



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:28 PM GMT

PDB ID : 1AW7  
Title : Q136A MUTANT OF TOXIC SHOCK SYNDROME TOXIN-1 FROM S. AU-REUS  
Authors : Earhart, C.A.; Mitchell, D.T.; Murray, D.L.; Pinheiro, D.M.; Matsumura, M.; Schlievert, P.M.; Ohlendorf, D.H.  
Deposited on : 1997-10-11  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

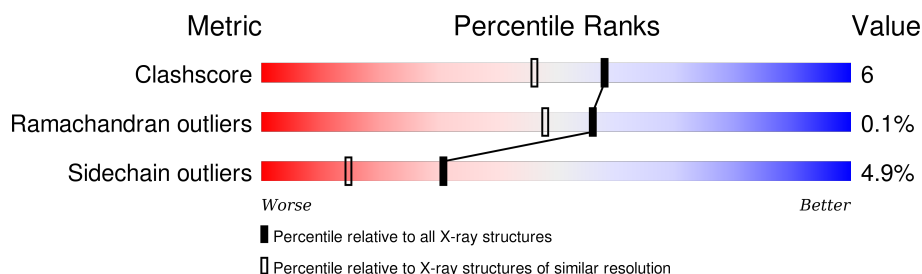
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	
1	B	194	
1	C	194	
1	D	194	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6539 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 TOXIC SHOCK SYNDROME TOXIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	B	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	C	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	D	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TRP	GLY	SEE REMARK 999	UNP P06886
A	136	ALA	GLN	ENGINEERED	UNP P06886
B	316	TRP	GLY	SEE REMARK 999	UNP P06886
B	336	ALA	GLN	ENGINEERED	UNP P06886
C	516	TRP	GLY	SEE REMARK 999	UNP P06886
C	536	ALA	GLN	ENGINEERED	UNP P06886
D	716	TRP	GLY	SEE REMARK 999	UNP P06886
D	736	ALA	GLN	ENGINEERED	UNP P06886

- Molecule 2 is water.

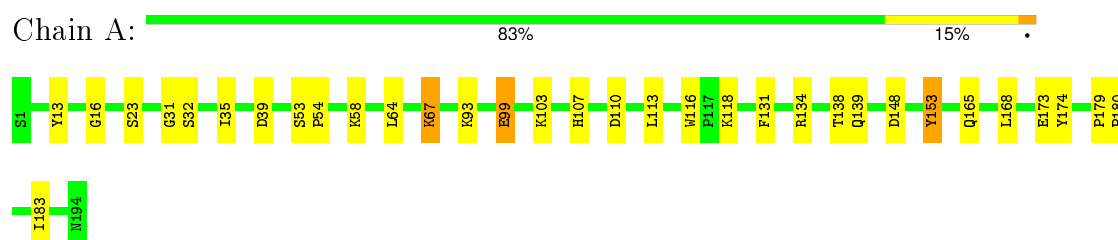
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	79	Total	O	0	0
			79	79		
2	C	64	Total	O	0	0
			64	64		
2	D	70	Total	O	0	0
			70	70		

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

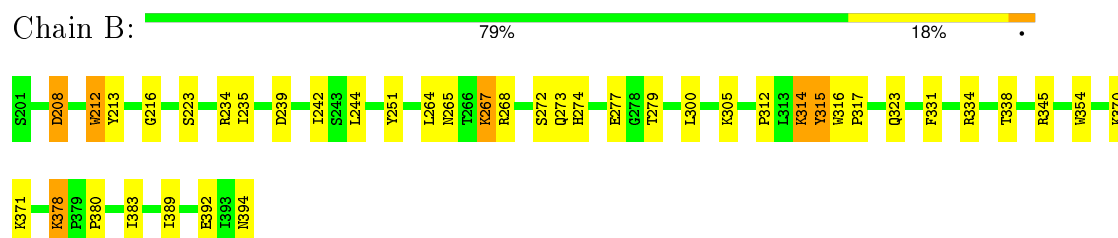
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

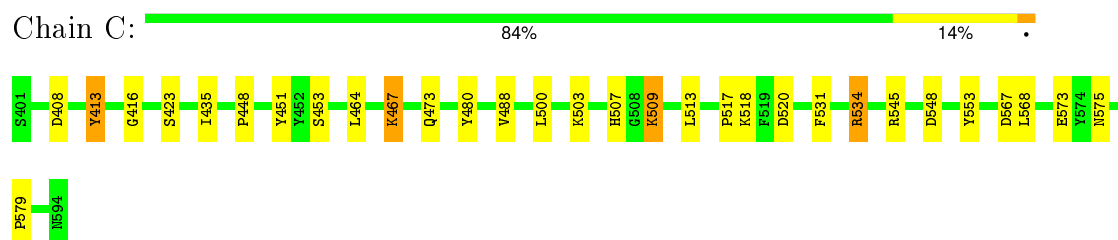
#### • Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



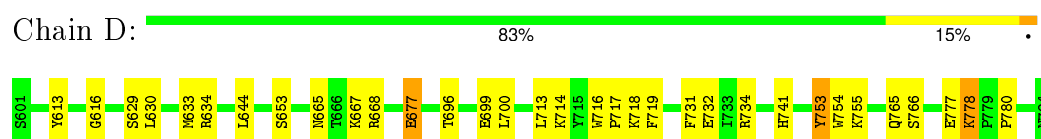
#### • Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



#### • Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



#### • Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.63 Å 99.28 Å 41.33 Å 88.50° 93.30° 91.10°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.95)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 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	1.18	0/1603	1.08	4/2168 (0.2%)
1	B	1.21	3/1603 (0.2%)	1.14	7/2168 (0.3%)
1	C	1.15	1/1603 (0.1%)	1.05	4/2168 (0.2%)
1	D	1.14	2/1603 (0.1%)	1.06	3/2168 (0.1%)
All	All	1.17	6/6412 (0.1%)	1.08	18/8672 (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	2
1	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	TYR	CE2-CZ	6.18	1.46	1.38
1	B	208	ASP	CB-CG	-5.88	1.39	1.51
1	B	354	TRP	CB-CG	5.41	1.59	1.50
1	B	212	TRP	CE3-CZ3	5.37	1.47	1.38
1	D	753	TYR	CD2-CE2	5.22	1.47	1.39
1	D	777	GLU	CD-OE2	-5.02	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	39	ASP	CB-CG-OD1	8.33	125.80	118.30
1	B	268	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	D	633	MET	CG-SD-CE	6.92	111.27	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	534	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	668	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	239	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	264	LEU	CA-CB-CG	6.26	129.70	115.30
1	C	567	ASP	CB-CG-OD1	6.19	123.87	118.30
1	D	665	ASN	N-CA-C	-5.57	95.96	111.00
1	C	545	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	345	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	545	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	39	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	265	ASN	N-CA-C	-5.06	97.34	111.00
1	A	31	GLY	N-CA-C	5.04	125.70	113.10
1	A	64	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain
1	A	174	TYR	Sidechain
1	B	251	TYR	Sidechain
1	B	315	TYR	Sidechain

## 5.2 Too-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 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	1562	0	1545	15	0
1	B	1562	0	1542	21	0
1	C	1562	0	1542	15	0
1	D	1562	0	1542	22	0
2	A	78	0	0	4	0
2	B	79	0	0	0	0
2	C	64	0	0	0	0
2	D	70	0	0	0	0
All	All	6539	0	6171	73	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 6.

All (73) 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:C:416:GLY:O	1:C:467:LYS:HE2	1.72	0.88
1:C:467:LYS:HE3	1:C:531[A]:PHE:CE2	2.21	0.75
1:B:216:GLY:O	1:B:267:LYS:HE2	1.93	0.68
2:A:196:HOH:O	1:B:274:HIS:HE1	1.74	0.68
1:D:616:GLY:O	1:D:667:LYS:HE2	1.94	0.68
1:B:212:TRP:CD2	1:B:371:LYS:HE3	2.31	0.65
1:D:755:LYS:HE2	1:D:765:GLN:NE2	2.16	0.61
1:B:223:SER:HB3	1:B:235:ILE:CG2	2.30	0.61
1:C:500:LEU:O	1:C:517:PRO:HD2	2.04	0.58
1:D:713:LEU:HD11	1:D:741:HIS:CE1	2.39	0.58
1:A:16:GLY:O	1:A:67:LYS:HE2	2.05	0.57
1:D:753:TYR:CD1	1:D:753:TYR:C	2.80	0.55
1:A:173:GLU:HG2	2:A:250:HOH:O	2.08	0.54
1:B:315:TYR:O	1:B:316:TRP:HD1	1.91	0.54
1:A:13:TYR:CZ	1:A:134:ARG:HD2	2.43	0.53
1:D:667:LYS:CE	1:D:731[A]:PHE:CE2	2.92	0.52
1:D:613:TYR:CZ	1:D:734:ARG:HD2	2.44	0.52
1:B:213:TYR:CZ	1:B:334:ARG:HD2	2.45	0.52
1:B:242:ILE:HG12	1:B:279:THR:HG21	1.92	0.52
1:C:467:LYS:CE	1:C:531[A]:PHE:CE2	2.93	0.51
1:C:451:TYR:O	1:C:579:PRO:HD3	2.11	0.51
1:B:267:LYS:CE	1:B:331[A]:PHE:CE2	2.93	0.50
1:B:267:LYS:HE3	1:B:331[A]:PHE:HE2	1.75	0.50
1:B:212:TRP:CE2	1:B:371:LYS:HE3	2.47	0.50
1:B:378:LYS:HD3	1:B:378:LYS:N	2.26	0.50
1:D:634:ARG:HG3	1:D:644:LEU:HD23	1.93	0.49
1:A:103:LYS:HE2	1:A:110:ASP:OD1	2.13	0.48
1:C:413:TYR:CZ	1:C:534:ARG:HD2	2.48	0.48
1:A:134:ARG:O	1:A:138:THR:HG23	2.13	0.48
1:C:553:TYR:HA	1:C:568:LEU:HG	1.95	0.48
1:C:507:HIS:CE1	1:C:548:ASP:O	2.67	0.48
1:B:272:SER:C	1:B:273:GLN:HG2	2.33	0.47
1:B:267:LYS:HE3	1:B:331[A]:PHE:CE2	2.50	0.47
2:A:196:HOH:O	1:B:274:HIS:CE1	2.59	0.47
1:D:667:LYS:HE3	1:D:731[A]:PHE:CE2	2.49	0.47
1:D:778:LYS:N	1:D:778:LYS:HD3	2.29	0.47
1:C:467:LYS:HE3	1:C:531[A]:PHE:HE2	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HG2	1:A:116:TRP:HB3	1.98	0.46
1:D:699:GLU:HG2	1:D:718:LYS:HG2	1.96	0.46
1:C:509:LYS:HB2	1:C:509:LYS:NZ	2.30	0.46
1:D:700:LEU:O	1:D:717:PRO:HD2	2.15	0.46
1:A:107:HIS:HE1	1:A:148:ASP:O	1.98	0.45
1:C:464:LEU:HD22	1:C:488:VAL:HG22	1.98	0.45
1:B:267:LYS:HE2	1:B:331[A]:PHE:CE2	2.51	0.45
1:D:667:LYS:HE2	1:D:731[A]:PHE:CE2	2.52	0.45
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.69	0.45
1:A:153:TYR:HA	1:A:168:LEU:HG	1.99	0.44
1:D:719:PHE:HZ	1:D:732:GLU:HG3	1.83	0.44
1:D:667:LYS:HE3	1:D:731[A]:PHE:HE2	1.82	0.44
1:D:716:TRP:HA	1:D:717:PRO:HD3	1.82	0.44
1:D:754:TRP:CE2	1:D:766:SER:HB3	2.53	0.44
1:D:677:GLU:H	1:D:677:GLU:HG3	1.40	0.44
1:C:448:PRO:HB2	1:C:575:ASN:ND2	2.32	0.44
1:B:305:LYS:HB3	1:B:392:GLU:HG2	2.00	0.43
1:A:53:SER:HA	1:A:54:PRO:HD3	1.86	0.43
1:A:118:LYS:HE3	1:A:118:LYS:HB3	1.71	0.43
1:B:334:ARG:O	1:B:338:THR:HG23	2.18	0.43
1:A:173:GLU:CG	2:A:250:HOH:O	2.66	0.43
1:D:613:TYR:CE1	1:D:734:ARG:HD2	2.53	0.43
1:D:718:LYS:HB3	1:D:718:LYS:HE3	1.64	0.43
1:A:23:SER:HB3	1:A:35:ILE:CG2	2.48	0.42
1:B:234:ARG:HG3	1:B:244:LEU:CD2	2.49	0.42
1:B:314:LYS:HG2	1:B:316:TRP:NE1	2.34	0.42
1:B:383:ILE:HG21	1:B:383:ILE:HD13	1.82	0.42
1:B:300:LEU:O	1:B:317:PRO:HD2	2.20	0.41
1:C:423:SER:HB3	1:C:435:ILE:CG2	2.50	0.41
1:A:179:PRO:HA	1:A:180:PRO:HD3	1.94	0.41
1:C:507:HIS:HE1	1:C:548:ASP:O	2.04	0.41
1:A:183:ILE:HG21	1:A:183:ILE:HD13	1.65	0.40
1:C:448:PRO:HB2	1:C:575:ASN:HD22	1.87	0.40
1:D:667:LYS:HD2	1:D:731[A]:PHE:CD2	2.57	0.40
1:D:630:LEU:HA	1:D:630:LEU:HD12	1.96	0.40
1:D:629:SER:HB3	1:D:630:LEU:H	1.60	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	193/194 (100%)	187 (97%)	6 (3%)	0	100	100
1	B	193/194 (100%)	187 (97%)	5 (3%)	1 (0%)	34	21
1	C	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
1	D	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
All	All	772/776 (100%)	744 (96%)	27 (4%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	PRO

### 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	180/179 (101%)	171 (95%)	9 (5%)	30	14
1	B	180/179 (101%)	170 (94%)	10 (6%)	26	11
1	C	180/179 (101%)	169 (94%)	11 (6%)	23	9
1	D	180/179 (101%)	174 (97%)	6 (3%)	45	32
All	All	720/716 (101%)	684 (95%)	36 (5%)	31	14

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	67	LYS
1	A	93	LYS
1	A	99	GLU
1	A	113	LEU
1	A	131[A]	PHE
1	A	131[B]	PHE
1	A	139	GLN
1	A	165	GLN
1	B	208	ASP
1	B	267	LYS
1	B	277	GLU
1	B	314	LYS
1	B	323	GLN
1	B	370	LYS
1	B	378	LYS
1	B	380	PRO
1	B	389	ILE
1	B	394	ASN
1	C	408	ASP
1	C	453	SER
1	C	467	LYS
1	C	473	GLN
1	C	480	TYR
1	C	503	LYS
1	C	509	LYS
1	C	513	LEU
1	C	518	LYS
1	C	520	ASP
1	C	573	GLU
1	D	653	SER
1	D	677	GLU
1	D	696	THR
1	D	714	LYS
1	D	778	LYS
1	D	780	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	139	GLN
1	A	165	GLN

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Mol	Chain	Res	Type
1	A	175	ASN
1	B	273	GLN
1	B	274	HIS
1	B	307	HIS
1	B	335	HIS
1	B	375	ASN
1	C	507	HIS
1	C	541	HIS
1	C	575	ASN
1	D	741	HIS
1	D	765	GLN
1	D	775	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 carbohydrates 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.