



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:31 PM BST

PDB ID : 6B7R  
Title : Truncated strand 11-less green fluorescent protein  
Authors : Deng, A.; Boxer, S.G.  
Deposited on : 2017-10-05  
Resolution : 1.73 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

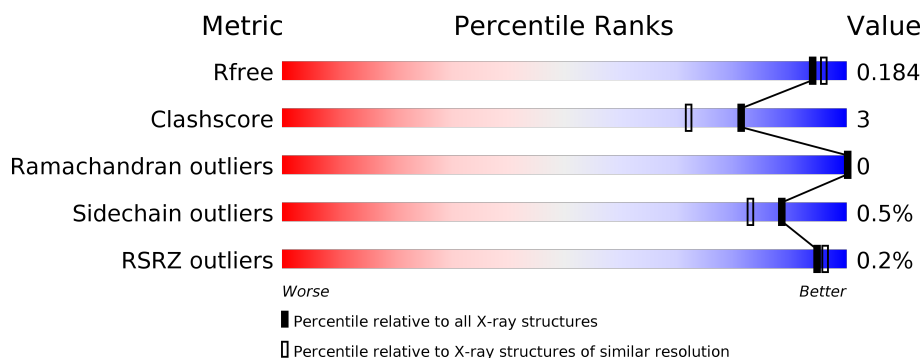
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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 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	236	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> <div>91% 6% .</div>
1	B	236	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> <div style="width: 2%;"></div> </div> <div>92% . .</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4005 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	228	Total	C	N	O	S	0	1	0
			1793	1134	317	338	4			
1	A	228	Total	C	N	O	S	0	1	0
			1794	1134	318	338	4			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP P42212
B	-22	GLY	-	expression tag	UNP P42212
B	-21	SER	-	expression tag	UNP P42212
B	-20	SER	-	expression tag	UNP P42212
B	-19	HIS	-	expression tag	UNP P42212
B	-18	HIS	-	expression tag	UNP P42212
B	-17	HIS	-	expression tag	UNP P42212
B	-16	HIS	-	expression tag	UNP P42212
B	-15	HIS	-	expression tag	UNP P42212
B	-14	HIS	-	expression tag	UNP P42212
B	-13	SER	-	expression tag	UNP P42212
B	-12	SER	-	expression tag	UNP P42212
B	-11	GLY	-	expression tag	UNP P42212
B	-10	LEU	-	expression tag	UNP P42212
B	-9	VAL	-	expression tag	UNP P42212
B	-8	PRO	-	expression tag	UNP P42212
B	-7	GLY	-	expression tag	UNP P42212
B	-6	GLY	-	expression tag	UNP P42212
B	-5	SER	-	expression tag	UNP P42212
B	-4	HIS	-	expression tag	UNP P42212
B	-3	MET	-	expression tag	UNP P42212
B	-2	GLY	-	expression tag	UNP P42212
B	-1	GLY	-	expression tag	UNP P42212
B	0	THR	-	expression tag	UNP P42212
B	1	SER	-	expression tag	UNP P42212

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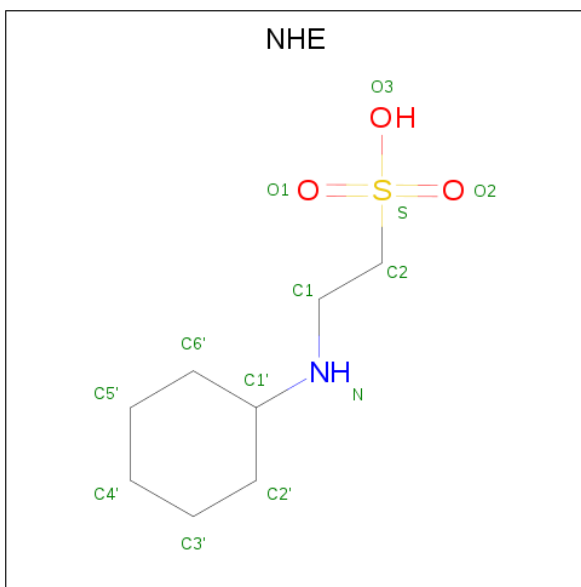
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ARG	SER	engineered mutation	UNP P42212
B	39	ILE	TYR	engineered mutation	UNP P42212
B	48	SER	CYS	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	GYS	SER	chromophore	UNP P42212
B	66	GYS	TYR	chromophore	UNP P42212
B	66	GYS	GLY	chromophore	UNP P42212
B	70	ALA	CYS	engineered mutation	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	105	LYS	ASN	engineered mutation	UNP P42212
B	111	VAL	GLU	engineered mutation	UNP P42212
B	128	THR	ILE	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	166	THR	LYS	engineered mutation	UNP P42212
B	167	VAL	ILE	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	205	THR	SER	conflict	UNP P42212
B	206	LYS	ALA	engineered mutation	UNP P42212
A	-23	MET	-	expression tag	UNP P42212
A	-22	GLY	-	expression tag	UNP P42212
A	-21	SER	-	expression tag	UNP P42212
A	-20	SER	-	expression tag	UNP P42212
A	-19	HIS	-	expression tag	UNP P42212
A	-18	HIS	-	expression tag	UNP P42212
A	-17	HIS	-	expression tag	UNP P42212
A	-16	HIS	-	expression tag	UNP P42212
A	-15	HIS	-	expression tag	UNP P42212
A	-14	HIS	-	expression tag	UNP P42212
A	-13	SER	-	expression tag	UNP P42212
A	-12	SER	-	expression tag	UNP P42212
A	-11	GLY	-	expression tag	UNP P42212
A	-10	LEU	-	expression tag	UNP P42212
A	-9	VAL	-	expression tag	UNP P42212
A	-8	PRO	-	expression tag	UNP P42212
A	-7	GLY	-	expression tag	UNP P42212
A	-6	GLY	-	expression tag	UNP P42212
A	-5	SER	-	expression tag	UNP P42212
A	-4	HIS	-	expression tag	UNP P42212
A	-3	MET	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P42212
A	-1	GLY	-	expression tag	UNP P42212
A	0	THR	-	expression tag	UNP P42212
A	1	SER	-	expression tag	UNP P42212
A	30	ARG	SER	engineered mutation	UNP P42212
A	39	ILE	TYR	engineered mutation	UNP P42212
A	48	SER	CYS	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
A	70	ALA	CYS	engineered mutation	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	105	LYS	ASN	engineered mutation	UNP P42212
A	111	VAL	GLU	engineered mutation	UNP P42212
A	128	THR	ILE	engineered mutation	UNP P42212
A	145	PHE	TYR	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	166	THR	LYS	engineered mutation	UNP P42212
A	167	VAL	ILE	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	205	THR	SER	conflict	UNP P42212
A	206	LYS	ALA	engineered mutation	UNP P42212

- Molecule 2 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	182	Total	O	0	0
			182	182		
3	A	184	Total	O	0	0
			184	184		

### 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: Green fluorescent protein

Chain B:  92% . .



- Molecule 1: Green fluorescent protein

Chain A:  91% 6% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.55Å 55.55Å 139.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 1.73 29.60 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.60-1.73) 99.7 (29.60-1.72)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.158 , 0.184 0.157 , 0.184	Depositor DCC
$R_{free}$ test set	2162 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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

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

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	0.35	0/1816	0.55	0/2453
1	B	0.36	0/1815	0.56	0/2451
All	All	0.35	0/3631	0.56	0/4904

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1794	0	1738	12	0
1	B	1793	0	1737	7	0
2	A	26	0	34	0	0
2	B	26	0	34	1	0
3	A	184	0	0	4	3
3	B	182	0	0	2	4
All	All	4005	0	3543	19	4

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 3.

All (19) 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:90:GLU:HG2	3:A:561:HOH:O	1.83	0.78
1:A:73:ARG:NH2	3:A:401:HOH:O	2.24	0.69
1:A:66:GYS:OH	1:A:148:HIS:HD2	1.77	0.67
1:A:148:HIS:HE1	1:A:168:ARG:H	1.46	0.63
1:A:147:SER:HB3	3:A:412:HOH:O	1.98	0.62
1:B:135:ASN:HA	1:B:140:LYS:HD2	1.82	0.60
1:A:148:HIS:CE1	1:A:168:ARG:H	2.19	0.59
1:B:155:ASP:OD2	1:B:184:GLN:NE2	2.36	0.57
1:B:17:GLU:HG3	1:B:30:ARG:CZ	2.38	0.53
1:B:80:ARG:HG3	2:B:302:NHE:H5'2	1.95	0.48
1:B:147:SER:HB3	3:B:412:HOH:O	2.13	0.47
1:B:184:GLN:HG3	3:B:401:HOH:O	2.14	0.47
1:B:3:LYS:HE3	1:B:6:GLU:OE2	2.14	0.47
1:A:17:GLU:OE2	1:A:122:ARG:NH1	2.49	0.46
1:A:17:GLU:CD	1:A:122:ARG:NH1	2.72	0.43
1:A:150:VAL:HB	1:A:201:LEU:HB2	2.02	0.42
1:A:3:LYS:HB3	1:A:3:LYS:HE3	1.93	0.41
1:A:150:VAL:O	1:A:200:TYR:HA	2.21	0.41
1:A:184:GLN:HG3	3:A:402:HOH:O	2.21	0.40

All (4) 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)
3:B:405:HOH:O	3:A:464:HOH:O[1_445]	1.85	0.35
3:B:571:HOH:O	3:A:553:HOH:O[3_544]	1.95	0.25
3:B:567:HOH:O	3:A:569:HOH:O[3_444]	2.02	0.18
3:B:427:HOH:O	3:B:537:HOH:O[4_545]	2.09	0.11

## 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	226/236 (96%)	223 (99%)	3 (1%)	0	100	100
1	B	226/236 (96%)	222 (98%)	4 (2%)	0	100	100
All	All	452/472 (96%)	445 (98%)	7 (2%)	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	193/203 (95%)	192 (100%)	1 (0%)	88	83
1	B	193/203 (95%)	192 (100%)	1 (0%)	88	83
All	All	386/406 (95%)	384 (100%)	2 (0%)	88	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	ARG
1	A	80	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	170	ASN

### 5.3.3 RNA ⓘ

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	GYS	A	66	1	22,22,23	1.35	3 (13%)	27,30,32	1.56	4 (14%)
1	GYS	B	66	1	22,22,23	1.38	4 (18%)	27,30,32	1.57	3 (11%)

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	GYS	A	66	1	-	1/9/29/30	0/2/2/2
1	GYS	B	66	1	-	2/9/29/30	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CA2-N2	3.07	1.45	1.38
1	B	66	GYS	O-C	3.04	1.37	1.19
1	B	66	GYS	C1-N3	2.94	1.42	1.37
1	A	66	GYS	O-C	2.81	1.35	1.19
1	A	66	GYS	C1-N3	2.61	1.41	1.37
1	B	66	GYS	CA2-N2	2.38	1.43	1.38
1	B	66	GYS	CE1-CZ	2.05	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	O-C-CA3	-5.72	109.12	126.39
1	A	66	GYS	O-C-CA3	-5.62	109.42	126.39
1	A	66	GYS	CA3-N3-C1	3.03	130.80	127.16
1	B	66	GYS	CA3-N3-C1	2.98	130.74	127.16
1	B	66	GYS	CA1-C1-N3	-2.24	121.93	124.85
1	A	66	GYS	N3-C1-N2	2.06	112.88	111.45
1	A	66	GYS	CA1-C1-N3	-2.01	122.23	124.85

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	GYS	N2-CA2-CB2-CG2
1	A	66	GYS	N2-CA2-CB2-CG2
1	B	66	GYS	C2-CA2-CB2-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	GYS	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z  > 2$
2	NHE	A	302	-	13,13,13	1.49	3 (23%)	16,17,17	1.73	6 (37%)
2	NHE	B	301	-	13,13,13	1.30	3 (23%)	16,17,17	2.06	4 (25%)
2	NHE	A	301	-	13,13,13	1.27	3 (23%)	16,17,17	2.00	5 (31%)
2	NHE	B	302	-	13,13,13	1.33	3 (23%)	16,17,17	1.61	5 (31%)

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	NHE	A	302	-	-	3/7/15/15	0/1/1/1
2	NHE	B	301	-	-	1/7/15/15	0/1/1/1
2	NHE	A	301	-	-	2/7/15/15	0/1/1/1
2	NHE	B	302	-	-	0/7/15/15	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	NHE	C2-S	3.91	1.83	1.77
2	B	302	NHE	C2-S	3.36	1.82	1.77
2	B	301	NHE	C2-S	2.91	1.81	1.77
2	A	301	NHE	C2-S	2.77	1.81	1.77
2	A	302	NHE	O1-S	2.22	1.51	1.45
2	A	301	NHE	O2-S	2.20	1.51	1.45
2	B	301	NHE	O1-S	2.20	1.51	1.45
2	B	301	NHE	O2-S	2.17	1.51	1.45
2	A	302	NHE	O2-S	2.14	1.51	1.45
2	B	302	NHE	O1-S	2.13	1.51	1.45
2	B	302	NHE	O2-S	2.07	1.51	1.45
2	A	301	NHE	O1-S	2.03	1.51	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NHE	O1-S-C2	4.58	112.43	106.92
2	A	301	NHE	O3-S-O2	-3.90	101.74	111.27
2	B	301	NHE	O2-S-O1	-3.76	100.94	113.95
2	A	301	NHE	O2-S-C2	3.47	111.09	106.92
2	A	301	NHE	O3-S-C2	3.46	111.36	105.77
2	A	302	NHE	O2-S-O1	-3.10	103.22	113.95
2	B	302	NHE	O1-S-C2	3.09	110.63	106.92
2	B	301	NHE	O2-S-C2	3.08	110.62	106.92
2	B	302	NHE	O2-S-O1	-2.97	103.66	113.95
2	A	302	NHE	O2-S-C2	2.81	110.30	106.92
2	B	301	NHE	O3-S-C2	2.62	110.01	105.77
2	A	302	NHE	O1-S-C2	2.61	110.05	106.92
2	A	302	NHE	C3'-C2'-C1'	2.56	115.92	111.11
2	A	301	NHE	O1-S-C2	2.55	109.99	106.92
2	A	302	NHE	O3-S-C2	2.34	109.56	105.77
2	A	301	NHE	C1-N-C1'	-2.23	109.75	114.14
2	B	302	NHE	O2-S-C2	2.17	109.52	106.92
2	A	302	NHE	C4'-C5'-C6'	2.06	115.62	111.42
2	B	302	NHE	C5'-C6'-C1'	2.03	114.94	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	302	NHE	O3-S-C2	2.03	109.04	105.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	NHE	C6'-C1'-N-C1
2	B	301	NHE	C1-C2-S-O2
2	A	301	NHE	C1-C2-S-O3
2	A	302	NHE	N-C1-C2-S
2	A	301	NHE	C1-C2-S-O1
2	A	302	NHE	C2'-C1'-N-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	NHE	1	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, 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	227/236 (96%)	-0.21	0	100   100	16, 24, 39, 48	0
1	B	227/236 (96%)	-0.23	1 (0%)	92   94	16, 24, 38, 47	0
All	All	454/472 (96%)	-0.22	1 (0%)	95   96	16, 24, 39, 48	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-18	HIS	2.0

### 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	GYS	B	66	21/22	0.95	0.07	14,17,20,23	0
1	GYS	A	66	21/22	0.96	0.08	13,15,20,22	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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
2	NHE	A	302	13/13	0.93	0.11	26,32,38,49	0
2	NHE	A	301	13/13	0.93	0.11	34,41,52,52	0
2	NHE	B	301	13/13	0.95	0.13	30,40,54,55	0
2	NHE	B	302	13/13	0.95	0.12	26,30,39,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.