B	23	HIS
1	B	56	ASN
1	B	95	GLN
1	B	216	GLN
1	B	239	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 [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

### 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	311/345 (90%)	0.31	18 (5%) 30 31	12, 21, 42, 57	0
1	B	313/345 (90%)	0.29	23 (7%) 22 23	11, 20, 44, 70	0
All	All	624/690 (90%)	0.30	41 (6%) 26 27	11, 20, 43, 70	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	TYR	7.9
1	B	323	VAL	6.6
1	A	325	TYR	5.9
1	A	229	PHE	5.8
1	B	3	GLY	5.4
1	B	217	TRP	4.6
1	B	235	ILE	4.6
1	B	237	ASP	4.5
1	B	312	HIS	4.3
1	A	169	TRP	4.3
1	A	233	PHE	4.1
1	B	231	GLY	3.7
1	B	228	PHE	3.6
1	B	311	GLN	3.5
1	B	105	TRP	3.3
1	A	238	ALA	3.0
1	B	243	PHE	2.9
1	B	236	THR	2.8
1	A	125	ASP	2.7
1	A	228	PHE	2.7
1	B	234	GLU	2.7
1	B	2	MET	2.7
1	A	3	GLY	2.7
1	A	261	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	324	GLU	2.6
1	A	105	TRP	2.6
1	B	124	GLY	2.6
1	A	217	TRP	2.5
1	A	2	MET	2.5
1	B	322	LYS	2.5
1	A	307	ALA	2.5
1	A	308	GLU	2.4
1	B	216	GLN	2.3
1	B	238	ALA	2.2
1	B	186	TYR	2.2
1	B	324	GLU	2.1
1	A	108	ASP	2.1
1	B	261	PHE	2.1
1	A	232	ALA	2.0
1	B	239	ASN	2.0
1	A	49	ALA	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 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.