



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:13 PM GMT

PDB ID : 1EMC  
Title : GREEN FLUORESCENT PROTEIN FROM AEQUOREA VICTORIA, MUTANT  
Authors : Palm, G.; Zdanov, A.; Wlodawer, A.  
Deposited on : 1997-03-31  
Resolution : 2.30 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.

---

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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

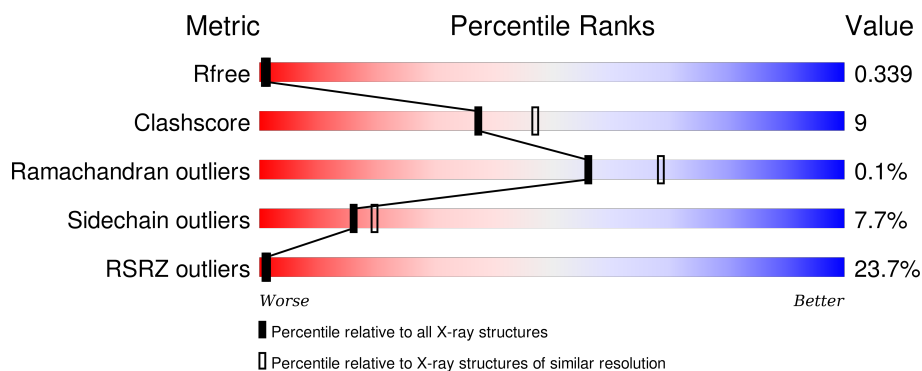
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>7%</div> <div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	B	237	<div> <div>4%</div> <div> <div>72%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	C	237	<div> <div>42%</div> <div> <div>64%</div> <div>29%</div> <div>• 5%</div> </div> </div>
1	D	237	<div> <div>36%</div> <div> <div>69%</div> <div>25%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7354 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	A	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			
1	B	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			
1	C	226	Total	C	N	O	S	0	1	0
			1811	1151	308	346	6			
1	D	225	Total	C	N	O	S	0	1	0
			1795	1142	302	345	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	PHE	ENGINEERED	UNP P42212
A	66	GYS	SER	CHROMOPHORE	UNP P42212
A	66	GYS	TYR	CHROMOPHORE	UNP P42212
A	66	GYS	GLY	CHROMOPHORE	UNP P42212
A	80	ARG	GLN	CONFLICT	UNP P42212
A	167	THR	ILE	ENGINEERED	UNP P42212
B	64	LEU	PHE	ENGINEERED	UNP P42212
B	66	GYS	SER	CHROMOPHORE	UNP P42212
B	66	GYS	TYR	CHROMOPHORE	UNP P42212
B	66	GYS	GLY	CHROMOPHORE	UNP P42212
B	80	ARG	GLN	CONFLICT	UNP P42212
B	167	THR	ILE	ENGINEERED	UNP P42212
C	64	LEU	PHE	ENGINEERED	UNP P42212
C	66	GYS	SER	CHROMOPHORE	UNP P42212
C	66	GYS	TYR	CHROMOPHORE	UNP P42212
C	66	GYS	GLY	CHROMOPHORE	UNP P42212
C	80	ARG	GLN	CONFLICT	UNP P42212
C	167	THR	ILE	ENGINEERED	UNP P42212
D	64	LEU	PHE	ENGINEERED	UNP P42212
D	66	GYS	SER	CHROMOPHORE	UNP P42212
D	66	GYS	TYR	CHROMOPHORE	UNP P42212

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	GYS	GLY	CHROMOPHORE	UNP P42212
D	80	ARG	GLN	CONFLICT	UNP P42212
D	167	THR	ILE	ENGINEERED	UNP P42212

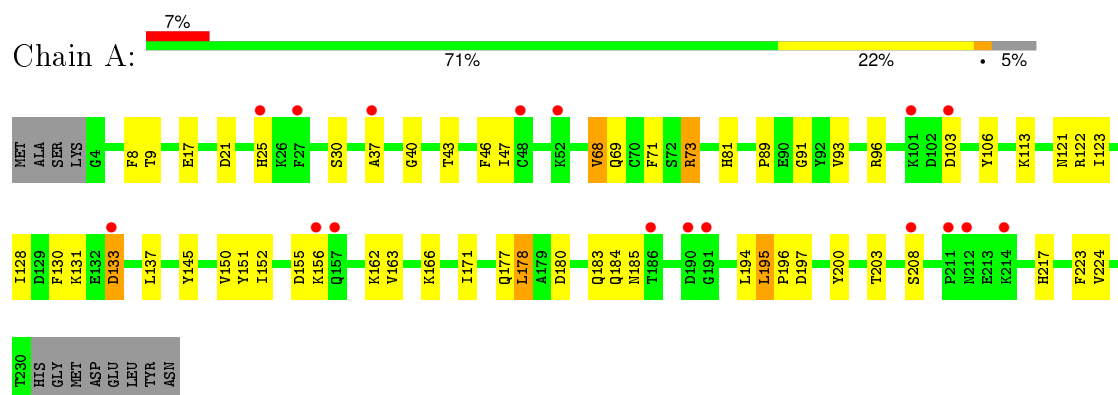
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	42	Total	O	0	0
			42	42		
2	C	38	Total	O	0	0
			38	38		
2	D	38	Total	O	0	0
			38	38		

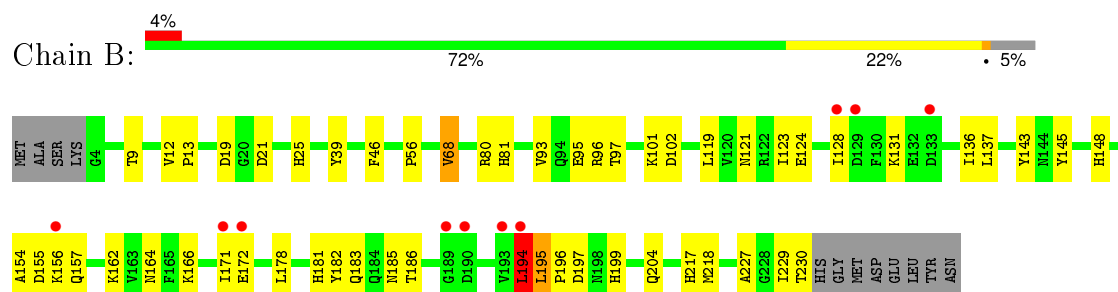
### 3 Residue-property plots [i](#)

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.

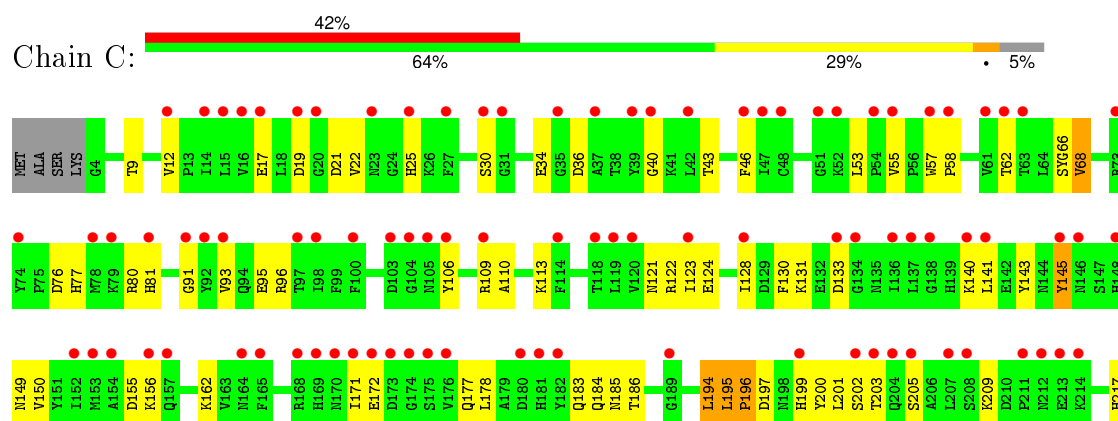
#### • Molecule 1: GREEN FLUORESCENT PROTEIN

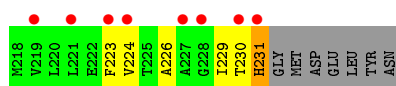


#### • Molecule 1: GREEN FLUORESCENT PROTEIN



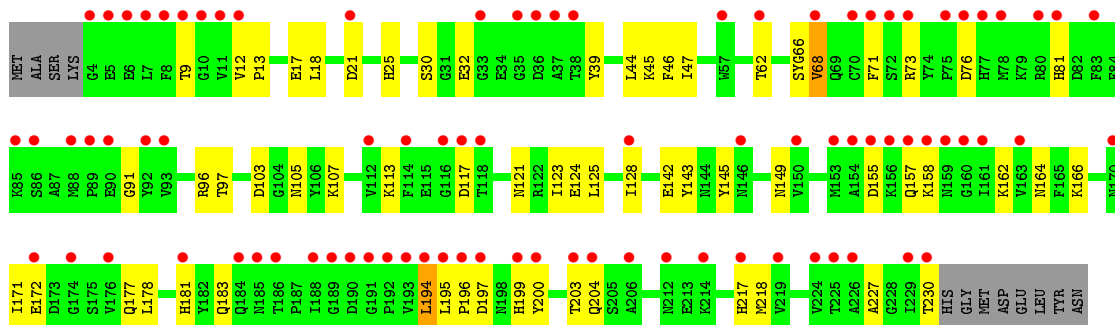
#### • Molecule 1: GREEN FLUORESCENT PROTEIN





● Molecule 1: GREEN FLUORESCENT PROTEIN

Chain D: 36% 69% 25% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.00 Å 52.00 Å 103.00 Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.05 – 2.29	Depositor EDS
% Data completeness (in resolution range)	72.5 (10.00-2.30) 71.5 (10.05-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.28 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.205 , 0.288 0.298 , 0.339	Depositor DCC
$R_{free}$ test set	2209 reflections (7.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 83.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31013 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	7354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.40 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.5076e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.86	0/1817	0.95	1/2458 (0.0%)
1	B	0.85	0/1817	0.92	2/2458 (0.1%)
1	C	0.81	0/1834	0.97	2/2480 (0.1%)
1	D	0.82	0/1817	0.94	3/2458 (0.1%)
All	All	0.83	0/7285	0.95	8/9854 (0.1%)

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	2
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	231	HIS	N-CA-C	6.51	128.57	111.00
1	C	194	LEU	CA-CB-CG	6.45	130.14	115.30
1	B	97	THR	N-CA-C	-6.44	93.61	111.00
1	D	44	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	73	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	D	97	THR	N-CA-C	-5.33	96.61	111.00
1	B	194	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	194	LEU	CA-CB-CG	5.11	127.05	115.30



There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	TYR	Sidechain
1	B	182	TYR	Sidechain
1	B	39	TYR	Sidechain
1	C	145	TYR	Sidechain
1	D	39	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	1795	0	1737	29	0
1	B	1795	0	1738	32	1
1	C	1811	0	1755	40	1
1	D	1795	0	1738	34	2
2	A	40	0	0	3	0
2	B	42	0	0	4	0
2	C	38	0	0	0	0
2	D	38	0	0	2	1
All	All	7354	0	6968	132	3

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 9.

All (132) 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:203[B]:THR:HG22	1:A:224:VAL:HG13	1.44	0.99
1:A:81:HIS:HD2	1:A:197:ASP:H	1.21	0.89
1:A:81:HIS:CD2	1:A:197:ASP:H	1.91	0.89
1:C:81:HIS:CD2	1:C:197:ASP:H	2.04	0.75
1:C:203[B]:THR:HG22	1:C:224:VAL:HG13	1.67	0.74
1:A:121:ASN:ND2	1:A:123:ILE:HD11	2.02	0.74
1:A:68:VAL:HG13	1:A:71:PHE:HD2	1.59	0.67
1:C:149:ASN:HD22	1:C:202:SER:HA	1.59	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PHE:O	1:B:217:HIS:HB2	1.98	0.63
1:C:53:LEU:HD23	1:C:55:VAL:O	2.00	0.61
1:D:155:ASP:OD2	1:D:162:LYS:HE2	1.99	0.61
1:B:156:LYS:HG2	1:B:195:LEU:HD23	1.83	0.61
1:A:156:LYS:HG2	1:A:195:LEU:HD23	1.81	0.61
1:C:96:ARG:HG2	1:C:183:GLN:HB2	1.82	0.61
1:B:81:HIS:CD2	1:B:197:ASP:H	2.18	0.61
1:A:178:LEU:HB2	2:A:261:HOH:O	2.02	0.60
1:D:81:HIS:CD2	1:D:197:ASP:H	2.18	0.60
1:C:155:ASP:OD2	1:C:162:LYS:HE2	2.01	0.60
1:C:81:HIS:HD2	1:C:197:ASP:H	1.49	0.59
1:A:21:ASP:HA	1:A:25:HIS:O	2.02	0.59
1:B:68:VAL:O	1:B:68:VAL:HG13	2.03	0.58
1:A:81:HIS:HD2	1:A:197:ASP:N	1.98	0.58
1:B:155:ASP:OD2	1:B:162:LYS:HE2	2.03	0.58
1:A:133:ASP:O	1:C:80:ARG:NH2	2.37	0.57
1:C:46:PHE:O	1:C:217:HIS:HB2	2.06	0.56
1:A:155:ASP:OD2	1:A:162:LYS:HE2	2.06	0.56
1:C:77:HIS:CD2	1:C:231:HIS:HA	2.40	0.56
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.88	0.56
1:D:121:ASN:ND2	1:D:123:ILE:HD11	2.21	0.55
1:D:203[B]:THR:HG21	2:D:241:HOH:O	2.05	0.55
1:C:21:ASP:HA	1:C:25:HIS:O	2.06	0.54
1:D:155:ASP:OD1	1:D:157:GLN:HB3	2.08	0.54
1:C:184:GLN:HG3	1:C:185:ASN:N	2.23	0.54
1:B:154:ALA:HB1	1:B:195:LEU:HG	1.88	0.54
1:C:149:ASN:ND2	1:C:202:SER:HA	2.23	0.54
1:B:204:GLN:NE2	2:B:259:HOH:O	2.41	0.53
1:A:91:GLY:HA3	1:A:113:LYS:HB3	1.89	0.53
1:C:68:VAL:HG13	1:C:68:VAL:O	2.09	0.53
1:A:68:VAL:HG13	1:A:71:PHE:CD2	2.40	0.53
1:D:68:VAL:O	1:D:68:VAL:HG13	2.09	0.53
1:C:140:LYS:O	1:C:172:GLU:HG3	2.09	0.52
1:B:199:HIS:HB3	1:B:229:ILE:HD11	1.90	0.52
1:D:142:GLU:HG2	1:D:172:GLU:OE2	2.10	0.52
1:D:96:ARG:HG2	1:D:183:GLN:HB2	1.90	0.52
1:C:123:ILE:HG22	1:C:124:GLU:N	2.25	0.52
1:B:155:ASP:OD1	1:B:157:GLN:HB3	2.10	0.52
1:A:152:ILE:HG12	1:A:163:VAL:HG22	1.91	0.52
1:B:148:HIS:HE1	2:B:252:HOH:O	1.92	0.51
1:A:150:VAL:O	1:A:200:TYR:HA	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:HD2	1:B:197:ASP:H	1.57	0.51
1:D:46:PHE:O	1:D:217:HIS:HB2	2.11	0.51
1:D:142:GLU:OE2	1:D:172:GLU:HA	2.10	0.51
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.92	0.51
1:C:201:LEU:HD23	1:C:226:ALA:HA	1.93	0.51
1:D:149:ASN:HD22	1:D:200:TYR:HD2	1.59	0.50
1:A:46:PHE:O	1:A:217:HIS:HB2	2.12	0.50
1:C:95:GLU:HG2	1:C:109:ARG:HG3	1.93	0.49
1:C:141:LEU:HD12	1:C:141:LEU:N	2.28	0.49
1:D:143:TYR:OH	1:D:218:MET:HG3	2.13	0.48
1:D:123:ILE:HG22	1:D:124:GLU:N	2.29	0.48
1:D:68:VAL:HG13	1:D:71:PHE:HD2	1.78	0.48
1:A:131:LYS:O	1:A:137:LEU:HD12	2.13	0.48
1:A:197:ASP:HB3	2:A:270:HOH:O	2.13	0.48
1:B:102:ASP:O	1:B:131:LYS:HE3	2.13	0.48
1:A:184:GLN:HG3	1:A:185:ASN:N	2.28	0.48
1:D:18:LEU:HD23	1:D:18:LEU:C	2.34	0.48
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.95	0.47
1:D:157:GLN:HE22	1:D:158:LYS:HE3	1.79	0.47
1:C:62:THR:O	1:C:96:ARG:NH1	2.44	0.47
1:C:143:TYR:CZ	1:C:209:LYS:HE2	2.48	0.47
1:B:96:ARG:HG2	1:B:183:GLN:HB2	1.96	0.47
1:B:95:GLU:O	1:B:183:GLN:HA	2.15	0.47
1:A:106:TYR:CE1	1:A:130:PHE:CZ	3.02	0.47
1:D:21:ASP:HA	1:D:25:HIS:O	2.15	0.47
1:C:110:ALA:HB2	1:C:123:ILE:HG23	1.96	0.46
1:A:73:ARG:HH22	1:B:124:GLU:CD	2.18	0.46
1:A:93:VAL:O	1:A:185:ASN:HA	2.14	0.46
1:D:164:ASN:HA	1:D:181:HIS:O	2.16	0.46
1:C:156:LYS:HG2	1:C:195:LEU:HD23	1.97	0.46
1:C:91:GLY:HA3	1:C:113:LYS:HB3	1.96	0.46
1:B:93:VAL:O	1:B:185:ASN:HA	2.17	0.45
1:B:199:HIS:HB2	1:B:227:ALA:O	2.17	0.45
1:B:121:ASN:ND2	1:B:123:ILE:HD11	2.31	0.45
1:A:171:ILE:HD11	1:A:177:GLN:HB2	1.98	0.45
1:C:36:ASP:OD2	1:D:107:LYS:NZ	2.49	0.44
1:A:166:LYS:HE3	1:A:166:LYS:HB2	1.78	0.44
1:D:204:GLN:NE2	2:D:255:HOH:O	2.50	0.44
1:C:66:GYS:HD1	1:C:66:GYS:N2	2.32	0.44
1:B:131:LYS:O	1:B:137:LEU:HD12	2.18	0.44
1:B:166:LYS:HB2	1:B:166:LYS:HE3	1.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:HA	1:C:201:LEU:O	2.18	0.44
1:C:40:GLY:O	1:C:223:PHE:HA	2.17	0.44
1:A:69:GLN:HG2	2:A:240:HOH:O	2.18	0.43
1:D:149:ASN:ND2	1:D:200:TYR:CD2	2.86	0.43
1:D:149:ASN:ND2	1:D:200:TYR:CE2	2.86	0.43
1:C:155:ASP:HB2	1:C:162:LYS:HG3	2.01	0.43
1:B:12:VAL:HA	1:B:13:PRO:HD3	1.92	0.43
1:B:123:ILE:HG22	1:B:124:GLU:N	2.34	0.43
1:C:57:TRP:N	1:C:58:PRO:CD	2.82	0.43
1:D:62:THR:HG22	1:D:66:GYS:CG2	2.48	0.43
1:C:93:VAL:O	1:C:185:ASN:HA	2.19	0.42
1:C:171:ILE:HG22	1:C:172:GLU:N	2.34	0.42
1:C:150:VAL:O	1:C:200:TYR:HA	2.19	0.42
1:B:21:ASP:HA	1:B:25:HIS:O	2.19	0.42
1:D:73:ARG:HG2	1:D:73:ARG:NH1	2.34	0.42
1:D:155:ASP:HB2	1:D:162:LYS:HG3	2.01	0.42
1:C:121:ASN:ND2	1:C:123:ILE:HD11	2.35	0.42
1:D:125:LEU:C	1:D:125:LEU:HD23	2.39	0.42
1:B:199:HIS:HB3	1:B:229:ILE:CD1	2.49	0.42
1:D:91:GLY:HA3	1:D:113:LYS:HB3	2.02	0.42
1:D:12:VAL:HA	1:D:13:PRO:HD3	1.92	0.42
1:B:80:ARG:O	1:B:194:LEU:HG	2.18	0.42
1:B:68:VAL:HG22	1:B:119:LEU:HD11	2.02	0.42
1:D:73:ARG:HH11	1:D:73:ARG:HG2	1.86	0.41
1:B:68:VAL:O	1:B:68:VAL:CG1	2.68	0.41
1:C:106:TYR:CE1	1:C:130:PHE:CZ	3.08	0.41
1:B:164:ASN:HA	1:B:181:HIS:O	2.21	0.41
1:A:8:PHE:HB3	1:A:37:ALA:CB	2.50	0.41
1:A:47:ILE:HD13	1:A:217:HIS:HB3	2.02	0.41
1:C:199:HIS:HB3	1:C:229:ILE:HD11	2.01	0.41
1:C:22:VAL:HG21	1:C:55:VAL:HG11	2.03	0.41
1:B:197:ASP:HB3	2:B:275:HOH:O	2.19	0.41
1:D:81:HIS:HD2	1:D:196:PRO:HA	1.84	0.41
1:A:40:GLY:O	1:A:223:PHE:HA	2.20	0.41
1:C:81:HIS:HD2	1:C:196:PRO:HA	1.85	0.41
1:C:12:VAL:O	1:C:34:GLU:HA	2.20	0.40
1:D:199:HIS:HB2	1:D:227:ALA:O	2.21	0.40
1:C:171:ILE:HD11	1:C:177:GLN:HB2	2.03	0.40
1:B:148:HIS:CE1	2:B:252:HOH:O	2.71	0.40
1:B:143:TYR:OH	1:B:218:MET:HG3	2.22	0.40
1:D:166:LYS:HB2	1:D:166:LYS:HE3	1.81	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ILE:HD13	1:B:171:ILE:HG21	1.85	0.40

All (3) 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)
1:D:32:GLU:OE2	1:D:76:ASP:N[2_646]	1.91	0.29
1:D:117:ASP:OD1	2:D:260:HOH:O[2_646]	2.06	0.14
1:B:101:LYS:NZ	1:C:131:LYS:NZ[1_564]	2.10	0.10

## 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	223/237 (94%)	215 (96%)	8 (4%)	0	100	100
1	B	223/237 (94%)	212 (95%)	10 (4%)	1 (0%)	39	48
1	C	224/237 (94%)	216 (96%)	8 (4%)	0	100	100
1	D	223/237 (94%)	216 (97%)	7 (3%)	0	100	100
All	All	893/948 (94%)	859 (96%)	33 (4%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	ILE

### 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	195/206 (95%)	178 (91%)	17 (9%)	13	15
1	B	195/206 (95%)	182 (93%)	13 (7%)	20	26
1	C	197/206 (96%)	179 (91%)	18 (9%)	12	13
1	D	195/206 (95%)	183 (94%)	12 (6%)	23	30
All	All	782/824 (95%)	722 (92%)	60 (8%)	16	20

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	17	GLU
1	A	30	SER
1	A	43	THR
1	A	68	VAL
1	A	89	PRO
1	A	103	ASP
1	A	122	ARG
1	A	128	ILE
1	A	133	ASP
1	A	145	TYR
1	A	178	LEU
1	A	180	ASP
1	A	194	LEU
1	A	195	LEU
1	A	196	PRO
1	A	208	SER
1	B	9	THR
1	B	19	ASP
1	B	56	PRO
1	B	68	VAL
1	B	128	ILE
1	B	145	TYR
1	B	172	GLU
1	B	178	LEU
1	B	186	THR
1	B	194	LEU
1	B	195	LEU
1	B	196	PRO
1	B	230	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	9	THR
1	C	17	GLU
1	C	19	ASP
1	C	30	SER
1	C	43	THR
1	C	68	VAL
1	C	76	ASP
1	C	122	ARG
1	C	128	ILE
1	C	133	ASP
1	C	145	TYR
1	C	178	LEU
1	C	186	THR
1	C	194	LEU
1	C	195	LEU
1	C	196	PRO
1	C	205	SER
1	C	230	THR
1	D	9	THR
1	D	17	GLU
1	D	30	SER
1	D	68	VAL
1	D	103	ASP
1	D	105	ASN
1	D	128	ILE
1	D	145	TYR
1	D	178	LEU
1	D	194	LEU
1	D	195	LEU
1	D	230	THR

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	81	HIS
1	A	149	ASN
1	A	204	GLN
1	B	81	HIS
1	B	105	ASN
1	B	149	ASN
1	B	204	GLN
1	C	81	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	149	ASN
1	D	81	HIS
1	D	105	ASN
1	D	121	ASN
1	D	149	ASN
1	D	157	GLN
1	D	204	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	1.20	3 (13%)	27,30,32	1.09	3 (11%)
1	GYS	B	66	1	22,22,23	1.24	3 (13%)	27,30,32	1.48	4 (14%)
1	GYS	C	66	1	22,22,23	1.44	3 (13%)	27,30,32	1.13	4 (14%)
1	GYS	D	66	1	22,22,23	1.25	2 (9%)	27,30,32	1.25	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	-	0/8/29/30	0/2/2/2
1	GYS	B	66	1	-	0/8/29/30	0/2/2/2
1	GYS	C	66	1	-	0/8/29/30	0/2/2/2
1	GYS	D	66	1	-	0/8/29/30	0/2/2/2



All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	GYS	C2-N3	-3.19	1.33	1.39
1	B	66	GYS	CB2-CA2	-2.63	1.32	1.35
1	A	66	GYS	CB2-CA2	-2.62	1.32	1.35
1	D	66	GYS	C2-N3	-2.61	1.34	1.39
1	D	66	GYS	CB2-CA2	-2.52	1.32	1.35
1	C	66	GYS	C2-N3	-2.39	1.34	1.39
1	A	66	GYS	C2-N3	-2.17	1.35	1.39
1	B	66	GYS	CA3-N3	-2.11	1.43	1.47
1	A	66	GYS	CE1-CD1	2.23	1.42	1.38
1	C	66	GYS	CE2-CD2	2.92	1.44	1.38
1	C	66	GYS	CE1-CD1	3.75	1.45	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	CA2-N2-C1	-2.69	103.27	105.71
1	C	66	GYS	CA3-N3-C1	-2.67	124.25	127.36
1	D	66	GYS	CA2-N2-C1	-2.18	103.73	105.71
1	C	66	GYS	CA2-N2-C1	-2.17	103.74	105.71
1	A	66	GYS	CA3-N3-C1	-2.07	124.95	127.36
1	B	66	GYS	CA3-N3-C1	-2.01	125.02	127.36
1	A	66	GYS	O2-C2-CA2	2.24	132.15	130.95
1	C	66	GYS	O2-C2-CA2	2.36	132.22	130.95
1	D	66	GYS	N3-C1-N2	2.80	113.72	111.56
1	A	66	GYS	N3-C1-N2	3.08	113.93	111.56
1	B	66	GYS	N3-C1-N2	3.09	113.94	111.56
1	C	66	GYS	N3-C1-N2	3.41	114.19	111.56
1	D	66	GYS	O2-C2-CA2	4.01	133.11	130.95
1	B	66	GYS	O2-C2-CA2	4.86	133.57	130.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	GYS	1	0
1	D	66	GYS	1	0

## 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

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	224/237 (94%)	0.91	17 (7%)	17 24	3, 14, 41, 56	0
1	B	224/237 (94%)	0.52	10 (4%)	37 46	2, 10, 39, 59	0
1	C	225/237 (94%)	2.02	100 (44%)	0 0	3, 13, 40, 60	0
1	D	224/237 (94%)	1.89	86 (38%)	0 0	2, 11, 40, 61	0
All	All	897/948 (94%)	1.33	213 (23%)	1 1	2, 12, 41, 61	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	GLY	9.2
1	D	4	GLY	8.0
1	C	174	GLY	6.5
1	C	133	ASP	6.1
1	D	157	GLN	5.8
1	C	208	SER	5.5
1	D	38	THR	5.3
1	D	156	LYS	5.1
1	D	155	ASP	4.8
1	D	196	PRO	4.7
1	A	211	PRO	4.6
1	A	103	ASP	4.5
1	C	25	HIS	4.4
1	D	203[A]	THR	4.3
1	D	37	ALA	4.3
1	C	211	PRO	4.3
1	C	48	CYS	4.2
1	D	229	ILE	4.2
1	A	214	LYS	4.2
1	A	190	ASP	4.0
1	C	118	THR	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	74	TYR	4.0
1	D	7	LEU	4.0
1	C	138	GLY	4.0
1	C	231	HIS	4.0
1	C	128	ILE	3.9
1	D	192	PRO	3.9
1	C	227	ALA	3.9
1	C	141	LEU	3.9
1	D	80	ARG	3.8
1	D	35	GLY	3.8
1	C	203[A]	THR	3.8
1	C	173	ASP	3.7
1	D	194	LEU	3.7
1	C	156	LYS	3.7
1	D	153	MET	3.7
1	D	159	ASN	3.6
1	C	228	GLY	3.6
1	D	10	GLY	3.6
1	C	212	ASN	3.6
1	D	9	THR	3.6
1	D	186	THR	3.6
1	D	160	GLY	3.6
1	C	221	LEU	3.5
1	D	78	MET	3.5
1	C	171	ILE	3.5
1	D	86	SER	3.4
1	D	193	VAL	3.4
1	C	103	ASP	3.4
1	D	70	CYS	3.4
1	C	134	GLY	3.4
1	C	152	ILE	3.4
1	D	114	PHE	3.4
1	C	19	ASP	3.4
1	D	89	PRO	3.4
1	C	114	PHE	3.3
1	D	92	TYR	3.3
1	B	190	ASP	3.3
1	D	83	PHE	3.2
1	D	200	TYR	3.2
1	D	116	GLY	3.2
1	D	190	ASP	3.2
1	D	189	GLY	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	163	VAL	3.2
1	C	14	ILE	3.1
1	C	223	PHE	3.1
1	C	98	ILE	3.1
1	C	164	ASN	3.1
1	D	172	GLU	3.1
1	C	16	VAL	3.1
1	C	61	VAL	3.1
1	C	145	TYR	3.1
1	D	117	ASP	3.0
1	C	78	MET	3.0
1	D	5	GLU	3.0
1	C	219	VAL	3.0
1	C	214	LYS	3.0
1	C	57	TRP	3.0
1	D	226	ALA	3.0
1	C	157	GLN	3.0
1	D	188	ILE	3.0
1	D	76	ASP	2.9
1	C	168	ARG	2.9
1	D	128	ILE	2.9
1	C	93	VAL	2.9
1	C	165	PHE	2.9
1	C	47	ILE	2.9
1	D	230	THR	2.9
1	A	133	ASP	2.9
1	C	106	TYR	2.9
1	C	58	PRO	2.9
1	D	75	PRO	2.8
1	D	212	ASN	2.8
1	C	104	GLY	2.8
1	D	154	ALA	2.8
1	C	170	ASN	2.8
1	C	39	TYR	2.8
1	C	51	GLY	2.8
1	B	189	GLY	2.8
1	B	129	ASP	2.8
1	C	17	GLU	2.8
1	D	72	SER	2.7
1	B	128	ILE	2.7
1	C	52	LYS	2.7
1	D	197	ASP	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	120	VAL	2.7
1	C	213	GLU	2.7
1	D	184	GLN	2.7
1	D	8	PHE	2.7
1	C	182	TYR	2.7
1	C	230	THR	2.7
1	D	71	PHE	2.6
1	D	11	VAL	2.6
1	C	42	LEU	2.6
1	C	199	HIS	2.6
1	D	33	GLY	2.6
1	C	73	ARG	2.6
1	D	93	VAL	2.6
1	D	214	LYS	2.6
1	C	79	LYS	2.6
1	A	212	ASN	2.6
1	C	181	HIS	2.6
1	C	119	LEU	2.6
1	D	68	VAL	2.6
1	D	36	ASP	2.5
1	C	153	MET	2.5
1	D	62	THR	2.5
1	C	30	SER	2.5
1	C	54	PRO	2.5
1	C	15	LEU	2.5
1	C	62	THR	2.5
1	C	172	GLU	2.5
1	C	189	GLY	2.5
1	A	27	PHE	2.5
1	D	118	THR	2.5
1	C	146	ASN	2.5
1	D	204	GLN	2.5
1	D	88	MET	2.4
1	C	109	ARG	2.4
1	D	57	TRP	2.4
1	D	176	VAL	2.4
1	A	156	LYS	2.4
1	B	133	ASP	2.4
1	C	180	ASP	2.4
1	C	224	VAL	2.4
1	D	195	LEU	2.4
1	D	73	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	2.4
1	D	224	VAL	2.4
1	A	48	CYS	2.4
1	D	77	HIS	2.4
1	A	37	ALA	2.4
1	D	206	ALA	2.4
1	D	225	THR	2.4
1	B	171	ILE	2.4
1	C	23	ASN	2.3
1	C	175	SER	2.3
1	A	25	HIS	2.3
1	C	204	GLN	2.3
1	C	105	ASN	2.3
1	D	174	GLY	2.3
1	D	158	LYS	2.3
1	D	219	VAL	2.3
1	A	101	LYS	2.3
1	C	140	LYS	2.3
1	C	92	TYR	2.3
1	C	176	VAL	2.3
1	C	154	ALA	2.3
1	D	170	ASN	2.3
1	C	27	PHE	2.3
1	C	205	SER	2.3
1	D	21	ASP	2.3
1	B	156	LYS	2.2
1	B	193	VAL	2.2
1	D	81	HIS	2.2
1	D	85	LYS	2.2
1	A	186	THR	2.2
1	C	97	THR	2.2
1	A	52	LYS	2.2
1	C	91	GLY	2.2
1	D	199	HIS	2.2
1	C	31	GLY	2.2
1	D	181	HIS	2.2
1	D	217	HIS	2.2
1	C	37	ALA	2.2
1	D	90	GLU	2.2
1	D	161	ILE	2.1
1	A	191	GLY	2.1
1	D	12	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	112	VAL	2.1
1	C	46	PHE	2.1
1	C	148	HIS	2.1
1	C	12	VAL	2.1
1	D	146	ASN	2.1
1	A	208	SER	2.1
1	C	81	HIS	2.1
1	C	137	LEU	2.1
1	C	35	GLY	2.1
1	D	150	VAL	2.1
1	C	40	GLY	2.1
1	C	202	SER	2.1
1	D	185	ASN	2.1
1	D	6	GLU	2.1
1	A	157	GLN	2.1
1	C	169	HIS	2.1
1	C	55	VAL	2.1
1	C	207	LEU	2.0
1	C	123	ILE	2.0
1	C	20	GLY	2.0
1	C	63	THR	2.0
1	B	194	LEU	2.0
1	B	172	GLU	2.0
1	C	100	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GYS	A	66	21/22	0.91	0.14	-	2,3,12,16	0
1	GYS	B	66	21/22	0.92	0.16	-	2,4,7,9	0
1	GYS	C	66	21/22	0.85	0.20	-	2,4,9,13	0
1	GYS	D	66	21/22	0.80	0.24	-	2,2,7,10	0



### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.