



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 21, 2022 – 07:52 pm GMT

PDB ID : 7BHG  
Title : Gene-engineered variant of FusionRed with Trp based chromophore - 2.1A  
Authors : Pletnev, V.Z.; Pletnev, S.V.; Pletneva, N.V.  
Deposited on : 2021-01-11  
Resolution : 2.09 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

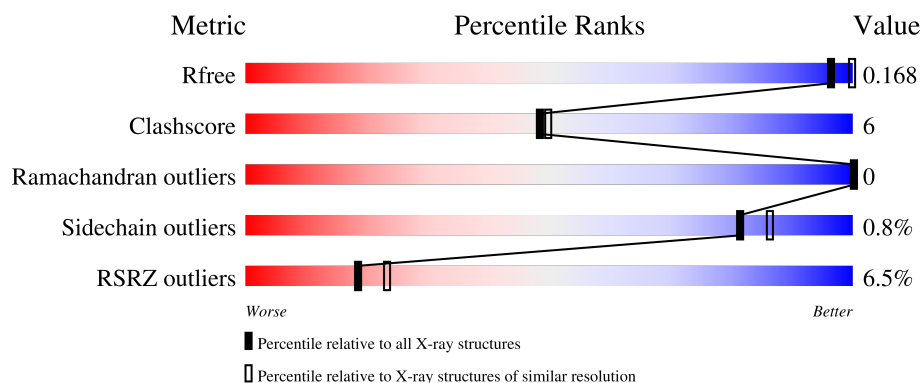
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	249	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	249	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TUK	A	65	X	-	-	-
1	TUK	B	65	X	-	-	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3688 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 Fluorescent protein FP480.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1773	1128	298	334	13			
1	B	223	Total	C	N	O	S	0	0	0
			1773	1128	298	334	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP D0VX33
A	-16	ARG	-	expression tag	UNP D0VX33
A	-15	GLY	-	expression tag	UNP D0VX33
A	-14	SER	-	expression tag	UNP D0VX33
A	-13	HIS	-	expression tag	UNP D0VX33
A	-12	HIS	-	expression tag	UNP D0VX33
A	-11	HIS	-	expression tag	UNP D0VX33
A	-10	HIS	-	expression tag	UNP D0VX33
A	-9	HIS	-	expression tag	UNP D0VX33
A	-8	HIS	-	expression tag	UNP D0VX33
A	-7	GLY	-	expression tag	UNP D0VX33
A	-6	SER	-	expression tag	UNP D0VX33
A	-5	LEU	-	expression tag	UNP D0VX33
A	-4	PRO	-	expression tag	UNP D0VX33
A	-3	VAL	-	expression tag	UNP D0VX33
A	-2	ALA	-	expression tag	UNP D0VX33
A	-1	THR	-	expression tag	UNP D0VX33
A	0	MET	-	expression tag	UNP D0VX33
A	1	VAL	-	expression tag	UNP D0VX33
A	6	LYS	THR	conflict	UNP D0VX33
A	10	PRO	HIS	conflict	UNP D0VX33
A	11	THR	MET	conflict	UNP D0VX33
A	41	MET	GLN	conflict	UNP D0VX33
A	65	TUK	MET	chromophore	UNP D0VX33
A	65	TUK	TYR	chromophore	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	65	TUK	GLY	chromophore	UNP D0VX33
A	67	ARG	HIS	conflict	UNP D0VX33
A	71	LYS	ASN	conflict	UNP D0VX33
A	73	PRO	THR	conflict	UNP D0VX33
A	74	PRO	GLN	conflict	UNP D0VX33
A	80	PHE	TRP	conflict	UNP D0VX33
A	121	VAL	ILE	conflict	UNP D0VX33
A	143	SER	HIS	conflict	UNP D0VX33
A	146	THR	MET	conflict	UNP D0VX33
A	147	MET	LEU	conflict	UNP D0VX33
A	158	CYS	ALA	conflict	UNP D0VX33
A	160	MET	LEU	conflict	UNP D0VX33
A	174	LEU	PHE	conflict	UNP D0VX33
A	185	THR	LYS	conflict	UNP D0VX33
A	186	LYS	ASN	conflict	UNP D0VX33
A	197	HIS	TYR	conflict	UNP D0VX33
A	207	ASP	LYS	conflict	UNP D0VX33
B	-17	MET	-	initiating methionine	UNP D0VX33
B	-16	ARG	-	expression tag	UNP D0VX33
B	-15	GLY	-	expression tag	UNP D0VX33
B	-14	SER	-	expression tag	UNP D0VX33
B	-13	HIS	-	expression tag	UNP D0VX33
B	-12	HIS	-	expression tag	UNP D0VX33
B	-11	HIS	-	expression tag	UNP D0VX33
B	-10	HIS	-	expression tag	UNP D0VX33
B	-9	HIS	-	expression tag	UNP D0VX33
B	-8	HIS	-	expression tag	UNP D0VX33
B	-7	GLY	-	expression tag	UNP D0VX33
B	-6	SER	-	expression tag	UNP D0VX33
B	-5	LEU	-	expression tag	UNP D0VX33
B	-4	PRO	-	expression tag	UNP D0VX33
B	-3	VAL	-	expression tag	UNP D0VX33
B	-2	ALA	-	expression tag	UNP D0VX33
B	-1	THR	-	expression tag	UNP D0VX33
B	0	MET	-	expression tag	UNP D0VX33
B	1	VAL	-	expression tag	UNP D0VX33
B	6	LYS	THR	conflict	UNP D0VX33
B	10	PRO	HIS	conflict	UNP D0VX33
B	11	THR	MET	conflict	UNP D0VX33
B	41	MET	GLN	conflict	UNP D0VX33
B	65	TUK	MET	chromophore	UNP D0VX33
B	65	TUK	TYR	chromophore	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	65	TUK	GLY	chromophore	UNP D0VX33
B	67	ARG	HIS	conflict	UNP D0VX33
B	71	LYS	ASN	conflict	UNP D0VX33
B	73	PRO	THR	conflict	UNP D0VX33
B	74	PRO	GLN	conflict	UNP D0VX33
B	80	PHE	TRP	conflict	UNP D0VX33
B	121	VAL	ILE	conflict	UNP D0VX33
B	143	SER	HIS	conflict	UNP D0VX33
B	146	THR	MET	conflict	UNP D0VX33
B	147	MET	LEU	conflict	UNP D0VX33
B	158	CYS	ALA	conflict	UNP D0VX33
B	160	MET	LEU	conflict	UNP D0VX33
B	174	LEU	PHE	conflict	UNP D0VX33
B	185	THR	LYS	conflict	UNP D0VX33
B	186	LYS	ASN	conflict	UNP D0VX33
B	197	HIS	TYR	conflict	UNP D0VX33
B	207	ASP	LYS	conflict	UNP D0VX33


- Molecule 2 is water.

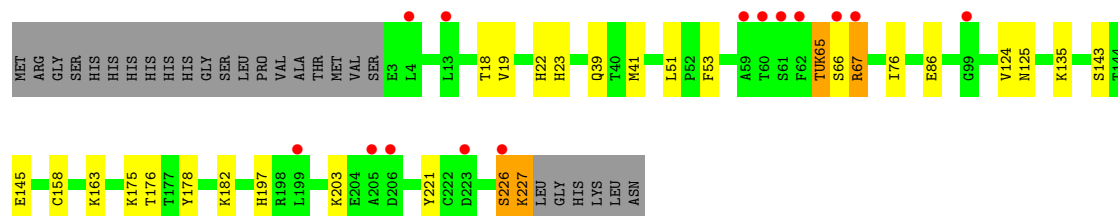
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	66	Total O 66 66	0	0

### 3 Residue-property plots


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.

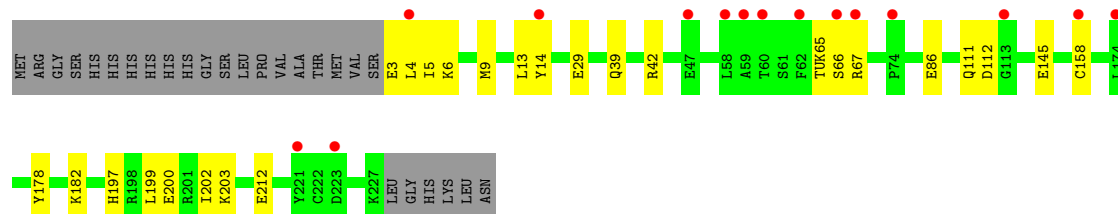
#### • Molecule 1: Fluorescent protein FP480

Chain A: 



#### • Molecule 1: Fluorescent protein FP480

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.85Å 92.23Å 58.00Å 90.00° 111.83° 90.00°	Depositor
Resolution (Å)	28.99 – 2.09 28.97 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.7 (28.99-2.09) 98.7 (28.97-2.09)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.163 , 0.230 0.173 , 0.168	Depositor DCC
$R_{free}$ test set	1332 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.87	1/1790 (0.1%)	0.83	0/2419
1	B	0.74	0/1790	0.85	0/2419
All	All	0.81	1/3580 (0.0%)	0.84	0/4838

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	1	1
1	B	1	0
All	All	2	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	SER	CB-OG	-14.08	1.24	1.42

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	65	TUK	C1
1	B	65	TUK	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	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	1773	0	1717	26	0
1	B	1773	0	1717	17	0
2	A	76	0	0	3	0
2	B	66	0	0	1	0
All	All	3688	0	3434	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 6.

The worst 5 of 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:67:ARG:HH12	1:A:197:HIS:CE1	1.66	1.14
1:A:67:ARG:NH1	1:A:197:HIS:HE1	1.63	0.96
1:A:41:MET:HG3	1:A:65:TUK:CE1	1.99	0.93
1:A:67:ARG:HH12	1:A:197:HIS:HE1	0.91	0.90
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.39	0.86

There are no symmetry-related clashes.

## 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	220/249 (88%)	216 (98%)	4 (2%)	0	100	100
1	B	220/249 (88%)	214 (97%)	6 (3%)	0	100	100
All	All	440/498 (88%)	430 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	191/213 (90%)	189 (99%)	2 (1%)	76	82
1	B	191/213 (90%)	190 (100%)	1 (0%)	88	92
All	All	382/426 (90%)	379 (99%)	3 (1%)	81	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	LYS
1	A	227	LYS
1	B	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	197	HIS
1	B	39	GLN
1	B	197	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z  > 2$
1	TUK	B	65	1	26,27,27	2.47	10 (38%)	24,37,37	5.08	16 (66%)
1	TUK	A	65	1	26,27,27	2.18	8 (30%)	24,37,37	5.44	14 (58%)

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
1	TUK	B	65	1	1/1/5/6	5/10/31/31	0/3/3/3
1	TUK	A	65	1	1/1/5/6	5/10/31/31	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	TUK	CB2-CA2	-7.01	1.43	1.50
1	A	65	TUK	CB2-CA2	-5.37	1.44	1.50
1	B	65	TUK	C1-N2	-4.85	1.34	1.46
1	A	65	TUK	C1-N2	-4.76	1.34	1.46
1	B	65	TUK	CA1-C1	-4.63	1.46	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	TUK	CA1-C1-N3	16.24	132.83	112.48
1	B	65	TUK	CA1-C1-N3	14.94	131.20	112.48
1	A	65	TUK	CB2-CA2-C2	11.18	142.31	128.44
1	B	65	TUK	CA3-N3-C1	11.08	133.29	124.24
1	A	65	TUK	CA3-N3-C1	9.20	131.76	124.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	65	TUK	C1
1	B	65	TUK	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	65	TUK	C2-CA2-CB2-CG2
1	A	65	TUK	N2-CA2-CB2-CG2
1	B	65	TUK	C2-CA2-CB2-CG2
1	B	65	TUK	N2-CA2-CB2-CG2
1	B	65	TUK	CA1-CB1-CG1-SD1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	65	TUK	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [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, 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	222/249 (89%)	0.04	14 (6%) 20 24	37, 46, 62, 90	0
1	B	222/249 (89%)	0.11	15 (6%) 17 21	36, 47, 67, 85	0
All	All	444/498 (89%)	0.08	29 (6%) 18 23	36, 47, 65, 90	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	THR	3.8
1	A	59	ALA	3.7
1	A	66	SER	3.6
1	A	62	PHE	3.3
1	A	60	THR	3.2

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TUK	A	65	25/25	0.90	0.36	61,72,86,88	0
1	TUK	B	65	25/25	0.92	0.37	63,75,81,84	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.