



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:25 AM GMT

PDB ID : 3IF5
Title : Crystal Structure Analysis of Mglu
Authors : Yoshimune, K.; Shirakihara, Y.
Deposited on : 2009-07-24
Resolution : 2.44 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
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

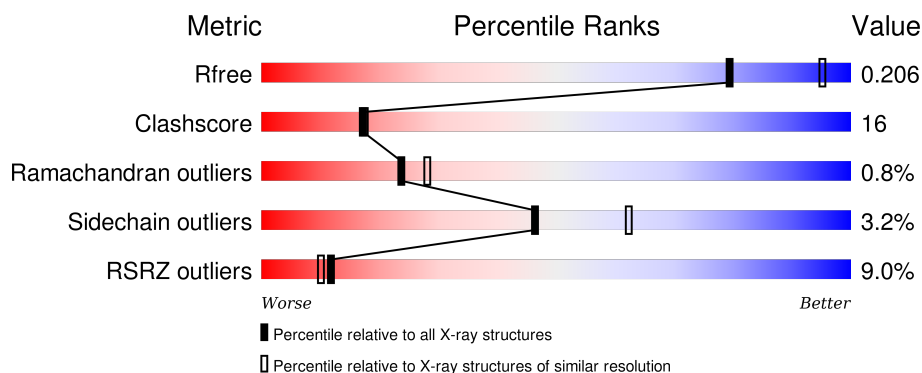
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	456	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3097 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 Salt-tolerant glutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			2982	1856	545	566	15			

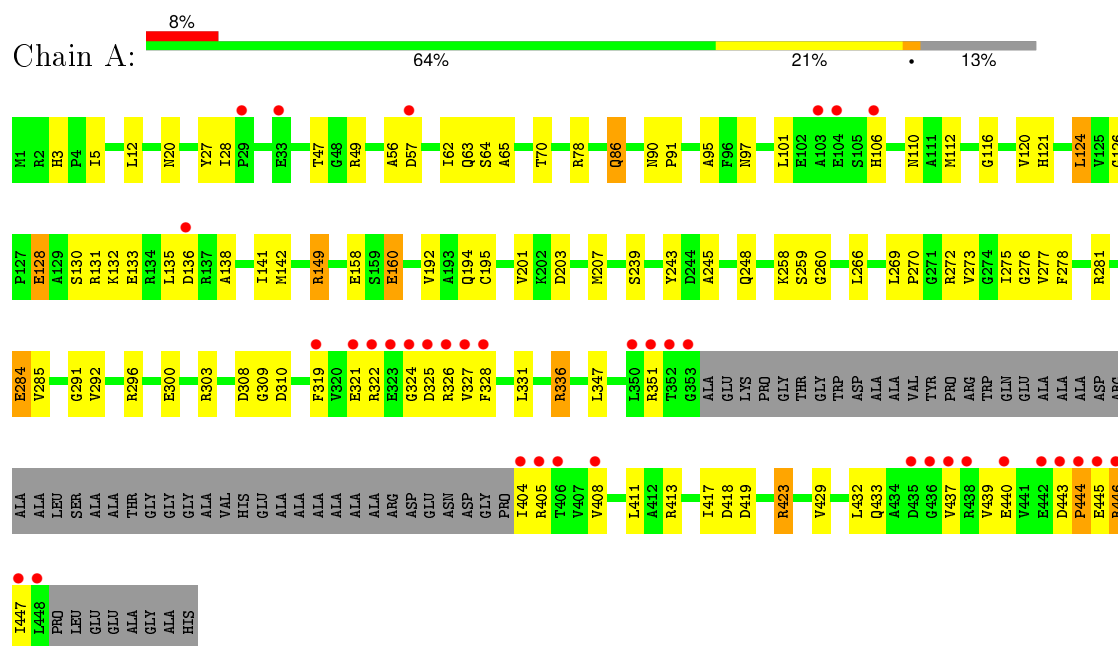
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		

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: Salt-tolerant glutaminase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	115.33Å 116.68Å 144.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.18 – 2.44 36.18 – 2.44	Depositor EDS
% Data completeness (in resolution range)	93.5 (36.18-2.44) 93.6 (36.18-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 2.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.204 , 0.256 0.206 , 0.206	Depositor DCC
R_{free} test set	868 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.5	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17155 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3097	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.63	1/3025 (0.0%)	0.66	3/4100 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	ARG	CZ-NH2	28.15	1.69	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	A	336	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	124	LEU	N-CA-C	5.18	124.99	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2982	0	2997	97	5
2	A	115	0	0	17	4
All	All	3097	0	2997	97	5

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 16.

All (97) 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:336:ARG:CZ	1:A:336:ARG:NH2	1.69	1.56
1:A:95:ALA:O	2:A:553:HOH:O	1.72	1.06
1:A:62:ILE:HD13	1:A:142:MET:HE3	1.34	1.05
1:A:112:MET:HE3	1:A:258:LYS:HD3	1.38	1.05
1:A:136:ASP:HB3	2:A:514:HOH:O	1.59	1.00
1:A:110:ASN:HD22	1:A:112:MET:H	1.18	0.86
1:A:445:GLU:O	1:A:447:ILE:HG13	1.79	0.83
1:A:260:GLY:O	2:A:503:HOH:O	1.96	0.83
1:A:259:SER:OG	2:A:503:HOH:O	2.04	0.75
1:A:112:MET:CE	1:A:258:LYS:HD3	2.15	0.74
1:A:132:LYS:HE2	2:A:514:HOH:O	1.87	0.74
1:A:110:ASN:ND2	1:A:112:MET:H	1.85	0.73
1:A:97:ASN:OD1	2:A:535:HOH:O	2.10	0.70
1:A:86:GLN:HE21	1:A:86:GLN:HA	1.56	0.69
1:A:347:LEU:HD22	1:A:432:LEU:HD11	1.74	0.69
1:A:57:ASP:OD1	1:A:57:ASP:O	2.14	0.66
1:A:429:VAL:HG13	1:A:439:VAL:HG11	1.78	0.66
1:A:47:THR:OG1	1:A:49:ARG:NH1	2.28	0.66
1:A:248:GLN:NE2	2:A:565:HOH:O	2.30	0.65
1:A:413:ARG:NH1	2:A:480:HOH:O	2.31	0.63
1:A:160:GLU:HG2	1:A:192:VAL:HG13	1.81	0.63
1:A:423:ARG:CB	1:A:423:ARG:HH11	2.13	0.61
1:A:319:PHE:CD2	1:A:321:GLU:HG2	2.36	0.60
1:A:284:GLU:OE1	1:A:285:VAL:HG13	2.00	0.60
1:A:128:GLU:OE2	2:A:471:HOH:O	2.16	0.59
1:A:201:VAL:HG22	1:A:278:PHE:HB2	1.85	0.59
1:A:62:ILE:HD13	1:A:142:MET:CE	2.22	0.58
1:A:423:ARG:HB2	1:A:423:ARG:HH11	1.68	0.57
1:A:160:GLU:HG2	1:A:192:VAL:CG1	2.34	0.57
1:A:408:VAL:HG22	1:A:440:GLU:HG3	1.87	0.56
1:A:327:VAL:HG21	1:A:404:ILE:HD13	1.88	0.56
1:A:3:HIS:HE1	1:A:5:ILE:HD13	1.71	0.55
1:A:201:VAL:HG22	1:A:278:PHE:CB	2.36	0.55
1:A:321:GLU:HB2	1:A:328:PHE:HB2	1.88	0.55
1:A:272:ARG:O	1:A:273:VAL:HG13	2.08	0.54
1:A:319:PHE:HD2	1:A:321:GLU:HG2	1.72	0.54
1:A:419:ASP:O	1:A:423:ARG:HG3	2.07	0.53
1:A:277:VAL:HG11	1:A:291:GLY:HA2	1.89	0.53
1:A:308:ASP:OD2	2:A:539:HOH:O	2.18	0.53
1:A:325:ASP:HB2	1:A:405:ARG:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ASN:O	1:A:116:GLY:HA3	2.09	0.52
1:A:3:HIS:CE1	1:A:5:ILE:HD13	2.45	0.52
1:A:149:ARG:HE	1:A:149:ARG:HA	1.73	0.52
1:A:158:GLU:HA	1:A:158:GLU:OE1	2.10	0.52
1:A:325:ASP:OD2	1:A:326:ARG:HG2	2.11	0.51
1:A:91:PRO:HB3	1:A:239:SER:O	2.10	0.51
1:A:149:ARG:NE	1:A:149:ARG:HA	2.27	0.50
1:A:423:ARG:NH1	1:A:423:ARG:HB2	2.27	0.50
1:A:90:ASN:OD1	1:A:91:PRO:O	2.30	0.50
1:A:27:TYR:CD1	1:A:28:ILE:HG23	2.46	0.50
1:A:296:ARG:O	1:A:300:GLU:HG3	2.11	0.50
1:A:78:ARG:NE	1:A:126:GLY:HA2	2.27	0.50
1:A:63:GLN:HA	1:A:195:CYS:HB3	1.93	0.49
1:A:62:ILE:CD1	1:A:142:MET:HE3	2.25	0.49
1:A:78:ARG:HE	1:A:126:GLY:HA2	1.79	0.48
1:A:296:ARG:HD2	2:A:536:HOH:O	2.13	0.48
1:A:133:GLU:HA	1:A:136:ASP:OD2	2.14	0.47
1:A:331:LEU:O	1:A:413:ARG:HB2	2.15	0.47
1:A:135:LEU:O	1:A:135:LEU:HD22	2.15	0.47
1:A:62:ILE:HG12	1:A:65:ALA:HB3	1.95	0.47
1:A:336:ARG:HA	1:A:418:ASP:OD1	2.15	0.47
1:A:62:ILE:CG1	1:A:65:ALA:HB3	2.45	0.47
1:A:136:ASP:CB	2:A:514:HOH:O	2.37	0.47
1:A:272:ARG:O	1:A:273:VAL:CG1	2.63	0.46
1:A:20:ASN:OD1	1:A:281:ARG:HD2	2.15	0.46
1:A:203:ASP:O	1:A:207:MET:HG3	2.15	0.46
1:A:130:SER:OG	1:A:133:GLU:HG3	2.15	0.46
1:A:138:ALA:O	1:A:141:ILE:HG22	2.16	0.46
1:A:444:PRO:HG2	1:A:445:GLU:H	1.81	0.46
1:A:272:ARG:HH22	1:A:308:ASP:HB3	1.81	0.45
1:A:70:THR:HG21	1:A:194:GLN:CD	2.37	0.45
1:A:303:ARG:NH2	2:A:538:HOH:O	2.09	0.45
1:A:325:ASP:OD2	1:A:326:ARG:N	2.50	0.45
1:A:269:LEU:HA	1:A:270:PRO:HD2	1.85	0.45
1:A:116:GLY:O	1:A:120:VAL:HG23	2.17	0.45
1:A:86:GLN:HE21	1:A:86:GLN:CA	2.27	0.45
1:A:417:ILE:HG22	1:A:447:ILE:HG22	1.99	0.45
1:A:243:TYR:OH	2:A:537:HOH:O	2.05	0.45
1:A:121:HIS:HE1	2:A:520:HOH:O	2.00	0.45
1:A:417:ILE:HG22	1:A:447:ILE:CG2	2.47	0.44
1:A:445:GLU:O	1:A:446:ARG:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:O	1:A:248:GLN:HG2	2.19	0.43
1:A:78:ARG:HD2	2:A:525:HOH:O	2.17	0.43
1:A:62:ILE:HG21	1:A:142:MET:CE	2.49	0.43
1:A:322:ARG:HG2	1:A:322:ARG:HH21	1.83	0.43
1:A:429:VAL:O	1:A:433:GLN:HG3	2.20	0.42
1:A:325:ASP:HB2	1:A:405:ARG:CD	2.49	0.42
1:A:275:ILE:HG22	1:A:276:GLY:N	2.35	0.42
1:A:56:ALA:HA	1:A:201:VAL:CG2	2.50	0.42
1:A:408:VAL:HG22	1:A:440:GLU:CG	2.48	0.41
1:A:309:GLY:N	2:A:532:HOH:O	2.49	0.41
1:A:411:LEU:HD12	1:A:443:ASP:OD2	2.21	0.41
1:A:101:LEU:O	1:A:106:HIS:HA	2.21	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.87	0.41
1:A:433:GLN:HA	1:A:437:VAL:O	2.20	0.41
1:A:12:LEU:HD23	1:A:12:LEU:HA	1.91	0.40
1:A:351:ARG:HA	1:A:351:ARG:HD3	1.82	0.40

All (5) 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:A:336:ARG:CZ	2:A:539:HOH:O[2_565]	1.14	1.06
1:A:336:ARG:NH2	2:A:539:HOH:O[2_565]	1.21	0.99
1:A:336:ARG:NH1	2:A:539:HOH:O[2_565]	1.89	0.31
1:A:336:ARG:NE	2:A:539:HOH:O[2_565]	2.06	0.14
1:A:310:ASP:O	1:A:310:ASP:O[2_565]	2.17	0.03

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	394/456 (86%)	375 (95%)	16 (4%)	3 (1%)	24	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ARG
1	A	444	PRO
1	A	324	GLY

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	309/341 (91%)	299 (97%)	10 (3%)	46	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	86	GLN
1	A	128	GLU
1	A	131	ARG
1	A	149	ARG
1	A	160	GLU
1	A	266	LEU
1	A	284	GLU
1	A	292	VAL
1	A	423	ARG

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

Mol	Chain	Res	Type
1	A	26	GLN
1	A	86	GLN
1	A	110	ASN
1	A	121	HIS

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	398/456 (87%)	0.32	36 (9%) 12 10	16, 32, 75, 101	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	ARG	6.0
1	A	448	LEU	5.5
1	A	322	ARG	5.3
1	A	404	ILE	5.1
1	A	323	GLU	4.7
1	A	351	ARG	4.6
1	A	328	PHE	4.5
1	A	406	THR	4.4
1	A	324	GLY	4.4
1	A	321	GLU	4.3
1	A	104	GLU	3.8
1	A	103	ALA	3.7
1	A	405	ARG	3.5
1	A	435	ASP	3.5
1	A	436	GLY	3.4
1	A	325	ASP	3.4
1	A	29	PRO	3.3
1	A	442	GLU	3.2
1	A	447	ILE	3.2
1	A	350	LEU	3.2
1	A	327	VAL	3.1
1	A	326	ARG	3.0
1	A	33	GLU	3.0
1	A	438	ARG	2.9
1	A	445	GLU	2.8
1	A	440	GLU	2.8
1	A	57	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	437	VAL	2.3
1	A	444	PRO	2.2
1	A	443	ASP	2.2
1	A	408	VAL	2.2
1	A	352	THR	2.2
1	A	353	GLY	2.1
1	A	106	HIS	2.1
1	A	136	ASP	2.0
1	A	319	PHE	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.