



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3C03 / pdb_00003c03
Title : Crystal structure of the EscU C-terminal domain with P263A mutation,space group P 1 21 1
Authors : Zarivach, R.; Deng, W.; Vuckovic, M.; Felise, H.B.; Nguyen, H.V.; Miller, S.I.; Finlay, B.B.; Strynadka, N.C.J.
Deposited on : 2008-01-18
Resolution : 1.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

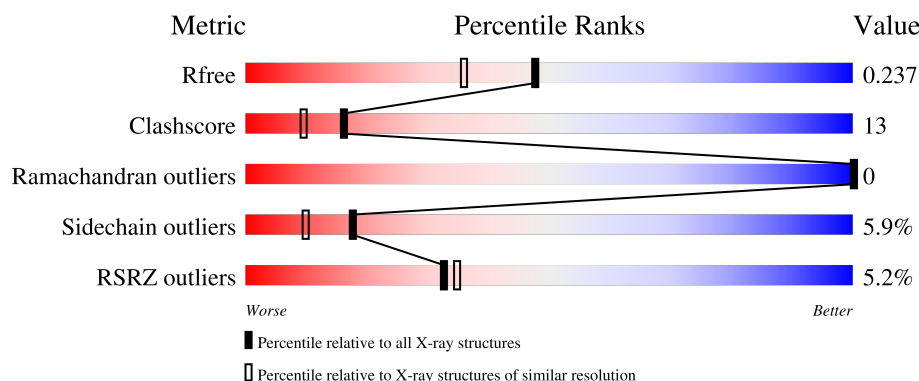
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	137	8% 53% 13% 29%
2	B	54	2% 15% 9% 9% 67%
3	C	83	8% 69% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1636 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 EscU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	4	0
			787	514	125	146	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	expression tag	UNP Q9AJ26
A	210	SER	-	expression tag	UNP Q9AJ26
A	211	HIS	-	expression tag	UNP Q9AJ26
A	212	MET	-	expression tag	UNP Q9AJ26
A	213	ALA	-	expression tag	UNP Q9AJ26
A	214	SER	-	expression tag	UNP Q9AJ26
A	263	ALA	PRO	engineered mutation	UNP Q9AJ26

- Molecule 2 is a protein called EscU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	0	0	0
			132	81	25	26			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	209	GLY	-	expression tag	UNP Q9AJ26
B	210	SER	-	expression tag	UNP Q9AJ26
B	211	HIS	-	expression tag	UNP Q9AJ26
B	212	MET	-	expression tag	UNP Q9AJ26
B	213	ALA	-	expression tag	UNP Q9AJ26
B	214	SER	-	expression tag	UNP Q9AJ26
B	262	SNN	ASN	SEE REMARK 999	UNP Q9AJ26

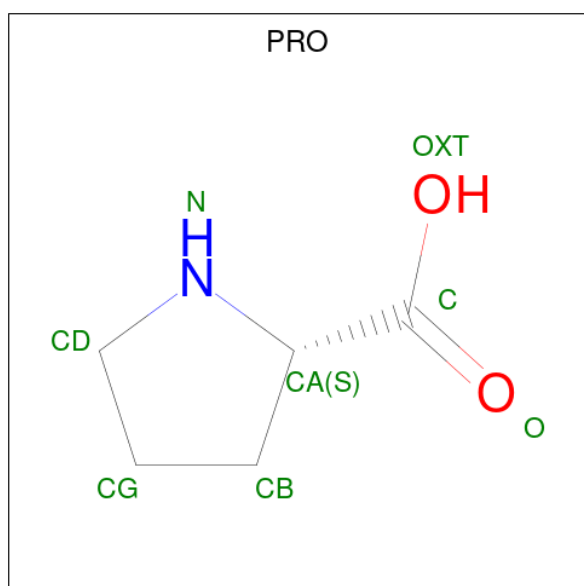
- Molecule 3 is a protein called EscU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total 646	C 428	N 100	O 117	S 1	3	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	263	ALA	PRO	engineered mutation	UNP Q9AJ26

- Molecule 4 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 8	C 5	N 1	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total 42	O 42	0	0
5	B	4	Total 4	O 4	0	0
5	C	17	Total 17	O 17	0	0

- Molecule 1: EscU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.11Å 55.48Å 50.45Å 90.00° 108.69° 90.00°	Depositor
Resolution (Å)	16.00 – 1.90 16.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (16.00-1.90) 97.3 (16.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.239 0.181 , 0.237	Depositor DCC
R_{free} test set	731 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1636	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SNN

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	1.06	2/806 (0.2%)	1.00	1/1095 (0.1%)
2	B	1.34	1/123 (0.8%)	1.52	5/163 (3.1%)
3	C	0.89	1/662 (0.2%)	1.01	1/900 (0.1%)
All	All	1.02	4/1591 (0.3%)	1.05	7/2158 (0.3%)

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
3	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	260	VAL	C-N	7.96	1.44	1.33
1	A	309	ILE	CA-CB	7.26	1.58	1.54
1	A	342	ASP	CG-OD2	5.97	1.36	1.25
3	C	339	ILE	CG1-CD1	5.59	1.73	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	265	HIS	N-CA-C	-11.18	91.42	109.76
2	B	250	ALA	N-CA-C	7.44	121.27	111.75
2	B	252	ASN	N-CA-C	-6.11	104.54	111.14
2	B	253	ILE	N-CA-C	-6.04	104.45	110.62
2	B	251	ASN	N-CA-C	5.77	117.65	111.36
1	A	288	ASP	CB-CA-C	-5.59	110.15	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	260	VAL	O-C-N	5.48	129.12	123.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	264	THR	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	787	0	830	17	0
2	B	132	0	139	14	0
3	C	646	0	675	17	0
4	A	8	0	7	2	0
5	A	42	0	0	1	0
5	B	4	0	0	2	0
5	C	17	0	0	1	0
All	All	1636	0	1651	42	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 13.

All (42) 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:256[B]:SER:HB3	1:A:269[B]:CYS:SG	2.15	0.86
4:A:4:PRO:O	5:A:362:HOH:O	1.93	0.86
1:A:256[A]:SER:OG	1:A:283:ILE:HD11	1.76	0.85
1:A:295:ILE:O	1:A:299:GLU:HG2	1.78	0.83
2:B:248:SER:O	5:B:80:HOH:O	2.03	0.76
2:B:259:ILE:CD1	3:C:298:ALA:HB2	2.16	0.75
1:A:256[B]:SER:CB	1:A:269[B]:CYS:SG	2.76	0.73
1:A:331[A]:GLU:HB3	1:A:332:PRO:HD3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLN:HE21	2:B:245:GLN:N	1.86	0.72
2:B:260:VAL:HG12	3:C:268:ILE:HB	1.75	0.68
2:B:245:GLN:N	2:B:245:GLN:NE2	2.45	0.64
3:C:327:GLU:HG2	3:C:330:PHE:CE1	2.34	0.62
1:A:320:HIS:CE1	4:A:4:PRO:HG2	2.35	0.62
3:C:335:GLN:NE2	5:C:75:HOH:O	2.33	0.61
2:B:259:ILE:HD12	3:C:298:ALA:CB	2.32	0.59
2:B:259:ILE:CD1	3:C:298:ALA:CB	2.81	0.57
1:A:264:THR:HG22	1:A:292:LEU:HD11	1.87	0.57
3:C:305:VAL:C	3:C:306:ILE:HD13	2.31	0.55
2:B:260:VAL:CG1	3:C:268:ILE:HB	2.38	0.54
2:B:260:VAL:HG11	3:C:315:LEU:HD12	1.90	0.54
3:C:265:HIS:HB2	3:C:288:ASP:HA	1.88	0.53
3:C:340:ALA:O	3:C:343:LEU:HB2	2.10	0.52
1:A:339:ILE:O	1:A:342:ASP:HB2	2.12	0.50
2:B:245:GLN:HG2	2:B:245:GLN:O	2.13	0.49
2:B:252:ASN:ND2	5:B:80:HOH:O	2.46	0.48
3:C:331:GLU:OE1	3:C:335:GLN:HG2	2.13	0.48
1:A:331[A]:GLU:HB3	1:A:332:PRO:CD	2.43	0.47
2:B:252:ASN:O	2:B:253:ILE:C	2.57	0.47
1:A:262:ASN:C	1:A:262:ASN:ND2	2.70	0.46
1:A:308:ASP:OD1	1:A:308:ASP:C	2.59	0.46
2:B:259:ILE:HD12	3:C:298:ALA:HB1	1.97	0.45
3:C:272:TYR:OH	3:C:274:LEU:HD13	2.17	0.44
1:A:265:HIS:O	1:A:287:LYS:HA	2.17	0.44
1:A:309:ILE:HB	1:A:310:PRO:HD3	1.99	0.44
1:A:305:VAL:C	1:A:306:ILE:HD12	2.44	0.42
3:C:331:GLU:N	3:C:332:PRO:CD	2.83	0.42
3:C:306:ILE:HD13	3:C:306:ILE:N	2.35	0.41
1:A:306:ILE:HD12	1:A:306:ILE:N	2.35	0.41
1:A:339:ILE:O	1:A:343:LEU:HG	2.20	0.41
3:C:311:LEU:HD23	3:C:336:LEU:HD11	2.02	0.41
1:A:304:PRO:HB3	1:A:343:LEU:HD12	2.03	0.41
2:B:247:GLY:O	2:B:250:ALA:HB3	2.20	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	99/137 (72%)	99 (100%)	0	0	100	100
2	B	16/54 (30%)	16 (100%)	0	0	100	100
3	C	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
All	All	194/274 (71%)	192 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	88/119 (74%)	82 (93%)	6 (7%)	14	7
2	B	15/46 (33%)	14 (93%)	1 (7%)	15	7
3	C	70/72 (97%)	66 (94%)	4 (6%)	18	11
All	All	173/237 (73%)	162 (94%)	11 (6%)	18	8

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	292	LEU
1	A	293	GLN
1	A	299	GLU
1	A	331[A]	GLU

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Mol	Chain	Res	Type
1	A	331[B]	GLU
2	B	245	GLN
3	C	274	LEU
3	C	302	ASP
3	C	328	ASP
3	C	338	ARG

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

Mol	Chain	Res	Type
1	A	262	ASN
1	A	320	HIS
1	A	335	GLN
2	B	245	GLN
2	B	251	ASN
3	C	265	HIS
3	C	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SNN	B	262	2	7,8,8	3.22	2 (28%)	10,11,11	1.53	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SNN	B	262	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	262	SNN	C5-N1	-6.53	1.26	1.37
2	B	262	SNN	C-N1	-5.13	1.31	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	262	SNN	C4-CA-C	-2.51	101.47	104.30
2	B	262	SNN	C5-N1-C	-2.45	111.50	113.96
2	B	262	SNN	CA-C-N1	2.05	108.90	107.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PRO	A	4	-	8,8,8	0.94	1 (12%)	10,10,10	1.39	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PRO	A	4	-	-	0/4/11/11	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4	PRO	OXT-C	-2.20	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	PRO	OXT-C-O	-2.40	118.63	124.08
4	A	4	PRO	OXT-C-CA	2.31	121.33	113.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4	PRO	2	0

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 [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	97/137 (70%)	0.03	2 (2%) 63 67	6, 19, 27, 34	5 (5%)
2	B	17/54 (31%)	0.30	1 (5%) 28 30	19, 33, 39, 48	0
3	C	80/83 (96%)	0.49	7 (8%) 15 16	15, 28, 37, 50	2 (2%)
All	All	194/274 (70%)	0.25	10 (5%) 33 35	6, 22, 37, 50	7 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	322	GLY	3.5
3	C	265	HIS	3.0
3	C	324	TYR	3.0
1	A	247	GLY	2.7
3	C	339	ILE	2.6
1	A	337	ILE	2.5
3	C	337	ILE	2.5
3	C	343	LEU	2.4
3	C	321	LYS	2.3
2	B	250	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SNN	B	262	8/8	0.74	0.12	49,52,54,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PRO	A	4	8/8	0.83	0.11	80,80,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.