



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:46 PM UTC

PDB ID : 5CNK / pdb_00005cnk
Title : mglur3 with glutamate
Authors : Monn, J.A.; Clawson, D.K.
Deposited on : 2015-07-17
Resolution : 3.15 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

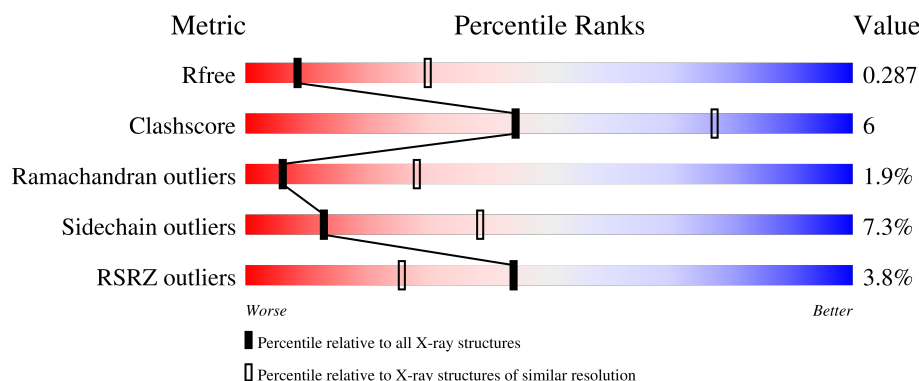
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

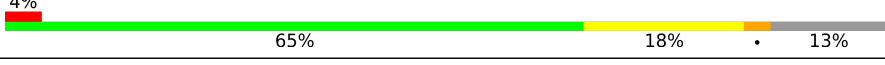
The reported resolution of this entry is 3.15 Å.

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 ≥ 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	517	
1	B	517	
1	C	517	

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
3	IOD	A	604	-	-	X	-
3	IOD	B	602	-	-	X	-
3	IOD	C	603	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10563 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 Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3518	2237	608	659	14			
1	B	438	Total	C	N	O	S	0	0	0
			3478	2210	600	654	14			
1	C	448	Total	C	N	O	S	0	0	0
			3525	2234	607	670	14			

There are 36 discrepancies between the modelled and reference sequences:

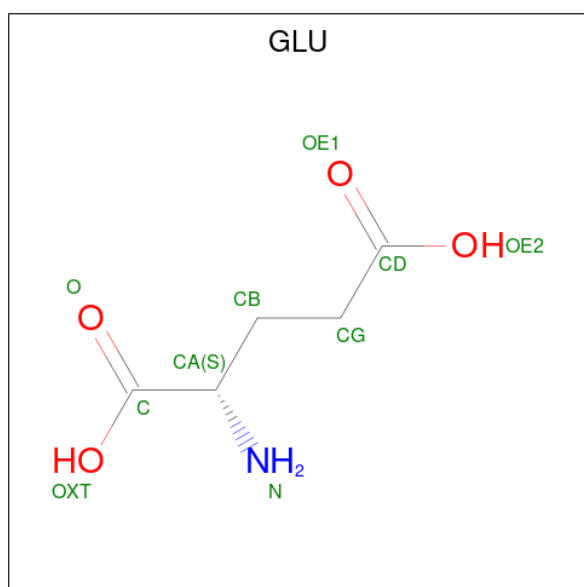
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q14832
A	0	ALA	-	expression tag	UNP Q14832
A	1	LEU	-	expression tag	UNP Q14832
A	240	SER	CYS	conflict	UNP Q14832
A	508	GLU	-	expression tag	UNP Q14832
A	509	GLY	-	expression tag	UNP Q14832
A	510	HIS	-	expression tag	UNP Q14832
A	511	HIS	-	expression tag	UNP Q14832
A	512	HIS	-	expression tag	UNP Q14832
A	513	HIS	-	expression tag	UNP Q14832
A	514	HIS	-	expression tag	UNP Q14832
A	515	HIS	-	expression tag	UNP Q14832
B	-1	MET	-	initiating methionine	UNP Q14832
B	0	ALA	-	expression tag	UNP Q14832
B	1	LEU	-	expression tag	UNP Q14832
B	240	SER	CYS	conflict	UNP Q14832
B	508	GLU	-	expression tag	UNP Q14832
B	509	GLY	-	expression tag	UNP Q14832
B	510	HIS	-	expression tag	UNP Q14832
B	511	HIS	-	expression tag	UNP Q14832
B	512	HIS	-	expression tag	UNP Q14832
B	513	HIS	-	expression tag	UNP Q14832
B	514	HIS	-	expression tag	UNP Q14832

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	515	HIS	-	expression tag	UNP Q14832
C	-1	MET	-	initiating methionine	UNP Q14832
C	0	ALA	-	expression tag	UNP Q14832
C	1	LEU	-	expression tag	UNP Q14832
C	240	SER	CYS	conflict	UNP Q14832
C	508	GLU	-	expression tag	UNP Q14832
C	509	GLY	-	expression tag	UNP Q14832
C	510	HIS	-	expression tag	UNP Q14832
C	511	HIS	-	expression tag	UNP Q14832
C	512	HIS	-	expression tag	UNP Q14832
C	513	HIS	-	expression tag	UNP Q14832
C	514	HIS	-	expression tag	UNP Q14832
C	515	HIS	-	expression tag	UNP Q14832

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	I	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total I 3 3	0	0
3	C	3	Total I 3 3	0	0

- Molecule 4 is water.

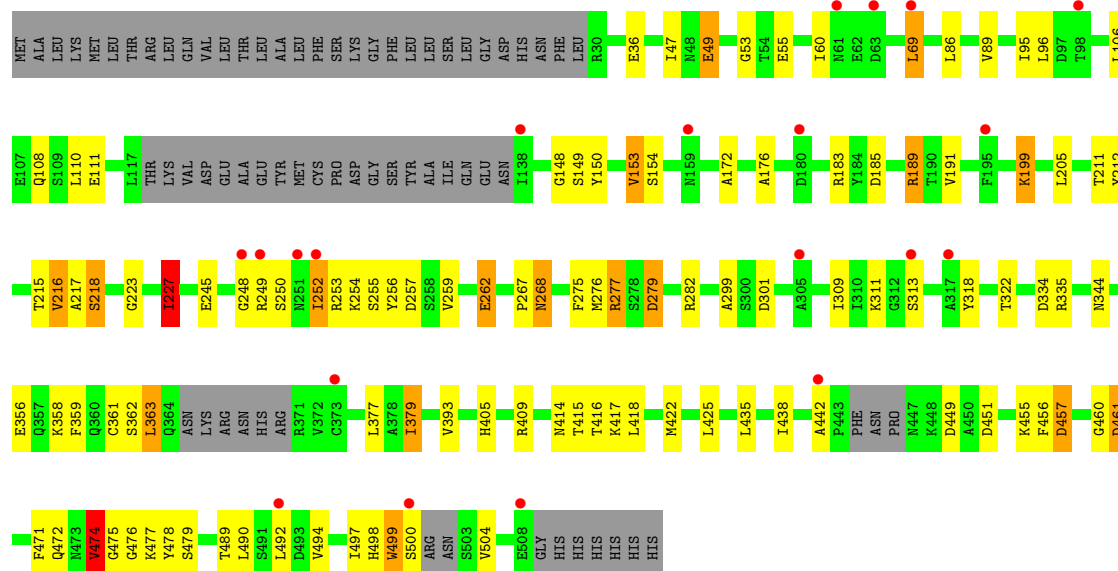
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	4	Total O 4 4	0	0
4	C	10	Total O 10 10	0	0

- Molecule 1: Metabotropic glutamate receptor 3





• Molecule 1: Metabotropic glutamate receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.34Å 80.00Å 206.86Å 90.00° 130.73° 90.00°	Depositor
Resolution (Å)	78.38 – 3.15 78.38 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.8 (78.38-3.15) 97.8 (78.38-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.221 , 0.258 0.243 , 0.287	Depositor DCC
R_{free} test set	873 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -1/2*h+3/2*k,1/2*h+1/2*k,-1/2* h-3/2*k-l 0.059 for -1/2*h-3/2*k,-1/2*h+1/2*k,-1/2* h+3/2*k-l 0.105 for 1/2*h+3/2*k,1/2*h-1/2*k,-3/2*h- 3/2*k-l 0.078 for 1/2*h-3/2*k,-1/2*h-1/2*k,-3/2*h +3/2*k-l 0.064 for -h,-k,2*h+l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10563	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 ⓘ

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

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	2/3592 (0.1%)	1.35	21/4856 (0.4%)
1	B	0.87	0/3551	1.43	33/4800 (0.7%)
1	C	0.89	1/3596 (0.0%)	1.45	35/4866 (0.7%)
All	All	0.87	3/10739 (0.0%)	1.41	89/14522 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	PRO	N-CD	14.95	1.68	1.47
1	A	473	ASN	CA-C	5.32	1.59	1.52
1	C	474	VAL	CA-C	5.16	1.59	1.52

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	SER	N-CA-C	-12.32	96.76	112.90
1	A	440	PHE	CA-CB-CG	10.79	124.59	113.80
1	A	310	ILE	N-CA-CB	-8.82	101.83	112.33
1	C	248	GLY	N-CA-C	8.59	125.19	114.37
1	B	439	ASN	CA-CB-CG	8.58	121.18	112.60

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	3518	0	3425	34	0
1	B	3478	0	3378	53	0
1	C	3525	0	3402	40	0
2	A	10	0	5	2	0
3	A	4	0	0	3	0
3	B	3	0	0	2	0
3	C	3	0	0	2	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
4	C	10	0	0	1	0
All	All	10563	0	10210	125	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 125 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:446:PRO:N	1:A:446:PRO:CD	1.68	1.43
1:B:216:VAL:HG22	1:B:245:GLU:HB2	1.38	1.03
1:C:216:VAL:HG22	1:C:245:GLU:HB2	1.42	0.98
1:C:438:ILE:HG22	1:C:455:LYS:HB3	1.50	0.92
1:B:247:VAL:HG23	1:B:248:GLY:H	1.38	0.89

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	436/517 (84%)	413 (95%)	17 (4%)	6 (1%)	9 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	430/517 (83%)	390 (91%)	30 (7%)	10 (2%)	5	24
1	C	438/517 (85%)	394 (90%)	35 (8%)	9 (2%)	5	26
All	All	1304/1551 (84%)	1197 (92%)	82 (6%)	25 (2%)	6	28

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	A	443	PRO
1	A	500	SER
1	B	253	ARG
1	B	441	THR

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	373/445 (84%)	350 (94%)	23 (6%)	16	44
1	B	368/445 (83%)	341 (93%)	27 (7%)	13	38
1	C	372/445 (84%)	341 (92%)	31 (8%)	10	34
All	All	1113/1335 (83%)	1032 (93%)	81 (7%)	13	38

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	153	VAL
1	C	313	SER
1	C	189	ARG
1	C	262	GLU
1	C	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	165	GLN
1	C	360	GLN
1	B	360	GLN
1	B	445	ASN
1	B	470	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	GLU	A	601	-	8,9,9	2.08	2 (25%)	8,11,11	1.53	2 (25%)

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	GLU	A	601	-	-	2/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GLU	O-C	5.04	1.37	1.22
2	A	601	GLU	OXT-C	-2.50	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GLU	CG-CB-CA	-2.42	108.31	113.86
2	A	601	GLU	OE2-CD-OE1	-2.16	117.77	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GLU	N-CA-CB-CG
2	A	601	GLU	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GLU	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	444/517 (85%)	0.61	18 (4%) 41 24	25, 55, 87, 119	0
1	B	438/517 (84%)	0.49	13 (2%) 52 32	17, 52, 80, 103	0
1	C	448/517 (86%)	0.60	20 (4%) 38 22	22, 53, 85, 101	0
All	All	1330/1551 (85%)	0.57	51 (3%) 44 26	17, 54, 85, 119	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	251	ASN	5.5
1	A	476	GLY	3.9
1	A	501	ARG	3.7
1	A	503	SER	3.6
1	A	147	GLY	3.3

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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	GLU	A	601	10/10	0.96	0.08	33,39,40,41	0
3	IOD	A	605	1/1	0.97	0.08	92,92,92,92	0
3	IOD	C	603	1/1	0.98	0.11	78,78,78,78	0
3	IOD	A	602	1/1	0.99	0.02	53,53,53,53	0
3	IOD	B	602	1/1	0.99	0.05	84,84,84,84	0
3	IOD	B	603	1/1	0.99	0.03	51,51,51,51	0
3	IOD	C	601	1/1	0.99	0.04	62,62,62,62	0
3	IOD	A	604	1/1	0.99	0.04	69,69,69,69	0
3	IOD	A	603	1/1	1.00	0.01	45,45,45,45	0
3	IOD	C	602	1/1	1.00	0.01	42,42,42,42	0
3	IOD	B	601	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.