



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:18 pm GMT

PDB ID : 4GCR
Title : STRUCTURE OF THE BOVINE EYE LENS PROTEIN GAMMA-B (GAMMA-II)-CRYSTALLIN AT 1.47 ANGSTROMS
Authors : Slingsby, C.; Najmudin, S.; Nalini, V.; Driessen, H.P.C.; Blundell, T.L.; Moss, D.S.; Lindley, P.
Deposited on : 1992-04-02
Resolution : 1.47 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

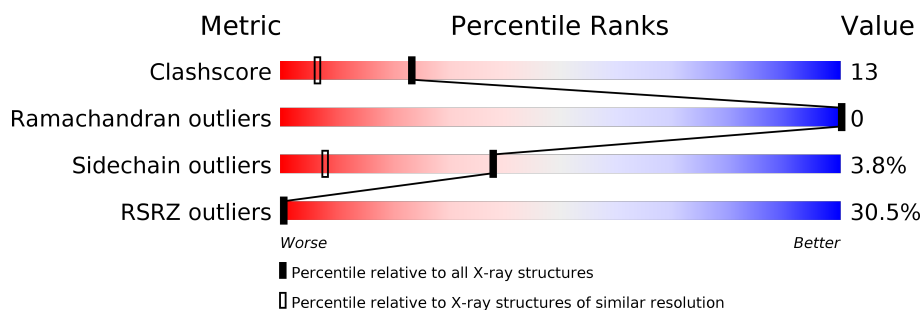
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	112137	3795 (1.50-1.46)
Ramachandran outliers	110173	3721 (1.50-1.46)
Sidechain outliers	110143	3719 (1.50-1.46)
RSRZ outliers	101464	3549 (1.50-1.46)

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 ≥ 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	174	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1786 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 GAMMA-B CRYSTALLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	11	0
			1556	974	278	287	17			

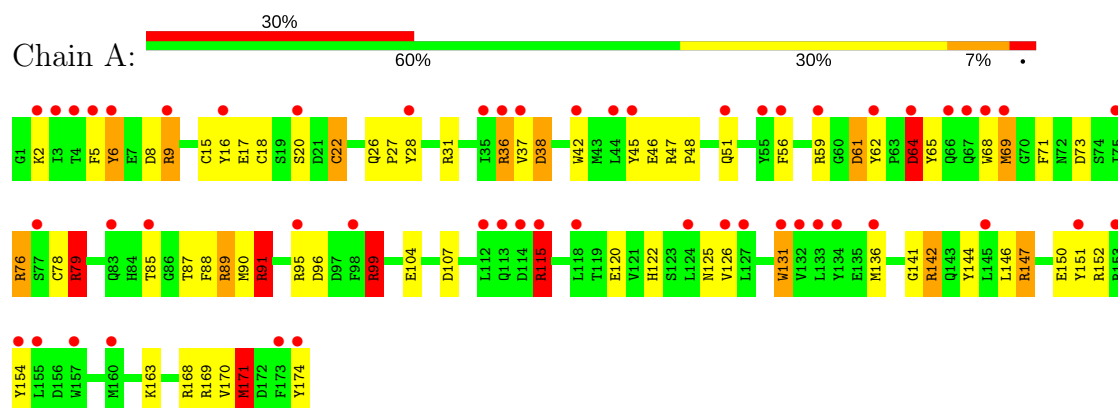
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		

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 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 ($\text{RSRZ} > 2$). 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: GAMMA-B CRYSTALLIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	57.53Å 57.53Å 97.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.47 8.00 – 1.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.47) 95.3 (8.00-1.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.49Å)	Xtriage
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.181 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1786	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.07% 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

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	1.38	2/1602 (0.1%)	2.18	69/2161 (3.2%)

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	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	TRP	NE1-CE2	-5.71	1.30	1.37
1	A	169	ARG	NE-CZ	5.42	1.40	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ASP	CB-CG-OD2	10.86	128.07	118.30
1	A	45	TYR	CB-CG-CD2	-10.54	114.68	121.00
1	A	6	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	A	45	TYR	CG-CD2-CE2	-9.70	113.54	121.30
1	A	62	TYR	CB-CG-CD2	-9.49	115.30	121.00
1	A	65	TYR	CB-CG-CD2	-9.34	115.40	121.00
1	A	47	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	A	152	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	A	56	PHE	CB-CG-CD2	-8.48	114.87	120.80
1	A	142	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	36	ARG	CD-NE-CZ	-8.30	111.98	123.60
1	A	147	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	16[A]	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	A	16[B]	TYR	CB-CG-CD2	-7.86	116.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	TYR	CG-CD2-CE2	-7.63	115.19	121.30
1	A	85	THR	C-N-CA	-7.55	106.44	122.30
1	A	36	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	A	144	TYR	CG-CD1-CE1	-7.12	115.60	121.30
1	A	9	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	A	174	TYR	CB-CG-CD1	-7.09	116.74	121.00
1	A	87	THR	O-C-N	6.99	133.89	122.70
1	A	65	TYR	CG-CD2-CE2	-6.86	115.81	121.30
1	A	6	TYR	CG-CD2-CE2	-6.40	116.18	121.30
1	A	131	TRP	CE3-CZ3-CH2	-6.38	114.18	121.20
1	A	45	TYR	CD1-CE1-CZ	-6.35	114.08	119.80
1	A	76	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	61	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	142	ARG	CG-CD-NE	-6.04	99.11	111.80
1	A	154	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	A	96	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	62	TYR	CD1-CE1-CZ	-5.92	114.47	119.80
1	A	144	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	37	VAL	O-C-N	5.83	132.02	122.70
1	A	38	ASP	CA-CB-CG	-5.75	100.74	113.40
1	A	171	MET	CG-SD-CE	5.73	109.37	100.20
1	A	71	PHE	CB-CG-CD2	5.73	124.81	120.80
1	A	16[A]	TYR	CD1-CG-CD2	5.72	124.19	117.90
1	A	16[B]	TYR	CD1-CG-CD2	5.72	124.19	117.90
1	A	64	ASP	CA-CB-CG	5.71	125.95	113.40
1	A	115	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	22[A]	CYS	N-CA-CB	5.62	120.72	110.60
1	A	22[B]	CYS	N-CA-CB	5.62	120.72	110.60
1	A	151	TYR	CD1-CG-CD2	5.58	124.04	117.90
1	A	131	TRP	CD1-CG-CD2	5.53	110.72	106.30
1	A	151	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	89	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	28	TYR	CG-CD1-CE1	-5.43	116.95	121.30
1	A	79	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	88	PHE	CG-CD2-CE2	-5.42	114.83	120.80
1	A	168	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	45	TYR	CD1-CG-CD2	5.40	123.84	117.90
1	A	65	TYR	CZ-CE2-CD2	5.35	124.62	119.80
1	A	46	GLU	N-CA-CB	-5.32	101.03	110.60
1	A	79	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	151	TYR	CG-CD2-CE2	-5.27	117.09	121.30
1	A	91	ARG	CD-NE-CZ	-5.26	116.23	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	170	VAL	O-C-N	5.22	131.05	122.70
1	A	88	PHE	CB-CG-CD2	-5.20	117.16	120.80
1	A	154	TYR	CG-CD2-CE2	-5.17	117.17	121.30
1	A	65	TYR	CB-CG-CD1	5.13	124.08	121.00
1	A	31	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	6	TYR	CB-CG-CD2	5.12	124.07	121.00
1	A	61	ASP	CB-CG-OD2	-5.11	113.71	118.30
1	A	99	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	168	ARG	CG-CD-NE	-5.07	101.15	111.80
1	A	171	MET	O-C-N	5.07	130.81	122.70
1	A	150	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	A	48	PRO	CA-N-CD	5.00	118.70	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ARG	Sidechain
1	A	147	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	91	ARG	Sidechain
1	A	99	ARG	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	1556	0	1435	38	0
2	A	230	0	0	13	3
All	All	1786	0	1435	38	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 13.

All (38) 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:51:GLN:NE2	2:A:400:HOH:O	1.81	1.10
1:A:59:ARG:HG3	2:A:234:HOH:O	1.57	1.03
1:A:89:ARG:CD	2:A:414:HOH:O	2.17	0.91
1:A:89:ARG:HD2	2:A:414:HOH:O	1.73	0.88
1:A:76:ARG:NH1	2:A:316:HOH:O	2.04	0.84
1:A:64:ASP:OD1	2:A:299:HOH:O	2.00	0.79
1:A:68:TRP:O	1:A:69:MET:HG2	1.88	0.74
1:A:89:ARG:HD3	2:A:414:HOH:O	1.86	0.69
1:A:68:TRP:C	1:A:69:MET:HG2	2.15	0.67
1:A:73:ASP:OD2	2:A:317:HOH:O	2.13	0.66
1:A:8:ASP:OD2	2:A:265:HOH:O	2.15	0.65
1:A:99:ARG:NH2	2:A:331:HOH:O	2.29	0.64
1:A:90:MET:HG2	1:A:131:TRP:CE2	2.35	0.62
1:A:36:ARG:HE	1:A:61:ASP:CG	2.04	0.61
1:A:171:MET:HE2	2:A:214:HOH:O	1.99	0.60
1:A:90:MET:HG2	1:A:131:TRP:CZ2	2.37	0.59
1:A:36:ARG:NE	1:A:61:ASP:OD1	2.40	0.55
1:A:107:ASP:OD1	1:A:115:ARG:NH2	2.39	0.54
1:A:89:ARG:NH1	1:A:104:GLU:OE2	2.40	0.54
1:A:18[A]:CYS:SG	1:A:20[A]:SER:O	2.68	0.52
1:A:136:MET:HE2	1:A:141:GLY:N	2.25	0.52
1:A:76:ARG:NE	2:A:371:HOH:O	2.46	0.49
1:A:136:MET:HE2	1:A:136:MET:HB2	1.78	0.46
1:A:5:PHE:O	1:A:15[B]:CYS:HA	2.16	0.45
1:A:79:ARG:NE	2:A:364:HOH:O	2.25	0.44
1:A:120:GLU:OE1	1:A:122:HIS:HE1	2.00	0.44
1:A:36:ARG:HH11	1:A:36:ARG:HD2	1.53	0.44
1:A:26:GLN:N	1:A:27:PRO:CD	2.81	0.43
1:A:9:ARG:HD3	1:A:9:ARG:HH11	1.55	0.43
1:A:69:MET:HE2	1:A:69:MET:HB3	1.60	0.43
1:A:2:LYS:HB3	1:A:38:ASP:HB2	1.99	0.43
1:A:91:ARG:HH11	1:A:91:ARG:HD2	1.73	0.42
1:A:22[B]:CYS:HB2	1:A:78:CYS:SG	2.60	0.41
1:A:126:VAL:HG21	1:A:146:LEU:HB3	2.03	0.41
1:A:6:TYR:CD2	1:A:15[A]:CYS:HB3	2.55	0.41
1:A:68:TRP:C	1:A:69:MET:CG	2.88	0.41
1:A:95:ARG:NH1	1:A:95:ARG:HG3	2.35	0.41
1:A:163:LYS:HB3	1:A:163:LYS:HE3	1.75	0.41

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)
2:A:393:HOH:O	2:A:393:HOH:O[7_556]	1.48	0.72
2:A:376:HOH:O	2:A:408:HOH:O[4_454]	1.92	0.28
2:A:235:HOH:O	2:A:294:HOH:O[4_454]	1.95	0.25

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	183/174 (105%)	182 (100%)	1 (0%)	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	169/158 (107%)	162 (96%)	7 (4%)	35 6

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17[A]	GLU
1	A	17[B]	GLU
1	A	64	ASP
1	A	69	MET
1	A	115	ARG
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	171	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	122	HIS
1	A	125	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

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	174/174 (100%)	1.65	53 (30%) 0 1	0, 0, 0, 1	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	TYR	7.0
1	A	173	PHE	4.8
1	A	160	MET	4.7
1	A	28	TYR	4.3
1	A	131	TRP	4.0
1	A	83	GLN	4.0
1	A	113	GLN	3.7
1	A	153	ARG	3.6
1	A	66	GLN	3.5
1	A	45	TYR	3.4
1	A	69	MET	3.3
1	A	55	TYR	3.3
1	A	59	ARG	3.3
1	A	132	VAL	3.2
1	A	85	THR	3.2
1	A	9	ARG	3.0
1	A	114	ASP	2.9
1	A	56	PHE	2.8
1	A	37	VAL	2.8
1	A	134	TYR	2.7
1	A	64	ASP	2.7
1	A	145	LEU	2.7
1	A	42	TRP	2.6
1	A	95	ARG	2.6
1	A	67	GLN	2.5
1	A	35	ILE	2.5
1	A	133	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	SER	2.5
1	A	136	MET	2.5
1	A	36	ARG	2.4
1	A	151	TYR	2.4
1	A	51	GLN	2.4
1	A	75	ILE	2.4
1	A	2	LYS	2.4
1	A	112	LEU	2.3
1	A	127	LEU	2.3
1	A	6	TYR	2.3
1	A	155	LEU	2.3
1	A	124	LEU	2.3
1	A	16[A]	TYR	2.3
1	A	20[A]	SER	2.2
1	A	44	LEU	2.2
1	A	115	ARG	2.1
1	A	118	LEU	2.1
1	A	157	TRP	2.1
1	A	4	THR	2.1
1	A	126	VAL	2.1
1	A	98	PHE	2.1
1	A	62	TYR	2.0
1	A	5	PHE	2.0
1	A	68	TRP	2.0
1	A	3	ILE	2.0
1	A	154	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.